



wwPDB X-ray Structure Validation Summary Report i

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PDB ID : 4U50
Title : Crystal structure of Verrucarin bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.20 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

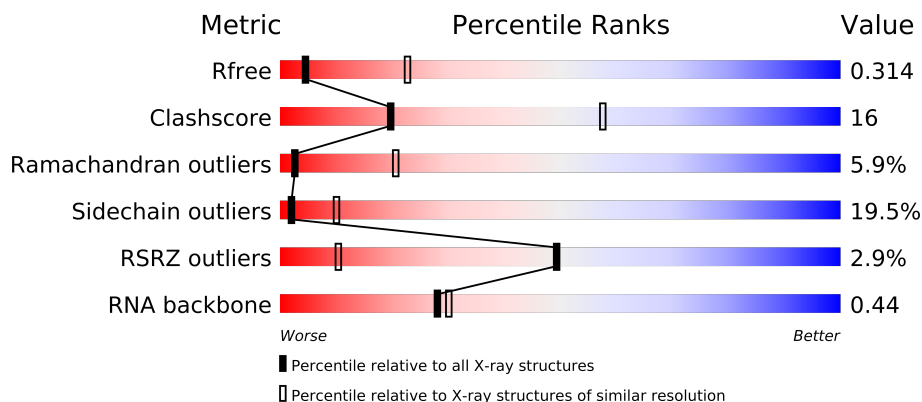
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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

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

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Mol	Chain	Length	Quality of chain
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
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	p0	311	
82	m2	160	
83	p1	47	
84	p2	46	

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

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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3414	-	X
85	MG	1	3415	-	X
85	MG	1	3417	-	X
85	MG	1	3418	-	X
85	MG	1	3419	-	X
85	MG	1	3421	-	X
85	MG	1	3423	-	X
85	MG	1	3424	-	X
85	MG	1	3427	-	X
85	MG	1	3429	-	X
85	MG	1	3430	-	X
85	MG	1	3431	-	X
85	MG	1	3432	-	X
85	MG	1	3433	-	X
85	MG	1	3435	-	X
85	MG	1	3437	-	X
85	MG	1	3438	-	X
85	MG	1	3439	-	X
85	MG	1	3440	-	X
85	MG	1	3441	-	X
85	MG	1	3442	-	X
85	MG	1	3444	-	X
85	MG	1	3446	-	X
85	MG	1	3447	-	X
85	MG	1	3449	-	X
85	MG	1	3450	-	X
85	MG	1	3451	-	X
85	MG	1	3452	-	X
85	MG	1	3453	-	X
85	MG	1	3454	-	X
85	MG	1	3455	-	X
85	MG	1	3456	-	X
85	MG	1	3457	-	X
85	MG	1	3458	-	X
85	MG	1	3459	-	X
85	MG	1	3460	-	X
85	MG	1	3461	-	X
85	MG	1	3462	-	X
85	MG	1	3464	-	X
85	MG	1	3467	-	X
85	MG	1	3468	-	X
85	MG	1	3469	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	3479	-	X
85	MG	1	3480	-	X
85	MG	1	3481	-	X
85	MG	1	3483	-	X
85	MG	1	3484	-	X
85	MG	1	3485	-	X
85	MG	1	3486	-	X
85	MG	1	3487	-	X
85	MG	1	3490	-	X
85	MG	1	3491	-	X
85	MG	1	3492	-	X
85	MG	1	3493	-	X
85	MG	1	3494	-	X
85	MG	1	3495	-	X
85	MG	1	3496	-	X
85	MG	1	3497	-	X
85	MG	1	3498	-	X
85	MG	1	3499	-	X
85	MG	1	3500	-	X
85	MG	1	3501	-	X
85	MG	1	3502	-	X
85	MG	1	3503	-	X
85	MG	1	3504	-	X
85	MG	1	3505	-	X
85	MG	1	3506	-	X
85	MG	1	3507	-	X
85	MG	1	3508	-	X
85	MG	1	3509	-	X
85	MG	1	3510	-	X
85	MG	1	3511	-	X
85	MG	1	3512	-	X
85	MG	1	3513	-	X
85	MG	1	3514	-	X
85	MG	1	3515	-	X
85	MG	1	3516	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3517	-	X
85	MG	1	3518	-	X
85	MG	1	3519	-	X
85	MG	1	3521	-	X
85	MG	1	3522	-	X
85	MG	1	3523	-	X
85	MG	1	3524	-	X
85	MG	1	3525	-	X
85	MG	1	3526	-	X
85	MG	1	3527	-	X
85	MG	1	3528	-	X
85	MG	1	3529	-	X
85	MG	1	3530	-	X
85	MG	1	3531	-	X
85	MG	1	3532	-	X
85	MG	1	3533	-	X
85	MG	1	3534	-	X
85	MG	1	3535	-	X
85	MG	1	3536	-	X
85	MG	1	3537	-	X
85	MG	1	3539	-	X
85	MG	1	3540	-	X
85	MG	1	3541	-	X
85	MG	1	3542	-	X
85	MG	1	3543	-	X
85	MG	1	3544	-	X
85	MG	1	3545	-	X
85	MG	1	3546	-	X
85	MG	1	3547	-	X
85	MG	1	3548	-	X
85	MG	1	3549	-	X
85	MG	1	3550	-	X
85	MG	1	3551	-	X
85	MG	1	3552	-	X
85	MG	1	3553	-	X
85	MG	1	3554	-	X
85	MG	1	3555	-	X
85	MG	1	3556	-	X
85	MG	1	3557	-	X
85	MG	1	3558	-	X
85	MG	1	3559	-	X
85	MG	1	3560	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	3577	-	X
85	MG	1	3578	-	X
85	MG	1	3579	-	X
85	MG	1	3580	-	X
85	MG	1	3582	-	X
85	MG	1	3583	-	X
85	MG	1	3584	-	X
85	MG	1	3585	-	X
85	MG	1	3586	-	X
85	MG	1	3587	-	X
85	MG	1	3588	-	X
85	MG	1	3589	-	X
85	MG	1	3590	-	X
85	MG	1	3591	-	X
85	MG	1	3592	-	X
85	MG	1	3593	-	X
85	MG	1	3594	-	X
85	MG	1	3595	-	X
85	MG	1	3596	-	X
85	MG	1	3597	-	X
85	MG	1	3598	-	X
85	MG	1	3599	-	X
85	MG	1	3600	-	X
85	MG	1	3602	-	X
85	MG	1	3605	-	X
85	MG	1	3606	-	X
85	MG	1	3607	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3609	-	X
85	MG	1	3610	-	X
85	MG	1	3613	-	X
85	MG	1	3614	-	X
85	MG	1	3616	-	X
85	MG	1	3617	-	X
85	MG	1	3618	-	X
85	MG	1	3619	-	X
85	MG	1	3620	-	X
85	MG	1	3621	-	X
85	MG	1	3622	-	X
85	MG	1	3624	-	X
85	MG	1	3625	-	X
85	MG	1	3626	-	X
85	MG	1	3628	-	X
85	MG	1	3629	-	X
85	MG	1	3630	-	X
85	MG	1	3633	-	X
85	MG	1	3634	-	X
85	MG	1	3636	-	X
85	MG	1	3637	-	X
85	MG	1	3639	-	X
85	MG	1	3640	-	X
85	MG	1	3641	-	X
85	MG	1	3642	-	X
85	MG	1	3643	-	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
85	MG	1	3660	-	X
85	MG	1	3662	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3663	-	X
85	MG	1	3664	-	X
85	MG	1	3665	-	X
85	MG	1	3666	-	X
85	MG	1	3667	-	X
85	MG	1	3668	-	X
85	MG	1	3669	-	X
85	MG	1	3670	-	X
85	MG	1	3672	-	X
85	MG	1	3673	-	X
85	MG	1	3675	-	X
85	MG	1	3676	-	X
85	MG	1	3677	-	X
85	MG	1	3680	-	X
85	MG	1	3681	-	X
85	MG	1	3682	-	X
85	MG	1	3684	-	X
85	MG	1	3686	-	X
85	MG	1	3687	-	X
85	MG	1	3688	-	X
85	MG	1	3689	-	X
85	MG	1	3690	-	X
85	MG	1	3691	-	X
85	MG	1	3693	-	X
85	MG	1	3694	-	X
85	MG	1	3695	-	X
85	MG	1	3696	-	X
85	MG	1	3697	-	X
85	MG	1	3698	-	X
85	MG	1	3699	-	X
85	MG	1	3700	-	X
85	MG	1	3702	-	X
85	MG	1	3703	-	X
85	MG	1	3704	-	X
85	MG	1	3705	-	X
85	MG	1	3707	-	X
85	MG	1	3708	-	X
85	MG	1	3710	-	X
85	MG	1	3711	-	X
85	MG	1	3713	-	X
85	MG	1	3716	-	X
85	MG	1	3718	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3719	-	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	3728	-	X
85	MG	1	3729	-	X
85	MG	1	3730	-	X
85	MG	1	3731	-	X
85	MG	1	3732	-	X
85	MG	1	3737	-	X
85	MG	1	3738	-	X
85	MG	1	3739	-	X
85	MG	1	3740	-	X
85	MG	1	3741	-	X
85	MG	1	3742	-	X
85	MG	1	3743	-	X
85	MG	1	3744	-	X
85	MG	1	3745	-	X
85	MG	1	3746	-	X
85	MG	1	3747	-	X
85	MG	1	3750	-	X
85	MG	1	3751	-	X
85	MG	1	3753	-	X
85	MG	1	3755	-	X
85	MG	1	3756	-	X
85	MG	1	3757	-	X
85	MG	1	3758	-	X
85	MG	1	3759	-	X
85	MG	1	3760	-	X
85	MG	1	3761	-	X
85	MG	1	3762	-	X
85	MG	1	3763	-	X
85	MG	1	3764	-	X
85	MG	1	3765	-	X
85	MG	1	3768	-	X
85	MG	1	3770	-	X
85	MG	1	3771	-	X
85	MG	1	3772	-	X
85	MG	1	3773	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3774	-	X
85	MG	1	3776	-	X
85	MG	1	3777	-	X
85	MG	1	3779	-	X
85	MG	1	3780	-	X
85	MG	1	3781	-	X
85	MG	1	3783	-	X
85	MG	1	3785	-	X
85	MG	1	3786	-	X
85	MG	1	3787	-	X
85	MG	1	3789	-	X
85	MG	1	3790	-	X
85	MG	1	3791	-	X
85	MG	1	3793	-	X
85	MG	1	3794	-	X
85	MG	1	3795	-	X
85	MG	1	3796	-	X
85	MG	1	3798	-	X
85	MG	1	3802	-	X
85	MG	1	3803	-	X
85	MG	1	3807	-	X
85	MG	1	3810	-	X
85	MG	1	3811	-	X
85	MG	1	3812	-	X
85	MG	1	3814	-	X
85	MG	1	3817	-	X
85	MG	1	3818	-	X
85	MG	1	3819	-	X
85	MG	1	3822	-	X
85	MG	1	3823	-	X
85	MG	1	3824	-	X
85	MG	1	3826	-	X
85	MG	1	3827	-	X
85	MG	1	3828	-	X
85	MG	1	3829	-	X
85	MG	1	3830	-	X
85	MG	1	3831	-	X
85	MG	1	3832	-	X
85	MG	1	3834	-	X
85	MG	1	3835	-	X
85	MG	1	3838	-	X
85	MG	1	3839	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3840	-	X
85	MG	1	3841	-	X
85	MG	1	3842	-	X
85	MG	1	3843	-	X
85	MG	1	3844	-	X
85	MG	1	3846	-	X
85	MG	1	3848	-	X
85	MG	1	3849	-	X
85	MG	1	3850	-	X
85	MG	1	3851	-	X
85	MG	1	3852	-	X
85	MG	1	3853	-	X
85	MG	1	3854	-	X
85	MG	1	3856	-	X
85	MG	1	3857	-	X
85	MG	1	3858	-	X
85	MG	1	3859	-	X
85	MG	1	3860	-	X
85	MG	1	3861	-	X
85	MG	1	3862	-	X
85	MG	1	4213	-	X
85	MG	1	4216	-	X
85	MG	1	4218	-	X
85	MG	1	4219	-	X
85	MG	1	4220	-	X
85	MG	2	1901	-	X
85	MG	2	1902	-	X
85	MG	2	1903	-	X
85	MG	2	1904	-	X
85	MG	2	1905	-	X
85	MG	2	1906	-	X
85	MG	2	1907	-	X
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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1918	-	X
85	MG	2	1919	-	X
85	MG	2	1920	-	X
85	MG	2	1922	-	X
85	MG	2	1923	-	X
85	MG	2	1924	-	X
85	MG	2	1925	-	X
85	MG	2	1926	-	X
85	MG	2	1928	-	X
85	MG	2	1929	-	X
85	MG	2	1930	-	X
85	MG	2	1931	-	X
85	MG	2	1932	-	X
85	MG	2	1933	-	X
85	MG	2	1934	-	X
85	MG	2	1935	-	X
85	MG	2	1936	-	X
85	MG	2	1937	-	X
85	MG	2	1938	-	X
85	MG	2	1939	-	X
85	MG	2	1940	-	X
85	MG	2	1941	-	X
85	MG	2	1943	-	X
85	MG	2	1944	-	X
85	MG	2	1945	-	X
85	MG	2	1947	-	X
85	MG	2	1948	-	X
85	MG	2	1949	-	X
85	MG	2	1950	-	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	1963	-	X
85	MG	2	1964	-	X
85	MG	2	1965	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1966	-	X
85	MG	2	1967	-	X
85	MG	2	1969	-	X
85	MG	2	1970	-	X
85	MG	2	1971	-	X
85	MG	2	1972	-	X
85	MG	2	1973	-	X
85	MG	2	1974	-	X
85	MG	2	1975	-	X
85	MG	2	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	1986	-	X
85	MG	2	1987	-	X
85	MG	2	1988	-	X
85	MG	2	1990	-	X
85	MG	2	1991	-	X
85	MG	2	1992	-	X
85	MG	2	1993	-	X
85	MG	2	1999	-	X
85	MG	2	2001	-	X
85	MG	2	2002	-	X
85	MG	2	2003	-	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	2012	-	X
85	MG	2	2013	-	X
85	MG	2	2014	-	X
85	MG	2	2015	-	X
85	MG	2	2016	-	X
85	MG	2	2017	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	208	-	X
85	MG	3	209	-	X
85	MG	3	210	-	X
85	MG	3	212	-	X
85	MG	3	213	-	X
85	MG	3	214	-	X
85	MG	4	201	-	X
85	MG	4	202	-	X
85	MG	4	203	-	X
85	MG	4	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	212	-	X
85	MG	4	213	-	X
85	MG	4	214	-	X
85	MG	4	215	-	X
85	MG	4	216	-	X
85	MG	4	217	-	X
85	MG	4	218	-	X
85	MG	4	219	-	X
85	MG	4	220	-	X
85	MG	4	221	-	X
85	MG	4	222	-	X
85	MG	4	223	-	X
85	MG	4	224	-	X
85	MG	4	225	-	X
85	MG	5	3402	-	X
85	MG	5	3403	-	X
85	MG	5	3405	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3406	-	X
85	MG	5	3409	-	X
85	MG	5	3411	-	X
85	MG	5	3413	-	X
85	MG	5	3414	-	X
85	MG	5	3415	-	X
85	MG	5	3417	-	X
85	MG	5	3418	-	X
85	MG	5	3420	-	X
85	MG	5	3421	-	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	3430	-	X
85	MG	5	3431	-	X
85	MG	5	3433	-	X
85	MG	5	3435	-	X
85	MG	5	3436	-	X
85	MG	5	3438	-	X
85	MG	5	3439	-	X
85	MG	5	3440	-	X
85	MG	5	3441	-	X
85	MG	5	3442	-	X
85	MG	5	3443	-	X
85	MG	5	3444	-	X
85	MG	5	3445	-	X
85	MG	5	3446	-	X
85	MG	5	3448	-	X
85	MG	5	3449	-	X
85	MG	5	3450	-	X
85	MG	5	3451	-	X
85	MG	5	3452	-	X
85	MG	5	3453	-	X
85	MG	5	3454	-	X
85	MG	5	3455	-	X
85	MG	5	3456	-	X
85	MG	5	3457	-	X
85	MG	5	3458	-	X
85	MG	5	3459	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3460	-	X
85	MG	5	3461	-	X
85	MG	5	3462	-	X
85	MG	5	3463	-	X
85	MG	5	3464	-	X
85	MG	5	3466	-	X
85	MG	5	3469	-	X
85	MG	5	3470	-	X
85	MG	5	3471	-	X
85	MG	5	3472	-	X
85	MG	5	3473	-	X
85	MG	5	3474	-	X
85	MG	5	3475	-	X
85	MG	5	3476	-	X
85	MG	5	3477	-	X
85	MG	5	3478	-	X
85	MG	5	3479	-	X
85	MG	5	3480	-	X
85	MG	5	3481	-	X
85	MG	5	3482	-	X
85	MG	5	3483	-	X
85	MG	5	3485	-	X
85	MG	5	3486	-	X
85	MG	5	3487	-	X
85	MG	5	3488	-	X
85	MG	5	3490	-	X
85	MG	5	3491	-	X
85	MG	5	3492	-	X
85	MG	5	3494	-	X
85	MG	5	3495	-	X
85	MG	5	3496	-	X
85	MG	5	3497	-	X
85	MG	5	3498	-	X
85	MG	5	3499	-	X
85	MG	5	3500	-	X
85	MG	5	3501	-	X
85	MG	5	3502	-	X
85	MG	5	3503	-	X
85	MG	5	3504	-	X
85	MG	5	3505	-	X
85	MG	5	3506	-	X
85	MG	5	3507	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3508	-	X
85	MG	5	3509	-	X
85	MG	5	3510	-	X
85	MG	5	3511	-	X
85	MG	5	3513	-	X
85	MG	5	3514	-	X
85	MG	5	3515	-	X
85	MG	5	3516	-	X
85	MG	5	3517	-	X
85	MG	5	3518	-	X
85	MG	5	3519	-	X
85	MG	5	3520	-	X
85	MG	5	3521	-	X
85	MG	5	3522	-	X
85	MG	5	3523	-	X
85	MG	5	3524	-	X
85	MG	5	3525	-	X
85	MG	5	3526	-	X
85	MG	5	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	3543	-	X
85	MG	5	3544	-	X
85	MG	5	3545	-	X
85	MG	5	3546	-	X
85	MG	5	3547	-	X
85	MG	5	3548	-	X
85	MG	5	3549	-	X
85	MG	5	3550	-	X
85	MG	5	3551	-	X
85	MG	5	3552	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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
85	MG	5	3592	-	X
85	MG	5	3593	-	X
85	MG	5	3594	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3595	-	X
85	MG	5	3596	-	X
85	MG	5	3597	-	X
85	MG	5	3598	-	X
85	MG	5	3602	-	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	3610	-	X
85	MG	5	3611	-	X
85	MG	5	3612	-	X
85	MG	5	3614	-	X
85	MG	5	3618	-	X
85	MG	5	3619	-	X
85	MG	5	3620	-	X
85	MG	5	3621	-	X
85	MG	5	3622	-	X
85	MG	5	3623	-	X
85	MG	5	3624	-	X
85	MG	5	3625	-	X
85	MG	5	3627	-	X
85	MG	5	3628	-	X
85	MG	5	3629	-	X
85	MG	5	3630	-	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	3642	-	X
85	MG	5	3644	-	X
85	MG	5	3645	-	X
85	MG	5	3648	-	X
85	MG	5	3650	-	X
85	MG	5	3651	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	3658	-	X
85	MG	5	3659	-	X
85	MG	5	3660	-	X
85	MG	5	3661	-	X
85	MG	5	3662	-	X
85	MG	5	3663	-	X
85	MG	5	3664	-	X
85	MG	5	3665	-	X
85	MG	5	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	3677	-	X
85	MG	5	3678	-	X
85	MG	5	3679	-	X
85	MG	5	3680	-	X
85	MG	5	3682	-	X
85	MG	5	3683	-	X
85	MG	5	3686	-	X
85	MG	5	3687	-	X
85	MG	5	3689	-	X
85	MG	5	3690	-	X
85	MG	5	3692	-	X
85	MG	5	3693	-	X
85	MG	5	3695	-	X
85	MG	5	3696	-	X
85	MG	5	3698	-	X
85	MG	5	3699	-	X
85	MG	5	3701	-	X
85	MG	5	3702	-	X
85	MG	5	3703	-	X
85	MG	5	3705	-	X
85	MG	5	3706	-	X
85	MG	5	3707	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3708	-	X
85	MG	5	3709	-	X
85	MG	5	3711	-	X
85	MG	5	3712	-	X
85	MG	5	3713	-	X
85	MG	5	3714	-	X
85	MG	5	3715	-	X
85	MG	5	3716	-	X
85	MG	5	3717	-	X
85	MG	5	3718	-	X
85	MG	5	3720	-	X
85	MG	5	3721	-	X
85	MG	5	3724	-	X
85	MG	5	3726	-	X
85	MG	5	3727	-	X
85	MG	5	3728	-	X
85	MG	5	3730	-	X
85	MG	5	3731	-	X
85	MG	5	3733	-	X
85	MG	5	3734	-	X
85	MG	5	3735	-	X
85	MG	5	3736	-	X
85	MG	5	3737	-	X
85	MG	5	3738	-	X
85	MG	5	3739	-	X
85	MG	5	3740	-	X
85	MG	5	3741	-	X
85	MG	5	3742	-	X
85	MG	5	3744	-	X
85	MG	5	3745	-	X
85	MG	5	3747	-	X
85	MG	5	3748	-	X
85	MG	5	3749	-	X
85	MG	5	3750	-	X
85	MG	5	3753	-	X
85	MG	5	3755	-	X
85	MG	5	3758	-	X
85	MG	5	3759	-	X
85	MG	5	3760	-	X
85	MG	5	3761	-	X
85	MG	5	3763	-	X
85	MG	5	3764	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3766	-	X
85	MG	5	3767	-	X
85	MG	5	3769	-	X
85	MG	5	3770	-	X
85	MG	5	3771	-	X
85	MG	5	3772	-	X
85	MG	5	3773	-	X
85	MG	5	3774	-	X
85	MG	5	3776	-	X
85	MG	5	3777	-	X
85	MG	5	3779	-	X
85	MG	5	3780	-	X
85	MG	5	3782	-	X
85	MG	5	3785	-	X
85	MG	5	3786	-	X
85	MG	5	3787	-	X
85	MG	5	3788	-	X
85	MG	5	3789	-	X
85	MG	5	3790	-	X
85	MG	5	3792	-	X
85	MG	5	3794	-	X
85	MG	5	3798	-	X
85	MG	5	3800	-	X
85	MG	5	3802	-	X
85	MG	5	3804	-	X
85	MG	5	3805	-	X
85	MG	5	3807	-	X
85	MG	5	3809	-	X
85	MG	5	3811	-	X
85	MG	5	3813	-	X
85	MG	5	3814	-	X
85	MG	5	3815	-	X
85	MG	5	3819	-	X
85	MG	5	3820	-	X
85	MG	5	3821	-	X
85	MG	5	3822	-	X
85	MG	5	3823	-	X
85	MG	5	3827	-	X
85	MG	5	3828	-	X
85	MG	5	3829	-	X
85	MG	5	3832	-	X
85	MG	5	3837	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3838	-	X
85	MG	5	3839	-	X
85	MG	5	3840	-	X
85	MG	5	3841	-	X
85	MG	5	3842	-	X
85	MG	5	3844	-	X
85	MG	5	3846	-	X
85	MG	5	3847	-	X
85	MG	5	3852	-	X
85	MG	5	3853	-	X
85	MG	5	3854	-	X
85	MG	5	3855	-	X
85	MG	5	3856	-	X
85	MG	5	3857	-	X
85	MG	5	3858	-	X
85	MG	5	3859	-	X
85	MG	5	3861	-	X
85	MG	5	3862	-	X
85	MG	5	3863	-	X
85	MG	5	3864	-	X
85	MG	5	3865	-	X
85	MG	5	3867	-	X
85	MG	5	3868	-	X
85	MG	5	3869	-	X
85	MG	5	3871	-	X
85	MG	5	3872	-	X
85	MG	5	3873	-	X
85	MG	5	3874	-	X
85	MG	5	3876	-	X
85	MG	5	3877	-	X
85	MG	5	3878	-	X
85	MG	5	3879	-	X
85	MG	5	3880	-	X
85	MG	5	3881	-	X
85	MG	5	3882	-	X
85	MG	5	3884	-	X
85	MG	5	3886	-	X
85	MG	5	3887	-	X
85	MG	5	3888	-	X
85	MG	5	3889	-	X
85	MG	5	3891	-	X
85	MG	5	4248	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	4249	-	X
85	MG	5	4251	-	X
85	MG	5	4252	-	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	1925	-	X
85	MG	6	1926	-	X
85	MG	6	1927	-	X
85	MG	6	1928	-	X
85	MG	6	1929	-	X
85	MG	6	1930	-	X
85	MG	6	1931	-	X
85	MG	6	1932	-	X
85	MG	6	1933	-	X
85	MG	6	1934	-	X
85	MG	6	1935	-	X
85	MG	6	1936	-	X
85	MG	6	1937	-	X
85	MG	6	1938	-	X
85	MG	6	1939	-	X
85	MG	6	1941	-	X
85	MG	6	1942	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	1964	-	X
85	MG	6	1965	-	X
85	MG	6	1966	-	X
85	MG	6	1967	-	X
85	MG	6	1968	-	X
85	MG	6	1970	-	X
85	MG	6	1971	-	X
85	MG	6	1972	-	X
85	MG	6	1973	-	X
85	MG	6	1974	-	X
85	MG	6	1975	-	X
85	MG	6	1976	-	X
85	MG	6	1977	-	X
85	MG	6	1978	-	X
85	MG	6	1979	-	X
85	MG	6	1980	-	X
85	MG	6	1983	-	X
85	MG	6	1985	-	X
85	MG	6	1986	-	X
85	MG	6	1987	-	X
85	MG	6	1989	-	X
85	MG	6	1990	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1991	-	X
85	MG	6	1992	-	X
85	MG	6	1993	-	X
85	MG	6	1994	-	X
85	MG	6	1997	-	X
85	MG	6	1999	-	X
85	MG	6	2000	-	X
85	MG	6	2001	-	X
85	MG	6	2002	-	X
85	MG	6	2003	-	X
85	MG	6	2004	-	X
85	MG	6	2005	-	X
85	MG	6	2007	-	X
85	MG	6	2008	-	X
85	MG	6	2009	-	X
85	MG	6	2010	-	X
85	MG	6	2011	-	X
85	MG	6	2012	-	X
85	MG	6	2013	-	X
85	MG	6	2014	-	X
85	MG	6	2017	-	X
85	MG	6	2018	-	X
85	MG	6	2020	-	X
85	MG	6	2021	-	X
85	MG	6	2022	-	X
85	MG	6	2023	-	X
85	MG	6	2027	-	X
85	MG	6	2028	-	X
85	MG	6	2029	-	X
85	MG	6	2031	-	X
85	MG	6	2032	-	X
85	MG	6	2033	-	X
85	MG	6	2034	-	X
85	MG	6	2035	-	X
85	MG	6	2038	-	X
85	MG	6	2040	-	X
85	MG	6	2041	-	X
85	MG	6	2042	-	X
85	MG	6	2043	-	X
85	MG	6	2044	-	X
85	MG	6	2203	-	X
85	MG	6	2204	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	209	-	X
85	MG	7	210	-	X
85	MG	7	211	-	X
85	MG	7	212	-	X
85	MG	7	214	-	X
85	MG	7	215	-	X
85	MG	7	216	-	X
85	MG	8	202	-	X
85	MG	8	203	-	X
85	MG	8	204	-	X
85	MG	8	205	-	X
85	MG	8	206	-	X
85	MG	8	207	-	X
85	MG	8	208	-	X
85	MG	8	209	-	X
85	MG	8	210	-	X
85	MG	8	212	-	X
85	MG	8	213	-	X
85	MG	8	214	-	X
85	MG	8	215	-	X
85	MG	C1	201	-	X
85	MG	D0	201	-	X
85	MG	L2	301	-	X
85	MG	L2	302	-	X
85	MG	L3	401	-	X
85	MG	L4	401	-	X
85	MG	L4	402	-	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	M0	301	-	X
85	MG	M1	201	-	X
85	MG	M3	203	-	X
85	MG	M5	301	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	M7	201	-	X
85	MG	N0	201	-	X
85	MG	N3	201	-	X
85	MG	N3	202	-	X
85	MG	N5	201	-	X
85	MG	N5	202	-	X
85	MG	N6	201	-	X
85	MG	N6	202	-	X
85	MG	N8	201	-	X
85	MG	N8	202	-	X
85	MG	N8	204	-	X
85	MG	O4	201	-	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	c8	201	-	X
85	MG	d3	201	-	X
85	MG	d3	202	-	X
85	MG	d4	201	-	X
85	MG	d6	102	-	X
85	MG	l2	301	-	X
85	MG	l2	302	-	X
85	MG	l2	303	-	X
85	MG	l3	401	-	X
85	MG	l3	402	-	X
85	MG	l3	403	-	X
85	MG	l4	402	-	X
85	MG	l7	301	-	X
85	MG	l7	302	-	X
85	MG	l8	301	-	X
85	MG	m1	201	-	X
85	MG	m5	301	-	X
85	MG	m5	302	-	X
85	MG	m5	303	-	X
85	MG	m7	201	-	X
85	MG	m7	203	-	X
85	MG	n0	202	-	X
85	MG	n0	203	-	X
85	MG	n3	201	-	X
85	MG	n6	201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	n8	201	-	X
85	MG	n8	202	-	X
85	MG	n8	203	-	X
85	MG	n8	204	-	X
85	MG	n9	101	-	X
85	MG	o3	201	-	X
85	MG	o4	202	-	X
85	MG	q0	202	-	X
85	MG	s1	301	-	X
85	MG	s8	301	-	X
86	OHX	1	3921	-	X
86	OHX	1	3952	-	X
86	OHX	1	3954	-	X
86	OHX	1	3966	-	X
86	OHX	1	3972	-	X
86	OHX	1	3977	-	X
86	OHX	1	3983	-	X
86	OHX	1	3984	-	X
86	OHX	1	3986	-	X
86	OHX	1	3990	-	X
86	OHX	1	3999	-	X
86	OHX	1	4002	-	X
86	OHX	1	4003	-	X
86	OHX	1	4004	-	X
86	OHX	1	4006	-	X
86	OHX	1	4007	-	X
86	OHX	1	4009	-	X
86	OHX	1	4012	-	X
86	OHX	1	4013	-	X
86	OHX	1	4014	-	X
86	OHX	1	4018	-	X
86	OHX	1	4019	-	X
86	OHX	1	4024	-	X
86	OHX	1	4026	-	X
86	OHX	1	4031	-	X
86	OHX	1	4034	-	X
86	OHX	1	4036	-	X
86	OHX	1	4040	-	X
86	OHX	1	4041	-	X
86	OHX	1	4043	-	X
86	OHX	1	4044	-	X
86	OHX	1	4047	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4049	-	X
86	OHX	1	4052	-	X
86	OHX	1	4054	-	X
86	OHX	1	4055	-	X
86	OHX	1	4059	-	X
86	OHX	1	4060	-	X
86	OHX	1	4061	-	X
86	OHX	1	4062	-	X
86	OHX	1	4064	-	X
86	OHX	1	4065	-	X
86	OHX	1	4066	-	X
86	OHX	1	4067	-	X
86	OHX	1	4068	-	X
86	OHX	1	4069	-	X
86	OHX	1	4070	-	X
86	OHX	1	4072	-	X
86	OHX	1	4073	-	X
86	OHX	1	4074	-	X
86	OHX	1	4075	-	X
86	OHX	1	4076	-	X
86	OHX	1	4077	-	X
86	OHX	1	4078	-	X
86	OHX	1	4079	-	X
86	OHX	1	4080	-	X
86	OHX	1	4084	-	X
86	OHX	1	4085	-	X
86	OHX	1	4086	-	X
86	OHX	1	4089	-	X
86	OHX	1	4092	-	X
86	OHX	1	4093	-	X
86	OHX	1	4094	-	X
86	OHX	1	4095	-	X
86	OHX	1	4096	-	X
86	OHX	1	4097	-	X
86	OHX	1	4102	-	X
86	OHX	1	4104	-	X
86	OHX	1	4105	-	X
86	OHX	1	4106	-	X
86	OHX	1	4107	-	X
86	OHX	1	4108	-	X
86	OHX	1	4109	-	X
86	OHX	1	4110	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4112	-	X
86	OHX	1	4113	-	X
86	OHX	1	4114	-	X
86	OHX	1	4116	-	X
86	OHX	1	4117	-	X
86	OHX	1	4118	-	X
86	OHX	1	4119	-	X
86	OHX	1	4120	-	X
86	OHX	1	4123	-	X
86	OHX	1	4124	-	X
86	OHX	1	4125	-	X
86	OHX	1	4126	-	X
86	OHX	1	4127	-	X
86	OHX	1	4128	-	X
86	OHX	1	4130	-	X
86	OHX	1	4131	-	X
86	OHX	1	4132	-	X
86	OHX	1	4133	-	X
86	OHX	1	4135	-	X
86	OHX	1	4136	-	X
86	OHX	1	4137	-	X
86	OHX	1	4138	-	X
86	OHX	1	4139	-	X
86	OHX	1	4140	-	X
86	OHX	1	4141	-	X
86	OHX	1	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	4151	-	X
86	OHX	1	4152	-	X
86	OHX	1	4153	-	X
86	OHX	1	4155	-	X
86	OHX	1	4156	-	X
86	OHX	1	4157	-	X
86	OHX	1	4158	-	X
86	OHX	1	4159	-	X
86	OHX	1	4161	-	X
86	OHX	1	4162	-	X
86	OHX	1	4163	-	X
86	OHX	1	4165	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4166	-	X
86	OHX	1	4167	-	X
86	OHX	1	4168	-	X
86	OHX	1	4169	-	X
86	OHX	1	4170	-	X
86	OHX	1	4172	-	X
86	OHX	1	4173	-	X
86	OHX	1	4174	-	X
86	OHX	1	4175	-	X
86	OHX	1	4176	-	X
86	OHX	1	4178	-	X
86	OHX	1	4179	-	X
86	OHX	1	4181	-	X
86	OHX	1	4182	-	X
86	OHX	1	4183	-	X
86	OHX	1	4184	-	X
86	OHX	1	4185	-	X
86	OHX	1	4187	-	X
86	OHX	1	4188	-	X
86	OHX	1	4190	-	X
86	OHX	1	4192	-	X
86	OHX	1	4193	-	X
86	OHX	1	4194	-	X
86	OHX	1	4195	-	X
86	OHX	1	4196	-	X
86	OHX	1	4197	-	X
86	OHX	1	4199	-	X
86	OHX	1	4200	-	X
86	OHX	1	4201	-	X
86	OHX	1	4202	-	X
86	OHX	1	4203	-	X
86	OHX	1	4204	-	X
86	OHX	1	4205	-	X
86	OHX	1	4206	-	X
86	OHX	1	4207	-	X
86	OHX	1	4208	-	X
86	OHX	1	4209	-	X
86	OHX	1	4210	-	X
86	OHX	1	4211	-	X
86	OHX	2	2057	-	X
86	OHX	2	2064	-	X
86	OHX	2	2068	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	2	2073	-	X
86	OHX	2	2075	-	X
86	OHX	2	2078	-	X
86	OHX	2	2080	-	X
86	OHX	2	2083	-	X
86	OHX	2	2085	-	X
86	OHX	2	2086	-	X
86	OHX	2	2089	-	X
86	OHX	2	2090	-	X
86	OHX	2	2091	-	X
86	OHX	2	2098	-	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	2110	-	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	2121	-	X
86	OHX	2	2122	-	X
86	OHX	2	2125	-	X
86	OHX	2	2126	-	X
86	OHX	2	2127	-	X
86	OHX	2	2128	-	X
86	OHX	2	2131	-	X
86	OHX	2	2134	-	X
86	OHX	2	2135	-	X
86	OHX	2	2136	-	X
86	OHX	2	2137	-	X
86	OHX	2	2139	-	X
86	OHX	2	2140	-	X
86	OHX	2	2143	-	X
86	OHX	2	2145	-	X
86	OHX	2	2146	-	X
86	OHX	2	2147	-	X
86	OHX	2	2148	-	X
86	OHX	2	2149	-	X
86	OHX	2	2150	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	2	2152	-	X
86	OHX	2	2153	-	X
86	OHX	2	2154	-	X
86	OHX	2	2157	-	X
86	OHX	2	2159	-	X
86	OHX	2	2160	-	X
86	OHX	2	2161	-	X
86	OHX	2	2162	-	X
86	OHX	2	2163	-	X
86	OHX	2	2167	-	X
86	OHX	2	2168	-	X
86	OHX	2	2169	-	X
86	OHX	2	2170	-	X
86	OHX	2	2171	-	X
86	OHX	2	2172	-	X
86	OHX	2	2173	-	X
86	OHX	2	2174	-	X
86	OHX	2	2176	-	X
86	OHX	2	2177	-	X
86	OHX	3	222	-	X
86	OHX	3	223	-	X
86	OHX	3	224	-	X
86	OHX	3	225	-	X
86	OHX	3	226	-	X
86	OHX	4	230	-	X
86	OHX	4	231	-	X
86	OHX	4	232	-	X
86	OHX	4	235	-	X
86	OHX	4	236	-	X
86	OHX	4	237	-	X
86	OHX	4	238	-	X
86	OHX	4	239	-	X
86	OHX	4	240	-	X
86	OHX	4	241	-	X
86	OHX	5	3946	-	X
86	OHX	5	3966	-	X
86	OHX	5	3977	-	X
86	OHX	5	3986	-	X
86	OHX	5	3995	-	X
86	OHX	5	4004	-	X
86	OHX	5	4005	-	X
86	OHX	5	4008	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4020	-	X
86	OHX	5	4023	-	X
86	OHX	5	4033	-	X
86	OHX	5	4036	-	X
86	OHX	5	4038	-	X
86	OHX	5	4039	-	X
86	OHX	5	4040	-	X
86	OHX	5	4041	-	X
86	OHX	5	4042	-	X
86	OHX	5	4043	-	X
86	OHX	5	4045	-	X
86	OHX	5	4048	-	X
86	OHX	5	4050	-	X
86	OHX	5	4053	-	X
86	OHX	5	4055	-	X
86	OHX	5	4056	-	X
86	OHX	5	4062	-	X
86	OHX	5	4063	-	X
86	OHX	5	4064	-	X
86	OHX	5	4065	-	X
86	OHX	5	4066	-	X
86	OHX	5	4067	-	X
86	OHX	5	4070	-	X
86	OHX	5	4073	-	X
86	OHX	5	4076	-	X
86	OHX	5	4079	-	X
86	OHX	5	4082	-	X
86	OHX	5	4083	-	X
86	OHX	5	4085	-	X
86	OHX	5	4086	-	X
86	OHX	5	4089	-	X
86	OHX	5	4090	-	X
86	OHX	5	4091	-	X
86	OHX	5	4093	-	X
86	OHX	5	4094	-	X
86	OHX	5	4096	-	X
86	OHX	5	4099	-	X
86	OHX	5	4101	-	X
86	OHX	5	4102	-	X
86	OHX	5	4103	-	X
86	OHX	5	4104	-	X
86	OHX	5	4105	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4106	-	X
86	OHX	5	4108	-	X
86	OHX	5	4109	-	X
86	OHX	5	4111	-	X
86	OHX	5	4112	-	X
86	OHX	5	4113	-	X
86	OHX	5	4114	-	X
86	OHX	5	4117	-	X
86	OHX	5	4119	-	X
86	OHX	5	4120	-	X
86	OHX	5	4121	-	X
86	OHX	5	4122	-	X
86	OHX	5	4124	-	X
86	OHX	5	4126	-	X
86	OHX	5	4127	-	X
86	OHX	5	4128	-	X
86	OHX	5	4129	-	X
86	OHX	5	4130	-	X
86	OHX	5	4131	-	X
86	OHX	5	4132	-	X
86	OHX	5	4133	-	X
86	OHX	5	4134	-	X
86	OHX	5	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
86	OHX	5	4143	-	X
86	OHX	5	4144	-	X
86	OHX	5	4145	-	X
86	OHX	5	4146	-	X
86	OHX	5	4147	-	X
86	OHX	5	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

