



wwPDB X-ray Structure Validation Summary Report i

Oct 9, 2014 – 10:28 PM BST

PDB ID : 4U4Q
Title : Crystal structure of Homoharringtonine bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.00 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>

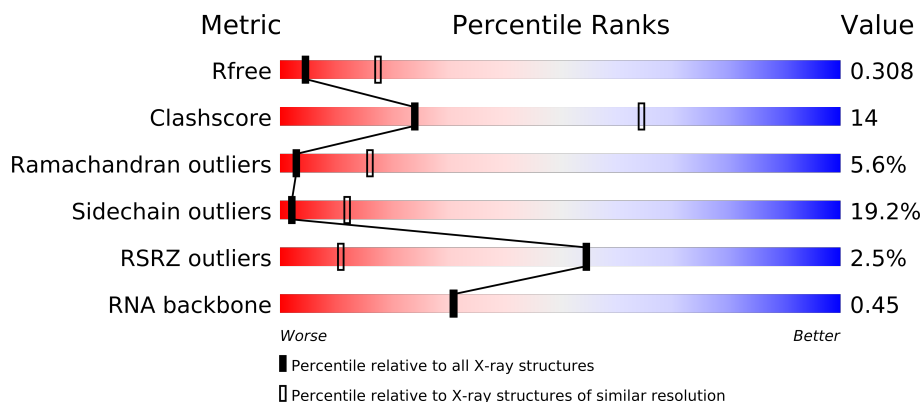
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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	120	

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Mol	Chain	Length	Quality of chain
70	o4	120	
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	3406	-	X
85	MG	1	3407	-	X
85	MG	1	3408	-	X
85	MG	1	3409	-	X
85	MG	1	3410	-	X
85	MG	1	3411	-	X
85	MG	1	3412	-	X
85	MG	1	3413	-	X
85	MG	1	3414	-	X

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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	3420	-	X
85	MG	1	3422	-	X
85	MG	1	3424	-	X
85	MG	1	3425	-	X
85	MG	1	3427	-	X
85	MG	1	3428	-	X
85	MG	1	3430	-	X
85	MG	1	3431	-	X
85	MG	1	3432	-	X
85	MG	1	3433	-	X
85	MG	1	3434	-	X
85	MG	1	3438	-	X
85	MG	1	3439	-	X
85	MG	1	3440	-	X
85	MG	1	3441	-	X
85	MG	1	3443	-	X
85	MG	1	3444	-	X
85	MG	1	3445	-	X
85	MG	1	3446	-	X
85	MG	1	3447	-	X
85	MG	1	3448	-	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	3464	-	X
85	MG	1	3465	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3467	-	X
85	MG	1	3469	-	X
85	MG	1	3470	-	X
85	MG	1	3471	-	X
85	MG	1	3472	-	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	3478	-	X
85	MG	1	3479	-	X
85	MG	1	3481	-	X
85	MG	1	3482	-	X
85	MG	1	3483	-	X
85	MG	1	3485	-	X
85	MG	1	3486	-	X
85	MG	1	3487	-	X
85	MG	1	3488	-	X
85	MG	1	3489	-	X
85	MG	1	3492	-	X
85	MG	1	3493	-	X
85	MG	1	3494	-	X
85	MG	1	3495	-	X
85	MG	1	3496	-	X
85	MG	1	3497	-	X
85	MG	1	3498	-	X
85	MG	1	3499	-	X
85	MG	1	3500	-	X
85	MG	1	3501	-	X
85	MG	1	3502	-	X
85	MG	1	3503	-	X
85	MG	1	3504	-	X
85	MG	1	3505	-	X
85	MG	1	3506	-	X
85	MG	1	3507	-	X
85	MG	1	3508	-	X
85	MG	1	3509	-	X
85	MG	1	3510	-	X
85	MG	1	3511	-	X
85	MG	1	3512	-	X
85	MG	1	3513	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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
85	MG	1	3519	-	X
85	MG	1	3520	-	X
85	MG	1	3521	-	X
85	MG	1	3523	-	X
85	MG	1	3524	-	X
85	MG	1	3525	-	X
85	MG	1	3526	-	X
85	MG	1	3527	-	X
85	MG	1	3528	-	X
85	MG	1	3529	-	X
85	MG	1	3530	-	X
85	MG	1	3531	-	X
85	MG	1	3532	-	X
85	MG	1	3533	-	X
85	MG	1	3534	-	X
85	MG	1	3535	-	X
85	MG	1	3536	-	X
85	MG	1	3537	-	X
85	MG	1	3538	-	X
85	MG	1	3539	-	X
85	MG	1	3540	-	X
85	MG	1	3541	-	X
85	MG	1	3542	-	X
85	MG	1	3543	-	X
85	MG	1	3544	-	X
85	MG	1	3545	-	X
85	MG	1	3546	-	X
85	MG	1	3547	-	X
85	MG	1	3548	-	X
85	MG	1	3549	-	X
85	MG	1	3550	-	X
85	MG	1	3551	-	X
85	MG	1	3552	-	X
85	MG	1	3553	-	X
85	MG	1	3554	-	X
85	MG	1	3555	-	X
85	MG	1	3556	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3557	-	X
85	MG	1	3558	-	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
85	MG	1	3565	-	X
85	MG	1	3566	-	X
85	MG	1	3567	-	X
85	MG	1	3568	-	X
85	MG	1	3569	-	X
85	MG	1	3570	-	X
85	MG	1	3571	-	X
85	MG	1	3572	-	X
85	MG	1	3573	-	X
85	MG	1	3574	-	X
85	MG	1	3575	-	X
85	MG	1	3576	-	X
85	MG	1	3577	-	X
85	MG	1	3578	-	X
85	MG	1	3579	-	X
85	MG	1	3580	-	X
85	MG	1	3581	-	X
85	MG	1	3582	-	X
85	MG	1	3583	-	X
85	MG	1	3585	-	X
85	MG	1	3586	-	X
85	MG	1	3587	-	X
85	MG	1	3588	-	X
85	MG	1	3589	-	X
85	MG	1	3590	-	X
85	MG	1	3591	-	X
85	MG	1	3592	-	X
85	MG	1	3593	-	X
85	MG	1	3594	-	X
85	MG	1	3595	-	X
85	MG	1	3596	-	X
85	MG	1	3597	-	X
85	MG	1	3598	-	X
85	MG	1	3599	-	X
85	MG	1	3600	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3601	-	X
85	MG	1	3603	-	X
85	MG	1	3604	-	X
85	MG	1	3605	-	X
85	MG	1	3606	-	X
85	MG	1	3608	-	X
85	MG	1	3609	-	X
85	MG	1	3610	-	X
85	MG	1	3611	-	X
85	MG	1	3612	-	X
85	MG	1	3613	-	X
85	MG	1	3615	-	X
85	MG	1	3616	-	X
85	MG	1	3617	-	X
85	MG	1	3620	-	X
85	MG	1	3621	-	X
85	MG	1	3623	-	X
85	MG	1	3625	-	X
85	MG	1	3626	-	X
85	MG	1	3628	-	X
85	MG	1	3629	-	X
85	MG	1	3632	-	X
85	MG	1	3634	-	X
85	MG	1	3636	-	X
85	MG	1	3638	-	X
85	MG	1	3639	-	X
85	MG	1	3640	-	X
85	MG	1	3641	-	X
85	MG	1	3644	-	X
85	MG	1	3645	-	X
85	MG	1	3646	-	X
85	MG	1	3647	-	X
85	MG	1	3648	-	X
85	MG	1	3649	-	X
85	MG	1	3650	-	X
85	MG	1	3651	-	X
85	MG	1	3652	-	X
85	MG	1	3653	-	X
85	MG	1	3654	-	X
85	MG	1	3655	-	X
85	MG	1	3656	-	X
85	MG	1	3657	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3658	-	X
85	MG	1	3659	-	X
85	MG	1	3660	-	X
85	MG	1	3661	-	X
85	MG	1	3662	-	X
85	MG	1	3663	-	X
85	MG	1	3664	-	X
85	MG	1	3668	-	X
85	MG	1	3669	-	X
85	MG	1	3670	-	X
85	MG	1	3671	-	X
85	MG	1	3672	-	X
85	MG	1	3673	-	X
85	MG	1	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	3681	-	X
85	MG	1	3684	-	X
85	MG	1	3685	-	X
85	MG	1	3686	-	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	3696	-	X
85	MG	1	3697	-	X
85	MG	1	3698	-	X
85	MG	1	3700	-	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	3710	-	X
85	MG	1	3712	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3714	-	X
85	MG	1	3716	-	X
85	MG	1	3717	-	X
85	MG	1	3720	-	X
85	MG	1	3721	-	X
85	MG	1	3722	-	X
85	MG	1	3723	-	X
85	MG	1	3724	-	X
85	MG	1	3726	-	X
85	MG	1	3727	-	X
85	MG	1	3729	-	X
85	MG	1	3730	-	X
85	MG	1	3731	-	X
85	MG	1	3732	-	X
85	MG	1	3733	-	X
85	MG	1	3735	-	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	3754	-	X
85	MG	1	3757	-	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	3766	-	X
85	MG	1	3767	-	X
85	MG	1	3768	-	X
85	MG	1	3769	-	X
85	MG	1	3772	-	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	3776	-	X
85	MG	1	3777	-	X
85	MG	1	3778	-	X
85	MG	1	3780	-	X
85	MG	1	3781	-	X
85	MG	1	3782	-	X
85	MG	1	3784	-	X
85	MG	1	3785	-	X
85	MG	1	3786	-	X
85	MG	1	3787	-	X
85	MG	1	3788	-	X
85	MG	1	3789	-	X
85	MG	1	3790	-	X
85	MG	1	3791	-	X
85	MG	1	3796	-	X
85	MG	1	3797	-	X
85	MG	1	3798	-	X
85	MG	1	3799	-	X
85	MG	1	3800	-	X
85	MG	1	3801	-	X
85	MG	1	3806	-	X
85	MG	1	3807	-	X
85	MG	1	3808	-	X
85	MG	1	3811	-	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	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	3838	-	X
85	MG	1	3841	-	X
85	MG	1	3842	-	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	3849	-	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	3857	-	X
85	MG	1	3858	-	X
85	MG	1	3859	-	X
85	MG	1	3860	-	X
85	MG	1	3861	-	X
85	MG	1	3863	-	X
85	MG	1	3864	-	X
85	MG	1	3865	-	X
85	MG	1	3866	-	X
85	MG	2	1901	-	X
85	MG	2	1902	-	X
85	MG	2	1903	-	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
85	MG	2	1916	-	X
85	MG	2	1917	-	X
85	MG	2	1918	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1919	-	X
85	MG	2	1921	-	X
85	MG	2	1922	-	X
85	MG	2	1923	-	X
85	MG	2	1924	-	X
85	MG	2	1925	-	X
85	MG	2	1926	-	X
85	MG	2	1927	-	X
85	MG	2	1928	-	X
85	MG	2	1929	-	X
85	MG	2	1930	-	X
85	MG	2	1931	-	X
85	MG	2	1932	-	X
85	MG	2	1933	-	X
85	MG	2	1934	-	X
85	MG	2	1935	-	X
85	MG	2	1936	-	X
85	MG	2	1937	-	X
85	MG	2	1938	-	X
85	MG	2	1939	-	X
85	MG	2	1940	-	X
85	MG	2	1941	-	X
85	MG	2	1942	-	X
85	MG	2	1943	-	X
85	MG	2	1944	-	X
85	MG	2	1945	-	X
85	MG	2	1946	-	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	1954	-	X
85	MG	2	1955	-	X
85	MG	2	1956	-	X
85	MG	2	1957	-	X
85	MG	2	1958	-	X
85	MG	2	1959	-	X
85	MG	2	1960	-	X
85	MG	2	1961	-	X
85	MG	2	1962	-	X
85	MG	2	1964	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1965	-	X
85	MG	2	1966	-	X
85	MG	2	1967	-	X
85	MG	2	1968	-	X
85	MG	2	1969	-	X
85	MG	2	1970	-	X
85	MG	2	1971	-	X
85	MG	2	1973	-	X
85	MG	2	1974	-	X
85	MG	2	1975	-	X
85	MG	2	1976	-	X
85	MG	2	1977	-	X
85	MG	2	1978	-	X
85	MG	2	1979	-	X
85	MG	2	1980	-	X
85	MG	2	1981	-	X
85	MG	2	1982	-	X
85	MG	2	1983	-	X
85	MG	2	1984	-	X
85	MG	2	1985	-	X
85	MG	2	1986	-	X
85	MG	2	1988	-	X
85	MG	2	1989	-	X
85	MG	2	1990	-	X
85	MG	2	1991	-	X
85	MG	2	1992	-	X
85	MG	2	1993	-	X
85	MG	2	1994	-	X
85	MG	2	1999	-	X
85	MG	2	2000	-	X
85	MG	2	2001	-	X
85	MG	2	2004	-	X
85	MG	2	2005	-	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	2013	-	X
85	MG	2	2014	-	X
85	MG	2	2015	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	2016	-	X
85	MG	2	2017	-	X
85	MG	2	2018	-	X
85	MG	2	2019	-	X
85	MG	2	2020	-	X
85	MG	2	2021	-	X
85	MG	3	201	-	X
85	MG	3	202	-	X
85	MG	3	204	-	X
85	MG	3	205	-	X
85	MG	3	206	-	X
85	MG	3	207	-	X
85	MG	3	209	-	X
85	MG	3	210	-	X
85	MG	3	211	-	X
85	MG	3	212	-	X
85	MG	3	213	-	X
85	MG	4	201	-	X
85	MG	4	202	-	X
85	MG	4	203	-	X
85	MG	4	204	-	X
85	MG	4	205	-	X
85	MG	4	206	-	X
85	MG	4	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	216	-	X
85	MG	4	217	-	X
85	MG	4	218	-	X
85	MG	4	220	-	X
85	MG	4	221	-	X
85	MG	4	222	-	X
85	MG	5	3402	-	X
85	MG	5	3403	-	X
85	MG	5	3405	-	X
85	MG	5	3406	-	X
85	MG	5	3409	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	3420	-	X
85	MG	5	3421	-	X
85	MG	5	3422	-	X
85	MG	5	3423	-	X
85	MG	5	3424	-	X
85	MG	5	3425	-	X
85	MG	5	3426	-	X
85	MG	5	3427	-	X
85	MG	5	3428	-	X
85	MG	5	3429	-	X
85	MG	5	3432	-	X
85	MG	5	3434	-	X
85	MG	5	3435	-	X
85	MG	5	3436	-	X
85	MG	5	3437	-	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	3446	-	X
85	MG	5	3447	-	X
85	MG	5	3449	-	X
85	MG	5	3450	-	X
85	MG	5	3451	-	X
85	MG	5	3452	-	X
85	MG	5	3453	-	X
85	MG	5	3454	-	X
85	MG	5	3455	-	X
85	MG	5	3456	-	X
85	MG	5	3457	-	X
85	MG	5	3458	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3459	-	X
85	MG	5	3460	-	X
85	MG	5	3461	-	X
85	MG	5	3463	-	X
85	MG	5	3464	-	X
85	MG	5	3465	-	X
85	MG	5	3466	-	X
85	MG	5	3467	-	X
85	MG	5	3468	-	X
85	MG	5	3469	-	X
85	MG	5	3471	-	X
85	MG	5	3473	-	X
85	MG	5	3474	-	X
85	MG	5	3475	-	X
85	MG	5	3476	-	X
85	MG	5	3477	-	X
85	MG	5	3478	-	X
85	MG	5	3479	-	X
85	MG	5	3480	-	X
85	MG	5	3481	-	X
85	MG	5	3482	-	X
85	MG	5	3483	-	X
85	MG	5	3484	-	X
85	MG	5	3486	-	X
85	MG	5	3487	-	X
85	MG	5	3488	-	X
85	MG	5	3489	-	X
85	MG	5	3490	-	X
85	MG	5	3491	-	X
85	MG	5	3492	-	X
85	MG	5	3493	-	X
85	MG	5	3494	-	X
85	MG	5	3495	-	X
85	MG	5	3496	-	X
85	MG	5	3497	-	X
85	MG	5	3498	-	X
85	MG	5	3499	-	X
85	MG	5	3500	-	X
85	MG	5	3501	-	X
85	MG	5	3502	-	X
85	MG	5	3503	-	X
85	MG	5	3504	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3505	-	X
85	MG	5	3506	-	X
85	MG	5	3507	-	X
85	MG	5	3508	-	X
85	MG	5	3509	-	X
85	MG	5	3510	-	X
85	MG	5	3511	-	X
85	MG	5	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	3522	-	X
85	MG	5	3523	-	X
85	MG	5	3524	-	X
85	MG	5	3525	-	X
85	MG	5	3526	-	X
85	MG	5	3527	-	X
85	MG	5	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	3542	-	X
85	MG	5	3543	-	X
85	MG	5	3544	-	X
85	MG	5	3545	-	X
85	MG	5	3546	-	X
85	MG	5	3547	-	X
85	MG	5	3548	-	X
85	MG	5	3549	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3550	-	X
85	MG	5	3551	-	X
85	MG	5	3552	-	X
85	MG	5	3553	-	X
85	MG	5	3554	-	X
85	MG	5	3555	-	X
85	MG	5	3556	-	X
85	MG	5	3557	-	X
85	MG	5	3558	-	X
85	MG	5	3559	-	X
85	MG	5	3560	-	X
85	MG	5	3561	-	X
85	MG	5	3562	-	X
85	MG	5	3563	-	X
85	MG	5	3564	-	X
85	MG	5	3565	-	X
85	MG	5	3566	-	X
85	MG	5	3567	-	X
85	MG	5	3568	-	X
85	MG	5	3569	-	X
85	MG	5	3570	-	X
85	MG	5	3571	-	X
85	MG	5	3572	-	X
85	MG	5	3573	-	X
85	MG	5	3574	-	X
85	MG	5	3575	-	X
85	MG	5	3576	-	X
85	MG	5	3577	-	X
85	MG	5	3578	-	X
85	MG	5	3579	-	X
85	MG	5	3580	-	X
85	MG	5	3581	-	X
85	MG	5	3582	-	X
85	MG	5	3583	-	X
85	MG	5	3584	-	X
85	MG	5	3585	-	X
85	MG	5	3586	-	X
85	MG	5	3587	-	X
85	MG	5	3588	-	X
85	MG	5	3589	-	X
85	MG	5	3590	-	X
85	MG	5	3591	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3592	-	X
85	MG	5	3593	-	X
85	MG	5	3594	-	X
85	MG	5	3595	-	X
85	MG	5	3596	-	X
85	MG	5	3597	-	X
85	MG	5	3598	-	X
85	MG	5	3603	-	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	3611	-	X
85	MG	5	3612	-	X
85	MG	5	3613	-	X
85	MG	5	3614	-	X
85	MG	5	3618	-	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	3629	-	X
85	MG	5	3630	-	X
85	MG	5	3631	-	X
85	MG	5	3632	-	X
85	MG	5	3633	-	X
85	MG	5	3634	-	X
85	MG	5	3635	-	X
85	MG	5	3636	-	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	3643	-	X
85	MG	5	3644	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3645	-	X
85	MG	5	3646	-	X
85	MG	5	3647	-	X
85	MG	5	3649	-	X
85	MG	5	3652	-	X
85	MG	5	3653	-	X
85	MG	5	3654	-	X
85	MG	5	3655	-	X
85	MG	5	3656	-	X
85	MG	5	3657	-	X
85	MG	5	3659	-	X
85	MG	5	3660	-	X
85	MG	5	3661	-	X
85	MG	5	3662	-	X
85	MG	5	3663	-	X
85	MG	5	3664	-	X
85	MG	5	3665	-	X
85	MG	5	3666	-	X
85	MG	5	3667	-	X
85	MG	5	3668	-	X
85	MG	5	3669	-	X
85	MG	5	3670	-	X
85	MG	5	3671	-	X
85	MG	5	3672	-	X
85	MG	5	3673	-	X
85	MG	5	3674	-	X
85	MG	5	3675	-	X
85	MG	5	3676	-	X
85	MG	5	3677	-	X
85	MG	5	3680	-	X
85	MG	5	3681	-	X
85	MG	5	3682	-	X
85	MG	5	3684	-	X
85	MG	5	3686	-	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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3697	-	X
85	MG	5	3698	-	X
85	MG	5	3701	-	X
85	MG	5	3705	-	X
85	MG	5	3708	-	X
85	MG	5	3709	-	X
85	MG	5	3710	-	X
85	MG	5	3711	-	X
85	MG	5	3713	-	X
85	MG	5	3714	-	X
85	MG	5	3715	-	X
85	MG	5	3717	-	X
85	MG	5	3719	-	X
85	MG	5	3720	-	X
85	MG	5	3722	-	X
85	MG	5	3724	-	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	3731	-	X
85	MG	5	3732	-	X
85	MG	5	3733	-	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	3741	-	X
85	MG	5	3742	-	X
85	MG	5	3743	-	X
85	MG	5	3744	-	X
85	MG	5	3745	-	X
85	MG	5	3747	-	X
85	MG	5	3748	-	X
85	MG	5	3750	-	X
85	MG	5	3752	-	X
85	MG	5	3756	-	X
85	MG	5	3758	-	X
85	MG	5	3761	-	X
85	MG	5	3762	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3763	-	X
85	MG	5	3764	-	X
85	MG	5	3766	-	X
85	MG	5	3767	-	X
85	MG	5	3770	-	X
85	MG	5	3772	-	X
85	MG	5	3774	-	X
85	MG	5	3775	-	X
85	MG	5	3776	-	X
85	MG	5	3777	-	X
85	MG	5	3779	-	X
85	MG	5	3780	-	X
85	MG	5	3781	-	X
85	MG	5	3783	-	X
85	MG	5	3784	-	X
85	MG	5	3785	-	X
85	MG	5	3786	-	X
85	MG	5	3789	-	X
85	MG	5	3791	-	X
85	MG	5	3792	-	X
85	MG	5	3793	-	X
85	MG	5	3794	-	X
85	MG	5	3795	-	X
85	MG	5	3796	-	X
85	MG	5	3797	-	X
85	MG	5	3798	-	X
85	MG	5	3800	-	X
85	MG	5	3801	-	X
85	MG	5	3802	-	X
85	MG	5	3803	-	X
85	MG	5	3804	-	X
85	MG	5	3808	-	X
85	MG	5	3809	-	X
85	MG	5	3810	-	X
85	MG	5	3812	-	X
85	MG	5	3813	-	X
85	MG	5	3814	-	X
85	MG	5	3815	-	X
85	MG	5	3818	-	X
85	MG	5	3820	-	X
85	MG	5	3822	-	X
85	MG	5	3825	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3826	-	X
85	MG	5	3827	-	X
85	MG	5	3828	-	X
85	MG	5	3829	-	X
85	MG	5	3830	-	X
85	MG	5	3835	-	X
85	MG	5	3838	-	X
85	MG	5	3839	-	X
85	MG	5	3840	-	X
85	MG	5	3843	-	X
85	MG	5	3844	-	X
85	MG	5	3845	-	X
85	MG	5	3846	-	X
85	MG	5	3847	-	X
85	MG	5	3848	-	X
85	MG	5	3849	-	X
85	MG	5	3851	-	X
85	MG	5	3853	-	X
85	MG	5	3854	-	X
85	MG	5	3855	-	X
85	MG	5	3858	-	X
85	MG	5	3860	-	X
85	MG	5	3861	-	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	3872	-	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	3880	-	X
85	MG	5	3881	-	X
85	MG	5	3882	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3883	-	X
85	MG	5	3884	-	X
85	MG	5	3885	-	X
85	MG	5	3887	-	X
85	MG	5	3888	-	X
85	MG	5	3889	-	X
85	MG	5	3890	-	X
85	MG	5	3891	-	X
85	MG	5	3892	-	X
85	MG	5	3893	-	X
85	MG	5	3894	-	X
85	MG	5	3895	-	X
85	MG	5	3896	-	X
85	MG	5	3897	-	X
85	MG	5	3898	-	X
85	MG	5	3899	-	X
85	MG	5	3900	-	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	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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1927	-	X
85	MG	6	1928	-	X
85	MG	6	1929	-	X
85	MG	6	1930	-	X
85	MG	6	1931	-	X
85	MG	6	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	1940	-	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	1966	-	X
85	MG	6	1967	-	X
85	MG	6	1968	-	X
85	MG	6	1969	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1971	-	X
85	MG	6	1973	-	X
85	MG	6	1974	-	X
85	MG	6	1975	-	X
85	MG	6	1976	-	X
85	MG	6	1977	-	X
85	MG	6	1978	-	X
85	MG	6	1979	-	X
85	MG	6	1980	-	X
85	MG	6	1981	-	X
85	MG	6	1982	-	X
85	MG	6	1984	-	X
85	MG	6	1985	-	X
85	MG	6	1986	-	X
85	MG	6	1987	-	X
85	MG	6	1988	-	X
85	MG	6	1989	-	X
85	MG	6	1990	-	X
85	MG	6	1991	-	X
85	MG	6	1992	-	X
85	MG	6	1993	-	X
85	MG	6	1994	-	X
85	MG	6	1995	-	X
85	MG	6	1996	-	X
85	MG	6	1999	-	X
85	MG	6	2001	-	X
85	MG	6	2003	-	X
85	MG	6	2004	-	X
85	MG	6	2005	-	X
85	MG	6	2006	-	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	2014	-	X
85	MG	6	2015	-	X
85	MG	6	2016	-	X
85	MG	6	2019	-	X
85	MG	6	2020	-	X
85	MG	6	2021	-	X
85	MG	6	2022	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	2023	-	X
85	MG	6	2024	-	X
85	MG	6	2025	-	X
85	MG	6	2026	-	X
85	MG	6	2027	-	X
85	MG	6	2029	-	X
85	MG	6	2030	-	X
85	MG	6	2031	-	X
85	MG	6	2032	-	X
85	MG	6	2033	-	X
85	MG	6	2034	-	X
85	MG	6	2036	-	X
85	MG	6	2037	-	X
85	MG	6	2038	-	X
85	MG	6	2039	-	X
85	MG	6	2041	-	X
85	MG	6	2043	-	X
85	MG	6	2044	-	X
85	MG	6	2046	-	X
85	MG	6	2047	-	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	210	-	X
85	MG	7	211	-	X
85	MG	7	212	-	X
85	MG	7	213	-	X
85	MG	7	214	-	X
85	MG	7	216	-	X
85	MG	8	201	-	X
85	MG	8	202	-	X
85	MG	8	203	-	X
85	MG	8	204	-	X
85	MG	8	205	-	X
85	MG	8	206	-	X
85	MG	8	208	-	X
85	MG	8	209	-	X
85	MG	8	210	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	8	212	-	X
85	MG	8	213	-	X
85	MG	8	214	-	X
85	MG	L2	301	-	X
85	MG	L2	302	-	X
85	MG	L3	402	-	X
85	MG	L3	403	-	X
85	MG	L5	301	-	X
85	MG	L7	301	-	X
85	MG	L7	302	-	X
85	MG	L7	303	-	X
85	MG	L7	304	-	X
85	MG	L8	301	-	X
85	MG	M0	301	-	X
85	MG	M0	303	-	X
85	MG	M3	201	-	X
85	MG	M3	203	-	X
85	MG	M5	302	-	X
85	MG	M7	201	-	X
85	MG	M7	203	-	X
85	MG	M7	204	-	X
85	MG	N0	201	-	X
85	MG	N3	201	-	X
85	MG	N3	202	-	X
85	MG	N8	201	-	X
85	MG	N8	202	-	X
85	MG	N8	204	-	X
85	MG	N8	205	-	X
85	MG	O1	201	-	X
85	MG	O3	201	-	X
85	MG	O4	201	-	X
85	MG	O7	102	-	X
85	MG	O7	103	-	X
85	MG	S2	301	-	X
85	MG	S2	302	-	X
85	MG	S4	301	-	X
85	MG	S8	301	-	X
85	MG	c1	201	-	X
85	MG	c7	201	-	X
85	MG	c9	201	-	X
85	MG	d3	201	-	X
85	MG	d3	202	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	l2	301	-	X
85	MG	l2	302	-	X
85	MG	l3	401	-	X
85	MG	l3	402	-	X
85	MG	l7	302	-	X
85	MG	l7	303	-	X
85	MG	l9	201	-	X
85	MG	m0	301	-	X
85	MG	m1	201	-	X
85	MG	m1	202	-	X
85	MG	m6	201	-	X
85	MG	m7	201	-	X
85	MG	m7	202	-	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	n8	203	-	X
85	MG	n8	204	-	X
85	MG	o1	201	-	X
85	MG	o3	201	-	X
85	MG	o3	202	-	X
85	MG	o4	202	-	X
85	MG	o7	502	-	X
85	MG	q1	101	-	X
85	MG	s1	301	-	X
85	MG	s4	301	-	X
85	MG	s8	301	-	X
85	MG	s9	201	-	X
86	OHX	1	3896	-	X
86	OHX	1	3911	-	X
86	OHX	1	3980	-	X
86	OHX	1	3987	-	X
86	OHX	1	3993	-	X
86	OHX	1	3994	-	X
86	OHX	1	4008	-	X
86	OHX	1	4009	-	X
86	OHX	1	4012	-	X
86	OHX	1	4017	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4019	-	X
86	OHX	1	4029	-	X
86	OHX	1	4031	-	X
86	OHX	1	4032	-	X
86	OHX	1	4037	-	X
86	OHX	1	4041	-	X
86	OHX	1	4046	-	X
86	OHX	1	4048	-	X
86	OHX	1	4049	-	X
86	OHX	1	4050	-	X
86	OHX	1	4055	-	X
86	OHX	1	4058	-	X
86	OHX	1	4060	-	X
86	OHX	1	4061	-	X
86	OHX	1	4065	-	X
86	OHX	1	4066	-	X
86	OHX	1	4067	-	X
86	OHX	1	4068	-	X
86	OHX	1	4070	-	X
86	OHX	1	4071	-	X
86	OHX	1	4073	-	X
86	OHX	1	4074	-	X
86	OHX	1	4075	-	X
86	OHX	1	4076	-	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	4083	-	X
86	OHX	1	4085	-	X
86	OHX	1	4086	-	X
86	OHX	1	4090	-	X
86	OHX	1	4093	-	X
86	OHX	1	4095	-	X
86	OHX	1	4098	-	X
86	OHX	1	4099	-	X
86	OHX	1	4100	-	X
86	OHX	1	4101	-	X
86	OHX	1	4102	-	X
86	OHX	1	4103	-	X
86	OHX	1	4104	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4111	-	X
86	OHX	1	4112	-	X
86	OHX	1	4113	-	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
86	OHX	1	4120	-	X
86	OHX	1	4122	-	X
86	OHX	1	4123	-	X
86	OHX	1	4124	-	X
86	OHX	1	4125	-	X
86	OHX	1	4126	-	X
86	OHX	1	4129	-	X
86	OHX	1	4130	-	X
86	OHX	1	4131	-	X
86	OHX	1	4132	-	X
86	OHX	1	4133	-	X
86	OHX	1	4134	-	X
86	OHX	1	4136	-	X
86	OHX	1	4137	-	X
86	OHX	1	4139	-	X
86	OHX	1	4141	-	X
86	OHX	1	4142	-	X
86	OHX	1	4143	-	X
86	OHX	1	4144	-	X
86	OHX	1	4145	-	X
86	OHX	1	4146	-	X
86	OHX	1	4147	-	X
86	OHX	1	4149	-	X
86	OHX	1	4150	-	X
86	OHX	1	4151	-	X
86	OHX	1	4152	-	X
86	OHX	1	4154	-	X
86	OHX	1	4156	-	X
86	OHX	1	4157	-	X
86	OHX	1	4158	-	X
86	OHX	1	4160	-	X
86	OHX	1	4161	-	X
86	OHX	1	4162	-	X
86	OHX	1	4163	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4164	-	X
86	OHX	1	4166	-	X
86	OHX	1	4167	-	X
86	OHX	1	4168	-	X
86	OHX	1	4170	-	X
86	OHX	1	4171	-	X
86	OHX	1	4172	-	X
86	OHX	1	4173	-	X
86	OHX	1	4174	-	X
86	OHX	1	4175	-	X
86	OHX	1	4177	-	X
86	OHX	1	4178	-	X
86	OHX	1	4179	-	X
86	OHX	1	4180	-	X
86	OHX	1	4181	-	X
86	OHX	1	4183	-	X
86	OHX	1	4184	-	X
86	OHX	1	4186	-	X
86	OHX	1	4187	-	X
86	OHX	1	4188	-	X
86	OHX	1	4189	-	X
86	OHX	1	4190	-	X
86	OHX	1	4192	-	X
86	OHX	1	4193	-	X
86	OHX	1	4195	-	X
86	OHX	1	4197	-	X
86	OHX	1	4198	-	X
86	OHX	1	4199	-	X
86	OHX	1	4200	-	X
86	OHX	1	4202	-	X
86	OHX	1	4203	-	X
86	OHX	1	4204	-	X
86	OHX	1	4205	-	X
86	OHX	1	4206	-	X
86	OHX	1	4207	-	X
86	OHX	1	4208	-	X
86	OHX	1	4209	-	X
86	OHX	1	4210	-	X
86	OHX	1	4211	-	X
86	OHX	1	4212	-	X
86	OHX	1	4213	-	X
86	OHX	1	4215	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4216	-	X
86	OHX	2	2061	-	X
86	OHX	2	2073	-	X
86	OHX	2	2074	-	X
86	OHX	2	2078	-	X
86	OHX	2	2083	-	X
86	OHX	2	2090	-	X
86	OHX	2	2095	-	X
86	OHX	2	2099	-	X
86	OHX	2	2100	-	X
86	OHX	2	2102	-	X
86	OHX	2	2104	-	X
86	OHX	2	2105	-	X
86	OHX	2	2107	-	X
86	OHX	2	2108	-	X
86	OHX	2	2110	-	X
86	OHX	2	2111	-	X
86	OHX	2	2112	-	X
86	OHX	2	2115	-	X
86	OHX	2	2116	-	X
86	OHX	2	2118	-	X
86	OHX	2	2119	-	X
86	OHX	2	2122	-	X
86	OHX	2	2125	-	X
86	OHX	2	2127	-	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	2140	-	X
86	OHX	2	2142	-	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	2152	-	X
86	OHX	2	2153	-	X
86	OHX	2	2154	-	X
86	OHX	2	2157	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	2	2159	-	X
86	OHX	2	2160	-	X
86	OHX	2	2162	-	X
86	OHX	2	2163	-	X
86	OHX	2	2164	-	X
86	OHX	2	2169	-	X
86	OHX	2	2171	-	X
86	OHX	2	2172	-	X
86	OHX	2	2173	-	X
86	OHX	2	2174	-	X
86	OHX	2	2175	-	X
86	OHX	2	2176	-	X
86	OHX	2	2178	-	X
86	OHX	2	2179	-	X
86	OHX	3	220	-	X
86	OHX	3	221	-	X
86	OHX	3	222	-	X
86	OHX	3	223	-	X
86	OHX	3	224	-	X
86	OHX	4	230	-	X
86	OHX	4	234	-	X
86	OHX	4	235	-	X
86	OHX	4	236	-	X
86	OHX	4	237	-	X
86	OHX	4	238	-	X
86	OHX	5	3912	-	X
86	OHX	5	3932	-	X
86	OHX	5	3995	-	X
86	OHX	5	4004	-	X
86	OHX	5	4028	-	X
86	OHX	5	4034	-	X
86	OHX	5	4041	-	X
86	OHX	5	4044	-	X
86	OHX	5	4046	-	X
86	OHX	5	4047	-	X
86	OHX	5	4049	-	X
86	OHX	5	4050	-	X
86	OHX	5	4051	-	X
86	OHX	5	4053	-	X
86	OHX	5	4054	-	X
86	OHX	5	4063	-	X
86	OHX	5	4064	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4071	-	X
86	OHX	5	4072	-	X
86	OHX	5	4073	-	X
86	OHX	5	4074	-	X
86	OHX	5	4075	-	X
86	OHX	5	4078	-	X
86	OHX	5	4084	-	X
86	OHX	5	4086	-	X
86	OHX	5	4087	-	X
86	OHX	5	4090	-	X
86	OHX	5	4091	-	X
86	OHX	5	4093	-	X
86	OHX	5	4094	-	X
86	OHX	5	4098	-	X
86	OHX	5	4099	-	X
86	OHX	5	4101	-	X
86	OHX	5	4102	-	X
86	OHX	5	4104	-	X
86	OHX	5	4107	-	X
86	OHX	5	4108	-	X
86	OHX	5	4110	-	X
86	OHX	5	4111	-	X
86	OHX	5	4113	-	X
86	OHX	5	4114	-	X
86	OHX	5	4115	-	X
86	OHX	5	4117	-	X
86	OHX	5	4118	-	X
86	OHX	5	4119	-	X
86	OHX	5	4120	-	X
86	OHX	5	4122	-	X
86	OHX	5	4125	-	X
86	OHX	5	4128	-	X
86	OHX	5	4129	-	X
86	OHX	5	4130	-	X
86	OHX	5	4135	-	X
86	OHX	5	4136	-	X
86	OHX	5	4137	-	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

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4143	-	X
86	OHX	5	4144	-	X
86	OHX	5	4145	-	X
86	OHX	5	4146	-	X
86	OHX	5	4148	-	X
86	OHX	5	4149	-	X
86	OHX	5	4150	-	X
86	OHX	5	4151	-	X
86	OHX	5	4152	-	X
86	OHX	5	4153	-	X
86	OHX	5	4154	-	X
86	OHX	5	4155	-	X
86	OHX	5	4156	-	X
86	OHX	5	4158	-	X
86	OHX	5	4159	-	X
86	OHX	5	4160	-	X
86	OHX	5	4161	-	X
86	OHX	5	4162	-	X
86	OHX	5	4163	-	X
86	OHX	5	4164	-	X
86	OHX	5	4165	-	X
86	OHX	5	4166	-	X
86	OHX	5	4167	-	X
86	OHX	5	4168	-	X
86	OHX	5	4169	-	X
86	OHX	5	4171	-	X
86	OHX	5	4172	-	X
86	OHX	5	4174	-	X
86	OHX	5	4175	-	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	4184	-	X
86	OHX	5	4186	-	X
86	OHX	5	4187	-	X
86	OHX	5	4188	-	X
86	OHX	5	4189	-	X
86	OHX	5	4190	-	X
86	OHX	5	4191	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4194	-	X
86	OHX	5	4195	-	X
86	OHX	5	4196	-	X
86	OHX	5	4198	-	X
86	OHX	5	4199	-	X
86	OHX	5	4200	-	X
86	OHX	5	4201	-	X
86	OHX	5	4202	-	X
86	OHX	5	4204	-	X
86	OHX	5	4205	-	X
86	OHX	5	4206	-	X
86	OHX	5	4207	-	X
86	OHX	5	4208	-	X
86	OHX	5	4209	-	X
86	OHX	5	4211	-	X
86	OHX	5	4212	-	X
86	OHX	5	4213	-	X
86	OHX	5	4215	-	X
86	OHX	5	4216	-	X
86	OHX	5	4218	-	X
86	OHX	5	4219	-	X
86	OHX	5	4220	-	X
86	OHX	5	4221	-	X
86	OHX	5	4222	-	X
86	OHX	5	4223	-	X
86	OHX	5	4224	-	X
86	OHX	5	4225	-	X
86	OHX	5	4226	-	X
86	OHX	5	4227	-	X
86	OHX	5	4229	-	X
86	OHX	5	4231	-	X
86	OHX	5	4232	-	X
86	OHX	5	4233	-	X
86	OHX	5	4234	-	X
86	OHX	5	4235	-	X
86	OHX	5	4236	-	X
86	OHX	5	4237	-	X
86	OHX	5	4238	-	X
86	OHX	5	4239	-	X
86	OHX	5	4240	-	X
86	OHX	5	4242	-	X
86	OHX	5	4243	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4246	-	X
86	OHX	5	4248	-	X
86	OHX	5	4249	-	X
86	OHX	5	4250	-	X
86	OHX	5	4251	-	X
86	OHX	5	4252	-	X
86	OHX	5	4253	-	X
86	OHX	5	4254	-	X
86	OHX	6	2105	-	X
86	OHX	6	2112	-	X
86	OHX	6	2115	-	X
86	OHX	6	2117	-	X
86	OHX	6	2119	-	X
86	OHX	6	2122	-	X
86	OHX	6	2125	-	X
86	OHX	6	2126	-	X
86	OHX	6	2127	-	X
86	OHX	6	2128	-	X
86	OHX	6	2129	-	X
86	OHX	6	2130	-	X
86	OHX	6	2134	-	X
86	OHX	6	2135	-	X
86	OHX	6	2136	-	X
86	OHX	6	2138	-	X
86	OHX	6	2142	-	X
86	OHX	6	2143	-	X
86	OHX	6	2146	-	X
86	OHX	6	2149	-	X
86	OHX	6	2150	-	X
86	OHX	6	2151	-	X
86	OHX	6	2153	-	X
86	OHX	6	2154	-	X
86	OHX	6	2158	-	X
86	OHX	6	2159	-	X
86	OHX	6	2160	-	X
86	OHX	6	2162	-	X
86	OHX	6	2163	-	X
86	OHX	6	2165	-	X
86	OHX	6	2167	-	X
86	OHX	6	2170	-	X
86	OHX	6	2171	-	X
86	OHX	6	2172	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	2179	-	X
86	OHX	6	2180	-	X
86	OHX	6	2182	-	X
86	OHX	6	2183	-	X
86	OHX	6	2185	-	X
86	OHX	6	2186	-	X
86	OHX	6	2187	-	X
86	OHX	6	2188	-	X
86	OHX	6	2189	-	X
86	OHX	6	2190	-	X
86	OHX	6	2191	-	X
86	OHX	6	2192	-	X
86	OHX	6	2193	-	X
86	OHX	6	2196	-	X
86	OHX	6	2197	-	X
86	OHX	6	2199	-	X
86	OHX	6	2200	-	X
86	OHX	6	2201	-	X
86	OHX	6	2202	-	X
86	OHX	6	2205	-	X
86	OHX	6	2206	-	X
86	OHX	7	226	-	X
86	OHX	7	227	-	X
86	OHX	7	228	-	X
86	OHX	8	222	-	X
86	OHX	8	226	-	X
86	OHX	8	227	-	X
86	OHX	8	228	-	X
86	OHX	8	229	-	X
86	OHX	8	230	-	X
86	OHX	D9	102	-	X
86	OHX	L4	402	-	X
86	OHX	M7	206	-	X
86	OHX	M7	207	-	X
86	OHX	M9	203	-	X
86	OHX	O3	202	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	O9	101	-	X
86	OHX	l4	402	-	X
86	OHX	l4	403	-	X
86	OHX	l5	304	-	X
86	OHX	m4	201	-	X
86	OHX	m7	206	-	X
86	OHX	o9	101	-	X
86	OHX	s1	302	-	X
86	OHX	s9	202	-	X
87	ZN	d7	101	-	X
88	HMT	5	4255	-	X

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411245 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	C	N	O	0	0	0
			1111	711	204	196			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
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	C	N	O	S	0	0	0
			959	617	168	172	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	4	Total	Mg	0	0
			4	4		
85	m6	2	Total	Mg	0	0
			2	2		
85	n8	5	Total	Mg	0	0
			5	5		
85	o1	1	Total	Mg	0	0
			1	1		
85	N5	1	Total	Mg	0	0
			1	1		
85	6	147	Total	Mg	0	0
			147	147		
85	sM	2	Total	Mg	0	0
			2	2		
85	O4	1	Total	Mg	0	0
			1	1		
85	q1	1	Total	Mg	0	0
			1	1		
85	l3	3	Total	Mg	0	0
			3	3		
85	M1	2	Total	Mg	0	0
			2	2		
85	n0	2	Total	Mg	0	0
			2	2		
85	d6	1	Total	Mg	0	0
			1	1		
85	C8	1	Total	Mg	0	0
			1	1		
85	O3	1	Total	Mg	0	0
			1	1		
85	S6	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L4	1	Total 1	Mg 1	0	0
85	l7	3	Total 3	Mg 3	0	0
85	M5	2	Total 2	Mg 2	0	0
85	c9	2	Total 2	Mg 2	0	0
85	S2	2	Total 2	Mg 2	0	0
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	M9	2	Total 2	Mg 2	0	0
85	q0	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0
85	M0	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	500	Total 500	Mg 500	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	s6	1	Total 1	Mg 1	0	0
85	l4	1	Total 1	Mg 1	0	0
85	1	466	Total 466	Mg 466	0	0
85	s4	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	S8	1	Total 1	Mg 1	0	0

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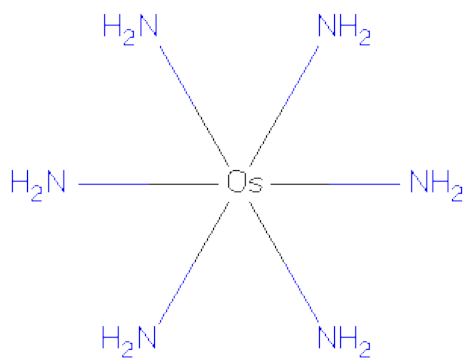
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	m1	2	Total 2	Mg 2	0	0
85	O2	1	Total 1	Mg 1	0	0
85	s9	1	Total 1	Mg 1	0	0
85	o3	2	Total 2	Mg 2	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	2	Total 2	Mg 2	0	0
85	N8	6	Total 6	Mg 6	0	0
85	4	23	Total 23	Mg 23	0	0
85	n6	2	Total 2	Mg 2	0	0
85	S4	2	Total 2	Mg 2	0	0
85	L2	2	Total 2	Mg 2	0	0
85	o7	1	Total 1	Mg 1	0	0
85	l5	1	Total 1	Mg 1	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	5	Total 5	Mg 5	0	0
85	L6	1	Total 1	Mg 1	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	O1	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c7	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	7	16	Total	Mg	0	0
			16	16		
85	n3	2	Total	Mg	0	0
			2	2		
85	L3	3	Total	Mg	0	0
			3	3		
85	2	121	Total	Mg	0	0
			121	121		
85	12	2	Total	Mg	0	0
			2	2		
85	8	15	Total	Mg	0	0
			15	15		
85	m0	1	Total	Mg	0	0
			1	1		
85	M6	1	Total	Mg	0	0
			1	1		
85	N0	1	Total	Mg	0	0
			1	1		
85	3	13	Total	Mg	0	0
			13	13		

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



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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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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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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
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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
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	M8	1	Total	N	Os	0	0
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86	M9	1	Total	N	Os	0	0
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86	N1	1	Total	N	Os	0	0
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86	N9	1	Total	N	Os	0	0
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86	O2	1	Total	N	Os	0	0
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86	O3	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O9	1	Total	N	Os	0	0
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86	Q2	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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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	s4	1	Total	N	Os	0	0
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86	s8	1	Total	N	Os	0	0
			7	6	1		
86	s9	1	Total	N	Os	0	0
			7	6	1		
86	c3	1	Total	N	Os	0	0
			7	6	1		
86	c5	1	Total	N	Os	0	0
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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
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		

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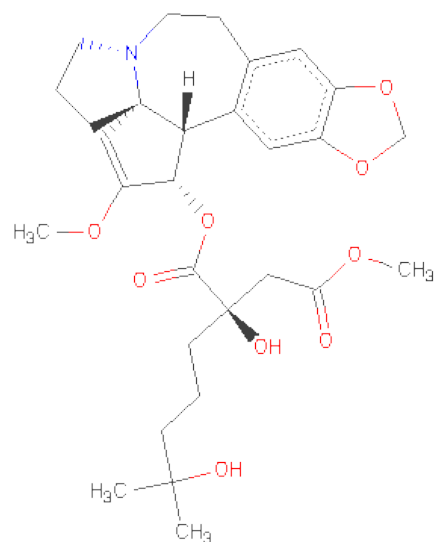
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	o9	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	q0	1	Total Zn 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
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)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano
yl]cephalotaxine (three-letter code: HMT) (formula: C₂₉H₃₉NO₉).