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4156	-	X
86	OHX	5	4157	-	X
86	OHX	5	4158	-	X
86	OHX	5	4159	-	X
86	OHX	5	4160	-	X
86	OHX	5	4161	-	X
86	OHX	5	4162	-	X
86	OHX	5	4163	-	X
86	OHX	5	4166	-	X
86	OHX	5	4169	-	X
86	OHX	5	4170	-	X
86	OHX	5	4171	-	X
86	OHX	5	4172	-	X
86	OHX	5	4173	-	X
86	OHX	5	4175	-	X
86	OHX	5	4177	-	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	4185	-	X
86	OHX	5	4186	-	X
86	OHX	5	4187	-	X
86	OHX	5	4189	-	X
86	OHX	5	4190	-	X
86	OHX	5	4191	-	X
86	OHX	5	4193	-	X
86	OHX	5	4195	-	X
86	OHX	5	4196	-	X
86	OHX	5	4197	-	X
86	OHX	5	4198	-	X
86	OHX	5	4199	-	X
86	OHX	5	4200	-	X
86	OHX	5	4201	-	X
86	OHX	5	4202	-	X
86	OHX	5	4203	-	X
86	OHX	5	4204	-	X
86	OHX	5	4205	-	X
86	OHX	5	4206	-	X
86	OHX	5	4207	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4209	-	X
86	OHX	5	4211	-	X
86	OHX	5	4212	-	X
86	OHX	5	4213	-	X
86	OHX	5	4214	-	X
86	OHX	5	4215	-	X
86	OHX	5	4216	-	X
86	OHX	5	4217	-	X
86	OHX	5	4218	-	X
86	OHX	5	4220	-	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	4228	-	X
86	OHX	5	4229	-	X
86	OHX	5	4230	-	X
86	OHX	5	4231	-	X
86	OHX	5	4233	-	X
86	OHX	5	4234	-	X
86	OHX	5	4237	-	X
86	OHX	5	4238	-	X
86	OHX	5	4239	-	X
86	OHX	5	4240	-	X
86	OHX	5	4241	-	X
86	OHX	5	4242	-	X
86	OHX	5	4243	-	X
86	OHX	5	4245	-	X
86	OHX	6	2070	-	X
86	OHX	6	2101	-	X
86	OHX	6	2104	-	X
86	OHX	6	2108	-	X
86	OHX	6	2111	-	X
86	OHX	6	2113	-	X
86	OHX	6	2115	-	X
86	OHX	6	2118	-	X
86	OHX	6	2121	-	X
86	OHX	6	2122	-	X
86	OHX	6	2124	-	X
86	OHX	6	2125	-	X
86	OHX	6	2126	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	6	2130	-	X
86	OHX	6	2131	-	X
86	OHX	6	2132	-	X
86	OHX	6	2134	-	X
86	OHX	6	2136	-	X
86	OHX	6	2137	-	X
86	OHX	6	2138	-	X
86	OHX	6	2139	-	X
86	OHX	6	2142	-	X
86	OHX	6	2145	-	X
86	OHX	6	2147	-	X
86	OHX	6	2149	-	X
86	OHX	6	2150	-	X
86	OHX	6	2154	-	X
86	OHX	6	2155	-	X
86	OHX	6	2156	-	X
86	OHX	6	2158	-	X
86	OHX	6	2159	-	X
86	OHX	6	2163	-	X
86	OHX	6	2164	-	X
86	OHX	6	2166	-	X
86	OHX	6	2167	-	X
86	OHX	6	2168	-	X
86	OHX	6	2169	-	X
86	OHX	6	2171	-	X
86	OHX	6	2172	-	X
86	OHX	6	2173	-	X
86	OHX	6	2174	-	X
86	OHX	6	2175	-	X
86	OHX	6	2176	-	X
86	OHX	6	2177	-	X
86	OHX	6	2178	-	X
86	OHX	6	2179	-	X
86	OHX	6	2181	-	X
86	OHX	6	2182	-	X
86	OHX	6	2184	-	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	2191	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	6	2194	-	X
86	OHX	6	2195	-	X
86	OHX	6	2196	-	X
86	OHX	6	2197	-	X
86	OHX	6	2198	-	X
86	OHX	6	2201	-	X
86	OHX	6	2202	-	X
86	OHX	7	225	-	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	229	-	X
86	OHX	8	230	-	X
86	OHX	8	231	-	X
86	OHX	D9	102	-	X
86	OHX	L3	403	-	X
86	OHX	L4	403	-	X
86	OHX	M7	204	-	X
86	OHX	M7	205	-	X
86	OHX	O3	201	-	X
86	OHX	d9	102	-	X
86	OHX	l3	405	-	X
86	OHX	l4	403	-	X
86	OHX	l4	404	-	X
86	OHX	m4	201	-	X
86	OHX	m7	206	-	X
86	OHX	o7	503	-	X
86	OHX	s1	303	-	X
86	OHX	s9	201	-	X
88	3L2	5	4246	-	X

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411230 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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C5	137	SER	ARG	conflict	UNP Q01855
c5	137	SER	ARG	conflict	UNP Q01855

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E1	77	ALA	GLY	conflict	UNP P05759
e1	77	ALA	GLY	conflict	UNP P05759

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	17	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	18	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	19	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
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 60S acidic ribosomal protein P0.

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

- Molecule 82 is a protein called UNKNOWN PROTEIN m2.

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

- Molecule 83 is a protein called UNKNOWN PROTEIN 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 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	n8	5	Total	Mg	0	0
			5	5		
85	o1	1	Total	Mg	0	0
			1	1		
85	N5	2	Total	Mg	0	0
			2	2		
85	6	146	Total	Mg	0	0
			146	146		
85	sM	2	Total	Mg	0	0
			2	2		
85	O4	1	Total	Mg	0	0
			1	1		
85	m5	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	l3	3	Total 3	Mg 3	0	0
85	C1	1	Total 1	Mg 1	0	0
85	M1	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	122	Total 122	Mg 122	0	0
85	n0	3	Total 3	Mg 3	0	0
85	L4	2	Total 2	Mg 2	0	0
85	l7	2	Total 2	Mg 2	0	0
85	M5	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0
85	S2	2	Total 2	Mg 2	0	0
85	L8	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	M0	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	497	Total 497	Mg 497	0	0
85	L5	1	Total 1	Mg 1	0	0

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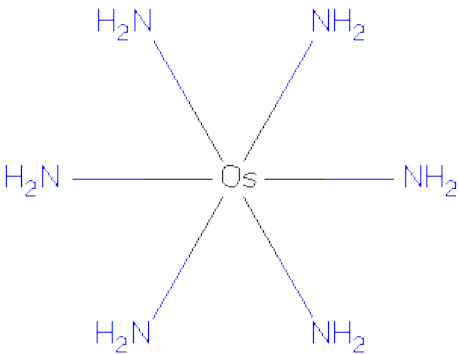
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	O7	1	Total 1	Mg 1	0	0
85	s6	1	Total 1	Mg 1	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	n9	1	Total 1	Mg 1	0	0
85	1	470	Total 470	Mg 470	0	0
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	3	Total 3	Mg 3	0	0
85	O2	1	Total 1	Mg 1	0	0
85	q3	2	Total 2	Mg 2	0	0
85	o3	1	Total 1	Mg 1	0	0
85	d3	3	Total 3	Mg 3	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	3	Total 3	Mg 3	0	0
85	4	25	Total 25	Mg 25	0	0
85	n6	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	2	Total 2	Mg 2	0	0
85	m1	2	Total 2	Mg 2	0	0
85	l5	1	Total 1	Mg 1	0	0
85	m7	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	M7	3	Total 3	Mg 3	0	0
85	N8	4	Total 4	Mg 4	0	0
85	s1	1	Total 1	Mg 1	0	0
85	m6	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	l8	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	16	Total 16	Mg 16	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	2	Total 2	Mg 2	0	0
85	d4	1	Total 1	Mg 1	0	0
85	N6	2	Total 2	Mg 2	0	0
85	8	15	Total 15	Mg 15	0	0
85	l4	2	Total 2	Mg 2	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0
85	3	14	Total 14	Mg 14	0	0

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



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		

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

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

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

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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		
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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	C3	1	Total	N	Os	0	0
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86	C5	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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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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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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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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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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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	3	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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	L4	1	Total	N	Os	0	0
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86	M0	1	Total	N	Os	0	0
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86	M5	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
			7	6	1		
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
			7	6	1		
86	O3	1	Total	N	Os	0	0
			7	6	1		
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	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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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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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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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	s1	1	Total	N	Os	0	0
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86	s1	1	Total	N	Os	0	0
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86	s4	1	Total	N	Os	0	0
			7	6	1		
86	s8	1	Total	N	Os	0	0
			7	6	1		
86	s9	1	Total	N	Os	0	0
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86	c3	1	Total	N	Os	0	0
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86	c5	1	Total	N	Os	0	0
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86	c8	1	Total	N	Os	0	0
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86	d4	1	Total	N	Os	0	0
			7	6	1		
86	d9	1	Total	N	Os	0	0
			7	6	1		
86	sR	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l4	1	Total 7	N 6	Os 1	0	0
86	l4	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	0	0
86	l9	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m1	1	Total 7	N 6	Os 1	0	0
86	m4	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m6	1	Total 7	N 6	Os 1	0	0
86	m7	1	Total 7	N 6	Os 1	0	0
86	m8	1	Total 7	N 6	Os 1	0	0
86	n3	1	Total 7	N 6	Os 1	0	0
86	n3	1	Total 7	N 6	Os 1	0	0
86	n6	1	Total 7	N 6	Os 1	0	0
86	n9	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

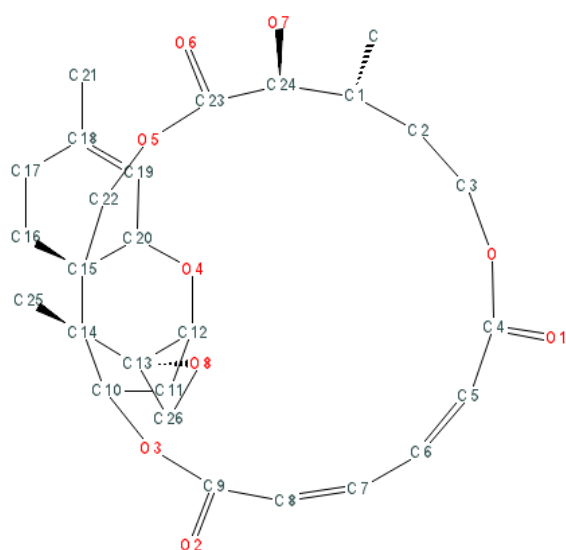
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		
87	q3	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		
87	D7	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
87	o7	1	Total	Zn	0	0
			1	1		

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

- Molecule 88 is (4S,5R,10E,12Z,16R,16aS,17S,18R,19aR,23aR)-4-hydroxy-5,16a,21-trimethyl-4,5,6,7,16,16a,22,23-octahydro-3H,18H,19aH-spiro[16,18-methano[1,6,12]trioxacyclooctadecino[3,4-d]chromene-17,2'-oxirane]-3,9,14-trione (three-letter code: 3L2) (formula: C₂₇H₃₄O₉).

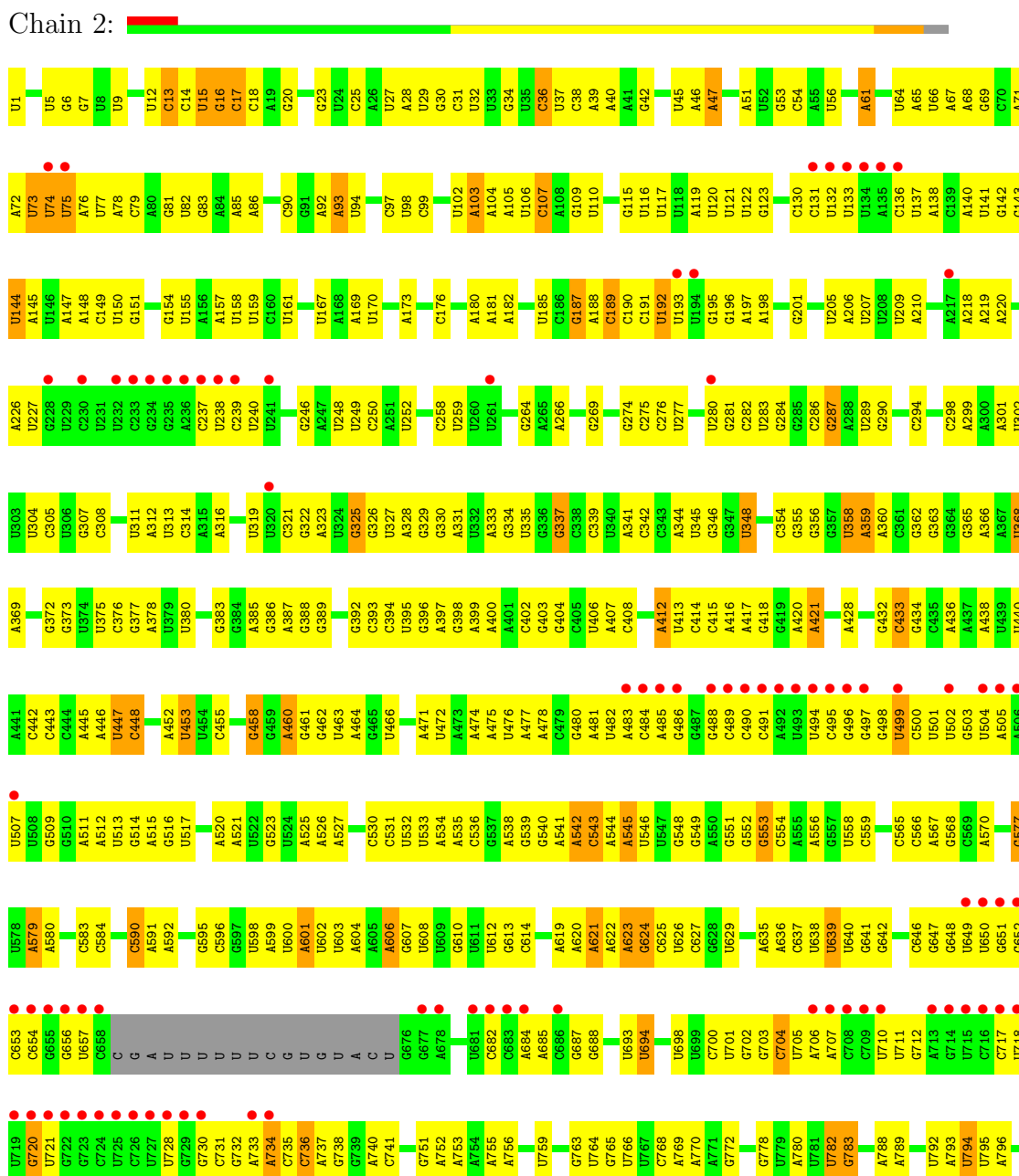


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			36	27	9		
88	5	1	Total	C	O	0	0
			36	27	9		

3 Residue-property plots

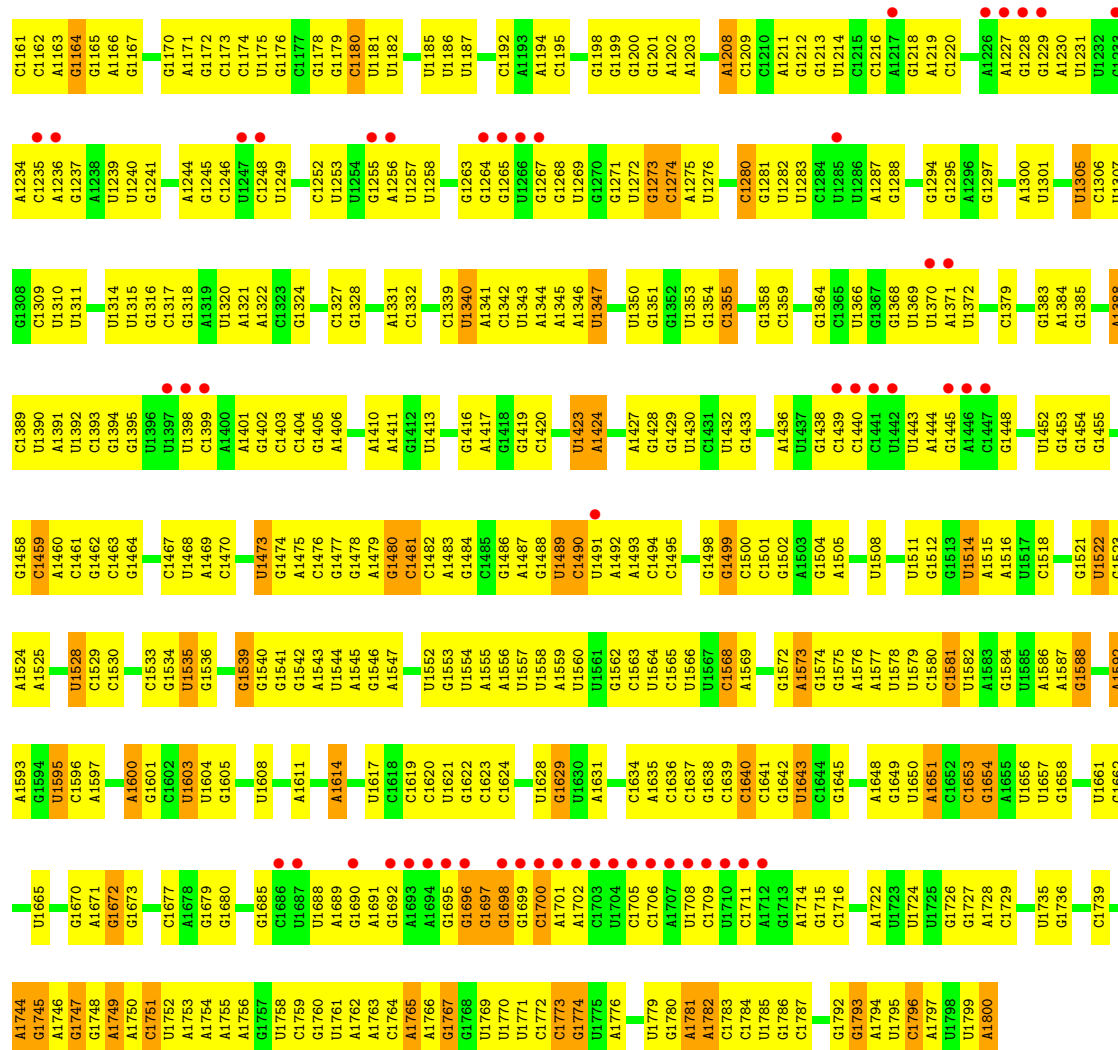
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



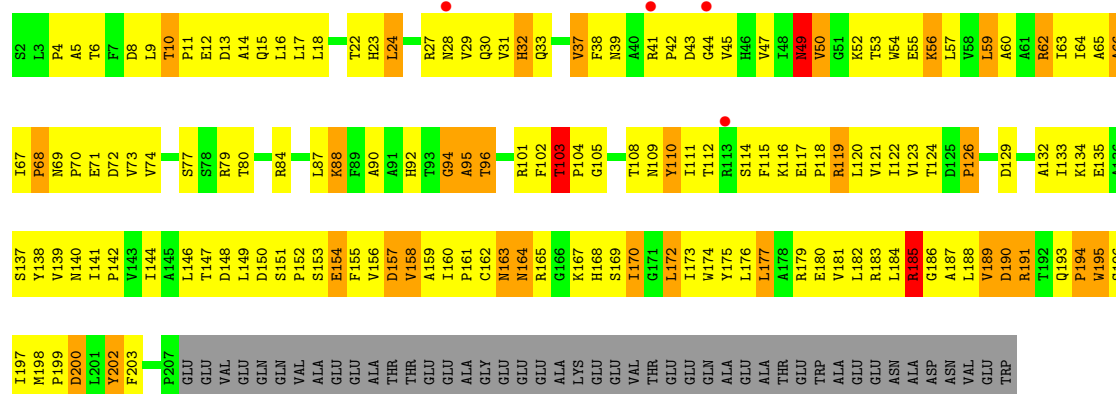


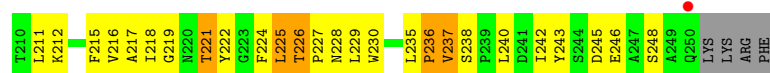




• Molecule 2: 40S ribosomal protein S0-A

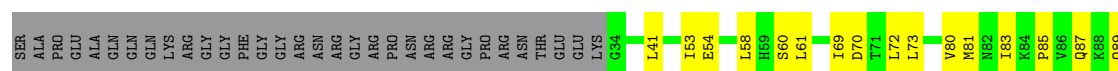
Chain S0:





• Molecule 4: 40S ribosomal protein S2

Chain s2:



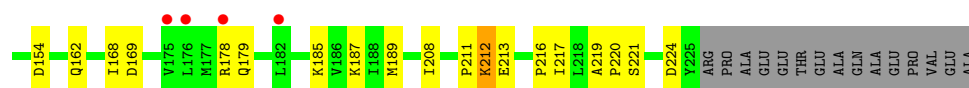
• Molecule 5: 40S ribosomal protein S3

Chain S3:



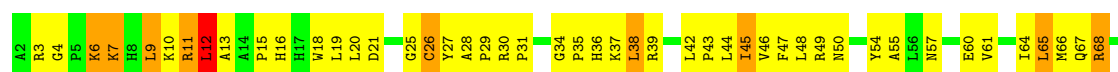
• Molecule 5: 40S ribosomal protein S3

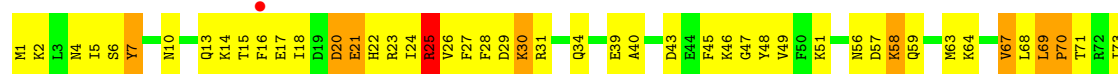
Chain s3:

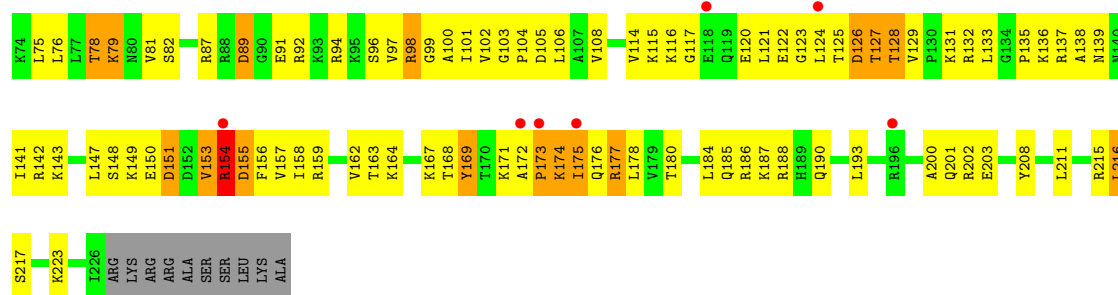


• Molecule 6: 40S ribosomal protein S4-A

Chain S4:

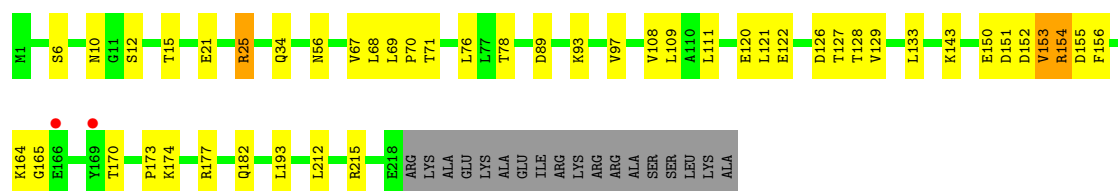






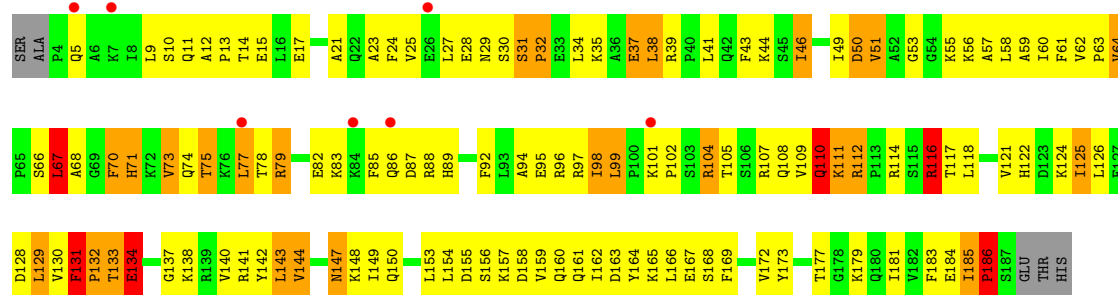
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



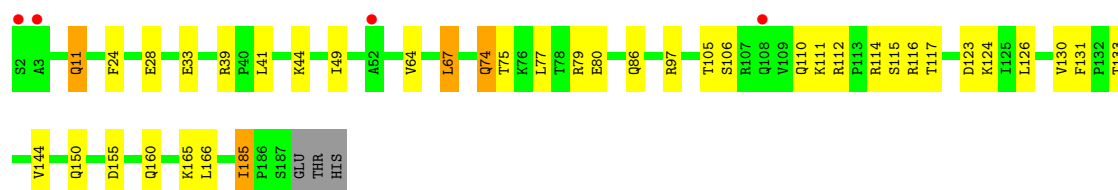
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



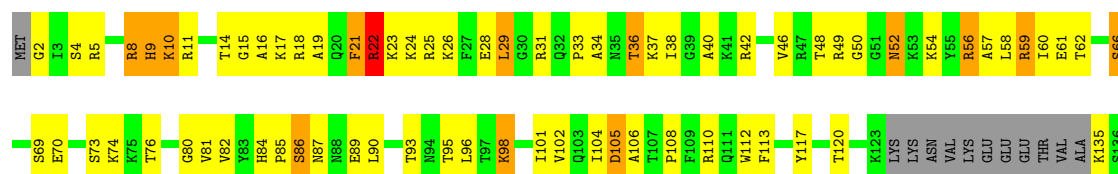
• Molecule 9: 40S ribosomal protein S7-A

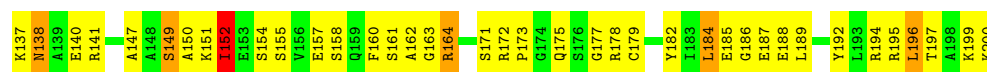
Chain s7:



• Molecule 10: 40S ribosomal protein S8-A

Chain S8:





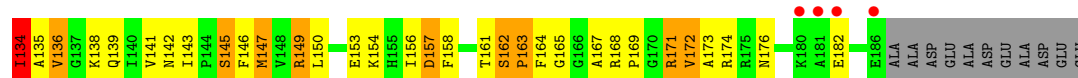
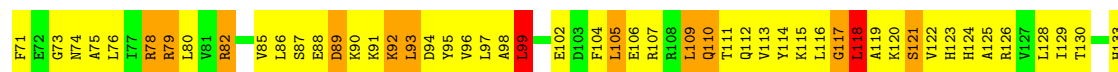
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



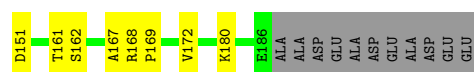
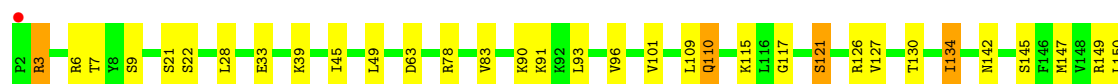
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



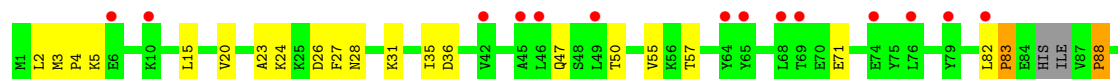
• Molecule 12: 40S ribosomal protein S10-A

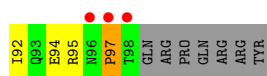
Chain C0:



• Molecule 12: 40S ribosomal protein S10-A

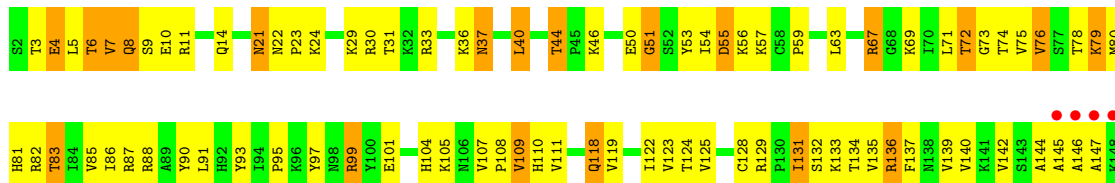
Chain c0:





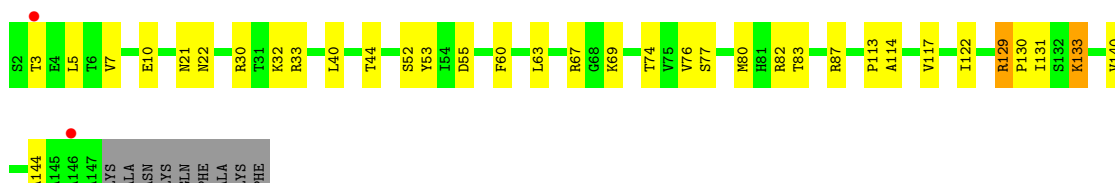
- Molecule 13: 40S ribosomal protein S11-A

Chain C1:



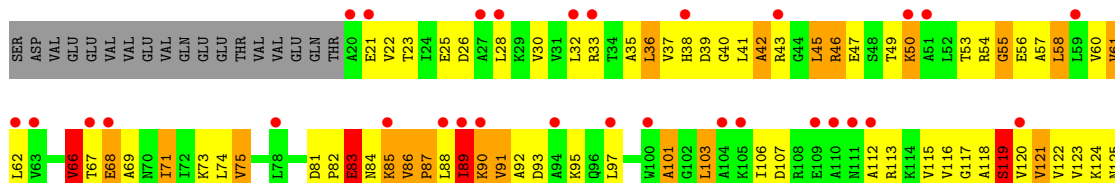
- Molecule 13: 40S ribosomal protein S11-A

Chain c1:



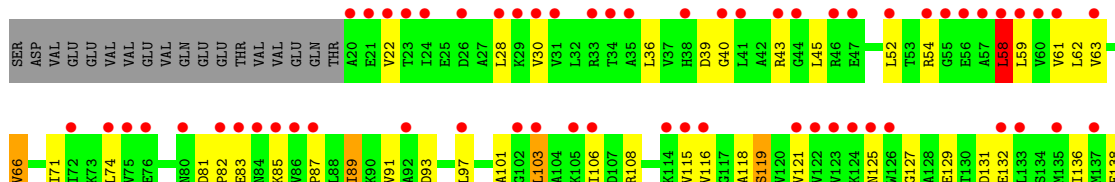
- Molecule 14: 40S ribosomal protein S12

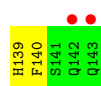
Chain C2:



- Molecule 14: 40S ribosomal protein S12

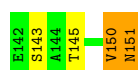
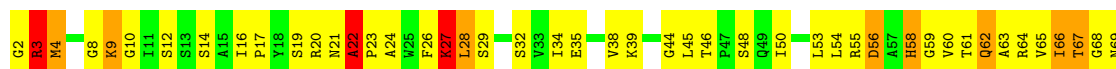
Chain c2:





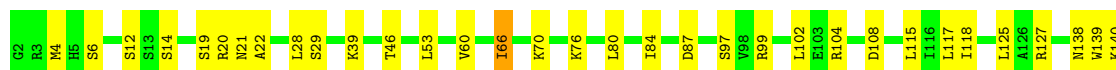
- Molecule 15: 40S ribosomal protein S13

Chain C3:



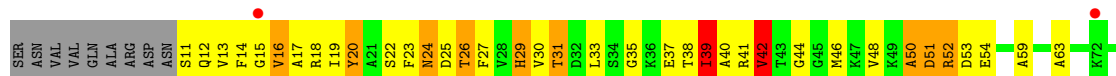
- Molecule 15: 40S ribosomal protein S13

Chain c3:



- Molecule 16: 40S ribosomal protein S14-A

Chain C4:



- Molecule 16: 40S ribosomal protein S14-A

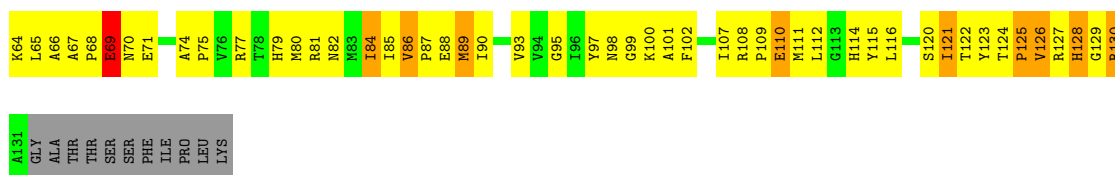
Chain c4:



- Molecule 17: 40S ribosomal protein S15

Chain C5:



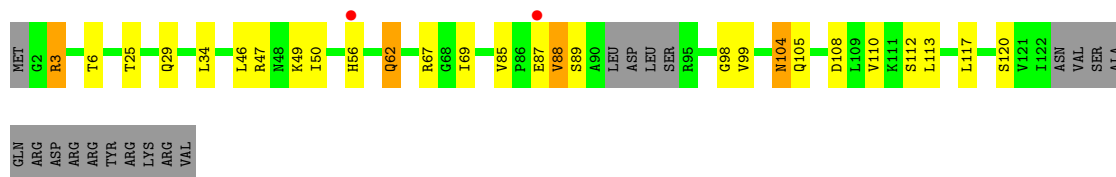


- Molecule 17: 40S ribosomal protein S15

Chain c5:

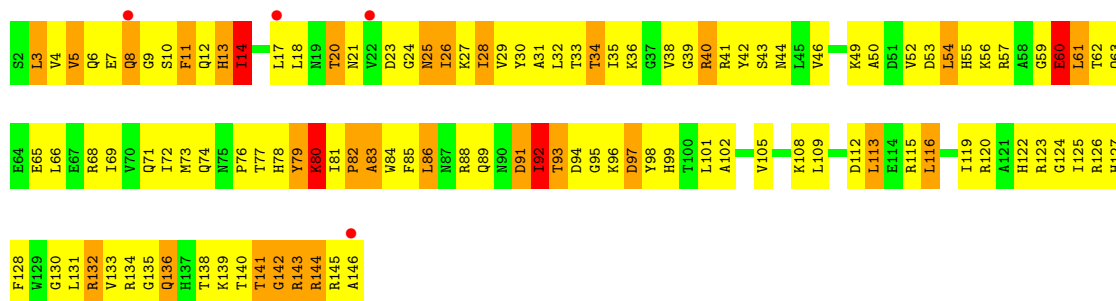
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:



- Molecule 20: 40S ribosomal protein S18-A

Chain C8:



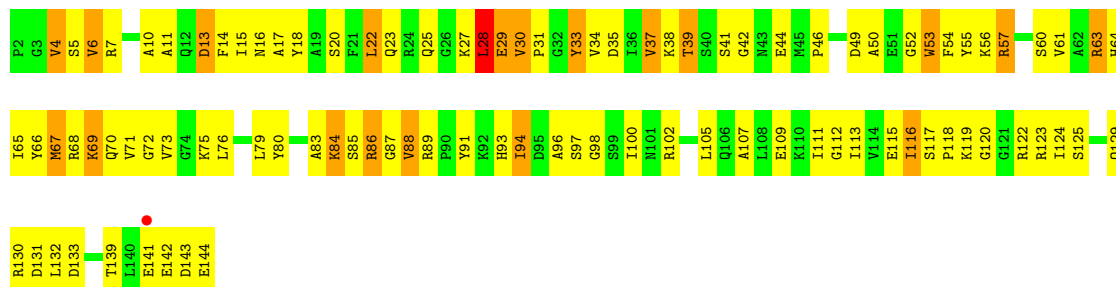
- Molecule 20: 40S ribosomal protein S18-A

Chain c8:



- Molecule 21: 40S ribosomal protein S19-A

Chain C9:



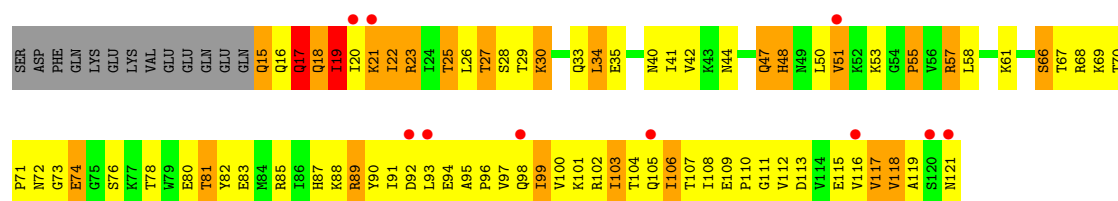
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



- Molecule 22: 40S ribosomal protein S20

Chain D0:



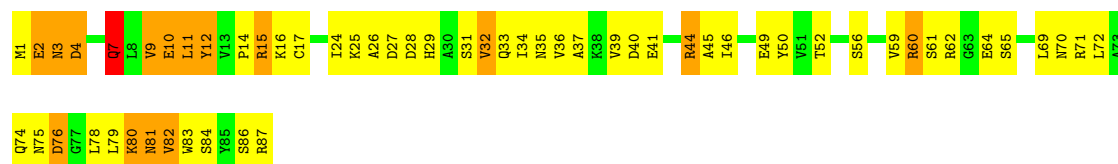
• Molecule 22: 40S ribosomal protein S20

Chain d0:



• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



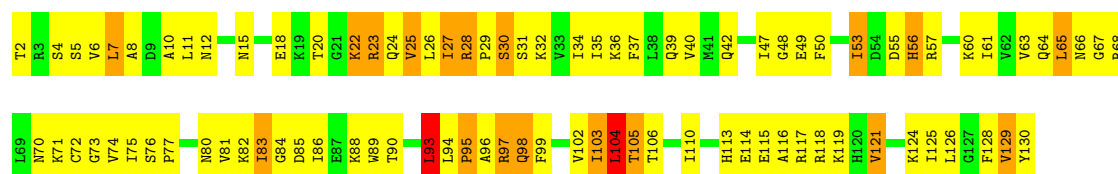
• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



• Molecule 24: 40S ribosomal protein S22-A

Chain D2:



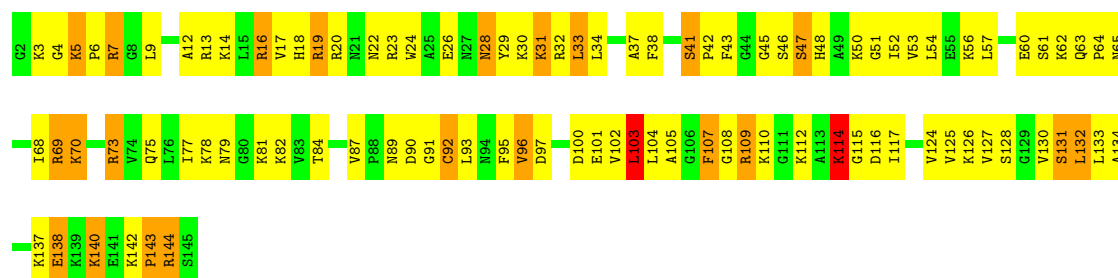
• Molecule 24: 40S ribosomal protein S22-A

Chain d2:



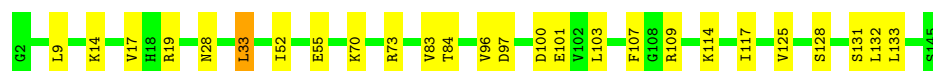
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



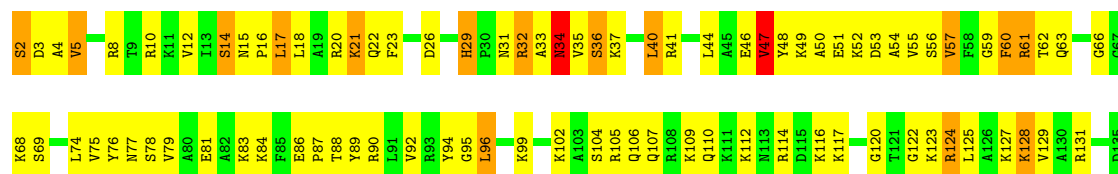
- Molecule 25: 40S ribosomal protein S23-A

Chain d3:



- Molecule 26: 40S ribosomal protein S24-A

Chain D4:



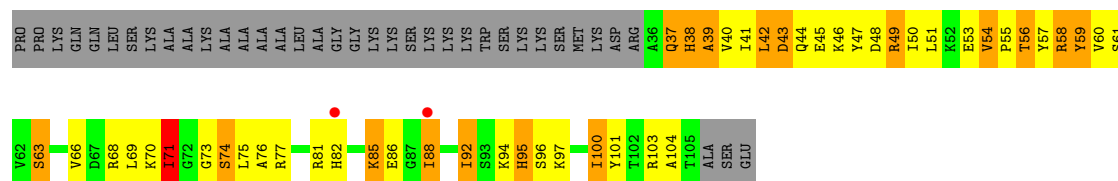
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:



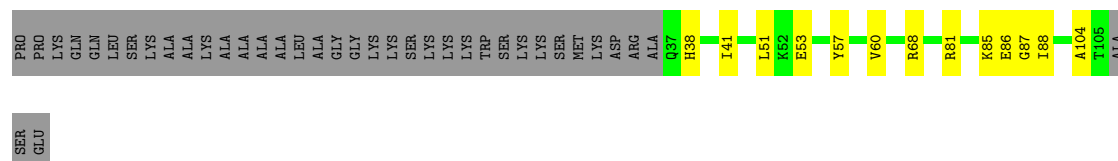
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:



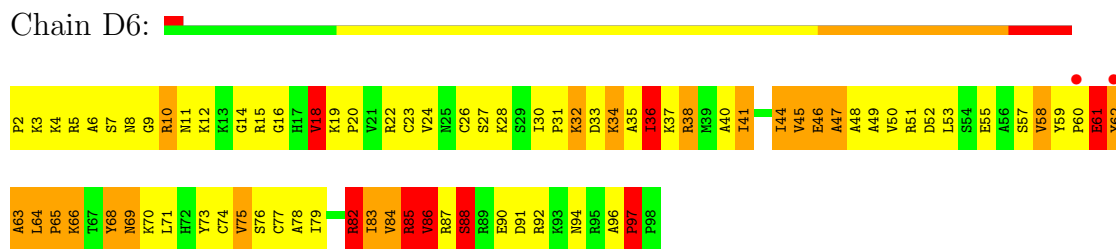
- Molecule 27: 40S ribosomal protein S25-A

Chain d5:



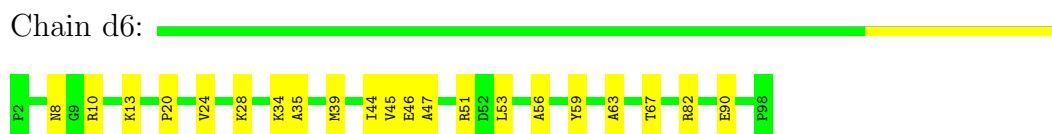
- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



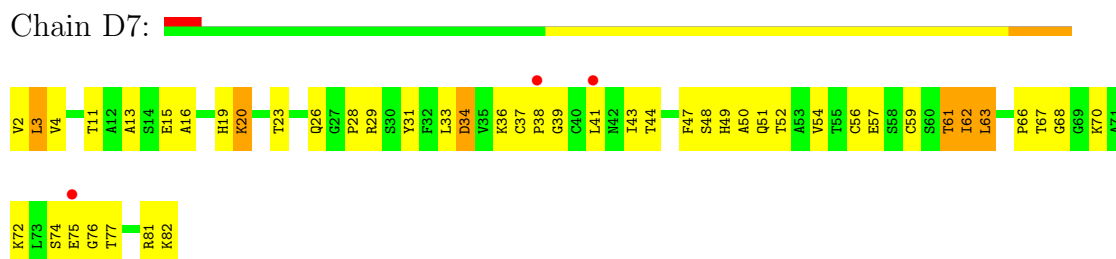
- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



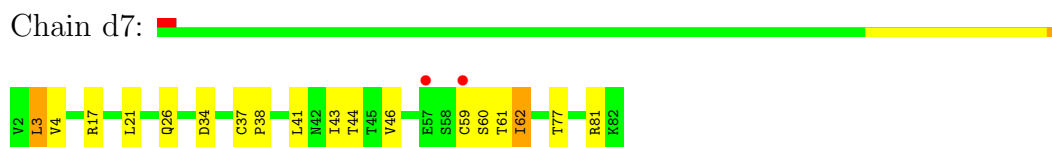
- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



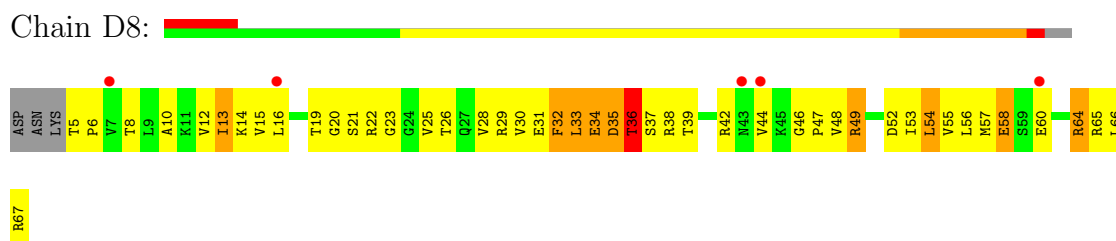
- Molecule 29: 40S ribosomal protein S27-A

Chain d7:



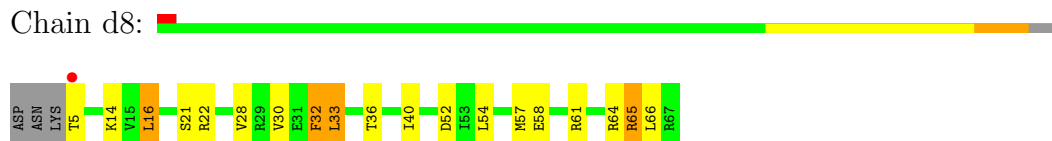
- Molecule 30: 40S ribosomal protein S28-A

Chain D8:



- Molecule 30: 40S ribosomal protein S28-A

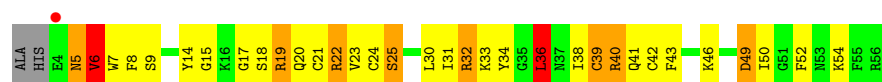
Chain d8:



- Molecule 31: 40S ribosomal protein S29-A

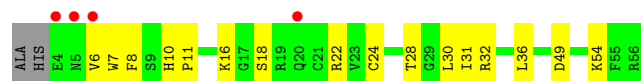
Chain D9:





- Molecule 31: 40S ribosomal protein S29-A

Chain d9:



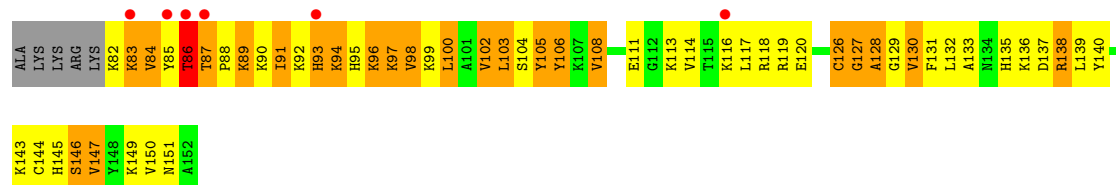
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:



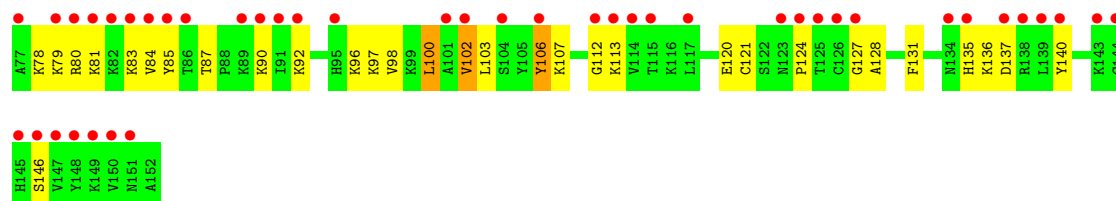
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



- Molecule 33: Ubiquitin-40S ribosomal protein S31

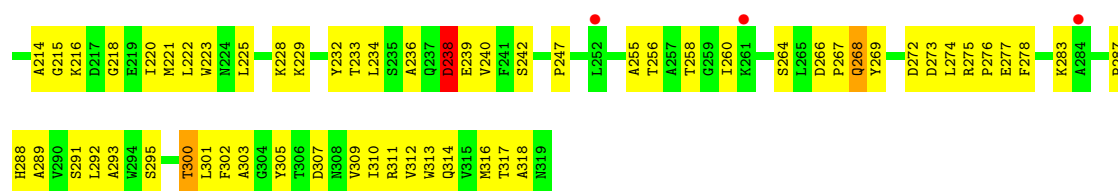
Chain e1:



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

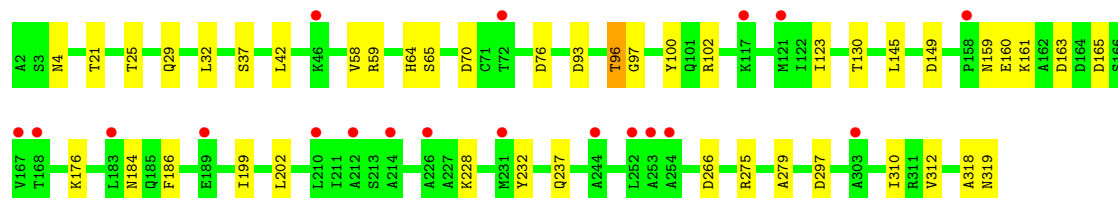
Chain SR:





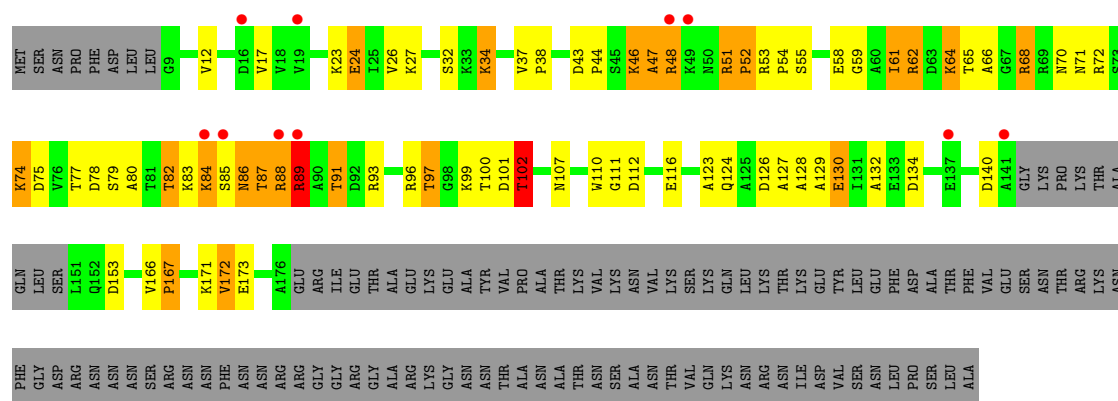
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



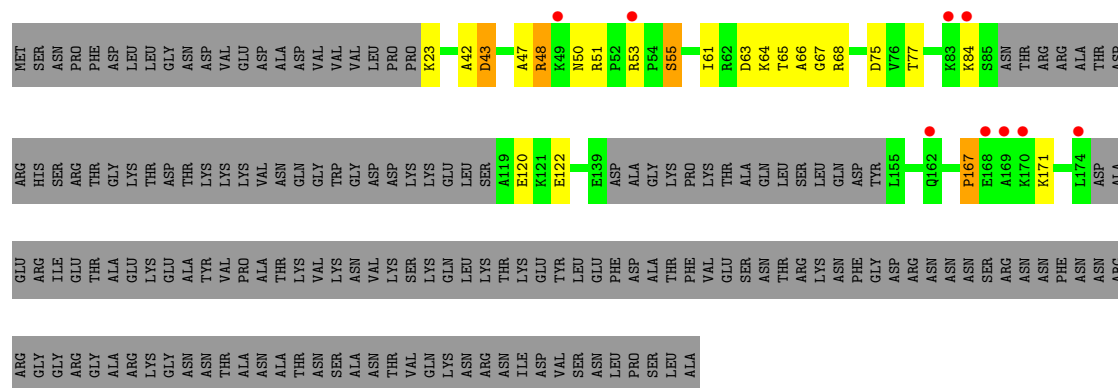
- Molecule 35: Suppressor protein STM1

Chain SM:



- Molecule 35: Suppressor protein STM1

Chain sM:



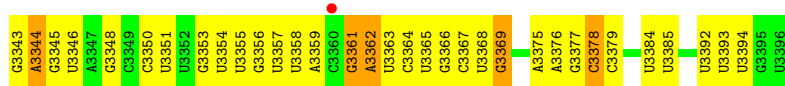
- Molecule 36: TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

Chain 1:

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A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101																																																																																																																																																																																																																																																																																																																																																								
U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024																																																																																																																																																																																																																																																																																																																																																														
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A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024																																																																																																																																																																																																																								
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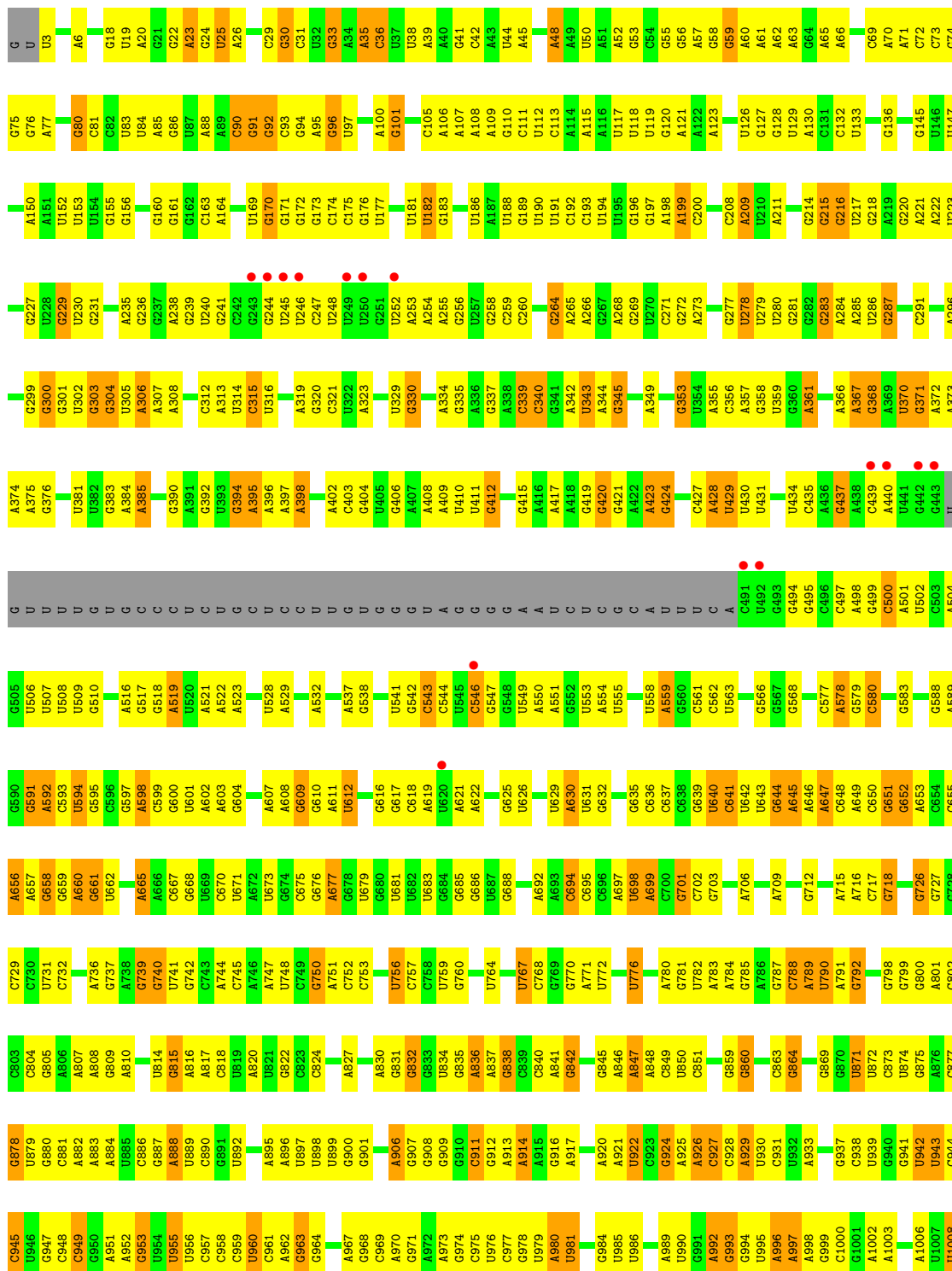


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C3272	G3188	U3118	A3046	G2898	U2829	C2755	U2688	G2620	U2541	U2410	C2344	A2263
		C3120	U3047	A2900	G2830		C2756	G2621	U2542	U2411		U2264
U3275	G3191	U3121	A3048	G2901	G2831	C2760	A2692	G2623	U2543	G2412	U2349	C2265
G3276	U3192	A3122	U3049	A2902	G2832	G2761	C2693	G2624	U2544	A2413	U2350	U2266
U3277	C3193	A3123	U3050	A2903	A2833	G2762	A2694	C2625	C2545	G2414	U2351	C2267
C3278	G3194	U3124	U3051		G2834	U2763	A2695	A2626	C2546	U2415	A2352	U2268
A3279	U3195	G3125	G3052	G2908	U2835	U2764	A2696	G2627	U2547	U2416	G2353	
U3280	G3196	C3126	G3053		U2836	C2765		A2628	C2549	G2417	G2354	U2274
U3281	G3197	U3054	U3054	U2911	G2840	U2766	G2699	U2629	U2550	A2419	A2355	
U3282	U3198	U3055	U3055	U2912	G2841	U2767	G2700	C2630			A2357	C2278
U3283	G3199	U3056	U3056	C2913	U2842	U2768	U2701	U2631	A2554	C2422	A2358	A2279
G3284	G3200	C3132	U3057		U2843	A2769	A2702	G2632		U2423	C2359	A2280
C3285	C3201	C3133	U3057	U2916	U2844		A2703	U2633	U2557	A2424	A2360	A2281
G3286	G3202	G3060	G3060	G2918	G2845	U2771	A2704	U2634		G2425	A2361	U2282
U3287	C3203	G3061	G3061	G2917	U2846	C2772	A2705	A2635	C2560	U2426	C2362	G2283
U3288	C3204	C3137	G3062	A2919	U2846	C2773	G2706	A2636	U2561	U2427	A2363	C2284
G3289		U3138	G3063	U2920		C2774	C2707	A2637	A2562	U2428	G2364	
		A3139	U3064	U2921	G2850	U2775	C2708	C2638	G2563	G2429	C2365	C2287
U3293	A3209	G3140	G3065	U2922	A2851	C2776	C2709	C2639			C2366	
A3294	A3141	U3066	U3066	U2923	U2852	G2777	C2710		C2567	U2433		U2294
A3295	C3142	C3067	C3067	U2924	U2853	G2778	C2711	A2642	A2569	U2434	G2369	A2295
	G3143			C2925	U2854		C2712	A2643	C2568		G2370	A2296
C3298	U3214	A3070	A3070	A2926	U2855	G2779	U2713	C2644	U2570	A2438	G2371	U2297
A3299	A3215	C3071	C3072	C2927	G2856		G2714	G2645	U2571	A2439	A2372	U2298
U3300	G3216	U3148	U3072	C2928	C2857		U2715	G2646	C2572	U2440	A2373	A2299
U3301	C3217	G3073	A3073	U2858	G2787		U2716	A2647	G2573	U2501	C2374	G2300
U3302	A3218	U3152	C3074	A2930	G2787		U2717	C2648	A2502	G2442	G2375	U2301
G3303	G3219	C3153	G3074	U2859	U2717		U2718		G2503	U2443	G2376	G2302
U3304	G3220	U3154	U3078	C3002	U2860	A2790	U2719		U2578	C2444	G2377	A2303
A3305		C3155	U3079	G3003	U2861			G2651	U2581	A2445	C2378	C2304
U3306		U3156	C3082	A2983	U2862	G2794	U2722	U2652	C2582	U	U2379	G2305
A3307	G3224	U3157	G3083	A2984	G2863	U2795	U2723	C2653	C2583	A	G2380	C2306
G3308	C3225	G3158	C3084	U2985	U2865	C2797	U2724	A2656	C2584	G	G2381	C2307
G3309	G3226	G3159	G3085	G2986	U2868	A2799	U2725	G2657	G2585	A	G2382	C2308
A3310	U3231	U3160	G3086	A2940	G2869	G2800	C2726	G2658	G2586	G	C2383	A2309
		C3161	A3087	C2942	C2870	A2801	G2727	G2659	U2587	G	A2384	U2310
U3313	A3234	C3164	G3088	G2943	G2871	A2802	U2729	G2660	C2592	U2513	G2385	
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A3316	A3167	C3166	C3092	G2945	U2873	A2804	U2731	G2663	C2594	U	U2388	U2314
U3317	G3242	A3167	C3093	A2946	G2874		G2732	C2664		A	G2391	A2317
G3318	A3243	A3168	A3094	G2947	U2875		A2733	U2665	A2601	G	C2392	
U3319	G3246	U3169	U3095	U2948	C2876		A2734	C2666	G2602	A	C2393	A2320
A3320		A3170	U3100	U2949			U2735		G2603	A	G2394	
	G3247	G3173	G3101	G2952	U2880	C2809	C2810	A2671	U2604	U	G2395	A2324
G3325	C3248	A3174	G3102	U2953	C2881	A2811	G2812	G2672	G2605	A	A2397	G2325
G3326		U3175	A3103	U2954	U2882	A2813	C2737	A2673	G2606	G	A2398	U2327
		G3176			C2884	G2814				U	A2399	
U3333	G3252	G3177	A3106	A2958	U2885	G2815	U2744	C2675	A2609	G	G2400	
U3334	G3259	A3178	U3107	G2959	U2886	A2816	G2745	A2676	G2610	U	C2401	C2333
A3335	C3260	U3179	G3108	C2960	U2887	U2817	A2746	G2677	U2611	G	A2402	U2334
G3336	C3261	U3180	G3109	C2961	U2888	U2818	A2747	A2678	G2612	A	G2403	G2335
U3337		C3181	G3112	A3085	A2890	U2819	G2748	A2679	U2613	G	A2404	
C3338		C3182	A3113	C3039	U2891	A2820	G2749	A2680	G2614	U	G2405	
A3339	G3265	A3183	A3114	U2965	A2892	A2821	U2750	U2681	G2615	C	C2406	C2340
	G3266	G3266	C3115	U2966	C2893	G2823	G2751	C2682	C2616	U	U2337	
A3342	A3267			G2966	C2894	U2752	U2752	U2683	U2617		U	A2341



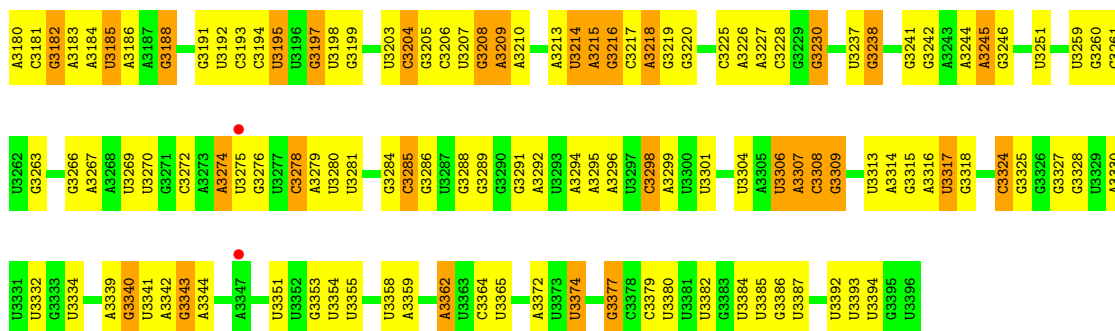
● Molecule 36: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 5:



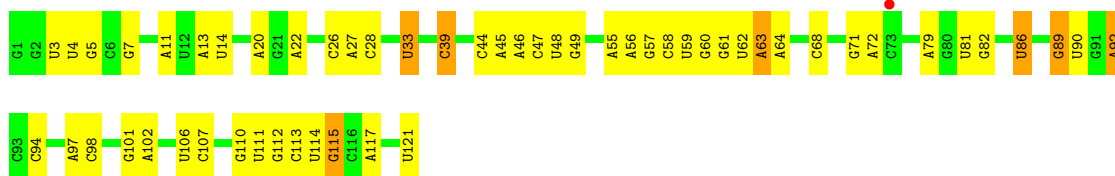
WORLDWIDE
PDB
PROTEIN DATA BANK

G3108	G3109	A3035	U2954	C2889	C2824	U2752	C2687	U2617	C2539	G	G2414	U2349	C2202	A2131
U2955	C2956	U2891	C2825	A2890	C2826	G2753	U2688	G2618	A2540	G	C2416	U2350	U2203	C2132
C2957	U2837	A2892	U2826	C2889	U2827	C2756	A2689	G2619	U2541	C	U2416	U2351	C2204	G2133
A2958	C2828	C2893	G2828	C2894	C2829	U2757	A2691	G2620	U2542	C	U2417	U2352	U2205	G2134
C2959	C2832	C2897	C2832	C2897	C2832	U2758	A2692	G2622	C2546	A	G2418	G2353	A2206	A2138
U2960	A2833	C2898	A2833	C2898	A2833	U2759	C2693	G2623	C2549	U	C2420	C2354	A2208	A2139
C2961	U2834	C2899	C2834	C2899	U2834	G2760	A2695	G2624	U2550	G	U2421	G2355	U2209	U2140
U2962	C2835	A2899	U2835	A2899	C2835	G2761	A2696	G2625	U2551	A	C2422	C2356	G2210	U2141
C2963	C2836	A2900	C2836	A2900	C2836	U2762	A2697	G2626	U2552	A	U2423	A2357	U2211	A2142
G3112	U2837	C2901	A2837	C2901	U2837	U2763	C2698	C2627	C2553	A	A2424	C2358	C2212	A2143
A3113	C2837	C2902	C2837	C2902	C2837	G2764	G2698	U2628	U2554	U	G2425	C2359	A2213	A2144
C3114	C2840	A2903	C2840	A2903	C2840	G2765	C2699	U2629	C2555	A	U2426	C2360	A2214	A2145
C3115	U2841	U2904	U2841	U2904	U2841	U2766	G2700	C2630	C2556	C	G2429	A2361	A2215	C2146
U3119	C2970	U2905	C2842	U2905	C2842	U2767	U2701	U2631	C2557	C	A2430	C2362	A2222	A2147
C3120	A2971	C2906	U2843	C2906	U2843	U2768	A2702	G2632	A2558	A	U2431	C2363	U2223	A2148
U3121	C2972	C2907	C2844	C2907	C2844	U2771	A2703	U2633	C2559	U	U2432	C2364	A2224	A2149
A3122	C2973	C2907	C2844	C2907	C2844	U2772	A2705	U2634	C2560	C	U2433	C2365	U2225	A2152
C3123	C2974	C2907	C2844	C2907	C2844	U2773	C2706	G2639	A2561	A	U2434	C2366	U2226	U2153
G3136	U2975	A2911	C2847	A2911	C2847	C2774	C2707	A2640	A2562	C	U2435	A2367	C2227	U2154
C3137	C2976	C2912	C2848	C2912	C2848	U2775	C2708	U2641	G2563	C	U2436	C2368	G2156	C2156
U3138	C2977	C2913	C2849	C2913	C2849	U2776	C2709	A2642	G2564	U	U2437	G2370	C2231	G2157
A3139	U2978	G2914	A2851	G2914	A2851	G2777	C2710	C2643	C2568	U	A2438	C2371	A2232	A2158
C3140	U2979	U2915	C2852	U2915	C2852	G2778	C2711	C2644	U2570	A	G2440	A2372	U2233	U2159
U3141	U2980	U2916	A2853	U2916	A2853	U2779	C2712	C2645	C2572	C	A2441	A2373	G2234	G2160
C3142	C2983	C2917	U2854	C2917	U2854	A2780	U2713	G2648	U2573	A	U2442	C2374	G2235	G2161
C3143	U2984	U2918	C2855	U2918	C2855	C2780	U2714	A2649	C2574	U	C2444	C2375	G2236	G2162
G3149	C2985	C2921	C2856	C2921	C2856	U2790	U2715	U2650	C2575	U	A	U2380	G2239	G2163
U3150	U2986	U2924	U2860	U2924	U2860	C2795	U2716	G2652	C2577	C	U	G2381	G2240	A2164
C3151	C2987	C2925	U2861	C2925	U2861	C2796	U2717	C2653	C2578	C	U	G2382	A2244	G2165
U3152	U2988	A2926	U2862	A2926	U2862	C2797	U2718	U2654	C2579	A	G	C2383	C2245	A2168
C3153	C2989	C2927	U2863	C2927	U2863	U2798	U2719	C2655	A2580	U	A	G2384	G2246	G2169
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C3155	C2991	C2929	U2865	C2929	U2865	U2799	U2721	C2657	C2585	U	G	A2386	G2248	G2171
U3156	U2992	A2930	C2867	A2930	C2867	C2798	U2722	U2658	C2586	U	A	G2387	G2249	U2172
C3157	C2993	C2931	U2868	C2931	U2868	U2799	U2723	U2659	C2587	C	U	G2388	G2250	U2173
G3158	A3000	C3001	C2869	A3000	C2869	C2798	U2724	C2660	U2588	U	G	C2389	A2255	G2174
C3159	C3001	C3002	C2870	C3001	C2870	U2799	U2725	C2661	C2589	C	U	C2390	A2256	G2177
U3160	U2935	U2936	C2871	U2935	C2871	U2806	U2726	C2662	C2594	U	A	G2391	C2257	A2178
C3069	A2936	A2936	C2872	A2936	C2872	U2807	U2727	C2663	C2595	U	G	U2327	U2258	C2179
A3163	C3004	A3005	U2873	C3004	U2873	C2812	U2730	C2664	C2596	C	A	C2328	G2261	G2180
C3164	U2874	C2874	C2874	U2874	C2874	U2813	U2731	U2665	U2597	U	U	C2329	G2262	C2181
A3165	C2875	C2875	C2875	C2875	C2875	C2814	U2732	C2666	C2598	A	A	C2330	A2263	U2186
C3166	U2876	C2876	C2876	U2876	C2876	C2815	U2733	C2667	C2599	C	U	C2331	U2264	U2190
A3167	C2877	C2877	C2877	C2877	C2877	C2816	U2734	C2668	C2600	U	A	A2332	G2265	U2191
U3168	C2878	C2878	C2878	C2878	C2878	C2817	U2735	C2669	C2601	C	U	A2333	U2266	C2192
C3169	U2879	C2879	C2879	U2879	C2879	C2818	U2736	C2670	C2602	U	G	U2334	G2267	U2193
A3173	U2880	C2880	C2880	U2880	C2880	C2819	U2737	C2671	C2603	U	G	C2335	U2268	G2194
C3174	C2881	C2881	C2881	C2881	C2881	C2820	U2738	C2672	C2604	C	U	U2336	G2269	C2195
U3175	U2882	C2882	C2882	U2882	C2882	C2821	U2739	C2673	C2605	U	G	C2337	U2270	A2198
C3176	U2883	C2883	C2883	U2883	C2883	C2822	U2740	C2674	C2606	U	G	U2338	G2271	G2199
U3177	U2884	C2884	C2884	U2884	C2884	C2823	U2741	C2675	C2607	C	U	C2339	A2272	U2200
C3178	U2885	C2885	C2885	U2885	C2885	C2824	U2742	C2676	C2608	U	G	U2340	G2273	G2201
U3179	U2886	C2886	C2886	U2886	C2886	C2825	U2743	C2677	C2609	C	U	U2341	G2274	
	U2887	C2887	C2887	U2887	C2887	C2826	U2744	C2678	C2610	U	G	U2342	G2275	
	U2888	C2888	C2888	U2888	C2888	C2827	U2745	C2679	C2611	C	U	U2343	G2276	
						C2828	U2746	C2680	C2612	U	G	C2344	G2277	
						C2829	U2747	C2681	C2613	C	U	U2345	G2278	
						C2830	U2748	C2682	C2614	U	G	C2346	A2279	
						C2831	U2749	C2683	C2615	C	U			
						C2832	U2750	C2684	C2616	C	U			
						C2833	U2751	C2685	C2617	C	U			