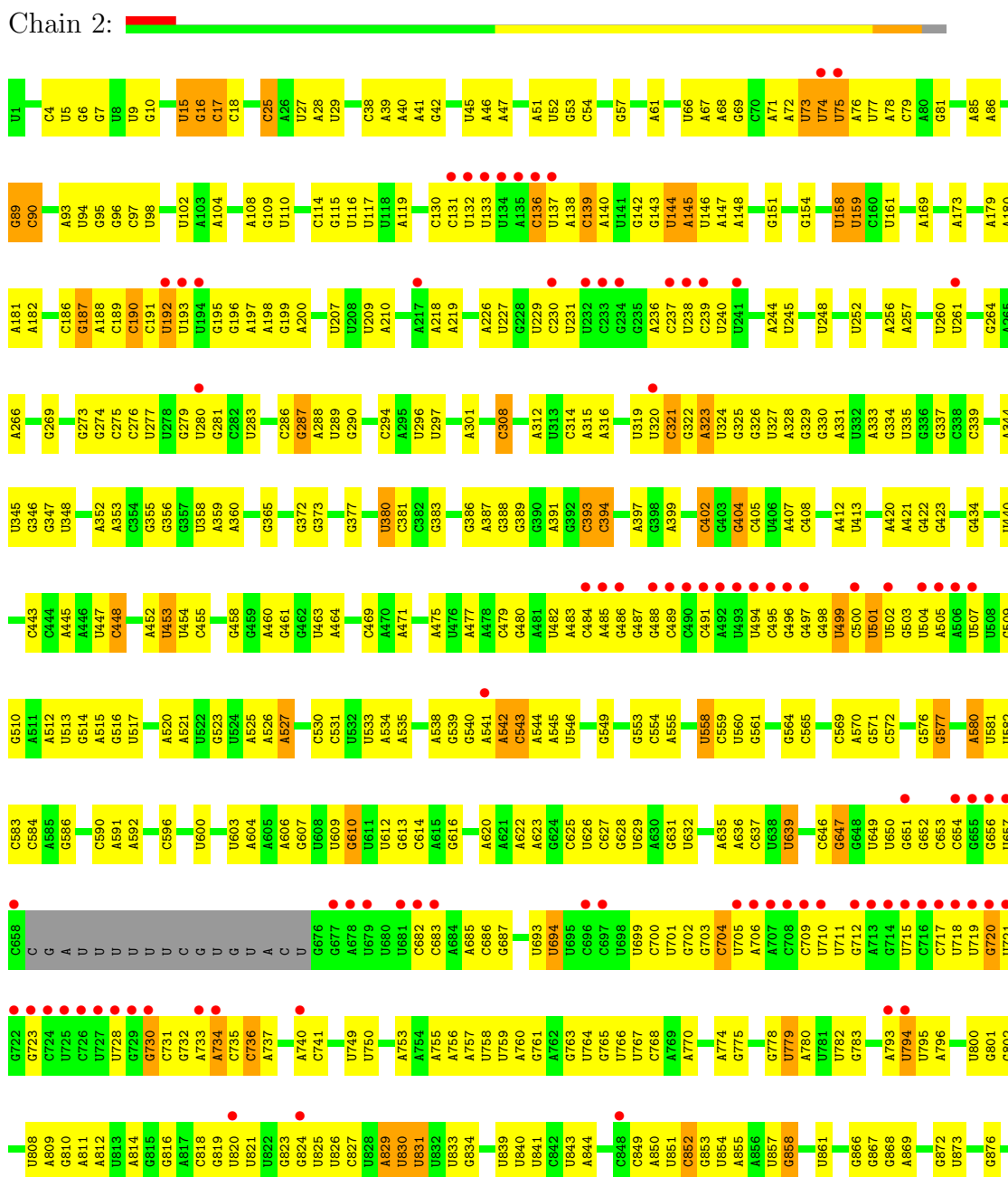


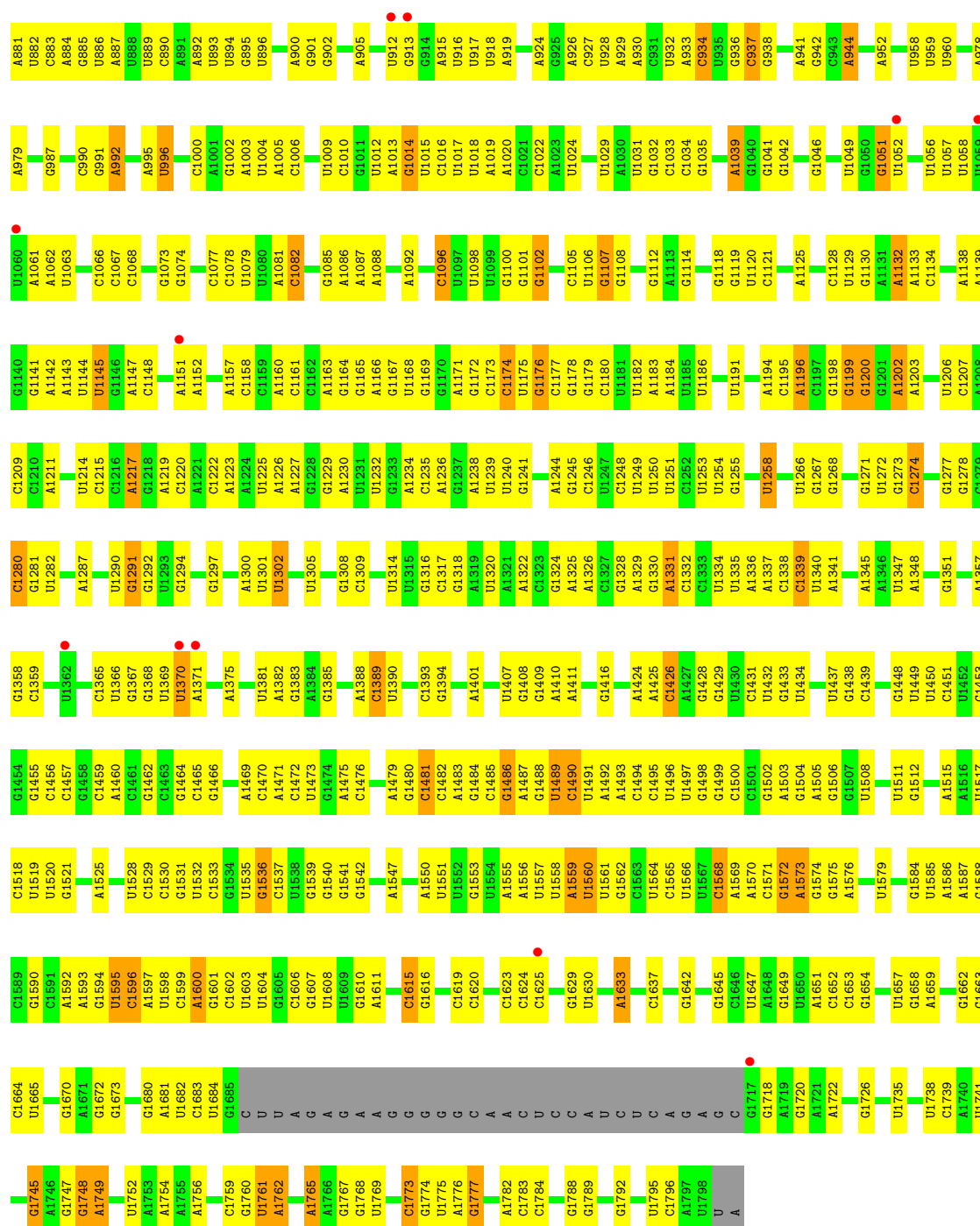
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
88	1	1	39	29	1	9	0	0
88	5	1	39	29	1	9	0	0

3 Residue-property plots

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

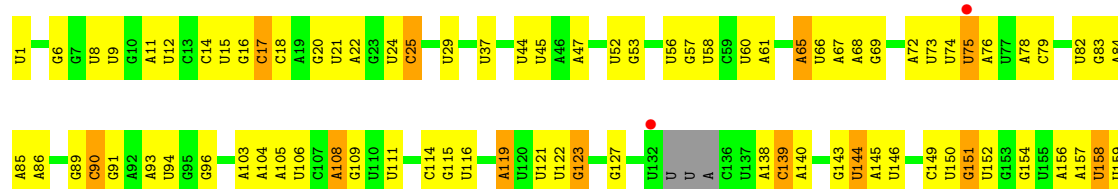
- Molecule 1: *Saccharomyces cerevisiae* chromosome XII cosmid 9634



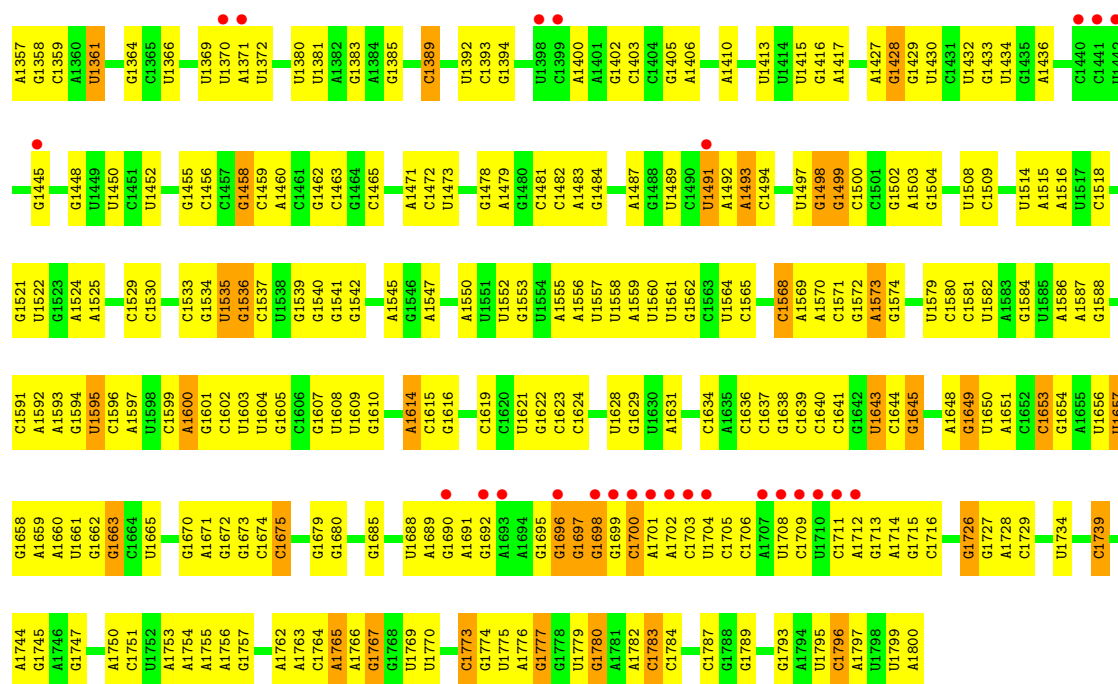


• Molecule 1: *Saccharomyces cerevisiae* chromosome XII cosmid 9634

Chain 6:

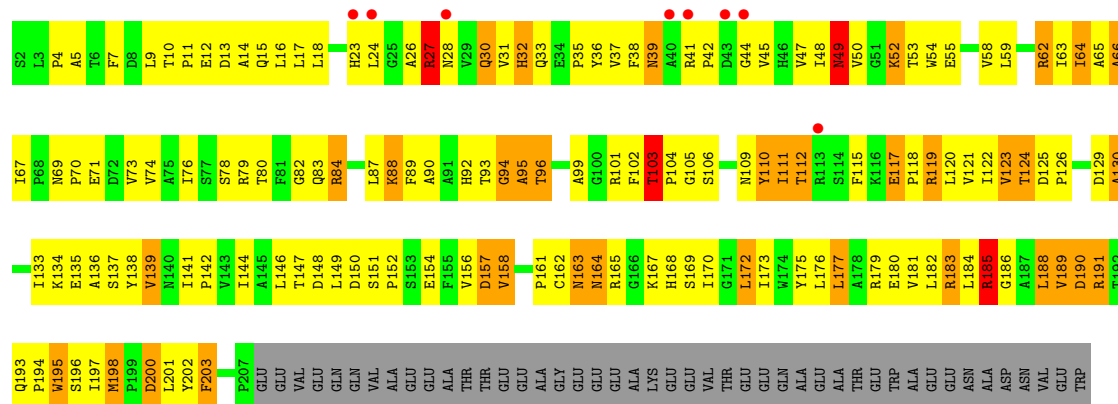


G1268	A1183	C1105	A1026	C950	A793	U711	G648	A570	U499	A421	A341	C283	C160
G1271	C1190	U1106	U1029	A951	U794	G712	U649	G571	C500	C424	G346	C283	U161
G1272	U1191	G1109	A1030	A952	U795	A713	U650	G574	U502	A425	G347	A266	G163
G1273	C1192	G1110	U1031	C956	U800	G714	U651	C575	U503	G426	U267	U267	A164
G1274	A1196	G1111	G1032	C957	G801	U717	C652	G576	U504	A432	U271	A271	G165
C1279	C1197	G1112	C1033	U959	A804	U718	C654	G577	A505	G433	U350	G166	C166
C1280	G1198	A1113	C1034	U959	U805	U719	G655	U578	A506	C433	C351	U272	A169
G1281	G1199	G1114	G1035	U960	U806	G720	G656	U579	U507	C434	A352	G273	U170
G1282	G1200	A1115	A1036	C962	A807	U721	U657	A580	U508	G437	C353	U277	A171
G1283	G1201	G1119	A1039	C962	U808	G722	C658	U581	A511	A437	G354	U278	C176
C1283	A1202	U1120	G1040	U964	U809	G723	C659	C584	A512	A438	G355	U279	A176
C1284	A1203	C1121	G1041	U965	G810	G724	C660	U588	A513	U439	G356	U280	C176
U1285	C1207	G1122	A966	A967	A811	U727	U662	U588	G514	A445	C357	U280	C176
G1288	A1208	G1126	A966	A967	U891	U728	U663	U588	G514	A446	U358	G281	A180
C1209	C1209	G1127	A967	A967	U894	U729	U664	A591	U517	A447	U359	G282	A181
U1293	C1210	G1130	C1045	A970	U895	G730	U665	A592	A518	C448	A360	U283	G187
A1296	A1211	A1131	U1049	A971	U896	G731	U666	U593	A521	C449	G361	U289	A188
A1300	G1212	A1132	G1050	G972	U897	A737	U667	A594	U522	U450	G362	G290	C189
A1309	G1213	A1133	U1054	G973	G824	G738	C668	G595	U523	A451	G363	G291	C190
G1308	A1217	U1135	U1055	G976	U825	G739	U669	G596	U524	U452	G364	U292	C191
C1309	G1218	C1134	U1058	A977	U826	A740	U670	G597	U524	U453	G371	U297	U192
C1220	A1219	U1136	U1059	A978	G901	U745	U671	U598	A525	U454	G372	C298	U193
U1314	G1228	A1137	U1059	A979	G902	U755	U672	U600	A526	C455	G373	A213	A217
U1315	A1224	A1143	A1065	U982	G903	A756	U673	U601	A527	A460	G377	A218	A219
G1316	U1225	U1144	C1066	U982	U829	A757	U674	A601	A528	A471	A378	A312	A220
C1317	G1317	U1145	C1067	G987	U830	U758	U675	G613	G539	U472	A387	A315	A221
G1318	A1227	U1146	U1068	U988	U831	G761	A684	A615	A541	A475	G382	A316	A222
A1321	G1228	A1151	C1068	U988	U832	A755	U678	G616	A542	U476	G383	G317	U223
A1322	G1229	A1152	C1072	C990	U836	A756	U679	A619	A544	U477	G384	C309	C224
C1323	A1230	G1153	G1073	G991	G837	U757	U680	A620	A545	A478	A385	U320	A225
G1324	U1231	G1154	C1074	A992	U841	U758	C682	A621	U546	C479	G386	C321	G228
A1325	A1234	G1155	C1075	A993	U842	G761	A685	A622	U547	G480	G388	A393	U229
A1326	C1235	U1156	U1079	C1000	U843	U765	U686	G624	G548	A483	G389	U324	C230
C1327	G1237	C1158	U1080	A1001	A844	U766	C687	C625	A550	C484	A401	G325	U231
G1330	A1238	U1159	G1002	G845	U845	U767	U688	U626	G553	A485	C402	A328	C232
C1332	U1239	C1161	A1003	U846	G846	U767	U689	C627	C554	G486	G403	G329	G234
U1341	U1240	A1166	U1004	A847	U847	U767	C700	U629	A555	G487	G404	G330	G235
G1342	G1241	G1167	A1005	C948	C948	A770	U701	A630	A556	C489	C405	A331	A236
A1343	A1244	U1167	U1009	C949	C949	A771	G702	A635	G557	C490	U406	U332	C237
U1344	G1245	A1171	C1010	G853	U854	G772	U695	A636	U558	C491	C408	U333	U238
C1336	C1246	G1172	G1011	U854	C696	C773	C697	C637	U563	A492	A412	U335	U240
G1339	U1248	C1173	U1012	A855	U698	G778	U699	C628	G554	U493	U336	G336	U241
U1340	U1249	A1091	A1013	A856	U699	U782	U700	G628	A555	U494	G337	C338	U242
A1341	U1250	C1174	G1014	U857	U699	U783	C701	U629	A556	C488	A416	G338	G246
U1342	U1251	U1175	U1015	G858	U699	U784	G702	A630	G557	C489	G417	C339	U247
U1343	C1252	G1176	C1016	A859	U699	U785	U701	A630	U558	C490	G418	U340	C1356
U1344	U1253	C1177	U1017	A862	U699	U786	G703	A635	U558	C491	A418	U341	C1355
U1345	U1254	U1178	U1018	A863	U699	U787	C704	A636	U558	C492	A419	U342	C1354
G1351	G1255	G1179	A1019	U864	U699	U788	U705	C637	U558	U493	A419	U343	C1353
A1256	A1256	C1180	U1100	U865	U699	U789	A706	U638	G564	U494	A419	U344	C1352
U1257	U1257	U1101	G1021	U866	U699	U790	A707	U639	G565	C495	A419	U345	C1351
U1258	U1258	U1102	C1022	U867	U699	U791	C708	U640	G566	C496	A419	U346	C1350
		U1103	U1023	U868	U699	U792	U710	G647	G569	C497	A419	U347	C1349



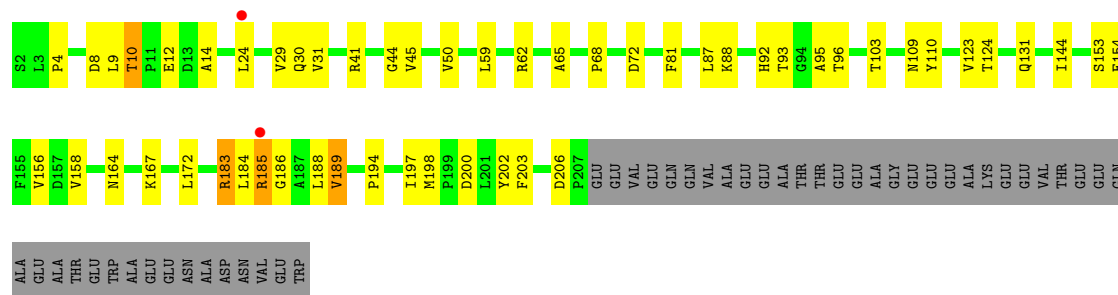
• Molecule 2: 40S ribosomal protein S0-A

Chain S0:



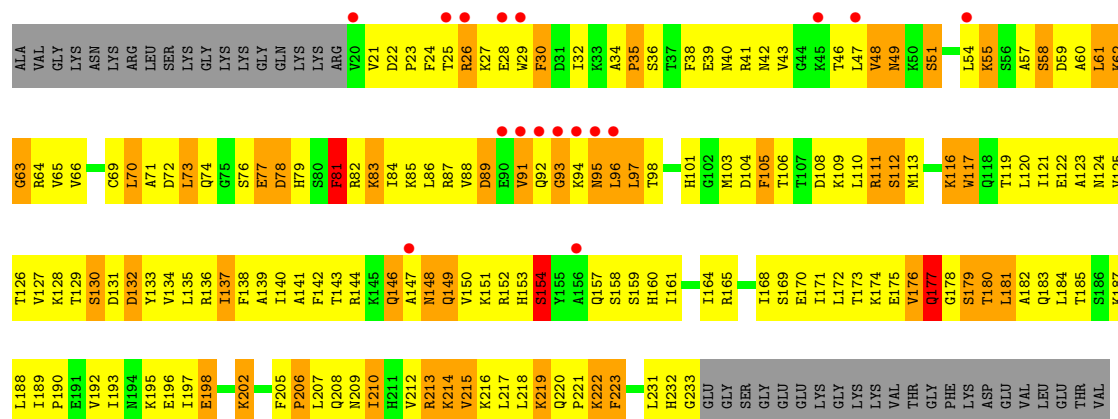
• Molecule 2: 40S ribosomal protein S0-A

Chain s0:



• Molecule 3: 40S ribosomal protein S1-A

Chain S1:



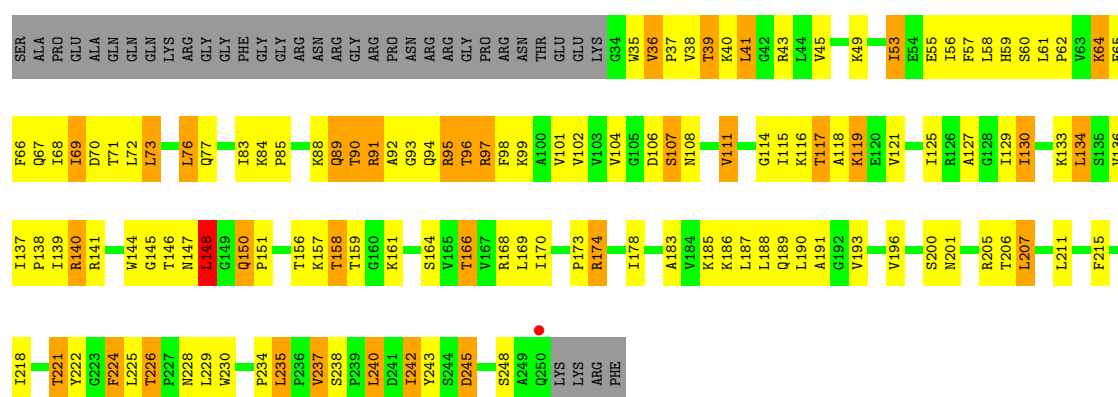
- Molecule 3: 40S ribosomal protein S1-A

Chain s1:



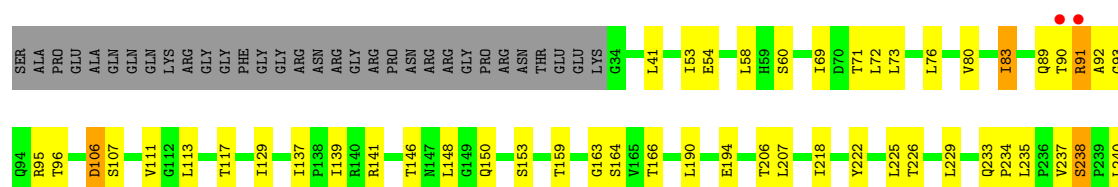
- Molecule 4: 40S ribosomal protein S2

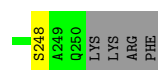
Chain S2:



- Molecule 4: 40S ribosomal protein S2

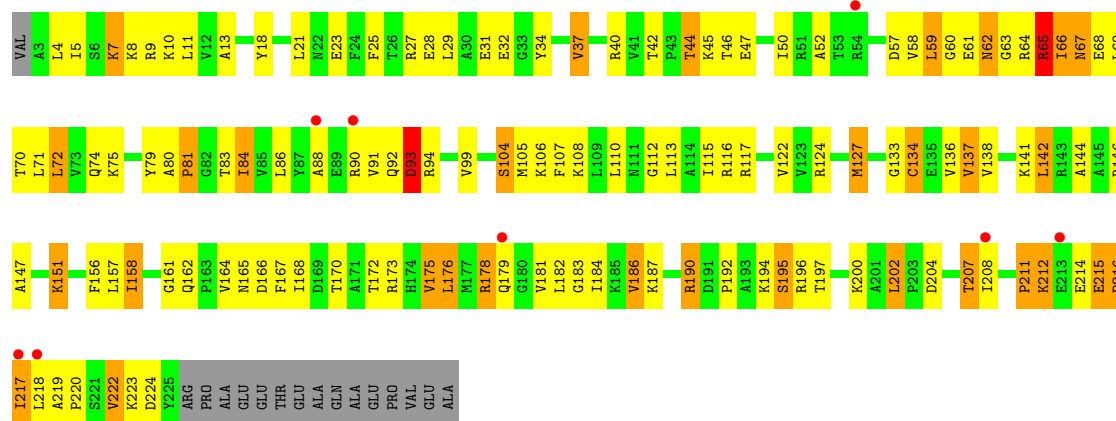
Chain s2:





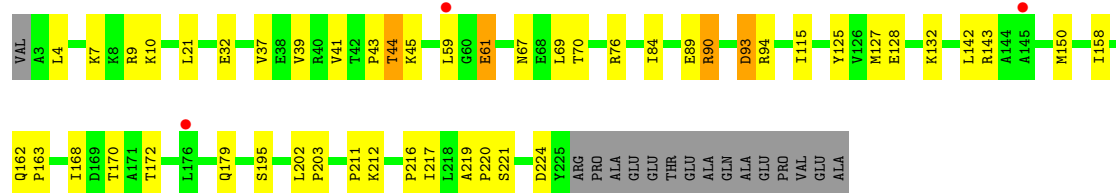
• Molecule 5: 40S ribosomal protein S3

Chain S3:



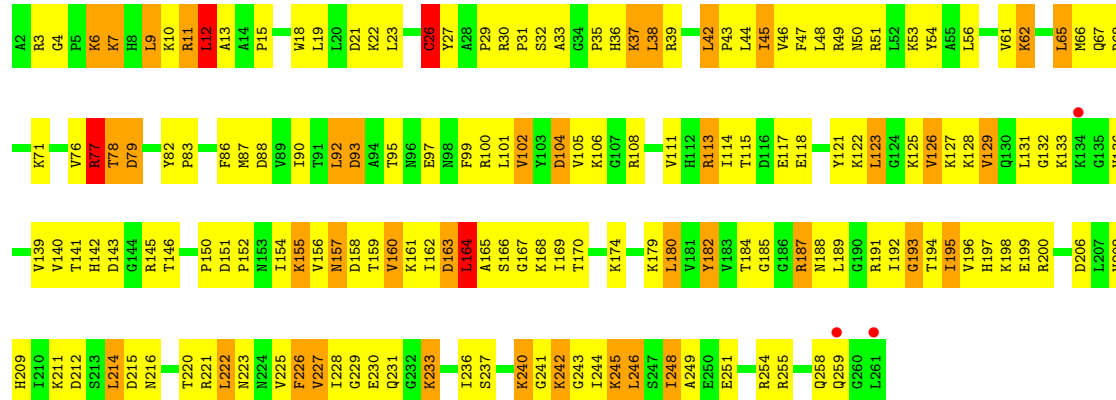
• Molecule 5: 40S ribosomal protein S3

Chain s3:



• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



• Molecule 6: 40S ribosomal protein S4-A

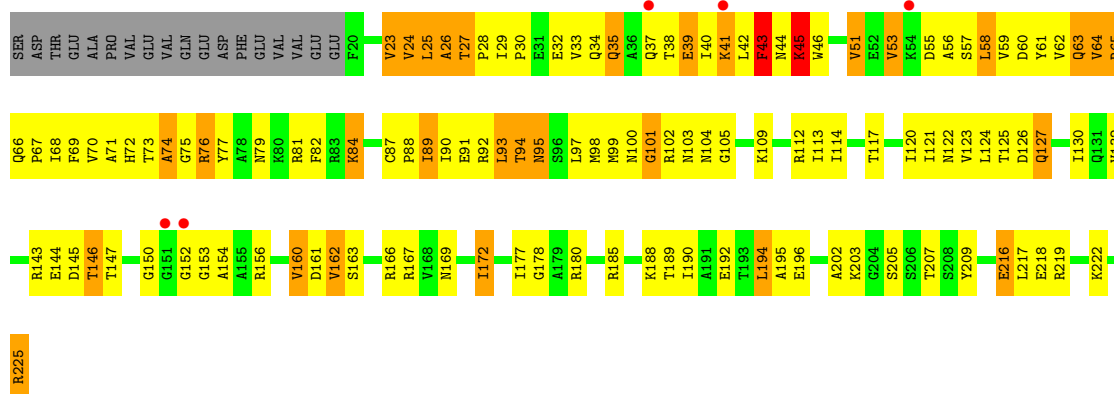
Chain s4:





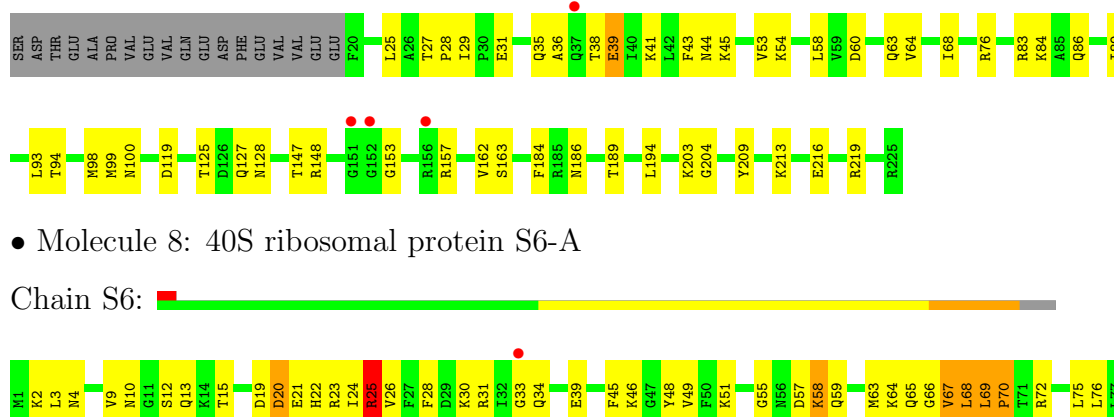
• Molecule 7: 40S ribosomal protein S5

Chain S5:



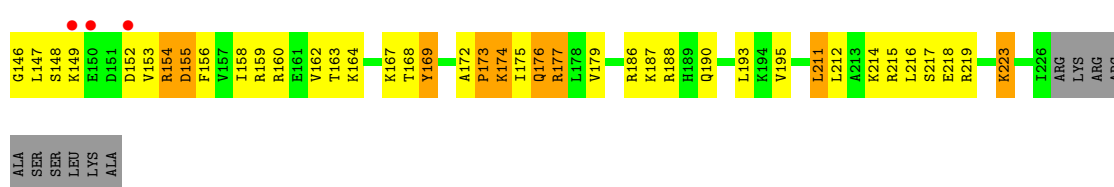
• Molecule 7: 40S ribosomal protein S5

Chain s5:



• Molecule 8: 40S ribosomal protein S6-A

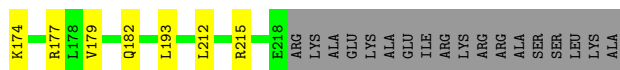
Chain S6:



• Molecule 8: 40S ribosomal protein S6-A

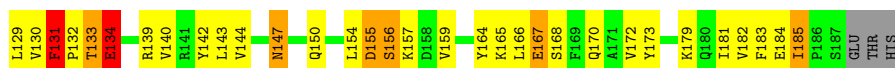
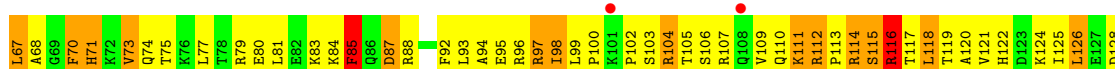
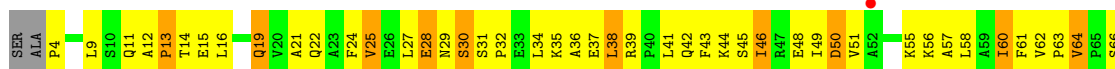
Chain s6:





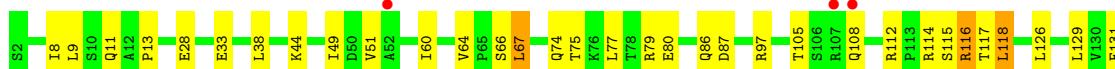
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



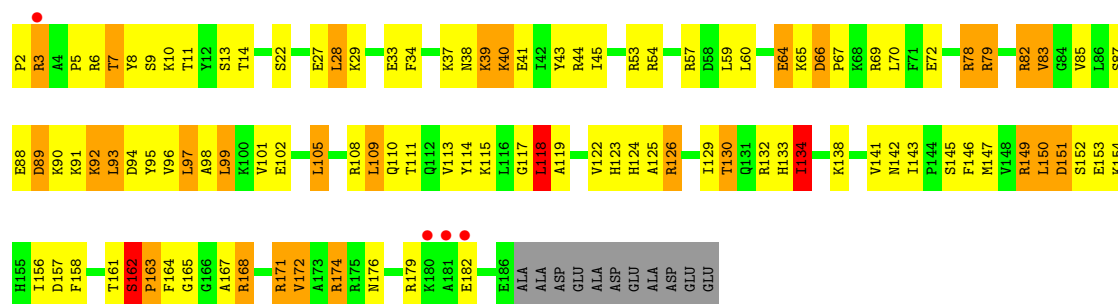
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



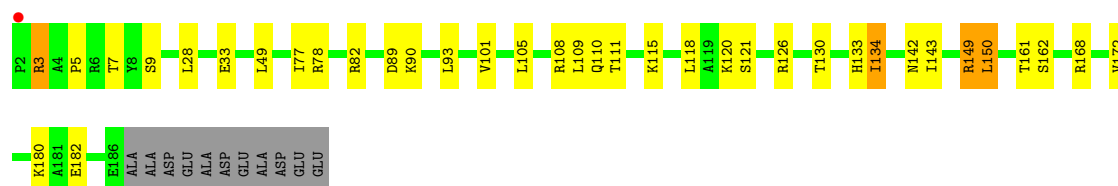
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



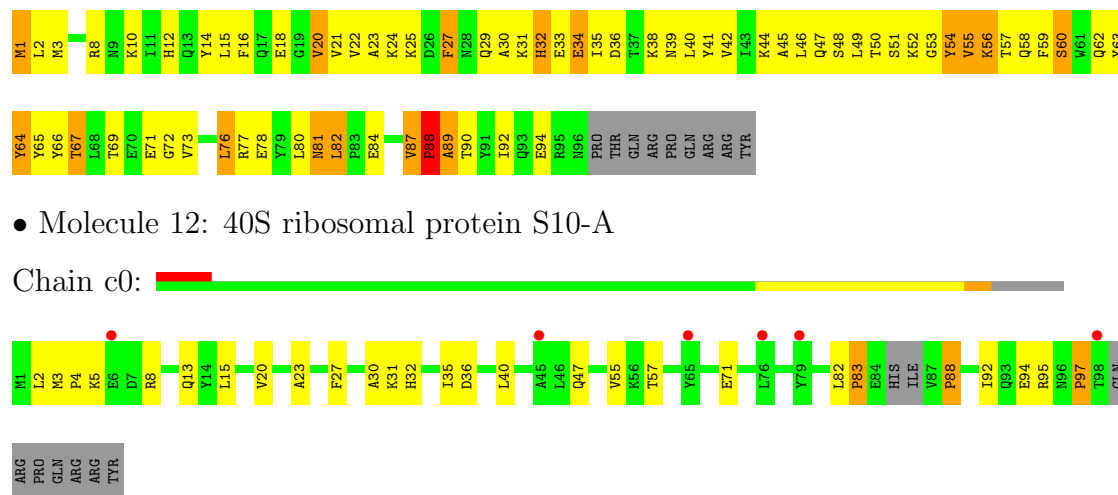
- Molecule 11: 40S ribosomal protein S9-A

Chain s9:



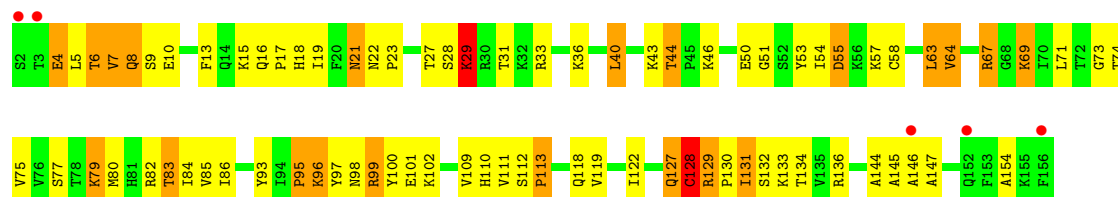
- Molecule 12: 40S ribosomal protein S10-A

Chain C0:



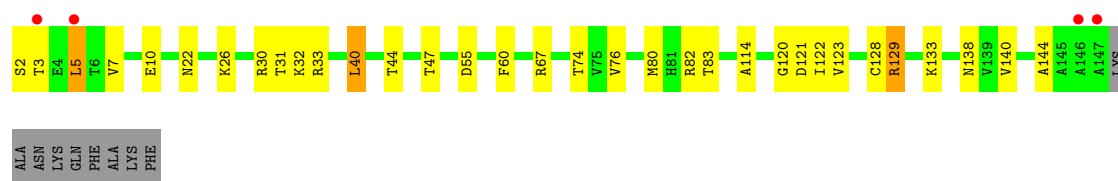
- Molecule 13: 40S ribosomal protein S11-A

Chain C1:



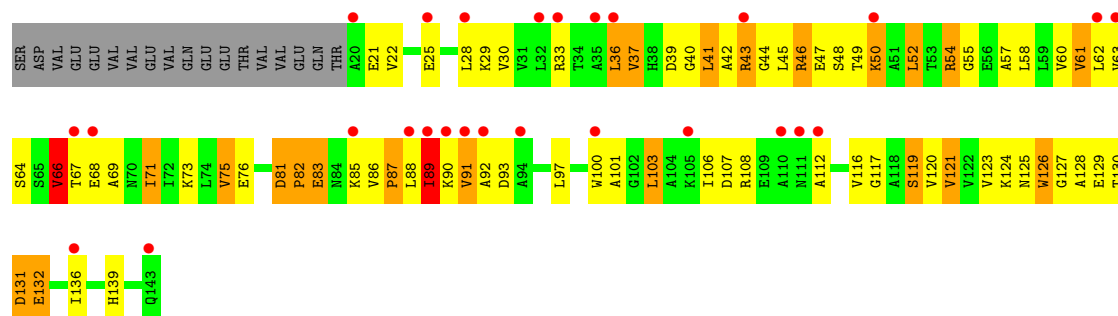
- Molecule 13: 40S ribosomal protein S11-A

Chain c1:



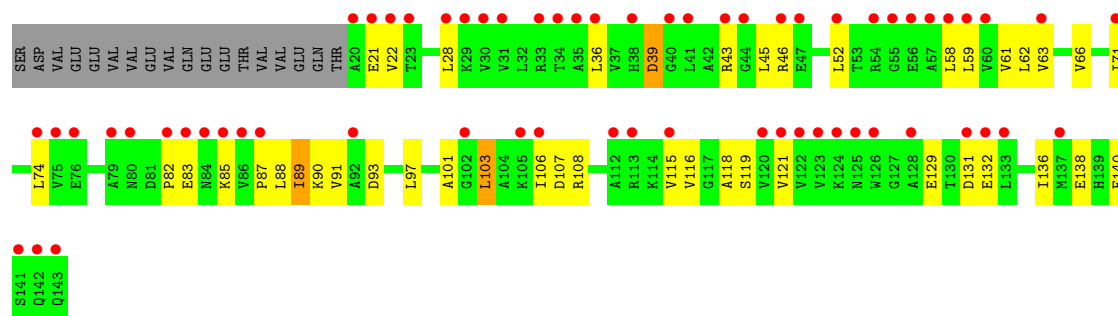
• Molecule 14: 40S ribosomal protein S12

Chain C2:



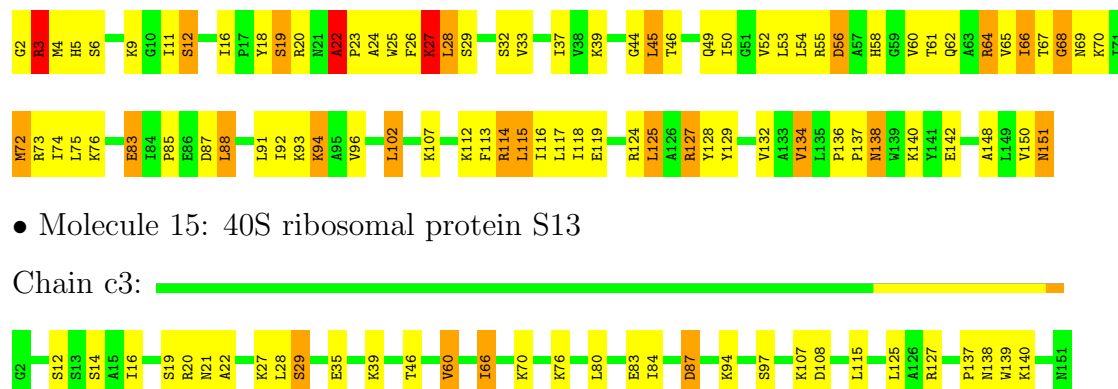
• Molecule 14: 40S ribosomal protein S12

Chain c2:



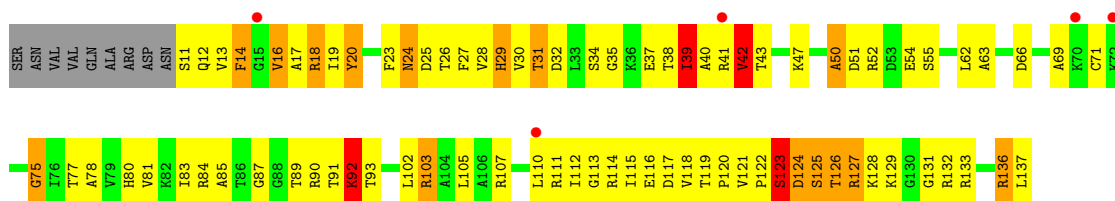
• Molecule 15: 40S ribosomal protein S13

Chain C3:



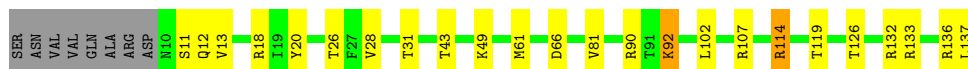
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



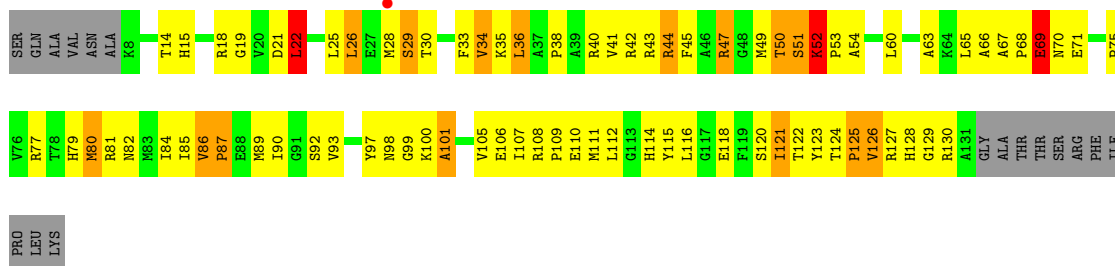
- Molecule 16: 40S ribosomal protein S14-A

Chain c4:



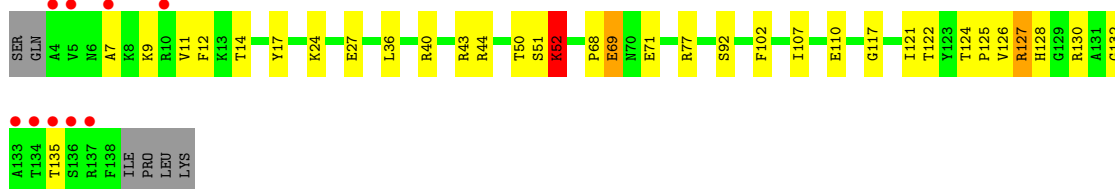
- Molecule 17: 40S ribosomal protein S15

Chain C5:



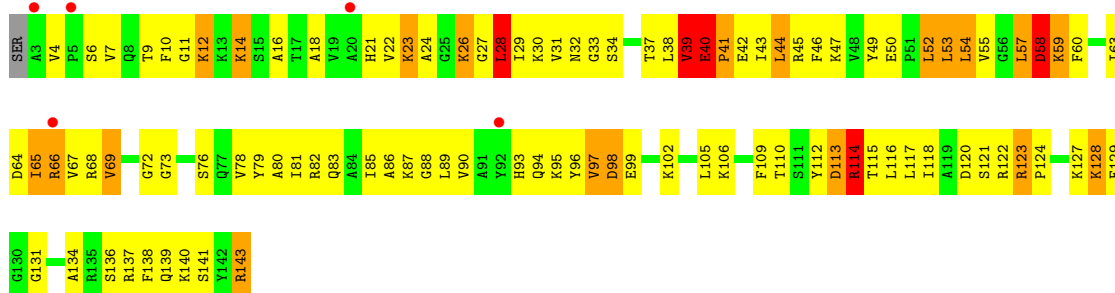
- Molecule 17: 40S ribosomal protein S15

Chain c5:



- Molecule 18: 40S ribosomal protein S16-A

Chain C6:



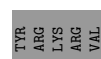
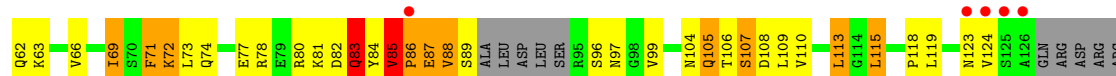
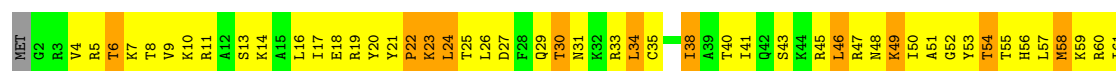
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:



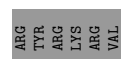
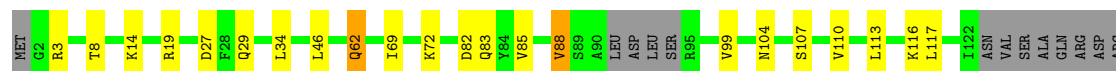
• Molecule 19: 40S ribosomal protein S17-A

Chain C7:



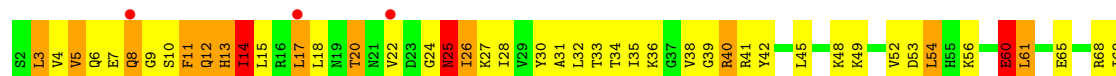
• Molecule 19: 40S ribosomal protein S17-A

Chain c7:



• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



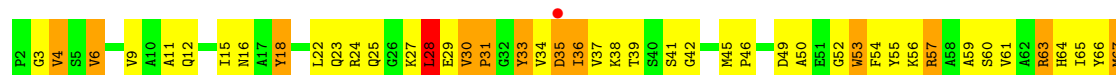
• Molecule 20: 40S ribosomal protein S18-A

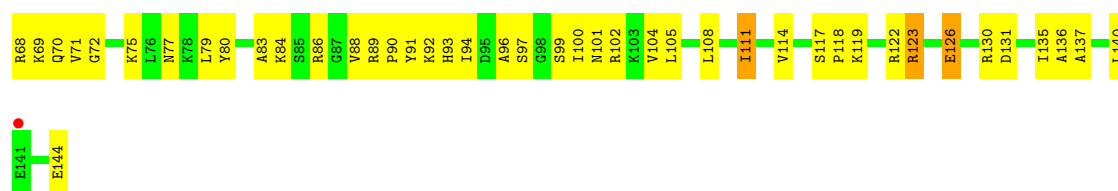
Chain c8:



• Molecule 21: 40S ribosomal protein S19-A

Chain C9:





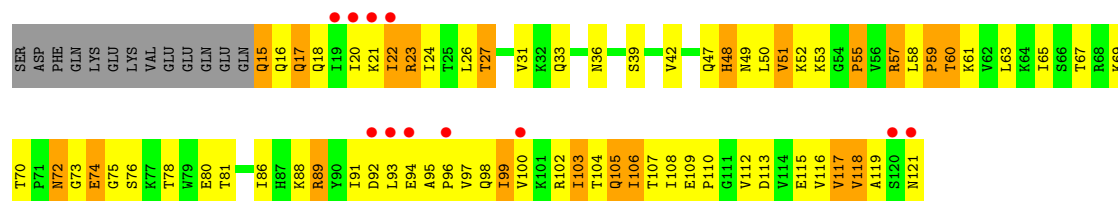
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



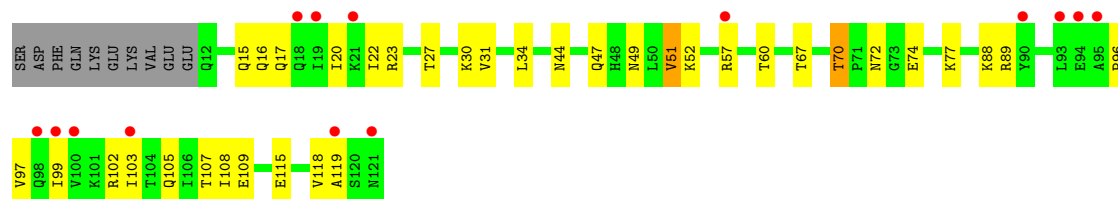
- Molecule 22: 40S ribosomal protein S20

Chain D0:



- Molecule 22: 40S ribosomal protein S20

Chain d0:



- Molecule 23: 40S ribosomal protein S21-A

Chain D1:



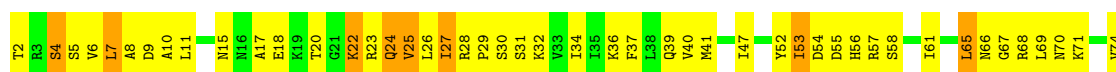
- Molecule 23: 40S ribosomal protein S21-A

Chain d1:



- Molecule 24: 40S ribosomal protein S22-A

Chain D2:



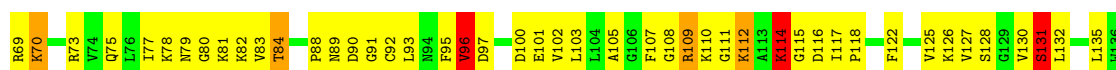
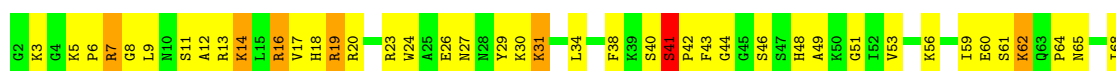
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:



- Molecule 25: 40S ribosomal protein S23-A

Chain D3:



- Molecule 25: 40S ribosomal protein S23-A

Chain d3:



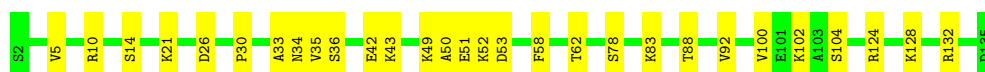
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:



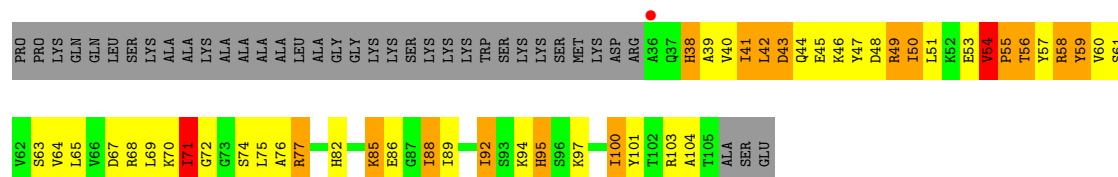
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:



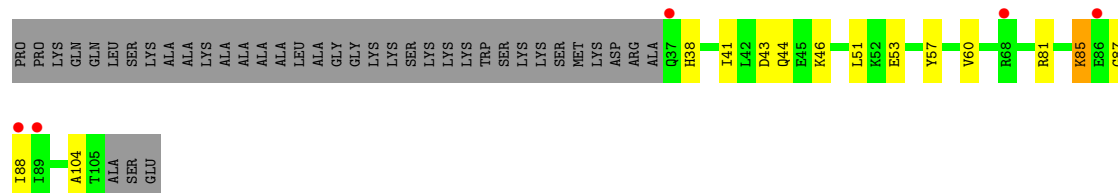
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:



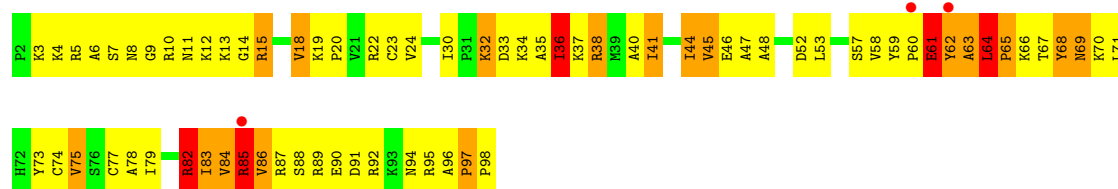
• Molecule 27: 40S ribosomal protein S25-A

Chain d5:



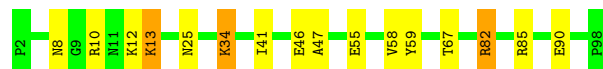
• Molecule 28: 40S ribosomal protein S26-B

Chain D6:



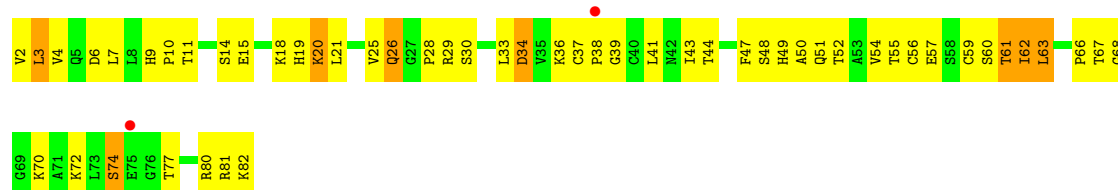
• Molecule 28: 40S ribosomal protein S26-B

Chain d6:



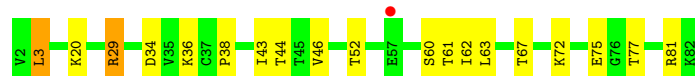
• Molecule 29: 40S ribosomal protein S27-A

Chain D7:



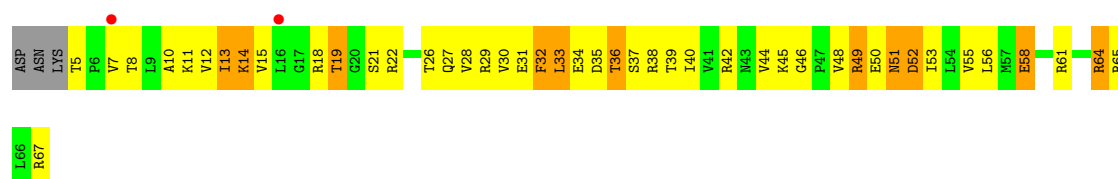
• Molecule 29: 40S ribosomal protein S27-A

Chain d7:



• Molecule 30: 40S ribosomal protein S28-A

Chain D8:



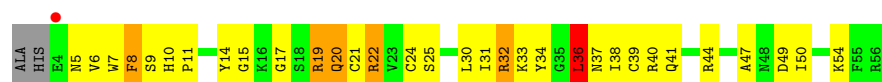
- Molecule 30: 40S ribosomal protein S28-A

Chain d8:



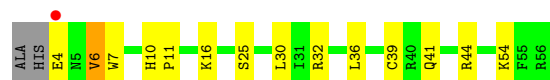
- Molecule 31: 40S ribosomal protein S29-A

Chain D9:



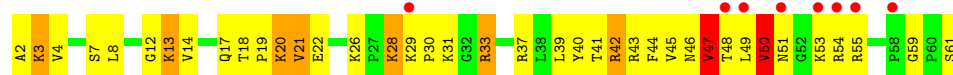
- Molecule 31: 40S ribosomal protein S29-A

Chain d9:



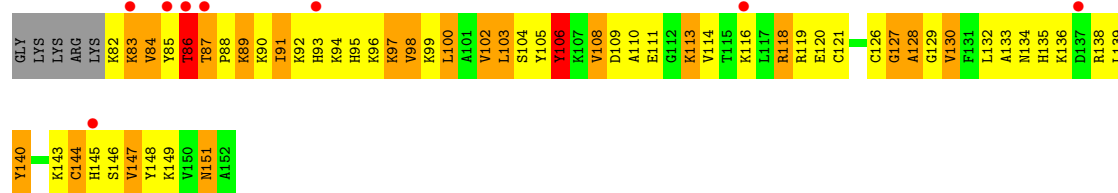
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:



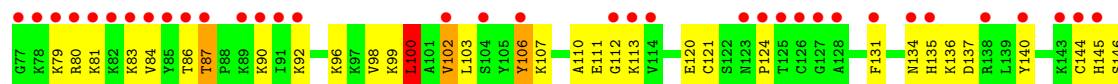
- Molecule 33: Ubiquitin-40S ribosomal protein S31

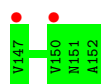
Chain E1:



- Molecule 33: Ubiquitin-40S ribosomal protein S31

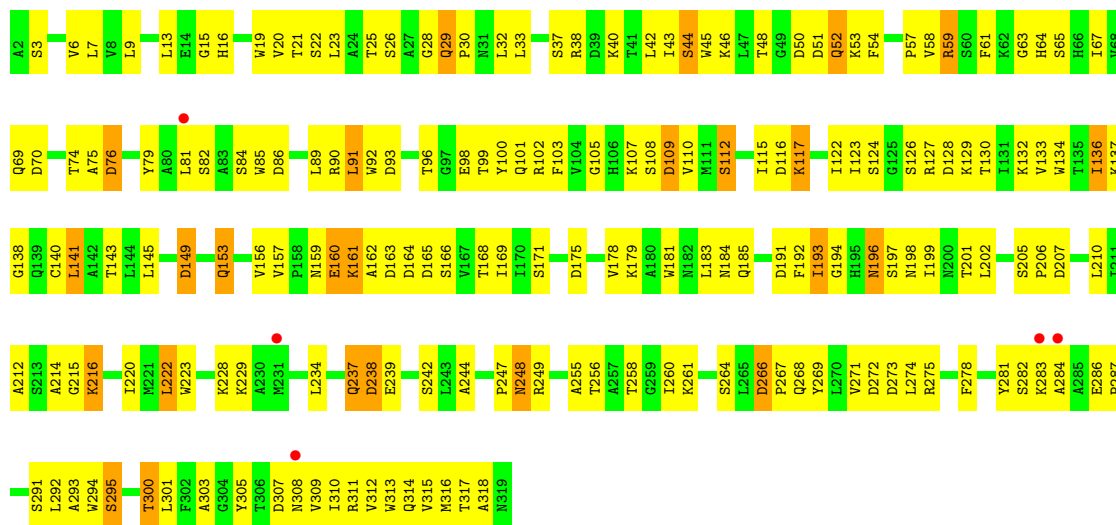
Chain e1:





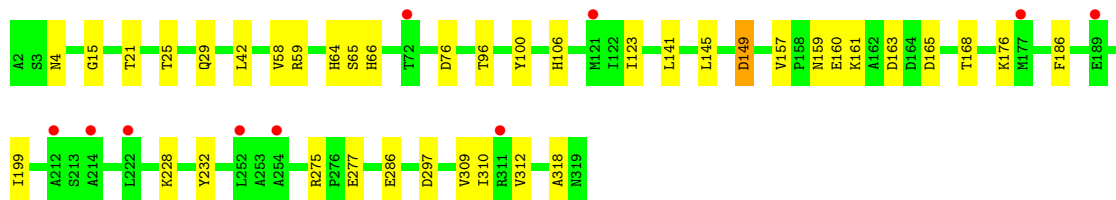
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