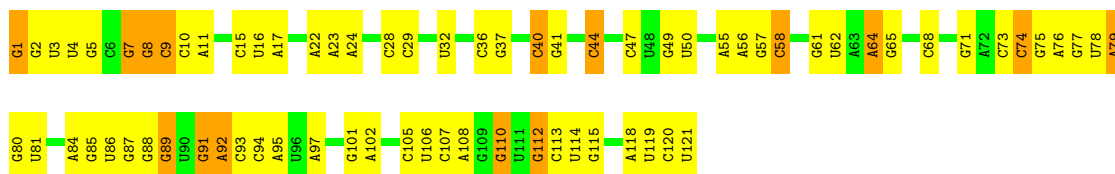
- Molecule 37: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 3:



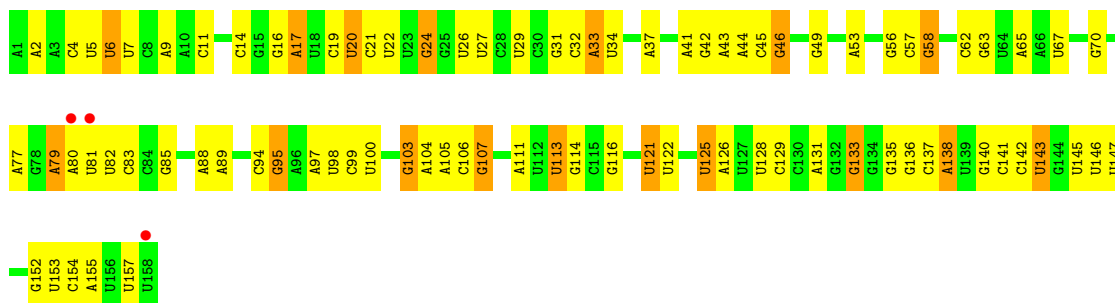
- Molecule 37: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 7:



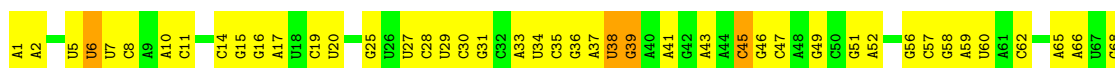
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

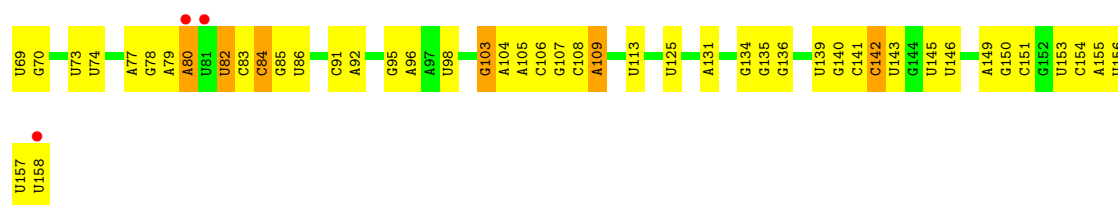
Chain 4:



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

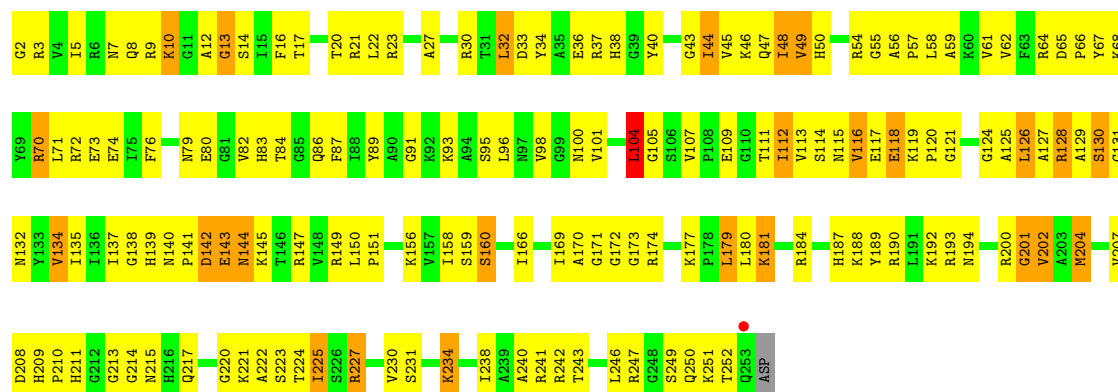
Chain 8:





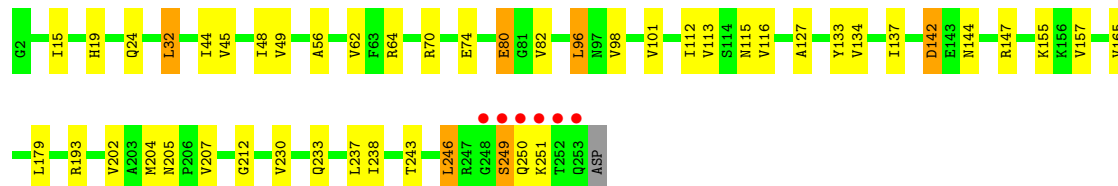
• Molecule 39: 60S ribosomal protein L2-A

Chain L2:



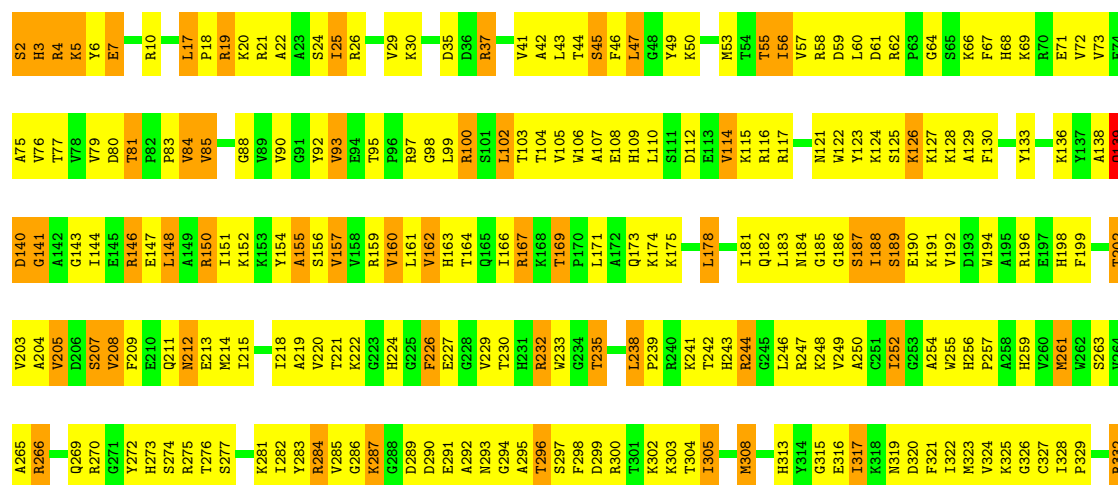
• Molecule 39: 60S ribosomal protein L2-A

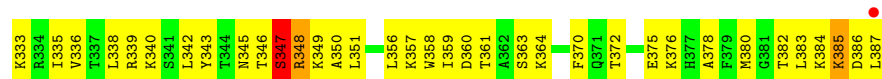
Chain L2:



• Molecule 40: 60S ribosomal protein L3

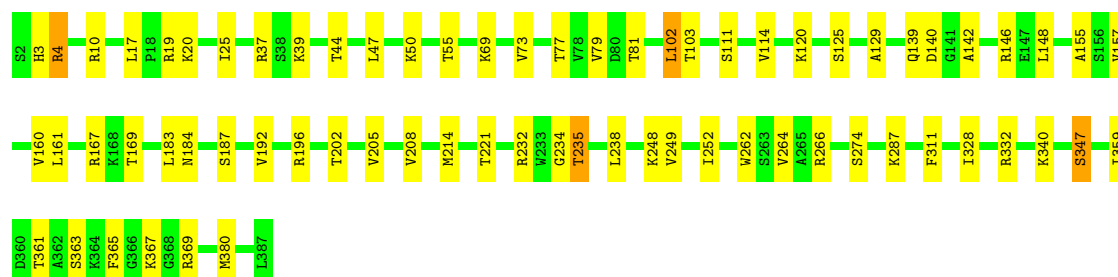
Chain L3:





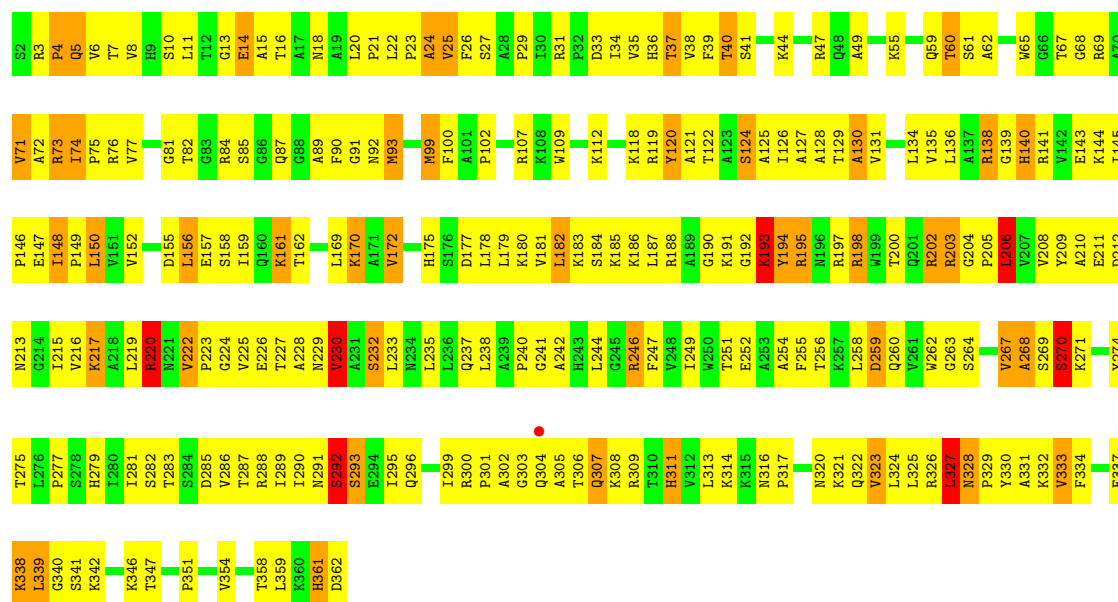
• Molecule 40: 60S ribosomal protein L3

Chain 13:



• Molecule 41: 60S ribosomal protein L4-A

Chain L4:

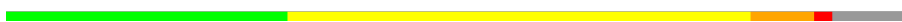
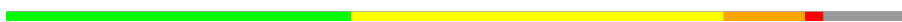


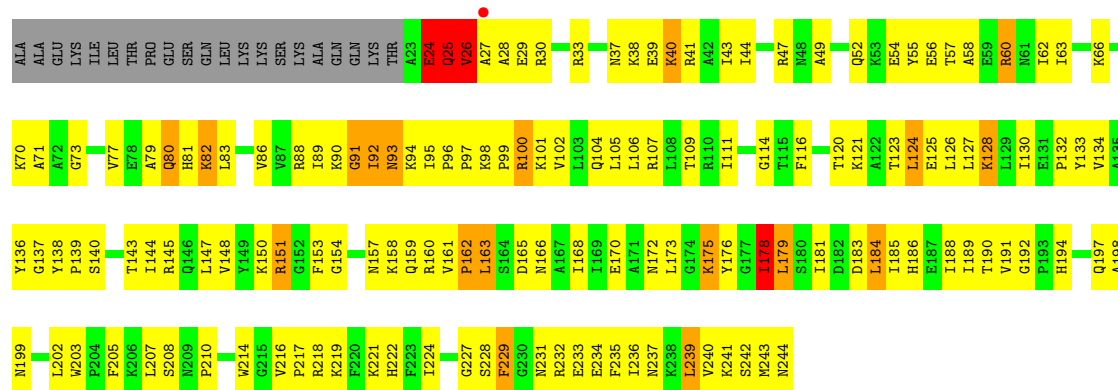
• Molecule 41: 60S ribosomal protein L4-A

Chain 14:



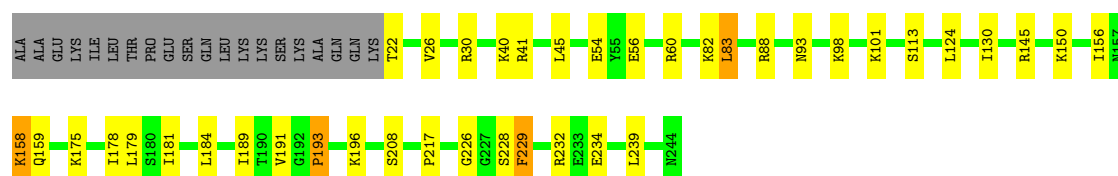
• Molecule 42: 60S ribosomal protein L5





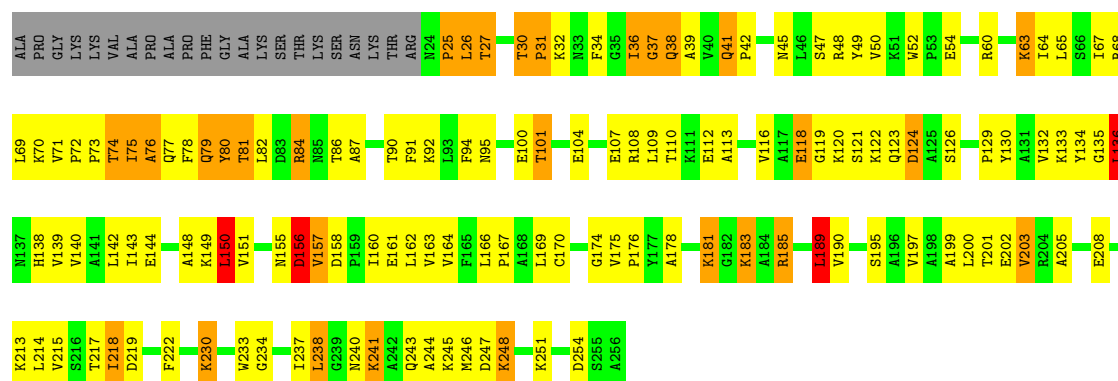
• Molecule 44: 60S ribosomal protein L7-A

Chain 17:



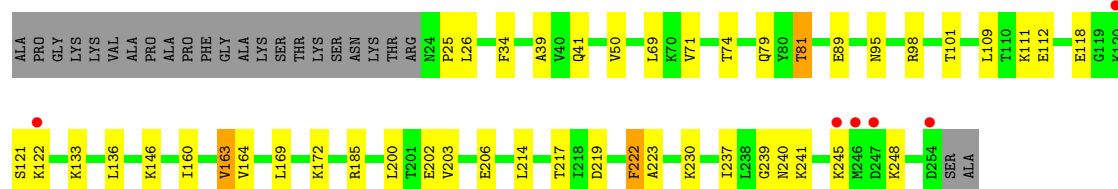
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



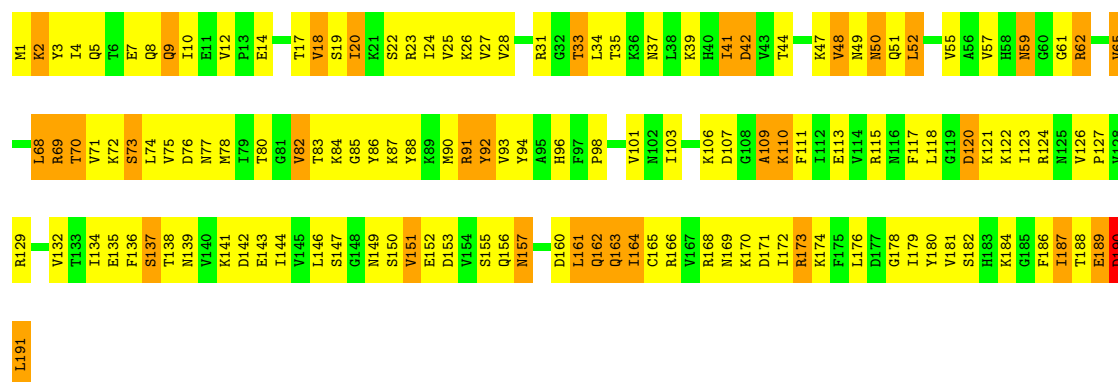
• Molecule 45: 60S ribosomal protein L8-A

Chain 18:



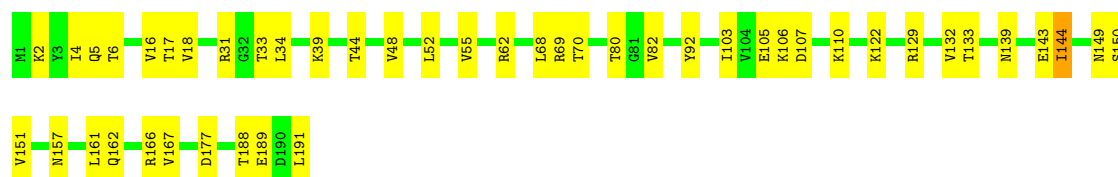
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



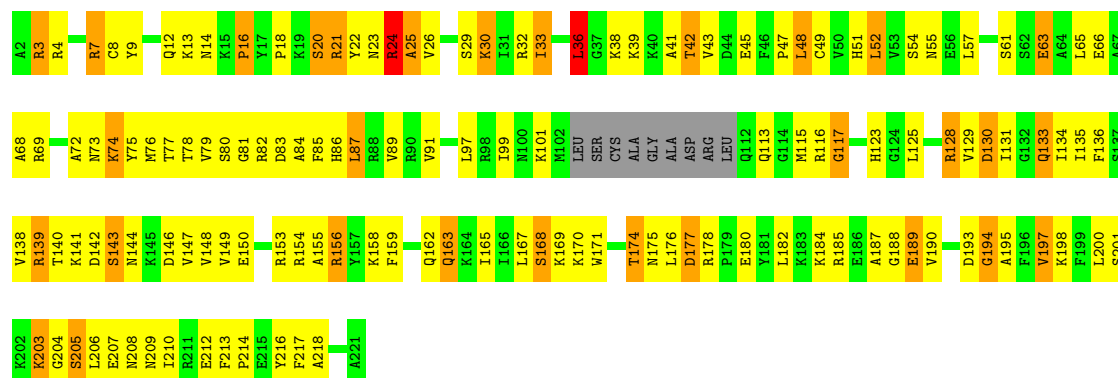
- Molecule 46: 60S ribosomal protein L9-A

Chain I9:



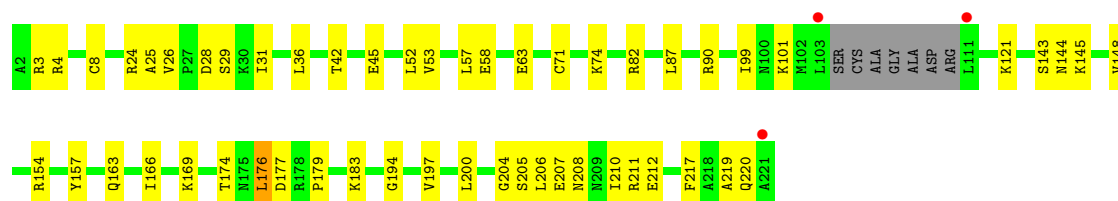
- Molecule 47: 60S ribosomal protein L10

Chain M0:



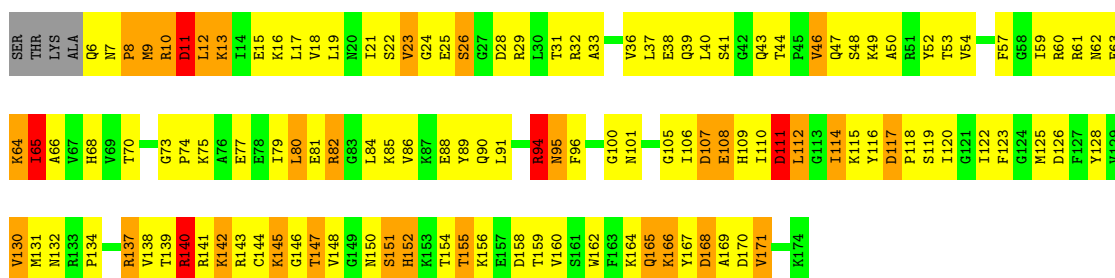
- Molecule 47: 60S ribosomal protein L10

Chain m0:



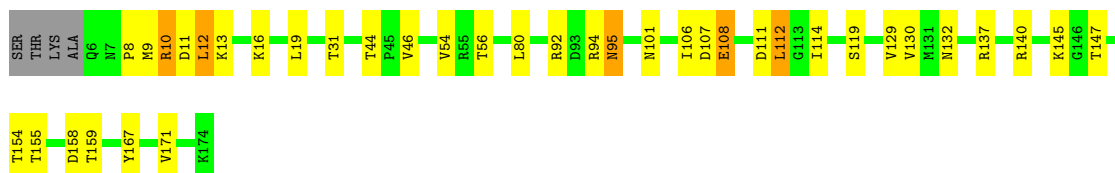
- Molecule 48: 60S ribosomal protein L11-B

Chain M1:



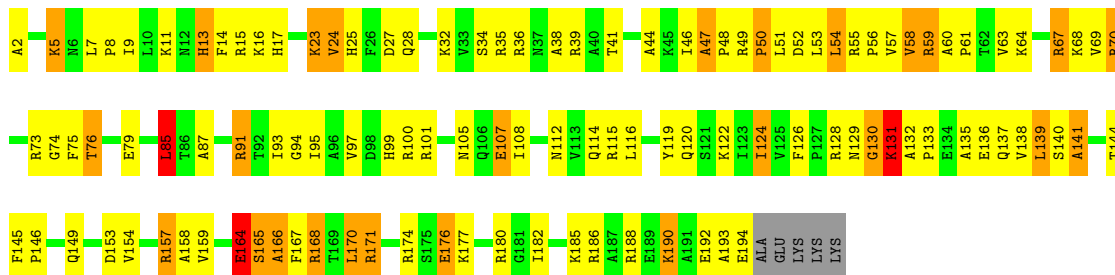
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



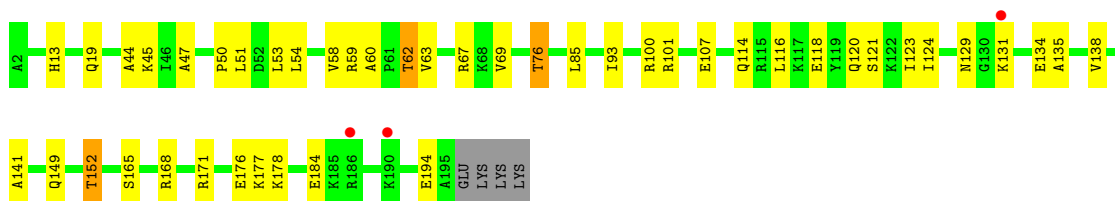
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



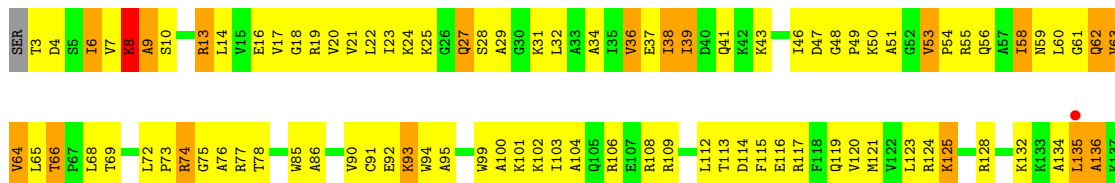
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



A138

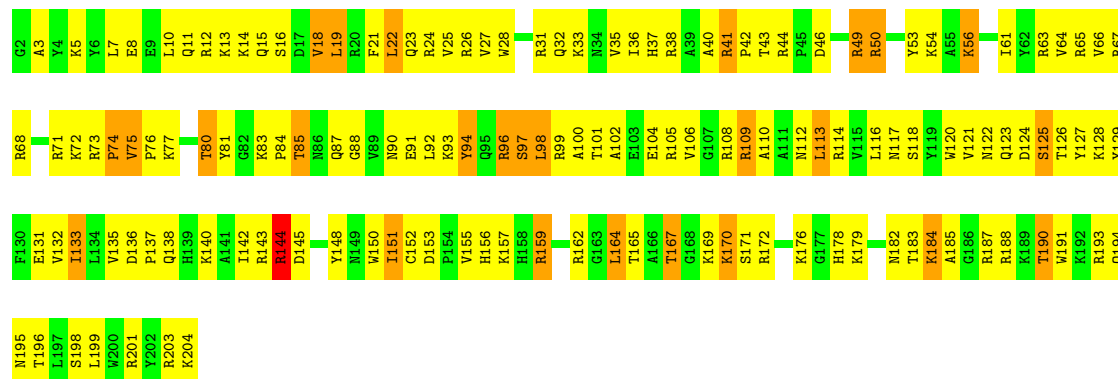
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:



- Molecule 51: 60S ribosomal protein L15-A

Chain M5:



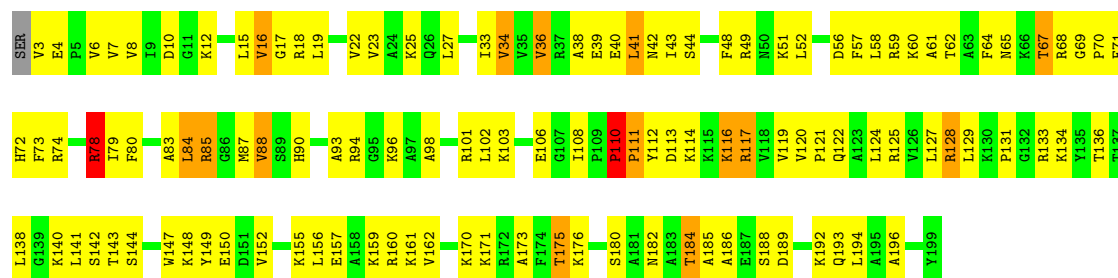
- Molecule 51: 60S ribosomal protein L15-A

Chain m5:



- Molecule 52: 60S ribosomal protein L16-A

Chain M6:



- Molecule 52: 60S ribosomal protein L16-A

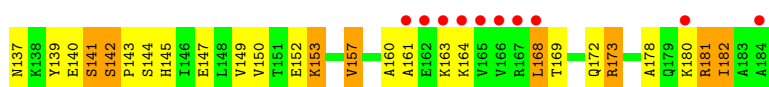
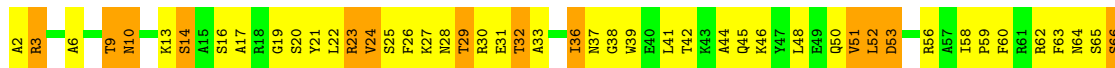
Chain m6:





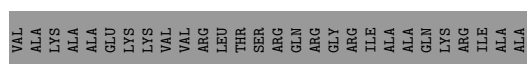
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:



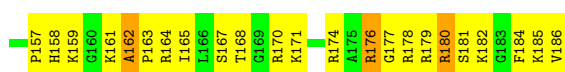
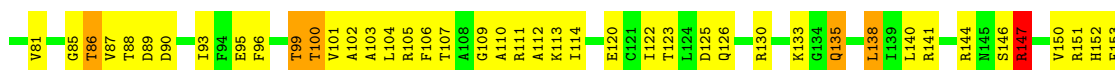
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:



- Molecule 54: 60S ribosomal protein L18-A

Chain M8:



- Molecule 54: 60S ribosomal protein L18-A

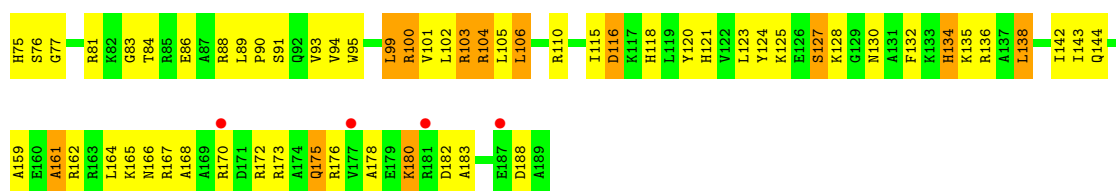
Chain m8:



- Molecule 55: 60S ribosomal protein L19-A

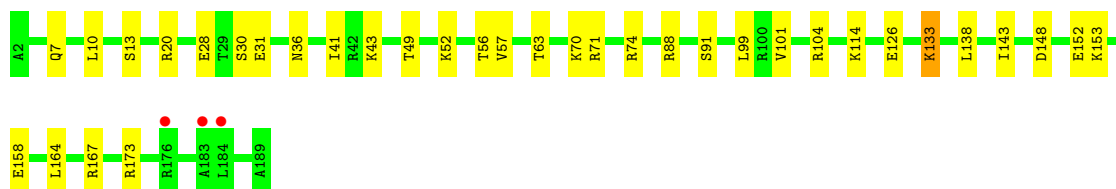
Chain M9:





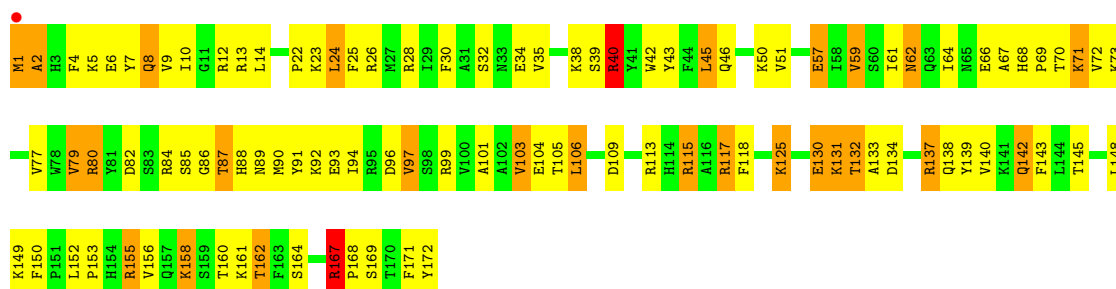
- Molecule 55: 60S ribosomal protein L19-A

Chain m9:



- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



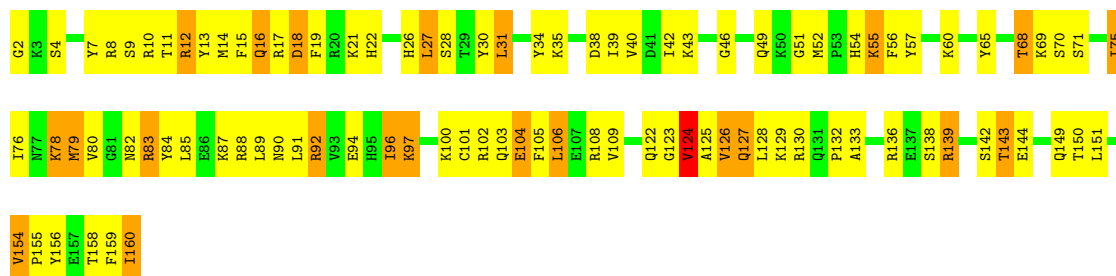
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:



- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



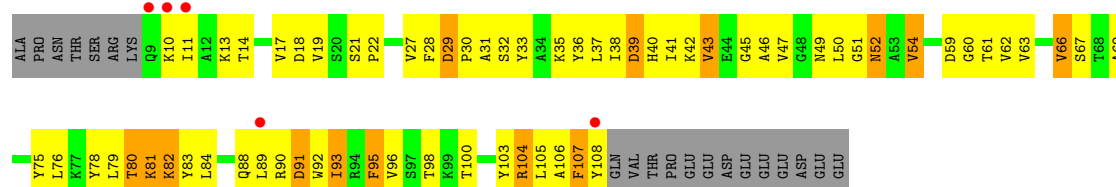
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:



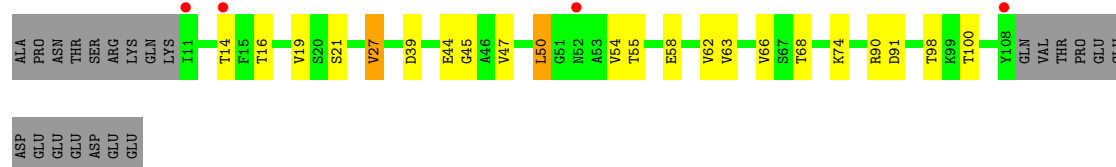
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



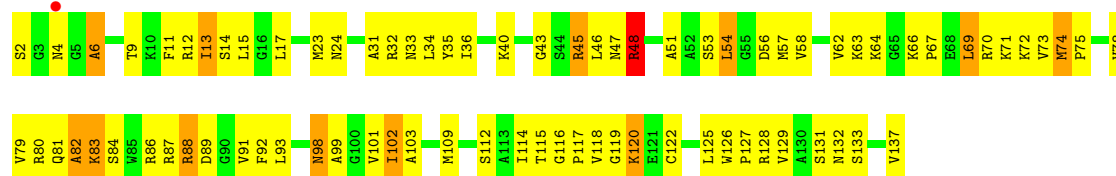
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



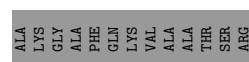
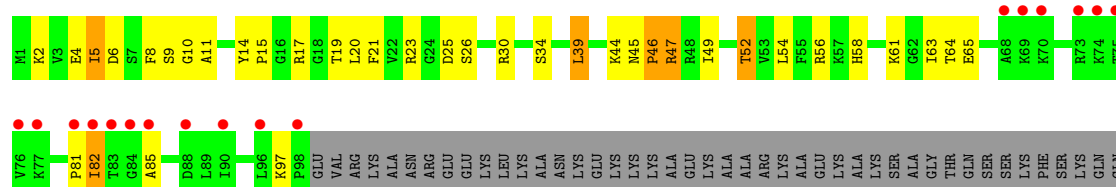
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



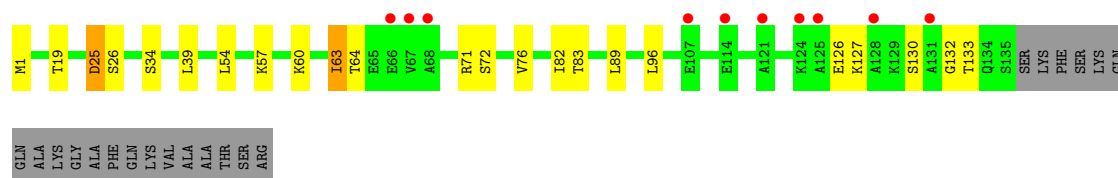
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



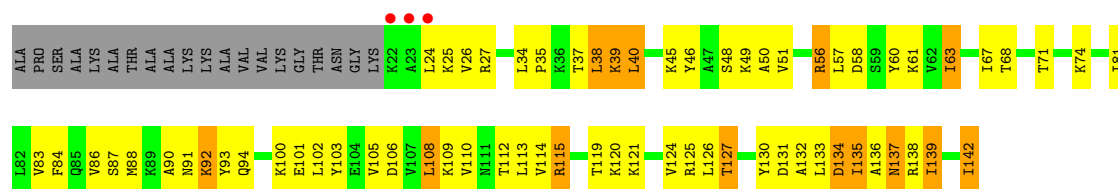
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:



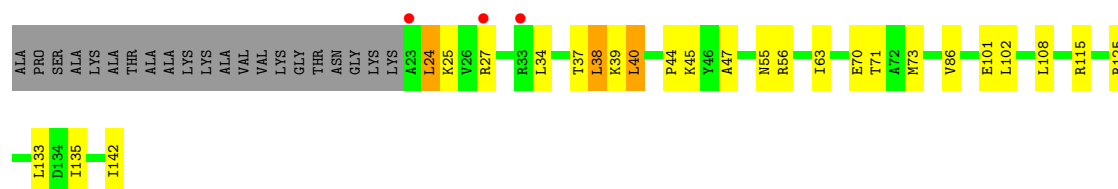
- Molecule 61: 60S ribosomal protein L25

Chain N5:



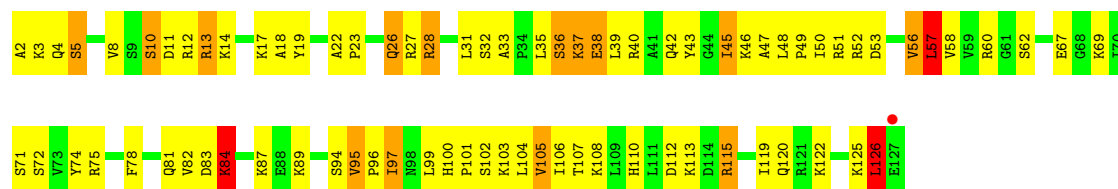
- Molecule 61: 60S ribosomal protein L25

Chain n5:



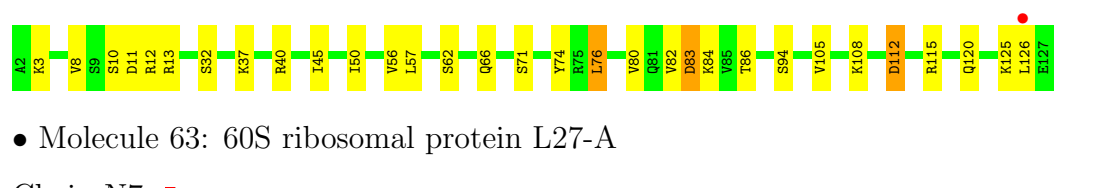
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



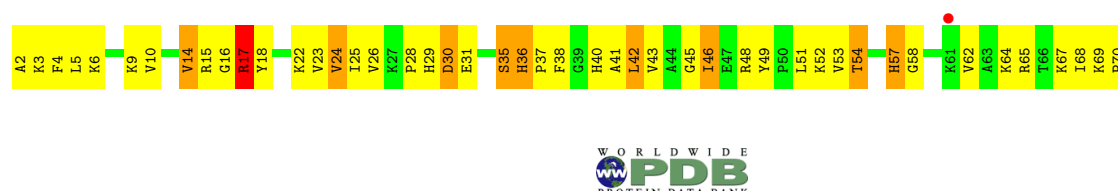
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



- Molecule 63: 60S ribosomal protein L27-A

Chain N7:





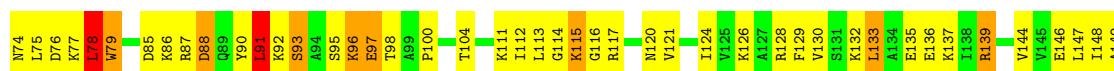
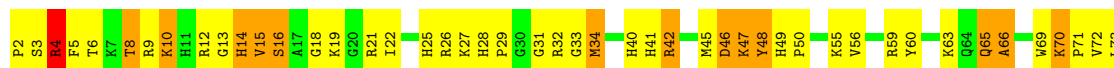
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:



- Molecule 64: 60S ribosomal protein L28

Chain N8:



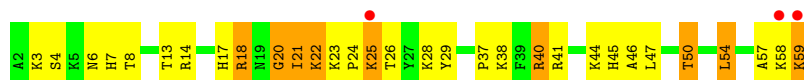
- Molecule 64: 60S ribosomal protein L28

Chain n8:



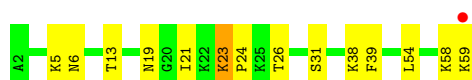
- Molecule 65: 60S ribosomal protein L29

Chain N9:



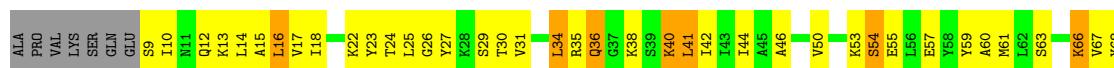
- Molecule 65: 60S ribosomal protein L29

Chain n9:



- Molecule 66: 60S ribosomal protein L30

Chain O0:



- Molecule 66: 60S ribosomal protein L30

Chain o0:



- Molecule 67: 60S ribosomal protein L31-A

Chain O1:



- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



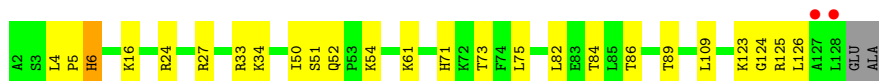
- Molecule 68: 60S ribosomal protein L32

Chain O2:



- Molecule 68: 60S ribosomal protein L32

Chain o2:



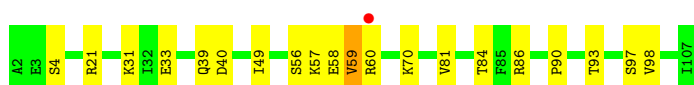
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



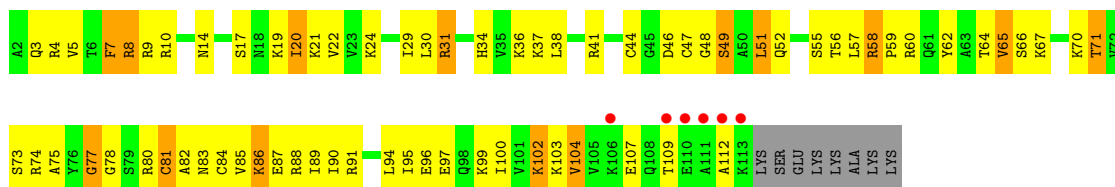
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



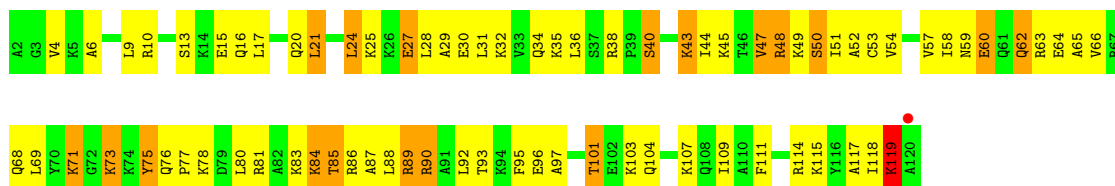
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



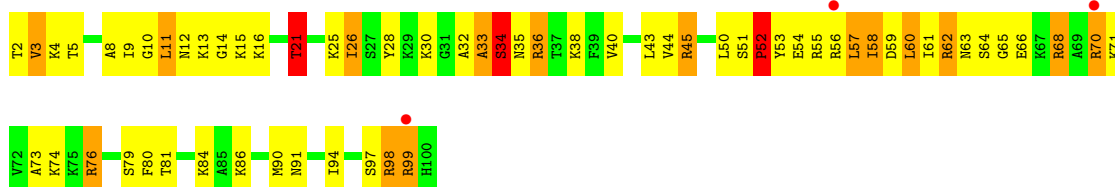
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:



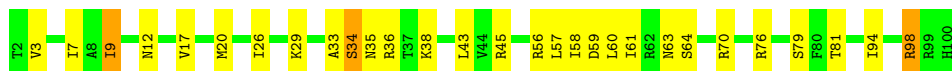
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:



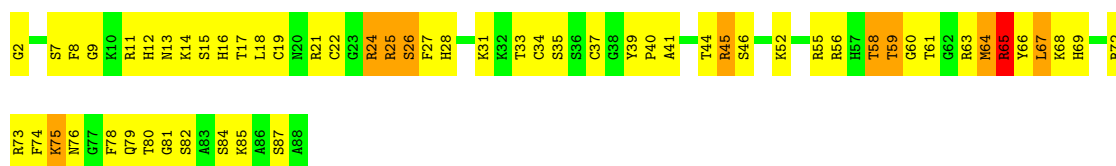
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



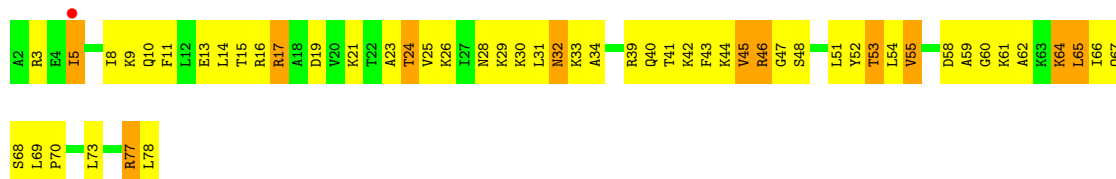
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



- Molecule 74: 60S ribosomal protein L38

Chain O8:



- Molecule 74: 60S ribosomal protein L38

Chain o8:



- Molecule 75: 60S ribosomal protein L39

Chain O9:



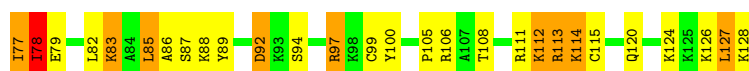
- Molecule 75: 60S ribosomal protein L39

Chain o9:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



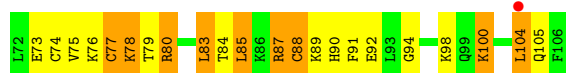
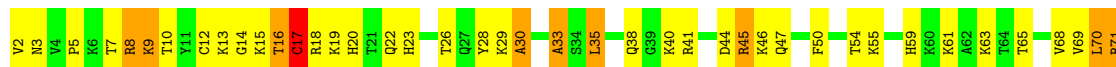
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:



- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



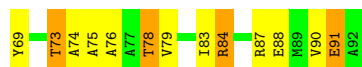
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:



- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



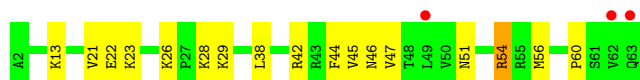
- Molecule 79: 60S ribosomal protein L43-A

Chain q3:



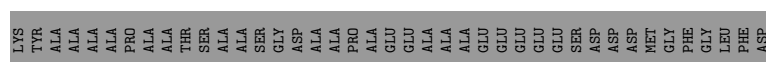
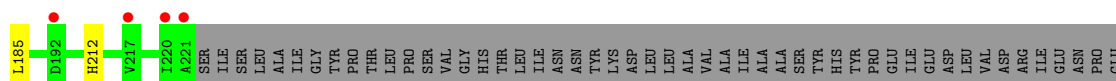
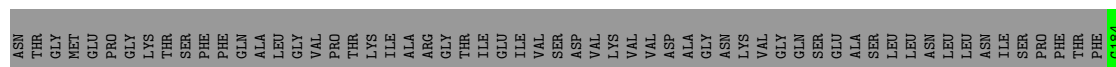
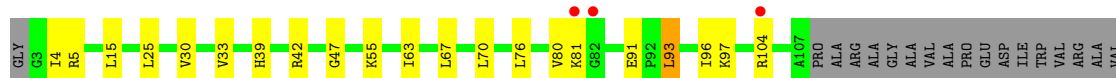
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:



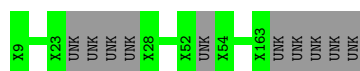
- Molecule 81: 60S acidic ribosomal protein P0

Chain p0:



- Molecule 82: UNKNOWN PROTEIN m2

Chain m2:



- Molecule 83: UNKNOWN PROTEIN p1

Chain p1:

There are no outlier residues recorded for this chain.

- Molecule 84: UNKNOWN PROTEIN p2

Chain p2:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	434.39Å 285.58Å 303.06Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	49.88 – 3.20 49.89 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.88-3.20) 99.8 (49.89-3.20)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.212 , 0.262 0.270 , 0.314	Depositor DCC
R_{free} test set	23650 reflections (1.98%)	DCC
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1195009 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	411230	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OHX, MG, 3L2

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	0.70	1/41698 (0.0%)	1.28	289/64972 (0.4%)
1	6	0.80	10/42765 (0.0%)	1.35	400/66634 (0.6%)
2	S0	0.45	0/1617	0.66	0/2215
2	s0	0.45	0/1623	0.68	0/2222
3	S1	0.38	0/1735	0.63	0/2335
3	s1	0.49	0/1748	0.69	0/2352
4	S2	0.48	0/1665	0.66	0/2263
4	s2	0.56	0/1665	0.74	0/2263
5	S3	0.47	0/1759	0.64	0/2368
5	s3	0.39	0/1759	0.59	0/2368
6	S4	0.46	0/2109	0.69	1/2839 (0.0%)
6	s4	0.49	0/2109	0.74	1/2839 (0.0%)
7	S5	0.37	0/1629	0.58	0/2202
7	s5	0.42	0/1629	0.66	1/2202 (0.0%)
8	S6	0.45	0/1823	0.65	0/2439
8	s6	0.49	0/1779	0.68	0/2379
9	S7	0.42	0/1506	0.65	0/2028
9	s7	0.43	0/1516	0.62	0/2043
10	S8	0.52	0/1514	0.67	0/2021
10	s8	0.58	0/1514	0.73	0/2021
11	S9	0.46	0/1519	0.65	0/2035
11	s9	0.52	0/1519	0.75	1/2035 (0.0%)
12	C0	0.43	0/790	0.70	1/1069 (0.1%)
12	c0	0.36	0/777	0.64	3/1049 (0.3%)
13	C1	0.55	0/1240	0.67	0/1675
13	c1	0.58	0/1194	0.71	0/1610
14	C2	0.35	0/900	0.63	0/1224
14	c2	0.30	0/900	0.60	1/1224 (0.1%)
15	C3	0.47	0/1215	0.69	2/1638 (0.1%)
15	c3	0.53	0/1215	0.69	0/1638
16	C4	0.40	0/901	0.70	0/1217
16	c4	0.49	0/960	0.74	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.43	0/998	0.64	0/1341
17	c5	0.44	0/1060	0.67	0/1426
18	C6	0.42	0/1125	0.69	2/1510 (0.1%)
18	c6	0.43	0/1131	0.67	0/1518
19	C7	0.43	0/935	0.64	0/1254
19	c7	0.43	0/914	0.67	0/1224
20	C8	0.41	0/1211	0.64	0/1628
20	c8	0.44	0/1211	0.68	1/1628 (0.1%)
21	C9	0.42	0/1130	0.65	0/1517
21	c9	0.44	0/1130	0.68	2/1517 (0.1%)
22	D0	0.42	0/865	0.64	0/1169
22	d0	0.43	0/892	0.64	0/1205
23	D1	0.44	0/693	0.63	0/935
23	d1	0.49	0/693	0.65	0/935
24	D2	0.50	0/1038	0.73	2/1395 (0.1%)
24	d2	0.56	0/1038	0.74	1/1395 (0.1%)
25	D3	0.59	0/1139	0.75	1/1518 (0.1%)
25	d3	0.66	0/1139	0.82	2/1518 (0.1%)
26	D4	0.43	0/1087	0.63	0/1449
26	d4	0.48	0/1087	0.69	0/1449
27	D5	0.38	0/571	0.69	0/768
27	d5	0.38	0/566	0.63	0/761
28	D6	0.48	0/782	0.73	0/1047
28	d6	0.59	0/782	0.73	0/1047
29	D7	0.42	0/620	0.65	0/838
29	d7	0.45	0/620	0.69	0/838
30	D8	0.35	0/499	0.59	0/670
30	d8	0.43	0/499	0.69	0/670
31	D9	0.52	0/452	0.71	1/600 (0.2%)
31	d9	0.45	0/452	0.67	0/600
32	E0	0.45	0/483	0.57	0/643
33	E1	0.42	0/577	0.76	0/770
33	e1	0.38	0/619	0.72	0/822
34	SR	0.36	0/2494	0.56	0/3393
34	sR	0.36	0/2495	0.58	0/3395
35	SM	0.51	0/1113	0.69	2/1502 (0.1%)
35	sM	0.47	0/683	0.67	1/923 (0.1%)
36	1	1.08	76/75394 (0.1%)	1.62	1625/117545 (1.4%)
36	5	1.10	110/75414 (0.1%)	1.64	1765/117575 (1.5%)
37	3	0.90	3/2883 (0.1%)	1.38	19/4491 (0.4%)
37	7	1.03	1/2883 (0.0%)	1.66	70/4491 (1.6%)
38	4	1.00	0/3746	1.57	67/5832 (1.1%)
38	8	0.90	2/3746 (0.1%)	1.41	29/5832 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.67	0/1948	0.81	1/2617 (0.0%)
39	l2	0.65	0/1946	0.82	1/2614 (0.0%)
40	L3	0.70	0/3146	0.81	1/4228 (0.0%)
40	l3	0.77	0/3146	0.85	3/4228 (0.1%)
41	L4	0.77	0/2800	0.91	5/3790 (0.1%)
41	l4	0.72	1/2800 (0.0%)	0.87	2/3790 (0.1%)
42	L5	0.52	0/2425	0.69	0/3271
42	l5	0.67	0/2408	0.77	1/3248 (0.0%)
43	L6	0.71	0/1260	0.82	1/1694 (0.1%)
43	l6	0.71	0/1269	0.78	0/1705
44	L7	0.73	0/1821	0.84	0/2451
44	l7	0.82	0/1828	0.86	2/2461 (0.1%)
45	L8	0.53	0/1836	0.68	1/2481 (0.0%)
45	l8	0.49	0/1795	0.66	0/2429
46	L9	0.64	0/1539	0.75	0/2073
46	l9	0.73	0/1539	0.81	0/2073
47	M0	0.69	1/1741 (0.1%)	0.81	5/2335 (0.2%)
47	m0	0.70	1/1758 (0.1%)	0.85	1/2358 (0.0%)
48	M1	0.51	0/1374	0.69	1/1842 (0.1%)
48	m1	0.64	0/1374	0.78	2/1842 (0.1%)
49	M3	0.71	0/1568	0.83	2/2106 (0.1%)
49	m3	0.62	0/1573	0.80	0/2113
50	M4	0.70	0/1068	0.79	0/1438
50	m4	0.76	0/1074	0.80	1/1446 (0.1%)
51	M5	0.72	1/1757 (0.1%)	0.84	2/2354 (0.1%)
51	m5	0.63	0/1757	0.83	3/2354 (0.1%)
52	M6	0.81	0/1585	0.84	2/2128 (0.1%)
52	m6	0.96	2/1585 (0.1%)	0.95	4/2128 (0.2%)
53	M7	0.73	0/1443	0.80	1/1944 (0.1%)
53	m7	0.86	0/1250	0.84	0/1683
54	M8	0.75	0/1465	0.88	0/1965
54	m8	0.67	0/1465	0.85	0/1965
55	M9	0.53	0/1538	0.66	0/2050
55	m9	0.54	0/1538	0.65	0/2050
56	N0	0.73	0/1481	0.79	1/1990 (0.1%)
56	n0	0.82	0/1481	0.86	0/1990
57	N1	0.71	0/1300	0.80	1/1743 (0.1%)
57	n1	0.80	1/1300 (0.1%)	0.83	2/1743 (0.1%)
58	N2	0.40	0/812	0.60	0/1099
58	n2	0.46	0/794	0.67	0/1076
59	N3	0.70	0/1018	0.87	2/1369 (0.1%)
59	n3	0.79	0/1018	0.84	0/1369
60	N4	0.52	0/712	0.67	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.58	0/1052	0.72	0/1398
61	N5	0.62	0/979	0.77	0/1321
61	n5	0.58	0/974	0.77	0/1314
62	N6	0.68	0/1004	0.85	2/1341 (0.1%)
62	n6	0.66	0/1004	0.82	1/1341 (0.1%)
63	N7	0.48	0/1118	0.67	0/1497
63	n7	0.47	0/1118	0.66	1/1497 (0.1%)
64	N8	0.73	0/1204	0.90	1/1612 (0.1%)
64	n8	0.72	0/1204	0.83	0/1612
65	N9	0.66	0/473	0.76	0/629
65	n9	0.71	0/473	0.94	1/629 (0.2%)
66	O0	0.49	0/751	0.63	0/1008
66	o0	0.46	0/775	0.63	0/1040
67	O1	0.61	0/890	0.73	0/1196
67	o1	0.72	0/897	0.80	0/1205
68	O2	0.76	0/1041	0.86	1/1394 (0.1%)
68	o2	0.79	0/1041	0.87	0/1394
69	O3	0.90	0/868	0.95	2/1168 (0.2%)
69	o3	0.87	0/868	0.90	0/1168
70	O4	0.56	0/890	0.75	1/1189 (0.1%)
70	o4	0.51	0/890	0.73	0/1189
71	O5	0.66	0/978	0.80	1/1301 (0.1%)
71	o5	0.53	0/974	0.68	0/1297
72	O6	0.62	0/778	0.78	0/1034
72	o6	0.54	0/777	0.72	0/1033
73	O7	0.73	0/696	1.03	4/923 (0.4%)
73	o7	0.61	0/696	0.80	0/923
74	O8	0.52	0/618	0.61	0/826
74	o8	0.45	0/614	0.59	0/822
75	O9	0.71	0/443	0.83	0/588
75	o9	0.67	0/443	0.81	0/588
76	Q0	0.65	0/423	0.80	0/562
76	q0	0.84	0/423	0.91	1/562 (0.2%)
77	Q1	0.63	0/234	0.93	0/300
77	q1	0.68	0/234	0.91	0/300
78	Q2	0.82	1/860 (0.1%)	0.80	0/1136
78	q2	0.76	1/860 (0.1%)	0.82	1/1136 (0.1%)
79	Q3	0.71	0/701	0.82	0/934
79	q3	0.66	0/701	0.76	2/934 (0.2%)
80	e0	0.56	0/499	0.72	0/665
81	p0	4.55	1/1091 (0.1%)	1.38	2/1472 (0.1%)
All	All	0.87	213/430073 (0.0%)	1.28	4359/631362 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	2
9	S7	0	1
9	s7	0	1
16	C4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	1
22	d0	0	1
27	D5	0	1
28	D6	0	1
33	E1	0	1
39	l2	0	1
40	l3	0	1
41	L4	0	1
42	l5	0	1
43	L6	0	1
43	l6	0	1
44	l7	0	1
45	L8	0	1
49	M3	0	1
52	M6	0	1
52	m6	0	1
54	m8	0	2
56	n0	0	2
57	N1	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
72	o6	0	1
81	p0	1	0
All	All	1	35

The worst 5 of 213 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	p0	212	HIS	CA-CB	149.59	4.83	1.53
78	Q2	17	CYS	CB-SG	13.09	2.04	1.82
36	5	1152	G	N9-C4	-11.55	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	9.39	1.98	1.82
36	1	656	A	N3-C4	-7.83	1.30	1.34

The worst 5 of 4359 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	p0	212	HIS	N-CA-CB	-47.24	25.57	110.60
36	5	1152	G	N3-C4-C5	23.22	140.21	128.60
36	5	1152	G	N3-C4-N9	-22.85	112.29	126.00
36	5	1152	G	C2-N3-C4	-18.92	102.44	111.90
36	5	780	A	O5'-P-OP1	-14.51	92.64	105.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
81	p0	212	HIS	CA

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	124	ASP	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
9	S7	131	PHE	Peptide

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	1016	0
1	6	38238	0	19239	992	0
2	S0	1577	0	1567	175	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	127	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	129	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	171	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	171	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1878	134	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	119	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	117	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	152	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	67	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	80	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	64	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	92	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	95	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	117	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	82	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	126	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	123	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	90	0
22	d0	882	0	939	0	0
23	D1	684	0	672	69	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	98	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	97	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	814	104	0
28	d6	769	0	815	0	0
29	D7	610	0	630	45	0
29	d7	610	0	631	0	0
30	D8	497	0	535	58	0
30	d8	497	0	535	0	0
31	D9	442	0	428	34	0
31	d9	442	0	428	0	0
32	E0	475	0	525	36	0
33	E1	566	0	602	56	0
33	e1	608	0	655	0	0
34	SR	2441	0	2397	151	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	74	0
35	sM	680	0	607	0	0
36	1	67355	0	33845	1373	1
36	5	67376	0	33860	1429	0
37	3	2579	0	1304	54	0
37	7	2579	0	1303	55	0
38	4	3353	0	1695	82	0
38	8	3353	0	1695	84	0
39	L2	1914	0	1981	170	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	267	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	249	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	183	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	96	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	146	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	142	0
45	l8	1763	0	1819	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	L9	1518	0	1587	132	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1735	140	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	117	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	127	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	103	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	154	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	139	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	113	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	105	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	114	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	108	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	119	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	54	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	75	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	32	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	76	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	91	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	117	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	40	0
65	n9	462	0	491	0	0
66	O0	743	0	797	55	0
66	o0	767	0	816	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	O1	876	0	912	60	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	89	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	69	0
69	o3	850	0	880	0	0
70	O4	880	0	945	78	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	80	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	70	0
72	o6	770	0	846	0	0
73	O7	681	0	682	63	0
73	o7	681	0	683	0	0
74	O8	612	0	682	43	0
74	o8	608	0	671	0	0
75	O9	436	0	475	45	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	28	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	31	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	56	0
78	q2	847	0	915	0	0
79	Q3	694	0	734	61	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	p0	1076	0	1040	0	0
82	m2	750	0	177	0	0
83	p1	235	0	50	0	0
84	p2	230	0	50	0	0
85	1	470	0	0	0	0
85	2	122	0	0	0	0
85	3	14	0	0	0	0
85	4	25	0	0	0	0
85	5	497	0	0	0	0
85	6	146	0	0	0	0
85	7	16	0	0	0	0
85	8	15	0	0	0	0
85	C1	1	0	0	0	0
85	D0	1	0	0	0	0
85	L2	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L3	2	0	0	0	0
85	L4	2	0	0	0	0
85	L5	1	0	0	0	0
85	L7	4	0	0	0	0
85	L8	1	0	0	0	0
85	M0	2	0	0	0	0
85	M1	1	0	0	0	0
85	M3	3	0	0	0	0
85	M5	1	0	0	0	0
85	M6	1	0	0	0	0
85	M7	3	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	3	0	0	0	0
85	N5	2	0	0	0	0
85	N6	2	0	0	0	0
85	N8	4	0	0	0	0
85	O2	1	0	0	0	0
85	O4	1	0	0	0	0
85	O7	1	0	0	0	0
85	Q2	1	0	0	0	0
85	S2	2	0	0	0	0
85	S4	1	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	1	0	0	0	0
85	c9	1	0	0	0	0
85	d3	3	0	0	0	0
85	d4	1	0	0	0	0
85	d6	1	0	0	0	0
85	l2	3	0	0	0	0
85	l3	3	0	0	0	0
85	l4	2	0	0	0	0
85	l5	1	0	0	0	0
85	l7	2	0	0	0	0
85	l8	1	0	0	0	0
85	m1	2	0	0	0	0
85	m5	3	0	0	0	0
85	m6	1	0	0	0	0
85	m7	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	n0	3	0	0	0	0
85	n3	2	0	0	0	0
85	n6	1	0	0	0	0
85	n8	5	0	0	0	0
85	n9	1	0	0	0	0
85	o1	1	0	0	0	0
85	o3	1	0	0	0	0
85	o4	2	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	2	0	0	0	0
85	s1	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2443	0	0	228	0
86	2	1099	0	0	110	0
86	3	84	0	0	4	0
86	4	112	0	0	12	0
86	5	2478	0	0	227	0
86	6	1106	0	0	118	0
86	7	84	0	0	4	0
86	8	112	0	0	15	0
86	C3	7	0	0	1	0
86	C5	7	0	0	3	0
86	C8	7	0	0	0	0
86	D9	7	0	0	1	0
86	L3	21	0	0	4	0
86	L4	7	0	0	2	0
86	M0	7	0	0	0	0
86	M5	7	0	0	0	0
86	M7	14	0	0	2	0
86	M9	7	0	0	1	0
86	N1	7	0	0	1	0
86	N9	7	0	0	0	0
86	O3	7	0	0	1	0
86	O7	14	0	0	3	0
86	Q2	7	0	0	2	0
86	S6	7	0	0	2	1
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	14	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	0	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	m8	7	0	0	0	0
86	n3	14	0	0	0	0
86	n6	7	0	0	0	0
86	n9	7	0	0	0	0
86	o2	7	0	0	0	0
86	o3	7	0	0	0	0
86	o7	14	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	0	0
86	sR	7	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	0	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	0	0
87	q2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	q3	1	0	0	0	0
88	1	36	0	0	0	0
88	5	36	0	0	1	0
All	All	411230	0	297281	10951	1

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

The worst 5 of 10951 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.04	1.43
28:D6:26:CYS:SG	28:D6:77:CYS:SG	3.33	1.26
62:N6:71:SER:HB3	62:N6:83:ASP:HB2	1.33	1.09
36:5:2273:G:O6	86:5:4192:OHX:N5	1.88	1.07
36:5:3274:A:H3'	36:5:3275:U:H5''	1.38	1.05

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:531:G:OP1	86:S6:301:OHX:N1[2_545]	2.17	0.03

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%)	150 (74%)	31 (15%)	23 (11%)	1	4
2	s0	204/251 (81%)	156 (76%)	28 (14%)	20 (10%)	1	7
3	S1	212/254 (84%)	148 (70%)	40 (19%)	24 (11%)	1	4
3	s1	214/254 (84%)	171 (80%)	31 (14%)	12 (6%)	3	23
4	S2	215/253 (85%)	180 (84%)	24 (11%)	11 (5%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	s2	215/253 (85%)	177 (82%)	28 (13%)	10 (5%)	4	27
5	S3	221/239 (92%)	183 (83%)	27 (12%)	11 (5%)	3	26
5	s3	221/239 (92%)	170 (77%)	35 (16%)	16 (7%)	2	13
6	S4	258/260 (99%)	205 (80%)	43 (17%)	10 (4%)	5	33
6	s4	258/260 (99%)	209 (81%)	28 (11%)	21 (8%)	1	10
7	S5	204/224 (91%)	156 (76%)	30 (15%)	18 (9%)	1	8
7	s5	204/224 (91%)	158 (78%)	27 (13%)	19 (9%)	1	8
8	S6	224/236 (95%)	192 (86%)	21 (9%)	11 (5%)	3	26
8	s6	216/236 (92%)	186 (86%)	18 (8%)	12 (6%)	3	23
9	S7	182/189 (96%)	132 (72%)	29 (16%)	21 (12%)	1	4
9	s7	184/189 (97%)	148 (80%)	24 (13%)	12 (6%)	2	17
10	S8	184/200 (92%)	153 (83%)	19 (10%)	12 (6%)	2	17
10	s8	184/200 (92%)	163 (89%)	16 (9%)	5 (3%)	8	46
11	S9	183/196 (93%)	147 (80%)	25 (14%)	11 (6%)	2	20
11	s9	183/196 (93%)	149 (81%)	24 (13%)	10 (6%)	3	23
12	C0	94/105 (90%)	72 (77%)	12 (13%)	10 (11%)	1	5
12	c0	92/105 (88%)	67 (73%)	11 (12%)	14 (15%)	0	1
13	C1	153/155 (99%)	119 (78%)	22 (14%)	12 (8%)	1	11
13	c1	144/155 (93%)	118 (82%)	17 (12%)	9 (6%)	2	18
14	C2	122/142 (86%)	68 (56%)	29 (24%)	25 (20%)	0	0
14	c2	122/142 (86%)	64 (52%)	36 (30%)	22 (18%)	0	1
15	C3	148/150 (99%)	122 (82%)	17 (12%)	9 (6%)	2	19
15	c3	148/150 (99%)	111 (75%)	28 (19%)	9 (6%)	2	19
16	C4	125/136 (92%)	88 (70%)	25 (20%)	12 (10%)	1	7
16	c4	126/136 (93%)	97 (77%)	19 (15%)	10 (8%)	1	11
17	C5	122/141 (86%)	86 (70%)	24 (20%)	12 (10%)	1	7
17	c5	133/141 (94%)	90 (68%)	27 (20%)	16 (12%)	1	4
18	C6	139/142 (98%)	119 (86%)	11 (8%)	9 (6%)	2	17
18	c6	140/142 (99%)	113 (81%)	17 (12%)	10 (7%)	2	13
19	C7	116/136 (85%)	90 (78%)	15 (13%)	11 (10%)	1	7
19	c7	113/136 (83%)	85 (75%)	17 (15%)	11 (10%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	C8	143/145 (99%)	112 (78%)	19 (13%)	12 (8%)	1	9
20	c8	143/145 (99%)	112 (78%)	23 (16%)	8 (6%)	3	23
21	C9	141/143 (99%)	122 (86%)	11 (8%)	8 (6%)	3	22
21	c9	141/143 (99%)	118 (84%)	18 (13%)	5 (4%)	6	37
22	D0	105/120 (88%)	81 (77%)	17 (16%)	7 (7%)	2	16
22	d0	108/120 (90%)	85 (79%)	12 (11%)	11 (10%)	1	6
23	D1	85/87 (98%)	59 (69%)	15 (18%)	11 (13%)	0	3
23	d1	85/87 (98%)	69 (81%)	11 (13%)	5 (6%)	2	20
24	D2	127/129 (98%)	108 (85%)	16 (13%)	3 (2%)	9	51
24	d2	127/129 (98%)	109 (86%)	17 (13%)	1 (1%)	27	77
25	D3	142/144 (99%)	109 (77%)	18 (13%)	15 (11%)	1	5
25	d3	142/144 (99%)	123 (87%)	15 (11%)	4 (3%)	8	44
26	D4	132/134 (98%)	107 (81%)	17 (13%)	8 (6%)	2	19
26	d4	132/134 (98%)	102 (77%)	17 (13%)	13 (10%)	1	7
27	D5	68/107 (64%)	45 (66%)	14 (21%)	9 (13%)	0	2
27	d5	67/107 (63%)	53 (79%)	10 (15%)	4 (6%)	2	20
28	D6	95/97 (98%)	59 (62%)	16 (17%)	20 (21%)	0	0
28	d6	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	1	9
29	D7	79/81 (98%)	63 (80%)	12 (15%)	4 (5%)	3	25
29	d7	79/81 (98%)	61 (77%)	13 (16%)	5 (6%)	2	18
30	D8	61/66 (92%)	50 (82%)	9 (15%)	2 (3%)	6	38
30	d8	61/66 (92%)	40 (66%)	15 (25%)	6 (10%)	1	7
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	2	20
31	d9	51/55 (93%)	43 (84%)	4 (8%)	4 (8%)	1	11
32	E0	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	3	25
33	E1	69/76 (91%)	38 (55%)	13 (19%)	18 (26%)	0	0
33	e1	74/76 (97%)	35 (47%)	19 (26%)	20 (27%)	0	0
34	SR	316/318 (99%)	277 (88%)	28 (9%)	11 (4%)	6	37
34	sR	316/318 (99%)	274 (87%)	31 (10%)	11 (4%)	6	37
35	SM	155/273 (57%)	106 (68%)	30 (19%)	19 (12%)	1	3
35	sM	98/273 (36%)	63 (64%)	18 (18%)	17 (17%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	L2	250/253 (99%)	220 (88%)	20 (8%)	10 (4%)	5	32
39	l2	250/253 (99%)	207 (83%)	31 (12%)	12 (5%)	4	27
40	L3	384/386 (100%)	326 (85%)	42 (11%)	16 (4%)	4	31
40	l3	384/386 (100%)	344 (90%)	31 (8%)	9 (2%)	10	52
41	L4	359/361 (99%)	286 (80%)	46 (13%)	27 (8%)	2	12
41	l4	359/361 (99%)	297 (83%)	36 (10%)	26 (7%)	2	13
42	L5	294/296 (99%)	245 (83%)	27 (9%)	22 (8%)	2	12
42	l5	292/296 (99%)	243 (83%)	39 (13%)	10 (3%)	6	38
43	L6	152/175 (87%)	133 (88%)	15 (10%)	4 (3%)	8	47
43	l6	153/175 (87%)	131 (86%)	17 (11%)	5 (3%)	6	38
44	L7	220/243 (90%)	189 (86%)	24 (11%)	7 (3%)	6	39
44	l7	221/243 (91%)	194 (88%)	18 (8%)	9 (4%)	4	32
45	L8	231/255 (91%)	181 (78%)	35 (15%)	15 (6%)	2	17
45	l8	229/255 (90%)	166 (72%)	45 (20%)	18 (8%)	1	11
46	L9	189/191 (99%)	156 (82%)	25 (13%)	8 (4%)	4	31
46	l9	189/191 (99%)	163 (86%)	19 (10%)	7 (4%)	5	34
47	M0	207/220 (94%)	166 (80%)	33 (16%)	8 (4%)	5	33
47	m0	209/220 (95%)	163 (78%)	32 (15%)	14 (7%)	2	16
48	M1	167/173 (96%)	127 (76%)	19 (11%)	21 (13%)	0	3
48	m1	167/173 (96%)	138 (83%)	20 (12%)	9 (5%)	3	24
49	M3	191/198 (96%)	155 (81%)	23 (12%)	13 (7%)	2	15
49	m3	192/198 (97%)	151 (79%)	22 (12%)	19 (10%)	1	7
50	M4	134/137 (98%)	115 (86%)	12 (9%)	7 (5%)	3	25
50	m4	135/137 (98%)	119 (88%)	13 (10%)	3 (2%)	10	53
51	M5	201/203 (99%)	181 (90%)	12 (6%)	8 (4%)	5	32
51	m5	201/203 (99%)	175 (87%)	21 (10%)	5 (2%)	9	49
52	M6	195/198 (98%)	181 (93%)	11 (6%)	3 (2%)	15	64
52	m6	195/198 (98%)	171 (88%)	17 (9%)	7 (4%)	5	36
53	M7	181/183 (99%)	151 (83%)	21 (12%)	9 (5%)	3	26
53	m7	153/183 (84%)	137 (90%)	14 (9%)	2 (1%)	18	68
54	M8	183/185 (99%)	156 (85%)	21 (12%)	6 (3%)	6	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	m8	183/185 (99%)	155 (85%)	23 (13%)	5 (3%)	8	46
55	M9	186/188 (99%)	163 (88%)	21 (11%)	2 (1%)	21	72
55	m9	186/188 (99%)	158 (85%)	26 (14%)	2 (1%)	21	72
56	N0	170/172 (99%)	157 (92%)	8 (5%)	5 (3%)	7	43
56	n0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	33	83
57	N1	157/159 (99%)	136 (87%)	16 (10%)	5 (3%)	6	39
57	n1	157/159 (99%)	134 (85%)	18 (12%)	5 (3%)	6	39
58	N2	98/120 (82%)	72 (74%)	22 (22%)	4 (4%)	4	32
58	n2	96/120 (80%)	79 (82%)	12 (12%)	5 (5%)	3	25
59	N3	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	10	53
59	n3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	15	64
60	N4	96/155 (62%)	70 (73%)	21 (22%)	5 (5%)	3	25
60	n4	133/155 (86%)	109 (82%)	14 (10%)	10 (8%)	2	12
61	N5	119/141 (84%)	107 (90%)	12 (10%)	0	100	100
61	n5	118/141 (84%)	97 (82%)	9 (8%)	12 (10%)	1	6
62	N6	124/126 (98%)	110 (89%)	11 (9%)	3 (2%)	9	51
62	n6	124/126 (98%)	102 (82%)	17 (14%)	5 (4%)	5	32
63	N7	133/135 (98%)	113 (85%)	12 (9%)	8 (6%)	2	20
63	n7	133/135 (98%)	111 (84%)	11 (8%)	11 (8%)	1	9
64	N8	146/148 (99%)	117 (80%)	19 (13%)	10 (7%)	2	15
64	n8	146/148 (99%)	113 (77%)	23 (16%)	10 (7%)	2	15
65	N9	56/58 (97%)	49 (88%)	6 (11%)	1 (2%)	13	60
65	n9	56/58 (97%)	43 (77%)	8 (14%)	5 (9%)	1	8
66	O0	95/104 (91%)	88 (93%)	6 (6%)	1 (1%)	21	72
66	o0	98/104 (94%)	85 (87%)	8 (8%)	5 (5%)	3	25
67	O1	107/112 (96%)	88 (82%)	11 (10%)	8 (8%)	2	12
67	o1	107/112 (96%)	89 (83%)	12 (11%)	6 (6%)	3	23
68	O2	125/129 (97%)	111 (89%)	12 (10%)	2 (2%)	14	63
68	o2	125/129 (97%)	105 (84%)	16 (13%)	4 (3%)	6	39
69	O3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	7	43
69	o3	104/106 (98%)	93 (89%)	7 (7%)	4 (4%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	O4	110/120 (92%)	96 (87%)	13 (12%)	1 (1%)	25	76
70	o4	110/120 (92%)	92 (84%)	14 (13%)	4 (4%)	5	36
71	O5	117/119 (98%)	104 (89%)	9 (8%)	4 (3%)	6	38
71	o5	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	8	47
72	O6	97/99 (98%)	73 (75%)	17 (18%)	7 (7%)	2	13
72	o6	97/99 (98%)	80 (82%)	11 (11%)	6 (6%)	2	19
73	O7	85/87 (98%)	73 (86%)	12 (14%)	0	100	100
73	o7	85/87 (98%)	71 (84%)	12 (14%)	2 (2%)	9	51
74	O8	75/77 (97%)	63 (84%)	11 (15%)	1 (1%)	18	68
74	o8	75/77 (97%)	59 (79%)	11 (15%)	5 (7%)	2	16
75	O9	48/50 (96%)	38 (79%)	9 (19%)	1 (2%)	11	55
75	o9	48/50 (96%)	43 (90%)	3 (6%)	2 (4%)	4	31
76	Q0	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	2	20
76	q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	5	32
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	17 (74%)	6 (26%)	0	100	100
78	Q2	103/105 (98%)	79 (77%)	15 (15%)	9 (9%)	1	8
78	q2	103/105 (98%)	90 (87%)	10 (10%)	3 (3%)	7	43
79	Q3	89/91 (98%)	77 (86%)	11 (12%)	1 (1%)	21	72
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	21	72
80	e0	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	2	16
81	p0	139/311 (45%)	120 (86%)	16 (12%)	3 (2%)	10	53
All	All	22333/24143 (92%)	18254 (82%)	2761 (12%)	1318 (6%)	2	20