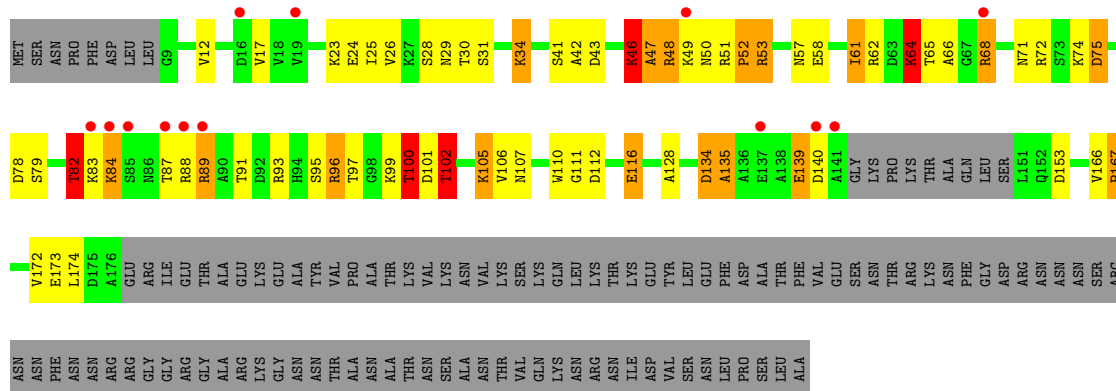
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



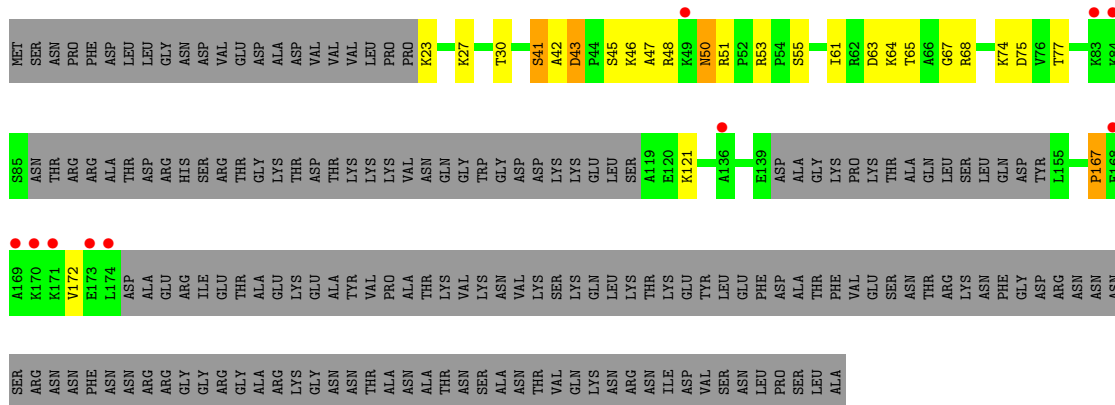
- Molecule 35: Suppressor protein STM1

Chain SM:



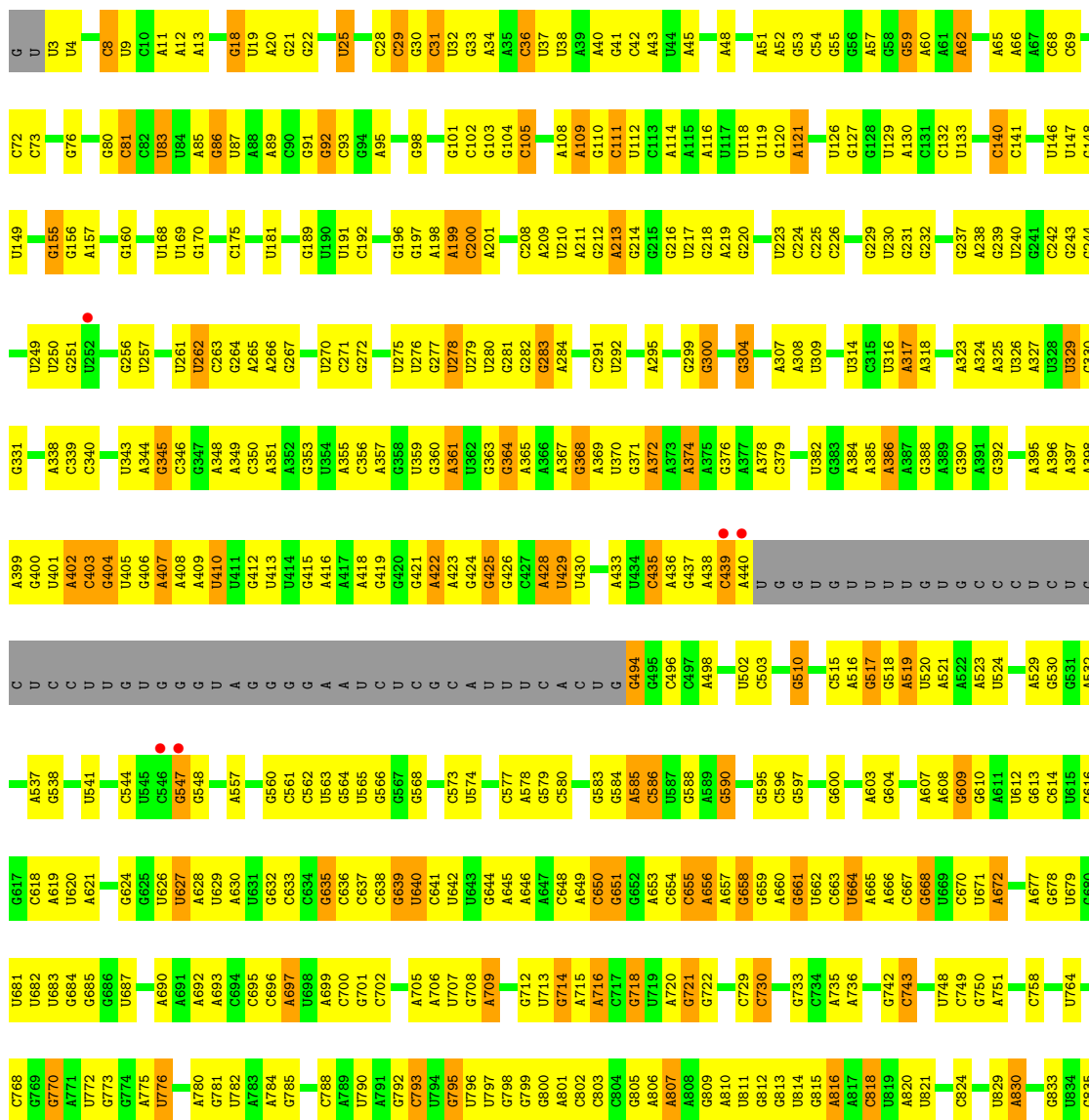
- Molecule 35: Suppressor protein STM1

Chain sM:



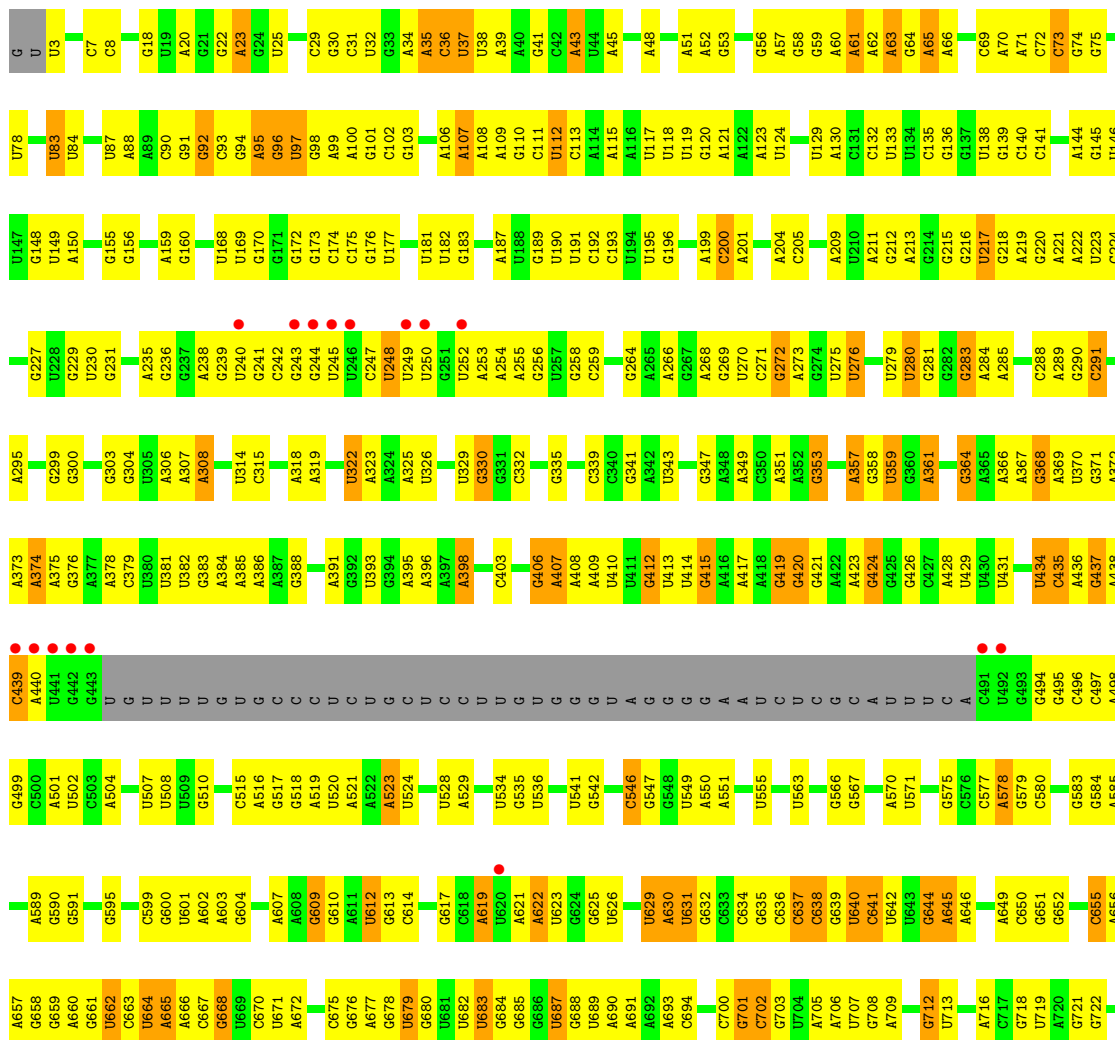
● Molecule 36: TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

Chain 1:



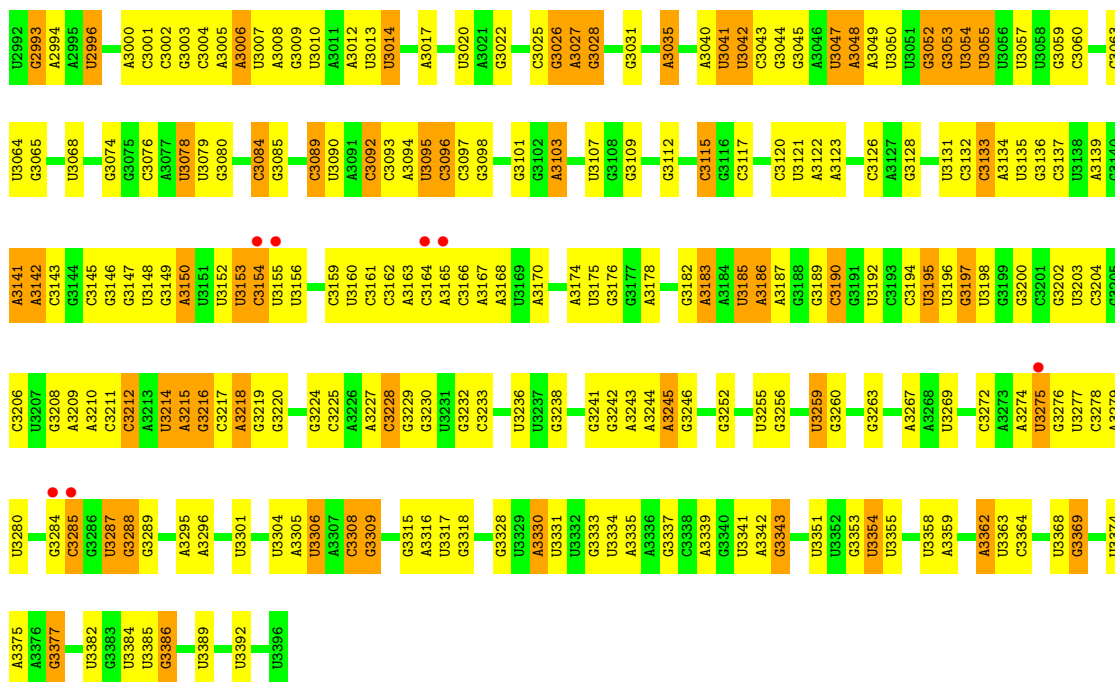
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A1913	U1632	U1741	C1556	C1478	G1408	C1390	A1273	A1204	C1140	A1064	C977	G910	A838
G1914	C1633	U1742	U1479	U1479	G1409	G1340	A1274	A1205	C1141	A1065	C978	C911	A839
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A1933	A1846	U1765	A1575	C1496	C1426	U1356	U1293	G1227	G1156	U1094	G999	A863	A864
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G1939	A1850	G1769	A1504	U1504	U1430	G1362	C1297	G1231	C1160	A1098	G934	A871	A872
C1940	G1851	C1770	A1505	A1506	G1431	A1363	U1298	C1232	G1161	A1099	U1007	A873	A874
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U3045	C2832	G2751	C2666	C2597	C	U2458	C2383	U2319	C2248	G2160	A	C
C3046	G2833	U2752	G2667	U2598	C	U2459	C2384	A2320	U2249	U2161	A	U
A3047	C2834	A2753	A2668	C2599	C	U2460	A2385	G2322	G2250	C2162	A	C
U3048	G2835	G2754	U2669	C2600	C	U2461	C2386	G2323	G2251	C2163	U	C
A3049	C2836	C2755	A2670	U2601	C	U2462	C2387	A2324	G2252	A2164	U	C
	A2837	U2756	U2603	G2602	C	U2463	C2388	G2325	G2253	G2165	A	U
	C2840	U2757	U2604	U2603	C	U2464	C2389	A2326	U2254	U2170	A2093	C
			U2605	G2605	C	U2465	C2390	U2328	A2255	G2094	G2095	C



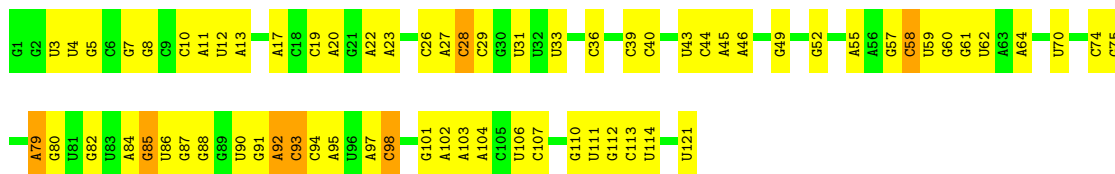






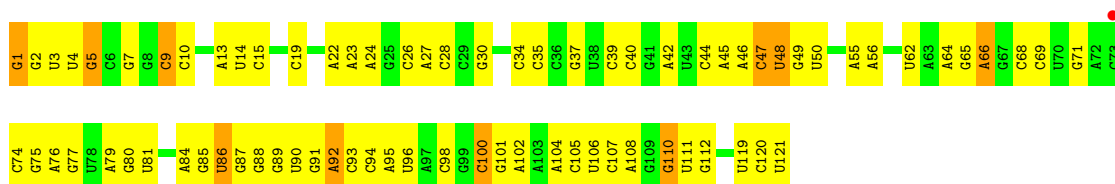
- Molecule 37: TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

Chain 3:



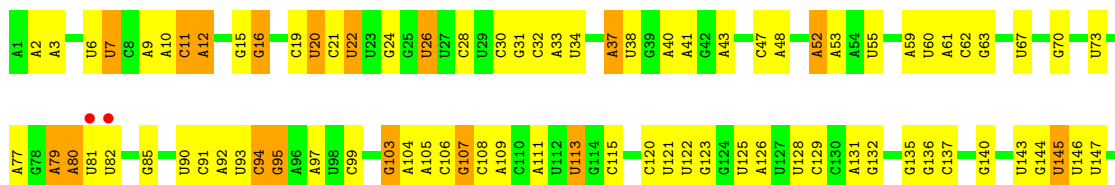
- Molecule 37: TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

Chain 7:



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

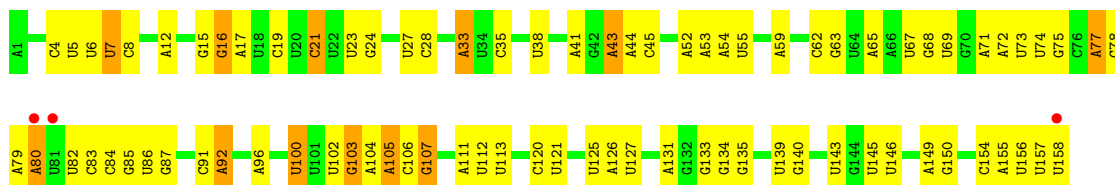
Chain 4:





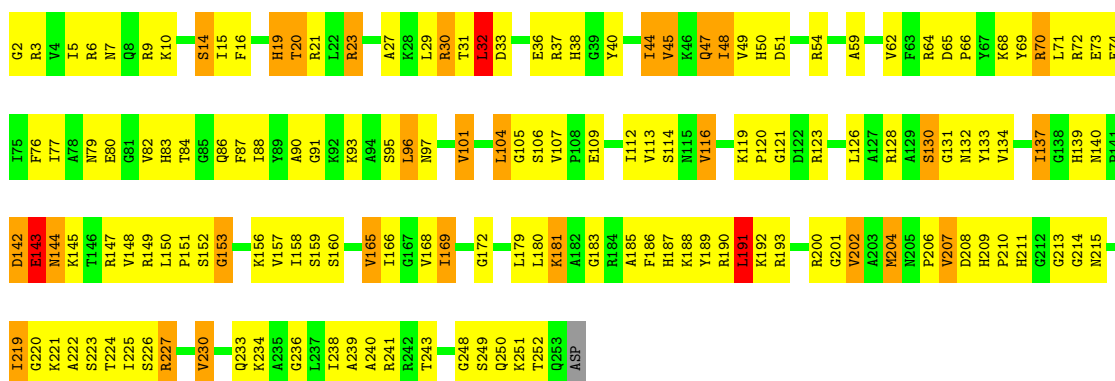
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 8:



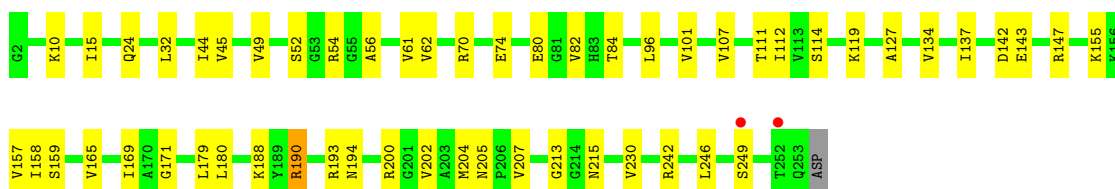
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



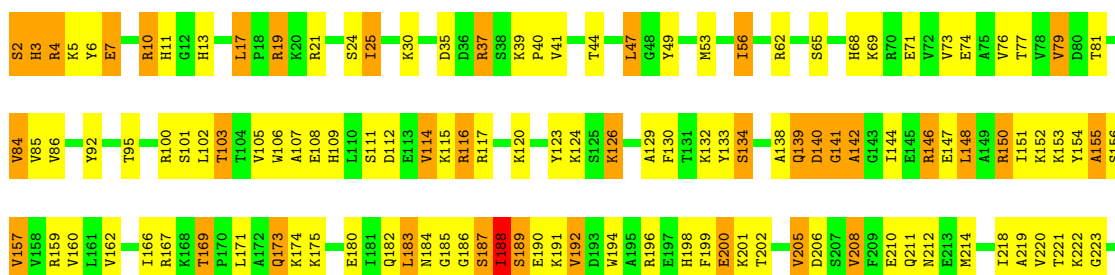
- Molecule 39: 60S ribosomal protein L2-A

Chain l2:



- Molecule 40: 60S ribosomal protein L3

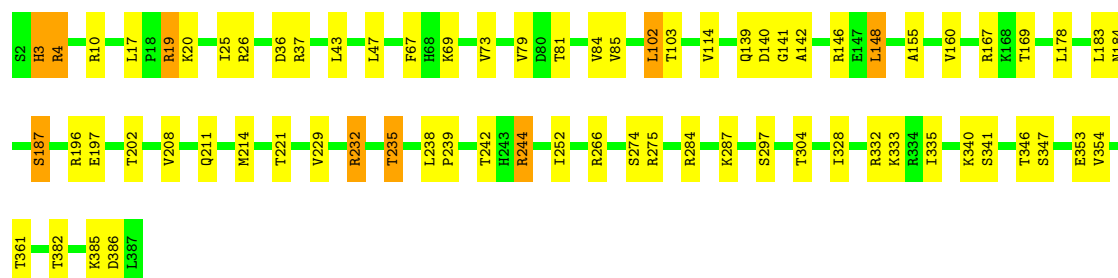
Chain L3:





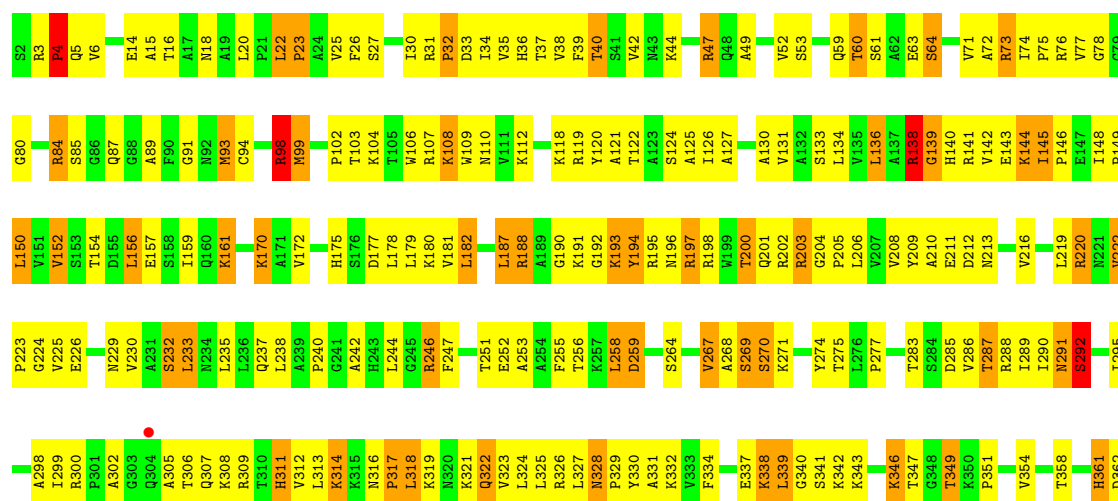
• Molecule 40: 60S ribosomal protein L3

Chain l3:



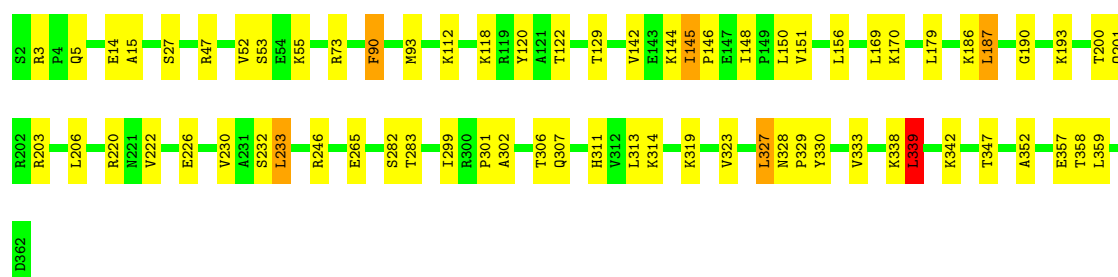
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



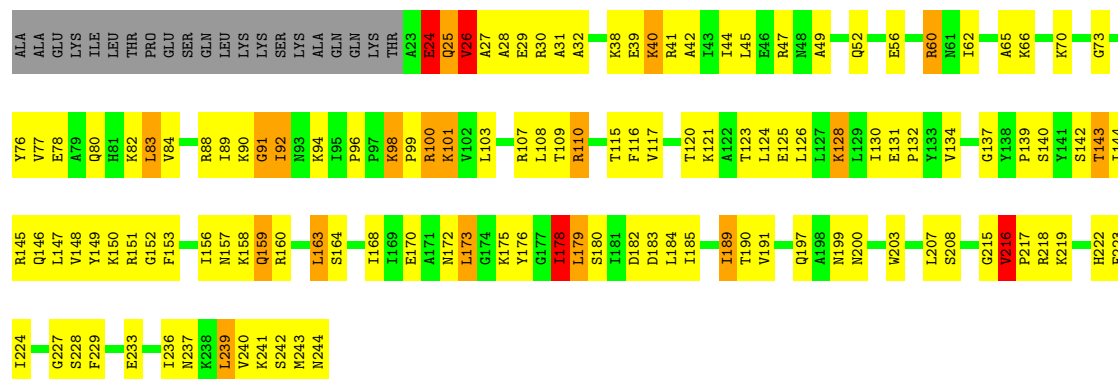
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:



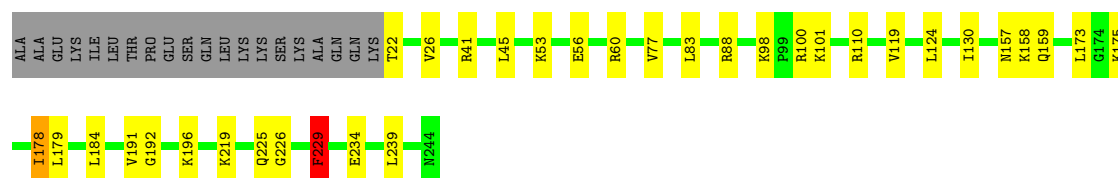
- Molecule 44: 60S ribosomal protein L7-A

Chain L7:



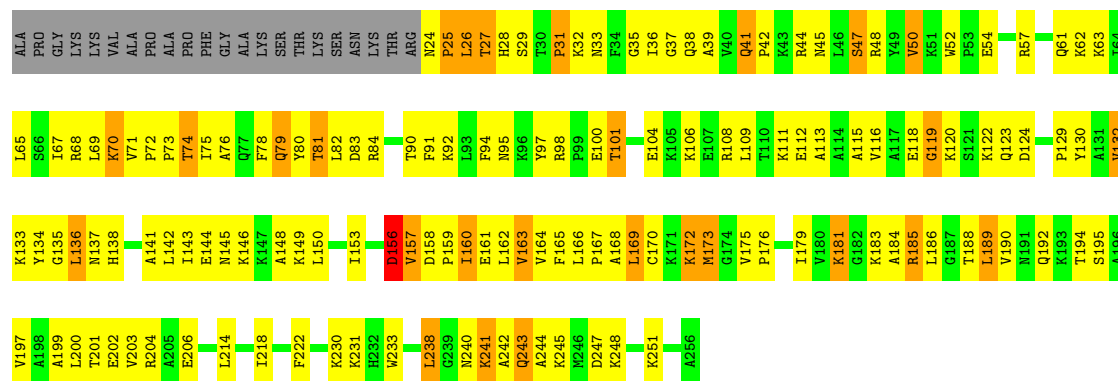
• Molecule 44: 60S ribosomal protein L7-A

Chain l7:



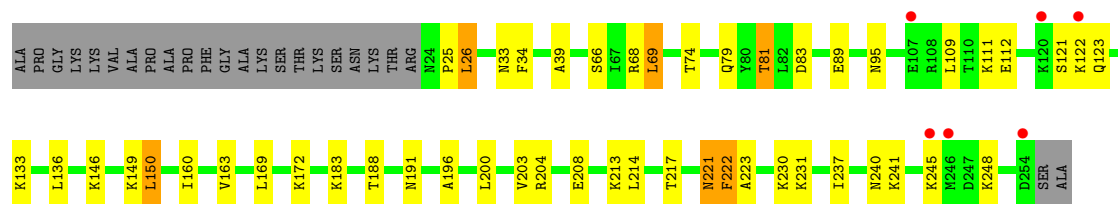
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



• Molecule 45: 60S ribosomal protein L8-A

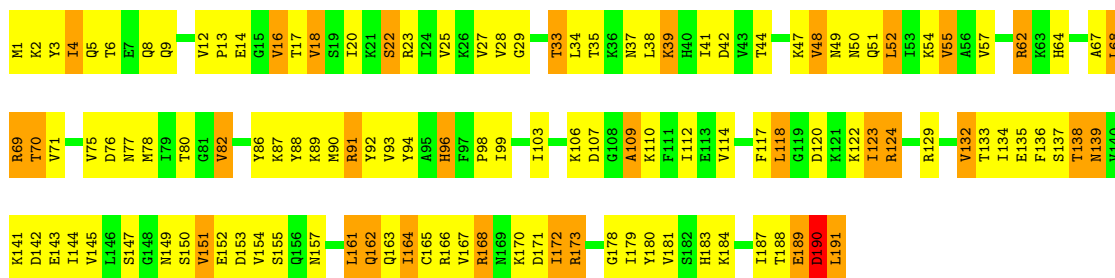
Chain l8:



• Molecule 46: 60S ribosomal protein L9-A

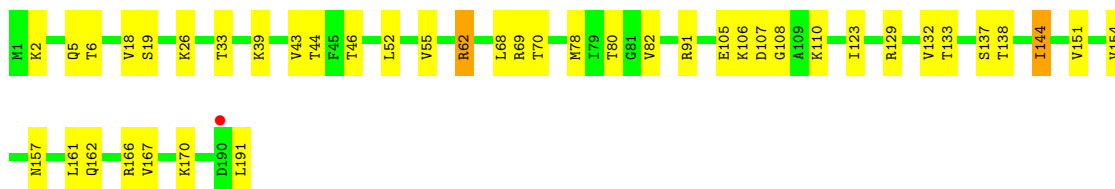
Chain L9:





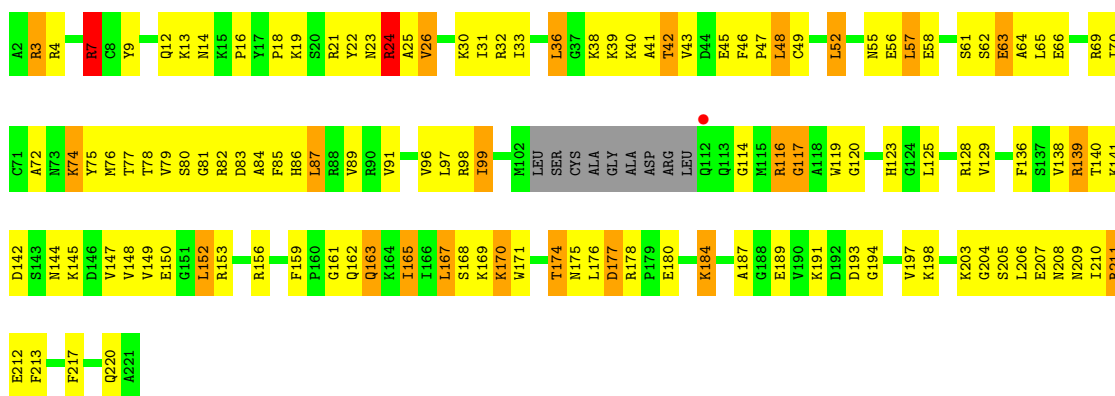
- Molecule 46: 60S ribosomal protein L9-A

Chain 19:



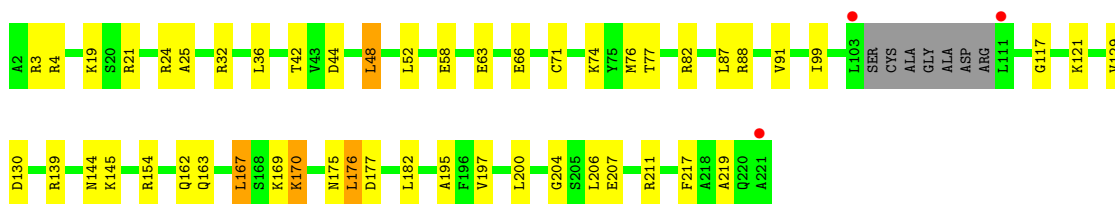
- Molecule 47: 60S ribosomal protein L10

Chain M0:



- Molecule 47: 60S ribosomal protein L10

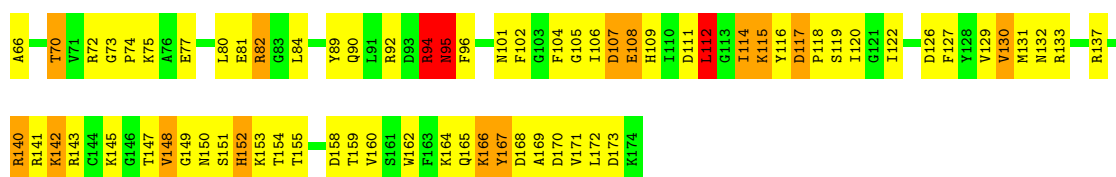
Chain m0: 



- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 





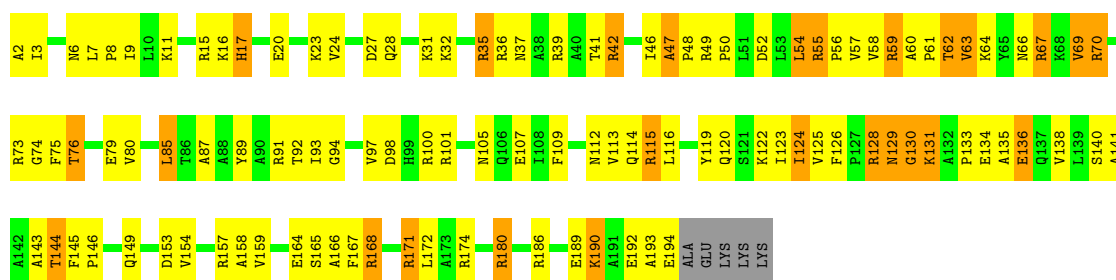
- Molecule 48: 60S ribosomal protein L11-B

Chain m1:



- Molecule 49: 60S ribosomal protein L13-A

Chain M3:



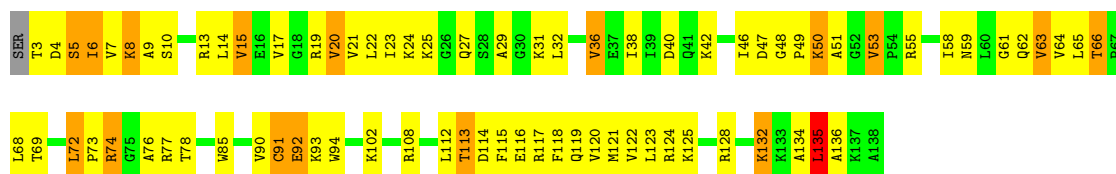
- Molecule 49: 60S ribosomal protein L13-A

Chain m3:



- Molecule 50: 60S ribosomal protein L14-A

Chain M4:



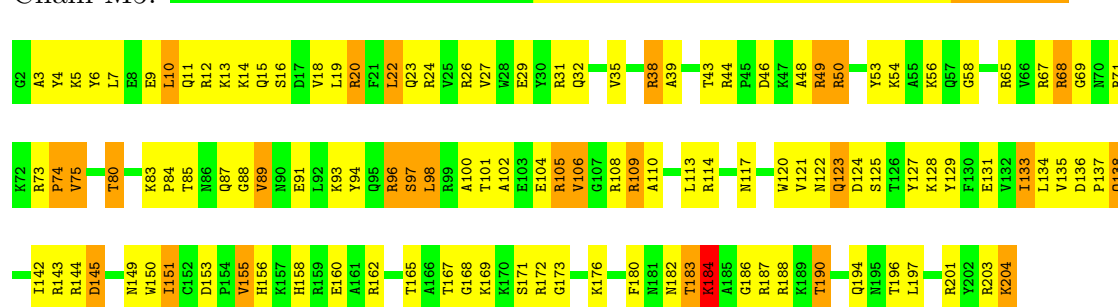
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:



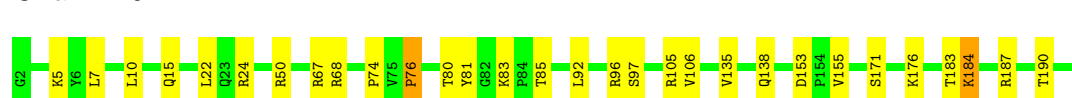
- Molecule 51: 60S ribosomal protein L15-A

Chain M5:



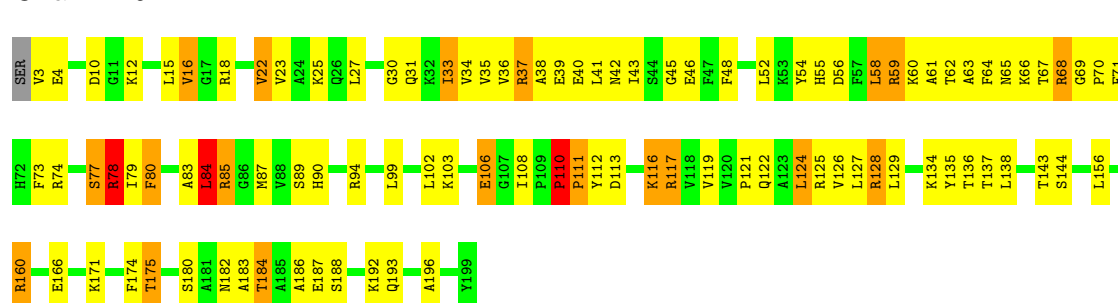
- Molecule 51: 60S ribosomal protein L15-A

Chain m5:



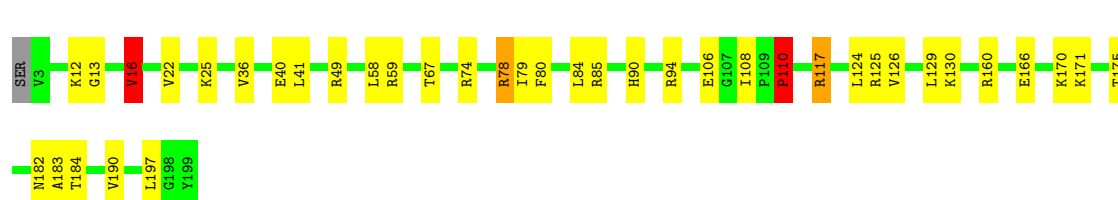
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:



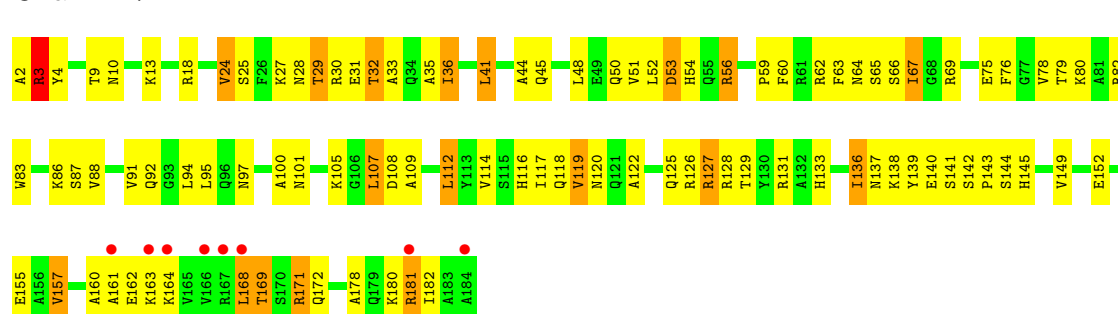
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:



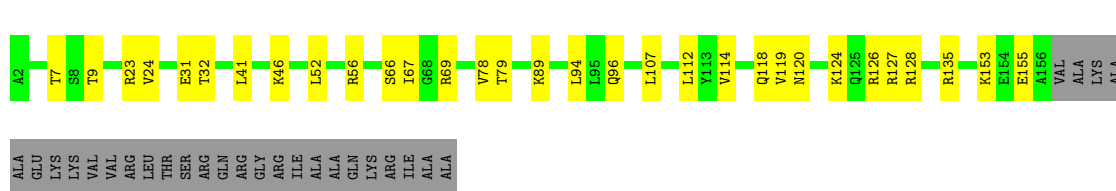
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:



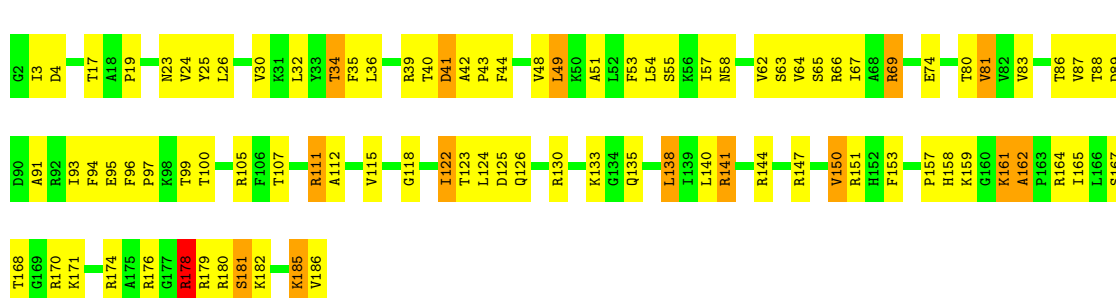
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:



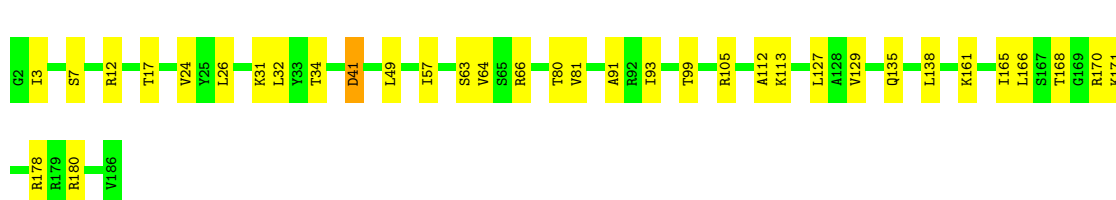
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:



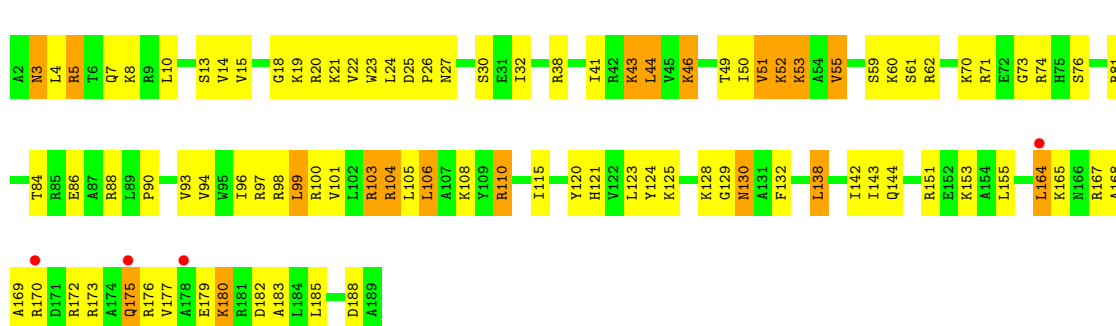
- Molecule 54: 60S ribosomal protein L18-A

Chain m8:



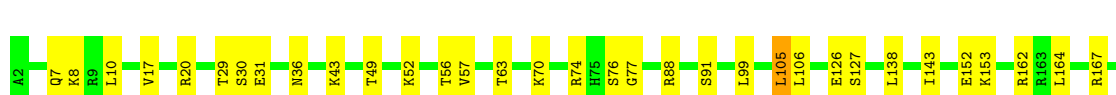
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:



- Molecule 55: 60S ribosomal protein L19-A

Chain m9:





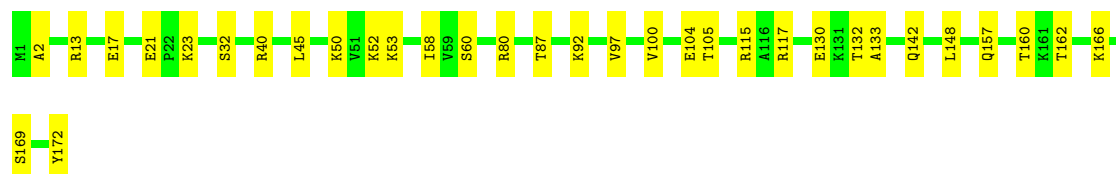
- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



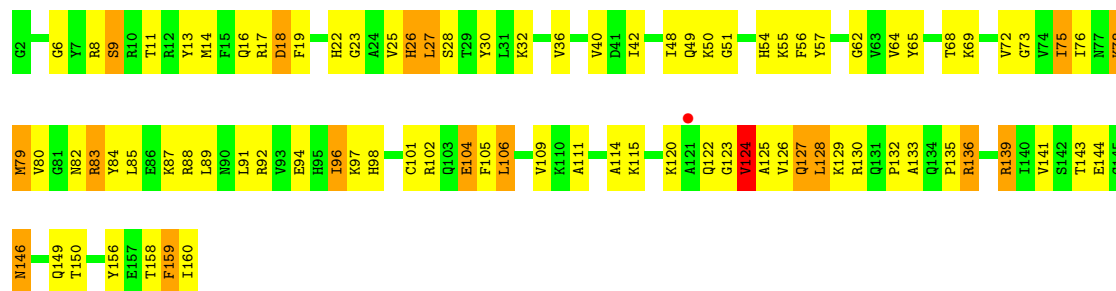
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:



- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



- Molecule 57: 60S ribosomal protein L21-A

Chain n1:



- Molecule 58: 60S ribosomal protein L22-A

Chain N2:





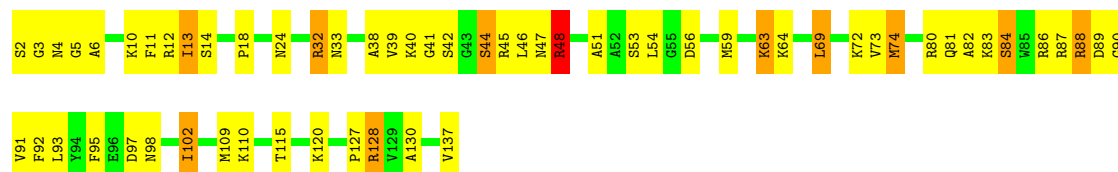
- Molecule 58: 60S ribosomal protein L22-A

Chain n2:



- Molecule 59: 60S ribosomal protein L23-A

Chain N3:



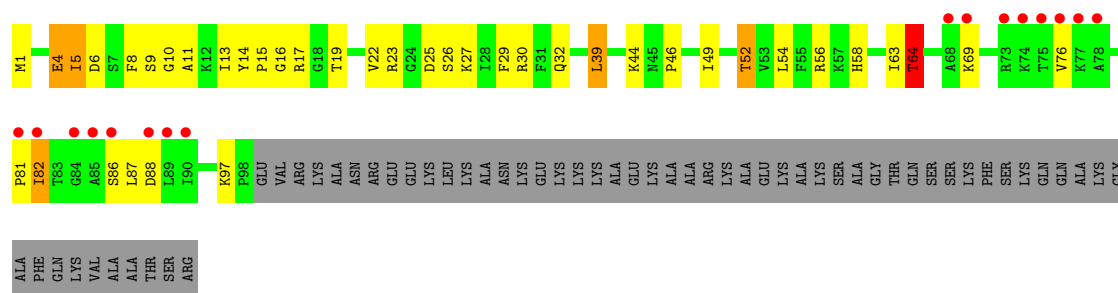
- Molecule 59: 60S ribosomal protein L23-A

Chain n3:



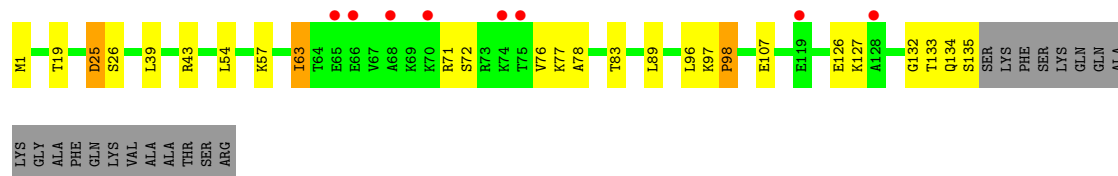
- Molecule 60: 60S ribosomal protein L24-A

Chain N4:



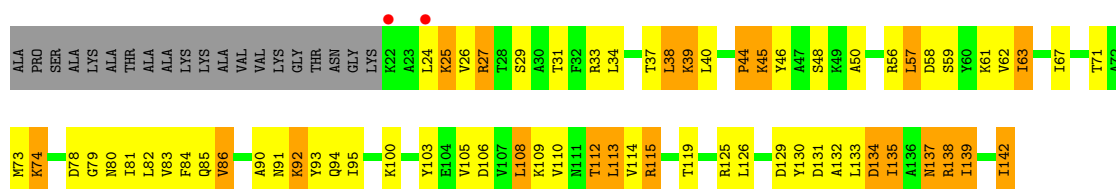
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:



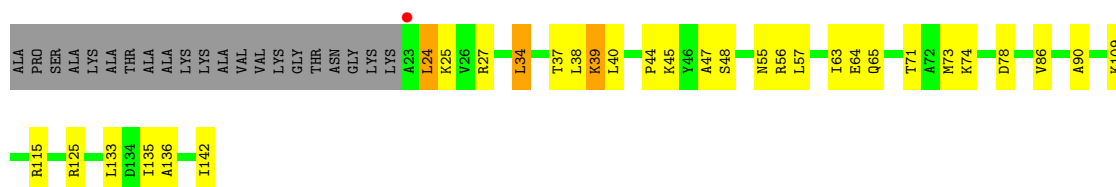
- Molecule 61: 60S ribosomal protein L25

Chain N5:



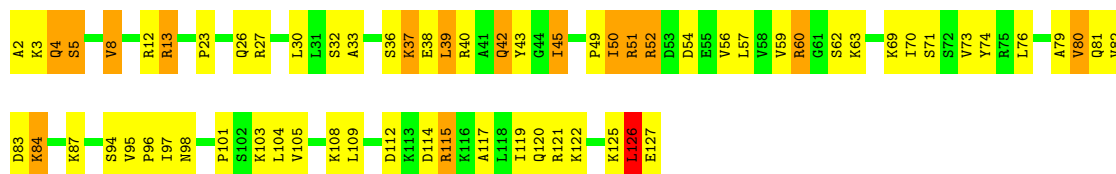
- Molecule 61: 60S ribosomal protein L25

Chain n5:



- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



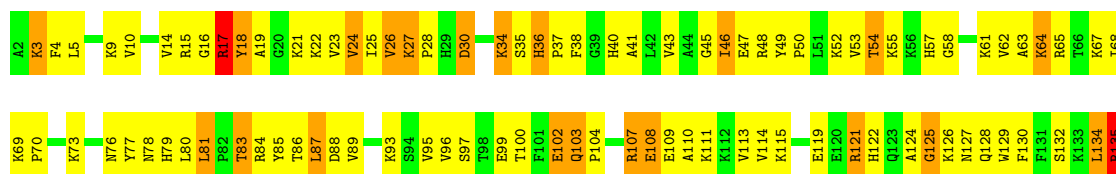
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



- Molecule 63: 60S ribosomal protein L27-A

Chain N7:



- Molecule 63: 60S ribosomal protein L27-A

Chain n7:



- Molecule 64: 60S ribosomal protein L28

Chain N8:



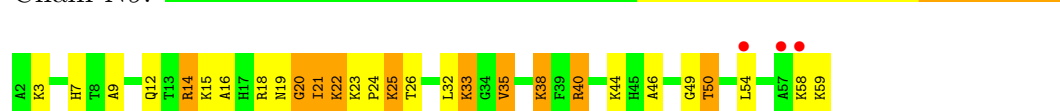
- Molecule 64: 60S ribosomal protein L28

Chain n8:



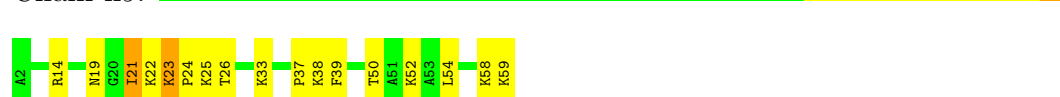
- Molecule 65: 60S ribosomal protein L29

Chain N9:



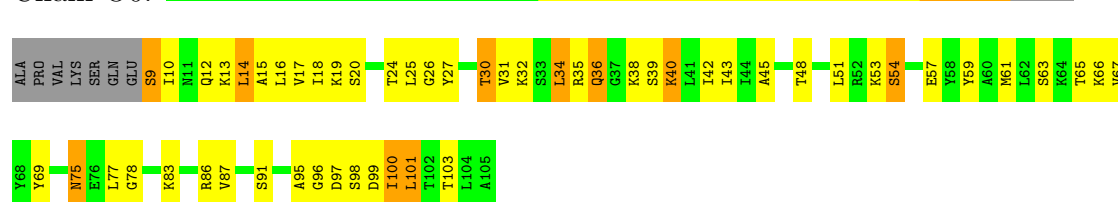
- Molecule 65: 60S ribosomal protein L29

Chain n9:



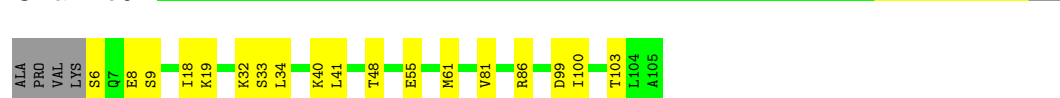
- Molecule 66: 60S ribosomal protein L30

Chain O0:



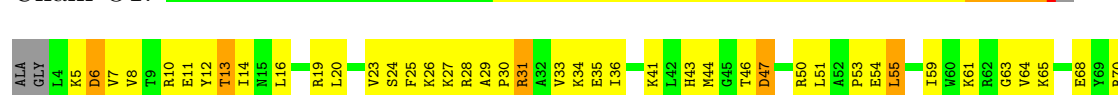
- Molecule 66: 60S ribosomal protein L30

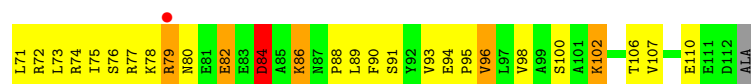
Chain o0:



- Molecule 67: 60S ribosomal protein L31-A

Chain O1:





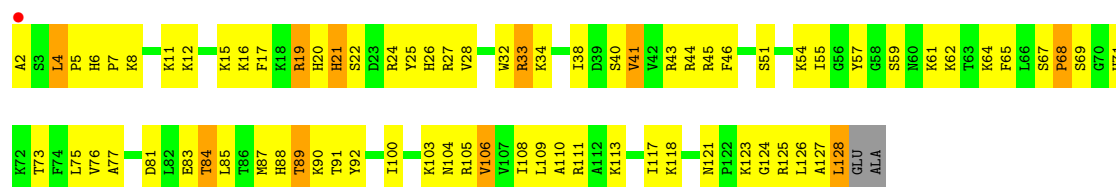
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



- Molecule 68: 60S ribosomal protein L32

Chain O2:



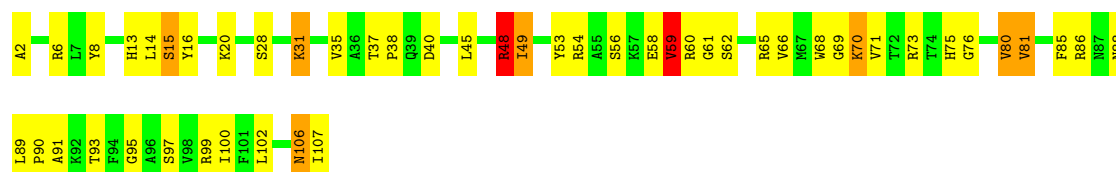
- Molecule 68: 60S ribosomal protein L32

Chain o2:



- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



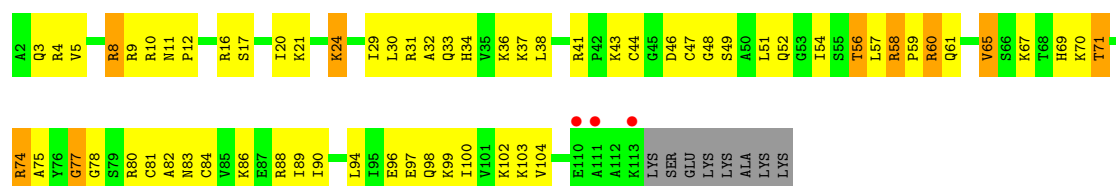
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



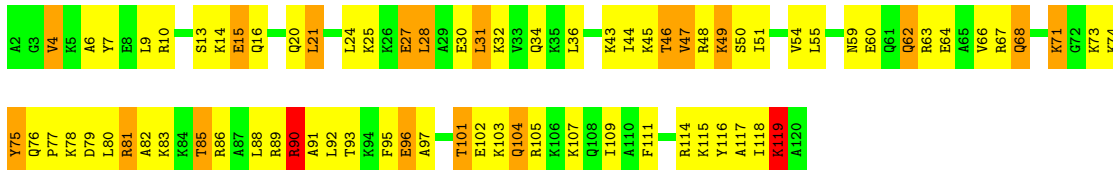
- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 



- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



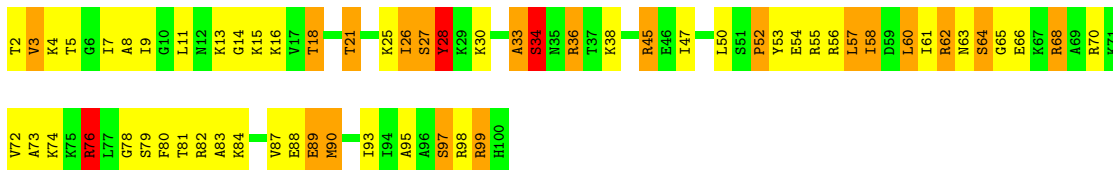
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:



- Molecule 72: 60S ribosomal protein L36-A

Chain O6:



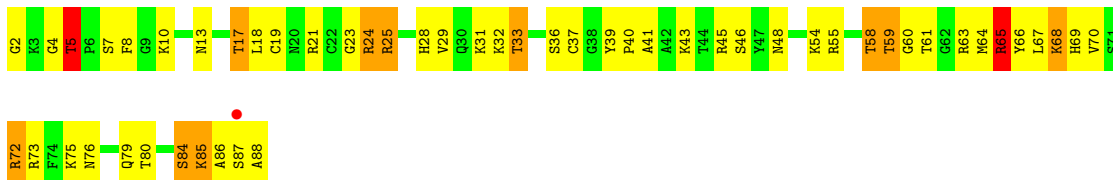
- Molecule 72: 60S ribosomal protein L36-A

Chain 06:



- Molecule 73: 60S ribosomal protein L37-A

Chain 07:



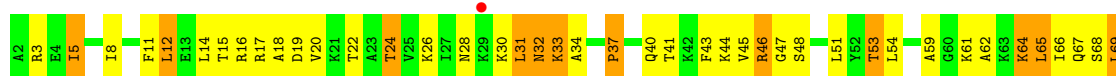
- Molecule 73: 60S ribosomal protein L37-A

Chain o7: 



- Molecule 74: 60S ribosomal protein L38

Chain O8:



- Molecule 74: 60S ribosomal protein L38

Chain o8:



- Molecule 75: 60S ribosomal protein L39

Chain O9:



- Molecule 75: 60S ribosomal protein L39

Chain o9:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:

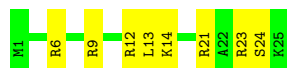


- Molecule 77: 60S ribosomal protein L41-A

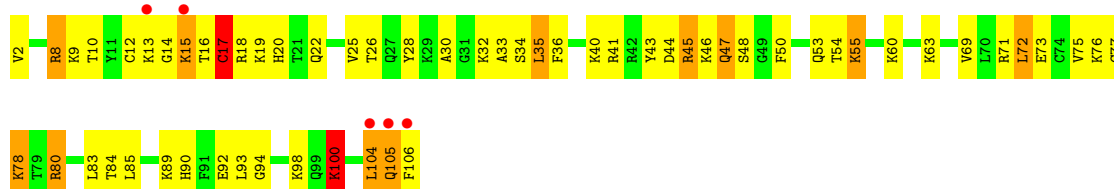
Chain Q1:



- Molecule 77: 60S ribosomal protein L41-A

Chain q1: 

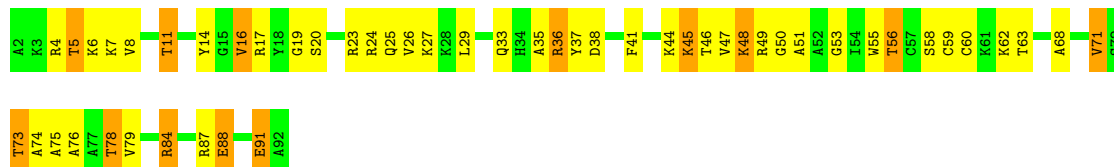
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 

- Molecule 78: 60S ribosomal protein L42-A

Chain q2: 

- Molecule 79: 60S ribosomal protein L43-A

Chain Q3: 

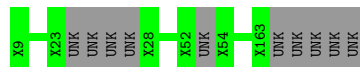
- Molecule 79: 60S ribosomal protein L43-A

Chain q3: 

- Molecule 80: 40S ribosomal protein S30-A

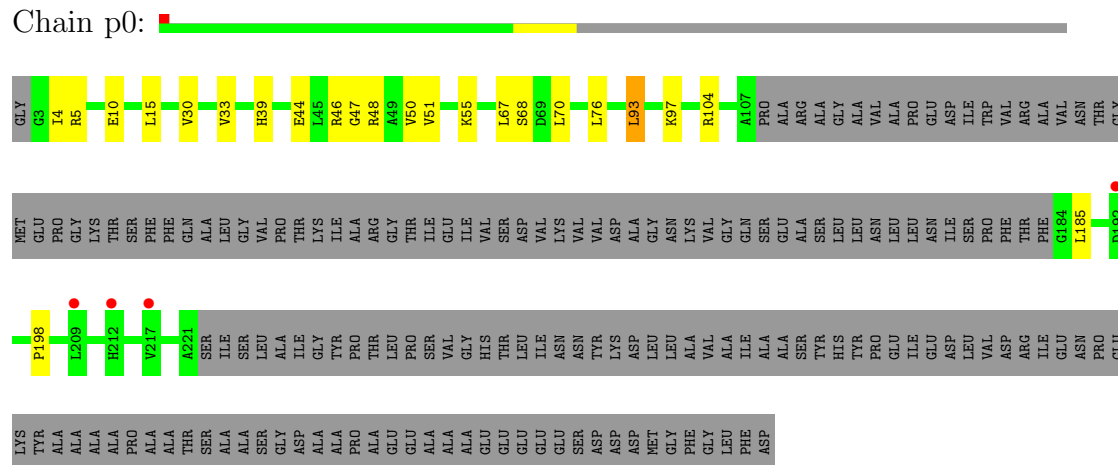
Chain e0: 

- Molecule 81: Unknown protein chain m2

Chain m2: 

- Molecule 82: 60S acidic ribosomal protein P0

Chain p0:



- Molecule 83: Unknown protein chain p1

Chain p1:

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein chain p2

Chain p2:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.25Å 286.92Å 303.84Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	49.69 – 3.00 49.89 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.69-3.00) 98.8 (49.89-3.00)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.208 , 0.255 0.269 , 0.308	Depositor DCC
R_{free} test set	28331 reflections (1.95%)	DCC
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 1451442 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	411245	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HMT, ZN, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.68	1/41698 (0.0%)	1.25	264/64972 (0.4%)
1	6	0.84	11/42765 (0.0%)	1.37	434/66634 (0.7%)
2	S0	0.46	0/1617	0.68	0/2215
2	s0	0.48	0/1623	0.70	0/2222
3	S1	0.37	0/1735	0.64	0/2335
3	s1	0.50	0/1748	0.66	0/2352
4	S2	0.48	0/1665	0.65	0/2263
4	s2	0.57	0/1665	0.75	0/2263
5	S3	0.47	0/1759	0.64	0/2368
5	s3	0.41	0/1759	0.60	0/2368
6	S4	0.45	0/2109	0.70	0/2839
6	s4	0.55	0/2109	0.78	1/2839 (0.0%)
7	S5	0.37	0/1629	0.58	0/2202
7	s5	0.45	0/1629	0.64	0/2202
8	S6	0.46	0/1823	0.64	0/2439
8	s6	0.56	0/1779	0.70	0/2379
9	S7	0.42	0/1506	0.64	1/2028 (0.0%)
9	s7	0.47	0/1516	0.67	1/2043 (0.0%)
10	S8	0.51	0/1514	0.72	1/2021 (0.0%)
10	s8	0.62	0/1514	0.76	1/2021 (0.0%)
11	S9	0.46	0/1519	0.63	0/2035
11	s9	0.53	0/1519	0.74	2/2035 (0.1%)
12	C0	0.42	0/790	0.69	1/1069 (0.1%)
12	c0	0.36	0/777	0.64	3/1049 (0.3%)
13	C1	0.58	1/1240 (0.1%)	0.67	0/1675
13	c1	0.65	1/1194 (0.1%)	0.78	1/1610 (0.1%)
14	C2	0.37	0/900	0.63	0/1224
14	c2	0.30	0/900	0.56	0/1224
15	C3	0.48	0/1215	0.67	2/1638 (0.1%)
15	c3	0.59	0/1215	0.71	0/1638
16	C4	0.39	0/901	0.65	0/1217
16	c4	0.54	0/960	0.76	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.43	0/998	0.65	0/1341
17	c5	0.49	0/1060	0.70	0/1426
18	C6	0.43	0/1125	0.69	3/1510 (0.2%)
18	c6	0.48	0/1131	0.67	0/1518
19	C7	0.44	0/935	0.63	0/1254
19	c7	0.49	0/914	0.72	0/1224
20	C8	0.42	0/1211	0.61	0/1628
20	c8	0.49	0/1211	0.71	2/1628 (0.1%)
21	C9	0.40	0/1130	0.59	0/1517
21	c9	0.49	0/1130	0.66	1/1517 (0.1%)
22	D0	0.44	0/865	0.63	0/1169
22	d0	0.48	0/892	0.66	0/1205
23	D1	0.45	0/693	0.64	0/935
23	d1	0.52	0/693	0.72	0/935
24	D2	0.49	0/1038	0.69	2/1395 (0.1%)
24	d2	0.60	0/1038	0.74	1/1395 (0.1%)
25	D3	0.62	0/1139	0.75	1/1518 (0.1%)
25	d3	0.70	0/1139	0.83	1/1518 (0.1%)
26	D4	0.44	0/1087	0.63	1/1449 (0.1%)
26	d4	0.55	0/1087	0.71	0/1449
27	D5	0.39	0/571	0.69	0/768
27	d5	0.41	0/566	0.63	0/761
28	D6	0.45	0/782	0.66	0/1047
28	d6	0.55	0/782	0.71	0/1047
29	D7	0.43	0/620	0.66	0/838
29	d7	0.50	0/620	0.75	1/838 (0.1%)
30	D8	0.36	0/499	0.59	0/670
30	d8	0.44	0/499	0.67	0/670
31	D9	0.47	0/452	0.72	1/600 (0.2%)
31	d9	0.48	0/452	0.64	0/600
32	E0	0.48	0/483	0.63	0/643
33	E1	0.45	0/577	0.77	0/770
33	e1	0.39	0/619	0.74	1/822 (0.1%)
34	SR	0.36	0/2494	0.58	0/3393
34	sR	0.37	0/2495	0.55	0/3395
35	SM	0.54	1/1113 (0.1%)	0.79	4/1502 (0.3%)
35	sM	0.49	0/683	0.70	1/923 (0.1%)
36	1	1.11	100/75394 (0.1%)	1.65	1834/117545 (1.6%)
36	5	1.17	147/75414 (0.2%)	1.69	1950/117575 (1.7%)
37	3	0.90	2/2883 (0.1%)	1.41	33/4491 (0.7%)
37	7	1.15	8/2883 (0.3%)	1.71	80/4491 (1.8%)
38	4	1.06	4/3746 (0.1%)	1.62	86/5832 (1.5%)
38	8	0.98	1/3746 (0.0%)	1.47	39/5832 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.73	0/1948	0.85	2/2617 (0.1%)
39	l2	0.75	1/1946 (0.1%)	0.90	3/2614 (0.1%)
40	L3	0.74	1/3146 (0.0%)	0.83	0/4228
40	l3	0.85	0/3146	0.93	11/4228 (0.3%)
41	L4	0.82	0/2800	0.96	7/3790 (0.2%)
41	l4	0.75	0/2800	0.90	3/3790 (0.1%)
42	L5	0.57	0/2425	0.69	0/3271
42	l5	0.74	0/2408	0.82	2/3248 (0.1%)
43	L6	0.76	0/1260	0.81	0/1694
43	l6	0.80	0/1269	0.87	2/1705 (0.1%)
44	L7	0.79	0/1821	0.89	2/2451 (0.1%)
44	l7	0.87	0/1828	0.89	1/2461 (0.0%)
45	L8	0.57	0/1836	0.70	2/2481 (0.1%)
45	l8	0.53	0/1795	0.67	1/2429 (0.0%)
46	L9	0.66	0/1539	0.77	0/2073
46	l9	0.80	0/1539	0.86	0/2073
47	M0	0.74	0/1741	0.84	4/2335 (0.2%)
47	m0	0.76	0/1758	0.86	3/2358 (0.1%)
48	M1	0.50	0/1374	0.71	1/1842 (0.1%)
48	m1	0.63	0/1374	0.82	1/1842 (0.1%)
49	M3	0.74	0/1568	0.85	0/2106
49	m3	0.71	0/1573	0.85	0/2113
50	M4	0.74	0/1068	0.84	1/1438 (0.1%)
50	m4	0.81	0/1074	0.82	0/1446
51	M5	0.75	0/1757	0.85	0/2354
51	m5	0.67	0/1757	0.82	0/2354
52	M6	0.89	1/1585 (0.1%)	0.91	4/2128 (0.2%)
52	m6	1.01	5/1585 (0.3%)	0.99	8/2128 (0.4%)
53	M7	0.80	0/1443	0.89	2/1944 (0.1%)
53	m7	0.90	0/1250	0.89	1/1683 (0.1%)
54	M8	0.82	0/1465	0.89	2/1965 (0.1%)
54	m8	0.75	0/1465	0.93	2/1965 (0.1%)
55	M9	0.55	0/1538	0.66	0/2050
55	m9	0.65	0/1538	0.70	1/2050 (0.0%)
56	N0	0.77	0/1481	0.89	0/1990
56	n0	0.86	0/1481	0.89	1/1990 (0.1%)
57	N1	0.76	0/1300	0.80	0/1743
57	n1	0.88	1/1300 (0.1%)	0.86	1/1743 (0.1%)
58	N2	0.43	0/812	0.62	0/1099
58	n2	0.51	0/794	0.66	0/1076
59	N3	0.72	0/1018	0.83	1/1369 (0.1%)
59	n3	0.83	0/1018	0.94	3/1369 (0.2%)
60	N4	0.55	0/712	0.67	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.68	0/1052	0.74	0/1398
61	N5	0.63	0/979	0.78	0/1321
61	n5	0.66	0/974	0.79	1/1314 (0.1%)
62	N6	0.70	0/1004	0.88	2/1341 (0.1%)
62	n6	0.69	0/1004	0.81	0/1341
63	N7	0.53	0/1118	0.68	1/1497 (0.1%)
63	n7	0.50	0/1118	0.67	0/1497
64	N8	0.80	0/1204	0.92	4/1612 (0.2%)
64	n8	0.76	0/1204	0.91	2/1612 (0.1%)
65	N9	0.76	0/473	0.81	0/629
65	n9	0.84	0/473	0.98	0/629
66	O0	0.50	0/751	0.67	0/1008
66	o0	0.54	0/775	0.68	0/1040
67	O1	0.62	0/890	0.68	0/1196
67	o1	0.80	0/897	0.87	1/1205 (0.1%)
68	O2	0.82	0/1041	0.85	0/1394
68	o2	0.85	0/1041	0.93	1/1394 (0.1%)
69	O3	0.91	0/868	0.92	2/1168 (0.2%)
69	o3	0.95	0/868	0.86	0/1168
70	O4	0.59	0/890	0.83	2/1189 (0.2%)
70	o4	0.60	0/890	0.80	0/1189
71	O5	0.72	0/978	0.82	1/1301 (0.1%)
71	o5	0.58	0/974	0.71	0/1297
72	O6	0.65	0/778	0.81	1/1034 (0.1%)
72	o6	0.61	0/777	0.72	0/1033
73	O7	0.81	0/696	0.94	2/923 (0.2%)
73	o7	0.76	0/696	0.90	1/923 (0.1%)
74	O8	0.53	0/618	0.64	0/826
74	o8	0.46	0/614	0.67	0/822
75	O9	0.79	1/443 (0.2%)	0.87	1/588 (0.2%)
75	o9	0.75	0/443	0.87	1/588 (0.2%)
76	Q0	0.78	0/423	0.81	0/562
76	q0	0.94	0/423	0.94	2/562 (0.4%)
77	Q1	0.57	0/234	1.04	1/300 (0.3%)
77	q1	0.82	0/234	1.05	1/300 (0.3%)
78	Q2	0.94	1/860 (0.1%)	0.84	0/1136
78	q2	0.82	1/860 (0.1%)	0.83	0/1136
79	Q3	0.72	0/701	0.83	0/934
79	q3	0.72	0/701	0.80	0/934
80	e0	0.54	0/499	0.72	0/665
82	p0	0.45	0/1092	0.62	0/1474
All	All	0.88	289/430074 (0.1%)	1.31	4853/631364 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	s3	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
11	s9	0	1
16	C4	0	1
17	c5	0	1
18	c6	0	2
19	C7	0	2
22	d0	0	1
25	d3	0	1
27	D5	0	2
27	d5	0	1
33	E1	0	1
39	L2	0	1
39	l2	0	2
42	l5	0	2
43	L6	0	3
43	l6	0	1
44	l7	0	2
45	l8	0	1
48	M1	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	2
60	n4	0	1
62	n6	0	1
63	n7	0	1
64	n8	0	3
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
All	All	0	45

The worst 5 of 289 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	16.24	2.09	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-11.04	1.29	1.38
36	1	3181	C	N3-C4	-10.76	1.26	1.33
78	q2	17	CYS	CB-SG	10.62	2.00	1.82
36	5	1152	G	C2-N3	-9.57	1.25	1.32

The worst 5 of 4853 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	26.65	141.93	128.60
36	5	1152	G	N3-C4-N9	-25.57	110.66	126.00
36	5	1152	G	C2-N3-C4	-18.36	102.72	111.90
36	5	2818	U	O5'-P-OP1	-17.90	89.22	110.70
36	5	1116	G	O5'-P-OP1	-16.32	91.01	105.70

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	Peptide

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	929	0
1	6	38238	0	19240	856	0
2	S0	1577	0	1567	152	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	183	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	121	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	117	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	155	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	143	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1878	128	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	111	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	102	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	116	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	65	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	69	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	50	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	82	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	103	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	92	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	100	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	81	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	112	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	91	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	78	0
22	d0	882	0	939	0	0
23	D1	684	0	672	59	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	83	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	84	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	82	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	61	0
27	d5	558	0	598	0	0
28	D6	769	0	815	93	0
28	d6	769	0	814	0	0
29	D7	610	0	631	52	0
29	d7	610	0	631	0	0
30	D8	497	0	535	46	0
30	d8	497	0	535	0	0
31	D9	442	0	428	41	0
31	d9	442	0	429	0	0
32	E0	475	0	525	40	0
33	E1	566	0	602	57	0
33	e1	608	0	657	0	0
34	SR	2441	0	2397	139	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	64	0
35	sM	680	0	607	0	0
36	1	67355	0	33848	1213	0
36	5	67376	0	33860	1225	0
37	3	2579	0	1304	56	0
37	7	2579	0	1303	41	0
38	4	3353	0	1695	62	0
38	8	3353	0	1695	73	0
39	L2	1914	0	1981	158	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	233	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	203	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	203	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	78	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	118	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	126	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	120	0
46	l9	1518	0	1587	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	M0	1705	0	1736	135	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	100	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	117	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	74	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	131	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	99	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	97	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	90	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	94	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	99	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	98	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	41	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	61	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	25	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	58	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	64	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	93	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1214	98	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	35	0
65	n9	462	0	491	0	0
66	O0	743	0	797	54	0
66	o0	767	0	816	0	0
67	O1	876	0	912	49	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	75	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	57	0
69	o3	850	0	880	0	0
70	O4	880	0	945	74	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	83	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	66	0
72	o6	770	0	846	0	0
73	O7	681	0	683	49	0
73	o7	681	0	683	0	0
74	O8	612	0	682	44	0
74	o8	608	0	671	0	0
75	O9	436	0	475	41	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	24	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	25	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	57	0
78	q2	847	0	916	0	0
79	Q3	694	0	734	50	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	750	0	179	0	0
82	p0	1077	0	1041	0	0
83	p1	235	0	51	0	0
84	p2	230	0	51	0	0
85	1	466	0	0	0	0
85	2	121	0	0	0	0
85	3	13	0	0	0	0
85	4	23	0	0	0	0
85	5	500	0	0	0	0
85	6	147	0	0	0	0
85	7	16	0	0	0	0
85	8	15	0	0	0	0
85	C8	1	0	0	0	0
85	D3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L5	1	0	0	0	0
85	L6	1	0	0	0	0
85	L7	4	0	0	0	0
85	L8	1	0	0	0	0
85	M0	3	0	0	0	0
85	M1	2	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	5	0	0	0	0
85	M9	2	0	0	0	0
85	N0	1	0	0	0	0
85	N3	2	0	0	0	0
85	N5	1	0	0	0	0
85	N8	6	0	0	0	0
85	O1	1	0	0	0	0
85	O2	1	0	0	0	0
85	O3	1	0	0	0	0
85	O4	1	0	0	0	0
85	O7	2	0	0	0	0
85	S2	2	0	0	0	0
85	S4	2	0	0	0	0
85	S6	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	c9	2	0	0	0	0
85	d3	2	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	1	0	0	0	0
85	l7	3	0	0	0	0
85	l9	1	0	0	0	0
85	m0	1	0	0	0	0
85	m1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	n8	5	0	0	0	0
85	o1	1	0	0	0	0
85	o3	2	0	0	0	0
85	o4	2	0	0	0	0
85	o7	1	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	s1	1	0	0	0	0
85	s4	1	0	0	0	0
85	s6	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	2450	0	0	237	0
86	2	1113	0	0	125	0
86	3	77	0	0	5	0
86	4	105	0	0	9	0
86	5	2478	0	0	249	0
86	6	1113	0	0	108	0
86	7	84	0	0	9	0
86	8	105	0	0	22	0
86	C3	7	0	0	2	0
86	C5	7	0	0	6	0
86	C8	7	0	0	0	0
86	D9	7	0	0	0	0
86	L3	14	0	0	2	0
86	L4	7	0	0	1	0
86	M0	7	0	0	1	0
86	M5	7	0	0	1	0
86	M7	14	0	0	2	0
86	M8	7	0	0	0	0
86	M9	7	0	0	1	0
86	N1	7	0	0	1	0
86	N9	7	0	0	1	0
86	O2	7	0	0	0	0
86	O3	7	0	0	1	0
86	O7	14	0	0	5	0
86	O9	7	0	0	1	0
86	Q2	7	0	0	6	0
86	S8	7	0	0	0	0
86	SR	7	0	0	0	0
86	c3	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	21	0	0	0	0
86	l4	14	0	0	0	0
86	l5	21	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	0	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	m8	7	0	0	0	0
86	n3	14	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	7	0	0	0	0
86	o9	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	7	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	0	0
86	sR	7	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	3	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	q3	1	0	0	0	0
88	1	39	0	39	4	0
88	5	39	0	39	3	0
All	All	411245	0	297375	9722	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 9722 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.09	1.40
78:Q2:17:CYS:CB	87:Q2:501:ZN:ZN	0.98	1.40
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.41	1.06
36:5:2836:C:H5	36:5:2852:C:H42	1.05	1.02
65:N9:50:THR:HG22	36:5:1073:U:H1'	205.84	1.02

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	145 (71%)	33 (16%)	26 (13%)	0	2
2	s0	204/251 (81%)	148 (72%)	33 (16%)	23 (11%)	1	3
3	S1	212/254 (84%)	147 (69%)	38 (18%)	27 (13%)	0	2
3	s1	214/254 (84%)	176 (82%)	22 (10%)	16 (8%)	2	8
4	S2	215/253 (85%)	179 (83%)	26 (12%)	10 (5%)	4	21
4	s2	215/253 (85%)	179 (83%)	25 (12%)	11 (5%)	3	18
5	S3	221/239 (92%)	178 (80%)	29 (13%)	14 (6%)	2	12
5	s3	221/239 (92%)	178 (80%)	27 (12%)	16 (7%)	2	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S4	258/260 (99%)	206 (80%)	39 (15%)	13 (5%)	3	19
6	s4	258/260 (99%)	214 (83%)	30 (12%)	14 (5%)	3	17
7	S5	204/224 (91%)	160 (78%)	26 (13%)	18 (9%)	1	5
7	s5	204/224 (91%)	162 (79%)	27 (13%)	15 (7%)	2	8
8	S6	224/236 (95%)	194 (87%)	19 (8%)	11 (5%)	3	20
8	s6	216/236 (92%)	187 (87%)	19 (9%)	10 (5%)	4	22
9	S7	182/189 (96%)	134 (74%)	28 (15%)	20 (11%)	1	3
9	s7	184/189 (97%)	141 (77%)	33 (18%)	10 (5%)	3	17
10	S8	184/200 (92%)	159 (86%)	13 (7%)	12 (6%)	2	11
10	s8	184/200 (92%)	159 (86%)	20 (11%)	5 (3%)	8	38
11	S9	183/196 (93%)	152 (83%)	21 (12%)	10 (6%)	3	16
11	s9	183/196 (93%)	142 (78%)	33 (18%)	8 (4%)	4	22
12	C0	94/105 (90%)	71 (76%)	13 (14%)	10 (11%)	1	3
12	c0	92/105 (88%)	64 (70%)	14 (15%)	14 (15%)	0	1
13	C1	153/155 (99%)	123 (80%)	18 (12%)	12 (8%)	1	7
13	c1	144/155 (93%)	120 (83%)	15 (10%)	9 (6%)	2	12
14	C2	122/142 (86%)	68 (56%)	28 (23%)	26 (21%)	0	0
14	c2	122/142 (86%)	69 (57%)	31 (25%)	22 (18%)	0	1
15	C3	148/150 (99%)	125 (84%)	15 (10%)	8 (5%)	3	17
15	c3	148/150 (99%)	114 (77%)	24 (16%)	10 (7%)	2	10
16	C4	125/136 (92%)	91 (73%)	22 (18%)	12 (10%)	1	4
16	c4	126/136 (93%)	104 (82%)	15 (12%)	7 (6%)	3	16
17	C5	122/141 (86%)	85 (70%)	26 (21%)	11 (9%)	1	5
17	c5	133/141 (94%)	93 (70%)	22 (16%)	18 (14%)	0	2
18	C6	139/142 (98%)	113 (81%)	16 (12%)	10 (7%)	2	8
18	c6	140/142 (99%)	117 (84%)	16 (11%)	7 (5%)	3	19
19	C7	116/136 (85%)	90 (78%)	14 (12%)	12 (10%)	1	4
19	c7	113/136 (83%)	88 (78%)	18 (16%)	7 (6%)	2	13
20	C8	143/145 (99%)	112 (78%)	20 (14%)	11 (8%)	1	7
20	c8	143/145 (99%)	112 (78%)	22 (15%)	9 (6%)	2	12
21	C9	141/143 (99%)	119 (84%)	17 (12%)	5 (4%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	c9	141/143 (99%)	118 (84%)	19 (14%)	4 (3%)	8	37
22	D0	105/120 (88%)	83 (79%)	14 (13%)	8 (8%)	2	7
22	d0	108/120 (90%)	83 (77%)	15 (14%)	10 (9%)	1	5
23	D1	85/87 (98%)	63 (74%)	14 (16%)	8 (9%)	1	5
23	d1	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	6	30
24	D2	127/129 (98%)	109 (86%)	17 (13%)	1 (1%)	27	76
24	d2	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	9	42
25	D3	142/144 (99%)	109 (77%)	21 (15%)	12 (8%)	1	6
25	d3	142/144 (99%)	128 (90%)	8 (6%)	6 (4%)	4	24
26	D4	132/134 (98%)	108 (82%)	14 (11%)	10 (8%)	2	7
26	d4	132/134 (98%)	108 (82%)	15 (11%)	9 (7%)	2	10
27	D5	68/107 (64%)	43 (63%)	14 (21%)	11 (16%)	0	1
27	d5	67/107 (63%)	55 (82%)	7 (10%)	5 (8%)	2	8
28	D6	95/97 (98%)	58 (61%)	19 (20%)	18 (19%)	0	0
28	d6	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	1	6
29	D7	79/81 (98%)	67 (85%)	8 (10%)	4 (5%)	3	18
29	d7	79/81 (98%)	66 (84%)	7 (9%)	6 (8%)	2	7
30	D8	61/66 (92%)	51 (84%)	7 (12%)	3 (5%)	3	20
30	d8	61/66 (92%)	46 (75%)	8 (13%)	7 (12%)	1	3
31	D9	51/55 (93%)	43 (84%)	6 (12%)	2 (4%)	5	26
31	d9	51/55 (93%)	42 (82%)	5 (10%)	4 (8%)	1	7
32	E0	58/60 (97%)	47 (81%)	7 (12%)	4 (7%)	2	9
33	E1	69/76 (91%)	36 (52%)	15 (22%)	18 (26%)	0	0
33	e1	74/76 (97%)	34 (46%)	20 (27%)	20 (27%)	0	0
34	SR	316/318 (99%)	277 (88%)	27 (8%)	12 (4%)	5	27
34	sR	316/318 (99%)	270 (85%)	36 (11%)	10 (3%)	6	33
35	SM	155/273 (57%)	113 (73%)	18 (12%)	24 (16%)	0	1
35	sM	98/273 (36%)	64 (65%)	20 (20%)	14 (14%)	0	1
39	L2	250/253 (99%)	225 (90%)	17 (7%)	8 (3%)	6	33
39	l2	250/253 (99%)	211 (84%)	33 (13%)	6 (2%)	9	42
40	L3	384/386 (100%)	336 (88%)	31 (8%)	17 (4%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	l3	384/386 (100%)	341 (89%)	31 (8%)	12 (3%)	7	34
41	L4	359/361 (99%)	293 (82%)	46 (13%)	20 (6%)	3	16
41	l4	359/361 (99%)	305 (85%)	35 (10%)	19 (5%)	3	18
42	L5	294/296 (99%)	245 (83%)	31 (10%)	18 (6%)	2	14
42	l5	292/296 (99%)	259 (89%)	23 (8%)	10 (3%)	6	31
43	L6	152/175 (87%)	135 (89%)	14 (9%)	3 (2%)	11	48
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	8	39
44	L7	220/243 (90%)	198 (90%)	14 (6%)	8 (4%)	5	29
44	l7	221/243 (91%)	199 (90%)	19 (9%)	3 (1%)	16	60
45	L8	231/255 (91%)	189 (82%)	34 (15%)	8 (4%)	6	30
45	l8	229/255 (90%)	183 (80%)	26 (11%)	20 (9%)	1	5
46	L9	189/191 (99%)	168 (89%)	15 (8%)	6 (3%)	6	33
46	l9	189/191 (99%)	174 (92%)	9 (5%)	6 (3%)	6	33
47	M0	207/220 (94%)	179 (86%)	20 (10%)	8 (4%)	5	26
47	m0	209/220 (95%)	168 (80%)	30 (14%)	11 (5%)	3	18
48	M1	167/173 (96%)	132 (79%)	17 (10%)	18 (11%)	1	3
48	m1	167/173 (96%)	140 (84%)	16 (10%)	11 (7%)	2	10
49	M3	191/198 (96%)	156 (82%)	28 (15%)	7 (4%)	5	28
49	m3	192/198 (97%)	156 (81%)	22 (12%)	14 (7%)	2	8
50	M4	134/137 (98%)	116 (87%)	10 (8%)	8 (6%)	2	14
50	m4	135/137 (98%)	121 (90%)	11 (8%)	3 (2%)	10	45
51	M5	201/203 (99%)	186 (92%)	10 (5%)	5 (2%)	9	40
51	m5	201/203 (99%)	181 (90%)	13 (6%)	7 (4%)	6	30
52	M6	195/198 (98%)	180 (92%)	12 (6%)	3 (2%)	15	58
52	m6	195/198 (98%)	174 (89%)	16 (8%)	5 (3%)	8	39
53	M7	181/183 (99%)	153 (84%)	20 (11%)	8 (4%)	4	22
53	m7	153/183 (84%)	140 (92%)	11 (7%)	2 (1%)	18	62
54	M8	183/185 (99%)	157 (86%)	21 (12%)	5 (3%)	8	38
54	m8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	6	32
55	M9	186/188 (99%)	161 (87%)	23 (12%)	2 (1%)	21	67
55	m9	186/188 (99%)	163 (88%)	22 (12%)	1 (0%)	38	84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	N0	170/172 (99%)	151 (89%)	14 (8%)	5 (3%)	7	35
56	n0	170/172 (99%)	154 (91%)	14 (8%)	2 (1%)	19	64
57	N1	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	6	33
57	n1	157/159 (99%)	139 (88%)	13 (8%)	5 (3%)	6	33
58	N2	98/120 (82%)	76 (78%)	15 (15%)	7 (7%)	2	9
58	n2	96/120 (80%)	82 (85%)	10 (10%)	4 (4%)	4	24
59	N3	134/136 (98%)	121 (90%)	11 (8%)	2 (2%)	15	58
59	n3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	15	58
60	N4	96/155 (62%)	77 (80%)	12 (12%)	7 (7%)	2	8
60	n4	133/155 (86%)	110 (83%)	12 (9%)	11 (8%)	1	6
61	N5	119/141 (84%)	107 (90%)	9 (8%)	3 (2%)	9	40
61	n5	118/141 (84%)	96 (81%)	10 (8%)	12 (10%)	1	4
62	N6	124/126 (98%)	114 (92%)	7 (6%)	3 (2%)	9	42
62	n6	124/126 (98%)	110 (89%)	8 (6%)	6 (5%)	4	20
63	N7	133/135 (98%)	113 (85%)	12 (9%)	8 (6%)	2	14
63	n7	133/135 (98%)	104 (78%)	18 (14%)	11 (8%)	1	6
64	N8	146/148 (99%)	123 (84%)	13 (9%)	10 (7%)	2	10
64	n8	146/148 (99%)	121 (83%)	20 (14%)	5 (3%)	6	31
65	N9	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	5	29
65	n9	56/58 (97%)	41 (73%)	9 (16%)	6 (11%)	1	3
66	O0	95/104 (91%)	87 (92%)	8 (8%)	0	100	100
66	o0	98/104 (94%)	88 (90%)	9 (9%)	1 (1%)	22	70
67	O1	107/112 (96%)	98 (92%)	4 (4%)	5 (5%)	4	21
67	o1	107/112 (96%)	88 (82%)	15 (14%)	4 (4%)	5	28
68	O2	125/129 (97%)	112 (90%)	11 (9%)	2 (2%)	14	56
68	o2	125/129 (97%)	108 (86%)	12 (10%)	5 (4%)	5	25
69	O3	104/106 (98%)	96 (92%)	7 (7%)	1 (1%)	22	70
69	o3	104/106 (98%)	96 (92%)	7 (7%)	1 (1%)	22	70
70	O4	110/120 (92%)	100 (91%)	7 (6%)	3 (3%)	8	38
70	o4	110/120 (92%)	99 (90%)	7 (6%)	4 (4%)	5	29
71	O5	117/119 (98%)	103 (88%)	9 (8%)	5 (4%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	o5	117/119 (98%)	98 (84%)	14 (12%)	5 (4%)	4	23
72	O6	97/99 (98%)	76 (78%)	14 (14%)	7 (7%)	2	8
72	o6	97/99 (98%)	80 (82%)	9 (9%)	8 (8%)	1	6
73	O7	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	9	42
73	o7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	9	42
74	O8	75/77 (97%)	59 (79%)	14 (19%)	2 (3%)	8	38
74	o8	75/77 (97%)	63 (84%)	8 (11%)	4 (5%)	3	18
75	O9	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	11	47
75	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
76	Q0	50/52 (96%)	44 (88%)	4 (8%)	2 (4%)	5	25
76	q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	5	25
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
78	Q2	103/105 (98%)	83 (81%)	16 (16%)	4 (4%)	5	26
78	q2	103/105 (98%)	92 (89%)	8 (8%)	3 (3%)	7	35
79	Q3	89/91 (98%)	70 (79%)	16 (18%)	3 (3%)	6	31
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	21	67
80	e0	60/62 (97%)	44 (73%)	10 (17%)	6 (10%)	1	4
82	p0	139/311 (45%)	115 (83%)	19 (14%)	5 (4%)	5	29
All	All	22333/24143 (92%)	18550 (83%)	2534 (11%)	1249 (6%)	3	16

5 of 1249 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	49	ASN
2	S0	66	ALA
2	S0	158	VAL

5.3.2 Protein sidechains ⓘ

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

conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	133 (81%)	31 (19%)	2	12
2	s0	165/209 (79%)	131 (79%)	34 (21%)	2	9
3	S1	191/223 (86%)	151 (79%)	40 (21%)	1	8
3	s1	192/223 (86%)	155 (81%)	37 (19%)	2	12
4	S2	176/204 (86%)	140 (80%)	36 (20%)	2	9
4	s2	176/204 (86%)	131 (74%)	45 (26%)	1	4
5	S3	182/194 (94%)	147 (81%)	35 (19%)	2	12
5	s3	182/194 (94%)	146 (80%)	36 (20%)	2	11
6	S4	221/221 (100%)	170 (77%)	51 (23%)	1	6
6	s4	221/221 (100%)	184 (83%)	37 (17%)	3	16
7	S5	173/190 (91%)	147 (85%)	26 (15%)	4	20
7	s5	173/190 (91%)	139 (80%)	34 (20%)	2	11
8	S6	188/201 (94%)	158 (84%)	30 (16%)	3	17
8	s6	187/201 (93%)	151 (81%)	36 (19%)	2	12
9	S7	165/169 (98%)	136 (82%)	29 (18%)	3	14
9	s7	165/169 (98%)	130 (79%)	35 (21%)	1	8
10	S8	150/161 (93%)	130 (87%)	20 (13%)	6	25
10	s8	150/161 (93%)	128 (85%)	22 (15%)	4	21
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1	7
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	12
12	C0	77/98 (79%)	65 (84%)	12 (16%)	4	18
12	c0	73/98 (74%)	60 (82%)	13 (18%)	2	14
13	C1	129/136 (95%)	107 (83%)	22 (17%)	3	15
13	c1	129/136 (95%)	104 (81%)	25 (19%)	2	11
14	C2	88/118 (75%)	67 (76%)	21 (24%)	1	5
14	c2	88/118 (75%)	64 (73%)	24 (27%)	0	3
15	C3	127/127 (100%)	102 (80%)	25 (20%)	2	11
15	c3	127/127 (100%)	101 (80%)	26 (20%)	2	9
16	C4	81/104 (78%)	66 (82%)	15 (18%)	2	13
16	c4	97/104 (93%)	78 (80%)	19 (20%)	2	11
17	C5	101/117 (86%)	82 (81%)	19 (19%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	c5	103/117 (88%)	84 (82%)	19 (18%)	2	13
18	C6	117/118 (99%)	89 (76%)	28 (24%)	1	5
18	c6	118/118 (100%)	96 (81%)	22 (19%)	2	13
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1	7
19	c7	92/124 (74%)	75 (82%)	17 (18%)	2	13
20	C8	128/128 (100%)	97 (76%)	31 (24%)	1	5
20	c8	128/128 (100%)	105 (82%)	23 (18%)	2	13
21	C9	115/115 (100%)	92 (80%)	23 (20%)	2	10
21	c9	115/115 (100%)	98 (85%)	17 (15%)	4	21
22	D0	100/113 (88%)	80 (80%)	20 (20%)	2	10
22	d0	103/113 (91%)	76 (74%)	27 (26%)	1	4
23	D1	74/74 (100%)	61 (82%)	13 (18%)	3	14
23	d1	74/74 (100%)	59 (80%)	15 (20%)	2	9
24	D2	110/110 (100%)	93 (84%)	17 (16%)	4	19
24	d2	110/110 (100%)	99 (90%)	11 (10%)	11	39
25	D3	119/119 (100%)	95 (80%)	24 (20%)	2	10
25	d3	119/119 (100%)	100 (84%)	19 (16%)	3	17
26	D4	112/112 (100%)	92 (82%)	20 (18%)	2	13
26	d4	112/112 (100%)	92 (82%)	20 (18%)	2	13
27	D5	61/88 (69%)	45 (74%)	16 (26%)	1	4
27	d5	61/88 (69%)	52 (85%)	9 (15%)	4	21
28	D6	83/83 (100%)	66 (80%)	17 (20%)	2	9
28	d6	83/83 (100%)	72 (87%)	11 (13%)	6	25
29	D7	70/70 (100%)	61 (87%)	9 (13%)	6	26
29	d7	70/70 (100%)	56 (80%)	14 (20%)	2	10
30	D8	56/59 (95%)	45 (80%)	11 (20%)	2	11
30	d8	56/59 (95%)	44 (79%)	12 (21%)	1	8
31	D9	47/48 (98%)	41 (87%)	6 (13%)	6	27
31	d9	47/48 (98%)	36 (77%)	11 (23%)	1	5
32	E0	51/51 (100%)	42 (82%)	9 (18%)	3	14
33	E1	62/66 (94%)	48 (77%)	14 (23%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	e1	66/66 (100%)	49 (74%)	17 (26%)	1	4
34	SR	260/261 (100%)	226 (87%)	34 (13%)	6	25
34	sR	260/261 (100%)	230 (88%)	30 (12%)	8	32
35	SM	97/228 (42%)	75 (77%)	22 (23%)	1	6
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	3
39	L2	193/195 (99%)	152 (79%)	41 (21%)	1	8
39	l2	192/195 (98%)	148 (77%)	44 (23%)	1	6
40	L3	319/322 (99%)	256 (80%)	63 (20%)	2	11
40	l3	321/322 (100%)	261 (81%)	60 (19%)	2	12
41	L4	288/288 (100%)	227 (79%)	61 (21%)	1	8
41	l4	288/288 (100%)	234 (81%)	54 (19%)	2	12
42	L5	244/244 (100%)	195 (80%)	49 (20%)	2	10
42	l5	243/244 (100%)	203 (84%)	40 (16%)	3	16
43	L6	134/152 (88%)	113 (84%)	21 (16%)	4	18
43	l6	135/152 (89%)	112 (83%)	23 (17%)	3	15
44	L7	186/204 (91%)	156 (84%)	30 (16%)	3	17
44	l7	187/204 (92%)	156 (83%)	31 (17%)	3	16
45	L8	187/207 (90%)	153 (82%)	34 (18%)	2	13
45	l8	177/207 (86%)	143 (81%)	34 (19%)	2	12
46	L9	171/171 (100%)	131 (77%)	40 (23%)	1	5
46	l9	171/171 (100%)	133 (78%)	38 (22%)	1	7
47	M0	177/186 (95%)	143 (81%)	34 (19%)	2	12
47	m0	179/186 (96%)	139 (78%)	40 (22%)	1	7
48	M1	147/150 (98%)	116 (79%)	31 (21%)	1	8
48	m1	147/150 (98%)	123 (84%)	24 (16%)	3	17
49	M3	154/158 (98%)	126 (82%)	28 (18%)	2	13
49	m3	154/158 (98%)	129 (84%)	25 (16%)	3	17
50	M4	107/108 (99%)	87 (81%)	20 (19%)	2	12
50	m4	108/108 (100%)	90 (83%)	18 (17%)	3	16
51	M5	175/175 (100%)	144 (82%)	31 (18%)	3	14
51	m5	175/175 (100%)	149 (85%)	26 (15%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	M6	160/161 (99%)	135 (84%)	25 (16%)	4	18
52	m6	160/161 (99%)	130 (81%)	30 (19%)	2	12
53	M7	140/145 (97%)	112 (80%)	28 (20%)	2	10
53	m7	125/145 (86%)	97 (78%)	28 (22%)	1	7
54	M8	150/150 (100%)	129 (86%)	21 (14%)	5	23
54	m8	150/150 (100%)	122 (81%)	28 (19%)	2	12
55	M9	153/153 (100%)	126 (82%)	27 (18%)	3	14
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	7
56	N0	156/156 (100%)	125 (80%)	31 (20%)	2	10
56	n0	156/156 (100%)	126 (81%)	30 (19%)	2	12
57	N1	136/136 (100%)	110 (81%)	26 (19%)	2	12
57	n1	136/136 (100%)	112 (82%)	24 (18%)	3	14
58	N2	87/106 (82%)	77 (88%)	10 (12%)	8	32
58	n2	85/106 (80%)	69 (81%)	16 (19%)	2	12
59	N3	104/104 (100%)	84 (81%)	20 (19%)	2	12
59	n3	104/104 (100%)	92 (88%)	12 (12%)	8	32
60	N4	57/129 (44%)	49 (86%)	8 (14%)	5	23
60	n4	100/129 (78%)	83 (83%)	17 (17%)	3	15
61	N5	104/117 (89%)	78 (75%)	26 (25%)	1	4
61	n5	104/117 (89%)	83 (80%)	21 (20%)	2	10
62	N6	109/109 (100%)	87 (80%)	22 (20%)	2	10
62	n6	109/109 (100%)	82 (75%)	27 (25%)	1	4
63	N7	115/115 (100%)	92 (80%)	23 (20%)	2	10
63	n7	115/115 (100%)	90 (78%)	25 (22%)	1	8
64	N8	118/118 (100%)	96 (81%)	22 (19%)	2	13
64	n8	118/118 (100%)	95 (80%)	23 (20%)	2	11
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1	8
65	n9	46/46 (100%)	34 (74%)	12 (26%)	1	4
66	O0	81/87 (93%)	66 (82%)	15 (18%)	2	13
66	o0	84/87 (97%)	67 (80%)	17 (20%)	2	10
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	o1	94/96 (98%)	71 (76%)	23 (24%)	1	5
68	O2	109/110 (99%)	92 (84%)	17 (16%)	4	18
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	7
69	O3	90/90 (100%)	80 (89%)	10 (11%)	9	34
69	o3	90/90 (100%)	75 (83%)	15 (17%)	3	16
70	O4	95/102 (93%)	82 (86%)	13 (14%)	5	24
70	o4	95/102 (93%)	74 (78%)	21 (22%)	1	7
71	O5	104/104 (100%)	81 (78%)	23 (22%)	1	7
71	o5	103/104 (99%)	81 (79%)	22 (21%)	1	8
72	O6	81/81 (100%)	59 (73%)	22 (27%)	0	3
72	o6	80/81 (99%)	53 (66%)	27 (34%)	0	1
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1	8
73	o7	70/70 (100%)	55 (79%)	15 (21%)	1	8
74	O8	68/68 (100%)	50 (74%)	18 (26%)	1	4
74	o8	67/68 (98%)	54 (81%)	13 (19%)	2	11
75	O9	45/45 (100%)	38 (84%)	7 (16%)	4	18
75	o9	45/45 (100%)	35 (78%)	10 (22%)	1	7
76	Q0	47/47 (100%)	36 (77%)	11 (23%)	1	5
76	q0	47/47 (100%)	35 (74%)	12 (26%)	1	4
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	2
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	1	5
78	q2	90/90 (100%)	74 (82%)	16 (18%)	2	14
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1	8
79	q3	71/71 (100%)	61 (86%)	10 (14%)	5	23
80	e0	53/53 (100%)	42 (79%)	11 (21%)	2	8
82	p0	105/253 (42%)	86 (82%)	19 (18%)	2	13
All	All	18728/20241 (92%)	15139 (81%)	3589 (19%)	2	12

5 of 3589 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	O3	70	LYS

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Mol	Chain	Res	Type
8	s6	71	THR
64	n8	82	ILE
72	O6	45	ARG
3	s1	58	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
69	O3	106	ASN
9	s7	86	GLN
64	n8	44	ASN
2	s0	23	HIS
7	s5	104	ASN

5.3.3 RNA ⓘ

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

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2562 ligands modelled in this entry, 1427 are monoatomic - leaving 1135 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	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	-
86	OHX	1	3897	-	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	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	-
86	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
86	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
86	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
86	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
86	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
86	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
86	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	HMT	1	4217	-	43,43,43	1.00	1 (2%)	66,66,66	1.30	6 (9%)
86	OHX	2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2088	-	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	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2131	-	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	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2147	-	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	86	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	-
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	-

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

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

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4252	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4253	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4254	-	0,6,6	0.00	-	0,15,15	0.00	-
88	HMT	5	4255	-	43,43,43	0.55	0	66,66,66	1.04	5 (7%)

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	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	402	-	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	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O2	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	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	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	201	-	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	l3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	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	203	-	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	301	-	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	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	203	-	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	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	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s4	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s9	202	-	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	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

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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4216	-	-	0/0/0/0	0/0/0/0
88	HMT	1	4217	-	-	0/27/74/74	0/5/5/5
86	OHX	2	2022	-	-	0/0/0/0	0/0/0/0
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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	3	214	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	3	215	-	-	0/0/0/0	0/0/0/0
86	OHX	3	216	-	-	0/0/0/0	0/0/0/0
86	OHX	3	217	-	-	0/0/0/0	0/0/0/0
86	OHX	3	218	-	-	0/0/0/0	0/0/0/0
86	OHX	3	219	-	-	0/0/0/0	0/0/0/0
86	OHX	3	220	-	-	0/0/0/0	0/0/0/0
86	OHX	3	221	-	-	0/0/0/0	0/0/0/0
86	OHX	3	222	-	-	0/0/0/0	0/0/0/0
86	OHX	3	223	-	-	0/0/0/0	0/0/0/0
86	OHX	3	224	-	-	0/0/0/0	0/0/0/0
86	OHX	4	224	-	-	0/0/0/0	0/0/0/0
86	OHX	4	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	227	-	-	0/0/0/0	0/0/0/0
86	OHX	4	228	-	-	0/0/0/0	0/0/0/0
86	OHX	4	229	-	-	0/0/0/0	0/0/0/0
86	OHX	4	230	-	-	0/0/0/0	0/0/0/0
86	OHX	4	231	-	-	0/0/0/0	0/0/0/0
86	OHX	4	232	-	-	0/0/0/0	0/0/0/0
86	OHX	4	233	-	-	0/0/0/0	0/0/0/0
86	OHX	4	234	-	-	0/0/0/0	0/0/0/0
86	OHX	4	235	-	-	0/0/0/0	0/0/0/0
86	OHX	4	236	-	-	0/0/0/0	0/0/0/0
86	OHX	4	237	-	-	0/0/0/0	0/0/0/0
86	OHX	4	238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3917	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3959	-	-	0/0/0/0	0/0/0/0

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	86	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4252	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4253	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4254	-	-	0/0/0/0	0/0/0/0
88	HMT	5	4255	-	-	0/27/74/74	0/5/5/5
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2087	-	-	0/0/0/0	0/0/0/0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2205	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2206	-	-	0/0/0/0	0/0/0/0
86	OHX	7	217	-	-	0/0/0/0	0/0/0/0
86	OHX	7	218	-	-	0/0/0/0	0/0/0/0
86	OHX	7	219	-	-	0/0/0/0	0/0/0/0
86	OHX	7	220	-	-	0/0/0/0	0/0/0/0
86	OHX	7	221	-	-	0/0/0/0	0/0/0/0
86	OHX	7	222	-	-	0/0/0/0	0/0/0/0
86	OHX	7	223	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	7	224	-	-	0/0/0/0	0/0/0/0
86	OHX	7	225	-	-	0/0/0/0	0/0/0/0
86	OHX	7	226	-	-	0/0/0/0	0/0/0/0
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	7	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	-	-	0/0/0/0	0/0/0/0
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0
86	OHX	8	219	-	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	-	-	0/0/0/0	0/0/0/0
86	OHX	8	222	-	-	0/0/0/0	0/0/0/0
86	OHX	8	223	-	-	0/0/0/0	0/0/0/0
86	OHX	8	224	-	-	0/0/0/0	0/0/0/0
86	OHX	8	225	-	-	0/0/0/0	0/0/0/0
86	OHX	8	226	-	-	0/0/0/0	0/0/0/0
86	OHX	8	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	229	-	-	0/0/0/0	0/0/0/0
86	OHX	8	230	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	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	402	-	-	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	206	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	203	-	-	0/0/0/0	0/0/0/0
86	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O2	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	105	-	-	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	S8	302	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	201	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	406	-	-	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	302	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	301	-	-	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	n9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	503	-	-	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	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4217	HMT	C4-C3	-5.23	1.46	1.54

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4217	HMT	O4-C3-C2	-6.53	98.35	109.08
88	5	4255	HMT	C1-C9-N1	-3.98	106.86	114.71
88	5	4255	HMT	O4-C3-C2	-3.81	102.81	109.08
88	1	4217	HMT	C8-N1-C9	3.31	124.16	117.27
88	1	4217	HMT	C9-C4-C5	2.92	121.79	116.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1750/1800 (97%)	0.08	102 (5%) 22 5	52, 89, 160, 248	0
1	6	1795/1800 (99%)	0.09	105 (5%) 22 5	38, 74, 169, 247	0
2	S0	206/251 (82%)	0.07	8 (3%) 37 7	92, 106, 118, 143	0
2	s0	206/251 (82%)	-0.15	2 (0%) 79 22	71, 90, 103, 116	0
3	S1	214/254 (84%)	0.53	17 (7%) 13 3	99, 126, 152, 160	0
3	s1	216/254 (85%)	-0.08	0 100 100	68, 82, 101, 110	0
4	S2	217/253 (85%)	-0.15	1 (0%) 88 36	71, 86, 102, 120	0
4	s2	217/253 (85%)	-0.11	2 (0%) 81 24	54, 70, 87, 97	0
5	S3	223/239 (93%)	0.12	8 (3%) 41 8	76, 91, 120, 132	0
5	s3	223/239 (93%)	0.17	3 (1%) 74 19	73, 104, 126, 134	0
6	S4	260/260 (100%)	0.05	3 (1%) 75 20	63, 89, 101, 126	0
6	s4	260/260 (100%)	-0.17	0 100 100	49, 73, 86, 113	0
7	S5	206/224 (91%)	0.17	5 (2%) 56 11	99, 117, 129, 138	0
7	s5	206/224 (91%)	-0.01	4 (1%) 64 13	69, 91, 111, 124	0
8	S6	226/236 (95%)	0.31	5 (2%) 59 12	64, 99, 119, 140	0
8	s6	218/236 (92%)	0.11	1 (0%) 88 36	49, 78, 100, 121	0
9	S7	184/189 (97%)	0.16	3 (1%) 68 16	86, 113, 137, 144	0
9	s7	186/189 (98%)	0.17	3 (1%) 68 16	68, 100, 132, 138	0
10	S8	188/200 (94%)	0.02	1 (0%) 88 36	56, 71, 111, 124	0
10	s8	188/200 (94%)	0.07	4 (2%) 60 12	43, 64, 111, 126	0
11	S9	185/196 (94%)	0.14	4 (2%) 59 12	83, 97, 132, 163	0
11	s9	185/196 (94%)	-0.06	1 (0%) 88 36	64, 77, 109, 140	0
12	C0	96/105 (91%)	-0.03	0 100 100	83, 104, 139, 152	0
12	c0	96/105 (91%)	0.46	6 (6%) 19 5	99, 134, 150, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	0.00	5 (3%)	45	9	60, 70, 114, 119	0
13	c1	146/155 (94%)	-0.09	4 (2%)	52	10	47, 62, 94, 115	0
14	C2	124/142 (87%)	1.28	27 (21%)	1	1	129, 139, 155, 163	0
14	c2	124/142 (87%)	2.07	62 (50%)	0	0	178, 189, 204, 208	0
15	C3	150/150 (100%)	-0.01	0	100	100	67, 87, 100, 107	0
15	c3	150/150 (100%)	-0.17	0	100	100	54, 69, 86, 97	0
16	C4	127/136 (93%)	0.27	5 (3%)	37	7	69, 122, 136, 138	0
16	c4	128/136 (94%)	0.02	0	100	100	48, 82, 90, 97	0
17	C5	124/141 (87%)	0.06	1 (0%)	83	26	80, 96, 129, 145	0
17	c5	135/141 (95%)	0.20	9 (6%)	17	4	77, 99, 117, 129	0
18	C6	141/142 (99%)	0.22	5 (3%)	42	8	82, 111, 116, 119	0
18	c6	142/142 (100%)	0.29	5 (3%)	42	8	64, 85, 102, 124	0
19	C7	120/136 (88%)	0.22	5 (4%)	35	7	94, 109, 130, 132	0
19	c7	117/136 (86%)	0.12	0	100	100	78, 92, 112, 116	0
20	C8	145/145 (100%)	0.23	6 (4%)	35	7	78, 108, 129, 137	0
20	c8	145/145 (100%)	0.01	3 (2%)	60	12	68, 88, 110, 122	0
21	C9	143/143 (100%)	0.17	2 (1%)	72	18	92, 107, 122, 133	0
21	c9	143/143 (100%)	-0.14	0	100	100	64, 77, 94, 114	0
22	D0	107/120 (89%)	0.64	11 (10%)	7	2	74, 108, 136, 139	0
22	d0	110/120 (91%)	0.72	14 (12%)	4	1	69, 105, 138, 148	0
23	D1	87/87 (100%)	0.02	0	100	100	89, 95, 111, 121	0
23	d1	87/87 (100%)	-0.09	1 (1%)	77	21	68, 76, 97, 107	0
24	D2	129/129 (100%)	-0.15	0	100	100	70, 81, 90, 101	0
24	d2	129/129 (100%)	-0.22	0	100	100	52, 63, 70, 81	0
25	D3	144/144 (100%)	-0.06	0	100	100	58, 63, 74, 86	0
25	d3	144/144 (100%)	-0.20	0	100	100	43, 48, 60, 73	0
26	D4	134/134 (100%)	0.27	2 (1%)	70	16	75, 102, 116, 122	0
26	d4	134/134 (100%)	-0.05	0	100	100	57, 81, 95, 115	0
27	D5	70/107 (65%)	0.18	1 (1%)	72	18	115, 129, 136, 137	0
27	d5	69/107 (64%)	0.57	5 (7%)	15	4	83, 106, 118, 121	0
28	D6	97/97 (100%)	0.31	3 (3%)	47	9	75, 90, 138, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	-0.10	0 100 100	53, 66, 93, 101	0
29	D7	81/81 (100%)	0.15	2 (2%) 54 11	84, 98, 125, 130	0
29	d7	81/81 (100%)	0.08	1 (1%) 75 20	65, 82, 120, 124	0
30	D8	63/66 (95%)	0.67	2 (3%) 45 9	111, 125, 136, 141	0
30	d8	63/66 (95%)	0.65	3 (4%) 29 6	88, 103, 116, 125	0
31	D9	53/55 (96%)	-0.04	1 (1%) 64 13	77, 82, 102, 109	0
31	d9	53/55 (96%)	0.26	1 (1%) 64 13	70, 82, 124, 134	0
32	E0	60/60 (100%)	0.79	8 (13%) 4 1	62, 95, 131, 137	0
33	E1	71/76 (93%)	0.81	8 (11%) 6 2	99, 126, 138, 141	0
33	e1	76/76 (100%)	2.30	37 (48%) 1 0	146, 165, 178, 179	0
34	SR	318/318 (100%)	0.20	5 (1%) 68 16	66, 115, 133, 150	0
34	sR	318/318 (100%)	0.29	10 (3%) 47 9	97, 115, 131, 147	0
35	SM	159/273 (58%)	0.32	13 (8%) 12 3	62, 88, 139, 144	0
35	sM	104/273 (38%)	0.48	10 (9%) 8 2	63, 100, 182, 188	0
36	1	3149/3396 (92%)	-0.15	105 (3%) 44 8	25, 49, 127, 239	0
36	5	3150/3396 (92%)	-0.19	68 (2%) 59 12	24, 47, 115, 209	0
37	3	121/121 (100%)	-0.33	0 100 100	38, 68, 85, 89	0
37	7	121/121 (100%)	-0.41	1 (0%) 83 26	31, 50, 63, 72	0
38	4	158/158 (100%)	-0.35	3 (1%) 64 13	32, 51, 91, 126	0
38	8	158/158 (100%)	-0.29	3 (1%) 64 13	35, 57, 96, 117	0
39	L2	252/253 (99%)	-0.26	0 100 100	32, 47, 64, 74	0
39	l2	252/253 (99%)	-0.19	2 (0%) 83 26	32, 50, 67, 78	0
40	L3	386/386 (100%)	-0.29	0 100 100	30, 54, 68, 104	0
40	l3	386/386 (100%)	-0.34	0 100 100	24, 39, 52, 83	0
41	L4	361/361 (100%)	-0.29	1 (0%) 91 48	27, 42, 60, 69	0
41	l4	361/361 (100%)	-0.22	0 100 100	28, 47, 66, 79	0
42	L5	296/296 (100%)	-0.02	1 (0%) 91 48	49, 74, 93, 118	0
42	l5	294/296 (99%)	-0.23	0 100 100	38, 54, 81, 121	0
43	L6	156/175 (89%)	-0.23	0 100 100	38, 45, 66, 87	0
43	l6	157/175 (89%)	-0.28	1 (0%) 86 32	39, 46, 67, 78	0
44	L7	222/243 (91%)	-0.37	0 100 100	31, 39, 68, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	-0.33	0 100 100	29, 36, 72, 113	0
45	L8	233/255 (91%)	-0.08	0 100 100	55, 69, 102, 116	0
45	l8	231/255 (90%)	0.26	6 (2%) 53 10	66, 79, 105, 117	0
46	L9	191/191 (100%)	-0.12	0 100 100	49, 61, 77, 93	0
46	l9	191/191 (100%)	-0.30	1 (0%) 88 36	33, 43, 61, 74	0
47	M0	211/220 (95%)	-0.23	1 (0%) 88 36	37, 50, 87, 99	0
47	m0	213/220 (96%)	-0.16	3 (1%) 72 18	33, 54, 79, 97	0
48	M1	169/173 (97%)	0.02	0 100 100	60, 79, 92, 98	0
48	m1	169/173 (97%)	-0.18	0 100 100	41, 60, 72, 83	0
49	M3	193/198 (97%)	-0.18	0 100 100	30, 51, 91, 119	0
49	m3	194/198 (97%)	-0.14	2 (1%) 79 22	39, 59, 97, 120	0
50	M4	136/137 (99%)	-0.20	0 100 100	41, 49, 62, 73	0
50	m4	137/137 (100%)	-0.37	0 100 100	36, 41, 60, 71	0
51	M5	203/203 (100%)	-0.28	0 100 100	30, 45, 55, 61	0
51	m5	203/203 (100%)	-0.19	0 100 100	37, 53, 64, 69	0
52	M6	197/198 (99%)	-0.29	0 100 100	30, 40, 57, 62	0
52	m6	197/198 (99%)	-0.38	0 100 100	25, 30, 57, 63	0
53	M7	183/183 (100%)	0.01	8 (4%) 33 7	34, 42, 96, 127	0
53	m7	155/183 (84%)	-0.28	0 100 100	29, 36, 49, 79	0
54	M8	185/185 (100%)	-0.34	0 100 100	33, 42, 57, 72	0
54	m8	185/185 (100%)	-0.34	0 100 100	36, 47, 55, 61	0
55	M9	188/188 (100%)	0.09	4 (2%) 60 12	50, 66, 148, 158	0
55	m9	188/188 (100%)	-0.00	0 100 100	44, 57, 127, 137	0
56	N0	172/172 (100%)	-0.34	0 100 100	40, 47, 63, 70	0
56	n0	172/172 (100%)	-0.37	0 100 100	30, 38, 49, 60	0
57	N1	159/159 (100%)	-0.27	1 (0%) 86 32	35, 47, 89, 97	0
57	n1	159/159 (100%)	-0.26	0 100 100	32, 39, 77, 84	0
58	N2	100/120 (83%)	0.41	3 (3%) 48 9	83, 96, 110, 122	0
58	n2	98/120 (81%)	0.28	1 (1%) 79 22	70, 83, 93, 100	0
59	N3	136/136 (100%)	-0.20	0 100 100	37, 48, 60, 69	0
59	n3	136/136 (100%)	-0.27	0 100 100	26, 37, 52, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	0.73	16 (16%) 2 1	48, 63, 145, 148	0
60	n4	135/155 (87%)	0.31	8 (5%) 22 5	38, 85, 117, 135	0
61	N5	121/141 (85%)	0.02	2 (1%) 67 15	43, 58, 73, 103	0
61	n5	120/141 (85%)	-0.03	1 (0%) 83 26	45, 61, 79, 88	0
62	N6	126/126 (100%)	-0.25	0 100 100	39, 51, 63, 73	0
62	n6	126/126 (100%)	-0.18	0 100 100	44, 56, 72, 80	0
63	N7	135/135 (100%)	0.06	0 100 100	68, 80, 96, 105	0
63	n7	135/135 (100%)	-0.05	1 (0%) 84 28	72, 86, 107, 114	0
64	N8	148/148 (100%)	-0.21	0 100 100	26, 44, 65, 76	0
64	n8	148/148 (100%)	-0.23	0 100 100	28, 49, 68, 73	0
65	N9	58/58 (100%)	0.13	3 (5%) 26 6	35, 52, 98, 114	0
65	n9	58/58 (100%)	-0.12	0 100 100	31, 48, 73, 84	0
66	O0	97/104 (93%)	-0.14	0 100 100	67, 75, 94, 100	0
66	o0	100/104 (96%)	-0.24	0 100 100	65, 77, 99, 106	0
67	O1	109/112 (97%)	-0.03	1 (0%) 81 24	48, 61, 92, 105	0
67	o1	109/112 (97%)	0.02	1 (0%) 81 24	38, 48, 82, 102	0
68	O2	127/129 (98%)	-0.23	1 (0%) 83 26	25, 39, 50, 65	0
68	o2	127/129 (98%)	-0.22	2 (1%) 68 16	26, 44, 57, 73	0
69	O3	106/106 (100%)	-0.29	0 100 100	31, 37, 59, 68	0
69	o3	106/106 (100%)	-0.27	0 100 100	29, 35, 59, 72	0
70	O4	112/120 (93%)	0.12	3 (2%) 52 10	45, 64, 100, 112	0
70	o4	112/120 (93%)	0.07	2 (1%) 65 14	45, 65, 110, 119	0
71	O5	119/119 (100%)	-0.12	0 100 100	43, 60, 68, 71	0
71	o5	119/119 (100%)	-0.15	0 100 100	50, 64, 76, 83	0
72	O6	99/99 (100%)	0.02	0 100 100	49, 59, 89, 103	0
72	o6	99/99 (100%)	0.02	0 100 100	53, 68, 91, 110	0
73	O7	87/87 (100%)	-0.08	1 (1%) 77 21	32, 37, 60, 85	0
73	o7	87/87 (100%)	-0.06	3 (3%) 43 8	33, 41, 70, 107	0
74	O8	77/77 (100%)	0.08	1 (1%) 74 19	72, 82, 104, 109	0
74	o8	77/77 (100%)	0.23	0 100 100	73, 85, 103, 106	0
75	O9	50/50 (100%)	-0.35	0 100 100	41, 44, 53, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	-0.27	0 100 100	43, 46, 58, 64	0
76	Q0	52/52 (100%)	-0.18	0 100 100	43, 50, 62, 73	0
76	q0	52/52 (100%)	-0.29	0 100 100	30, 34, 46, 51	0
77	Q1	25/25 (100%)	-0.12	0 100 100	54, 56, 59, 61	0
77	q1	25/25 (100%)	-0.29	0 100 100	41, 43, 55, 63	0
78	Q2	105/105 (100%)	0.28	5 (4%) 29 6	35, 52, 72, 100	0
78	q2	105/105 (100%)	0.20	1 (0%) 79 22	38, 50, 69, 93	0
79	Q3	91/91 (100%)	-0.18	0 100 100	40, 50, 68, 81	0
79	q3	91/91 (100%)	-0.23	0 100 100	36, 50, 65, 75	0
80	e0	62/62 (100%)	0.50	5 (8%) 12 3	52, 78, 106, 115	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	0.24	4 (2%) 50 10	84, 102, 180, 188	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35346 (93%)	-0.03	841 (2%) 54 11	24, 65, 129, 248	0