5 of 1318 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	66	ALA
2	S0	95	ALA
2	S0	139	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	11
2	s0	165/209 (79%)	132 (80%)	33 (20%)	2	9
3	S1	191/223 (86%)	146 (76%)	45 (24%)	1	4
3	s1	192/223 (86%)	146 (76%)	46 (24%)	1	4
4	S2	176/204 (86%)	138 (78%)	38 (22%)	1	7
4	s2	176/204 (86%)	126 (72%)	50 (28%)	0	2
5	S3	182/194 (94%)	146 (80%)	36 (20%)	2	9
5	s3	182/194 (94%)	144 (79%)	38 (21%)	1	8
6	S4	221/221 (100%)	175 (79%)	46 (21%)	2	8
6	s4	221/221 (100%)	189 (86%)	32 (14%)	5	22
7	S5	173/190 (91%)	142 (82%)	31 (18%)	2	12
7	s5	173/190 (91%)	139 (80%)	34 (20%)	2	10
8	S6	188/201 (94%)	154 (82%)	34 (18%)	2	12
8	s6	187/201 (93%)	149 (80%)	38 (20%)	2	9
9	S7	165/169 (98%)	134 (81%)	31 (19%)	2	11
9	s7	165/169 (98%)	135 (82%)	30 (18%)	2	12
10	S8	150/161 (93%)	126 (84%)	24 (16%)	3	16
10	s8	150/161 (93%)	122 (81%)	28 (19%)	2	11
11	S9	158/165 (96%)	127 (80%)	31 (20%)	2	10
11	s9	158/165 (96%)	124 (78%)	34 (22%)	1	7
12	C0	77/98 (79%)	63 (82%)	14 (18%)	2	12
12	c0	73/98 (74%)	61 (84%)	12 (16%)	3	15
13	C1	129/136 (95%)	109 (84%)	20 (16%)	4	17
13	c1	129/136 (95%)	101 (78%)	28 (22%)	1	7
14	C2	88/118 (75%)	63 (72%)	25 (28%)	0	2
14	c2	88/118 (75%)	60 (68%)	28 (32%)	0	1
15	C3	127/127 (100%)	99 (78%)	28 (22%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	c3	127/127 (100%)	101 (80%)	26 (20%)	2	8
16	C4	81/104 (78%)	62 (76%)	19 (24%)	1	5
16	c4	97/104 (93%)	73 (75%)	24 (25%)	1	3
17	C5	101/117 (86%)	80 (79%)	21 (21%)	2	8
17	c5	103/117 (88%)	79 (77%)	24 (23%)	1	5
18	C6	117/118 (99%)	90 (77%)	27 (23%)	1	5
18	c6	118/118 (100%)	99 (84%)	19 (16%)	3	16
19	C7	94/124 (76%)	75 (80%)	19 (20%)	2	9
19	c7	92/124 (74%)	73 (79%)	19 (21%)	2	8
20	C8	128/128 (100%)	96 (75%)	32 (25%)	1	3
20	c8	128/128 (100%)	102 (80%)	26 (20%)	2	9
21	C9	115/115 (100%)	92 (80%)	23 (20%)	2	9
21	c9	115/115 (100%)	97 (84%)	18 (16%)	4	17
22	D0	100/113 (88%)	77 (77%)	23 (23%)	1	5
22	d0	103/113 (91%)	80 (78%)	23 (22%)	1	6
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	7
23	d1	74/74 (100%)	61 (82%)	13 (18%)	3	13
24	D2	110/110 (100%)	88 (80%)	22 (20%)	2	9
24	d2	110/110 (100%)	96 (87%)	14 (13%)	6	29
25	D3	119/119 (100%)	97 (82%)	22 (18%)	2	11
25	d3	119/119 (100%)	98 (82%)	21 (18%)	3	13
26	D4	112/112 (100%)	93 (83%)	19 (17%)	3	14
26	d4	112/112 (100%)	90 (80%)	22 (20%)	2	10
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	5
27	d5	61/88 (69%)	52 (85%)	9 (15%)	4	20
28	D6	83/83 (100%)	63 (76%)	20 (24%)	1	4
28	d6	83/83 (100%)	70 (84%)	13 (16%)	4	17
29	D7	70/70 (100%)	64 (91%)	6 (9%)	15	52
29	d7	70/70 (100%)	55 (79%)	15 (21%)	1	7
30	D8	56/59 (95%)	42 (75%)	14 (25%)	1	3
30	d8	56/59 (95%)	39 (70%)	17 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	D9	47/48 (98%)	34 (72%)	13 (28%)	0	2
31	d9	47/48 (98%)	35 (74%)	12 (26%)	1	3
32	E0	51/51 (100%)	43 (84%)	8 (16%)	4	17
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	4
33	e1	66/66 (100%)	52 (79%)	14 (21%)	1	8
34	SR	260/261 (100%)	228 (88%)	32 (12%)	7	31
34	sR	260/261 (100%)	227 (87%)	33 (13%)	6	29
35	SM	97/228 (42%)	77 (79%)	20 (21%)	2	8
35	sM	54/228 (24%)	45 (83%)	9 (17%)	3	14
39	L2	193/195 (99%)	161 (83%)	32 (17%)	3	14
39	l2	192/195 (98%)	152 (79%)	40 (21%)	2	8
40	L3	321/322 (100%)	249 (78%)	72 (22%)	1	6
40	l3	318/322 (99%)	256 (80%)	62 (20%)	2	10
41	L4	288/288 (100%)	231 (80%)	57 (20%)	2	9
41	l4	288/288 (100%)	231 (80%)	57 (20%)	2	9
42	L5	244/244 (100%)	197 (81%)	47 (19%)	2	10
42	l5	243/244 (100%)	195 (80%)	48 (20%)	2	9
43	L6	134/152 (88%)	111 (83%)	23 (17%)	3	14
43	l6	135/152 (89%)	113 (84%)	22 (16%)	3	15
44	L7	186/204 (91%)	160 (86%)	26 (14%)	5	23
44	l7	187/204 (92%)	155 (83%)	32 (17%)	3	14
45	L8	187/207 (90%)	156 (83%)	31 (17%)	3	14
45	l8	177/207 (86%)	146 (82%)	31 (18%)	3	13
46	L9	171/171 (100%)	131 (77%)	40 (23%)	1	5
46	l9	171/171 (100%)	131 (77%)	40 (23%)	1	5
47	M0	177/186 (95%)	140 (79%)	37 (21%)	1	8
47	m0	179/186 (96%)	141 (79%)	38 (21%)	1	8
48	M1	147/150 (98%)	120 (82%)	27 (18%)	2	11
48	m1	147/150 (98%)	115 (78%)	32 (22%)	1	7
49	M3	154/158 (98%)	125 (81%)	29 (19%)	2	11
49	m3	154/158 (98%)	125 (81%)	29 (19%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	M4	107/108 (99%)	89 (83%)	18 (17%)	3	14
50	m4	108/108 (100%)	89 (82%)	19 (18%)	3	13
51	M5	175/175 (100%)	145 (83%)	30 (17%)	3	14
51	m5	175/175 (100%)	150 (86%)	25 (14%)	5	22
52	M6	160/161 (99%)	140 (88%)	20 (12%)	7	30
52	m6	160/161 (99%)	126 (79%)	34 (21%)	1	7
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	7
53	m7	125/145 (86%)	94 (75%)	31 (25%)	1	3
54	M8	150/150 (100%)	125 (83%)	25 (17%)	3	14
54	m8	150/150 (100%)	123 (82%)	27 (18%)	2	12
55	M9	153/153 (100%)	132 (86%)	21 (14%)	5	25
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	6
56	N0	156/156 (100%)	124 (80%)	32 (20%)	2	8
56	n0	156/156 (100%)	130 (83%)	26 (17%)	3	14
57	N1	136/136 (100%)	110 (81%)	26 (19%)	2	11
57	n1	136/136 (100%)	109 (80%)	27 (20%)	2	9
58	N2	87/106 (82%)	69 (79%)	18 (21%)	2	8
58	n2	85/106 (80%)	66 (78%)	19 (22%)	1	6
59	N3	104/104 (100%)	85 (82%)	19 (18%)	2	12
59	n3	104/104 (100%)	93 (89%)	11 (11%)	10	38
60	N4	57/129 (44%)	51 (90%)	6 (10%)	10	39
60	n4	100/129 (78%)	85 (85%)	15 (15%)	4	19
61	N5	104/117 (89%)	82 (79%)	22 (21%)	1	8
61	n5	104/117 (89%)	87 (84%)	17 (16%)	3	15
62	N6	109/109 (100%)	87 (80%)	22 (20%)	2	9
62	n6	109/109 (100%)	81 (74%)	28 (26%)	1	2
63	N7	115/115 (100%)	93 (81%)	22 (19%)	2	11
63	n7	115/115 (100%)	94 (82%)	21 (18%)	2	12
64	N8	118/118 (100%)	95 (80%)	23 (20%)	2	10
64	n8	118/118 (100%)	99 (84%)	19 (16%)	3	16
65	N9	46/46 (100%)	37 (80%)	9 (20%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	n9	46/46 (100%)	38 (83%)	8 (17%)	3	13
66	O0	81/87 (93%)	64 (79%)	17 (21%)	1	8
66	o0	84/87 (97%)	69 (82%)	15 (18%)	2	12
67	O1	92/96 (96%)	74 (80%)	18 (20%)	2	10
67	o1	94/96 (98%)	77 (82%)	17 (18%)	2	12
68	O2	109/110 (99%)	85 (78%)	24 (22%)	1	7
68	o2	109/110 (99%)	87 (80%)	22 (20%)	2	9
69	O3	90/90 (100%)	79 (88%)	11 (12%)	7	31
69	o3	90/90 (100%)	73 (81%)	17 (19%)	2	11
70	O4	95/102 (93%)	76 (80%)	19 (20%)	2	9
70	o4	95/102 (93%)	74 (78%)	21 (22%)	1	7
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1	8
71	o5	103/104 (99%)	78 (76%)	25 (24%)	1	3
72	O6	81/81 (100%)	61 (75%)	20 (25%)	1	3
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	1
73	O7	70/70 (100%)	57 (81%)	13 (19%)	2	11
73	o7	70/70 (100%)	60 (86%)	10 (14%)	5	22
74	O8	68/68 (100%)	51 (75%)	17 (25%)	1	3
74	o8	67/68 (98%)	56 (84%)	11 (16%)	3	15
75	O9	45/45 (100%)	38 (84%)	7 (16%)	4	17
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	13
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	1	3
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1	5
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	72 (80%)	18 (20%)	2	9
78	q2	90/90 (100%)	70 (78%)	20 (22%)	1	6
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	3	14
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	6
80	e0	53/53 (100%)	39 (74%)	14 (26%)	1	2
81	p0	105/253 (42%)	85 (81%)	20 (19%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	18727/20241 (92%)	15073 (80%)	3654 (20%)	2 10

5 of 3654 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	O3	98	VAL
8	s6	78	THR
63	n7	121	ARG
72	O6	45	ARG
3	s1	116	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
55	M9	130	ASN
5	s3	74	GLN
52	m6	90	HIS
57	N1	49	GLN
65	N9	45	HIS

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 2560 ligands modelled in this entry, 1426 are monoatomic - leaving 1134 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	3863	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

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

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3L2	1	4212	-	40,40,40	0.64	1 (2%)	62,62,62	1.37	8 (12%)
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	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	4	239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
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	-
86	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3L2	5	4246	-	40,40,40	1.15	5 (12%)	62,62,62	1.71	10 (16%)
86	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
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	1	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
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	1	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	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
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	8	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	103	-	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	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S6	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	202	-	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	d4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	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	l3	406	-	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	l4	404	-	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	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	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	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s4	301	-	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	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3863	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3864	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3865	-	-	0/0/0/0	0/0/0/0

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
88	3L2	1	4212	-	-	0/31/89/89	0/1/5/5
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
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

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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	3	225	-	-	0/0/0/0	0/0/0/0
86	OHX	3	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	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	4	239	-	-	0/0/0/0	0/0/0/0
86	OHX	4	240	-	-	0/0/0/0	0/0/0/0
86	OHX	4	241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3892	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3893	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3894	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3895	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3896	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3897	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3947	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
86	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
88	3L2	5	4246	-	-	0/31/89/89	0/1/5/5
86	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
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	1	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
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	1	-	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	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	7	222	-	-	0/0/0/0	0/0/0/0
86	OHX	7	223	-	-	0/0/0/0	0/0/0/0
86	OHX	7	224	-	-	0/0/0/0	0/0/0/0
86	OHX	7	225	-	-	0/0/0/0	0/0/0/0
86	OHX	7	226	-	-	0/0/0/0	0/0/0/0
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	7	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	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	8	231	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	302	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	204	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	205	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	S6	301	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	202	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	202	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	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	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	404	-	-	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	l9	600	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	m6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	204	-	-	0/0/0/0	0/0/0/0
86	OHX	n6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	503	-	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	4246	3L2	O8-C13	-2.34	1.39	1.44
88	5	4246	3L2	C25-C14	-2.34	1.47	1.52
88	1	4212	3L2	O8-C13	2.30	1.49	1.44
88	5	4246	3L2	O3-C9	-2.26	1.29	1.34
88	5	4246	3L2	C22-C15	2.26	1.57	1.53

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	4246	3L2	C16-C15-C20	6.20	111.97	107.73
88	5	4246	3L2	O7-C24-C1	-5.49	98.81	110.24
88	5	4246	3L2	C13-C14-C10	-4.47	97.19	100.11
88	1	4212	3L2	C7-C8-C9	3.92	133.81	123.55
88	1	4212	3L2	C1-C24-C23	3.56	117.41	110.84

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%)	0.14	103 (5%) 22 5	43, 78, 163, 262	0
1	6	1795/1800 (99%)	0.24	143 (7%) 12 3	33, 68, 187, 266	0
2	S0	206/251 (82%)	0.09	4 (1%) 64 18	77, 95, 109, 131	0
2	s0	206/251 (82%)	-0.11	0 100 100	64, 86, 106, 112	0
3	S1	214/254 (84%)	0.39	10 (4%) 30 6	84, 113, 145, 154	0
3	s1	216/254 (85%)	-0.09	0 100 100	58, 72, 92, 104	0
4	S2	217/253 (85%)	-0.14	1 (0%) 88 46	59, 72, 90, 106	0
4	s2	217/253 (85%)	-0.04	2 (0%) 81 32	45, 62, 83, 104	0
5	S3	223/239 (93%)	0.18	7 (3%) 47 10	65, 79, 111, 133	0
5	s3	223/239 (93%)	0.48	12 (5%) 25 5	70, 121, 151, 161	0
6	S4	260/260 (100%)	0.22	6 (2%) 57 13	53, 78, 92, 131	0
6	s4	260/260 (100%)	-0.06	2 (0%) 83 35	44, 71, 84, 124	0
7	S5	206/224 (91%)	0.15	4 (1%) 64 18	86, 107, 128, 144	0
7	s5	206/224 (91%)	0.11	4 (1%) 64 18	64, 85, 110, 128	0
8	S6	226/236 (95%)	0.35	8 (3%) 42 8	54, 88, 113, 157	0
8	s6	218/236 (92%)	0.29	2 (0%) 81 32	46, 75, 99, 128	0
9	S7	184/189 (97%)	0.32	7 (3%) 38 7	72, 102, 133, 143	0
9	s7	186/189 (98%)	0.21	4 (2%) 59 14	64, 100, 133, 144	0
10	S8	188/200 (94%)	0.02	0 100 100	46, 60, 103, 122	0
10	s8	188/200 (94%)	-0.05	1 (0%) 88 46	38, 60, 108, 123	0
11	S9	185/196 (94%)	0.24	4 (2%) 59 14	70, 87, 130, 160	0
11	s9	185/196 (94%)	0.06	1 (0%) 88 46	56, 71, 111, 149	0
12	C0	96/105 (91%)	0.10	1 (1%) 79 29	73, 95, 134, 155	0
12	c0	96/105 (91%)	1.03	17 (17%) 2 1	112, 152, 164, 188	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	0.23	6 (3%) 37 7	49, 60, 128, 141	0
13	c1	146/155 (94%)	0.05	2 (1%) 72 22	41, 56, 96, 120	0
14	C2	124/142 (87%)	1.49	32 (25%) 1 1	127, 139, 170, 183	0
14	c2	124/142 (87%)	2.23	62 (50%) 0 0	187, 199, 218, 222	0
15	C3	150/150 (100%)	-0.04	0 100 100	55, 75, 88, 95	0
15	c3	150/150 (100%)	-0.11	0 100 100	48, 66, 85, 98	0
16	C4	127/136 (93%)	0.16	2 (1%) 68 20	54, 104, 121, 124	0
16	c4	128/136 (94%)	0.08	1 (0%) 83 35	43, 71, 81, 94	0
17	C5	124/141 (87%)	0.02	0 100 100	70, 89, 132, 155	0
17	c5	135/141 (95%)	0.40	7 (5%) 26 5	76, 101, 132, 143	0
18	C6	141/142 (99%)	0.19	4 (2%) 50 11	72, 98, 104, 108	0
18	c6	142/142 (100%)	0.23	7 (4%) 28 6	58, 80, 104, 128	0
19	C7	120/136 (88%)	0.38	9 (7%) 14 3	78, 98, 125, 132	0
19	c7	117/136 (86%)	0.26	2 (1%) 67 19	71, 89, 114, 124	0
20	C8	145/145 (100%)	0.35	4 (2%) 50 11	69, 99, 127, 138	0
20	c8	145/145 (100%)	0.20	6 (4%) 35 7	66, 86, 110, 126	0
21	C9	143/143 (100%)	0.24	1 (0%) 84 38	80, 95, 115, 129	0
21	c9	143/143 (100%)	0.03	0 100 100	59, 72, 95, 118	0
22	D0	107/120 (89%)	0.62	10 (9%) 9 2	66, 101, 141, 147	0
22	d0	110/120 (91%)	0.80	15 (13%) 4 1	65, 113, 156, 165	0
23	D1	87/87 (100%)	-0.09	0 100 100	76, 81, 100, 114	0
23	d1	87/87 (100%)	-0.14	0 100 100	60, 71, 100, 112	0
24	D2	129/129 (100%)	-0.16	0 100 100	56, 68, 76, 91	0
24	d2	129/129 (100%)	-0.21	0 100 100	45, 57, 66, 80	0
25	D3	144/144 (100%)	-0.11	0 100 100	45, 51, 65, 84	0
25	d3	144/144 (100%)	-0.14	0 100 100	35, 41, 53, 68	0
26	D4	134/134 (100%)	0.24	0 100 100	65, 92, 108, 118	0
26	d4	134/134 (100%)	-0.07	0 100 100	53, 79, 96, 127	0
27	D5	70/107 (65%)	0.32	2 (2%) 49 10	103, 124, 131, 135	0
27	d5	69/107 (64%)	0.28	0 100 100	81, 102, 116, 119	0
28	D6	97/97 (100%)	0.24	2 (2%) 60 15	57, 69, 127, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	-0.15	0 100 100	42, 51, 86, 94	0
29	D7	81/81 (100%)	0.15	3 (3%) 39 8	71, 88, 127, 135	0
29	d7	81/81 (100%)	0.09	2 (2%) 54 12	59, 76, 121, 130	0
30	D8	63/66 (95%)	0.93	5 (7%) 13 3	101, 115, 130, 142	0
30	d8	63/66 (95%)	0.53	1 (1%) 68 20	79, 97, 116, 129	0
31	D9	53/55 (96%)	-0.05	1 (1%) 64 18	66, 71, 94, 100	0
31	d9	53/55 (96%)	0.39	4 (7%) 14 3	64, 83, 142, 155	0
32	E0	60/60 (100%)	0.74	6 (10%) 8 2	52, 83, 133, 142	0
33	E1	71/76 (93%)	0.81	6 (8%) 11 3	96, 121, 141, 143	0
33	e1	76/76 (100%)	2.34	43 (56%) 0 0	134, 184, 193, 196	0
34	SR	318/318 (100%)	0.31	10 (3%) 47 10	67, 106, 126, 150	0
34	sR	318/318 (100%)	0.58	19 (5%) 21 5	94, 117, 140, 157	0
35	SM	159/273 (58%)	0.35	10 (6%) 19 4	55, 79, 139, 145	0
35	sM	104/273 (38%)	0.52	9 (8%) 10 3	55, 103, 184, 196	0
36	1	3149/3396 (92%)	-0.12	123 (3%) 37 7	21, 40, 130, 244	0
36	5	3150/3396 (92%)	-0.16	80 (2%) 54 12	20, 40, 114, 234	0
37	3	121/121 (100%)	-0.25	1 (0%) 83 35	29, 57, 74, 80	0
37	7	121/121 (100%)	-0.36	0 100 100	25, 42, 57, 66	0
38	4	158/158 (100%)	-0.32	3 (1%) 64 18	27, 43, 83, 135	0
38	8	158/158 (100%)	-0.22	3 (1%) 64 18	28, 51, 93, 123	0
39	L2	252/253 (99%)	-0.20	1 (0%) 90 51	27, 37, 54, 68	0
39	l2	252/253 (99%)	-0.09	6 (2%) 56 13	25, 42, 62, 73	0
40	L3	386/386 (100%)	-0.25	1 (0%) 91 58	22, 41, 57, 95	0
40	l3	386/386 (100%)	-0.31	0 100 100	17, 31, 47, 86	0
41	L4	361/361 (100%)	-0.25	1 (0%) 91 58	22, 35, 53, 65	0
41	l4	361/361 (100%)	-0.23	0 100 100	24, 39, 60, 91	0
42	L5	296/296 (100%)	-0.02	1 (0%) 91 58	40, 64, 83, 121	0
42	l5	294/296 (99%)	-0.17	1 (0%) 91 58	30, 46, 80, 131	0
43	L6	156/175 (89%)	-0.15	0 100 100	30, 36, 59, 80	0
43	l6	157/175 (89%)	-0.22	2 (1%) 74 24	28, 38, 60, 78	0
44	L7	222/243 (91%)	-0.29	1 (0%) 88 46	22, 29, 64, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	-0.26	0 100 100	20, 27, 69, 127	0
45	L8	233/255 (91%)	0.00	0 100 100	45, 60, 102, 139	0
45	l8	231/255 (90%)	0.21	6 (2%) 53 11	60, 73, 106, 122	0
46	L9	191/191 (100%)	-0.09	0 100 100	36, 47, 62, 81	0
46	l9	191/191 (100%)	-0.35	0 100 100	27, 36, 58, 74	0
47	M0	211/220 (95%)	-0.19	0 100 100	31, 40, 76, 96	0
47	m0	213/220 (96%)	-0.05	3 (1%) 72 22	32, 50, 77, 101	0
48	M1	169/173 (97%)	0.12	0 100 100	51, 70, 85, 94	0
48	m1	169/173 (97%)	-0.08	0 100 100	34, 50, 63, 75	0
49	M3	193/198 (97%)	-0.11	0 100 100	28, 45, 94, 126	0
49	m3	194/198 (97%)	0.02	3 (1%) 70 21	30, 54, 104, 147	0
50	M4	136/137 (99%)	-0.18	1 (0%) 84 38	34, 38, 52, 63	0
50	m4	137/137 (100%)	-0.30	1 (0%) 84 38	26, 32, 53, 67	0
51	M5	203/203 (100%)	-0.28	0 100 100	22, 36, 47, 53	0
51	m5	203/203 (100%)	-0.19	0 100 100	30, 47, 58, 65	0
52	M6	197/198 (99%)	-0.30	0 100 100	22, 29, 47, 51	0
52	m6	197/198 (99%)	-0.32	0 100 100	17, 21, 48, 54	0
53	M7	183/183 (100%)	0.09	10 (5%) 24 5	26, 33, 105, 153	0
53	m7	155/183 (84%)	-0.23	0 100 100	23, 30, 40, 79	0
54	M8	185/185 (100%)	-0.31	0 100 100	24, 33, 52, 73	0
54	m8	185/185 (100%)	-0.29	0 100 100	32, 38, 48, 53	0
55	M9	188/188 (100%)	0.16	4 (2%) 60 15	40, 56, 144, 149	0
55	m9	188/188 (100%)	0.17	3 (1%) 68 20	38, 51, 133, 143	0
56	N0	172/172 (100%)	-0.29	1 (0%) 86 41	27, 36, 49, 60	0
56	n0	172/172 (100%)	-0.30	0 100 100	23, 28, 41, 55	0
57	N1	159/159 (100%)	-0.20	0 100 100	28, 37, 85, 96	0
57	n1	159/159 (100%)	-0.25	0 100 100	27, 32, 68, 70	0
58	N2	100/120 (83%)	0.45	5 (5%) 28 5	72, 88, 106, 122	0
58	n2	98/120 (81%)	0.30	4 (4%) 35 7	63, 78, 90, 93	0
59	N3	136/136 (100%)	-0.19	1 (0%) 84 38	29, 36, 50, 62	0
59	n3	136/136 (100%)	-0.23	0 100 100	20, 29, 42, 48	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	0.71	17 (17%) 2 1	40, 53, 164, 168	0
60	n4	135/155 (87%)	0.36	10 (7%) 14 3	34, 82, 131, 151	0
61	N5	121/141 (85%)	-0.04	3 (2%) 54 12	36, 48, 66, 110	0
61	n5	120/141 (85%)	0.09	3 (2%) 54 12	39, 54, 76, 86	0
62	N6	126/126 (100%)	-0.16	1 (0%) 83 35	32, 44, 54, 65	0
62	n6	126/126 (100%)	-0.07	1 (0%) 83 35	39, 48, 67, 73	0
63	N7	135/135 (100%)	0.15	1 (0%) 84 38	58, 71, 86, 100	0
63	n7	135/135 (100%)	0.11	1 (0%) 84 38	66, 81, 105, 116	0
64	N8	148/148 (100%)	-0.28	0 100 100	17, 34, 59, 73	0
64	n8	148/148 (100%)	-0.27	0 100 100	29, 41, 60, 65	0
65	N9	58/58 (100%)	0.19	3 (5%) 26 5	28, 42, 98, 120	0
65	n9	58/58 (100%)	0.03	1 (1%) 67 19	28, 41, 71, 89	0
66	O0	97/104 (93%)	0.00	0 100 100	56, 66, 88, 98	0
66	o0	100/104 (96%)	-0.20	0 100 100	59, 70, 97, 107	0
67	O1	109/112 (97%)	-0.12	0 100 100	37, 49, 86, 100	0
67	o1	109/112 (97%)	-0.11	1 (0%) 81 32	31, 42, 83, 107	0
68	O2	127/129 (98%)	-0.17	0 100 100	20, 32, 44, 60	0
68	o2	127/129 (98%)	-0.15	2 (1%) 68 20	19, 36, 50, 70	0
69	O3	106/106 (100%)	-0.23	0 100 100	25, 28, 53, 68	0
69	o3	106/106 (100%)	-0.21	1 (0%) 81 32	20, 26, 53, 68	0
70	O4	112/120 (93%)	0.18	6 (5%) 25 5	39, 53, 95, 107	0
70	o4	112/120 (93%)	0.10	2 (1%) 65 18	37, 57, 95, 103	0
71	O5	119/119 (100%)	-0.10	1 (0%) 83 35	37, 51, 61, 63	0
71	o5	119/119 (100%)	-0.09	0 100 100	44, 57, 69, 77	0
72	O6	99/99 (100%)	-0.03	3 (3%) 48 10	43, 51, 87, 106	0
72	o6	99/99 (100%)	0.02	0 100 100	49, 63, 85, 107	0
73	O7	87/87 (100%)	-0.13	0 100 100	27, 31, 54, 85	0
73	o7	87/87 (100%)	-0.01	3 (3%) 43 9	31, 36, 65, 115	0
74	O8	77/77 (100%)	0.14	1 (1%) 74 24	61, 70, 98, 105	0
74	o8	77/77 (100%)	0.48	0 100 100	67, 77, 95, 99	0
75	O9	50/50 (100%)	-0.28	0 100 100	34, 37, 42, 49	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	-0.20	0 100 100	40, 42, 51, 60	0
76	Q0	52/52 (100%)	-0.24	0 100 100	33, 38, 53, 68	0
76	q0	52/52 (100%)	-0.25	0 100 100	23, 26, 39, 45	0
77	Q1	25/25 (100%)	0.04	0 100 100	42, 44, 48, 51	0
77	q1	25/25 (100%)	-0.17	0 100 100	33, 38, 51, 58	0
78	Q2	105/105 (100%)	0.14	1 (0%) 79 29	30, 43, 66, 107	0
78	q2	105/105 (100%)	0.09	0 100 100	33, 41, 60, 91	0
79	Q3	91/91 (100%)	-0.23	0 100 100	31, 40, 57, 78	0
79	q3	91/91 (100%)	-0.28	0 100 100	29, 42, 57, 68	0
80	e0	62/62 (100%)	0.35	3 (4%) 29 6	41, 70, 116, 140	0
81	p0	143/311 (45%)	0.45	7 (4%) 28 6	76, 97, 175, 186	0
82	m2	0/160	-	-	-	-
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35346 (93%)	0.02	974 (2%) 49 10	17, 57, 130, 266	0

The worst 5 of 974 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	c2	20	ALA	12.6
1	6	656	G	10.0
36	1	1237	G	10.0
60	N4	75	THR	9.4
1	6	662	U	9.2