The worst 5 of 841 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	6	662	U	11.6
33	e1	85	TYR	10.5
1	6	663	U	9.9
33	e1	77	GLY	9.8
60	N4	76	VAL	9.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	3594	1/1	0.76	1199.00	58,58,58,58	0
85	MG	1	3747	1/1	0.73	363.00	59,59,59,59	0
85	MG	5	3781	1/1	0.44	269.00	76,76,76,76	0
85	MG	1	3826	1/1	0.56	261.00	47,47,47,47	0
85	MG	4	222	1/1	0.84	231.67	90,90,90,90	0
85	MG	6	2034	1/1	0.74	227.97	66,66,66,66	0
85	MG	5	3866	1/1	0.74	227.00	56,56,56,56	0
85	MG	1	3686	1/1	0.35	205.00	43,43,43,43	0
85	MG	6	1920	1/1	0.57	199.50	61,61,61,61	0
85	MG	1	3814	1/1	0.49	153.50	39,39,39,39	0
85	MG	6	1924	1/1	1.38	149.25	97,97,97,97	0
85	MG	7	216	1/1	0.31	141.00	47,47,47,47	0
85	MG	5	3731	1/1	0.45	139.00	61,61,61,61	0
85	MG	5	3604	1/1	0.56	137.23	40,40,40,40	0
85	MG	1	3735	1/1	0.25	136.00	81,81,81,81	0
85	MG	2	1958	1/1	0.92	133.33	85,85,85,85	0
85	MG	5	3853	1/1	0.44	130.00	62,62,62,62	0
86	OHX	5	4182	7/7	0.47	126.84	140,140,140,140	0
85	MG	3	205	1/1	0.64	121.82	44,44,44,44	0
85	MG	5	3454	1/1	0.59	119.73	45,45,45,45	0
85	MG	1	3679	1/1	0.57	113.00	72,72,72,72	0
85	MG	5	3695	1/1	1.32	111.87	74,74,74,74	0
85	MG	1	3581	1/1	0.68	108.89	34,34,34,34	0
85	MG	1	3662	1/1	0.52	100.31	42,42,42,42	0
85	MG	5	3725	1/1	0.45	99.53	37,37,37,37	0
85	MG	1	3649	1/1	0.45	99.33	38,38,38,38	0
85	MG	2	2013	1/1	0.75	98.82	72,72,72,72	0
85	MG	5	3562	1/1	0.73	98.43	26,26,26,26	0
85	MG	1	3762	1/1	0.37	97.80	54,54,54,54	0
85	MG	5	3855	1/1	0.63	95.44	54,54,54,54	0
85	MG	5	3666	1/1	0.49	93.00	53,53,53,53	0
85	MG	1	3494	1/1	0.63	92.64	83,83,83,83	0
85	MG	2	1909	1/1	0.91	91.99	77,77,77,77	0
86	OHX	5	4231	7/7	0.53	91.65	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	5	3481	1/1	0.84	91.40	68,68,68,68	0
85	MG	1	3536	1/1	0.62	91.08	29,29,29,29	0
85	MG	1	3853	1/1	0.68	89.51	56,56,56,56	0
85	MG	17	303	1/1	0.45	87.00	39,39,39,39	0
85	MG	L3	403	1/1	1.06	85.38	52,52,52,52	0
85	MG	5	3458	1/1	0.45	84.43	34,34,34,34	0
85	MG	5	3493	1/1	0.78	84.35	59,59,59,59	0
85	MG	2	1926	1/1	0.69	83.77	96,96,96,96	0
85	MG	4	201	1/1	0.59	83.55	55,55,55,55	0
85	MG	1	3451	1/1	0.49	81.02	36,36,36,36	0
85	MG	6	1948	1/1	0.69	79.56	42,42,42,42	0
85	MG	6	1981	1/1	0.54	78.24	67,67,67,67	0
85	MG	2	1982	1/1	1.03	77.88	90,90,90,90	0
85	MG	7	206	1/1	0.49	76.33	27,27,27,27	0
85	MG	5	3474	1/1	0.48	76.33	67,67,67,67	0
85	MG	2	1981	1/1	0.92	74.73	61,61,61,61	0
85	MG	1	3689	1/1	0.66	73.00	82,82,82,82	0
85	MG	2	2015	1/1	0.60	72.09	70,70,70,70	0
85	MG	2	1990	1/1	0.88	72.05	111,111,111,111	0
85	MG	5	3537	1/1	0.45	71.67	34,34,34,34	0
85	MG	2	1925	1/1	0.93	71.61	67,67,67,67	0
85	MG	1	3481	1/1	0.77	70.85	78,78,78,78	0
85	MG	6	1928	1/1	0.67	70.20	71,71,71,71	0
85	MG	1	3470	1/1	0.49	69.56	48,48,48,48	0
85	MG	1	3508	1/1	0.64	69.44	37,37,37,37	0
85	MG	1	3778	1/1	0.46	69.43	61,61,61,61	0
85	MG	5	3502	1/1	0.55	68.50	46,46,46,46	0
85	MG	1	3528	1/1	0.51	67.13	28,28,28,28	0
85	MG	1	3835	1/1	0.42	66.53	28,28,28,28	0
85	MG	5	3530	1/1	0.69	65.17	26,26,26,26	0
85	MG	4	202	1/1	0.81	63.75	50,50,50,50	0
85	MG	6	2039	1/1	0.64	63.61	58,58,58,58	0
85	MG	5	3598	1/1	0.69	61.80	28,28,28,28	0
85	MG	1	3638	1/1	0.48	61.55	72,72,72,72	0
85	MG	5	3443	1/1	0.28	61.00	31,31,31,31	0
85	MG	6	2020	1/1	0.56	60.54	53,53,53,53	0
85	MG	5	3483	1/1	0.34	60.50	71,71,71,71	0
86	OHX	1	4199	7/7	0.44	59.20	155,155,155,155	0
85	MG	1	3449	1/1	0.36	59.18	29,29,29,29	0
85	MG	5	3849	1/1	0.36	59.00	46,46,46,46	0
85	MG	2	2010	1/1	0.47	58.71	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	1982	1/1	0.68	58.33	78,78,78,78	0
85	MG	6	1915	1/1	0.63	58.04	56,56,56,56	0
85	MG	5	3622	1/1	0.87	57.84	35,35,35,35	0
85	MG	5	3538	1/1	0.47	56.68	33,33,33,33	0
85	MG	5	3556	1/1	0.49	55.73	36,36,36,36	0
85	MG	5	3591	1/1	0.41	54.56	43,43,43,43	0
85	MG	5	3898	1/1	1.17	54.05	94,94,94,94	0
85	MG	2	2021	1/1	0.73	53.88	97,97,97,97	0
86	OHX	6	2192	7/7	0.41	53.86	142,142,142,142	0
85	MG	5	3578	1/1	0.93	53.25	44,44,44,44	0
85	MG	8	214	1/1	0.55	52.87	56,56,56,56	0
85	MG	1	3419	1/1	0.47	52.84	56,56,56,56	0
85	MG	2	1917	1/1	0.68	52.40	64,64,64,64	0
85	MG	5	3883	1/1	0.47	52.19	50,50,50,50	0
85	MG	5	3733	1/1	0.29	52.14	68,68,68,68	0
85	MG	2	1913	1/1	1.45	51.69	82,82,82,82	0
85	MG	5	3896	1/1	0.61	51.62	52,52,52,52	0
86	OHX	5	4224	7/7	0.44	51.03	165,165,165,165	0
85	MG	5	3436	1/1	0.42	50.80	33,33,33,33	0
85	MG	2	1975	1/1	1.31	50.79	87,87,87,87	0
85	MG	1	3527	1/1	0.38	50.63	28,28,28,28	0
85	MG	5	3708	1/1	0.98	50.56	91,91,91,91	0
85	MG	1	3525	1/1	0.35	50.24	25,25,25,25	0
85	MG	1	3620	1/1	0.31	48.50	51,51,51,51	0
85	MG	5	3513	1/1	0.61	48.11	61,61,61,61	0
85	MG	5	3575	1/1	0.50	47.87	24,24,24,24	0
85	MG	2	1957	1/1	0.99	47.69	72,72,72,72	0
85	MG	1	3847	1/1	0.70	47.42	51,51,51,51	0
85	MG	2	1935	1/1	0.58	47.33	60,60,60,60	0
85	MG	1	3514	1/1	0.63	47.26	27,27,27,27	0
85	MG	5	3596	1/1	0.52	47.13	26,26,26,26	0
85	MG	1	3529	1/1	0.53	46.79	32,32,32,32	0
85	MG	1	3706	1/1	0.65	46.20	42,42,42,42	0
85	MG	5	3577	1/1	0.40	45.95	34,34,34,34	0
85	MG	7	202	1/1	0.49	45.77	40,40,40,40	0
85	MG	2	1928	1/1	0.82	45.56	86,86,86,86	0
85	MG	1	3563	1/1	0.62	45.30	41,41,41,41	0
85	MG	1	3430	1/1	0.57	45.14	41,41,41,41	0
85	MG	5	3571	1/1	0.52	45.08	23,23,23,23	0
85	MG	5	3539	1/1	0.39	45.03	25,25,25,25	0
85	MG	1	3500	1/1	0.59	44.66	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1989	1/1	0.89	44.44	61,61,61,61	0
85	MG	6	1959	1/1	0.63	44.37	60,60,60,60	0
85	MG	6	1958	1/1	0.69	44.06	53,53,53,53	0
85	MG	5	3621	1/1	0.30	44.04	48,48,48,48	0
85	MG	5	3518	1/1	0.53	43.36	22,22,22,22	0
85	MG	2	1905	1/1	0.65	43.29	65,65,65,65	0
85	MG	6	2036	1/1	1.11	43.27	67,67,67,67	0
85	MG	2	2016	1/1	0.78	42.59	78,78,78,78	0
85	MG	1	3600	1/1	0.59	42.43	22,22,22,22	0
85	MG	1	3564	1/1	0.48	42.29	26,26,26,26	0
85	MG	5	3632	1/1	0.54	41.62	90,90,90,90	0
85	MG	6	1939	1/1	0.91	41.16	66,66,66,66	0
85	MG	5	3464	1/1	0.38	41.12	51,51,51,51	0
85	MG	1	3599	1/1	0.64	40.60	42,42,42,42	0
86	OHX	5	4118	7/7	0.24	40.50	141,141,141,141	0
85	MG	1	3754	1/1	0.72	40.35	61,61,61,61	0
85	MG	5	3889	1/1	0.59	40.32	53,53,53,53	0
85	MG	6	2037	1/1	0.76	40.20	87,87,87,87	0
85	MG	6	1933	1/1	0.49	40.11	65,65,65,65	0
85	MG	2	2018	1/1	1.49	40.05	79,79,79,79	0
85	MG	5	3643	1/1	0.66	40.02	56,56,56,56	0
85	MG	5	3553	1/1	0.72	39.25	47,47,47,47	0
85	MG	1	3539	1/1	0.80	38.83	37,37,37,37	0
85	MG	2	1906	1/1	0.44	38.78	54,54,54,54	0
85	MG	1	3790	1/1	0.29	38.75	38,38,38,38	0
85	MG	1	3651	1/1	0.71	38.71	46,46,46,46	0
85	MG	1	3692	1/1	0.42	38.69	60,60,60,60	0
85	MG	5	3549	1/1	0.69	38.57	43,43,43,43	0
85	MG	5	3585	1/1	0.64	38.41	30,30,30,30	0
85	MG	6	1945	1/1	0.62	38.24	52,52,52,52	0
85	MG	5	3672	1/1	0.49	37.92	57,57,57,57	0
85	MG	5	3868	1/1	0.26	37.67	49,49,49,49	0
85	MG	5	3880	1/1	0.46	37.48	24,24,24,24	0
85	MG	1	3410	1/1	0.50	37.33	26,26,26,26	0
85	MG	5	3446	1/1	0.34	37.20	42,42,42,42	0
85	MG	6	1951	1/1	0.69	37.12	75,75,75,75	0
85	MG	5	3507	1/1	0.54	37.04	35,35,35,35	0
85	MG	5	3526	1/1	0.55	36.96	46,46,46,46	0
85	MG	1	3787	1/1	0.33	36.60	43,43,43,43	0
86	OHX	1	4150	7/7	0.34	36.27	135,135,135,135	0
85	MG	6	1904	1/1	0.68	36.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	3	206	1/1	0.58	36.19	31,31,31,31	0
86	OHX	1	4116	7/7	0.53	35.75	108,108,108,108	0
85	MG	1	3557	1/1	0.59	35.74	28,28,28,28	0
85	MG	1	3501	1/1	0.59	35.69	77,77,77,77	0
85	MG	1	3516	1/1	0.43	35.65	28,28,28,28	0
85	MG	5	3567	1/1	0.43	35.29	25,25,25,25	0
85	MG	1	3863	1/1	0.43	35.22	42,42,42,42	0
85	MG	6	1926	1/1	0.58	35.20	49,49,49,49	0
85	MG	1	3460	1/1	0.50	35.14	63,63,63,63	0
85	MG	1	3462	1/1	0.46	35.12	27,27,27,27	0
85	MG	2	1994	1/1	0.80	35.11	72,72,72,72	0
85	MG	1	3463	1/1	0.45	34.76	28,28,28,28	0
85	MG	5	3764	1/1	0.70	34.75	41,41,41,41	0
85	MG	6	1907	1/1	0.51	34.05	70,70,70,70	0
85	MG	3	202	1/1	0.35	33.99	44,44,44,44	0
85	MG	2	1915	1/1	1.01	33.60	73,73,73,73	0
85	MG	1	3554	1/1	0.67	33.49	38,38,38,38	0
85	MG	1	3580	1/1	0.52	33.44	26,26,26,26	0
85	MG	1	3807	1/1	0.74	33.29	37,37,37,37	0
85	MG	1	3515	1/1	0.51	33.28	26,26,26,26	0
85	MG	1	3729	1/1	0.96	33.23	35,35,35,35	0
85	MG	1	3765	1/1	0.79	33.03	49,49,49,49	0
85	MG	N3	201	1/1	0.49	32.99	32,32,32,32	0
85	MG	2	2014	1/1	0.79	32.79	65,65,65,65	0
85	MG	6	1974	1/1	0.45	32.68	52,52,52,52	0
85	MG	5	3418	1/1	0.50	32.52	24,24,24,24	0
85	MG	5	3888	1/1	0.54	32.48	54,54,54,54	0
85	MG	5	3561	1/1	0.69	32.44	31,31,31,31	0
85	MG	1	3568	1/1	0.54	32.33	34,34,34,34	0
85	MG	5	3437	1/1	0.71	32.28	45,45,45,45	0
85	MG	5	3794	1/1	0.45	32.16	48,48,48,48	0
85	MG	1	3832	1/1	0.40	31.96	26,26,26,26	0
85	MG	1	3623	1/1	0.39	31.93	42,42,42,42	0
86	OHX	1	4193	7/7	0.61	31.93	131,131,131,131	0
85	MG	5	3684	1/1	0.27	31.85	33,33,33,33	0
85	MG	2	1918	1/1	0.78	31.73	57,57,57,57	0
86	OHX	2	2159	7/7	0.47	31.73	148,148,148,148	0
85	MG	l3	402	1/1	0.73	31.61	24,24,24,24	0
85	MG	2	2007	1/1	0.47	31.57	58,58,58,58	0
85	MG	6	1916	1/1	1.40	31.57	65,65,65,65	0
85	MG	5	3861	1/1	0.51	31.33	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	8	212	1/1	0.65	31.29	56,56,56,56	0
85	MG	5	3750	1/1	0.58	31.15	40,40,40,40	0
85	MG	5	3550	1/1	0.65	31.06	53,53,53,53	0
85	MG	2	1938	1/1	0.54	30.76	62,62,62,62	0
85	MG	1	3657	1/1	0.36	30.72	32,32,32,32	0
85	MG	1	3476	1/1	0.42	30.47	73,73,73,73	0
85	MG	1	3513	1/1	0.47	30.47	41,41,41,41	0
85	MG	2	1946	1/1	0.69	30.45	94,94,94,94	0
85	MG	5	3563	1/1	0.74	30.27	34,34,34,34	0
85	MG	5	3574	1/1	0.80	30.26	35,35,35,35	0
85	MG	2	1903	1/1	0.53	30.21	50,50,50,50	0
85	MG	5	3626	1/1	0.50	30.15	28,28,28,28	0
85	MG	2	1979	1/1	0.64	30.13	59,59,59,59	0
85	MG	1	3857	1/1	0.45	30.03	41,41,41,41	0
85	MG	1	3697	1/1	0.47	29.99	39,39,39,39	0
85	MG	1	3545	1/1	0.46	29.96	37,37,37,37	0
85	MG	2	1911	1/1	0.75	29.91	60,60,60,60	0
85	MG	2	1983	1/1	0.42	29.83	78,78,78,78	0
85	MG	5	3846	1/1	0.42	29.77	32,32,32,32	0
85	MG	1	3589	1/1	0.52	29.74	29,29,29,29	0
85	MG	1	3576	1/1	0.53	29.69	41,41,41,41	0
85	MG	1	3553	1/1	0.56	29.60	32,32,32,32	0
85	MG	2	1936	1/1	0.67	29.57	49,49,49,49	0
85	MG	5	3421	1/1	0.41	29.54	97,97,97,97	0
86	OHX	5	4189	7/7	0.35	29.38	121,121,121,121	0
85	MG	5	3739	1/1	0.41	29.35	35,35,35,35	0
85	MG	L7	304	1/1	0.41	29.31	36,36,36,36	0
85	MG	1	3722	1/1	0.32	29.31	54,54,54,54	0
85	MG	1	3524	1/1	0.54	29.29	36,36,36,36	0
85	MG	1	3502	1/1	0.57	29.21	28,28,28,28	0
85	MG	5	3830	1/1	0.48	29.20	50,50,50,50	0
85	MG	5	3536	1/1	0.55	29.14	40,40,40,40	0
85	MG	6	1910	1/1	0.51	29.08	48,48,48,48	0
85	MG	1	3769	1/1	0.49	28.75	56,56,56,56	0
86	OHX	6	2183	7/7	0.39	28.74	135,135,135,135	0
85	MG	4	212	1/1	0.41	28.73	50,50,50,50	0
85	MG	5	3582	1/1	0.49	28.67	30,30,30,30	0
85	MG	5	3557	1/1	0.54	28.62	24,24,24,24	0
85	MG	6	2012	1/1	0.64	28.60	58,58,58,58	0
85	MG	6	1984	1/1	0.34	28.58	53,53,53,53	0
85	MG	6	1944	1/1	0.89	28.53	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3562	1/1	0.52	28.28	38,38,38,38	0
85	MG	1	3493	1/1	0.58	28.24	62,62,62,62	0
85	MG	5	3457	1/1	0.40	28.18	24,24,24,24	0
85	MG	1	3859	1/1	0.43	28.13	58,58,58,58	0
85	MG	6	2006	1/1	0.45	28.10	95,95,95,95	0
85	MG	5	3527	1/1	0.48	27.98	30,30,30,30	0
85	MG	4	205	1/1	0.54	27.97	46,46,46,46	0
85	MG	8	204	1/1	0.64	27.96	48,48,48,48	0
85	MG	1	3542	1/1	0.59	27.82	65,65,65,65	0
85	MG	1	3503	1/1	0.95	27.82	49,49,49,49	0
86	OHX	5	4153	7/7	0.40	27.79	110,110,110,110	0
85	MG	1	3696	1/1	0.57	27.77	53,53,53,53	0
85	MG	5	3737	1/1	0.27	27.71	41,41,41,41	0
85	MG	6	1912	1/1	0.84	27.69	51,51,51,51	0
85	MG	6	1955	1/1	0.62	27.53	42,42,42,42	0
85	MG	5	3545	1/1	0.64	27.51	50,50,50,50	0
85	MG	1	3464	1/1	0.54	27.49	28,28,28,28	0
85	MG	5	3808	1/1	0.33	27.45	38,38,38,38	0
85	MG	5	3663	1/1	0.73	27.45	66,66,66,66	0
85	MG	5	3541	1/1	0.52	27.35	32,32,32,32	0
85	MG	5	3584	1/1	0.50	27.28	33,33,33,33	0
85	MG	5	3872	1/1	0.66	27.25	38,38,38,38	0
85	MG	5	3588	1/1	0.96	27.09	56,56,56,56	0
85	MG	5	3509	1/1	0.51	27.08	35,35,35,35	0
85	MG	1	3598	1/1	0.47	27.00	26,26,26,26	0
85	MG	5	3776	1/1	0.27	27.00	82,82,82,82	0
85	MG	1	3672	1/1	0.70	26.80	41,41,41,41	0
85	MG	1	3414	1/1	0.65	26.76	58,58,58,58	0
85	MG	1	3761	1/1	0.57	26.69	37,37,37,37	0
85	MG	5	3653	1/1	0.54	26.42	35,35,35,35	0
85	MG	1	3544	1/1	0.45	26.41	32,32,32,32	0
85	MG	1	3676	1/1	0.38	26.36	65,65,65,65	0
85	MG	1	3577	1/1	0.50	26.27	19,19,19,19	0
85	MG	7	211	1/1	0.60	26.26	41,41,41,41	0
85	MG	7	214	1/1	0.28	26.24	41,41,41,41	0
85	MG	5	3532	1/1	0.38	26.24	33,33,33,33	0
85	MG	1	3838	1/1	0.56	26.17	34,34,34,34	0
85	MG	1	3454	1/1	0.42	26.16	44,44,44,44	0
85	MG	5	3756	1/1	0.25	26.14	41,41,41,41	0
85	MG	5	3612	1/1	0.32	26.09	49,49,49,49	0
85	MG	5	3714	1/1	0.34	26.03	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	1992	1/1	0.54	25.83	80,80,80,80	0
85	MG	6	2031	1/1	0.71	25.66	89,89,89,89	0
85	MG	5	3576	1/1	0.63	25.65	45,45,45,45	0
85	MG	5	3867	1/1	0.51	25.60	55,55,55,55	0
85	MG	6	2033	1/1	0.68	25.47	71,71,71,71	0
85	MG	1	3823	1/1	0.22	25.46	59,59,59,59	0
85	MG	3	209	1/1	0.65	25.44	62,62,62,62	0
85	MG	1	3714	1/1	0.26	25.40	57,57,57,57	0
85	MG	1	3685	1/1	0.26	25.39	45,45,45,45	0
85	MG	5	3445	1/1	0.26	25.29	33,33,33,33	0
85	MG	1	3834	1/1	0.90	25.10	47,47,47,47	0
85	MG	n3	201	1/1	0.55	24.98	24,24,24,24	0
85	MG	6	1905	1/1	0.87	24.95	53,53,53,53	0
85	MG	1	3852	1/1	0.35	24.86	36,36,36,36	0
85	MG	6	1946	1/1	0.65	24.82	66,66,66,66	0
85	MG	6	1931	1/1	0.44	24.79	59,59,59,59	0
85	MG	5	3815	1/1	0.58	24.79	59,59,59,59	0
85	MG	5	3876	1/1	0.49	24.75	48,48,48,48	0
85	MG	4	215	1/1	0.41	24.71	56,56,56,56	0
85	MG	1	3487	1/1	0.43	24.59	41,41,41,41	0
85	MG	5	3535	1/1	0.62	24.54	38,38,38,38	0
85	MG	6	2044	1/1	0.35	24.50	47,47,47,47	0
85	MG	6	1935	1/1	1.05	24.37	59,59,59,59	0
85	MG	1	3731	1/1	0.38	24.36	32,32,32,32	0
85	MG	5	3466	1/1	0.43	24.35	51,51,51,51	0
85	MG	5	3636	1/1	0.35	24.35	49,49,49,49	0
85	MG	6	1922	1/1	0.94	24.34	57,57,57,57	0
86	OHX	1	4179	7/7	0.34	24.30	143,143,143,143	0
85	MG	1	3597	1/1	0.59	24.26	24,24,24,24	0
85	MG	2	1969	1/1	0.50	24.14	84,84,84,84	0
85	MG	2	1965	1/1	0.76	24.12	63,63,63,63	0
85	MG	1	3441	1/1	0.45	23.92	36,36,36,36	0
85	MG	1	3830	1/1	0.52	23.92	48,48,48,48	0
85	MG	1	3707	1/1	0.87	23.91	63,63,63,63	0
85	MG	1	3588	1/1	0.49	23.75	36,36,36,36	0
86	OHX	1	4123	7/7	0.39	23.74	108,108,108,108	0
85	MG	3	204	1/1	0.62	23.71	59,59,59,59	0
85	MG	5	3892	1/1	0.46	23.60	21,21,21,21	0
85	MG	1	3644	1/1	0.45	23.59	42,42,42,42	0
86	OHX	1	4174	7/7	0.41	23.52	157,157,157,157	0
85	MG	5	3761	1/1	0.48	23.49	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3669	1/1	0.36	23.43	38,38,38,38	0
86	OHX	5	4142	7/7	0.21	23.42	134,134,134,134	0
85	MG	1	3724	1/1	0.43	23.39	37,37,37,37	0
85	MG	5	3822	1/1	0.48	23.34	40,40,40,40	0
85	MG	1	3420	1/1	1.27	23.32	90,90,90,90	0
85	MG	2	1939	1/1	0.59	23.32	70,70,70,70	0
85	MG	1	3402	1/1	0.56	23.17	52,52,52,52	0
85	MG	5	3862	1/1	0.29	23.17	57,57,57,57	0
85	MG	5	3792	1/1	0.28	23.15	90,90,90,90	0
85	MG	5	3572	1/1	0.42	23.14	37,37,37,37	0
85	MG	5	3531	1/1	0.43	23.12	48,48,48,48	0
85	MG	5	3447	1/1	0.60	23.11	38,38,38,38	0
85	MG	5	3489	1/1	0.63	23.08	25,25,25,25	0
85	MG	2	2009	1/1	0.59	23.07	75,75,75,75	0
86	OHX	5	4161	7/7	0.30	22.87	105,105,105,105	0
85	MG	5	3786	1/1	0.75	22.84	81,81,81,81	0
85	MG	1	3432	1/1	0.55	22.80	45,45,45,45	0
85	MG	1	3636	1/1	0.27	22.80	56,56,56,56	0
85	MG	1	3608	1/1	0.96	22.72	53,53,53,53	0
85	MG	L7	301	1/1	0.52	22.71	37,37,37,37	0
85	MG	1	3457	1/1	0.86	22.66	58,58,58,58	0
85	MG	5	3758	1/1	0.60	22.63	64,64,64,64	0
85	MG	4	206	1/1	0.56	22.63	39,39,39,39	0
85	MG	1	3815	1/1	0.33	22.63	54,54,54,54	0
85	MG	1	3424	1/1	0.43	22.62	44,44,44,44	0
85	MG	6	1943	1/1	0.44	22.56	40,40,40,40	0
85	MG	1	3592	1/1	0.48	22.36	35,35,35,35	0
86	OHX	1	4175	7/7	0.41	22.26	133,133,133,133	0
85	MG	1	3796	1/1	0.42	22.09	40,40,40,40	0
85	MG	1	3605	1/1	0.30	22.09	35,35,35,35	0
85	MG	6	1903	1/1	0.62	22.08	44,44,44,44	0
85	MG	5	3554	1/1	0.47	22.08	32,32,32,32	0
86	OHX	1	4192	7/7	0.46	22.07	122,122,122,122	0
85	MG	5	3406	1/1	0.59	22.06	36,36,36,36	0
85	MG	5	3581	1/1	0.47	21.98	35,35,35,35	0
86	OHX	1	4180	7/7	0.42	21.95	113,113,113,113	0
85	MG	2	1933	1/1	0.35	21.95	71,71,71,71	0
86	OHX	1	4167	7/7	0.36	21.90	158,158,158,158	0
85	MG	5	3623	1/1	0.39	21.88	68,68,68,68	0
85	MG	1	3543	1/1	0.35	21.86	25,25,25,25	0
85	MG	5	3809	1/1	0.45	21.85	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4131	7/7	0.51	21.81	146,146,146,146	0
85	MG	5	3747	1/1	0.42	21.79	36,36,36,36	0
85	MG	5	3595	1/1	0.77	21.71	34,34,34,34	0
85	MG	1	3560	1/1	0.41	21.70	47,47,47,47	0
85	MG	5	3641	1/1	0.42	21.69	47,47,47,47	0
85	MG	1	3575	1/1	0.54	21.62	31,31,31,31	0
85	MG	6	1956	1/1	0.54	21.59	50,50,50,50	0
85	MG	1	3558	1/1	0.46	21.56	38,38,38,38	0
85	MG	2	1937	1/1	0.56	21.54	59,59,59,59	0
86	OHX	2	2137	7/7	0.27	21.47	157,157,157,157	0
85	MG	5	3813	1/1	0.23	21.40	39,39,39,39	0
85	MG	1	3596	1/1	0.54	21.39	25,25,25,25	0
85	MG	1	3655	1/1	0.43	21.38	70,70,70,70	0
85	MG	5	3564	1/1	0.52	21.33	28,28,28,28	0
85	MG	5	3460	1/1	0.32	21.27	31,31,31,31	0
85	MG	5	3428	1/1	0.83	21.22	44,44,44,44	0
85	MG	5	3796	1/1	0.56	21.18	53,53,53,53	0
85	MG	5	3865	1/1	0.28	21.16	42,42,42,42	0
85	MG	1	3645	1/1	0.49	21.10	38,38,38,38	0
85	MG	2	1978	1/1	0.49	21.09	99,99,99,99	0
85	MG	2	1924	1/1	0.66	21.04	85,85,85,85	0
86	OHX	5	4234	7/7	0.42	20.98	128,128,128,128	0
85	MG	6	2021	1/1	0.46	20.97	49,49,49,49	0
85	MG	5	3770	1/1	0.37	20.96	71,71,71,71	0
85	MG	5	3440	1/1	0.29	20.93	33,33,33,33	0
85	MG	2	1929	1/1	0.57	20.89	72,72,72,72	0
85	MG	q1	101	1/1	0.57	20.86	42,42,42,42	0
85	MG	1	3595	1/1	0.52	20.77	30,30,30,30	0
86	OHX	5	4090	7/7	0.49	20.75	104,104,104,104	0
85	MG	5	3878	1/1	0.56	20.71	38,38,38,38	0
85	MG	6	1911	1/1	0.66	20.61	83,83,83,83	0
85	MG	1	3475	1/1	0.45	20.60	23,23,23,23	0
85	MG	5	3569	1/1	0.49	20.57	36,36,36,36	0
85	MG	1	3461	1/1	0.42	20.57	30,30,30,30	0
86	OHX	1	4101	7/7	0.30	20.48	144,144,144,144	0
85	MG	6	1919	1/1	0.50	20.47	42,42,42,42	0
86	OHX	6	2176	7/7	0.39	20.46	123,123,123,123	0
86	OHX	5	4242	7/7	0.47	20.30	139,139,139,139	0
85	MG	5	3459	1/1	0.45	20.28	65,65,65,65	0
85	MG	6	1977	1/1	0.70	20.25	68,68,68,68	0
85	MG	5	3522	1/1	0.58	20.24	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3698	1/1	0.24	20.24	44,44,44,44	0
86	OHX	1	4112	7/7	0.34	20.23	121,121,121,121	0
85	MG	5	3414	1/1	0.52	20.21	30,30,30,30	0
85	MG	5	3900	1/1	0.43	20.05	36,36,36,36	0
85	MG	5	3640	1/1	0.28	20.03	37,37,37,37	0
86	OHX	5	4101	7/7	0.35	20.02	115,115,115,115	0
85	MG	1	3763	1/1	0.33	19.91	33,33,33,33	0
85	MG	2	1902	1/1	0.30	19.81	36,36,36,36	0
85	MG	5	3498	1/1	0.44	19.73	31,31,31,31	0
85	MG	1	3732	1/1	0.42	19.72	24,24,24,24	0
85	MG	5	3705	1/1	0.62	19.72	46,46,46,46	0
86	OHX	1	4166	7/7	0.46	19.72	141,141,141,141	0
85	MG	6	1960	1/1	0.64	19.64	41,41,41,41	0
85	MG	3	212	1/1	0.61	19.54	58,58,58,58	0
85	MG	5	3455	1/1	0.25	19.51	41,41,41,41	0
85	MG	2	1934	1/1	0.77	19.48	81,81,81,81	0
85	MG	1	3520	1/1	0.55	19.43	30,30,30,30	0
85	MG	5	3525	1/1	0.47	19.42	27,27,27,27	0
85	MG	5	3655	1/1	0.37	19.42	56,56,56,56	0
85	MG	1	3866	1/1	0.42	19.42	29,29,29,29	0
85	MG	4	207	1/1	0.46	19.35	34,34,34,34	0
85	MG	1	3615	1/1	0.33	19.33	36,36,36,36	0
85	MG	5	3504	1/1	0.56	19.27	31,31,31,31	0
85	MG	1	3865	1/1	0.48	19.24	65,65,65,65	0
85	MG	2	1919	1/1	0.70	19.23	71,71,71,71	0
85	MG	5	3664	1/1	0.55	19.20	55,55,55,55	0
85	MG	1	3499	1/1	0.43	19.16	32,32,32,32	0
85	MG	13	401	1/1	0.58	19.09	24,24,24,24	0
85	MG	5	3608	1/1	0.40	19.08	31,31,31,31	0
85	MG	6	1996	1/1	0.37	19.07	43,43,43,43	0
85	MG	5	3552	1/1	0.38	19.06	45,45,45,45	0
85	MG	4	203	1/1	0.65	18.98	55,55,55,55	0
85	MG	7	212	1/1	0.48	18.92	61,61,61,61	0
86	OHX	1	4076	7/7	0.39	18.92	97,97,97,97	0
85	MG	6	2047	1/1	0.37	18.89	76,76,76,76	0
85	MG	5	3803	1/1	0.38	18.81	52,52,52,52	0
85	MG	1	3517	1/1	0.60	18.73	34,34,34,34	0
86	OHX	1	4066	7/7	0.50	18.73	125,125,125,125	0
85	MG	1	3521	1/1	0.53	18.70	41,41,41,41	0
85	MG	2	1908	1/1	0.51	18.67	78,78,78,78	0
85	MG	2	2020	1/1	0.54	18.64	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3752	1/1	0.44	18.61	36,36,36,36	0
86	OHX	1	4209	7/7	0.45	18.59	121,121,121,121	0
86	OHX	5	4248	7/7	0.36	18.59	145,145,145,145	0
85	MG	5	3486	1/1	0.40	18.56	45,45,45,45	0
85	MG	2	2008	1/1	0.75	18.56	77,77,77,77	0
85	MG	1	3498	1/1	0.50	18.54	45,45,45,45	0
85	MG	5	3665	1/1	0.35	18.52	42,42,42,42	0
85	MG	5	3680	1/1	0.41	18.50	41,41,41,41	0
85	MG	1	3586	1/1	0.71	18.47	52,52,52,52	0
85	MG	1	3482	1/1	0.46	18.47	41,41,41,41	0
85	MG	4	217	1/1	0.42	18.45	65,65,65,65	0
85	MG	1	3512	1/1	0.41	18.42	31,31,31,31	0
86	OHX	5	4162	7/7	0.41	18.42	125,125,125,125	0
85	MG	1	3842	1/1	0.50	18.41	62,62,62,62	0
85	MG	2	2006	1/1	0.75	18.39	53,53,53,53	0
85	MG	1	3531	1/1	0.83	18.35	33,33,33,33	0
85	MG	5	3559	1/1	0.57	18.31	31,31,31,31	0
85	MG	5	3675	1/1	0.41	18.31	44,44,44,44	0
86	OHX	1	4198	7/7	0.54	18.12	129,129,129,129	0
85	MG	5	3439	1/1	0.47	18.10	62,62,62,62	0
85	MG	1	3661	1/1	0.45	18.10	26,26,26,26	0
85	MG	5	3560	1/1	0.51	18.06	33,33,33,33	0
85	MG	12	301	1/1	0.62	18.05	49,49,49,49	0
85	MG	5	3542	1/1	0.49	17.90	31,31,31,31	0
85	MG	1	3690	1/1	0.40	17.88	47,47,47,47	0
85	MG	6	1988	1/1	0.69	17.72	69,69,69,69	0
85	MG	1	3864	1/1	0.35	17.69	70,70,70,70	0
85	MG	2	1910	1/1	0.50	17.66	56,56,56,56	0
85	MG	8	208	1/1	0.39	17.62	59,59,59,59	0
85	MG	1	3617	1/1	0.32	17.61	36,36,36,36	0
85	MG	4	221	1/1	0.52	17.54	52,52,52,52	0
85	MG	1	3413	1/1	0.37	17.53	39,39,39,39	0
85	MG	1	3797	1/1	0.32	17.49	26,26,26,26	0
85	MG	7	207	1/1	0.32	17.47	44,44,44,44	0
85	MG	2	1999	1/1	0.39	17.39	87,87,87,87	0
85	MG	6	1986	1/1	0.37	17.38	82,82,82,82	0
85	MG	6	1966	1/1	0.53	17.38	67,67,67,67	0
85	MG	6	1921	1/1	0.42	17.36	44,44,44,44	0
86	OHX	5	4181	7/7	0.51	17.35	107,107,107,107	0
85	MG	1	3766	1/1	0.36	17.30	41,41,41,41	0
85	MG	5	3573	1/1	0.49	17.30	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	7	205	1/1	0.34	17.24	71,71,71,71	0
85	MG	5	3682	1/1	0.70	17.24	83,83,83,83	0
85	MG	1	3507	1/1	0.52	17.23	37,37,37,37	0
85	MG	5	3555	1/1	0.61	17.14	40,40,40,40	0
86	OHX	2	2157	7/7	0.43	17.13	113,113,113,113	0
85	MG	5	3698	1/1	0.32	17.11	41,41,41,41	0
85	MG	5	3875	1/1	0.49	17.05	41,41,41,41	0
85	MG	1	3443	1/1	0.39	17.03	25,25,25,25	0
85	MG	1	3846	1/1	0.54	17.01	58,58,58,58	0
85	MG	S2	301	1/1	0.76	17.00	57,57,57,57	0
85	MG	5	3568	1/1	0.34	17.00	27,27,27,27	0
85	MG	5	3519	1/1	0.36	16.96	25,25,25,25	0
85	MG	2	1914	1/1	0.67	16.95	71,71,71,71	0
85	MG	5	3646	1/1	0.47	16.94	34,34,34,34	0
85	MG	L3	402	1/1	0.41	16.90	35,35,35,35	0
85	MG	5	3413	1/1	0.71	16.86	43,43,43,43	0
85	MG	1	3681	1/1	0.33	16.85	46,46,46,46	0
85	MG	6	1942	1/1	0.39	16.83	32,32,32,32	0
85	MG	1	3422	1/1	0.36	16.79	39,39,39,39	0
85	MG	6	1918	1/1	0.59	16.78	69,69,69,69	0
86	OHX	1	4049	7/7	0.29	16.75	104,104,104,104	0
85	MG	5	3693	1/1	0.38	16.75	50,50,50,50	0
85	MG	6	1949	1/1	0.74	16.72	54,54,54,54	0
85	MG	5	3784	1/1	0.37	16.70	30,30,30,30	0
85	MG	5	3583	1/1	0.48	16.70	38,38,38,38	0
85	MG	5	3524	1/1	0.47	16.70	34,34,34,34	0
85	MG	5	3594	1/1	0.66	16.68	37,37,37,37	0
85	MG	3	213	1/1	0.33	16.64	61,61,61,61	0
85	MG	1	3851	1/1	0.45	16.61	57,57,57,57	0
85	MG	5	3597	1/1	0.45	16.58	32,32,32,32	0
85	MG	6	1971	1/1	0.29	16.57	63,63,63,63	0
86	OHX	O9	101	7/7	0.51	16.54	118,118,118,118	0
85	MG	o7	502	1/1	0.31	16.41	34,34,34,34	0
85	MG	5	3529	1/1	0.39	16.30	28,28,28,28	0
85	MG	2	1976	1/1	0.43	16.30	58,58,58,58	0
85	MG	5	3551	1/1	0.38	16.28	30,30,30,30	0
86	OHX	6	2185	7/7	0.43	16.28	141,141,141,141	0
86	OHX	5	4205	7/7	0.39	16.26	130,130,130,130	0
85	MG	2	1931	1/1	0.77	16.25	79,79,79,79	0
85	MG	6	2027	1/1	0.40	16.22	67,67,67,67	0
85	MG	6	1917	1/1	0.64	16.21	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4237	7/7	0.41	16.21	148,148,148,148	0
85	MG	1	3509	1/1	0.44	16.20	29,29,29,29	0
85	MG	1	3855	1/1	0.39	16.12	21,21,21,21	0
85	MG	1	3663	1/1	0.32	16.11	34,34,34,34	0
85	MG	1	3629	1/1	0.37	16.06	35,35,35,35	0
85	MG	1	3660	1/1	0.39	16.04	39,39,39,39	0
85	MG	5	3546	1/1	0.51	15.95	43,43,43,43	0
86	OHX	1	4208	7/7	0.40	15.91	128,128,128,128	0
85	MG	1	3533	1/1	0.38	15.90	26,26,26,26	0
85	MG	1	3818	1/1	0.37	15.86	53,53,53,53	0
86	OHX	6	2191	7/7	0.23	15.86	129,129,129,129	0
85	MG	N8	204	1/1	0.53	15.80	38,38,38,38	0
85	MG	1	3495	1/1	0.28	15.75	43,43,43,43	0
85	MG	5	3508	1/1	0.47	15.74	26,26,26,26	0
85	MG	1	3551	1/1	0.39	15.73	34,34,34,34	0
85	MG	5	3851	1/1	0.44	15.69	45,45,45,45	0
85	MG	6	1901	1/1	0.47	15.64	46,46,46,46	0
85	MG	1	3439	1/1	0.49	15.63	50,50,50,50	0
85	MG	1	3680	1/1	0.44	15.62	47,47,47,47	0
85	MG	6	1913	1/1	0.44	15.62	39,39,39,39	0
85	MG	1	3519	1/1	0.51	15.62	34,34,34,34	0
85	MG	2	1912	1/1	0.53	15.58	72,72,72,72	0
85	MG	6	1961	1/1	0.56	15.56	86,86,86,86	0
86	OHX	5	4159	7/7	0.29	15.54	129,129,129,129	0
85	MG	5	3671	1/1	0.43	15.51	31,31,31,31	0
86	OHX	5	4207	7/7	0.44	15.50	137,137,137,137	0
85	MG	6	1999	1/1	0.40	15.48	60,60,60,60	0
85	MG	5	3405	1/1	0.45	15.47	30,30,30,30	0
85	MG	2	1916	1/1	0.41	15.44	58,58,58,58	0
85	MG	5	3427	1/1	0.39	15.43	40,40,40,40	0
85	MG	5	3818	1/1	0.34	15.43	37,37,37,37	0
86	OHX	5	4155	7/7	0.38	15.42	107,107,107,107	0
85	MG	2	1945	1/1	0.56	15.40	70,70,70,70	0
85	MG	1	3606	1/1	0.37	15.37	39,39,39,39	0
85	MG	5	3674	1/1	0.22	15.37	63,63,63,63	0
85	MG	5	3637	1/1	0.44	15.36	51,51,51,51	0
85	MG	2	1961	1/1	0.51	15.35	59,59,59,59	0
85	MG	5	3894	1/1	0.37	15.31	66,66,66,66	0
85	MG	2	2001	1/1	0.39	15.30	119,119,119,119	0
85	MG	6	2046	1/1	0.60	15.30	86,86,86,86	0
85	MG	1	3671	1/1	0.26	15.25	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	7	204	1/1	0.43	15.22	53,53,53,53	0
85	MG	5	3625	1/1	0.38	15.22	40,40,40,40	0
85	MG	5	3503	1/1	0.36	15.18	40,40,40,40	0
86	OHX	5	4240	7/7	0.45	15.17	147,147,147,147	0
86	OHX	5	4087	7/7	0.23	15.11	112,112,112,112	0
85	MG	5	3726	1/1	0.22	15.10	96,96,96,96	0
85	MG	1	3632	1/1	0.40	15.10	41,41,41,41	0
85	MG	1	3433	1/1	0.57	15.08	48,48,48,48	0
85	MG	2	2017	1/1	0.61	15.06	79,79,79,79	0
85	MG	5	3452	1/1	0.32	15.05	40,40,40,40	0
85	MG	5	3510	1/1	0.64	15.05	29,29,29,29	0
86	OHX	8	227	7/7	0.31	15.04	123,123,123,123	0
85	MG	5	3858	1/1	0.27	15.03	45,45,45,45	0
85	MG	1	3860	1/1	0.50	15.03	61,61,61,61	0
85	MG	1	3578	1/1	0.59	15.00	29,29,29,29	0
85	MG	1	3571	1/1	0.43	14.88	26,26,26,26	0
85	MG	1	3613	1/1	0.22	14.87	44,44,44,44	0
85	MG	5	3661	1/1	0.44	14.87	31,31,31,31	0
85	MG	1	3721	1/1	0.34	14.83	34,34,34,34	0
86	OHX	5	4223	7/7	0.47	14.80	137,137,137,137	0
85	MG	1	3537	1/1	0.37	14.80	47,47,47,47	0
85	MG	5	3587	1/1	0.31	14.77	27,27,27,27	0
86	OHX	1	4145	7/7	0.38	14.76	129,129,129,129	0
85	MG	1	3833	1/1	0.46	14.73	20,20,20,20	0
85	MG	2	1974	1/1	0.41	14.70	70,70,70,70	0
85	MG	5	3548	1/1	0.46	14.66	45,45,45,45	0
86	OHX	1	4202	7/7	0.36	14.57	120,120,120,120	0
85	MG	1	3781	1/1	0.29	14.54	32,32,32,32	0
85	MG	1	3455	1/1	0.50	14.53	32,32,32,32	0
85	MG	8	202	1/1	0.51	14.51	39,39,39,39	0
85	MG	5	3477	1/1	0.42	14.51	34,34,34,34	0
85	MG	2	1907	1/1	0.69	14.51	59,59,59,59	0
86	OHX	5	4220	7/7	0.37	14.50	142,142,142,142	0
85	MG	2	1922	1/1	0.48	14.50	65,65,65,65	0
85	MG	1	3561	1/1	0.35	14.49	26,26,26,26	0
85	MG	2	1962	1/1	0.50	14.44	76,76,76,76	0
85	MG	5	3620	1/1	0.23	14.41	41,41,41,41	0
85	MG	1	3540	1/1	0.29	14.35	37,37,37,37	0
86	OHX	1	4206	7/7	0.29	14.35	125,125,125,125	0
85	MG	S8	301	1/1	0.39	14.33	62,62,62,62	0
85	MG	o3	202	1/1	0.74	14.29	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3573	1/1	0.56	14.27	44,44,44,44	0
85	MG	7	203	1/1	0.30	14.23	26,26,26,26	0
85	MG	S2	302	1/1	0.72	14.20	73,73,73,73	0
85	MG	6	1973	1/1	0.37	14.19	73,73,73,73	0
86	OHX	5	4152	7/7	0.38	14.14	142,142,142,142	0
86	OHX	5	4195	7/7	0.40	14.14	115,115,115,115	0
85	MG	5	3592	1/1	0.48	14.09	26,26,26,26	0
85	MG	1	3523	1/1	0.32	14.05	82,82,82,82	0
85	MG	1	3504	1/1	0.43	14.02	28,28,28,28	0
85	MG	6	1930	1/1	0.41	13.99	61,61,61,61	0
85	MG	5	3881	1/1	0.58	13.99	34,34,34,34	0
85	MG	6	1929	1/1	0.46	13.94	57,57,57,57	0
85	MG	1	3733	1/1	0.41	13.93	41,41,41,41	0
85	MG	1	3550	1/1	0.41	13.92	41,41,41,41	0
85	MG	6	1954	1/1	0.43	13.90	47,47,47,47	0
86	OHX	1	4146	7/7	0.37	13.90	139,139,139,139	0
85	MG	1	3817	1/1	0.33	13.89	63,63,63,63	0
85	MG	5	3673	1/1	0.62	13.86	28,28,28,28	0
86	OHX	6	2199	7/7	0.37	13.85	132,132,132,132	0
86	OHX	1	4210	7/7	0.45	13.82	129,129,129,129	0
86	OHX	5	4178	7/7	0.38	13.81	134,134,134,134	0
86	OHX	1	4143	7/7	0.46	13.80	109,109,109,109	0
85	MG	6	1994	1/1	0.42	13.80	53,53,53,53	0
86	OHX	5	4184	7/7	0.38	13.77	132,132,132,132	0
86	OHX	2	2162	7/7	0.38	13.74	160,160,160,160	0
85	MG	s9	201	1/1	0.60	13.62	70,70,70,70	0
86	OHX	5	4084	7/7	0.41	13.61	103,103,103,103	0
85	MG	1	3566	1/1	0.34	13.61	38,38,38,38	0
85	MG	7	201	1/1	0.53	13.60	45,45,45,45	0
85	MG	5	3520	1/1	0.33	13.59	34,34,34,34	0
85	MG	m1	202	1/1	0.28	13.57	57,57,57,57	0
85	MG	6	1937	1/1	0.39	13.57	43,43,43,43	0
85	MG	o1	201	1/1	1.14	13.57	62,62,62,62	0
85	MG	1	3587	1/1	0.94	13.53	53,53,53,53	0
85	MG	1	3705	1/1	0.45	13.50	45,45,45,45	0
85	MG	5	3589	1/1	0.40	13.48	25,25,25,25	0
85	MG	1	3565	1/1	0.40	13.46	49,49,49,49	0
85	MG	6	1925	1/1	0.50	13.40	42,42,42,42	0
86	OHX	1	4172	7/7	0.33	13.40	109,109,109,109	0
86	OHX	2	2083	7/7	0.30	13.39	121,121,121,121	0
85	MG	1	3552	1/1	0.46	13.38	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3473	1/1	0.50	13.36	39,39,39,39	0
85	MG	1	3844	1/1	0.50	13.36	55,55,55,55	0
86	OHX	1	4207	7/7	0.46	13.31	125,125,125,125	0
85	MG	2	1960	1/1	0.50	13.30	63,63,63,63	0
85	MG	5	3515	1/1	0.52	13.28	37,37,37,37	0
85	MG	1	3703	1/1	0.41	13.28	44,44,44,44	0
85	MG	6	2011	1/1	0.33	13.24	50,50,50,50	0
85	MG	1	3511	1/1	0.38	13.19	45,45,45,45	0
85	MG	1	3469	1/1	0.35	13.18	43,43,43,43	0
85	MG	3	207	1/1	0.40	13.17	66,66,66,66	0
85	MG	2	1967	1/1	0.78	13.13	52,52,52,52	0
85	MG	1	3843	1/1	0.36	13.12	43,43,43,43	0
85	MG	5	3411	1/1	0.46	13.10	33,33,33,33	0
86	OHX	6	2129	7/7	0.32	13.08	113,113,113,113	0
85	MG	1	3591	1/1	0.63	13.07	45,45,45,45	0
86	OHX	1	4082	7/7	0.29	13.06	116,116,116,116	0
86	OHX	2	2122	7/7	0.32	13.02	137,137,137,137	0
85	MG	5	3835	1/1	0.37	13.02	36,36,36,36	0
85	MG	2	1971	1/1	0.50	12.98	69,69,69,69	0
85	MG	1	3788	1/1	0.62	12.97	54,54,54,54	0
86	OHX	1	4048	7/7	0.28	12.92	105,105,105,105	0
86	OHX	5	4252	7/7	0.39	12.88	154,154,154,154	0
86	OHX	1	4149	7/7	0.32	12.86	141,141,141,141	0
86	OHX	5	4156	7/7	0.47	12.82	111,111,111,111	0
85	MG	5	3890	1/1	0.46	12.80	37,37,37,37	0
85	MG	5	3791	1/1	0.30	12.79	35,35,35,35	0
85	MG	6	1968	1/1	0.38	12.77	82,82,82,82	0
86	OHX	1	4171	7/7	0.29	12.73	113,113,113,113	0
85	MG	1	3821	1/1	0.33	12.73	55,55,55,55	0
86	OHX	5	4151	7/7	0.34	12.72	129,129,129,129	0
86	OHX	5	4221	7/7	0.43	12.71	124,124,124,124	0
85	MG	5	3624	1/1	0.44	12.71	38,38,38,38	0
85	MG	o3	201	1/1	0.37	12.71	45,45,45,45	0
86	OHX	2	2164	7/7	0.42	12.71	133,133,133,133	0
86	OHX	1	4129	7/7	0.38	12.70	112,112,112,112	0
86	OHX	2	2178	7/7	0.41	12.69	168,168,168,168	0
85	MG	2	1973	1/1	0.29	12.66	73,73,73,73	0
85	MG	5	3491	1/1	0.35	12.66	40,40,40,40	0
85	MG	8	205	1/1	0.38	12.63	49,49,49,49	0
85	MG	1	3625	1/1	0.36	12.52	49,49,49,49	0
85	MG	5	3429	1/1	0.31	12.48	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1923	1/1	0.38	12.45	61,61,61,61	0
85	MG	1	3407	1/1	0.53	12.42	38,38,38,38	0
85	MG	5	3783	1/1	0.21	12.41	59,59,59,59	0
85	MG	1	3777	1/1	0.34	12.36	53,53,53,53	0
86	OHX	5	4212	7/7	0.28	12.36	137,137,137,137	0
85	MG	1	3534	1/1	0.47	12.36	37,37,37,37	0
85	MG	5	3701	1/1	0.27	12.33	36,36,36,36	0
85	MG	1	3750	1/1	0.40	12.31	51,51,51,51	0
86	OHX	1	4162	7/7	0.31	12.28	125,125,125,125	0
85	MG	5	3722	1/1	0.53	12.23	43,43,43,43	0
85	MG	5	3689	1/1	0.35	12.23	48,48,48,48	0
85	MG	N3	202	1/1	0.23	12.19	68,68,68,68	0
85	MG	1	3472	1/1	0.27	12.18	43,43,43,43	0
85	MG	5	3610	1/1	0.33	12.17	32,32,32,32	0
86	OHX	5	4160	7/7	0.31	12.11	132,132,132,132	0
85	MG	1	3726	1/1	0.21	12.09	52,52,52,52	0
85	MG	5	3656	1/1	0.32	12.07	42,42,42,42	0
85	MG	1	3674	1/1	0.32	12.05	49,49,49,49	0
86	OHX	5	4128	7/7	0.30	12.04	133,133,133,133	0
85	MG	6	2030	1/1	0.40	12.03	66,66,66,66	0
85	MG	1	3849	1/1	0.32	12.03	50,50,50,50	0
86	OHX	1	4204	7/7	0.37	12.00	130,130,130,130	0
85	MG	4	220	1/1	0.24	11.92	37,37,37,37	0
85	MG	1	3609	1/1	0.74	11.92	65,65,65,65	0
86	OHX	2	2118	7/7	0.29	11.90	142,142,142,142	0
85	MG	1	3820	1/1	0.36	11.88	39,39,39,39	0
85	MG	5	3873	1/1	0.42	11.84	25,25,25,25	0
85	MG	1	3616	1/1	0.37	11.83	38,38,38,38	0
85	MG	1	3751	1/1	0.51	11.83	48,48,48,48	0
85	MG	n8	203	1/1	0.38	11.82	45,45,45,45	0
86	OHX	14	403	7/7	0.55	11.82	143,143,143,143	0
85	MG	5	3425	1/1	0.27	11.79	37,37,37,37	0
86	OHX	5	4074	7/7	0.26	11.75	108,108,108,108	0
85	MG	1	3506	1/1	0.34	11.75	36,36,36,36	0
86	OHX	2	2172	7/7	0.40	11.72	143,143,143,143	0
85	MG	1	3727	1/1	0.32	11.69	47,47,47,47	0
86	OHX	4	238	7/7	0.52	11.69	139,139,139,139	0
85	MG	3	201	1/1	0.45	11.68	74,74,74,74	0
86	OHX	1	4177	7/7	0.39	11.67	165,165,165,165	0
85	MG	5	3810	1/1	0.20	11.67	74,74,74,74	0
85	MG	1	3488	1/1	0.32	11.64	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3441	1/1	0.33	11.63	36,36,36,36	0
86	OHX	1	4060	7/7	0.28	11.63	94,94,94,94	0
85	MG	6	1938	1/1	0.42	11.62	43,43,43,43	0
85	MG	1	3716	1/1	0.50	11.60	76,76,76,76	0
86	OHX	2	2143	7/7	0.53	11.52	123,123,123,123	0
85	MG	1	3621	1/1	0.35	11.49	57,57,57,57	0
86	OHX	5	4239	7/7	0.40	11.47	126,126,126,126	0
85	MG	5	3738	1/1	0.37	11.45	71,71,71,71	0
86	OHX	4	236	7/7	0.32	11.43	131,131,131,131	0
85	MG	5	3844	1/1	0.39	11.43	47,47,47,47	0
85	MG	5	3432	1/1	0.46	11.43	35,35,35,35	0
85	MG	5	3870	1/1	0.27	11.43	23,23,23,23	0
85	MG	6	1906	1/1	0.39	11.41	44,44,44,44	0
85	MG	1	3401	1/1	0.51	11.39	41,41,41,41	0
85	MG	5	3476	1/1	0.35	11.37	73,73,73,73	0
85	MG	5	3766	1/1	0.44	11.36	40,40,40,40	0
85	MG	5	3505	1/1	0.29	11.33	52,52,52,52	0
86	OHX	6	2128	7/7	0.42	11.33	99,99,99,99	0
85	MG	1	3486	1/1	0.35	11.32	43,43,43,43	0
85	MG	5	3777	1/1	0.80	11.32	55,55,55,55	0
86	OHX	1	4213	7/7	0.39	11.27	121,121,121,121	0
86	OHX	2	2107	7/7	0.31	11.26	136,136,136,136	0
85	MG	5	3570	1/1	0.52	11.24	28,28,28,28	0
85	MG	1	3774	1/1	0.32	11.23	52,52,52,52	0
85	MG	1	3780	1/1	0.21	11.22	57,57,57,57	0
86	OHX	5	4117	7/7	0.26	11.20	112,112,112,112	0
85	MG	1	3841	1/1	0.37	11.19	29,29,29,29	0
85	MG	5	3523	1/1	0.47	11.19	44,44,44,44	0
85	MG	5	3590	1/1	0.43	11.19	33,33,33,33	0
85	MG	2	1970	1/1	0.40	11.14	76,76,76,76	0
85	MG	8	206	1/1	0.38	11.10	69,69,69,69	0
85	MG	M0	303	1/1	0.50	11.07	34,34,34,34	0
85	MG	2	1942	1/1	0.41	11.07	71,71,71,71	0
85	MG	5	3639	1/1	0.31	11.05	40,40,40,40	0
85	MG	1	3691	1/1	0.38	11.04	39,39,39,39	0
85	MG	6	1950	1/1	0.33	11.04	45,45,45,45	0
85	MG	1	3798	1/1	0.39	11.02	51,51,51,51	0
85	MG	5	3710	1/1	0.22	11.00	90,90,90,90	0
85	MG	6	1963	1/1	0.75	10.99	83,83,83,83	0
85	MG	n0	202	1/1	0.41	10.99	41,41,41,41	0
85	MG	6	1947	1/1	0.43	10.97	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2023	1/1	0.24	10.97	81,81,81,81	0
85	MG	1	3538	1/1	0.42	10.97	48,48,48,48	0
85	MG	1	3444	1/1	0.37	10.97	83,83,83,83	0
86	OHX	1	4163	7/7	0.52	10.95	145,145,145,145	0
86	OHX	1	4144	7/7	0.28	10.93	127,127,127,127	0
85	MG	2	1932	1/1	0.56	10.87	61,61,61,61	0
85	MG	5	3586	1/1	0.64	10.85	23,23,23,23	0
86	OHX	2	2112	7/7	0.29	10.85	128,128,128,128	0
85	MG	1	3709	1/1	0.28	10.81	40,40,40,40	0
85	MG	2	1985	1/1	0.38	10.80	65,65,65,65	0
85	MG	1	3497	1/1	0.32	10.80	30,30,30,30	0
85	MG	1	3789	1/1	0.26	10.80	40,40,40,40	0
85	MG	1	3811	1/1	0.32	10.78	38,38,38,38	0
85	MG	N0	201	1/1	0.42	10.75	45,45,45,45	0
85	MG	5	3657	1/1	0.34	10.71	47,47,47,47	0
86	OHX	5	4144	7/7	0.42	10.70	123,123,123,123	0
85	MG	2	2011	1/1	0.43	10.69	78,78,78,78	0
86	OHX	6	2149	7/7	0.26	10.64	105,105,105,105	0
85	MG	5	3501	1/1	0.32	10.62	26,26,26,26	0
85	MG	1	3425	1/1	0.36	10.53	48,48,48,48	0
86	OHX	2	2153	7/7	0.30	10.51	167,167,167,167	0
85	MG	1	3459	1/1	0.37	10.51	39,39,39,39	0
86	OHX	1	4170	7/7	0.36	10.49	98,98,98,98	0
85	MG	5	3487	1/1	0.41	10.49	35,35,35,35	0
86	OHX	2	2169	7/7	0.36	10.48	149,149,149,149	0
85	MG	5	3732	1/1	0.24	10.45	38,38,38,38	0
85	MG	5	3780	1/1	0.45	10.42	81,81,81,81	0
85	MG	1	3434	1/1	0.34	10.39	34,34,34,34	0
86	OHX	5	4254	7/7	0.33	10.39	153,153,153,153	0
86	OHX	3	222	7/7	0.30	10.38	150,150,150,150	0
85	MG	2	1964	1/1	0.43	10.37	100,100,100,100	0
85	MG	2	1980	1/1	0.45	10.35	66,66,66,66	0
86	OHX	1	4188	7/7	0.40	10.35	121,121,121,121	0
85	MG	5	3609	1/1	0.30	10.34	29,29,29,29	0
85	MG	5	3453	1/1	0.16	10.33	34,34,34,34	0
85	MG	6	2015	1/1	0.44	10.32	70,70,70,70	0
85	MG	1	3742	1/1	0.24	10.32	52,52,52,52	0
85	MG	4	216	1/1	0.30	10.27	52,52,52,52	0
86	OHX	5	4172	7/7	0.33	10.25	128,128,128,128	0
85	MG	2	1941	1/1	0.35	10.24	64,64,64,64	0
85	MG	5	3839	1/1	0.45	10.21	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3482	1/1	0.44	10.16	42,42,42,42	0
85	MG	5	3882	1/1	0.31	10.16	34,34,34,34	0
85	MG	1	3415	1/1	0.40	10.16	34,34,34,34	0
85	MG	1	3626	1/1	0.27	10.16	55,55,55,55	0
85	MG	5	3711	1/1	0.34	10.12	40,40,40,40	0
85	MG	5	3860	1/1	0.34	10.11	39,39,39,39	0
85	MG	6	1969	1/1	0.43	10.07	73,73,73,73	0
86	OHX	1	4156	7/7	0.44	10.05	136,136,136,136	0
85	MG	1	3505	1/1	0.41	9.99	40,40,40,40	0
86	OHX	5	4209	7/7	0.44	9.98	139,139,139,139	0
85	MG	1	3604	1/1	0.24	9.93	32,32,32,32	0
85	MG	1	3822	1/1	0.33	9.93	47,47,47,47	0
86	OHX	1	4173	7/7	0.45	9.93	153,153,153,153	0
85	MG	2	1944	1/1	0.50	9.90	69,69,69,69	0
85	MG	5	3516	1/1	0.33	9.90	28,28,28,28	0
85	MG	1	3556	1/1	0.42	9.88	32,32,32,32	0
86	OHX	5	4204	7/7	0.35	9.87	113,113,113,113	0
85	MG	5	3614	1/1	0.29	9.82	31,31,31,31	0
86	OHX	6	2146	7/7	0.36	9.82	128,128,128,128	0
85	MG	5	3475	1/1	0.69	9.80	51,51,51,51	0
85	MG	5	3871	1/1	0.34	9.79	27,27,27,27	0
86	OHX	1	4122	7/7	0.35	9.78	124,124,124,124	0
85	MG	1	3656	1/1	0.32	9.73	39,39,39,39	0
86	OHX	1	4186	7/7	0.36	9.72	136,136,136,136	0
85	MG	5	3727	1/1	0.33	9.70	29,29,29,29	0
86	OHX	1	4184	7/7	0.28	9.67	128,128,128,128	0
85	MG	1	3492	1/1	0.33	9.64	27,27,27,27	0
86	OHX	2	2073	7/7	0.27	9.64	111,111,111,111	0
85	MG	1	3786	1/1	0.45	9.63	33,33,33,33	0
85	MG	M5	302	1/1	0.66	9.63	50,50,50,50	0
85	MG	6	1979	1/1	0.34	9.62	46,46,46,46	0
85	MG	2	1955	1/1	0.42	9.62	64,64,64,64	0
85	MG	1	3510	1/1	0.54	9.61	25,25,25,25	0
85	MG	5	3820	1/1	0.38	9.61	61,61,61,61	0
86	OHX	5	3932	7/7	0.32	9.60	109,109,109,109	0
86	OHX	2	2179	7/7	0.56	9.60	145,145,145,145	0
86	OHX	5	4113	7/7	0.44	9.59	131,131,131,131	0
86	OHX	5	4216	7/7	0.32	9.58	114,114,114,114	0
85	MG	5	3611	1/1	0.39	9.58	35,35,35,35	0
85	MG	5	3534	1/1	0.43	9.57	37,37,37,37	0
85	MG	1	3477	1/1	0.26	9.57	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4175	7/7	0.36	9.56	95,95,95,95	0
85	MG	17	302	1/1	0.40	9.56	40,40,40,40	0
85	MG	1	3547	1/1	0.37	9.56	52,52,52,52	0
86	OHX	6	2189	7/7	0.30	9.54	154,154,154,154	0
86	OHX	5	4164	7/7	0.36	9.51	109,109,109,109	0
85	MG	2	1986	1/1	0.35	9.50	104,104,104,104	0
86	OHX	1	4103	7/7	0.28	9.50	113,113,113,113	0
85	MG	5	3676	1/1	0.36	9.50	41,41,41,41	0
85	MG	6	2004	1/1	0.42	9.49	79,79,79,79	0
85	MG	2	1993	1/1	0.70	9.43	100,100,100,100	0
85	MG	5	3800	1/1	0.16	9.40	36,36,36,36	0
85	MG	5	3763	1/1	0.32	9.38	36,36,36,36	0
85	MG	1	3428	1/1	0.56	9.38	42,42,42,42	0
86	OHX	2	2148	7/7	0.30	9.38	109,109,109,109	0
85	MG	5	3420	1/1	0.40	9.37	72,72,72,72	0
86	OHX	1	4215	7/7	0.52	9.35	130,130,130,130	0
85	MG	s4	301	1/1	0.46	9.35	58,58,58,58	0
85	MG	5	3874	1/1	0.47	9.31	54,54,54,54	0
86	OHX	5	4226	7/7	0.38	9.31	118,118,118,118	0
85	MG	1	3861	1/1	0.48	9.30	64,64,64,64	0
85	MG	5	3465	1/1	0.23	9.29	34,34,34,34	0
85	MG	1	3748	1/1	0.30	9.29	29,29,29,29	0
85	MG	5	3449	1/1	0.26	9.23	52,52,52,52	0
85	MG	1	3567	1/1	0.37	9.23	36,36,36,36	0
86	OHX	7	228	7/7	0.27	9.22	137,137,137,137	0
85	MG	1	3574	1/1	0.43	9.21	33,33,33,33	0
85	MG	1	3694	1/1	0.26	9.21	39,39,39,39	0
85	MG	5	3735	1/1	0.33	9.21	38,38,38,38	0
85	MG	5	3638	1/1	0.27	9.20	56,56,56,56	0
85	MG	6	2022	1/1	0.22	9.17	112,112,112,112	0
85	MG	O7	102	1/1	0.60	9.17	60,60,60,60	0
85	MG	1	3639	1/1	0.40	9.14	71,71,71,71	0
85	MG	5	3690	1/1	0.39	9.13	43,43,43,43	0
85	MG	1	3704	1/1	0.33	9.13	42,42,42,42	0
86	OHX	5	4073	7/7	0.21	9.12	124,124,124,124	0
85	MG	5	3442	1/1	0.45	9.10	32,32,32,32	0
85	MG	5	3607	1/1	0.30	9.10	48,48,48,48	0
85	MG	5	3500	1/1	0.44	9.08	37,37,37,37	0
86	OHX	6	2206	7/7	0.45	9.07	145,145,145,145	0
85	MG	1	3458	1/1	0.34	9.07	27,27,27,27	0
85	MG	1	3854	1/1	0.33	9.06	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3603	1/1	0.43	9.03	31,31,31,31	0
85	MG	2	2004	1/1	0.34	9.03	59,59,59,59	0
86	OHX	M7	206	7/7	0.53	9.02	103,103,103,103	0
86	OHX	5	4215	7/7	0.28	9.01	145,145,145,145	0
86	OHX	1	4132	7/7	0.24	9.00	118,118,118,118	0
85	MG	1	3610	1/1	0.59	8.99	63,63,63,63	0
85	MG	5	3593	1/1	0.33	8.95	30,30,30,30	0
85	MG	1	3741	1/1	0.35	8.91	52,52,52,52	0
86	OHX	1	4115	7/7	0.42	8.90	138,138,138,138	0
85	MG	1	3409	1/1	0.29	8.90	34,34,34,34	0
86	OHX	5	4034	7/7	0.21	8.88	107,107,107,107	0
86	OHX	5	4233	7/7	0.31	8.88	149,149,149,149	0
86	OHX	1	4071	7/7	0.32	8.85	125,125,125,125	0
86	OHX	8	222	7/7	0.23	8.85	111,111,111,111	0
85	MG	1	3518	1/1	0.47	8.83	37,37,37,37	0
85	MG	6	1941	1/1	0.37	8.83	48,48,48,48	0
85	MG	5	3463	1/1	0.50	8.81	33,33,33,33	0
85	MG	5	3686	1/1	0.34	8.78	73,73,73,73	0
85	MG	5	3670	1/1	0.28	8.76	36,36,36,36	0
86	OHX	5	4028	7/7	0.28	8.76	102,102,102,102	0
85	MG	2	2000	1/1	0.52	8.75	87,87,87,87	0
86	OHX	2	2125	7/7	0.28	8.73	125,125,125,125	0
85	MG	1	3593	1/1	0.46	8.72	51,51,51,51	0
85	MG	1	3546	1/1	0.33	8.67	34,34,34,34	0
85	MG	5	3795	1/1	0.29	8.67	55,55,55,55	0
86	OHX	8	229	7/7	0.34	8.65	119,119,119,119	0
85	MG	5	3741	1/1	0.27	8.64	25,25,25,25	0
85	MG	5	3745	1/1	0.27	8.60	62,62,62,62	0
85	MG	5	3775	1/1	0.25	8.56	27,27,27,27	0
86	OHX	1	4133	7/7	0.37	8.56	155,155,155,155	0
85	MG	5	3847	1/1	0.34	8.53	32,32,32,32	0
86	OHX	6	2167	7/7	0.36	8.53	143,143,143,143	0
85	MG	5	3424	1/1	0.46	8.52	60,60,60,60	0
86	OHX	5	4140	7/7	0.40	8.51	116,116,116,116	0
86	OHX	1	4065	7/7	0.35	8.51	144,144,144,144	0
86	OHX	1	4187	7/7	0.29	8.51	145,145,145,145	0
85	MG	5	3403	1/1	0.56	8.50	49,49,49,49	0
85	MG	6	1975	1/1	0.33	8.49	51,51,51,51	0
86	OHX	6	2205	7/7	0.40	8.49	148,148,148,148	0
85	MG	1	3569	1/1	0.46	8.47	29,29,29,29	0
85	MG	1	3744	1/1	0.29	8.47	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3659	1/1	0.24	8.47	30,30,30,30	0
85	MG	5	3692	1/1	0.33	8.47	48,48,48,48	0
86	OHX	5	4190	7/7	0.45	8.45	108,108,108,108	0
86	OHX	5	4206	7/7	0.34	8.45	126,126,126,126	0
85	MG	6	2032	1/1	0.36	8.43	98,98,98,98	0
86	OHX	5	4122	7/7	0.33	8.43	117,117,117,117	0
85	MG	1	3757	1/1	0.30	8.42	24,24,24,24	0
86	OHX	5	4165	7/7	0.27	8.42	115,115,115,115	0
86	OHX	1	4095	7/7	0.31	8.42	113,113,113,113	0
85	MG	5	3829	1/1	0.27	8.40	27,27,27,27	0
85	MG	5	3634	1/1	0.22	8.39	35,35,35,35	0
86	OHX	4	235	7/7	0.43	8.37	143,143,143,143	0
86	OHX	1	4181	7/7	0.41	8.37	142,142,142,142	0
85	MG	6	2025	1/1	0.33	8.36	56,56,56,56	0
85	MG	1	3408	1/1	0.33	8.36	43,43,43,43	0
86	OHX	5	4187	7/7	0.37	8.35	115,115,115,115	0
85	MG	5	3789	1/1	0.26	8.31	23,23,23,23	0
85	MG	6	1914	1/1	0.39	8.28	73,73,73,73	0
85	MG	5	3511	1/1	0.49	8.26	25,25,25,25	0
85	MG	1	3659	1/1	0.26	8.26	32,32,32,32	0
85	MG	6	2010	1/1	0.27	8.26	48,48,48,48	0
85	MG	6	1965	1/1	0.38	8.24	58,58,58,58	0
85	MG	5	3869	1/1	0.26	8.20	28,28,28,28	0
86	OHX	5	4130	7/7	0.29	8.20	127,127,127,127	0
85	MG	5	3402	1/1	0.35	8.19	25,25,25,25	0
86	OHX	1	4157	7/7	0.31	8.16	128,128,128,128	0
85	MG	1	3541	1/1	0.43	8.15	23,23,23,23	0
86	OHX	M9	203	7/7	0.31	8.10	154,154,154,154	0
85	MG	6	1957	1/1	1.10	8.09	58,58,58,58	0
86	OHX	1	4098	7/7	0.32	8.07	125,125,125,125	0
85	MG	5	3488	1/1	0.23	8.02	51,51,51,51	0
85	MG	6	1953	1/1	0.42	8.01	63,63,63,63	0
85	MG	5	3409	1/1	0.35	7.99	48,48,48,48	0
85	MG	5	3579	1/1	0.38	7.98	28,28,28,28	0
85	MG	5	3629	1/1	0.30	7.97	62,62,62,62	0
85	MG	5	3469	1/1	0.29	7.96	34,34,34,34	0
85	MG	1	3670	1/1	0.33	7.95	82,82,82,82	0
85	MG	8	213	1/1	0.37	7.92	88,88,88,88	0
85	MG	5	3885	1/1	0.26	7.92	28,28,28,28	0
85	MG	1	3658	1/1	0.40	7.90	45,45,45,45	0
85	MG	1	3590	1/1	0.29	7.89	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4108	7/7	0.25	7.88	111,111,111,111	0
85	MG	4	213	1/1	0.26	7.87	52,52,52,52	0
86	OHX	6	2163	7/7	0.28	7.85	124,124,124,124	0
85	MG	5	3580	1/1	0.43	7.83	33,33,33,33	0
85	MG	1	3845	1/1	0.47	7.82	36,36,36,36	0
85	MG	5	3540	1/1	0.48	7.82	27,27,27,27	0
85	MG	1	3406	1/1	0.59	7.80	116,116,116,116	0
86	OHX	1	4031	7/7	0.32	7.80	109,109,109,109	0
85	MG	5	3468	1/1	0.24	7.80	35,35,35,35	0
86	OHX	5	4238	7/7	0.55	7.80	139,139,139,139	0
85	MG	5	3631	1/1	0.21	7.78	43,43,43,43	0
85	MG	M3	203	1/1	0.42	7.78	32,32,32,32	0
85	MG	l2	302	1/1	0.56	7.78	40,40,40,40	0
85	MG	S4	301	1/1	0.46	7.78	70,70,70,70	0
86	OHX	5	4198	7/7	0.34	7.78	125,125,125,125	0
86	OHX	5	4250	7/7	0.40	7.76	137,137,137,137	0
86	OHX	1	4009	7/7	0.29	7.76	112,112,112,112	0
86	OHX	6	2112	7/7	0.24	7.75	105,105,105,105	0
85	MG	5	3660	1/1	0.30	7.74	39,39,39,39	0
86	OHX	5	4200	7/7	0.28	7.73	114,114,114,114	0
85	MG	2	1951	1/1	0.78	7.73	102,102,102,102	0
85	MG	5	3828	1/1	0.35	7.72	34,34,34,34	0
85	MG	1	3440	1/1	0.53	7.65	32,32,32,32	0
86	OHX	5	4188	7/7	0.34	7.63	116,116,116,116	0
85	MG	5	3514	1/1	0.52	7.61	27,27,27,27	0
86	OHX	6	2162	7/7	0.39	7.57	124,124,124,124	0
85	MG	1	3411	1/1	0.47	7.54	43,43,43,43	0
85	MG	1	3723	1/1	0.28	7.54	45,45,45,45	0
85	MG	2	1930	1/1	0.34	7.51	67,67,67,67	0
86	OHX	2	2104	7/7	0.24	7.50	120,120,120,120	0
85	MG	1	3712	1/1	0.32	7.48	34,34,34,34	0
85	MG	6	1934	1/1	0.43	7.46	80,80,80,80	0
86	OHX	2	2146	7/7	0.25	7.45	132,132,132,132	0
85	MG	m6	201	1/1	0.34	7.45	35,35,35,35	0
85	MG	1	3555	1/1	0.38	7.45	49,49,49,49	0
85	MG	1	3418	1/1	0.40	7.44	47,47,47,47	0
85	MG	5	3547	1/1	0.47	7.42	47,47,47,47	0
86	OHX	5	4136	7/7	0.26	7.42	120,120,120,120	0
85	MG	6	2014	1/1	0.33	7.42	48,48,48,48	0
86	OHX	2	2111	7/7	0.36	7.41	153,153,153,153	0
86	OHX	6	2188	7/7	0.37	7.40	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4081	7/7	0.41	7.39	113,113,113,113	0
86	OHX	6	2179	7/7	0.35	7.38	112,112,112,112	0
85	MG	1	3474	1/1	0.29	7.37	29,29,29,29	0
86	OHX	1	4200	7/7	0.38	7.37	123,123,123,123	0
85	MG	5	3434	1/1	0.31	7.35	79,79,79,79	0
85	MG	1	3801	1/1	0.40	7.33	49,49,49,49	0
85	MG	2	1956	1/1	0.51	7.33	60,60,60,60	0
86	OHX	1	4216	7/7	0.35	7.33	141,141,141,141	0
85	MG	2	1954	1/1	0.37	7.32	105,105,105,105	0
85	MG	5	3630	1/1	0.29	7.31	40,40,40,40	0
86	OHX	5	4251	7/7	0.32	7.30	121,121,121,121	0
85	MG	1	3548	1/1	0.24	7.29	65,65,65,65	0
86	OHX	5	4213	7/7	0.33	7.28	107,107,107,107	0
85	MG	6	1952	1/1	0.56	7.28	63,63,63,63	0
86	OHX	4	234	7/7	0.30	7.27	111,111,111,111	0
86	OHX	1	4114	7/7	0.35	7.26	106,106,106,106	0
85	MG	5	3517	1/1	0.29	7.25	36,36,36,36	0
85	MG	1	3650	1/1	0.26	7.21	39,39,39,39	0
86	OHX	5	4115	7/7	0.31	7.19	105,105,105,105	0
85	MG	1	3684	1/1	0.33	7.17	63,63,63,63	0
85	MG	6	2026	1/1	0.34	7.13	42,42,42,42	0
85	MG	1	3646	1/1	0.30	7.12	46,46,46,46	0
86	OHX	1	4067	7/7	0.30	7.11	122,122,122,122	0
85	MG	5	3422	1/1	0.41	7.10	37,37,37,37	0
85	MG	1	3579	1/1	0.20	7.07	27,27,27,27	0
86	OHX	5	4143	7/7	0.23	7.06	123,123,123,123	0
85	MG	1	3496	1/1	0.30	7.05	48,48,48,48	0
85	MG	6	2009	1/1	0.24	7.04	51,51,51,51	0
86	OHX	5	4053	7/7	0.32	7.03	100,100,100,100	0
85	MG	1	3445	1/1	0.31	7.02	63,63,63,63	0
85	MG	4	218	1/1	0.22	7.01	61,61,61,61	0
85	MG	1	3530	1/1	0.36	7.01	47,47,47,47	0
85	MG	N8	205	1/1	0.38	7.00	28,28,28,28	0
85	MG	2	1950	1/1	0.77	6.99	88,88,88,88	0
85	MG	5	3544	1/1	0.25	6.96	30,30,30,30	0
85	MG	1	3799	1/1	0.27	6.94	31,31,31,31	0
85	MG	6	1995	1/1	0.36	6.94	56,56,56,56	0
86	OHX	5	4168	7/7	0.30	6.94	128,128,128,128	0
85	MG	2	1921	1/1	0.43	6.90	56,56,56,56	0
86	OHX	5	4179	7/7	0.30	6.89	134,134,134,134	0
85	MG	5	3484	1/1	0.53	6.88	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4075	7/7	0.28	6.84	107,107,107,107	0
86	OHX	5	4191	7/7	0.32	6.83	153,153,153,153	0
85	MG	1	3403	1/1	0.28	6.83	37,37,37,37	0
85	MG	5	3895	1/1	0.24	6.79	102,102,102,102	0
85	MG	5	3729	1/1	0.25	6.77	51,51,51,51	0
86	OHX	1	4189	7/7	0.38	6.76	138,138,138,138	0
85	MG	1	3583	1/1	0.61	6.75	38,38,38,38	0
85	MG	6	2019	1/1	0.27	6.75	41,41,41,41	0
85	MG	5	3736	1/1	0.18	6.74	50,50,50,50	0
86	OHX	5	4086	7/7	0.29	6.66	113,113,113,113	0
85	MG	5	3558	1/1	0.30	6.65	46,46,46,46	0
85	MG	1	3479	1/1	0.30	6.65	38,38,38,38	0
86	OHX	1	4136	7/7	0.30	6.65	111,111,111,111	0
86	OHX	1	4142	7/7	0.34	6.65	133,133,133,133	0
86	OHX	1	4139	7/7	0.25	6.63	110,110,110,110	0
85	MG	2	1977	1/1	0.32	6.63	88,88,88,88	0
85	MG	6	2013	1/1	0.35	6.62	59,59,59,59	0
85	MG	1	3634	1/1	0.23	6.61	33,33,33,33	0
85	MG	5	3565	1/1	0.24	6.60	25,25,25,25	0
85	MG	1	3535	1/1	0.22	6.59	31,31,31,31	0
86	OHX	6	2173	7/7	0.36	6.58	106,106,106,106	0
85	MG	1	3453	1/1	0.29	6.54	35,35,35,35	0
85	MG	1	3570	1/1	0.37	6.52	29,29,29,29	0
85	MG	6	1940	1/1	0.48	6.51	89,89,89,89	0
86	OHX	1	3980	7/7	0.33	6.50	87,87,87,87	0
86	OHX	5	4169	7/7	0.23	6.49	124,124,124,124	0
86	OHX	6	2119	7/7	0.37	6.47	137,137,137,137	0
86	OHX	6	2143	7/7	0.28	6.45	165,165,165,165	0
85	MG	1	3831	1/1	0.29	6.45	22,22,22,22	0
86	OHX	5	4129	7/7	0.30	6.43	121,121,121,121	0
85	MG	5	3717	1/1	0.33	6.43	47,47,47,47	0
85	MG	1	3585	1/1	0.52	6.42	39,39,39,39	0
85	MG	1	3447	1/1	0.28	6.41	46,46,46,46	0
85	MG	5	3451	1/1	0.39	6.41	30,30,30,30	0
86	OHX	6	2135	7/7	0.34	6.41	155,155,155,155	0
85	MG	1	3471	1/1	0.27	6.40	39,39,39,39	0
86	OHX	1	4090	7/7	0.26	6.39	127,127,127,127	0
85	MG	2	2019	1/1	0.65	6.39	84,84,84,84	0
86	OHX	5	4208	7/7	0.27	6.38	132,132,132,132	0
85	MG	2	1901	1/1	1.33	6.37	83,83,83,83	0
86	OHX	5	4249	7/7	0.27	6.34	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3897	1/1	0.25	6.34	58,58,58,58	0
86	OHX	1	4111	7/7	0.28	6.33	128,128,128,128	0
85	MG	5	3456	1/1	0.50	6.32	86,86,86,86	0
85	MG	M7	203	1/1	0.34	6.29	33,33,33,33	0
85	MG	5	3492	1/1	0.28	6.29	52,52,52,52	0
86	OHX	1	4211	7/7	0.41	6.27	117,117,117,117	0
86	OHX	1	4161	7/7	0.34	6.27	137,137,137,137	0
86	OHX	1	4205	7/7	0.49	6.23	135,135,135,135	0
85	MG	s1	301	1/1	0.27	6.22	74,74,74,74	0
86	OHX	5	4229	7/7	0.29	6.19	127,127,127,127	0
86	OHX	6	2158	7/7	0.38	6.19	169,169,169,169	0
85	MG	5	3899	1/1	0.29	6.18	52,52,52,52	0
85	MG	5	3450	1/1	0.34	6.16	62,62,62,62	0
85	MG	5	3728	1/1	0.56	6.14	76,76,76,76	0
85	MG	6	2043	1/1	0.42	6.12	75,75,75,75	0
86	OHX	1	4085	7/7	0.32	6.08	137,137,137,137	0
86	OHX	5	4141	7/7	0.43	6.08	122,122,122,122	0
86	OHX	1	4178	7/7	0.33	6.07	141,141,141,141	0
85	MG	1	3572	1/1	0.31	6.05	23,23,23,23	0
86	OHX	6	2187	7/7	0.27	6.05	161,161,161,161	0
86	OHX	5	4093	7/7	0.25	6.04	111,111,111,111	0
85	MG	5	3662	1/1	0.32	6.03	47,47,47,47	0
85	MG	1	3785	1/1	0.33	6.02	47,47,47,47	0
85	MG	5	3426	1/1	0.26	6.01	41,41,41,41	0
85	MG	6	1927	1/1	0.34	6.00	47,47,47,47	0
86	OHX	1	4099	7/7	0.29	6.00	139,139,139,139	0
85	MG	5	3652	1/1	0.28	5.98	27,27,27,27	0
85	MG	5	3697	1/1	0.28	5.98	54,54,54,54	0
86	OHX	1	4061	7/7	0.29	5.97	114,114,114,114	0
85	MG	1	3668	1/1	0.30	5.97	53,53,53,53	0
86	OHX	6	2165	7/7	0.27	5.95	127,127,127,127	0
86	OHX	6	2122	7/7	0.32	5.95	107,107,107,107	0
85	MG	1	3743	1/1	0.39	5.95	67,67,67,67	0
85	MG	2	1959	1/1	0.65	5.94	101,101,101,101	0
86	OHX	m4	201	7/7	0.38	5.93	197,197,197,197	0
86	OHX	6	2125	7/7	0.26	5.93	101,101,101,101	0
86	OHX	2	2136	7/7	0.42	5.90	128,128,128,128	0
86	OHX	1	4050	7/7	0.28	5.88	111,111,111,111	0
85	MG	5	3884	1/1	0.41	5.87	90,90,90,90	0
85	MG	5	3677	1/1	0.27	5.86	41,41,41,41	0
85	MG	m1	201	1/1	0.35	5.85	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3478	1/1	0.27	5.85	26,26,26,26	0
86	OHX	2	2127	7/7	0.28	5.85	133,133,133,133	0
85	MG	n6	201	1/1	0.48	5.83	55,55,55,55	0
85	MG	1	3702	1/1	0.30	5.80	43,43,43,43	0
85	MG	5	3417	1/1	0.28	5.80	25,25,25,25	0
86	OHX	6	2170	7/7	0.43	5.79	114,114,114,114	0
85	MG	5	3633	1/1	0.41	5.79	46,46,46,46	0
85	MG	1	3582	1/1	0.34	5.79	37,37,37,37	0
86	OHX	5	4199	7/7	0.27	5.79	142,142,142,142	0
86	OHX	2	2105	7/7	0.24	5.77	132,132,132,132	0
85	MG	1	3417	1/1	0.35	5.77	32,32,32,32	0
85	MG	5	3804	1/1	0.32	5.76	47,47,47,47	0
85	MG	5	3767	1/1	0.32	5.76	39,39,39,39	0
86	OHX	1	4124	7/7	0.22	5.75	129,129,129,129	0
85	MG	5	3444	1/1	0.28	5.75	25,25,25,25	0
85	MG	5	3412	1/1	0.25	5.73	30,30,30,30	0
85	MG	1	3549	1/1	0.24	5.71	40,40,40,40	0
86	OHX	6	2178	7/7	0.29	5.71	99,99,99,99	0
86	OHX	5	4102	7/7	0.29	5.68	126,126,126,126	0
86	OHX	4	230	7/7	0.21	5.65	103,103,103,103	0
86	OHX	1	4120	7/7	0.33	5.65	122,122,122,122	0
85	MG	5	3471	1/1	0.33	5.64	35,35,35,35	0
86	OHX	1	4079	7/7	0.26	5.59	117,117,117,117	0
86	OHX	5	4167	7/7	0.29	5.57	166,166,166,166	0
85	MG	1	3772	1/1	0.28	5.57	28,28,28,28	0
85	MG	1	3746	1/1	0.32	5.56	44,44,44,44	0
85	MG	5	3566	1/1	0.42	5.55	47,47,47,47	0
85	MG	5	3649	1/1	0.17	5.53	42,42,42,42	0
85	MG	5	3802	1/1	0.16	5.52	49,49,49,49	0
85	MG	M7	204	1/1	0.25	5.52	39,39,39,39	0
86	OHX	1	4195	7/7	0.43	5.51	143,143,143,143	0
85	MG	5	3742	1/1	0.25	5.51	33,33,33,33	0
85	MG	6	1980	1/1	0.21	5.51	77,77,77,77	0
85	MG	1	3669	1/1	0.31	5.47	39,39,39,39	0
85	MG	6	1989	1/1	0.20	5.46	46,46,46,46	0
86	OHX	5	4218	7/7	0.43	5.46	133,133,133,133	0
86	OHX	1	4070	7/7	0.33	5.45	107,107,107,107	0
86	OHX	5	4111	7/7	0.30	5.44	105,105,105,105	0
85	MG	1	3438	1/1	0.26	5.44	33,33,33,33	0
85	MG	5	3490	1/1	0.27	5.44	27,27,27,27	0
85	MG	1	3532	1/1	0.41	5.40	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4227	7/7	0.34	5.40	146,146,146,146	0
85	MG	5	3772	1/1	0.26	5.39	31,31,31,31	0
85	MG	1	3467	1/1	0.32	5.39	59,59,59,59	0
85	MG	5	3720	1/1	0.26	5.38	42,42,42,42	0
85	MG	2	1966	1/1	0.27	5.38	89,89,89,89	0
85	MG	5	3613	1/1	0.33	5.36	33,33,33,33	0
86	OHX	2	2102	7/7	0.23	5.36	142,142,142,142	0
85	MG	5	3793	1/1	0.33	5.36	42,42,42,42	0
85	MG	5	3667	1/1	0.31	5.33	31,31,31,31	0
86	OHX	5	4154	7/7	0.25	5.32	140,140,140,140	0
85	MG	1	3654	1/1	0.45	5.32	92,92,92,92	0
85	MG	7	210	1/1	0.34	5.32	45,45,45,45	0
86	OHX	5	3995	7/7	0.24	5.31	93,93,93,93	0
85	MG	1	3489	1/1	0.23	5.30	36,36,36,36	0
85	MG	1	3483	1/1	0.28	5.30	31,31,31,31	0
86	OHX	1	3993	7/7	0.27	5.29	101,101,101,101	0
85	MG	m7	201	1/1	0.38	5.29	31,31,31,31	0
86	OHX	2	2160	7/7	0.50	5.28	129,129,129,129	0
85	MG	1	3693	1/1	0.28	5.28	41,41,41,41	0
86	OHX	5	4222	7/7	0.36	5.25	166,166,166,166	0
86	OHX	6	2202	7/7	0.33	5.23	148,148,148,148	0
86	OHX	5	4246	7/7	0.27	5.23	158,158,158,158	0
85	MG	6	2038	1/1	0.75	5.21	78,78,78,78	0
85	MG	5	3877	1/1	0.36	5.19	47,47,47,47	0
85	MG	s8	301	1/1	0.30	5.18	51,51,51,51	0
86	OHX	2	2119	7/7	0.29	5.18	131,131,131,131	0
86	OHX	5	4041	7/7	0.30	5.17	86,86,86,86	0
86	OHX	6	2186	7/7	0.47	5.16	132,132,132,132	0
86	OHX	6	2138	7/7	0.31	5.15	130,130,130,130	0
86	OHX	1	4212	7/7	0.41	5.15	126,126,126,126	0
86	OHX	1	4100	7/7	0.25	5.14	137,137,137,137	0
86	OHX	5	4044	7/7	0.26	5.12	127,127,127,127	0
85	MG	5	3499	1/1	0.27	5.10	31,31,31,31	0
85	MG	1	3677	1/1	0.28	5.09	24,24,24,24	0
85	MG	5	3743	1/1	0.17	5.08	29,29,29,29	0
85	MG	L2	301	1/1	0.34	5.05	29,29,29,29	0
85	MG	O3	201	1/1	0.17	5.05	38,38,38,38	0
85	MG	1	3456	1/1	0.46	5.05	58,58,58,58	0
85	MG	1	3829	1/1	0.25	5.03	27,27,27,27	0
85	MG	5	3744	1/1	0.26	5.03	41,41,41,41	0
85	MG	5	3709	1/1	0.24	5.02	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4107	7/7	0.26	5.02	100,100,100,100	0
85	MG	1	3446	1/1	0.48	5.02	47,47,47,47	0
86	OHX	6	2200	7/7	0.30	5.01	133,133,133,133	0
86	OHX	1	4058	7/7	0.23	5.01	102,102,102,102	0
85	MG	5	3840	1/1	0.11	5.00	59,59,59,59	0
86	OHX	1	4126	7/7	0.30	4.99	103,103,103,103	0
85	MG	L2	302	1/1	0.34	4.99	40,40,40,40	0
85	MG	1	3653	1/1	0.26	4.98	72,72,72,72	0
85	MG	5	3891	1/1	0.29	4.98	34,34,34,34	0
86	OHX	5	4211	7/7	0.31	4.96	149,149,149,149	0
85	MG	1	3611	1/1	0.24	4.94	42,42,42,42	0
85	MG	n8	201	1/1	0.32	4.94	37,37,37,37	0
85	MG	5	3838	1/1	0.24	4.93	33,33,33,33	0
86	OHX	1	4190	7/7	0.48	4.93	181,181,181,181	0
86	OHX	6	2172	7/7	0.39	4.93	147,147,147,147	0
85	MG	6	1987	1/1	0.30	4.92	55,55,55,55	0
86	OHX	2	2163	7/7	0.30	4.91	168,168,168,168	0
86	OHX	5	4232	7/7	0.31	4.88	167,167,167,167	0
85	MG	2	1927	1/1	0.43	4.87	64,64,64,64	0
85	MG	5	3605	1/1	0.23	4.86	28,28,28,28	0
85	MG	3	211	1/1	0.37	4.86	74,74,74,74	0
85	MG	2	1984	1/1	0.29	4.86	62,62,62,62	0
86	OHX	2	2078	7/7	0.25	4.85	117,117,117,117	0
86	OHX	2	2145	7/7	0.32	4.84	143,143,143,143	0
85	MG	1	3782	1/1	0.18	4.82	62,62,62,62	0
85	MG	5	3893	1/1	0.22	4.82	82,82,82,82	0
85	MG	4	208	1/1	0.26	4.82	27,27,27,27	0
86	OHX	5	4194	7/7	0.28	4.81	119,119,119,119	0
86	OHX	5	4243	7/7	0.27	4.80	171,171,171,171	0
86	OHX	5	4098	7/7	0.26	4.80	145,145,145,145	0
86	OHX	1	4113	7/7	0.32	4.78	131,131,131,131	0
85	MG	2	1992	1/1	0.30	4.75	70,70,70,70	0
86	OHX	1	4012	7/7	0.17	4.73	120,120,120,120	0
86	OHX	5	4235	7/7	0.25	4.73	158,158,158,158	0
86	OHX	6	2182	7/7	0.39	4.71	133,133,133,133	0
86	OHX	2	2173	7/7	0.44	4.71	144,144,144,144	0
85	MG	6	2041	1/1	0.55	4.70	110,110,110,110	0
86	OHX	1	4137	7/7	0.29	4.68	133,133,133,133	0
86	OHX	2	2134	7/7	0.28	4.68	138,138,138,138	0
86	OHX	5	4046	7/7	0.24	4.68	98,98,98,98	0
85	MG	5	3506	1/1	0.33	4.68	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3700	1/1	0.30	4.64	55,55,55,55	0
86	OHX	6	2171	7/7	0.28	4.63	148,148,148,148	0
86	OHX	5	4158	7/7	0.40	4.63	137,137,137,137	0
85	MG	5	3826	1/1	0.25	4.63	36,36,36,36	0
86	OHX	6	2105	7/7	0.26	4.62	117,117,117,117	0
86	OHX	o9	101	7/7	0.31	4.62	114,114,114,114	0
86	OHX	5	4049	7/7	0.21	4.61	122,122,122,122	0
85	MG	2	1991	1/1	0.18	4.60	55,55,55,55	0
85	MG	1	3825	1/1	0.21	4.60	60,60,60,60	0
85	MG	1	3526	1/1	0.23	4.55	39,39,39,39	0
85	MG	1	3431	1/1	0.44	4.54	47,47,47,47	0
85	MG	6	1908	1/1	0.23	4.53	48,48,48,48	0
85	MG	5	3647	1/1	0.29	4.53	52,52,52,52	0
86	OHX	1	3896	7/7	0.23	4.52	101,101,101,101	0
86	OHX	3	224	7/7	0.26	4.51	136,136,136,136	0
85	MG	5	3779	1/1	0.22	4.50	44,44,44,44	0
86	OHX	5	4149	7/7	0.31	4.50	107,107,107,107	0
85	MG	5	3497	1/1	0.22	4.47	33,33,33,33	0
86	OHX	2	2171	7/7	0.25	4.46	141,141,141,141	0
85	MG	5	3461	1/1	0.29	4.45	27,27,27,27	0
85	MG	1	3717	1/1	0.21	4.45	32,32,32,32	0
86	OHX	s1	302	7/7	0.38	4.44	158,158,158,158	0
85	MG	5	3694	1/1	0.22	4.43	43,43,43,43	0
86	OHX	3	223	7/7	0.32	4.41	126,126,126,126	0
86	OHX	5	4094	7/7	0.24	4.40	107,107,107,107	0
85	MG	c9	201	1/1	0.45	4.40	72,72,72,72	0
86	OHX	1	4130	7/7	0.28	4.39	143,143,143,143	0
86	OHX	1	4134	7/7	0.30	4.39	143,143,143,143	0
85	MG	1	3427	1/1	0.30	4.39	59,59,59,59	0
85	MG	6	1990	1/1	0.27	4.39	88,88,88,88	0
86	OHX	5	4196	7/7	0.24	4.36	114,114,114,114	0
86	OHX	1	3994	7/7	0.28	4.32	118,118,118,118	0
85	MG	M7	201	1/1	0.27	4.31	33,33,33,33	0
85	MG	1	3760	1/1	0.18	4.29	47,47,47,47	0
86	OHX	1	4019	7/7	0.24	4.29	107,107,107,107	0
86	OHX	2	2140	7/7	0.29	4.28	154,154,154,154	0
86	OHX	6	2159	7/7	0.31	4.27	139,139,139,139	0
86	OHX	5	4072	7/7	0.24	4.25	130,130,130,130	0
85	MG	n8	204	1/1	0.26	4.25	41,41,41,41	0
86	OHX	5	4051	7/7	0.24	4.23	102,102,102,102	0
85	MG	2	1948	1/1	0.69	4.23	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	1993	1/1	0.29	4.21	51,51,51,51	0
86	OHX	5	4201	7/7	0.24	4.21	87,87,87,87	0
86	OHX	7	226	7/7	0.29	4.18	150,150,150,150	0
85	MG	6	1923	1/1	0.35	4.17	67,67,67,67	0
85	MG	6	2003	1/1	0.26	4.15	54,54,54,54	0
85	MG	6	1936	1/1	0.27	4.14	77,77,77,77	0
86	OHX	5	4146	7/7	0.29	4.12	110,110,110,110	0
85	MG	5	3479	1/1	0.21	4.11	58,58,58,58	0
85	MG	1	3673	1/1	0.17	4.10	80,80,80,80	0
85	MG	5	3864	1/1	0.19	4.10	38,38,38,38	0
86	OHX	5	4150	7/7	0.27	4.09	125,125,125,125	0
85	MG	2	2005	1/1	0.34	4.06	81,81,81,81	0
86	OHX	1	4197	7/7	0.47	4.03	131,131,131,131	0
86	OHX	1	4068	7/7	0.27	4.03	99,99,99,99	0
86	OHX	1	4037	7/7	0.21	4.03	104,104,104,104	0
86	OHX	1	4160	7/7	0.22	4.02	110,110,110,110	0
85	MG	1	3647	1/1	0.26	4.01	45,45,45,45	0
86	OHX	2	2154	7/7	0.29	4.00	149,149,149,149	0
85	MG	2	1952	1/1	0.51	3.98	102,102,102,102	0
85	MG	N8	201	1/1	0.28	3.98	29,29,29,29	0
85	MG	5	3713	1/1	0.24	3.98	43,43,43,43	0
86	OHX	7	227	7/7	0.26	3.97	112,112,112,112	0
86	OHX	1	4080	7/7	0.17	3.95	130,130,130,130	0
85	MG	1	3720	1/1	0.25	3.94	72,72,72,72	0
86	OHX	5	4071	7/7	0.18	3.93	137,137,137,137	0
85	MG	6	1967	1/1	0.31	3.93	85,85,85,85	0
86	OHX	1	4152	7/7	0.27	3.92	135,135,135,135	0
85	MG	1	3800	1/1	0.24	3.91	48,48,48,48	0
86	OHX	5	4054	7/7	0.26	3.90	95,95,95,95	0
86	OHX	5	4236	7/7	0.24	3.90	97,97,97,97	0
85	MG	2	1949	1/1	0.24	3.89	59,59,59,59	0
85	MG	5	3533	1/1	0.20	3.88	52,52,52,52	0
86	OHX	1	4041	7/7	0.25	3.87	111,111,111,111	0
86	OHX	2	2061	7/7	0.26	3.85	131,131,131,131	0
85	MG	5	3774	1/1	0.21	3.84	32,32,32,32	0
86	OHX	5	4219	7/7	0.25	3.82	99,99,99,99	0
85	MG	5	3691	1/1	0.30	3.82	43,43,43,43	0
86	OHX	6	2150	7/7	0.26	3.82	127,127,127,127	0
85	MG	5	3416	1/1	0.24	3.81	34,34,34,34	0
86	OHX	6	2136	7/7	0.23	3.81	129,129,129,129	0
85	MG	1	3412	1/1	0.23	3.81	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	n0	201	1/1	0.29	3.80	42,42,42,42	0
86	OHX	1	4102	7/7	0.41	3.80	107,107,107,107	0
85	MG	6	2001	1/1	0.40	3.80	55,55,55,55	0
86	OHX	6	2193	7/7	0.40	3.79	153,153,153,153	0
85	MG	n6	202	1/1	0.37	3.79	44,44,44,44	0
86	OHX	6	2190	7/7	0.37	3.77	142,142,142,142	0
86	OHX	1	4046	7/7	0.25	3.74	96,96,96,96	0
86	OHX	1	4151	7/7	0.30	3.71	140,140,140,140	0
86	OHX	5	4174	7/7	0.31	3.69	158,158,158,158	0
86	OHX	3	221	7/7	0.29	3.69	115,115,115,115	0
86	OHX	5	4139	7/7	0.38	3.69	126,126,126,126	0
85	MG	1	3710	1/1	0.22	3.67	55,55,55,55	0
86	OHX	l5	304	7/7	0.41	3.66	140,140,140,140	0
85	MG	6	1978	1/1	0.24	3.66	42,42,42,42	0
86	OHX	5	4135	7/7	0.27	3.63	114,114,114,114	0
85	MG	5	3688	1/1	0.19	3.63	42,42,42,42	0
86	OHX	2	2149	7/7	0.30	3.63	161,161,161,161	0
86	OHX	1	4154	7/7	0.28	3.62	108,108,108,108	0
85	MG	1	3775	1/1	0.27	3.62	51,51,51,51	0
86	OHX	6	2154	7/7	0.23	3.59	148,148,148,148	0
85	MG	1	3752	1/1	0.22	3.59	47,47,47,47	0
85	MG	m0	301	1/1	0.34	3.59	28,28,28,28	0
85	MG	5	3814	1/1	0.21	3.57	81,81,81,81	0
85	MG	2	1968	1/1	0.59	3.56	123,123,123,123	0
86	OHX	5	4166	7/7	0.21	3.55	140,140,140,140	0
86	OHX	2	2142	7/7	0.19	3.54	136,136,136,136	0
86	OHX	2	2176	7/7	0.35	3.54	141,141,141,141	0
86	OHX	1	4141	7/7	0.21	3.53	117,117,117,117	0
86	OHX	M7	207	7/7	0.33	3.53	133,133,133,133	0
86	OHX	5	4050	7/7	0.20	3.52	114,114,114,114	0
86	OHX	2	2100	7/7	0.23	3.52	139,139,139,139	0
85	MG	1	3450	1/1	0.25	3.51	37,37,37,37	0
85	MG	d3	202	1/1	0.39	3.51	53,53,53,53	0
85	MG	5	3801	1/1	0.23	3.50	31,31,31,31	0
86	OHX	1	4008	7/7	0.19	3.49	120,120,120,120	0
86	OHX	5	4099	7/7	0.21	3.49	121,121,121,121	0
85	MG	5	3603	1/1	0.26	3.48	38,38,38,38	0
86	OHX	1	4158	7/7	0.28	3.48	125,125,125,125	0
85	MG	5	3848	1/1	0.56	3.46	56,56,56,56	0
85	MG	1	3808	1/1	0.23	3.44	34,34,34,34	0
85	MG	5	3654	1/1	0.27	3.44	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2201	7/7	0.30	3.43	139,139,139,139	0
85	MG	5	3797	1/1	0.23	3.43	38,38,38,38	0
85	MG	1	3767	1/1	0.22	3.42	42,42,42,42	0
85	MG	1	3848	1/1	0.25	3.39	42,42,42,42	0
86	OHX	2	2099	7/7	0.32	3.39	154,154,154,154	0
86	OHX	8	226	7/7	0.25	3.37	135,135,135,135	0
86	OHX	s9	202	7/7	0.37	3.37	121,121,121,121	0
86	OHX	8	230	7/7	0.28	3.36	132,132,132,132	0
85	MG	5	3719	1/1	0.22	3.36	61,61,61,61	0
85	MG	5	3606	1/1	0.22	3.36	35,35,35,35	0
86	OHX	1	4093	7/7	0.18	3.35	131,131,131,131	0
85	MG	5	3854	1/1	0.29	3.34	46,46,46,46	0
86	OHX	1	4203	7/7	0.32	3.33	143,143,143,143	0
86	OHX	2	2174	7/7	0.29	3.33	158,158,158,158	0
86	OHX	1	4125	7/7	0.32	3.32	140,140,140,140	0
85	MG	4	210	1/1	0.22	3.32	47,47,47,47	0
86	OHX	2	2152	7/7	0.38	3.32	142,142,142,142	0
86	OHX	1	4168	7/7	0.32	3.31	119,119,119,119	0
86	OHX	1	4183	7/7	0.51	3.29	131,131,131,131	0
86	OHX	6	2197	7/7	0.38	3.27	156,156,156,156	0
85	MG	8	201	1/1	0.31	3.24	33,33,33,33	0
86	OHX	5	4225	7/7	0.37	3.24	137,137,137,137	0
85	MG	6	1985	1/1	0.25	3.23	79,79,79,79	0
85	MG	L7	303	1/1	0.20	3.20	47,47,47,47	0
86	OHX	6	2130	7/7	0.38	3.20	145,145,145,145	0
85	MG	1	3485	1/1	0.23	3.19	42,42,42,42	0
86	OHX	5	4171	7/7	0.29	3.19	126,126,126,126	0
86	OHX	6	2142	7/7	0.23	3.17	130,130,130,130	0
85	MG	o4	202	1/1	0.59	3.17	69,69,69,69	0
85	MG	1	3816	1/1	0.22	3.16	52,52,52,52	0
86	OHX	5	4104	7/7	0.24	3.16	95,95,95,95	0
85	MG	1	3768	1/1	0.20	3.12	52,52,52,52	0
85	MG	6	1962	1/1	0.25	3.12	45,45,45,45	0
85	MG	5	3410	1/1	0.21	3.12	55,55,55,55	0
85	MG	5	3785	1/1	0.18	3.11	36,36,36,36	0
86	OHX	5	4120	7/7	0.25	3.11	117,117,117,117	0
86	OHX	2	2115	7/7	0.32	3.10	146,146,146,146	0
86	OHX	1	4078	7/7	0.29	3.10	117,117,117,117	0
85	MG	5	3495	1/1	0.21	3.09	39,39,39,39	0
85	MG	1	3601	1/1	0.23	3.09	36,36,36,36	0
85	MG	m7	202	1/1	0.33	3.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1940	1/1	0.39	3.08	68,68,68,68	0
86	OHX	6	2151	7/7	0.28	3.08	106,106,106,106	0
86	OHX	6	2175	7/7	0.32	3.07	145,145,145,145	0
86	OHX	5	4119	7/7	0.33	3.05	95,95,95,95	0
86	OHX	1	3987	7/7	0.24	3.04	102,102,102,102	0
85	MG	5	3423	1/1	0.21	3.03	39,39,39,39	0
86	OHX	14	402	7/7	0.28	3.02	153,153,153,153	0
85	MG	8	203	1/1	0.23	3.01	55,55,55,55	0
86	OHX	5	4176	7/7	0.26	3.01	87,87,87,87	0
86	OHX	2	2108	7/7	0.23	3.00	149,149,149,149	0
85	MG	1	3806	1/1	0.28	2.98	59,59,59,59	0
86	OHX	1	4118	7/7	0.24	2.98	113,113,113,113	0
85	MG	1	3478	1/1	0.21	2.97	48,48,48,48	0
85	MG	19	201	1/1	0.23	2.96	42,42,42,42	0
85	MG	3	210	1/1	0.28	2.96	67,67,67,67	0
86	OHX	5	4163	7/7	0.28	2.96	114,114,114,114	0
86	OHX	D9	102	7/7	0.36	2.95	147,147,147,147	0
85	MG	5	3724	1/1	0.25	2.95	55,55,55,55	0
86	OHX	6	2115	7/7	0.19	2.95	97,97,97,97	0
85	MG	5	3827	1/1	0.23	2.94	41,41,41,41	0
85	MG	n3	202	1/1	0.39	2.93	44,44,44,44	0
85	MG	1	3858	1/1	0.25	2.93	88,88,88,88	0
86	OHX	5	4148	7/7	0.23	2.93	111,111,111,111	0
86	OHX	5	4125	7/7	0.28	2.91	127,127,127,127	0
85	MG	5	3435	1/1	0.22	2.89	29,29,29,29	0
85	MG	1	3759	1/1	0.24	2.88	50,50,50,50	0
86	OHX	2	2090	7/7	0.36	2.88	138,138,138,138	0
85	MG	5	3543	1/1	0.41	2.87	69,69,69,69	0
86	OHX	2	2135	7/7	0.28	2.87	124,124,124,124	0
86	OHX	6	2127	7/7	0.26	2.86	131,131,131,131	0
86	OHX	4	237	7/7	0.26	2.86	135,135,135,135	0
85	MG	6	2016	1/1	0.53	2.85	133,133,133,133	0
85	MG	L7	302	1/1	0.26	2.85	40,40,40,40	0
85	MG	1	3612	1/1	0.29	2.84	43,43,43,43	0
85	MG	1	3708	1/1	0.17	2.83	54,54,54,54	0
85	MG	5	3843	1/1	0.25	2.82	50,50,50,50	0
85	MG	5	3681	1/1	0.17	2.82	33,33,33,33	0
85	MG	5	3812	1/1	0.20	2.81	28,28,28,28	0
86	OHX	1	4086	7/7	0.21	2.79	119,119,119,119	0
86	OHX	5	3912	7/7	0.19	2.78	66,66,66,66	0
85	MG	2	1988	1/1	0.15	2.78	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4114	7/7	0.21	2.77	120,120,120,120	0
85	MG	5	3748	1/1	0.24	2.75	46,46,46,46	0
86	OHX	1	4073	7/7	0.27	2.75	112,112,112,112	0
85	MG	8	209	1/1	0.22	2.74	43,43,43,43	0
85	MG	5	3635	1/1	0.35	2.73	74,74,74,74	0
85	MG	6	1902	1/1	0.24	2.71	54,54,54,54	0
86	OHX	1	4119	7/7	0.25	2.70	119,119,119,119	0
85	MG	5	3845	1/1	0.35	2.70	49,49,49,49	0
86	OHX	5	4078	7/7	0.29	2.69	119,119,119,119	0
86	OHX	2	2175	7/7	0.32	2.66	161,161,161,161	0
86	OHX	5	4110	7/7	0.30	2.66	119,119,119,119	0
85	MG	5	3825	1/1	0.20	2.66	42,42,42,42	0
85	MG	1	3452	1/1	0.37	2.63	44,44,44,44	0
86	OHX	6	2196	7/7	0.36	2.63	174,174,174,174	0
85	MG	5	3496	1/1	0.30	2.62	26,26,26,26	0
85	MG	1	3784	1/1	0.18	2.62	51,51,51,51	0
85	MG	O1	201	1/1	0.28	2.61	70,70,70,70	0
85	MG	5	3798	1/1	0.29	2.61	37,37,37,37	0
85	MG	5	3644	1/1	0.21	2.61	33,33,33,33	0
86	OHX	5	4186	7/7	0.40	2.60	132,132,132,132	0
85	MG	1	3628	1/1	0.24	2.59	30,30,30,30	0
85	MG	4	209	1/1	0.22	2.59	40,40,40,40	0
86	OHX	6	2174	7/7	0.31	2.57	143,143,143,143	0
86	OHX	8	228	7/7	0.23	2.57	135,135,135,135	0
85	MG	M3	201	1/1	0.22	2.56	44,44,44,44	0
85	MG	2	1943	1/1	0.23	2.56	70,70,70,70	0
85	MG	7	213	1/1	0.15	2.55	70,70,70,70	0
86	OHX	5	4202	7/7	0.21	2.55	110,110,110,110	0
85	MG	5	3618	1/1	0.15	2.55	43,43,43,43	0
86	OHX	2	2131	7/7	0.33	2.55	131,131,131,131	0
85	MG	6	2024	1/1	0.35	2.55	61,61,61,61	0
86	OHX	6	2160	7/7	0.23	2.53	135,135,135,135	0
85	MG	1	3791	1/1	0.29	2.53	25,25,25,25	0
86	OHX	5	4180	7/7	0.18	2.51	120,120,120,120	0
85	MG	5	3668	1/1	0.23	2.51	27,27,27,27	0
86	OHX	5	4253	7/7	0.32	2.50	135,135,135,135	0
85	MG	N8	202	1/1	0.21	2.50	30,30,30,30	0
85	MG	6	1976	1/1	0.19	2.49	60,60,60,60	0
85	MG	5	3494	1/1	0.27	2.47	45,45,45,45	0
86	OHX	1	4029	7/7	0.21	2.47	124,124,124,124	0
85	MG	4	211	1/1	0.22	2.47	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3645	1/1	0.23	2.47	44,44,44,44	0
86	OHX	1	4075	7/7	0.21	2.46	139,139,139,139	0
86	OHX	5	4137	7/7	0.30	2.44	113,113,113,113	0
86	OHX	L4	402	7/7	0.30	2.44	138,138,138,138	0
85	MG	L5	301	1/1	0.66	2.44	68,68,68,68	0
85	MG	5	3715	1/1	0.24	2.43	48,48,48,48	0
85	MG	1	3827	1/1	0.16	2.42	43,43,43,43	0
85	MG	O7	103	1/1	0.28	2.42	34,34,34,34	0
86	OHX	1	4074	7/7	0.24	2.42	134,134,134,134	0
86	OHX	5	4063	7/7	0.21	2.42	104,104,104,104	0
85	MG	1	3652	1/1	0.27	2.42	46,46,46,46	0
85	MG	1	3641	1/1	0.30	2.42	55,55,55,55	0
86	OHX	6	2177	7/7	0.34	2.41	148,148,148,148	0
86	OHX	2	2110	7/7	0.21	2.39	114,114,114,114	0
86	OHX	5	4047	7/7	0.26	2.38	119,119,119,119	0
86	OHX	2	2074	7/7	0.20	2.38	139,139,139,139	0
85	MG	5	3762	1/1	0.38	2.38	44,44,44,44	0
86	OHX	1	4017	7/7	0.23	2.37	115,115,115,115	0
86	OHX	6	2153	7/7	0.27	2.35	110,110,110,110	0
86	OHX	6	2117	7/7	0.24	2.34	124,124,124,124	0
85	MG	5	3467	1/1	0.34	2.34	93,93,93,93	0
86	OHX	1	4147	7/7	0.21	2.32	108,108,108,108	0
86	OHX	1	4104	7/7	0.33	2.32	151,151,151,151	0
86	OHX	1	4055	7/7	0.17	2.31	136,136,136,136	0
86	OHX	3	220	7/7	0.21	2.29	137,137,137,137	0
86	OHX	5	4138	7/7	0.23	2.28	133,133,133,133	0
86	OHX	2	2095	7/7	0.27	2.27	134,134,134,134	0
86	OHX	m7	206	7/7	0.33	2.27	115,115,115,115	0
85	MG	5	3473	1/1	0.20	2.25	33,33,33,33	0
86	OHX	1	4083	7/7	0.26	2.25	119,119,119,119	0
88	HMT	5	4255	39/39	0.20	2.25	28,28,28,28	0
85	MG	1	3664	1/1	0.26	2.24	33,33,33,33	0
86	OHX	5	4004	7/7	0.25	2.23	75,75,75,75	0
85	MG	1	3640	1/1	0.36	2.23	51,51,51,51	0
85	MG	1	3764	1/1	0.22	2.23	43,43,43,43	0
85	MG	1	3465	1/1	0.15	2.22	44,44,44,44	0
86	OHX	2	2116	7/7	0.30	2.22	139,139,139,139	0
86	OHX	1	3911	7/7	0.23	2.22	83,83,83,83	0
85	MG	6	2029	1/1	0.26	2.20	88,88,88,88	0
85	MG	O4	201	1/1	0.32	2.20	60,60,60,60	0
86	OHX	6	2126	7/7	0.23	2.19	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4032	7/7	0.19	2.18	130,130,130,130	0
85	MG	L8	301	1/1	0.33	2.18	53,53,53,53	0
85	MG	c7	201	1/1	0.29	2.18	74,74,74,74	0
86	OHX	O3	202	7/7	0.28	2.18	106,106,106,106	0
85	MG	M0	301	1/1	0.23	2.17	40,40,40,40	0
85	MG	5	3480	1/1	0.38	2.17	62,62,62,62	0
86	OHX	5	4145	7/7	0.23	2.16	128,128,128,128	0
85	MG	c1	201	1/1	0.30	2.16	50,50,50,50	0
85	MG	4	204	1/1	0.50	2.16	70,70,70,70	0
85	MG	1	3648	1/1	0.20	2.13	64,64,64,64	0
85	MG	6	2005	1/1	0.26	2.11	73,73,73,73	0
85	MG	6	1964	1/1	0.28	2.11	99,99,99,99	0
86	OHX	5	4064	7/7	0.22	2.11	125,125,125,125	0
85	MG	d3	201	1/1	0.26	2.10	47,47,47,47	0
86	OHX	6	2134	7/7	0.31	2.09	123,123,123,123	0
85	MG	1	3404	1/1	0.57	2.08	62,62,62,62	0
86	OHX	1	4164	7/7	0.36	2.06	148,148,148,148	0
86	OHX	2	2139	7/7	0.31	2.06	152,152,152,152	0
85	MG	1	3448	1/1	0.43	2.06	45,45,45,45	0
85	MG	1	3776	1/1	0.31	2.06	53,53,53,53	0
85	MG	8	210	1/1	0.30	2.05	59,59,59,59	0
85	MG	6	1991	1/1	0.37	2.04	72,72,72,72	0
86	OHX	6	2180	7/7	0.28	2.04	135,135,135,135	0
85	MG	1	3730	1/1	0.23	2.04	61,61,61,61	0
86	OHX	5	4091	7/7	0.26	2.03	98,98,98,98	0
85	MG	5	3887	1/1	0.21	2.03	71,71,71,71	0
86	OHX	5	4123	7/7	0.26	2.00	140,140,140,140	0
85	MG	1	3436	1/1	0.18	1.99	40,40,40,40	0
86	OHX	1	4084	7/7	0.40	1.98	112,112,112,112	0
85	MG	5	3433	1/1	0.18	1.98	42,42,42,42	0
85	MG	5	3836	1/1	0.20	1.98	39,39,39,39	0
86	OHX	5	4095	7/7	0.23	1.97	109,109,109,109	0
86	OHX	1	4011	7/7	0.18	1.97	103,103,103,103	0
85	MG	5	3658	1/1	0.21	1.97	44,44,44,44	0
86	OHX	5	4203	7/7	0.28	1.96	117,117,117,117	0
86	OHX	5	3986	7/7	0.19	1.94	94,94,94,94	0
86	OHX	1	4106	7/7	0.18	1.93	137,137,137,137	0
85	MG	5	3734	1/1	0.21	1.93	43,43,43,43	0
86	OHX	2	2170	7/7	0.36	1.92	139,139,139,139	0
85	MG	6	1909	1/1	0.34	1.91	111,111,111,111	0
86	OHX	5	4214	7/7	0.28	1.91	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1947	1/1	0.19	1.90	63,63,63,63	0
85	MG	5	3462	1/1	0.22	1.90	38,38,38,38	0
86	OHX	5	4058	7/7	0.18	1.89	105,105,105,105	0
86	OHX	1	4053	7/7	0.21	1.89	110,110,110,110	0
86	OHX	5	4121	7/7	0.22	1.89	107,107,107,107	0
86	OHX	6	2141	7/7	0.17	1.87	129,129,129,129	0
85	MG	1	3701	1/1	0.41	1.87	68,68,68,68	0
86	OHX	1	4191	7/7	0.31	1.86	135,135,135,135	0
86	OHX	1	4024	7/7	0.22	1.82	119,119,119,119	0
85	MG	1	3794	1/1	0.16	1.82	58,58,58,58	0
86	OHX	5	4210	7/7	0.28	1.81	136,136,136,136	0
85	MG	5	3602	1/1	0.22	1.81	58,58,58,58	0
86	OHX	2	2068	7/7	0.22	1.81	111,111,111,111	0
85	MG	5	3700	1/1	0.21	1.79	54,54,54,54	0
85	MG	5	3599	1/1	0.19	1.78	37,37,37,37	0
85	MG	5	3754	1/1	0.24	1.78	50,50,50,50	0
86	OHX	6	2195	7/7	0.35	1.78	168,168,168,168	0
86	OHX	2	2089	7/7	0.21	1.78	122,122,122,122	0
85	MG	1	3718	1/1	0.20	1.77	40,40,40,40	0
85	MG	5	3816	1/1	0.17	1.75	62,62,62,62	0
86	OHX	1	4108	7/7	0.25	1.75	120,120,120,120	0
85	MG	6	2035	1/1	0.22	1.74	52,52,52,52	0
85	MG	1	3695	1/1	0.26	1.72	43,43,43,43	0
85	MG	5	3627	1/1	0.20	1.71	58,58,58,58	0
85	MG	6	1932	1/1	0.21	1.71	45,45,45,45	0
86	OHX	5	4109	7/7	0.29	1.71	114,114,114,114	0
85	MG	5	3707	1/1	0.16	1.70	50,50,50,50	0
85	MG	1	3687	1/1	0.21	1.69	46,46,46,46	0
86	OHX	5	4247	7/7	0.27	1.68	136,136,136,136	0
85	MG	1	3631	1/1	0.19	1.67	61,61,61,61	0
86	OHX	5	4022	7/7	0.19	1.66	96,96,96,96	0
85	MG	2	1920	1/1	0.33	1.66	65,65,65,65	0
85	MG	5	3730	1/1	0.19	1.66	47,47,47,47	0
85	MG	14	401	1/1	0.31	1.65	31,31,31,31	0
86	OHX	1	4194	7/7	0.20	1.65	141,141,141,141	0
86	OHX	1	3873	7/7	0.16	1.65	58,58,58,58	0
85	MG	8	207	1/1	0.25	1.64	53,53,53,53	0
86	OHX	5	4092	7/7	0.30	1.64	103,103,103,103	0
86	OHX	1	4072	7/7	0.20	1.64	117,117,117,117	0
85	MG	1	3584	1/1	0.38	1.62	39,39,39,39	0
85	MG	2	1972	1/1	0.32	1.60	89,89,89,89	0
85	MG	5	3685	1/1	0.25	1.60	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	8	211	1/1	0.28	1.60	38,38,38,38	0
86	OHX	6	2198	7/7	0.28	1.59	163,163,163,163	0
86	OHX	2	2168	7/7	0.23	1.57	118,118,118,118	0
85	MG	1	3602	1/1	0.18	1.56	28,28,28,28	0
85	MG	o4	201	1/1	0.36	1.55	52,52,52,52	0
86	OHX	6	2194	7/7	0.27	1.53	149,149,149,149	0
86	OHX	m8	201	7/7	0.27	1.53	123,123,123,123	0
85	MG	5	3799	1/1	0.28	1.52	71,71,71,71	0
85	MG	2	1995	1/1	0.21	1.52	96,96,96,96	0
86	OHX	1	4007	7/7	0.20	1.51	103,103,103,103	0
85	MG	1	3683	1/1	0.27	1.51	66,66,66,66	0
86	OHX	2	2129	7/7	0.34	1.48	188,188,188,188	0
86	OHX	5	4147	7/7	0.22	1.48	126,126,126,126	0
85	MG	1	3755	1/1	0.27	1.47	59,59,59,59	0
87	ZN	D7	101	1/1	0.39	1.47	144,144,144,144	0
85	MG	1	3637	1/1	0.26	1.46	42,42,42,42	0
86	OHX	M8	201	7/7	0.33	1.46	134,134,134,134	0
86	OHX	5	4177	7/7	0.21	1.46	111,111,111,111	0
87	ZN	d7	101	1/1	0.55	1.45	139,139,139,139	0
86	OHX	1	3955	7/7	0.17	1.45	96,96,96,96	0
86	OHX	1	4042	7/7	0.27	1.44	114,114,114,114	0
85	MG	5	3528	1/1	0.17	1.43	26,26,26,26	0
85	MG	5	3472	1/1	0.19	1.41	43,43,43,43	0
85	MG	m7	204	1/1	0.24	1.40	34,34,34,34	0
85	MG	5	3832	1/1	0.22	1.39	51,51,51,51	0
85	MG	1	3630	1/1	0.30	1.39	69,69,69,69	0
86	OHX	6	2110	7/7	0.22	1.38	108,108,108,108	0
86	OHX	2	2091	7/7	0.21	1.37	111,111,111,111	0
86	OHX	6	2074	7/7	0.20	1.37	89,89,89,89	0
85	MG	M7	202	1/1	0.32	1.36	29,29,29,29	0
86	OHX	5	4088	7/7	0.19	1.36	126,126,126,126	0
86	OHX	2	2166	7/7	0.27	1.35	155,155,155,155	0
86	OHX	1	4002	7/7	0.18	1.35	104,104,104,104	0
86	OHX	1	4110	7/7	0.27	1.33	114,114,114,114	0
86	OHX	5	4061	7/7	0.18	1.33	105,105,105,105	0
86	OHX	d4	201	7/7	0.23	1.32	145,145,145,145	0
86	OHX	1	4004	7/7	0.28	1.28	110,110,110,110	0
85	MG	5	3841	1/1	0.18	1.28	68,68,68,68	0
86	OHX	2	2147	7/7	0.22	1.28	166,166,166,166	0
85	MG	d6	102	1/1	0.29	1.27	55,55,55,55	0
86	OHX	1	3974	7/7	0.17	1.27	97,97,97,97	0
86	OHX	5	4059	7/7	0.22	1.27	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4096	7/7	0.24	1.26	126,126,126,126	0
85	MG	1	3771	1/1	0.20	1.26	83,83,83,83	0
86	OHX	5	4025	7/7	0.18	1.24	101,101,101,101	0
85	MG	l3	403	1/1	0.24	1.23	31,31,31,31	0
86	OHX	2	2087	7/7	0.22	1.23	130,130,130,130	0
85	MG	1	3667	1/1	0.18	1.21	52,52,52,52	0
85	MG	1	3736	1/1	0.23	1.20	60,60,60,60	0
86	OHX	d9	102	7/7	0.42	1.20	161,161,161,161	0
86	OHX	6	2203	7/7	0.44	1.19	142,142,142,142	0
86	OHX	1	4153	7/7	0.36	1.19	145,145,145,145	0
85	MG	1	3633	1/1	0.19	1.19	33,33,33,33	0
85	MG	m7	205	1/1	0.26	1.19	35,35,35,35	0
86	OHX	2	2128	7/7	0.21	1.17	147,147,147,147	0
85	MG	5	3419	1/1	0.23	1.16	33,33,33,33	0
85	MG	1	3688	1/1	0.20	1.16	38,38,38,38	0
86	OHX	5	4133	7/7	0.15	1.16	108,108,108,108	0
88	HMT	1	4217	39/39	0.21	1.14	30,30,30,30	0
86	OHX	5	3987	7/7	0.20	1.14	90,90,90,90	0
85	MG	1	3783	1/1	0.20	1.13	43,43,43,43	0
85	MG	M7	205	1/1	0.23	1.13	39,39,39,39	0
86	OHX	5	4127	7/7	0.22	1.11	144,144,144,144	0
85	MG	1	3770	1/1	0.23	1.11	65,65,65,65	0
86	OHX	2	2084	7/7	0.29	1.11	141,141,141,141	0
86	OHX	2	2121	7/7	0.33	1.11	141,141,141,141	0
86	OHX	5	4077	7/7	0.29	1.09	117,117,117,117	0
86	OHX	5	4192	7/7	0.36	1.08	119,119,119,119	0
86	OHX	1	4091	7/7	0.24	1.08	122,122,122,122	0
86	OHX	6	2184	7/7	0.40	1.06	131,131,131,131	0
86	OHX	2	2133	7/7	0.20	1.04	154,154,154,154	0
86	OHX	s4	302	7/7	0.20	1.00	142,142,142,142	0
85	MG	1	3745	1/1	0.16	1.00	38,38,38,38	0
85	MG	1	3682	1/1	0.21	1.00	41,41,41,41	0
86	OHX	5	4035	7/7	0.18	1.00	100,100,100,100	0
86	OHX	2	2150	7/7	0.36	0.98	154,154,154,154	0
86	OHX	5	4055	7/7	0.18	0.98	93,93,93,93	0
85	MG	5	3702	1/1	0.19	0.98	60,60,60,60	0
86	OHX	1	4096	7/7	0.22	0.97	141,141,141,141	0
86	OHX	5	4031	7/7	0.19	0.95	93,93,93,93	0
85	MG	5	3601	1/1	0.18	0.95	41,41,41,41	0
86	OHX	1	4097	7/7	0.16	0.95	141,141,141,141	0
86	OHX	5	4193	7/7	0.34	0.94	138,138,138,138	0
86	OHX	1	4045	7/7	0.20	0.93	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	7	208	1/1	0.13	0.93	54,54,54,54	0
86	OHX	2	2075	7/7	0.22	0.91	126,126,126,126	0
85	MG	1	3442	1/1	0.18	0.91	44,44,44,44	0
86	OHX	1	4127	7/7	0.21	0.91	133,133,133,133	0