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	5	3630	1/1	0.50	728.32	83,83,83,83	0
85	MG	1	3861	1/1	0.32	329.00	55,55,55,55	0
85	MG	2	1990	1/1	0.25	255.00	44,44,44,44	0
85	MG	5	3436	1/1	0.55	206.09	35,35,35,35	0
85	MG	5	3877	1/1	0.63	191.40	36,36,36,36	0
85	MG	5	3844	1/1	0.59	178.60	49,49,49,49	0
85	MG	1	3493	1/1	0.46	177.50	67,67,67,67	0
85	MG	4	204	1/1	0.64	171.67	37,37,37,37	0
85	MG	1	3402	1/1	0.64	158.95	60,60,60,60	0
85	MG	7	216	1/1	0.31	150.00	44,44,44,44	0
85	MG	6	1921	1/1	0.65	134.08	38,38,38,38	0
85	MG	4	208	1/1	0.49	133.23	18,18,18,18	0
85	MG	5	3859	1/1	0.28	133.00	34,34,34,34	0
85	MG	5	3734	1/1	0.42	129.15	29,29,29,29	0
85	MG	2	1917	1/1	0.58	123.41	40,40,40,40	0
85	MG	n0	202	1/1	0.21	119.00	26,26,26,26	0
85	MG	5	3677	1/1	0.41	113.61	35,35,35,35	0
85	MG	5	3731	1/1	0.36	103.80	70,70,70,70	0
85	MG	6	1933	1/1	0.79	102.17	63,63,63,63	0
85	MG	5	3420	1/1	0.34	101.00	86,86,86,86	0
85	MG	6	1945	1/1	0.53	95.67	34,34,34,34	0
85	MG	1	3405	1/1	0.78	94.38	56,56,56,56	0
85	MG	2	1956	1/1	0.83	94.07	70,70,70,70	0
85	MG	5	3777	1/1	0.53	91.25	77,77,77,77	0
85	MG	1	3596	1/1	0.56	91.14	24,24,24,24	0
85	MG	6	1922	1/1	0.82	90.01	47,47,47,47	0
85	MG	1	3578	1/1	0.59	89.96	15,15,15,15	0
85	MG	2	1988	1/1	0.62	82.67	98,98,98,98	0
85	MG	5	3815	1/1	0.80	77.31	36,36,36,36	0
85	MG	3	204	1/1	0.57	75.76	43,43,43,43	0
85	MG	1	3459	1/1	0.44	72.89	19,19,19,19	0
85	MG	1	3449	1/1	0.52	72.20	32,32,32,32	0
85	MG	5	3448	1/1	0.51	71.69	45,45,45,45	0
85	MG	1	3720	1/1	0.48	69.65	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3847	1/1	0.64	68.88	48,48,48,48	0
85	MG	6	1959	1/1	0.75	67.81	51,51,51,51	0
85	MG	1	3546	1/1	0.25	66.14	54,54,54,54	0
85	MG	1	3536	1/1	0.29	64.00	40,40,40,40	0
85	MG	2	1979	1/1	0.72	62.79	52,52,52,52	0
85	MG	6	1926	1/1	0.55	61.69	39,39,39,39	0
85	MG	5	3530	1/1	0.57	61.60	11,11,11,11	0
85	MG	5	3446	1/1	0.45	61.00	23,23,23,23	0
85	MG	2	1980	1/1	0.45	59.16	69,69,69,69	0
85	MG	2	1945	1/1	0.49	58.82	69,69,69,69	0
85	MG	5	3767	1/1	0.36	58.39	51,51,51,51	0
85	MG	6	1951	1/1	0.95	58.36	75,75,75,75	0
85	MG	1	3460	1/1	0.47	55.27	17,17,17,17	0
85	MG	2	2021	1/1	1.14	54.85	90,90,90,90	0
85	MG	1	3468	1/1	0.53	54.62	32,32,32,32	0
85	MG	5	3872	1/1	0.53	53.69	20,20,20,20	0
85	MG	2	1934	1/1	0.52	52.61	47,47,47,47	0
85	MG	1	3681	1/1	0.33	52.14	35,35,35,35	0
85	MG	5	3858	1/1	0.56	51.35	64,64,64,64	0
85	MG	1	3860	1/1	0.55	50.55	49,49,49,49	0
85	MG	5	3839	1/1	0.43	49.97	23,23,23,23	0
85	MG	3	209	1/1	0.68	49.91	51,51,51,51	0
85	MG	2	2011	1/1	0.43	49.85	48,48,48,48	0
85	MG	1	3548	1/1	0.27	49.33	30,30,30,30	0
85	MG	5	3552	1/1	0.57	49.10	29,29,29,29	0
85	MG	2	2012	1/1	0.40	49.00	69,69,69,69	0
85	MG	5	3792	1/1	0.62	48.69	51,51,51,51	0
86	OHX	5	4222	7/7	0.48	48.47	125,125,125,125	0
85	MG	2	2018	1/1	0.94	47.90	55,55,55,55	0
85	MG	5	3577	1/1	0.81	47.86	25,25,25,25	0
85	MG	4	213	1/1	0.43	47.78	35,35,35,35	0
85	MG	5	3570	1/1	0.51	47.77	16,16,16,16	0
85	MG	6	2028	1/1	1.01	47.51	85,85,85,85	0
85	MG	5	3561	1/1	0.68	47.42	14,14,14,14	0
85	MG	5	3888	1/1	0.53	47.33	46,46,46,46	0
85	MG	5	3472	1/1	0.46	47.07	27,27,27,27	0
85	MG	5	3701	1/1	0.40	46.45	36,36,36,36	0
85	MG	1	3619	1/1	0.36	46.00	36,36,36,36	0
85	MG	6	1979	1/1	0.95	45.96	61,61,61,61	0
85	MG	1	3512	1/1	0.62	45.27	16,16,16,16	0
85	MG	7	205	1/1	0.47	45.06	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	8	229	7/7	0.46	44.91	131,131,131,131	0
85	MG	5	3406	1/1	0.54	44.71	30,30,30,30	0
85	MG	5	3853	1/1	0.25	44.50	53,53,53,53	0
85	MG	3	206	1/1	0.57	43.47	26,26,26,26	0
85	MG	2	1936	1/1	0.60	43.21	43,43,43,43	0
85	MG	6	2017	1/1	0.42	43.18	38,38,38,38	0
85	MG	5	3661	1/1	0.91	43.05	56,56,56,56	0
85	MG	1	3703	1/1	0.61	42.92	32,32,32,32	0
85	MG	1	3500	1/1	0.58	42.60	53,53,53,53	0
85	MG	2	1918	1/1	0.70	42.50	42,42,42,42	0
85	MG	4	203	1/1	0.67	42.18	41,41,41,41	0
85	MG	5	3724	1/1	0.27	42.12	24,24,24,24	0
85	MG	5	3716	1/1	0.57	42.09	53,53,53,53	0
85	MG	6	1910	1/1	0.48	42.09	38,38,38,38	0
85	MG	5	4252	1/1	0.42	41.66	26,26,26,26	0
85	MG	1	3432	1/1	0.59	41.52	30,30,30,30	0
85	MG	1	3440	1/1	0.43	41.29	25,25,25,25	0
85	MG	1	3648	1/1	0.36	41.26	61,61,61,61	0
85	MG	5	3560	1/1	0.54	40.85	17,17,17,17	0
85	MG	5	3588	1/1	0.62	40.49	16,16,16,16	0
85	MG	6	2032	1/1	0.76	40.38	51,51,51,51	0
85	MG	5	3583	1/1	0.52	40.37	18,18,18,18	0
85	MG	1	3551	1/1	0.62	40.08	25,25,25,25	0
85	MG	5	3867	1/1	0.57	39.64	43,43,43,43	0
85	MG	1	3513	1/1	0.52	39.26	15,15,15,15	0
85	MG	5	3693	1/1	0.90	38.92	56,56,56,56	0
85	MG	1	3594	1/1	0.62	38.62	13,13,13,13	0
85	MG	6	1965	1/1	0.58	38.57	62,62,62,62	0
85	MG	4	224	1/1	0.46	38.50	52,52,52,52	0
85	MG	5	3491	1/1	0.37	38.45	37,37,37,37	0
85	MG	1	3423	1/1	0.38	38.44	28,28,28,28	0
85	MG	5	3823	1/1	0.58	38.26	38,38,38,38	0
85	MG	5	3535	1/1	0.45	38.20	26,26,26,26	0
85	MG	6	2042	1/1	0.23	37.80	41,41,41,41	0
85	MG	S2	302	1/1	0.74	37.29	55,55,55,55	0
85	MG	6	1944	1/1	0.77	37.25	53,53,53,53	0
85	MG	1	3561	1/1	0.56	37.23	15,15,15,15	0
85	MG	1	3689	1/1	0.40	37.09	49,49,49,49	0
85	MG	6	1915	1/1	0.46	36.96	32,32,32,32	0
85	MG	2	1937	1/1	0.69	36.95	48,48,48,48	0
85	MG	1	3796	1/1	0.39	36.77	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1993	1/1	0.56	36.42	45,45,45,45	0
85	MG	1	3810	1/1	0.43	36.29	26,26,26,26	0
85	MG	2	1906	1/1	0.37	36.19	45,45,45,45	0
85	MG	1	3770	1/1	0.27	35.86	36,36,36,36	0
85	MG	1	3514	1/1	0.29	35.84	17,17,17,17	0
85	MG	l3	401	1/1	0.59	35.79	11,11,11,11	0
85	MG	1	3655	1/1	0.50	35.72	32,32,32,32	0
85	MG	1	3726	1/1	0.80	35.71	27,27,27,27	0
85	MG	2	1924	1/1	0.71	35.66	72,72,72,72	0
85	MG	1	3857	1/1	0.69	35.48	55,55,55,55	0
85	MG	1	3559	1/1	0.53	35.42	27,27,27,27	0
86	OHX	1	4175	7/7	0.45	35.40	117,117,117,117	0
85	MG	6	2018	1/1	0.62	35.31	44,44,44,44	0
85	MG	1	3591	1/1	0.67	35.21	70,70,70,70	0
85	MG	5	3730	1/1	0.39	35.20	36,36,36,36	0
85	MG	5	3733	1/1	0.22	35.18	34,34,34,34	0
85	MG	5	3852	1/1	0.46	35.11	70,70,70,70	0
85	MG	1	3785	1/1	0.55	35.11	29,29,29,29	0
85	MG	1	3852	1/1	0.47	34.89	15,15,15,15	0
85	MG	L7	304	1/1	0.48	34.65	35,35,35,35	0
85	MG	5	3548	1/1	0.71	34.64	32,32,32,32	0
85	MG	1	3407	1/1	0.70	34.50	29,29,29,29	0
85	MG	5	3486	1/1	0.49	34.26	34,34,34,34	0
85	MG	5	3807	1/1	0.80	33.92	47,47,47,47	0
85	MG	6	1993	1/1	0.38	33.89	43,43,43,43	0
86	OHX	1	4204	7/7	0.58	33.81	127,127,127,127	0
85	MG	1	3849	1/1	0.51	33.56	30,30,30,30	0
85	MG	2	1905	1/1	0.62	33.53	45,45,45,45	0
85	MG	5	3507	1/1	0.43	33.50	25,25,25,25	0
86	OHX	5	4197	7/7	0.62	33.15	155,155,155,155	0
86	OHX	5	4215	7/7	0.46	32.99	183,183,183,183	0
85	MG	5	3863	1/1	0.59	32.90	24,24,24,24	0
85	MG	6	2009	1/1	0.25	32.75	41,41,41,41	0
86	OHX	5	4146	7/7	0.45	32.75	117,117,117,117	0
85	MG	1	3666	1/1	0.34	32.59	38,38,38,38	0
86	OHX	5	4067	7/7	0.35	32.34	109,109,109,109	0
85	MG	1	3499	1/1	0.69	32.26	56,56,56,56	0
85	MG	1	3790	1/1	0.40	32.25	45,45,45,45	0
85	MG	1	3597	1/1	0.51	32.12	11,11,11,11	0
85	MG	2	1915	1/1	0.85	32.06	61,61,61,61	0
85	MG	2	1973	1/1	1.27	32.04	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	5	3571	1/1	0.42	32.04	27,27,27,27	0
86	OHX	5	4231	7/7	0.44	32.03	143,143,143,143	0
85	MG	5	3749	1/1	0.43	31.80	21,21,21,21	0
85	MG	5	3619	1/1	0.40	31.57	36,36,36,36	0
85	MG	5	3566	1/1	0.55	31.49	14,14,14,14	0
85	MG	2	1938	1/1	0.56	31.36	56,56,56,56	0
85	MG	6	1946	1/1	0.69	31.36	56,56,56,56	0
85	MG	1	3568	1/1	0.42	31.34	15,15,15,15	0
85	MG	5	3586	1/1	0.39	31.30	17,17,17,17	0
85	MG	1	3687	1/1	0.74	31.16	35,35,35,35	0
85	MG	1	3527	1/1	0.61	30.92	17,17,17,17	0
85	MG	5	3536	1/1	0.48	30.91	25,25,25,25	0
85	MG	6	2035	1/1	0.64	30.82	49,49,49,49	0
85	MG	2	1978	1/1	0.85	30.78	56,56,56,56	0
85	MG	5	3480	1/1	0.51	30.71	55,55,55,55	0
85	MG	5	3809	1/1	0.40	30.55	29,29,29,29	0
85	MG	5	3521	1/1	0.39	30.47	25,25,25,25	0
85	MG	n3	201	1/1	0.47	30.42	14,14,14,14	0
85	MG	1	3446	1/1	0.43	30.40	22,22,22,22	0
85	MG	5	3856	1/1	0.34	30.35	26,26,26,26	0
85	MG	2	1908	1/1	0.48	30.34	64,64,64,64	0
85	MG	1	3672	1/1	0.31	30.33	38,38,38,38	0
85	MG	5	3509	1/1	0.47	30.32	26,26,26,26	0
85	MG	1	3757	1/1	0.58	30.29	25,25,25,25	0
85	MG	6	1939	1/1	0.69	30.16	63,63,63,63	0
85	MG	1	3503	1/1	0.41	30.13	18,18,18,18	0
85	MG	7	210	1/1	0.56	30.11	29,29,29,29	0
85	MG	5	3641	1/1	0.66	29.87	43,43,43,43	0
85	MG	5	3518	1/1	0.44	29.85	12,12,12,12	0
85	MG	5	3842	1/1	0.36	29.80	32,32,32,32	0
85	MG	2	2009	1/1	0.57	29.64	53,53,53,53	0
85	MG	1	3646	1/1	0.65	29.53	35,35,35,35	0
85	MG	5	3403	1/1	0.60	29.36	41,41,41,41	0
85	MG	5	3672	1/1	0.42	29.26	45,45,45,45	0
85	MG	6	1931	1/1	0.52	29.10	50,50,50,50	0
85	MG	1	3765	1/1	0.36	29.01	47,47,47,47	0
85	MG	7	201	1/1	0.68	28.96	35,35,35,35	0
85	MG	2	1919	1/1	0.53	28.73	51,51,51,51	0
86	OHX	6	2124	7/7	0.54	28.72	110,110,110,110	0
86	OHX	1	4139	7/7	0.46	28.66	134,134,134,134	0
85	MG	1	3667	1/1	0.63	28.63	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2185	7/7	0.40	28.49	148,148,148,148	0
85	MG	1	3522	1/1	0.52	28.43	25,25,25,25	0
85	MG	5	3857	1/1	0.48	28.39	48,48,48,48	0
85	MG	1	3586	1/1	0.55	28.17	14,14,14,14	0
85	MG	1	3728	1/1	0.51	28.10	25,25,25,25	0
85	MG	2	1975	1/1	0.49	28.05	70,70,70,70	0
86	OHX	1	4169	7/7	0.47	28.00	168,168,168,168	0
85	MG	1	3783	1/1	0.21	27.94	25,25,25,25	0
85	MG	5	3621	1/1	0.38	27.91	50,50,50,50	0
85	MG	5	3557	1/1	0.35	27.88	36,36,36,36	0
85	MG	5	3469	1/1	0.57	27.73	30,30,30,30	0
85	MG	5	3880	1/1	0.68	27.73	56,56,56,56	0
85	MG	1	3560	1/1	0.49	27.68	23,23,23,23	0
85	MG	5	3541	1/1	0.43	27.62	20,20,20,20	0
86	OHX	1	4170	7/7	0.43	27.60	134,134,134,134	0
85	MG	5	3832	1/1	0.54	27.57	36,36,36,36	0
85	MG	1	3413	1/1	0.30	27.54	28,28,28,28	0
85	MG	1	3589	1/1	0.66	27.51	39,39,39,39	0
85	MG	5	3761	1/1	0.54	27.40	32,32,32,32	0
85	MG	5	3576	1/1	0.39	27.29	18,18,18,18	0
85	MG	1	3844	1/1	0.74	27.28	45,45,45,45	0
85	MG	2	1939	1/1	0.38	27.27	54,54,54,54	0
85	MG	6	2010	1/1	0.62	27.15	48,48,48,48	0
85	MG	2	1912	1/1	0.55	27.04	59,59,59,59	0
85	MG	6	1925	1/1	0.55	26.79	32,32,32,32	0
85	MG	5	3585	1/1	0.61	26.64	11,11,11,11	0
85	MG	5	3742	1/1	0.30	26.59	52,52,52,52	0
86	OHX	1	4140	7/7	0.48	26.58	154,154,154,154	0
85	MG	5	3788	1/1	0.46	26.51	80,80,80,80	0
85	MG	1	3502	1/1	0.81	26.40	38,38,38,38	0
85	MG	6	1942	1/1	0.31	26.23	27,27,27,27	0
85	MG	5	3544	1/1	0.76	26.10	44,44,44,44	0
85	MG	2	1928	1/1	0.72	26.03	69,69,69,69	0
86	OHX	6	2184	7/7	0.40	25.84	141,141,141,141	0
85	MG	1	3588	1/1	0.98	25.82	37,37,37,37	0
85	MG	1	3534	1/1	0.61	25.76	15,15,15,15	0
85	MG	2	2006	1/1	0.64	25.71	41,41,41,41	0
85	MG	1	3419	1/1	1.10	25.69	85,85,85,85	0
86	OHX	1	4162	7/7	0.55	25.56	159,159,159,159	0
85	MG	2	1909	1/1	0.74	25.22	54,54,54,54	0
85	MG	1	3573	1/1	0.57	25.18	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	3637	1/1	0.28	25.06	50,50,50,50	0
85	MG	5	3490	1/1	0.17	25.00	30,30,30,30	0
85	MG	1	3552	1/1	0.65	24.97	24,24,24,24	0
85	MG	2	2020	1/1	0.73	24.89	83,83,83,83	0
85	MG	6	1916	1/1	1.24	24.84	51,51,51,51	0
85	MG	5	3428	1/1	0.33	24.75	19,19,19,19	0
85	MG	6	1948	1/1	0.47	24.73	36,36,36,36	0
85	MG	1	3585	1/1	0.56	24.73	28,28,28,28	0
85	MG	1	4216	1/1	0.58	24.70	24,24,24,24	0
85	MG	6	1917	1/1	0.56	24.66	48,48,48,48	0
86	OHX	4	232	7/7	0.35	24.65	114,114,114,114	0
85	MG	1	3831	1/1	0.91	24.64	43,43,43,43	0
85	MG	1	3554	1/1	0.54	24.61	17,17,17,17	0
85	MG	5	3774	1/1	0.97	24.60	47,47,47,47	0
85	MG	1	3682	1/1	0.32	24.57	29,29,29,29	0
85	MG	5	3780	1/1	0.30	24.56	18,18,18,18	0
85	MG	1	3464	1/1	0.46	24.52	40,40,40,40	0
86	OHX	2	2161	7/7	0.36	24.49	167,167,167,167	0
85	MG	3	205	1/1	0.41	24.48	22,22,22,22	0
85	MG	4	220	1/1	0.29	24.43	30,30,30,30	0
85	MG	5	3513	1/1	0.50	24.36	55,55,55,55	0
85	MG	2	1913	1/1	1.15	24.30	65,65,65,65	0
85	MG	5	3556	1/1	0.47	24.25	16,16,16,16	0
86	OHX	6	2179	7/7	0.42	24.19	128,128,128,128	0
85	MG	5	3662	1/1	0.82	24.15	49,49,49,49	0
86	OHX	5	4233	7/7	0.44	24.13	147,147,147,147	0
85	MG	5	3549	1/1	0.63	24.06	39,39,39,39	0
85	MG	1	3473	1/1	0.60	24.05	14,14,14,14	0
85	MG	6	2014	1/1	0.26	24.00	41,41,41,41	0
85	MG	5	3545	1/1	0.46	23.99	32,32,32,32	0
85	MG	5	3874	1/1	0.55	23.92	48,48,48,48	0
85	MG	6	1972	1/1	0.43	23.91	45,45,45,45	0
85	MG	1	3572	1/1	0.56	23.87	16,16,16,16	0
85	MG	1	3583	1/1	0.84	23.85	42,42,42,42	0
86	OHX	5	4135	7/7	0.40	23.81	127,127,127,127	0
85	MG	5	3568	1/1	0.48	23.76	22,22,22,22	0
85	MG	1	3758	1/1	0.45	23.67	46,46,46,46	0
85	MG	5	3717	1/1	0.71	23.62	40,40,40,40	0
85	MG	1	3622	1/1	0.38	23.60	39,39,39,39	0
85	MG	1	3537	1/1	0.76	23.51	22,22,22,22	0
85	MG	6	1904	1/1	0.65	23.51	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3851	1/1	0.57	23.44	62,62,62,62	0
86	OHX	5	4173	7/7	0.39	23.42	143,143,143,143	0
85	MG	1	3803	1/1	0.60	23.32	27,27,27,27	0
85	MG	1	3525	1/1	0.41	23.30	13,13,13,13	0
85	MG	5	3580	1/1	0.48	23.30	23,23,23,23	0
85	MG	1	3461	1/1	0.47	23.28	19,19,19,19	0
85	MG	5	3758	1/1	0.25	23.25	72,72,72,72	0
85	MG	2	2013	1/1	0.79	23.24	61,61,61,61	0
85	MG	8	205	1/1	0.63	23.17	41,41,41,41	0
85	MG	5	3669	1/1	0.54	23.09	48,48,48,48	0
85	MG	5	3537	1/1	0.36	23.07	26,26,26,26	0
86	OHX	5	3946	7/7	0.55	23.07	102,102,102,102	0
85	MG	6	1935	1/1	1.13	23.03	48,48,48,48	0
85	MG	5	3529	1/1	0.35	23.02	20,20,20,20	0
85	MG	6	1913	1/1	0.48	22.99	28,28,28,28	0
85	MG	o4	202	1/1	0.65	22.99	54,54,54,54	0
86	OHX	1	4196	7/7	0.25	22.91	130,130,130,130	0
86	OHX	5	4180	7/7	0.39	22.91	131,131,131,131	0
85	MG	8	202	1/1	0.48	22.85	35,35,35,35	0
85	MG	6	1928	1/1	0.66	22.76	62,62,62,62	0
85	MG	1	3526	1/1	0.40	22.76	13,13,13,13	0
86	OHX	1	4106	7/7	0.34	22.71	119,119,119,119	0
85	MG	5	3595	1/1	0.53	22.64	12,12,12,12	0
85	MG	1	3835	1/1	0.53	22.39	26,26,26,26	0
86	OHX	5	4091	7/7	0.29	22.33	120,120,120,120	0
85	MG	2	1914	1/1	0.71	22.33	57,57,57,57	0
85	MG	2	1987	1/1	0.88	22.26	47,47,47,47	0
85	MG	5	3887	1/1	0.33	22.23	112,112,112,112	0
85	MG	14	402	1/1	0.38	22.22	33,33,33,33	0
85	MG	1	3410	1/1	0.32	22.18	16,16,16,16	0
85	MG	1	3755	1/1	0.50	22.09	34,34,34,34	0
85	MG	1	3523	1/1	0.40	22.07	16,16,16,16	0
85	MG	1	3832	1/1	0.38	22.07	17,17,17,17	0
85	MG	5	3488	1/1	0.57	22.03	14,14,14,14	0
85	MG	5	3451	1/1	0.49	21.88	27,27,27,27	0
86	OHX	1	4055	7/7	0.48	21.83	108,108,108,108	0
85	MG	1	3656	1/1	0.53	21.81	18,18,18,18	0
85	MG	2	1911	1/1	0.73	21.77	45,45,45,45	0
85	MG	5	3435	1/1	0.40	21.76	24,24,24,24	0
85	MG	5	3427	1/1	0.67	21.71	38,38,38,38	0
85	MG	1	3455	1/1	0.82	21.63	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	1	3841	1/1	0.57	21.52	42,42,42,42	0
85	MG	1	3479	1/1	0.39	21.48	64,64,64,64	0
85	MG	2	1960	1/1	0.56	21.40	58,58,58,58	0
85	MG	1	3574	1/1	0.52	21.37	13,13,13,13	0
85	MG	5	3526	1/1	0.46	21.35	38,38,38,38	0
85	MG	1	3657	1/1	0.38	21.29	30,30,30,30	0
85	MG	5	3846	1/1	0.41	21.25	69,69,69,69	0
85	MG	5	3608	1/1	0.26	21.17	22,22,22,22	0
86	OHX	6	2159	7/7	0.35	21.13	123,123,123,123	0
85	MG	2	1941	1/1	0.54	21.12	62,62,62,62	0
85	MG	1	3694	1/1	0.45	21.11	37,37,37,37	0
85	MG	5	3587	1/1	0.63	21.10	46,46,46,46	0
86	OHX	1	4054	7/7	0.28	21.04	95,95,95,95	0
85	MG	5	3414	1/1	0.42	20.94	22,22,22,22	0
85	MG	1	3723	1/1	0.30	20.94	39,39,39,39	0
85	MG	6	1920	1/1	0.31	20.86	36,36,36,36	0
86	OHX	5	4243	7/7	0.50	20.85	148,148,148,148	0
85	MG	1	3839	1/1	0.47	20.74	51,51,51,51	0
85	MG	1	3640	1/1	0.40	20.73	27,27,27,27	0
85	MG	1	3738	1/1	0.34	20.73	43,43,43,43	0
85	MG	5	3442	1/1	0.37	20.68	32,32,32,32	0
85	MG	5	3770	1/1	0.37	20.64	96,96,96,96	0
85	MG	5	3871	1/1	0.40	20.56	16,16,16,16	0
86	OHX	5	4147	7/7	0.52	20.42	117,117,117,117	0
85	MG	5	3573	1/1	0.74	20.42	27,27,27,27	0
86	OHX	5	4237	7/7	0.29	20.37	162,162,162,162	0
85	MG	1	3403	1/1	0.38	20.35	25,25,25,25	0
86	OHX	5	4145	7/7	0.35	20.34	150,150,150,150	0
85	MG	5	3581	1/1	0.54	20.33	36,36,36,36	0
85	MG	5	3574	1/1	0.31	20.31	11,11,11,11	0
85	MG	5	3596	1/1	0.55	20.31	23,23,23,23	0
85	MG	5	3878	1/1	0.45	20.29	40,40,40,40	0
85	MG	1	3593	1/1	0.54	20.19	13,13,13,13	0
85	MG	5	3735	1/1	0.43	20.18	56,56,56,56	0
85	MG	5	3597	1/1	0.64	20.17	18,18,18,18	0
85	MG	1	3811	1/1	0.30	20.12	34,34,34,34	0
85	MG	1	3484	1/1	0.42	20.08	34,34,34,34	0
85	MG	1	3737	1/1	0.40	19.95	40,40,40,40	0
85	MG	2	2014	1/1	0.60	19.91	53,53,53,53	0
85	MG	5	3550	1/1	0.39	19.80	16,16,16,16	0
85	MG	1	3704	1/1	0.74	19.71	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4230	7/7	0.37	19.69	125,125,125,125	0
85	MG	1	3504	1/1	0.35	19.69	27,27,27,27	0
85	MG	5	3443	1/1	0.33	19.68	16,16,16,16	0
85	MG	1	3575	1/1	0.54	19.66	17,17,17,17	0
86	OHX	1	4123	7/7	0.44	19.63	117,117,117,117	0
86	OHX	1	4085	7/7	0.31	19.61	121,121,121,121	0
85	MG	5	3584	1/1	0.59	19.57	17,17,17,17	0
85	MG	5	3575	1/1	0.63	19.55	24,24,24,24	0
85	MG	1	3476	1/1	0.24	19.51	35,35,35,35	0
86	OHX	4	240	7/7	0.47	19.48	128,128,128,128	0
85	MG	5	3635	1/1	0.41	19.44	41,41,41,41	0
85	MG	5	3494	1/1	0.38	19.42	30,30,30,30	0
86	OHX	4	235	7/7	0.38	19.39	118,118,118,118	0
85	MG	1	3563	1/1	0.30	19.28	29,29,29,29	0
85	MG	N3	201	1/1	0.48	19.22	20,20,20,20	0
85	MG	5	3481	1/1	0.45	19.17	31,31,31,31	0
85	MG	5	3508	1/1	0.47	19.16	18,18,18,18	0
85	MG	5	3884	1/1	0.54	19.07	14,14,14,14	0
85	MG	1	3584	1/1	0.74	19.02	31,31,31,31	0
85	MG	5	3525	1/1	0.42	19.01	17,17,17,17	0
85	MG	1	3771	1/1	0.46	18.92	39,39,39,39	0
85	MG	5	3805	1/1	0.22	18.91	27,27,27,27	0
85	MG	3	208	1/1	0.42	18.89	33,33,33,33	0
85	MG	5	3562	1/1	0.59	18.88	19,19,19,19	0
86	OHX	5	4172	7/7	0.54	18.88	108,108,108,108	0
85	MG	6	1943	1/1	0.36	18.86	30,30,30,30	0
85	MG	5	3590	1/1	0.31	18.84	37,37,37,37	0
85	MG	1	3507	1/1	0.45	18.83	21,21,21,21	0
85	MG	5	3736	1/1	0.42	18.82	25,25,25,25	0
85	MG	m5	303	1/1	0.51	18.82	37,37,37,37	0
85	MG	6	1980	1/1	0.33	18.80	64,64,64,64	0
85	MG	5	3492	1/1	0.56	18.78	43,43,43,43	0
85	MG	5	3554	1/1	0.58	18.76	27,27,27,27	0
85	MG	1	3447	1/1	0.31	18.75	21,21,21,21	0
85	MG	5	3706	1/1	0.60	18.74	77,77,77,77	0
85	MG	N5	201	1/1	0.44	18.74	39,39,39,39	0
85	MG	1	3634	1/1	0.43	18.70	67,67,67,67	0
85	MG	1	3492	1/1	0.36	18.70	45,45,45,45	0
86	OHX	5	4020	7/7	0.36	18.68	110,110,110,110	0
85	MG	6	1947	1/1	0.44	18.68	36,36,36,36	0
85	MG	L4	401	1/1	0.49	18.64	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1925	1/1	0.93	18.59	53,53,53,53	0
85	MG	5	3558	1/1	0.54	18.57	21,21,21,21	0
86	OHX	2	2143	7/7	0.52	18.53	120,120,120,120	0
85	MG	M1	201	1/1	0.32	18.51	61,61,61,61	0
85	MG	1	3675	1/1	0.34	18.50	56,56,56,56	0
85	MG	5	3523	1/1	0.55	18.39	31,31,31,31	0
85	MG	6	1990	1/1	0.51	18.34	77,77,77,77	0
85	MG	6	1911	1/1	0.59	18.29	89,89,89,89	0
86	OHX	5	4240	7/7	0.34	18.27	142,142,142,142	0
86	OHX	1	4060	7/7	0.46	18.23	121,121,121,121	0
85	MG	1	3511	1/1	0.47	18.22	31,31,31,31	0
85	MG	2	1963	1/1	0.61	18.17	40,40,40,40	0
85	MG	5	3869	1/1	0.48	17.99	34,34,34,34	0
85	MG	1	3409	1/1	0.37	17.98	23,23,23,23	0
85	MG	5	3567	1/1	0.31	17.85	16,16,16,16	0
85	MG	1	3731	1/1	0.20	17.82	69,69,69,69	0
85	MG	5	3620	1/1	0.47	17.69	25,25,25,25	0
85	MG	1	3535	1/1	0.40	17.68	34,34,34,34	0
85	MG	1	3515	1/1	0.66	17.67	22,22,22,22	0
86	OHX	7	226	7/7	0.31	17.65	161,161,161,161	0
85	MG	3	202	1/1	0.42	17.64	36,36,36,36	0
85	MG	1	3570	1/1	0.58	17.64	32,32,32,32	0
85	MG	1	3713	1/1	0.38	17.60	70,70,70,70	0
86	OHX	2	2153	7/7	0.41	17.58	174,174,174,174	0
85	MG	5	3524	1/1	0.46	17.58	28,28,28,28	0
85	MG	5	3445	1/1	0.34	17.52	31,31,31,31	0
85	MG	5	3714	1/1	0.34	17.48	47,47,47,47	0
85	MG	N8	204	1/1	0.54	17.48	28,28,28,28	0
86	OHX	4	241	7/7	0.52	17.48	132,132,132,132	0
86	OHX	1	4117	7/7	0.44	17.47	118,118,118,118	0
85	MG	8	210	1/1	0.35	17.46	53,53,53,53	0
85	MG	5	3592	1/1	0.37	17.45	19,19,19,19	0
86	OHX	5	4224	7/7	0.33	17.45	155,155,155,155	0
85	MG	1	3590	1/1	0.48	17.45	33,33,33,33	0
86	OHX	1	4110	7/7	0.53	17.44	113,113,113,113	0
85	MG	1	3639	1/1	0.36	17.41	26,26,26,26	0
85	MG	1	3647	1/1	0.43	17.37	41,41,41,41	0
85	MG	5	3411	1/1	0.66	17.35	30,30,30,30	0
85	MG	1	3614	1/1	0.36	17.32	20,20,20,20	0
86	OHX	6	2181	7/7	0.51	17.32	148,148,148,148	0
85	MG	4	216	1/1	0.42	17.32	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	1	3592	1/1	0.46	17.30	20,20,20,20	0
85	MG	1	3518	1/1	0.49	17.30	17,17,17,17	0
85	MG	1	3497	1/1	0.41	17.28	35,35,35,35	0
85	MG	4	202	1/1	0.58	17.28	48,48,48,48	0
85	MG	5	4249	1/1	0.32	17.26	33,33,33,33	0
85	MG	5	3864	1/1	0.43	17.21	14,14,14,14	0
86	OHX	5	4133	7/7	0.26	17.19	139,139,139,139	0
86	OHX	2	2122	7/7	0.34	17.06	143,143,143,143	0
85	MG	5	3624	1/1	0.39	17.05	20,20,20,20	0
85	MG	5	3790	1/1	0.46	17.04	38,38,38,38	0
85	MG	1	3541	1/1	0.37	17.01	21,21,21,21	0
85	MG	2	1903	1/1	0.49	16.98	28,28,28,28	0
85	MG	5	3415	1/1	0.46	16.93	43,43,43,43	0
85	MG	5	3747	1/1	0.53	16.92	32,32,32,32	0
86	OHX	5	4214	7/7	0.41	16.89	139,139,139,139	0
85	MG	8	208	1/1	0.44	16.86	57,57,57,57	0
85	MG	1	3617	1/1	0.37	16.85	48,48,48,48	0
86	OHX	1	4167	7/7	0.44	16.84	110,110,110,110	0
86	OHX	5	3966	7/7	0.37	16.79	103,103,103,103	0
85	MG	5	3663	1/1	0.54	16.78	27,27,27,27	0
86	OHX	1	4201	7/7	0.32	16.74	120,120,120,120	0
85	MG	5	3539	1/1	0.48	16.68	16,16,16,16	0
85	MG	1	3768	1/1	0.39	16.59	18,18,18,18	0
85	MG	8	215	1/1	0.40	16.56	37,37,37,37	0
85	MG	1	3846	1/1	0.25	16.54	36,36,36,36	0
85	MG	2	2008	1/1	0.71	16.53	63,63,63,63	0
85	MG	7	203	1/1	0.36	16.51	42,42,42,42	0
85	MG	1	3414	1/1	0.57	16.48	41,41,41,41	0
85	MG	5	3546	1/1	0.50	16.45	39,39,39,39	0
85	MG	4	201	1/1	0.34	16.44	30,30,30,30	0
86	OHX	5	4206	7/7	0.30	16.43	139,139,139,139	0
85	MG	1	3431	1/1	0.33	16.39	32,32,32,32	0
85	MG	2	2016	1/1	0.37	16.36	62,62,62,62	0
85	MG	1	3829	1/1	0.42	16.31	15,15,15,15	0
86	OHX	2	2157	7/7	0.35	16.26	111,111,111,111	0
85	MG	5	3594	1/1	0.71	16.26	25,25,25,25	0
85	MG	5	3766	1/1	0.47	16.25	85,85,85,85	0
86	OHX	2	2159	7/7	0.50	16.25	146,146,146,146	0
85	MG	1	3543	1/1	0.38	16.18	23,23,23,23	0
85	MG	5	3504	1/1	0.47	16.17	19,19,19,19	0
85	MG	1	3724	1/1	0.38	16.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4199	7/7	0.40	16.13	135,135,135,135	0
85	MG	1	3862	1/1	0.36	16.08	54,54,54,54	0
85	MG	1	3579	1/1	0.39	16.05	26,26,26,26	0
85	MG	5	3459	1/1	0.35	16.05	20,20,20,20	0
85	MG	1	3761	1/1	0.61	16.02	35,35,35,35	0
86	OHX	6	2131	7/7	0.47	16.00	162,162,162,162	0
85	MG	1	3605	1/1	0.72	15.93	36,36,36,36	0
85	MG	5	3787	1/1	0.52	15.93	27,27,27,27	0
85	MG	2	1907	1/1	0.62	15.92	45,45,45,45	0
85	MG	1	3429	1/1	0.50	15.90	28,28,28,28	0
86	OHX	2	2125	7/7	0.37	15.89	122,122,122,122	0
85	MG	2	1969	1/1	0.44	15.86	56,56,56,56	0
85	MG	5	3622	1/1	0.40	15.85	33,33,33,33	0
85	MG	6	1903	1/1	0.64	15.75	28,28,28,28	0
85	MG	6	1971	1/1	0.51	15.72	63,63,63,63	0
85	MG	1	3421	1/1	0.39	15.69	26,26,26,26	0
85	MG	5	3855	1/1	0.31	15.66	32,32,32,32	0
86	OHX	1	4144	7/7	0.39	15.66	148,148,148,148	0
85	MG	12	302	1/1	0.66	15.65	25,25,25,25	0
85	MG	1	3817	1/1	0.31	15.64	37,37,37,37	0
85	MG	1	3791	1/1	0.38	15.61	19,19,19,19	0
86	OHX	1	4187	7/7	0.40	15.59	124,124,124,124	0
85	MG	5	3881	1/1	0.49	15.58	50,50,50,50	0
85	MG	6	1908	1/1	0.32	15.57	44,44,44,44	0
85	MG	1	3565	1/1	0.45	15.55	16,16,16,16	0
85	MG	5	3538	1/1	0.44	15.51	14,14,14,14	0
86	OHX	7	225	7/7	0.28	15.50	119,119,119,119	0
86	OHX	1	4208	7/7	0.53	15.50	126,126,126,126	0
85	MG	5	3418	1/1	0.48	15.49	15,15,15,15	0
85	MG	1	3472	1/1	0.32	15.49	19,19,19,19	0
85	MG	5	3540	1/1	0.53	15.49	21,21,21,21	0
85	MG	5	3658	1/1	0.35	15.49	28,28,28,28	0
85	MG	1	3663	1/1	0.46	15.48	40,40,40,40	0
86	OHX	5	4189	7/7	0.34	15.47	129,129,129,129	0
86	OHX	5	4142	7/7	0.39	15.46	132,132,132,132	0
85	MG	1	3645	1/1	0.35	15.44	34,34,34,34	0
85	MG	5	3522	1/1	0.54	15.42	21,21,21,21	0
86	OHX	6	2166	7/7	0.45	15.40	119,119,119,119	0
86	OHX	6	2154	7/7	0.40	15.34	191,191,191,191	0
85	MG	5	3424	1/1	0.36	15.27	21,21,21,21	0
85	MG	5	3582	1/1	0.38	15.23	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3703	1/1	0.57	15.21	39,39,39,39	0
85	MG	1	3519	1/1	0.36	15.18	23,23,23,23	0
85	MG	5	3744	1/1	0.40	15.08	28,28,28,28	0
86	OHX	5	4093	7/7	0.42	15.07	134,134,134,134	0
85	MG	2	1916	1/1	0.48	15.03	35,35,35,35	0
85	MG	7	211	1/1	0.22	15.00	74,74,74,74	0
85	MG	1	3644	1/1	0.23	15.00	16,16,16,16	0
85	MG	6	1958	1/1	0.48	15.00	40,40,40,40	0
85	MG	2	1972	1/1	0.50	14.97	54,54,54,54	0
86	OHX	5	4186	7/7	0.41	14.95	114,114,114,114	0
85	MG	1	3759	1/1	0.37	14.91	18,18,18,18	0
85	MG	6	2011	1/1	0.56	14.88	42,42,42,42	0
85	MG	1	3498	1/1	0.45	14.85	23,23,23,23	0
86	OHX	5	4220	7/7	0.33	14.85	136,136,136,136	0
85	MG	1	3750	1/1	0.49	14.82	38,38,38,38	0
86	OHX	5	4175	7/7	0.37	14.80	137,137,137,137	0
85	MG	5	3461	1/1	0.56	14.79	21,21,21,21	0