86	OHX	2	2126	7/7	0.18	0.90	135,135,135,135	0
86	OHX	5	4070	7/7	0.26	0.90	105,105,105,105	0
86	OHX	2	2180	7/7	0.33	0.90	164,164,164,164	0
85	MG	6	1983	1/1	0.31	0.90	46,46,46,46	0
85	MG	5	3755	1/1	0.16	0.89	57,57,57,57	0
85	MG	1	3622	1/1	0.17	0.88	69,69,69,69	0
86	OHX	1	4185	7/7	0.23	0.87	99,99,99,99	0
86	OHX	2	2098	7/7	0.15	0.87	116,116,116,116	0
86	OHX	1	4018	7/7	0.21	0.86	121,121,121,121	0
85	MG	n8	202	1/1	0.19	0.86	35,35,35,35	0
86	OHX	l9	202	7/7	0.22	0.84	121,121,121,121	0
86	OHX	5	4170	7/7	0.20	0.83	139,139,139,139	0
86	OHX	5	3917	7/7	0.15	0.83	61,61,61,61	0
85	MG	M6	201	1/1	0.22	0.81	44,44,44,44	0
85	MG	S6	301	1/1	0.26	0.79	90,90,90,90	0
86	OHX	n3	204	7/7	0.18	0.79	105,105,105,105	0
86	OHX	6	2133	7/7	0.20	0.79	139,139,139,139	0
86	OHX	5	4124	7/7	0.23	0.79	132,132,132,132	0
86	OHX	6	2155	7/7	0.19	0.79	141,141,141,141	0
86	OHX	2	2101	7/7	0.20	0.78	144,144,144,144	0
86	OHX	5	4230	7/7	0.31	0.78	151,151,151,151	0
85	MG	5	3699	1/1	0.18	0.77	33,33,33,33	0
86	OHX	6	2181	7/7	0.17	0.77	143,143,143,143	0
86	OHX	5	4024	7/7	0.17	0.76	108,108,108,108	0
85	MG	L6	201	1/1	0.22	0.76	47,47,47,47	0
85	MG	5	3753	1/1	0.19	0.75	46,46,46,46	0
85	MG	1	3713	1/1	0.17	0.74	37,37,37,37	0
86	OHX	L3	405	7/7	0.43	0.69	153,153,153,153	0
85	MG	1	3642	1/1	0.18	0.69	60,60,60,60	0
86	OHX	5	3903	7/7	0.16	0.67	43,43,43,43	0
86	OHX	2	2165	7/7	0.24	0.66	168,168,168,168	0
86	OHX	6	2109	7/7	0.30	0.65	134,134,134,134	0
85	MG	2	2012	1/1	0.19	0.65	61,61,61,61	0
85	MG	1	3665	1/1	0.18	0.65	45,45,45,45	0
85	MG	1	3435	1/1	0.18	0.65	46,46,46,46	0
85	MG	M9	202	1/1	0.27	0.64	72,72,72,72	0
86	OHX	6	2108	7/7	0.21	0.64	111,111,111,111	0
85	MG	O2	201	1/1	0.22	0.63	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2079	7/7	0.23	0.63	167,167,167,167	0
86	OHX	6	2169	7/7	0.21	0.62	171,171,171,171	0
86	OHX	2	2120	7/7	0.28	0.62	147,147,147,147	0
86	OHX	5	4048	7/7	0.20	0.61	101,101,101,101	0
86	OHX	6	2168	7/7	0.28	0.57	147,147,147,147	0
86	OHX	6	2164	7/7	0.24	0.57	117,117,117,117	0
85	MG	1	3624	1/1	0.18	0.57	38,38,38,38	0
86	OHX	O2	202	7/7	0.21	0.56	94,94,94,94	0
86	OHX	6	2161	7/7	0.19	0.56	107,107,107,107	0
86	OHX	6	2107	7/7	0.16	0.56	116,116,116,116	0
86	OHX	5	4228	7/7	0.32	0.56	138,138,138,138	0
86	OHX	5	4013	7/7	0.19	0.54	100,100,100,100	0
86	OHX	6	2049	7/7	0.20	0.53	74,74,74,74	0
86	OHX	5	4006	7/7	0.17	0.53	100,100,100,100	0
85	MG	2	1998	1/1	0.40	0.53	73,73,73,73	0
85	MG	1	3675	1/1	0.32	0.52	57,57,57,57	0
85	MG	1	3484	1/1	0.24	0.52	52,52,52,52	0
86	OHX	5	4081	7/7	0.18	0.51	121,121,121,121	0
85	MG	5	3448	1/1	0.16	0.51	42,42,42,42	0
86	OHX	l3	405	7/7	0.18	0.51	113,113,113,113	0
85	MG	5	3746	1/1	0.18	0.51	60,60,60,60	0
86	OHX	1	3985	7/7	0.26	0.50	104,104,104,104	0
86	OHX	2	2130	7/7	0.20	0.50	113,113,113,113	0
85	MG	6	1970	1/1	0.19	0.50	60,60,60,60	0
86	OHX	2	2024	7/7	0.20	0.49	90,90,90,90	0
86	OHX	1	4176	7/7	0.17	0.49	100,100,100,100	0
86	OHX	2	2085	7/7	0.15	0.49	111,111,111,111	0
85	MG	5	3619	1/1	0.21	0.49	43,43,43,43	0
86	OHX	1	3973	7/7	0.23	0.47	110,110,110,110	0
85	MG	1	3805	1/1	0.26	0.46	60,60,60,60	0
85	MG	5	3415	1/1	0.19	0.45	51,51,51,51	0
85	MG	1	3862	1/1	0.17	0.45	115,115,115,115	0
86	OHX	5	4039	7/7	0.15	0.45	115,115,115,115	0
85	MG	1	3737	1/1	0.15	0.45	36,36,36,36	0
86	OHX	1	4214	7/7	0.28	0.45	160,160,160,160	0
86	OHX	2	2094	7/7	0.18	0.44	146,146,146,146	0
86	OHX	1	4135	7/7	0.40	0.44	154,154,154,154	0
86	OHX	1	4117	7/7	0.23	0.44	163,163,163,163	0
85	MG	5	3782	1/1	0.22	0.43	77,77,77,77	0
86	OHX	5	4131	7/7	0.32	0.42	144,144,144,144	0
86	OHX	2	2161	7/7	0.39	0.42	144,144,144,144	0
86	OHX	5	4185	7/7	0.34	0.42	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3969	7/7	0.17	0.41	97,97,97,97	0
85	MG	s6	301	1/1	0.27	0.41	75,75,75,75	0
85	MG	1	3793	1/1	0.19	0.41	81,81,81,81	0
86	OHX	6	2145	7/7	0.28	0.40	138,138,138,138	0
85	MG	2	2003	1/1	0.29	0.40	66,66,66,66	0
86	OHX	1	4022	7/7	0.19	0.39	128,128,128,128	0
86	OHX	2	2151	7/7	0.21	0.39	177,177,177,177	0
85	MG	4	214	1/1	0.18	0.37	37,37,37,37	0
86	OHX	5	4067	7/7	0.17	0.37	108,108,108,108	0
86	OHX	1	4034	7/7	0.22	0.37	103,103,103,103	0
85	MG	5	3430	1/1	0.22	0.36	29,29,29,29	0
86	OHX	S8	302	7/7	0.28	0.36	157,157,157,157	0
86	OHX	1	4039	7/7	0.24	0.33	124,124,124,124	0
86	OHX	4	231	7/7	0.13	0.33	114,114,114,114	0
86	OHX	5	4100	7/7	0.16	0.32	130,130,130,130	0
86	OHX	1	4054	7/7	0.20	0.32	109,109,109,109	0
85	MG	1	3837	1/1	0.44	0.31	49,49,49,49	0
85	MG	M9	201	1/1	0.16	0.31	61,61,61,61	0
85	MG	4	223	1/1	0.16	0.31	46,46,46,46	0
85	MG	6	2018	1/1	0.14	0.30	68,68,68,68	0
86	OHX	6	2111	7/7	0.18	0.30	115,115,115,115	0
85	MG	1	3719	1/1	0.21	0.30	47,47,47,47	0
86	OHX	6	2093	7/7	0.18	0.29	111,111,111,111	0
85	MG	5	3431	1/1	0.24	0.29	74,74,74,74	0
86	OHX	5	3929	7/7	0.17	0.29	70,70,70,70	0
86	OHX	6	2144	7/7	0.35	0.29	127,127,127,127	0
86	OHX	2	2050	7/7	0.15	0.28	104,104,104,104	0
86	OHX	1	4105	7/7	0.26	0.27	136,136,136,136	0
86	OHX	1	3891	7/7	0.15	0.27	79,79,79,79	0
85	MG	5	3706	1/1	0.22	0.26	39,39,39,39	0
85	MG	1	3635	1/1	0.25	0.26	56,56,56,56	0
86	OHX	1	3957	7/7	0.17	0.26	99,99,99,99	0
86	OHX	1	3952	7/7	0.12	0.26	119,119,119,119	0
85	MG	5	3824	1/1	0.16	0.25	64,64,64,64	0
85	MG	M3	202	1/1	0.36	0.25	93,93,93,93	0
86	OHX	2	2177	7/7	0.26	0.25	168,168,168,168	0
86	OHX	6	2114	7/7	0.19	0.25	115,115,115,115	0
85	MG	5	3408	1/1	0.17	0.25	26,26,26,26	0
85	MG	5	3438	1/1	0.19	0.23	52,52,52,52	0
85	MG	1	3836	1/1	0.18	0.22	43,43,43,43	0
86	OHX	1	4077	7/7	0.20	0.22	119,119,119,119	0
86	OHX	5	4065	7/7	0.19	0.21	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4169	7/7	0.33	0.18	201,201,201,201	0
86	OHX	1	4138	7/7	0.19	0.18	101,101,101,101	0
85	MG	5	3771	1/1	0.21	0.17	66,66,66,66	0
85	MG	M1	201	1/1	0.19	0.17	79,79,79,79	0
87	ZN	q2	501	1/1	0.31	0.16	82,82,82,82	0
86	OHX	1	4201	7/7	0.26	0.15	128,128,128,128	0
86	OHX	1	4047	7/7	0.21	0.15	106,106,106,106	0
86	OHX	5	4007	7/7	0.17	0.15	99,99,99,99	0
86	OHX	l5	303	7/7	0.29	0.15	134,134,134,134	0
85	MG	1	3819	1/1	0.34	0.13	119,119,119,119	0
85	MG	1	3813	1/1	0.19	0.12	51,51,51,51	0
86	OHX	1	4040	7/7	0.14	0.11	140,140,140,140	0
86	OHX	5	3910	7/7	0.17	0.10	58,58,58,58	0
86	OHX	2	2088	7/7	0.18	0.09	108,108,108,108	0
86	OHX	1	3986	7/7	0.15	0.08	95,95,95,95	0
86	OHX	1	4087	7/7	0.24	0.08	138,138,138,138	0
86	OHX	2	2144	7/7	0.34	0.08	168,168,168,168	0
85	MG	5	3716	1/1	0.18	0.08	63,63,63,63	0
85	MG	6	2007	1/1	0.18	0.08	58,58,58,58	0
86	OHX	5	4126	7/7	0.18	0.07	140,140,140,140	0
86	OHX	1	4165	7/7	0.21	0.07	134,134,134,134	0
86	OHX	1	4107	7/7	0.23	0.07	119,119,119,119	0
86	OHX	2	2155	7/7	0.20	0.07	143,143,143,143	0
85	MG	5	3616	1/1	0.14	0.07	38,38,38,38	0
85	MG	1	3468	1/1	0.15	0.06	48,48,48,48	0
85	MG	2	1987	1/1	0.31	0.06	80,80,80,80	0
86	OHX	5	3901	7/7	0.20	0.05	49,49,49,49	0
86	OHX	5	4021	7/7	0.16	0.04	99,99,99,99	0
86	OHX	5	4197	7/7	0.26	0.01	164,164,164,164	0
85	MG	1	3699	1/1	0.14	-0.00	46,46,46,46	0
86	OHX	4	233	7/7	0.14	-0.01	129,129,129,129	0
85	MG	1	3711	1/1	0.15	-0.02	51,51,51,51	0
86	OHX	5	4056	7/7	0.16	-0.03	90,90,90,90	0
86	OHX	6	2139	7/7	0.27	-0.03	118,118,118,118	0
85	MG	M1	202	1/1	0.18	-0.04	75,75,75,75	0
86	OHX	1	4013	7/7	0.16	-0.04	125,125,125,125	0
86	OHX	1	4056	7/7	0.21	-0.05	139,139,139,139	0
85	MG	1	3490	1/1	0.30	-0.06	52,52,52,52	0
85	MG	5	3600	1/1	0.16	-0.07	39,39,39,39	0
86	OHX	m1	203	7/7	0.30	-0.07	142,142,142,142	0
86	OHX	5	4245	7/7	0.34	-0.08	100,100,100,100	0
86	OHX	2	2053	7/7	0.17	-0.08	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	3429	1/1	0.24	-0.08	50,50,50,50	0
86	OHX	l3	406	7/7	0.24	-0.09	131,131,131,131	0
85	MG	sM	302	1/1	0.22	-0.10	43,43,43,43	0
86	OHX	5	4016	7/7	0.19	-0.10	95,95,95,95	0
85	MG	5	3856	1/1	0.18	-0.11	71,71,71,71	0
86	OHX	6	2148	7/7	0.20	-0.12	129,129,129,129	0
86	OHX	2	2080	7/7	0.16	-0.12	132,132,132,132	0
86	OHX	c3	201	7/7	0.27	-0.12	146,146,146,146	0
86	OHX	1	3884	7/7	0.16	-0.13	67,67,67,67	0
86	OHX	1	4033	7/7	0.16	-0.13	125,125,125,125	0
86	OHX	1	4027	7/7	0.19	-0.13	143,143,143,143	0
86	OHX	1	4059	7/7	0.17	-0.14	144,144,144,144	0
86	OHX	2	2082	7/7	0.15	-0.14	130,130,130,130	0
86	OHX	1	3975	7/7	0.15	-0.14	103,103,103,103	0
86	OHX	1	3959	7/7	0.18	-0.14	92,92,92,92	0
86	OHX	2	2167	7/7	0.20	-0.15	153,153,153,153	0
85	MG	1	3824	1/1	0.21	-0.16	36,36,36,36	0
86	OHX	2	2123	7/7	0.25	-0.16	148,148,148,148	0
86	OHX	1	3897	7/7	0.17	-0.17	76,76,76,76	0
86	OHX	s8	303	7/7	0.40	-0.19	156,156,156,156	0
86	OHX	5	3926	7/7	0.15	-0.19	70,70,70,70	0
86	OHX	5	3916	7/7	0.14	-0.20	65,65,65,65	0
86	OHX	1	4051	7/7	0.15	-0.20	116,116,116,116	0
86	OHX	1	3871	7/7	0.21	-0.21	59,59,59,59	0
86	OHX	1	4062	7/7	0.21	-0.21	166,166,166,166	0
86	OHX	5	4157	7/7	0.17	-0.21	112,112,112,112	0
85	MG	c9	202	1/1	0.29	-0.22	66,66,66,66	0
86	OHX	6	2056	7/7	0.13	-0.22	85,85,85,85	0
86	OHX	5	4066	7/7	0.16	-0.23	142,142,142,142	0
86	OHX	1	3979	7/7	0.17	-0.25	91,91,91,91	0
86	OHX	8	216	7/7	0.15	-0.26	57,57,57,57	0
86	OHX	5	4003	7/7	0.20	-0.26	94,94,94,94	0
86	OHX	c5	201	7/7	0.24	-0.26	155,155,155,155	0
86	OHX	1	4148	7/7	0.24	-0.26	147,147,147,147	0
86	OHX	1	4010	7/7	0.18	-0.27	103,103,103,103	0
86	OHX	2	2092	7/7	0.19	-0.29	147,147,147,147	0
86	OHX	3	217	7/7	0.15	-0.30	118,118,118,118	0
85	MG	2	2002	1/1	0.20	-0.30	83,83,83,83	0
86	OHX	m0	303	7/7	0.27	-0.30	120,120,120,120	0
86	OHX	4	229	7/7	0.16	-0.30	118,118,118,118	0
86	OHX	3	215	7/7	0.16	-0.31	107,107,107,107	0
86	OHX	5	3976	7/7	0.16	-0.31	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3902	7/7	0.16	-0.31	43,43,43,43	0
86	OHX	1	4094	7/7	0.23	-0.32	151,151,151,151	0
86	OHX	4	232	7/7	0.12	-0.33	142,142,142,142	0
86	OHX	sR	401	7/7	0.22	-0.33	156,156,156,156	0
86	OHX	5	4037	7/7	0.16	-0.33	119,119,119,119	0
86	OHX	1	3991	7/7	0.16	-0.34	101,101,101,101	0
85	MG	1	3416	1/1	0.16	-0.34	49,49,49,49	0
86	OHX	6	2097	7/7	0.17	-0.36	127,127,127,127	0
85	MG	5	3704	1/1	0.12	-0.36	51,51,51,51	0
86	OHX	3	219	7/7	0.15	-0.36	124,124,124,124	0
86	OHX	1	3921	7/7	0.15	-0.37	114,114,114,114	0
86	OHX	5	4097	7/7	0.16	-0.37	127,127,127,127	0
86	OHX	2	2114	7/7	0.18	-0.38	120,120,120,120	0
86	OHX	1	4014	7/7	0.16	-0.38	121,121,121,121	0
86	OHX	2	2056	7/7	0.18	-0.39	140,140,140,140	0
86	OHX	2	2071	7/7	0.20	-0.40	117,117,117,117	0
86	OHX	1	3881	7/7	0.15	-0.40	65,65,65,65	0
86	OHX	5	3968	7/7	0.17	-0.41	96,96,96,96	0
86	OHX	5	3909	7/7	0.14	-0.41	62,62,62,62	0
86	OHX	1	3971	7/7	0.13	-0.41	102,102,102,102	0
86	OHX	5	4040	7/7	0.13	-0.42	126,126,126,126	0
86	OHX	5	3988	7/7	0.15	-0.44	80,80,80,80	0
86	OHX	6	2070	7/7	0.14	-0.44	92,92,92,92	0
86	OHX	5	3996	7/7	0.18	-0.44	128,128,128,128	0
86	OHX	5	3905	7/7	0.17	-0.46	54,54,54,54	0
86	OHX	1	3989	7/7	0.15	-0.46	109,109,109,109	0
86	OHX	1	3867	7/7	0.16	-0.47	44,44,44,44	0
86	OHX	2	2064	7/7	0.18	-0.48	107,107,107,107	0
86	OHX	5	4014	7/7	0.17	-0.48	103,103,103,103	0
86	OHX	5	4029	7/7	0.15	-0.48	98,98,98,98	0
86	OHX	2	2117	7/7	0.14	-0.50	152,152,152,152	0
85	MG	5	3760	1/1	0.18	-0.52	49,49,49,49	0
86	OHX	1	4026	7/7	0.15	-0.52	135,135,135,135	0
86	OHX	1	4035	7/7	0.19	-0.52	128,128,128,128	0
86	OHX	2	2054	7/7	0.15	-0.52	112,112,112,112	0
85	MG	s8	302	1/1	0.15	-0.52	50,50,50,50	0
86	OHX	1	3876	7/7	0.14	-0.53	59,59,59,59	0
86	OHX	2	2066	7/7	0.15	-0.53	138,138,138,138	0
85	MG	5	3485	1/1	0.17	-0.53	68,68,68,68	0
86	OHX	1	4025	7/7	0.14	-0.54	113,113,113,113	0
85	MG	6	1972	1/1	0.21	-0.54	70,70,70,70	0
86	OHX	2	2022	7/7	0.14	-0.54	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	5	3958	7/7	0.18	-0.55	91,91,91,91	0
86	OHX	6	2066	7/7	0.13	-0.55	94,94,94,94	0
85	MG	m7	203	1/1	0.13	-0.56	41,41,41,41	0
86	OHX	6	2131	7/7	0.15	-0.56	134,134,134,134	0
86	OHX	1	4052	7/7	0.14	-0.56	134,134,134,134	0
86	OHX	1	3869	7/7	0.14	-0.57	46,46,46,46	0
86	OHX	5	3977	7/7	0.11	-0.57	103,103,103,103	0
86	OHX	o2	201	7/7	0.17	-0.57	95,95,95,95	0
86	OHX	6	2156	7/7	0.17	-0.57	131,131,131,131	0
85	MG	5	3404	1/1	0.16	-0.58	45,45,45,45	0
85	MG	1	3809	1/1	0.48	-0.59	193,193,193,193	0
86	OHX	1	4057	7/7	0.16	-0.59	128,128,128,128	0
86	OHX	5	4027	7/7	0.15	-0.59	103,103,103,103	0
86	OHX	6	2157	7/7	0.16	-0.59	108,108,108,108	0
87	ZN	Q2	501	1/1	0.20	-0.59	82,82,82,82	0
85	MG	3	203	1/1	0.17	-0.60	96,96,96,96	0
86	OHX	2	2059	7/7	0.15	-0.60	101,101,101,101	0
86	OHX	2	2057	7/7	0.14	-0.60	108,108,108,108	0
86	OHX	1	3870	7/7	0.14	-0.60	54,54,54,54	0
86	OHX	8	225	7/7	0.20	-0.62	119,119,119,119	0
86	OHX	6	2048	7/7	0.15	-0.63	56,56,56,56	0
87	ZN	Q3	501	1/1	0.11	-0.63	60,60,60,60	0
85	MG	5	3650	1/1	0.15	-0.63	89,89,89,89	0
85	MG	D3	201	1/1	0.16	-0.63	57,57,57,57	0
86	OHX	8	223	7/7	0.11	-0.64	118,118,118,118	0
86	OHX	5	4089	7/7	0.18	-0.65	108,108,108,108	0
86	OHX	1	3968	7/7	0.12	-0.65	116,116,116,116	0
86	OHX	2	2081	7/7	0.13	-0.65	147,147,147,147	0
86	OHX	2	2063	7/7	0.16	-0.67	110,110,110,110	0
86	OHX	1	4088	7/7	0.15	-0.68	124,124,124,124	0
85	MG	N8	203	1/1	0.19	-0.69	48,48,48,48	0
85	MG	1	3779	1/1	0.14	-0.69	75,75,75,75	0
85	MG	1	3421	1/1	0.24	-0.69	74,74,74,74	0
86	OHX	6	2121	7/7	0.18	-0.69	113,113,113,113	0
86	OHX	2	2141	7/7	0.21	-0.69	160,160,160,160	0
86	OHX	n9	101	7/7	0.13	-0.70	66,66,66,66	0
86	OHX	5	3983	7/7	0.15	-0.72	103,103,103,103	0
86	OHX	1	4015	7/7	0.14	-0.72	125,125,125,125	0
86	OHX	5	3941	7/7	0.13	-0.73	81,81,81,81	0
85	MG	7	209	1/1	0.12	-0.74	65,65,65,65	0
86	OHX	O7	105	7/7	0.16	-0.74	94,94,94,94	0
85	MG	5	3615	1/1	0.14	-0.74	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4028	7/7	0.15	-0.75	107,107,107,107	0
85	MG	5	3642	1/1	0.13	-0.76	38,38,38,38	0
86	OHX	1	4128	7/7	0.15	-0.77	144,144,144,144	0
85	MG	6	1997	1/1	0.15	-0.77	74,74,74,74	0
86	OHX	1	3981	7/7	0.11	-0.78	104,104,104,104	0
85	MG	5	3751	1/1	0.17	-0.78	49,49,49,49	0
87	ZN	d6	101	1/1	0.14	-0.78	60,60,60,60	0
86	OHX	1	4021	7/7	0.15	-0.80	114,114,114,114	0
86	OHX	5	3935	7/7	0.14	-0.80	89,89,89,89	0
85	MG	5	3811	1/1	0.21	-0.80	67,67,67,67	0
86	OHX	1	3960	7/7	0.16	-0.80	78,78,78,78	0
86	OHX	2	2023	7/7	0.14	-0.80	83,83,83,83	0
86	OHX	1	3894	7/7	0.12	-0.81	74,74,74,74	0
86	OHX	O7	104	7/7	0.12	-0.82	94,94,94,94	0
86	OHX	6	2069	7/7	0.14	-0.82	89,89,89,89	0
86	OHX	5	4038	7/7	0.16	-0.82	127,127,127,127	0
86	OHX	1	4044	7/7	0.16	-0.83	126,126,126,126	0
86	OHX	2	2077	7/7	0.17	-0.83	126,126,126,126	0
86	OHX	1	3875	7/7	0.14	-0.83	61,61,61,61	0
86	OHX	2	2138	7/7	0.17	-0.84	139,139,139,139	0
85	MG	5	3723	1/1	0.15	-0.85	40,40,40,40	0
86	OHX	L3	404	7/7	0.16	-0.87	106,106,106,106	0
87	ZN	q3	501	1/1	0.11	-0.87	63,63,63,63	0
86	OHX	1	4182	7/7	0.25	-0.87	216,216,216,216	0
86	OHX	8	224	7/7	0.14	-0.87	138,138,138,138	0
85	MG	6	2028	1/1	0.13	-0.88	86,86,86,86	0
86	OHX	5	4060	7/7	0.13	-0.89	136,136,136,136	0
86	OHX	6	2054	7/7	0.13	-0.89	75,75,75,75	0
85	MG	5	3833	1/1	0.16	-0.90	71,71,71,71	0
87	ZN	Q0	500	1/1	0.13	-0.91	47,47,47,47	0
86	OHX	1	3997	7/7	0.16	-0.92	96,96,96,96	0
86	OHX	5	4105	7/7	0.15	-0.94	143,143,143,143	0
86	OHX	2	2124	7/7	0.17	-0.94	136,136,136,136	0
86	OHX	5	4116	7/7	0.17	-0.94	108,108,108,108	0
86	OHX	6	2079	7/7	0.12	-0.95	110,110,110,110	0
86	OHX	1	3940	7/7	0.09	-0.95	113,113,113,113	0
85	MG	l5	301	1/1	0.13	-0.96	61,61,61,61	0
86	OHX	1	3888	7/7	0.16	-0.96	67,67,67,67	0
86	OHX	7	223	7/7	0.11	-0.96	101,101,101,101	0
85	MG	1	3619	1/1	0.15	-0.96	55,55,55,55	0
86	OHX	1	3992	7/7	0.17	-0.97	105,105,105,105	0
85	MG	L4	401	1/1	0.16	-0.97	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3426	1/1	0.16	-0.97	29,29,29,29	0
86	OHX	5	4080	7/7	0.15	-0.97	91,91,91,91	0
86	OHX	5	4033	7/7	0.14	-0.98	129,129,129,129	0
85	MG	1	3728	1/1	0.14	-0.98	62,62,62,62	0
86	OHX	1	3995	7/7	0.15	-0.98	127,127,127,127	0
86	OHX	m5	301	7/7	0.15	-0.99	126,126,126,126	0
86	OHX	5	4076	7/7	0.16	-1.00	108,108,108,108	0
85	MG	1	3618	1/1	0.11	-1.01	62,62,62,62	0
85	MG	5	3817	1/1	0.10	-1.02	44,44,44,44	0
86	OHX	5	4083	7/7	0.15	-1.02	98,98,98,98	0
85	MG	M5	301	1/1	0.14	-1.02	45,45,45,45	0
85	MG	6	1998	1/1	0.15	-1.03	52,52,52,52	0
87	ZN	q0	201	1/1	0.13	-1.03	32,32,32,32	0
85	MG	1	3423	1/1	0.13	-1.04	32,32,32,32	0
85	MG	n8	205	1/1	0.14	-1.05	36,36,36,36	0
86	OHX	2	2032	7/7	0.14	-1.05	111,111,111,111	0
86	OHX	1	3872	7/7	0.12	-1.06	53,53,53,53	0
86	OHX	2	2097	7/7	0.10	-1.09	157,157,157,157	0
86	OHX	1	3958	7/7	0.09	-1.09	99,99,99,99	0
86	OHX	2	2113	7/7	0.15	-1.09	154,154,154,154	0
86	OHX	5	4068	7/7	0.13	-1.10	112,112,112,112	0
86	OHX	4	227	7/7	0.14	-1.11	98,98,98,98	0
87	ZN	d9	101	1/1	0.12	-1.11	82,82,82,82	0
85	MG	1	3480	1/1	0.15	-1.11	80,80,80,80	0
86	OHX	5	3978	7/7	0.13	-1.12	93,93,93,93	0
86	OHX	1	3925	7/7	0.09	-1.13	85,85,85,85	0
85	MG	C8	201	1/1	0.14	-1.14	106,106,106,106	0
85	MG	5	3648	1/1	0.16	-1.14	46,46,46,46	0
85	MG	5	3703	1/1	0.16	-1.14	69,69,69,69	0
85	MG	N8	206	1/1	0.14	-1.14	34,34,34,34	0
85	MG	5	3712	1/1	0.11	-1.15	68,68,68,68	0
86	OHX	1	3898	7/7	0.12	-1.15	81,81,81,81	0
86	OHX	5	4244	7/7	0.24	-1.15	207,207,207,207	0
86	OHX	8	218	7/7	0.06	-1.16	110,110,110,110	0
85	MG	M0	302	1/1	0.19	-1.17	46,46,46,46	0
86	OHX	1	4005	7/7	0.17	-1.17	97,97,97,97	0
86	OHX	c8	201	7/7	0.14	-1.19	142,142,142,142	0
86	OHX	1	3936	7/7	0.12	-1.19	100,100,100,100	0
85	MG	5	3850	1/1	0.16	-1.19	54,54,54,54	0
86	OHX	6	2055	7/7	0.16	-1.20	77,77,77,77	0
86	OHX	2	2106	7/7	0.12	-1.20	111,111,111,111	0
86	OHX	5	4106	7/7	0.12	-1.21	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3990	7/7	0.14	-1.21	114,114,114,114	0
85	MG	5	3823	1/1	0.14	-1.21	90,90,90,90	0
86	OHX	2	2132	7/7	0.14	-1.22	150,150,150,150	0
86	OHX	M5	303	7/7	0.18	-1.22	113,113,113,113	0
86	OHX	5	4173	7/7	0.21	-1.22	180,180,180,180	0
86	OHX	2	2062	7/7	0.12	-1.23	129,129,129,129	0
85	MG	1	3773	1/1	0.14	-1.24	66,66,66,66	0
85	MG	5	3651	1/1	0.18	-1.25	71,71,71,71	0
86	OHX	2	2030	7/7	0.11	-1.26	114,114,114,114	0
86	OHX	8	219	7/7	0.14	-1.27	105,105,105,105	0
86	OHX	6	2050	7/7	0.14	-1.28	66,66,66,66	0
86	OHX	5	3934	7/7	0.15	-1.29	73,73,73,73	0
85	MG	5	3749	1/1	0.08	-1.29	50,50,50,50	0
86	OHX	2	2109	7/7	0.08	-1.29	124,124,124,124	0
86	OHX	8	220	7/7	0.10	-1.29	126,126,126,126	0
85	MG	sM	301	1/1	0.12	-1.31	44,44,44,44	0
86	OHX	6	2152	7/7	0.18	-1.31	134,134,134,134	0
86	OHX	1	4092	7/7	0.14	-1.32	82,82,82,82	0
85	MG	5	3768	1/1	0.10	-1.32	47,47,47,47	0
86	OHX	N9	101	7/7	0.13	-1.32	63,63,63,63	0
87	ZN	D6	500	1/1	0.10	-1.33	85,85,85,85	0
86	OHX	1	3889	7/7	0.14	-1.33	78,78,78,78	0
85	MG	5	3687	1/1	0.11	-1.34	44,44,44,44	0
86	OHX	1	4109	7/7	0.14	-1.35	138,138,138,138	0
86	OHX	6	2166	7/7	0.25	-1.35	179,179,179,179	0
86	OHX	1	4016	7/7	0.10	-1.35	133,133,133,133	0
86	OHX	5	4001	7/7	0.10	-1.36	107,107,107,107	0
86	OHX	1	4038	7/7	0.08	-1.36	146,146,146,146	0
86	OHX	6	2204	7/7	0.18	-1.36	185,185,185,185	0
85	MG	1	3810	1/1	0.13	-1.38	49,49,49,49	0
86	OHX	5	4069	7/7	0.11	-1.38	122,122,122,122	0
86	OHX	5	4241	7/7	0.17	-1.40	139,139,139,139	0
86	OHX	6	2132	7/7	0.17	-1.41	119,119,119,119	0
86	OHX	5	4042	7/7	0.13	-1.42	117,117,117,117	0
86	OHX	6	2100	7/7	0.11	-1.42	117,117,117,117	0
86	OHX	5	4008	7/7	0.14	-1.42	109,109,109,109	0
86	OHX	l5	302	7/7	0.10	-1.42	128,128,128,128	0
86	OHX	2	2072	7/7	0.17	-1.43	142,142,142,142	0
86	OHX	6	2123	7/7	0.09	-1.44	140,140,140,140	0
85	MG	1	3559	1/1	0.13	-1.44	52,52,52,52	0
86	OHX	4	225	7/7	0.13	-1.44	64,64,64,64	0
86	OHX	6	2137	7/7	0.14	-1.45	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	o7	503	7/7	0.12	-1.46	99,99,99,99	0
85	MG	1	3666	1/1	0.10	-1.47	60,60,60,60	0
86	OHX	2	2036	7/7	0.11	-1.47	128,128,128,128	0
86	OHX	5	4019	7/7	0.15	-1.48	145,145,145,145	0
86	OHX	5	4134	7/7	0.19	-1.48	177,177,177,177	0
86	OHX	m0	302	7/7	0.08	-1.48	117,117,117,117	0
86	OHX	5	4043	7/7	0.08	-1.49	151,151,151,151	0
86	OHX	5	3906	7/7	0.13	-1.49	54,54,54,54	0
85	MG	1	3437	1/1	0.15	-1.49	40,40,40,40	0
86	OHX	5	4009	7/7	0.14	-1.49	118,118,118,118	0
85	MG	1	3856	1/1	0.10	-1.49	69,69,69,69	0
85	MG	5	3512	1/1	0.12	-1.50	29,29,29,29	0
87	ZN	o7	501	1/1	0.11	-1.50	43,43,43,43	0
87	ZN	O7	101	1/1	0.09	-1.51	36,36,36,36	0
86	OHX	5	4032	7/7	0.11	-1.51	110,110,110,110	0
86	OHX	1	3948	7/7	0.14	-1.51	85,85,85,85	0
86	OHX	5	4183	7/7	0.24	-1.53	148,148,148,148	0
85	MG	5	3819	1/1	0.12	-1.54	63,63,63,63	0
86	OHX	5	3959	7/7	0.12	-1.54	84,84,84,84	0
86	OHX	1	3965	7/7	0.15	-1.54	94,94,94,94	0
86	OHX	1	3933	7/7	0.12	-1.54	101,101,101,101	0
86	OHX	6	2061	7/7	0.11	-1.55	96,96,96,96	0
86	OHX	2	2035	7/7	0.06	-1.55	92,92,92,92	0
87	ZN	e1	501	1/1	0.16	-1.57	172,172,172,172	0
86	OHX	1	4023	7/7	0.15	-1.57	108,108,108,108	0
86	OHX	5	3908	7/7	0.16	-1.57	56,56,56,56	0
86	OHX	7	217	7/7	0.11	-1.61	85,85,85,85	0
87	ZN	D9	101	1/1	0.08	-1.62	84,84,84,84	0
86	OHX	o3	203	7/7	0.11	-1.63	98,98,98,98	0
86	OHX	1	3909	7/7	0.11	-1.63	90,90,90,90	0
86	OHX	6	2102	7/7	0.14	-1.63	169,169,169,169	0
86	OHX	1	3916	7/7	0.09	-1.63	99,99,99,99	0
86	OHX	1	3900	7/7	0.16	-1.64	89,89,89,89	0
86	OHX	2	2039	7/7	0.13	-1.64	102,102,102,102	0
86	OHX	6	2116	7/7	0.14	-1.64	123,123,123,123	0
86	OHX	6	2092	7/7	0.12	-1.65	111,111,111,111	0
86	OHX	5	3982	7/7	0.11	-1.66	88,88,88,88	0
86	OHX	SR	401	7/7	0.12	-1.66	164,164,164,164	0
85	MG	5	3407	1/1	0.11	-1.67	37,37,37,37	0
86	OHX	1	4036	7/7	0.11	-1.68	94,94,94,94	0
86	OHX	C5	201	7/7	0.16	-1.68	155,155,155,155	0
86	OHX	1	3988	7/7	0.17	-1.69	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2027	7/7	0.12	-1.70	99,99,99,99	0
86	OHX	C3	201	7/7	0.15	-1.71	151,151,151,151	0
86	OHX	Q2	502	7/7	0.10	-1.71	77,77,77,77	0
85	MG	L3	401	1/1	0.14	-1.72	70,70,70,70	0
86	OHX	1	3949	7/7	0.12	-1.72	111,111,111,111	0
86	OHX	5	4085	7/7	0.14	-1.72	134,134,134,134	0
86	OHX	5	3991	7/7	0.09	-1.73	116,116,116,116	0
86	OHX	5	3946	7/7	0.12	-1.73	79,79,79,79	0
86	OHX	2	2042	7/7	0.08	-1.74	114,114,114,114	0
86	OHX	5	3939	7/7	0.07	-1.74	68,68,68,68	0
85	MG	5	3834	1/1	0.13	-1.74	40,40,40,40	0
86	OHX	1	3908	7/7	0.12	-1.75	84,84,84,84	0
86	OHX	6	2052	7/7	0.15	-1.77	74,74,74,74	0
86	OHX	2	2034	7/7	0.14	-1.78	100,100,100,100	0
85	MG	5	3628	1/1	0.17	-1.78	52,52,52,52	0
86	OHX	1	3887	7/7	0.12	-1.80	70,70,70,70	0
85	MG	1	3627	1/1	0.25	-1.80	77,77,77,77	0
86	OHX	5	4132	7/7	0.11	-1.83	133,133,133,133	0
86	OHX	6	2073	7/7	0.10	-1.83	104,104,104,104	0
85	MG	5	3788	1/1	0.11	-1.83	45,45,45,45	0
86	OHX	2	2076	7/7	0.13	-1.84	118,118,118,118	0
86	OHX	7	224	7/7	0.10	-1.84	127,127,127,127	0
86	OHX	5	4062	7/7	0.09	-1.85	134,134,134,134	0
85	MG	1	3740	1/1	0.11	-1.85	67,67,67,67	0
86	OHX	5	3913	7/7	0.13	-1.86	55,55,55,55	0
86	OHX	1	3924	7/7	0.08	-1.86	85,85,85,85	0
86	OHX	5	4217	7/7	0.18	-1.88	185,185,185,185	0
86	OHX	6	2053	7/7	0.12	-1.88	70,70,70,70	0
86	OHX	1	3934	7/7	0.07	-1.89	99,99,99,99	0
86	OHX	1	3970	7/7	0.09	-1.91	125,125,125,125	0
86	OHX	C8	202	7/7	0.08	-1.91	121,121,121,121	0
86	OHX	2	2067	7/7	0.18	-1.92	153,153,153,153	0
86	OHX	5	3973	7/7	0.10	-1.94	96,96,96,96	0
86	OHX	1	3904	7/7	0.13	-1.94	85,85,85,85	0
86	OHX	1	4006	7/7	0.13	-1.94	116,116,116,116	0
86	OHX	6	2118	7/7	0.13	-1.95	132,132,132,132	0
86	OHX	1	4196	7/7	0.10	-1.95	168,168,168,168	0
86	OHX	2	2070	7/7	0.12	-1.96	127,127,127,127	0
86	OHX	1	3927	7/7	0.10	-1.96	109,109,109,109	0
86	OHX	1	3868	7/7	0.13	-1.96	50,50,50,50	0
86	OHX	5	3969	7/7	0.11	-1.96	101,101,101,101	0
86	OHX	5	3990	7/7	0.08	-1.97	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	ZN	E1	501	1/1	0.04	-1.98	122,122,122,122	0
86	OHX	6	2060	7/7	0.11	-1.99	89,89,89,89	0
85	MG	2	1996	1/1	0.16	-2.00	83,83,83,83	0
86	OHX	7	219	7/7	0.10	-2.00	98,98,98,98	0
85	MG	1	3749	1/1	0.14	-2.02	38,38,38,38	0
86	OHX	7	222	7/7	0.08	-2.02	101,101,101,101	0
86	OHX	2	2029	7/7	0.12	-2.02	98,98,98,98	0
85	MG	5	3790	1/1	0.14	-2.03	55,55,55,55	0
86	OHX	5	3942	7/7	0.08	-2.03	86,86,86,86	0
86	OHX	1	3917	7/7	0.10	-2.05	88,88,88,88	0
86	OHX	13	404	7/7	0.10	-2.07	95,95,95,95	0
86	OHX	5	3961	7/7	0.10	-2.07	88,88,88,88	0
86	OHX	6	2106	7/7	0.12	-2.08	118,118,118,118	0
86	OHX	1	4064	7/7	0.11	-2.08	147,147,147,147	0
86	OHX	1	3998	7/7	0.09	-2.08	125,125,125,125	0
86	OHX	5	3993	7/7	0.11	-2.08	99,99,99,99	0
86	OHX	1	3929	7/7	0.14	-2.08	99,99,99,99	0
86	OHX	1	3901	7/7	0.10	-2.09	81,81,81,81	0
86	OHX	6	2147	7/7	0.11	-2.09	129,129,129,129	0
86	OHX	6	2113	7/7	0.11	-2.09	124,124,124,124	0
86	OHX	2	2028	7/7	0.09	-2.09	106,106,106,106	0
86	OHX	2	2047	7/7	0.09	-2.09	115,115,115,115	0
86	OHX	5	3970	7/7	0.12	-2.13	93,93,93,93	0
86	OHX	4	224	7/7	0.14	-2.14	55,55,55,55	0
85	MG	5	3721	1/1	0.12	-2.14	54,54,54,54	0
86	OHX	4	226	7/7	0.07	-2.14	82,82,82,82	0
86	OHX	2	2026	7/7	0.11	-2.14	78,78,78,78	0
85	MG	1	3522	1/1	0.11	-2.15	33,33,33,33	0
85	MG	N5	201	1/1	0.14	-2.15	68,68,68,68	0
86	OHX	2	2046	7/7	0.05	-2.16	129,129,129,129	0
86	OHX	5	4052	7/7	0.10	-2.17	128,128,128,128	0
85	MG	5	3769	1/1	0.22	-2.17	98,98,98,98	0
86	OHX	1	3886	7/7	0.10	-2.17	73,73,73,73	0
86	OHX	1	4043	7/7	0.16	-2.17	105,105,105,105	0
86	OHX	5	3915	7/7	0.10	-2.19	62,62,62,62	0
86	OHX	1	3880	7/7	0.09	-2.19	65,65,65,65	0
86	OHX	5	3920	7/7	0.13	-2.19	62,62,62,62	0
86	OHX	5	3933	7/7	0.11	-2.20	62,62,62,62	0
86	OHX	1	3877	7/7	0.13	-2.22	65,65,65,65	0
85	MG	6	2008	1/1	0.12	-2.22	56,56,56,56	0
85	MG	5	3852	1/1	0.13	-2.22	46,46,46,46	0
86	OHX	1	3923	7/7	0.07	-2.23	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3943	7/7	0.12	-2.23	96,96,96,96	0
85	MG	5	3696	1/1	0.12	-2.23	41,41,41,41	0
86	OHX	6	2075	7/7	0.09	-2.23	137,137,137,137	0
86	OHX	q2	502	7/7	0.10	-2.24	79,79,79,79	0
85	MG	5	3765	1/1	0.12	-2.24	57,57,57,57	0
86	OHX	6	2091	7/7	0.05	-2.25	130,130,130,130	0
85	MG	5	3821	1/1	0.13	-2.25	54,54,54,54	0
86	OHX	2	2096	7/7	0.10	-2.26	163,163,163,163	0
85	MG	5	3831	1/1	0.14	-2.26	72,72,72,72	0
85	MG	1	3803	1/1	0.14	-2.26	55,55,55,55	0
86	OHX	N1	201	7/7	0.11	-2.26	65,65,65,65	0
85	MG	1	3607	1/1	0.11	-2.27	56,56,56,56	0
86	OHX	1	3913	7/7	0.08	-2.27	84,84,84,84	0
86	OHX	5	4082	7/7	0.11	-2.28	113,113,113,113	0
86	OHX	6	2104	7/7	0.10	-2.28	114,114,114,114	0
86	OHX	1	4121	7/7	0.15	-2.29	118,118,118,118	0
86	OHX	7	225	7/7	0.15	-2.30	102,102,102,102	0
86	OHX	1	4069	7/7	0.08	-2.31	143,143,143,143	0
86	OHX	1	4155	7/7	0.13	-2.32	124,124,124,124	0
85	MG	1	3812	1/1	0.10	-2.33	35,35,35,35	0
85	MG	5	3859	1/1	0.16	-2.33	69,69,69,69	0
86	OHX	n3	203	7/7	0.05	-2.35	90,90,90,90	0
86	OHX	M0	304	7/7	0.13	-2.35	108,108,108,108	0
85	MG	5	3806	1/1	0.09	-2.36	34,34,34,34	0
86	OHX	2	2052	7/7	0.09	-2.36	131,131,131,131	0
86	OHX	1	3944	7/7	0.14	-2.36	84,84,84,84	0
86	OHX	1	3951	7/7	0.10	-2.36	122,122,122,122	0
86	OHX	1	3984	7/7	0.06	-2.37	113,113,113,113	0
86	OHX	1	3883	7/7	0.13	-2.38	63,63,63,63	0
86	OHX	3	216	7/7	0.10	-2.39	105,105,105,105	0
85	MG	1	3756	1/1	0.14	-2.39	43,43,43,43	0
86	OHX	2	2093	7/7	0.06	-2.41	149,149,149,149	0
86	OHX	1	3956	7/7	0.13	-2.41	98,98,98,98	0
85	MG	5	3857	1/1	0.07	-2.43	56,56,56,56	0
86	OHX	1	3946	7/7	0.12	-2.45	89,89,89,89	0
86	OHX	5	3921	7/7	0.11	-2.47	71,71,71,71	0
86	OHX	2	2038	7/7	0.07	-2.50	96,96,96,96	0
86	OHX	1	3977	7/7	0.11	-2.50	101,101,101,101	0
86	OHX	5	4112	7/7	0.12	-2.50	83,83,83,83	0
85	MG	q0	202	1/1	0.13	-2.51	39,39,39,39	0
86	OHX	1	3947	7/7	0.08	-2.51	102,102,102,102	0
86	OHX	1	3919	7/7	0.08	-2.53	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2051	7/7	0.11	-2.53	74,74,74,74	0
86	OHX	5	4026	7/7	0.08	-2.54	113,113,113,113	0
85	MG	5	3807	1/1	0.09	-2.55	96,96,96,96	0
86	OHX	3	218	7/7	0.12	-2.56	119,119,119,119	0
86	OHX	1	3941	7/7	0.09	-2.57	101,101,101,101	0
86	OHX	1	3982	7/7	0.13	-2.57	100,100,100,100	0
86	OHX	5	3960	7/7	0.06	-2.58	80,80,80,80	0
86	OHX	6	2068	7/7	0.09	-2.61	115,115,115,115	0
86	OHX	6	2082	7/7	0.11	-2.62	99,99,99,99	0
86	OHX	5	4015	7/7	0.04	-2.64	145,145,145,145	0
86	OHX	1	3999	7/7	0.13	-2.66	94,94,94,94	0
86	OHX	5	3924	7/7	0.10	-2.68	64,64,64,64	0
86	OHX	5	4079	7/7	0.07	-2.68	150,150,150,150	0
85	MG	5	3470	1/1	0.09	-2.71	107,107,107,107	0
86	OHX	1	3938	7/7	0.14	-2.71	95,95,95,95	0
85	MG	5	3759	1/1	0.11	-2.72	41,41,41,41	0
86	OHX	1	3961	7/7	0.08	-2.72	106,106,106,106	0
86	OHX	5	3955	7/7	0.09	-2.72	101,101,101,101	0
86	OHX	6	2076	7/7	0.07	-2.72	136,136,136,136	0
86	OHX	1	3954	7/7	0.11	-2.73	107,107,107,107	0
86	OHX	5	3951	7/7	0.07	-2.74	92,92,92,92	0
86	OHX	6	2088	7/7	0.13	-2.74	102,102,102,102	0
86	OHX	1	3910	7/7	0.12	-2.75	74,74,74,74	0
86	OHX	2	2033	7/7	0.11	-2.75	104,104,104,104	0
86	OHX	5	4002	7/7	0.07	-2.76	111,111,111,111	0
86	OHX	6	2058	7/7	0.11	-2.77	83,83,83,83	0
86	OHX	1	4030	7/7	0.12	-2.80	124,124,124,124	0
86	OHX	6	2057	7/7	0.11	-2.81	72,72,72,72	0
86	OHX	6	2084	7/7	0.05	-2.82	101,101,101,101	0
86	OHX	2	2041	7/7	0.05	-2.83	97,97,97,97	0
86	OHX	2	2156	7/7	0.32	-2.84	227,227,227,227	0
86	OHX	5	3972	7/7	0.07	-2.85	98,98,98,98	0
86	OHX	6	2099	7/7	0.09	-2.87	152,152,152,152	0
86	OHX	5	3945	7/7	0.09	-2.88	89,89,89,89	0
86	OHX	6	2120	7/7	0.14	-2.89	138,138,138,138	0
86	OHX	1	3905	7/7	0.13	-2.91	81,81,81,81	0
86	OHX	2	2086	7/7	0.14	-2.94	122,122,122,122	0
86	OHX	5	3922	7/7	0.11	-2.94	66,66,66,66	0
86	OHX	6	2072	7/7	0.10	-2.97	87,87,87,87	0
86	OHX	3	214	7/7	0.07	-2.99	95,95,95,95	0
86	OHX	1	3967	7/7	0.14	-3.00	98,98,98,98	0
86	OHX	1	4140	7/7	0.13	-3.01	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	3939	7/7	0.10	-3.05	91,91,91,91	0
86	OHX	6	2103	7/7	0.05	-3.06	162,162,162,162	0
86	OHX	1	3930	7/7	0.09	-3.06	103,103,103,103	0
86	OHX	1	4089	7/7	0.14	-3.06	189,189,189,189	0
86	OHX	6	2094	7/7	0.08	-3.09	112,112,112,112	0
86	OHX	5	4017	7/7	0.13	-3.11	103,103,103,103	0
86	OHX	5	3985	7/7	0.10	-3.11	83,83,83,83	0
86	OHX	5	4020	7/7	0.06	-3.11	118,118,118,118	0
86	OHX	7	218	7/7	0.11	-3.17	90,90,90,90	0
86	OHX	6	2098	7/7	0.06	-3.18	123,123,123,123	0
86	OHX	1	4063	7/7	0.12	-3.18	121,121,121,121	0
86	OHX	5	3963	7/7	0.09	-3.20	71,71,71,71	0
86	OHX	2	2069	7/7	0.06	-3.21	130,130,130,130	0
86	OHX	5	3956	7/7	0.12	-3.21	79,79,79,79	0
86	OHX	5	4011	7/7	0.11	-3.21	88,88,88,88	0
86	OHX	5	4000	7/7	0.07	-3.22	104,104,104,104	0
86	OHX	1	3937	7/7	0.08	-3.22	93,93,93,93	0
86	OHX	1	3879	7/7	0.10	-3.23	60,60,60,60	0
86	OHX	1	4020	7/7	0.07	-3.23	153,153,153,153	0
86	OHX	5	4030	7/7	0.09	-3.26	84,84,84,84	0
86	OHX	5	3907	7/7	0.10	-3.27	56,56,56,56	0
86	OHX	5	3914	7/7	0.12	-3.28	57,57,57,57	0
86	OHX	6	2087	7/7	0.07	-3.30	128,128,128,128	0
86	OHX	2	2031	7/7	0.08	-3.30	102,102,102,102	0
85	MG	5	3757	1/1	0.11	-3.32	50,50,50,50	0
86	OHX	1	3882	7/7	0.10	-3.32	64,64,64,64	0
86	OHX	6	2067	7/7	0.07	-3.38	103,103,103,103	0
86	OHX	1	3928	7/7	0.07	-3.39	83,83,83,83	0
86	OHX	5	3964	7/7	0.05	-3.46	90,90,90,90	0
85	MG	1	3739	1/1	0.13	-3.47	36,36,36,36	0
86	OHX	1	4000	7/7	0.08	-3.48	157,157,157,157	0
86	OHX	7	220	7/7	0.12	-3.49	89,89,89,89	0
86	OHX	5	3952	7/7	0.06	-3.50	99,99,99,99	0
86	OHX	5	3965	7/7	0.06	-3.50	88,88,88,88	0
86	OHX	5	3953	7/7	0.10	-3.52	78,78,78,78	0
86	OHX	5	3999	7/7	0.05	-3.52	111,111,111,111	0
86	OHX	2	2044	7/7	0.06	-3.54	101,101,101,101	0
85	MG	m6	202	1/1	0.06	-3.60	31,31,31,31	0
86	OHX	2	2040	7/7	0.06	-3.60	96,96,96,96	0
86	OHX	1	3907	7/7	0.10	-3.61	91,91,91,91	0
86	OHX	5	3980	7/7	0.11	-3.62	96,96,96,96	0
86	OHX	5	3943	7/7	0.11	-3.62	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	3996	7/7	0.08	-3.62	123,123,123,123	0
86	OHX	2	2060	7/7	0.07	-3.63	130,130,130,130	0
86	OHX	6	2140	7/7	0.15	-3.63	116,116,116,116	0
86	OHX	1	4159	7/7	0.11	-3.65	97,97,97,97	0
86	OHX	2	2058	7/7	0.07	-3.67	121,121,121,121	0
86	OHX	1	3893	7/7	0.08	-3.67	67,67,67,67	0
86	OHX	5	3904	7/7	0.11	-3.70	46,46,46,46	0
86	OHX	1	3874	7/7	0.10	-3.71	53,53,53,53	0
86	OHX	1	3964	7/7	0.08	-3.72	118,118,118,118	0
86	OHX	1	3966	7/7	0.08	-3.72	69,69,69,69	0
86	OHX	6	2071	7/7	0.06	-3.73	98,98,98,98	0
86	OHX	1	3950	7/7	0.07	-3.74	103,103,103,103	0
86	OHX	1	3983	7/7	0.10	-3.76	78,78,78,78	0
86	OHX	5	3936	7/7	0.10	-3.76	70,70,70,70	0
86	OHX	1	3945	7/7	0.07	-3.76	102,102,102,102	0
86	OHX	1	3963	7/7	0.10	-3.76	92,92,92,92	0
86	OHX	1	3878	7/7	0.11	-3.77	61,61,61,61	0
86	OHX	5	3940	7/7	0.08	-3.85	78,78,78,78	0
85	MG	1	3643	1/1	0.11	-3.85	67,67,67,67	0
85	MG	1	3725	1/1	0.10	-3.86	56,56,56,56	0
86	OHX	5	3950	7/7	0.10	-3.88	87,87,87,87	0
86	OHX	4	228	7/7	0.06	-3.89	114,114,114,114	0
85	MG	1	3804	1/1	0.12	-3.92	58,58,58,58	0
86	OHX	6	2086	7/7	0.06	-3.93	113,113,113,113	0
86	OHX	2	2037	7/7	0.10	-3.97	100,100,100,100	0
86	OHX	5	3947	7/7	0.11	-3.97	84,84,84,84	0
85	MG	1	3678	1/1	0.09	-3.98	67,67,67,67	0
86	OHX	2	2025	7/7	0.08	-4.01	89,89,89,89	0
86	OHX	5	4103	7/7	0.11	-4.07	140,140,140,140	0
86	OHX	5	3957	7/7	0.08	-4.08	89,89,89,89	0
86	OHX	1	3962	7/7	0.08	-4.13	110,110,110,110	0
86	OHX	1	3922	7/7	0.09	-4.14	91,91,91,91	0
86	OHX	1	4001	7/7	0.07	-4.22	144,144,144,144	0
86	OHX	5	3974	7/7	0.09	-4.23	91,91,91,91	0
86	OHX	1	3885	7/7	0.08	-4.23	59,59,59,59	0
86	OHX	5	3911	7/7	0.12	-4.23	47,47,47,47	0
86	OHX	2	2103	7/7	0.23	-4.24	195,195,195,195	0
86	OHX	1	3892	7/7	0.11	-4.27	70,70,70,70	0
86	OHX	5	4045	7/7	0.10	-4.30	105,105,105,105	0
85	MG	5	3863	1/1	0.10	-4.31	65,65,65,65	0
86	OHX	5	3998	7/7	0.12	-4.33	91,91,91,91	0
86	OHX	5	3989	7/7	0.09	-4.34	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3899	7/7	0.09	-4.36	77,77,77,77	0
86	OHX	5	3938	7/7	0.09	-4.43	77,77,77,77	0
85	MG	5	3678	1/1	0.07	-4.49	91,91,91,91	0
86	OHX	5	4010	7/7	0.07	-4.53	69,69,69,69	0
85	MG	5	3787	1/1	0.08	-4.54	40,40,40,40	0
86	OHX	5	3919	7/7	0.07	-4.54	59,59,59,59	0
85	MG	5	3837	1/1	0.11	-4.57	64,64,64,64	0
86	OHX	1	3903	7/7	0.06	-4.58	79,79,79,79	0
86	OHX	5	3918	7/7	0.10	-4.64	70,70,70,70	0
85	MG	1	3828	1/1	0.11	-4.66	61,61,61,61	0
86	OHX	5	4018	7/7	0.13	-4.67	103,103,103,103	0
86	OHX	6	2080	7/7	0.09	-4.68	88,88,88,88	0
86	OHX	6	2124	7/7	0.11	-4.68	136,136,136,136	0
86	OHX	5	3954	7/7	0.11	-4.68	106,106,106,106	0
86	OHX	5	4012	7/7	0.07	-4.70	100,100,100,100	0
86	OHX	1	3912	7/7	0.07	-4.72	94,94,94,94	0
85	MG	5	3740	1/1	0.12	-4.73	55,55,55,55	0
86	OHX	6	2078	7/7	0.06	-4.74	104,104,104,104	0
86	OHX	5	4005	7/7	0.08	-4.75	105,105,105,105	0
86	OHX	6	2101	7/7	0.13	-4.77	155,155,155,155	0
86	OHX	5	4057	7/7	0.05	-4.78	93,93,93,93	0
86	OHX	6	2065	7/7	0.06	-4.80	87,87,87,87	0
86	OHX	5	3928	7/7	0.10	-4.80	61,61,61,61	0
86	OHX	5	4023	7/7	0.08	-4.81	110,110,110,110	0
86	OHX	5	3931	7/7	0.05	-4.83	77,77,77,77	0
86	OHX	2	2043	7/7	0.06	-4.86	102,102,102,102	0
85	MG	1	3753	1/1	0.13	-4.87	53,53,53,53	0
86	OHX	1	3978	7/7	0.09	-4.88	97,97,97,97	0
85	MG	1	3802	1/1	0.10	-5.00	88,88,88,88	0
86	OHX	5	3925	7/7	0.09	-5.01	67,67,67,67	0
86	OHX	6	2085	7/7	0.09	-5.01	112,112,112,112	0
86	OHX	6	2062	7/7	0.06	-5.06	82,82,82,82	0
86	OHX	1	3902	7/7	0.09	-5.06	70,70,70,70	0
86	OHX	2	2048	7/7	0.07	-5.10	126,126,126,126	0
86	OHX	2	2065	7/7	0.08	-5.10	131,131,131,131	0
86	OHX	6	2089	7/7	0.10	-5.13	106,106,106,106	0
86	OHX	5	3979	7/7	0.08	-5.14	96,96,96,96	0
86	OHX	6	2059	7/7	0.09	-5.25	78,78,78,78	0
86	OHX	5	3992	7/7	0.05	-5.34	80,80,80,80	0
86	OHX	6	2081	7/7	0.07	-5.37	102,102,102,102	0
86	OHX	5	3944	7/7	0.08	-5.52	80,80,80,80	0
85	MG	5	3842	1/1	0.10	-5.55	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	3890	7/7	0.09	-5.65	71,71,71,71	0
86	OHX	5	3981	7/7	0.07	-5.67	77,77,77,77	0
86	OHX	1	3972	7/7	0.08	-5.87	107,107,107,107	0
86	OHX	1	3918	7/7	0.09	-5.90	94,94,94,94	0
86	OHX	5	3927	7/7	0.08	-5.95	66,66,66,66	0
86	OHX	1	3935	7/7	0.07	-6.03	79,79,79,79	0
86	OHX	5	3962	7/7	0.11	-6.05	70,70,70,70	0
86	OHX	5	3966	7/7	0.09	-6.06	94,94,94,94	0
86	OHX	8	217	7/7	0.08	-6.06	86,86,86,86	0
86	OHX	5	3997	7/7	0.09	-6.12	104,104,104,104	0
86	OHX	1	4003	7/7	0.10	-6.13	88,88,88,88	0
86	OHX	5	3949	7/7	0.09	-6.18	73,73,73,73	0
86	OHX	2	2045	7/7	0.08	-6.31	119,119,119,119	0
86	OHX	6	2096	7/7	0.09	-6.33	133,133,133,133	0
86	OHX	5	3971	7/7	0.09	-6.44	88,88,88,88	0
86	OHX	1	3942	7/7	0.08	-6.44	96,96,96,96	0
85	MG	5	3683	1/1	0.14	-6.53	27,27,27,27	0
86	OHX	5	3994	7/7	0.07	-6.58	101,101,101,101	0
86	OHX	6	2077	7/7	0.07	-6.58	83,83,83,83	0
86	OHX	2	2051	7/7	0.09	-6.70	110,110,110,110	0
86	OHX	6	2095	7/7	0.09	-6.71	102,102,102,102	0
86	OHX	m6	203	7/7	0.06	-6.74	93,93,93,93	0
86	OHX	1	3895	7/7	0.06	-6.74	74,74,74,74	0
86	OHX	5	4036	7/7	0.07	-6.87	104,104,104,104	0
85	MG	1	3734	1/1	0.06	-6.87	54,54,54,54	0
86	OHX	5	3930	7/7	0.06	-7.02	75,75,75,75	0
86	OHX	5	3975	7/7	0.11	-7.08	78,78,78,78	0
86	OHX	2	2049	7/7	0.12	-7.19	116,116,116,116	0
86	OHX	8	221	7/7	0.07	-7.19	112,112,112,112	0
86	OHX	1	3914	7/7	0.07	-7.21	81,81,81,81	0
86	OHX	7	221	7/7	0.13	-7.50	95,95,95,95	0
86	OHX	1	3915	7/7	0.07	-7.70	85,85,85,85	0
86	OHX	5	3967	7/7	0.08	-7.87	76,76,76,76	0
86	OHX	1	3920	7/7	0.08	-7.99	85,85,85,85	0
86	OHX	6	2063	7/7	0.08	-8.13	83,83,83,83	0
86	OHX	6	2083	7/7	0.06	-8.21	96,96,96,96	0
86	OHX	2	2055	7/7	0.09	-8.39	127,127,127,127	0
86	OHX	5	3937	7/7	0.06	-8.69	78,78,78,78	0
86	OHX	6	2064	7/7	0.08	-8.93	86,86,86,86	0
85	MG	1	3715	1/1	0.14	-9.00	54,54,54,54	0
86	OHX	1	3931	7/7	0.07	-9.11	84,84,84,84	0
85	MG	17	301	1/1	0.13	-9.60	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3401	1/1	0.07	-10.30	59,59,59,59	0
86	OHX	1	3953	7/7	0.07	-11.97	94,94,94,94	0
85	MG	5	3805	1/1	0.08	-12.05	152,152,152,152	0
86	OHX	1	3906	7/7	0.10	-12.14	84,84,84,84	0
86	OHX	1	3926	7/7	0.06	-12.22	77,77,77,77	0
86	OHX	1	3932	7/7	0.06	-12.57	87,87,87,87	0
85	MG	6	2002	1/1	0.07	-13.67	94,94,94,94	0
86	OHX	5	3984	7/7	0.07	-14.71	81,81,81,81	0
86	OHX	5	3923	7/7	0.09	-16.12	67,67,67,67	0
86	OHX	5	3948	7/7	0.08	-16.15	74,74,74,74	0
85	MG	2	1963	1/1	0.05	-19.00	143,143,143,143	0
86	OHX	6	2090	7/7	0.11	-20.71	117,117,117,117	0
86	OHX	1	3976	7/7	0.07	-43.84	121,121,121,121	0
85	MG	5	3617	1/1	0.48	-	39,39,39,39	0
85	MG	1	3839	1/1	0.56	-	49,49,49,49	0
85	MG	1	3840	1/1	0.84	-	63,63,63,63	0
85	MG	5	3521	1/1	0.52	-	41,41,41,41	0
85	MG	6	2045	1/1	0.40	-	58,58,58,58	0
85	MG	4	219	1/1	0.51	-	48,48,48,48	0
85	MG	1	3614	1/1	0.42	-	49,49,49,49	0
85	MG	5	3679	1/1	0.23	-	40,40,40,40	0
85	MG	2	1904	1/1	0.39	-	74,74,74,74	0
85	MG	6	2042	1/1	0.50	-	71,71,71,71	0
85	MG	1	3466	1/1	0.66	-	48,48,48,48	0
85	MG	6	2040	1/1	0.45	-	87,87,87,87	0
85	MG	6	2000	1/1	0.35	-	114,114,114,114	0
85	MG	1	3758	1/1	0.22	-	99,99,99,99	0
85	MG	7	215	1/1	0.27	-	61,61,61,61	0
85	MG	2	1997	1/1	0.18	-	103,103,103,103	0
86	OHX	2	2158	7/7	0.18	-	281,281,281,281	0
85	MG	5	3879	1/1	0.87	-	57,57,57,57	0
85	MG	1	3491	1/1	0.48	-	49,49,49,49	0
85	MG	3	208	1/1	0.68	-	78,78,78,78	0
85	MG	1	3738	1/1	0.34	-	58,58,58,58	0
85	MG	1	3795	1/1	0.28	-	66,66,66,66	0
85	MG	S4	302	1/1	0.92	-	74,74,74,74	0
85	MG	5	3773	1/1	0.54	-	102,102,102,102	0
85	MG	6	2017	1/1	0.17	-	42,42,42,42	0
85	MG	5	3778	1/1	0.48	-	71,71,71,71	0
85	MG	5	3886	1/1	0.48	-	57,57,57,57	0
85	MG	2	1953	1/1	0.62	-	89,89,89,89	0
85	MG	1	3405	1/1	0.53	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	8	215	1/1	0.46	-	36,36,36,36	0
85	MG	1	3850	1/1	0.70	-	58,58,58,58	0
85	MG	1	3792	1/1	0.12	-	67,67,67,67	0
85	MG	5	3718	1/1	0.67	-	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.