86	OHX	5	4153	7/7	0.36	14.72	126,126,126,126	0
85	MG	2	2001	1/1	0.29	14.71	98,98,98,98	0
86	OHX	1	4176	7/7	0.49	14.69	139,139,139,139	0
85	MG	1	3558	1/1	0.29	14.66	16,16,16,16	0
85	MG	5	3687	1/1	0.37	14.66	45,45,45,45	0
86	OHX	5	4196	7/7	0.36	14.64	137,137,137,137	0
86	OHX	1	4141	7/7	0.32	14.51	141,141,141,141	0
85	MG	7	202	1/1	0.34	14.49	18,18,18,18	0
85	MG	5	3514	1/1	0.47	14.48	17,17,17,17	0
85	MG	2	1962	1/1	0.59	14.46	81,81,81,81	0
86	OHX	6	2125	7/7	0.29	14.46	111,111,111,111	0
85	MG	1	3557	1/1	0.48	14.45	51,51,51,51	0
85	MG	5	3637	1/1	0.44	14.39	35,35,35,35	0
86	OHX	1	4168	7/7	0.45	14.39	161,161,161,161	0
85	MG	2	1929	1/1	0.53	14.33	60,60,60,60	0
86	OHX	6	2188	7/7	0.32	14.29	150,150,150,150	0
86	OHX	6	2178	7/7	0.43	14.28	131,131,131,131	0
86	OHX	5	4042	7/7	0.23	14.26	117,117,117,117	0
85	MG	1	3690	1/1	0.41	14.25	23,23,23,23	0
85	MG	n9	101	1/1	0.30	14.25	21,21,21,21	0
85	MG	1	3739	1/1	0.45	14.22	42,42,42,42	0
85	MG	5	3559	1/1	0.48	14.20	22,22,22,22	0
85	MG	1	3516	1/1	0.57	14.19	27,27,27,27	0
85	MG	1	3838	1/1	0.40	14.18	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	3756	1/1	0.38	14.17	40,40,40,40	0
86	OHX	1	4193	7/7	0.51	14.15	135,135,135,135	0
85	MG	2	1944	1/1	0.37	14.10	56,56,56,56	0
86	OHX	1	4070	7/7	0.40	14.08	102,102,102,102	0
85	MG	5	3444	1/1	0.26	14.08	20,20,20,20	0
85	MG	6	1907	1/1	0.42	14.07	65,65,65,65	0
85	MG	2	1935	1/1	0.44	13.99	39,39,39,39	0
86	OHX	1	4197	7/7	0.39	13.97	121,121,121,121	0
86	OHX	1	4132	7/7	0.41	13.97	120,120,120,120	0
86	OHX	5	4228	7/7	0.42	13.96	153,153,153,153	0
85	MG	N0	201	1/1	0.51	13.92	33,33,33,33	0
85	MG	1	3529	1/1	0.75	13.92	21,21,21,21	0
85	MG	5	3828	1/1	0.28	13.86	26,26,26,26	0
85	MG	4	209	1/1	0.49	13.81	27,27,27,27	0
85	MG	5	3458	1/1	0.34	13.81	19,19,19,19	0
86	OHX	5	4151	7/7	0.37	13.80	126,126,126,126	0
85	MG	5	3607	1/1	0.37	13.80	19,19,19,19	0
85	MG	1	3486	1/1	0.38	13.79	19,19,19,19	0
85	MG	1	3827	1/1	0.44	13.69	39,39,39,39	0
86	OHX	5	4076	7/7	0.32	13.66	110,110,110,110	0
85	MG	2	1986	1/1	0.28	13.63	79,79,79,79	0
85	MG	6	1906	1/1	0.42	13.61	36,36,36,36	0
86	OHX	2	2171	7/7	0.44	13.61	142,142,142,142	0
86	OHX	5	4203	7/7	0.35	13.60	154,154,154,154	0
86	OHX	5	4131	7/7	0.35	13.60	122,122,122,122	0
85	MG	1	3532	1/1	0.42	13.59	25,25,25,25	0
85	MG	13	402	1/1	0.56	13.58	19,19,19,19	0
85	MG	6	1937	1/1	0.38	13.58	34,34,34,34	0
85	MG	5	3639	1/1	0.28	13.57	45,45,45,45	0
85	MG	2	2017	1/1	0.48	13.56	67,67,67,67	0
86	OHX	1	4194	7/7	0.40	13.51	166,166,166,166	0
85	MG	6	1912	1/1	0.63	13.49	37,37,37,37	0
85	MG	5	3510	1/1	0.54	13.49	20,20,20,20	0
85	MG	6	1974	1/1	0.41	13.42	51,51,51,51	0
85	MG	1	3697	1/1	0.32	13.42	53,53,53,53	0
85	MG	5	3527	1/1	0.40	13.39	15,15,15,15	0
86	OHX	5	4106	7/7	0.36	13.36	112,112,112,112	0
85	MG	1	3528	1/1	0.38	13.36	33,33,33,33	0
85	MG	1	3462	1/1	0.37	13.34	14,14,14,14	0
85	MG	1	3506	1/1	0.50	13.34	26,26,26,26	0
85	MG	1	3427	1/1	0.54	13.33	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3466	1/1	0.25	13.31	22,22,22,22	0
86	OHX	6	2149	7/7	0.39	13.31	119,119,119,119	0
85	MG	5	3502	1/1	0.37	13.30	27,27,27,27	0
85	MG	1	3780	1/1	0.36	13.29	36,36,36,36	0
86	OHX	5	4239	7/7	0.41	13.27	168,168,168,168	0
85	MG	5	3759	1/1	0.41	13.27	27,27,27,27	0
86	OHX	2	2176	7/7	0.48	13.26	175,175,175,175	0
86	OHX	3	224	7/7	0.38	13.24	171,171,171,171	0
85	MG	5	3563	1/1	0.42	13.24	22,22,22,22	0
85	MG	2	1923	1/1	0.25	13.24	47,47,47,47	0
85	MG	5	3645	1/1	0.39	13.21	38,38,38,38	0
86	OHX	2	2135	7/7	0.41	13.21	135,135,135,135	0
85	MG	L7	301	1/1	0.36	13.18	23,23,23,23	0
85	MG	6	1905	1/1	0.64	13.15	36,36,36,36	0
86	OHX	1	4210	7/7	0.52	13.10	137,137,137,137	0
86	OHX	8	227	7/7	0.30	13.08	126,126,126,126	0
85	MG	4	219	1/1	0.28	13.06	50,50,50,50	0
85	MG	6	2041	1/1	0.30	13.01	41,41,41,41	0
85	MG	5	3659	1/1	0.38	12.91	21,21,21,21	0
85	MG	n8	201	1/1	0.43	12.91	26,26,26,26	0
85	MG	1	3485	1/1	0.38	12.90	26,26,26,26	0
85	MG	6	2038	1/1	0.54	12.89	105,105,105,105	0
86	OHX	1	4165	7/7	0.41	12.86	109,109,109,109	0
85	MG	1	3501	1/1	0.46	12.84	16,16,16,16	0
85	MG	5	3726	1/1	0.39	12.84	19,19,19,19	0
85	MG	1	3853	1/1	0.89	12.81	48,48,48,48	0
85	MG	1	3496	1/1	0.26	12.81	23,23,23,23	0
86	OHX	1	4184	7/7	0.37	12.77	149,149,149,149	0
85	MG	2	1910	1/1	0.47	12.72	42,42,42,42	0
85	MG	1	3843	1/1	0.27	12.72	52,52,52,52	0
85	MG	2	1983	1/1	0.34	12.65	55,55,55,55	0
85	MG	5	3572	1/1	0.44	12.65	17,17,17,17	0
86	OHX	5	4085	7/7	0.36	12.64	111,111,111,111	0
85	MG	5	3652	1/1	0.39	12.63	60,60,60,60	0
85	MG	2	1955	1/1	0.36	12.61	55,55,55,55	0
85	MG	1	3854	1/1	0.47	12.60	29,29,29,29	0
86	OHX	1	4152	7/7	0.30	12.60	133,133,133,133	0
85	MG	1	3781	1/1	0.32	12.59	28,28,28,28	0
86	OHX	1	4125	7/7	0.41	12.59	154,154,154,154	0
86	OHX	6	2163	7/7	0.36	12.57	143,143,143,143	0
86	OHX	6	2202	7/7	0.44	12.55	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3595	1/1	0.42	12.52	14,14,14,14	0
85	MG	1	3544	1/1	0.26	12.51	31,31,31,31	0
85	MG	5	3657	1/1	0.26	12.50	16,16,16,16	0
85	MG	o3	201	1/1	0.49	12.49	24,24,24,24	0
86	OHX	5	4156	7/7	0.43	12.49	115,115,115,115	0
86	OHX	5	4132	7/7	0.49	12.43	137,137,137,137	0
85	MG	5	3679	1/1	0.47	12.42	69,69,69,69	0
86	OHX	2	2163	7/7	0.39	12.36	131,131,131,131	0
85	MG	1	3798	1/1	0.48	12.32	42,42,42,42	0
85	MG	6	1975	1/1	0.52	12.31	56,56,56,56	0
85	MG	1	3582	1/1	0.64	12.28	30,30,30,30	0
85	MG	1	3676	1/1	0.37	12.20	32,32,32,32	0
85	MG	5	3692	1/1	0.19	12.20	40,40,40,40	0
85	MG	5	3837	1/1	0.43	12.20	38,38,38,38	0
86	OHX	5	4211	7/7	0.37	12.19	144,144,144,144	0
86	OHX	5	4152	7/7	0.33	12.18	111,111,111,111	0
85	MG	5	3814	1/1	0.35	12.17	50,50,50,50	0
86	OHX	5	4055	7/7	0.29	12.13	120,120,120,120	0
86	OHX	5	4082	7/7	0.51	12.12	110,110,110,110	0
85	MG	1	3510	1/1	0.49	12.09	19,19,19,19	0
85	MG	1	3610	1/1	0.18	12.08	33,33,33,33	0
85	MG	5	3431	1/1	0.26	12.08	22,22,22,22	0
85	MG	1	3490	1/1	0.29	12.07	32,32,32,32	0
86	OHX	1	4127	7/7	0.31	12.04	159,159,159,159	0
86	OHX	5	4122	7/7	0.32	12.03	153,153,153,153	0
85	MG	1	3710	1/1	0.39	11.98	22,22,22,22	0
86	OHX	2	2177	7/7	0.54	11.98	147,147,147,147	0
85	MG	5	3413	1/1	0.55	11.96	31,31,31,31	0
86	OHX	8	230	7/7	0.48	11.92	124,124,124,124	0
85	MG	5	3591	1/1	0.43	11.90	15,15,15,15	0
85	MG	5	3644	1/1	0.39	11.90	24,24,24,24	0
85	MG	4	212	1/1	0.36	11.86	42,42,42,42	0
86	OHX	1	4151	7/7	0.43	11.85	140,140,140,140	0
85	MG	1	3633	1/1	0.35	11.85	38,38,38,38	0
85	MG	1	3600	1/1	0.52	11.84	23,23,23,23	0
85	MG	3	214	1/1	0.30	11.83	56,56,56,56	0
85	MG	5	3463	1/1	0.33	11.81	20,20,20,20	0
86	OHX	1	4043	7/7	0.29	11.78	103,103,103,103	0
85	MG	2	1940	1/1	0.36	11.77	52,52,52,52	0
85	MG	5	3763	1/1	0.41	11.75	21,21,21,21	0
86	OHX	3	225	7/7	0.33	11.71	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	1	3508	1/1	0.46	11.70	10,10,10,10	0
85	MG	1	3418	1/1	0.39	11.68	42,42,42,42	0
86	OHX	6	2134	7/7	0.36	11.67	143,143,143,143	0
85	MG	5	3862	1/1	0.37	11.64	19,19,19,19	0
86	OHX	5	4169	7/7	0.44	11.63	137,137,137,137	0
86	OHX	2	2173	7/7	0.31	11.63	167,167,167,167	0
85	MG	2	1932	1/1	0.40	11.62	56,56,56,56	0
85	MG	5	3628	1/1	0.38	11.60	26,26,26,26	0
85	MG	5	3405	1/1	0.38	11.55	18,18,18,18	0
86	OHX	5	4161	7/7	0.30	11.54	134,134,134,134	0
85	MG	1	3654	1/1	0.33	11.53	21,21,21,21	0
85	MG	5	3668	1/1	0.40	11.53	22,22,22,22	0
85	MG	5	3642	1/1	0.54	11.52	31,31,31,31	0
85	MG	N8	202	1/1	0.36	11.51	21,21,21,21	0
85	MG	1	3691	1/1	0.35	11.50	28,28,28,28	0
85	MG	5	3477	1/1	0.35	11.50	17,17,17,17	0
85	MG	8	214	1/1	0.46	11.46	86,86,86,86	0
85	MG	6	1902	1/1	0.43	11.46	39,39,39,39	0
86	OHX	1	4161	7/7	0.37	11.44	145,145,145,145	0
86	OHX	5	4108	7/7	0.22	11.41	115,115,115,115	0
85	MG	5	3579	1/1	0.30	11.41	17,17,17,17	0
85	MG	17	302	1/1	0.57	11.38	37,37,37,37	0
86	OHX	1	4026	7/7	0.39	11.37	115,115,115,115	0
85	MG	1	3795	1/1	0.35	11.36	43,43,43,43	0
85	MG	6	1955	1/1	0.56	11.36	31,31,31,31	0
85	MG	1	3453	1/1	0.33	11.35	24,24,24,24	0
85	MG	5	3515	1/1	0.61	11.34	28,28,28,28	0
85	MG	4	206	1/1	0.33	11.33	35,35,35,35	0
85	MG	3	201	1/1	0.35	11.33	57,57,57,57	0
85	MG	1	3830	1/1	0.42	11.33	11,11,11,11	0
85	MG	5	3453	1/1	0.34	11.32	34,34,34,34	0
85	MG	1	3556	1/1	0.34	11.29	42,42,42,42	0
86	OHX	5	4212	7/7	0.38	11.29	121,121,121,121	0
85	MG	5	3721	1/1	0.42	11.29	29,29,29,29	0
85	MG	1	3553	1/1	0.39	11.28	24,24,24,24	0
85	MG	5	3673	1/1	0.39	11.28	34,34,34,34	0
86	OHX	6	2182	7/7	0.48	11.26	131,131,131,131	0
86	OHX	5	4179	7/7	0.41	11.26	118,118,118,118	0
86	OHX	5	4144	7/7	0.44	11.26	110,110,110,110	0
85	MG	1	3793	1/1	0.33	11.26	31,31,31,31	0
85	MG	6	1954	1/1	0.44	11.24	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4076	7/7	0.31	11.21	129,129,129,129	0
85	MG	1	3415	1/1	0.41	11.16	22,22,22,22	0
85	MG	5	3876	1/1	0.37	11.15	24,24,24,24	0
85	MG	2	1984	1/1	0.36	11.13	93,93,93,93	0
85	MG	5	3547	1/1	0.41	11.12	40,40,40,40	0
85	MG	2	2002	1/1	0.53	11.11	75,75,75,75	0
85	MG	5	3655	1/1	0.28	11.09	27,27,27,27	0
86	OHX	5	4209	7/7	0.43	11.08	135,135,135,135	0
85	MG	1	3457	1/1	0.29	11.07	29,29,29,29	0
85	MG	2	1922	1/1	0.50	11.07	51,51,51,51	0
86	OHX	5	4199	7/7	0.46	11.01	145,145,145,145	0
85	MG	1	3764	1/1	0.22	11.00	39,39,39,39	0
85	MG	1	3458	1/1	0.32	11.00	55,55,55,55	0
85	MG	1	3859	1/1	0.38	11.00	99,99,99,99	0
86	OHX	5	4159	7/7	0.41	10.99	180,180,180,180	0
86	OHX	5	4113	7/7	0.33	10.95	122,122,122,122	0
86	OHX	1	4146	7/7	0.30	10.85	141,141,141,141	0
86	OHX	1	4097	7/7	0.32	10.79	119,119,119,119	0
85	MG	5	3520	1/1	0.35	10.78	22,22,22,22	0
86	OHX	1	4166	7/7	0.33	10.76	112,112,112,112	0
85	MG	6	1970	1/1	0.26	10.75	57,57,57,57	0
85	MG	1	3722	1/1	0.42	10.73	51,51,51,51	0
85	MG	4	223	1/1	0.42	10.72	34,34,34,34	0
85	MG	c8	201	1/1	0.61	10.72	71,71,71,71	0
85	MG	1	3467	1/1	0.28	10.70	29,29,29,29	0
86	OHX	5	4225	7/7	0.30	10.70	136,136,136,136	0
85	MG	1	3818	1/1	0.27	10.69	46,46,46,46	0
86	OHX	6	2145	7/7	0.22	10.67	107,107,107,107	0
85	MG	1	3693	1/1	0.35	10.66	37,37,37,37	0
85	MG	1	3408	1/1	0.32	10.64	34,34,34,34	0
86	OHX	4	236	7/7	0.41	10.62	141,141,141,141	0
86	OHX	5	4048	7/7	0.50	10.61	117,117,117,117	0
85	MG	1	3451	1/1	0.32	10.61	26,26,26,26	0
85	MG	5	3433	1/1	0.31	10.57	65,65,65,65	0
85	MG	5	3739	1/1	0.27	10.53	26,26,26,26	0
85	MG	5	3464	1/1	0.28	10.53	46,46,46,46	0
85	MG	5	3511	1/1	0.46	10.53	15,15,15,15	0
85	MG	5	3813	1/1	0.40	10.50	53,53,53,53	0
85	MG	5	3718	1/1	0.30	10.50	41,41,41,41	0
86	OHX	1	4084	7/7	0.33	10.49	126,126,126,126	0
85	MG	1	3411	1/1	0.50	10.49	38,38,38,38	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	0.35	10.47	27,27,27,27	0
86	OHX	6	2172	7/7	0.39	10.46	125,125,125,125	0
86	OHX	5	4050	7/7	0.29	10.46	105,105,105,105	0
86	OHX	5	4120	7/7	0.33	10.44	120,120,120,120	0
85	MG	1	3438	1/1	0.47	10.43	34,34,34,34	0
85	MG	5	3506	1/1	0.39	10.39	16,16,16,16	0
85	MG	1	3562	1/1	0.35	10.39	36,36,36,36	0
85	MG	4	221	1/1	0.31	10.38	29,29,29,29	0
85	MG	7	215	1/1	0.26	10.37	36,36,36,36	0
85	MG	5	3782	1/1	0.67	10.36	78,78,78,78	0
85	MG	5	3606	1/1	0.31	10.32	36,36,36,36	0
85	MG	5	3457	1/1	0.34	10.32	58,58,58,58	0
86	OHX	5	4178	7/7	0.41	10.30	119,119,119,119	0
85	MG	1	3517	1/1	0.46	10.27	24,24,24,24	0
85	MG	5	3636	1/1	0.25	10.24	35,35,35,35	0
86	OHX	5	4140	7/7	0.31	10.23	107,107,107,107	0
85	MG	1	3452	1/1	0.33	10.23	32,32,32,32	0
85	MG	1	3848	1/1	0.39	10.22	40,40,40,40	0
85	MG	5	3519	1/1	0.34	10.20	14,14,14,14	0
85	MG	1	3555	1/1	0.36	10.20	28,28,28,28	0
85	MG	1	3524	1/1	0.27	10.19	31,31,31,31	0
86	OHX	1	4062	7/7	0.33	10.19	105,105,105,105	0
86	OHX	1	4157	7/7	0.32	10.19	125,125,125,125	0
86	OHX	4	237	7/7	0.30	10.19	137,137,137,137	0
85	MG	2	1952	1/1	0.39	10.14	93,93,93,93	0
86	OHX	m4	201	7/7	0.49	10.14	209,209,209,209	0
85	MG	1	3684	1/1	0.48	10.07	29,29,29,29	0
86	OHX	1	4059	7/7	0.37	10.07	141,141,141,141	0
86	OHX	1	4153	7/7	0.33	10.07	122,122,122,122	0
85	MG	5	3789	1/1	0.48	10.05	29,29,29,29	0
85	MG	6	2022	1/1	0.38	10.05	46,46,46,46	0
85	MG	1	3587	1/1	0.33	10.05	18,18,18,18	0
86	OHX	1	4133	7/7	0.28	10.04	110,110,110,110	0
85	MG	8	204	1/1	0.40	10.04	44,44,44,44	0
86	OHX	1	4183	7/7	0.47	10.02	127,127,127,127	0
85	MG	1	3652	1/1	0.29	10.00	19,19,19,19	0
85	MG	1	3550	1/1	0.46	10.00	33,33,33,33	0
85	MG	5	3772	1/1	0.34	9.99	18,18,18,18	0
85	MG	5	3532	1/1	0.33	9.98	25,25,25,25	0
85	MG	d3	202	1/1	0.66	9.97	44,44,44,44	0
85	MG	1	3662	1/1	0.29	9.97	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3571	1/1	0.52	9.95	19,19,19,19	0
86	OHX	5	4190	7/7	0.38	9.93	152,152,152,152	0
86	OHX	7	228	7/7	0.28	9.91	133,133,133,133	0
86	OHX	1	4174	7/7	0.33	9.90	138,138,138,138	0
85	MG	1	3858	1/1	0.47	9.86	29,29,29,29	0
85	MG	1	3505	1/1	0.32	9.84	23,23,23,23	0
85	MG	5	3505	1/1	0.35	9.84	34,34,34,34	0
85	MG	1	3456	1/1	0.32	9.84	16,16,16,16	0
85	MG	2	1926	1/1	0.43	9.83	79,79,79,79	0
85	MG	5	3476	1/1	0.41	9.82	28,28,28,28	0
85	MG	6	2020	1/1	0.30	9.80	76,76,76,76	0
86	OHX	8	226	7/7	0.26	9.79	135,135,135,135	0
86	OHX	6	2158	7/7	0.44	9.79	128,128,128,128	0
86	OHX	5	4056	7/7	0.29	9.73	128,128,128,128	0
85	MG	1	3729	1/1	0.36	9.71	15,15,15,15	0
85	MG	6	2027	1/1	0.63	9.71	80,80,80,80	0
85	MG	1	4218	1/1	0.35	9.70	25,25,25,25	0
85	MG	1	3480	1/1	0.40	9.69	33,33,33,33	0
85	MG	6	2043	1/1	0.54	9.69	70,70,70,70	0
85	MG	1	3531	1/1	0.27	9.69	15,15,15,15	0
86	OHX	8	222	7/7	0.28	9.67	112,112,112,112	0
85	MG	5	4251	1/1	0.38	9.66	20,20,20,20	0
85	MG	5	3456	1/1	0.26	9.61	28,28,28,28	0
85	MG	6	1987	1/1	0.32	9.54	40,40,40,40	0
86	OHX	5	4104	7/7	0.43	9.52	138,138,138,138	0
85	MG	1	3626	1/1	0.28	9.52	27,27,27,27	0
86	OHX	1	4077	7/7	0.35	9.51	123,123,123,123	0
85	MG	1	3412	1/1	0.30	9.50	16,16,16,16	0
85	MG	1	3665	1/1	0.41	9.48	68,68,68,68	0
85	MG	5	3517	1/1	0.32	9.46	28,28,28,28	0
86	OHX	6	2187	7/7	0.22	9.45	132,132,132,132	0
86	OHX	6	2169	7/7	0.41	9.45	111,111,111,111	0
85	MG	5	3873	1/1	0.32	9.41	20,20,20,20	0
86	OHX	2	2102	7/7	0.33	9.40	142,142,142,142	0
85	MG	1	3794	1/1	0.23	9.39	18,18,18,18	0
85	MG	6	1967	1/1	0.37	9.38	87,87,87,87	0
86	OHX	5	4064	7/7	0.32	9.37	128,128,128,128	0
85	MG	6	1952	1/1	0.50	9.33	54,54,54,54	0
86	OHX	1	4137	7/7	0.44	9.32	107,107,107,107	0
85	MG	6	2029	1/1	0.44	9.31	64,64,64,64	0
85	MG	5	3497	1/1	0.36	9.31	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	3424	1/1	0.38	9.29	38,38,38,38	0
85	MG	1	3539	1/1	0.47	9.29	11,11,11,11	0
85	MG	5	3439	1/1	0.26	9.28	22,22,22,22	0
86	OHX	5	4094	7/7	0.38	9.27	129,129,129,129	0
85	MG	5	3627	1/1	0.33	9.26	47,47,47,47	0
86	OHX	5	4114	7/7	0.34	9.25	147,147,147,147	0
86	OHX	1	4207	7/7	0.48	9.24	129,129,129,129	0
86	OHX	1	4205	7/7	0.39	9.23	123,123,123,123	0
85	MG	5	3798	1/1	0.19	9.21	51,51,51,51	0
86	OHX	5	4191	7/7	0.30	9.21	107,107,107,107	0
85	MG	5	3503	1/1	0.29	9.20	32,32,32,32	0
85	MG	5	3654	1/1	0.32	9.19	27,27,27,27	0
85	MG	6	1927	1/1	0.27	9.17	43,43,43,43	0
85	MG	1	3649	1/1	0.57	9.16	90,90,90,90	0
85	MG	5	3712	1/1	0.28	9.16	37,37,37,37	0
85	MG	2	2019	1/1	0.78	9.16	83,83,83,83	0
85	MG	1	3477	1/1	0.28	9.16	30,30,30,30	0
86	OHX	5	4086	7/7	0.28	9.16	111,111,111,111	0
85	MG	5	3485	1/1	0.28	9.16	33,33,33,33	0
85	MG	2	1957	1/1	0.45	9.15	86,86,86,86	0
86	OHX	1	4067	7/7	0.35	9.13	117,117,117,117	0
85	MG	5	3602	1/1	0.43	9.10	26,26,26,26	0
86	OHX	5	4171	7/7	0.24	9.10	137,137,137,137	0
85	MG	1	3542	1/1	0.36	9.08	18,18,18,18	0
85	MG	5	3865	1/1	0.48	9.06	44,44,44,44	0
86	OHX	1	4092	7/7	0.33	9.06	126,126,126,126	0
85	MG	5	3409	1/1	0.31	9.05	34,34,34,34	0
86	OHX	5	4241	7/7	0.39	9.04	142,142,142,142	0
86	OHX	1	4136	7/7	0.34	8.91	135,135,135,135	0
86	OHX	1	4069	7/7	0.25	8.89	143,143,143,143	0
86	OHX	6	2195	7/7	0.39	8.89	140,140,140,140	0
85	MG	5	3786	1/1	0.31	8.87	46,46,46,46	0
85	MG	1	3442	1/1	0.34	8.87	16,16,16,16	0
85	MG	2	2007	1/1	0.27	8.85	38,38,38,38	0
86	OHX	2	2091	7/7	0.38	8.85	118,118,118,118	0
85	MG	1	3741	1/1	0.25	8.81	28,28,28,28	0
86	OHX	5	4157	7/7	0.26	8.77	111,111,111,111	0
85	MG	2	1901	1/1	1.16	8.77	64,64,64,64	0
85	MG	8	203	1/1	0.42	8.71	28,28,28,28	0
85	MG	5	3441	1/1	0.42	8.71	19,19,19,19	0
85	MG	m5	301	1/1	0.42	8.71	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4211	7/7	0.35	8.71	157,157,157,157	0
85	MG	1	3628	1/1	0.31	8.68	51,51,51,51	0
85	MG	6	2034	1/1	0.84	8.67	74,74,74,74	0
86	OHX	5	4141	7/7	0.28	8.66	130,130,130,130	0
85	MG	5	3438	1/1	0.42	8.66	44,44,44,44	0
86	OHX	5	4181	7/7	0.50	8.65	114,114,114,114	0
86	OHX	5	4045	7/7	0.34	8.64	106,106,106,106	0
86	OHX	6	2155	7/7	0.31	8.63	148,148,148,148	0
85	MG	5	3760	1/1	0.27	8.63	28,28,28,28	0
85	MG	5	3474	1/1	0.52	8.61	35,35,35,35	0
86	OHX	1	4138	7/7	0.24	8.61	123,123,123,123	0
85	MG	5	3713	1/1	0.35	8.60	40,40,40,40	0
86	OHX	1	4105	7/7	0.29	8.59	129,129,129,129	0
85	MG	D0	201	1/1	0.57	8.59	65,65,65,65	0
85	MG	5	3455	1/1	0.27	8.58	16,16,16,16	0
86	OHX	o7	503	7/7	0.43	8.55	123,123,123,123	0
85	MG	5	3779	1/1	0.24	8.55	49,49,49,49	0
86	OHX	1	4107	7/7	0.35	8.55	135,135,135,135	0
85	MG	S2	301	1/1	0.57	8.51	43,43,43,43	0
85	MG	5	3421	1/1	0.44	8.49	29,29,29,29	0
85	MG	1	3569	1/1	0.32	8.49	14,14,14,14	0
85	MG	5	3614	1/1	0.29	8.49	30,30,30,30	0
86	OHX	6	2118	7/7	0.35	8.49	111,111,111,111	0
85	MG	6	1932	1/1	0.28	8.45	36,36,36,36	0
85	MG	2	2004	1/1	0.28	8.44	50,50,50,50	0
85	MG	5	3475	1/1	0.32	8.44	76,76,76,76	0
85	MG	1	3607	1/1	0.54	8.44	49,49,49,49	0
85	MG	6	1961	1/1	0.37	8.42	84,84,84,84	0
85	MG	1	3718	1/1	0.35	8.39	28,28,28,28	0
85	MG	5	3822	1/1	0.26	8.38	17,17,17,17	0
85	MG	2	1943	1/1	0.45	8.38	54,54,54,54	0
86	OHX	1	4119	7/7	0.44	8.37	144,144,144,144	0
85	MG	1	3826	1/1	0.25	8.37	20,20,20,20	0
86	OHX	1	3984	7/7	0.32	8.36	104,104,104,104	0
86	OHX	s9	201	7/7	0.49	8.36	132,132,132,132	0
85	MG	M5	301	1/1	0.33	8.35	25,25,25,25	0
86	OHX	1	4075	7/7	0.44	8.28	112,112,112,112	0
85	MG	6	1934	1/1	0.46	8.27	73,73,73,73	0
86	OHX	2	2104	7/7	0.26	8.27	118,118,118,118	0
86	OHX	5	4166	7/7	0.33	8.26	102,102,102,102	0
86	OHX	2	2148	7/7	0.34	8.24	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2128	7/7	0.32	8.23	144,144,144,144	0
85	MG	5	3555	1/1	0.44	8.20	19,19,19,19	0
85	MG	1	3509	1/1	0.28	8.19	33,33,33,33	0
85	MG	5	3665	1/1	0.31	8.18	22,22,22,22	0
85	MG	2	1970	1/1	0.40	8.17	74,74,74,74	0
85	MG	18	301	1/1	0.50	8.15	55,55,55,55	0
85	MG	2	1981	1/1	0.28	8.15	53,53,53,53	0
86	OHX	5	4207	7/7	0.26	8.15	113,113,113,113	0
85	MG	6	2004	1/1	0.20	8.12	93,93,93,93	0
85	MG	6	1914	1/1	0.42	8.11	47,47,47,47	0
85	MG	1	3708	1/1	0.29	8.11	39,39,39,39	0
85	MG	5	3531	1/1	0.37	8.10	27,27,27,27	0
86	OHX	5	4036	7/7	0.30	8.10	123,123,123,123	0
86	OHX	2	2089	7/7	0.29	8.09	125,125,125,125	0
86	OHX	1	4114	7/7	0.37	8.05	132,132,132,132	0
86	OHX	5	4185	7/7	0.28	8.04	119,119,119,119	0
85	MG	1	3651	1/1	0.28	8.04	32,32,32,32	0
86	OHX	3	226	7/7	0.29	7.99	136,136,136,136	0
85	MG	5	3670	1/1	0.40	7.99	19,19,19,19	0
86	OHX	6	2113	7/7	0.35	7.99	126,126,126,126	0
85	MG	1	3814	1/1	0.26	7.96	37,37,37,37	0
85	MG	7	212	1/1	0.32	7.95	58,58,58,58	0
85	MG	1	3630	1/1	0.29	7.93	23,23,23,23	0
86	OHX	5	4121	7/7	0.31	7.89	136,136,136,136	0
86	OHX	14	404	7/7	0.47	7.89	164,164,164,164	0
86	OHX	1	4108	7/7	0.36	7.88	109,109,109,109	0
85	MG	1	3444	1/1	0.24	7.88	46,46,46,46	0
85	MG	3	207	1/1	0.35	7.87	48,48,48,48	0
85	MG	5	3487	1/1	0.29	7.84	41,41,41,41	0
85	MG	1	3774	1/1	0.26	7.83	52,52,52,52	0
85	MG	1	3673	1/1	0.26	7.81	19,19,19,19	0
86	OHX	1	4173	7/7	0.37	7.80	142,142,142,142	0
85	MG	2	1949	1/1	0.55	7.79	87,87,87,87	0
86	OHX	2	2172	7/7	0.50	7.79	166,166,166,166	0
86	OHX	2	2107	7/7	0.28	7.77	138,138,138,138	0
85	MG	m7	201	1/1	0.44	7.77	19,19,19,19	0
85	MG	5	3516	1/1	0.30	7.76	21,21,21,21	0
85	MG	4	218	1/1	0.39	7.72	37,37,37,37	0
85	MG	5	3711	1/1	0.25	7.72	40,40,40,40	0
85	MG	6	1929	1/1	0.32	7.72	50,50,50,50	0
85	MG	5	3423	1/1	0.51	7.71	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	5	3664	1/1	0.36	7.70	36,36,36,36	0
85	MG	5	3682	1/1	0.37	7.68	34,34,34,34	0
85	MG	1	3677	1/1	0.27	7.67	32,32,32,32	0
85	MG	5	3499	1/1	0.29	7.65	22,22,22,22	0
86	OHX	1	4188	7/7	0.60	7.65	148,148,148,148	0
85	MG	O4	201	1/1	0.38	7.64	30,30,30,30	0
86	OHX	2	2168	7/7	0.31	7.63	148,148,148,148	0
85	MG	5	3650	1/1	0.24	7.63	21,21,21,21	0
86	OHX	6	2176	7/7	0.40	7.58	141,141,141,141	0
85	MG	5	3440	1/1	0.41	7.57	27,27,27,27	0
86	OHX	2	2170	7/7	0.27	7.54	138,138,138,138	0
86	OHX	M7	204	7/7	0.51	7.54	106,106,106,106	0
85	MG	5	3450	1/1	0.28	7.50	21,21,21,21	0
85	MG	5	3501	1/1	0.31	7.45	18,18,18,18	0
85	MG	1	3469	1/1	0.27	7.45	36,36,36,36	0
86	OHX	5	4150	7/7	0.33	7.39	134,134,134,134	0
86	OHX	7	227	7/7	0.30	7.39	123,123,123,123	0
86	OHX	5	4213	7/7	0.32	7.38	179,179,179,179	0
86	OHX	1	4044	7/7	0.34	7.36	110,110,110,110	0
86	OHX	5	4109	7/7	0.27	7.35	146,146,146,146	0
86	OHX	6	2189	7/7	0.41	7.33	179,179,179,179	0
85	MG	1	3786	1/1	0.29	7.33	27,27,27,27	0
86	OHX	6	2138	7/7	0.27	7.32	131,131,131,131	0
85	MG	1	3743	1/1	0.40	7.31	48,48,48,48	0
85	MG	6	1986	1/1	0.34	7.24	59,59,59,59	0
85	MG	1	3566	1/1	0.53	7.21	17,17,17,17	0
85	MG	1	3401	1/1	0.40	7.21	30,30,30,30	0
86	OHX	2	2118	7/7	0.28	7.20	146,146,146,146	0
86	OHX	6	2139	7/7	0.34	7.20	191,191,191,191	0
85	MG	1	3650	1/1	0.33	7.20	61,61,61,61	0
85	MG	d4	201	1/1	0.31	7.18	45,45,45,45	0
85	MG	6	1977	1/1	0.32	7.16	38,38,38,38	0
85	MG	5	3589	1/1	0.40	7.12	23,23,23,23	0
85	MG	1	3776	1/1	0.27	7.11	41,41,41,41	0
85	MG	1	3807	1/1	0.26	7.11	30,30,30,30	0
85	MG	5	3551	1/1	0.28	7.10	35,35,35,35	0
85	MG	1	4219	1/1	0.40	7.09	53,53,53,53	0
85	MG	7	206	1/1	0.23	7.08	33,33,33,33	0
86	OHX	5	4039	7/7	0.36	7.06	124,124,124,124	0
86	OHX	1	4126	7/7	0.26	7.06	118,118,118,118	0
85	MG	1	3664	1/1	0.38	7.05	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	5	3638	1/1	0.24	7.03	29,29,29,29	0
86	OHX	s1	303	7/7	0.44	7.01	161,161,161,161	0
85	MG	5	3879	1/1	0.17	7.00	58,58,58,58	0
86	OHX	5	4200	7/7	0.36	6.99	134,134,134,134	0
86	OHX	1	4158	7/7	0.51	6.98	159,159,159,159	0
85	MG	1	3779	1/1	0.21	6.97	32,32,32,32	0
86	OHX	1	4124	7/7	0.37	6.97	139,139,139,139	0
86	OHX	1	4135	7/7	0.27	6.94	124,124,124,124	0
86	OHX	1	4080	7/7	0.23	6.93	131,131,131,131	0
85	MG	6	1956	1/1	0.46	6.93	34,34,34,34	0
85	MG	6	2003	1/1	0.54	6.93	79,79,79,79	0
86	OHX	6	2142	7/7	0.34	6.92	129,129,129,129	0
86	OHX	1	4094	7/7	0.26	6.91	156,156,156,156	0
85	MG	2	1931	1/1	0.41	6.91	45,45,45,45	0
86	OHX	3	223	7/7	0.34	6.89	117,117,117,117	0
85	MG	1	3530	1/1	0.49	6.87	63,63,63,63	0
86	OHX	2	2139	7/7	0.36	6.86	179,179,179,179	0
86	OHX	4	231	7/7	0.23	6.86	117,117,117,117	0
85	MG	6	2008	1/1	0.33	6.83	39,39,39,39	0
85	MG	6	1936	1/1	0.35	6.82	74,74,74,74	0
85	MG	2	1902	1/1	0.28	6.81	30,30,30,30	0
85	MG	8	207	1/1	0.33	6.79	33,33,33,33	0
86	OHX	2	2119	7/7	0.30	6.79	137,137,137,137	0
86	OHX	1	4116	7/7	0.37	6.78	129,129,129,129	0
85	MG	l2	301	1/1	0.35	6.77	25,25,25,25	0
85	MG	6	1960	1/1	0.58	6.77	40,40,40,40	0
86	OHX	1	4190	7/7	0.42	6.73	140,140,140,140	0
85	MG	1	3680	1/1	0.29	6.70	47,47,47,47	0
85	MG	1	3773	1/1	0.23	6.70	54,54,54,54	0
86	OHX	5	4229	7/7	0.79	6.68	148,148,148,148	0
85	MG	5	3671	1/1	0.18	6.68	58,58,58,58	0
86	OHX	1	4004	7/7	0.29	6.67	116,116,116,116	0
85	MG	1	3491	1/1	0.25	6.64	20,20,20,20	0
85	MG	2	1959	1/1	0.33	6.62	48,48,48,48	0
85	MG	2	2005	1/1	0.43	6.60	68,68,68,68	0
85	MG	M7	201	1/1	0.40	6.60	21,21,21,21	0
85	MG	n8	203	1/1	0.36	6.58	35,35,35,35	0
85	MG	6	1901	1/1	0.39	6.55	35,35,35,35	0
85	MG	5	3653	1/1	0.30	6.55	45,45,45,45	0
85	MG	n0	203	1/1	0.33	6.54	25,25,25,25	0
85	MG	N3	202	1/1	0.21	6.50	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4109	7/7	0.46	6.49	147,147,147,147	0
85	MG	5	3889	1/1	0.34	6.47	44,44,44,44	0
85	MG	5	3482	1/1	0.19	6.46	37,37,37,37	0
85	MG	5	3727	1/1	0.28	6.45	48,48,48,48	0
85	MG	1	3494	1/1	0.24	6.44	33,33,33,33	0
86	OHX	6	2070	7/7	0.30	6.44	100,100,100,100	0
85	MG	1	3545	1/1	0.28	6.41	40,40,40,40	0
85	MG	5	3496	1/1	0.33	6.40	24,24,24,24	0
85	MG	5	3471	1/1	0.32	6.40	32,32,32,32	0
85	MG	6	1918	1/1	0.52	6.39	64,64,64,64	0
85	MG	5	3470	1/1	0.39	6.39	26,26,26,26	0
85	MG	2	1992	1/1	0.55	6.39	81,81,81,81	0
85	MG	2	1920	1/1	0.42	6.38	47,47,47,47	0
85	MG	1	3521	1/1	0.34	6.37	64,64,64,64	0
85	MG	1	3547	1/1	0.33	6.37	27,27,27,27	0
85	MG	5	3728	1/1	0.24	6.34	32,32,32,32	0
85	MG	8	213	1/1	0.29	6.34	43,43,43,43	0
86	OHX	5	4043	7/7	0.24	6.34	103,103,103,103	0
86	OHX	5	4119	7/7	0.29	6.33	132,132,132,132	0
85	MG	5	3819	1/1	0.32	6.32	22,22,22,22	0
85	MG	2	1991	1/1	0.26	6.32	52,52,52,52	0
85	MG	5	3610	1/1	0.24	6.32	34,34,34,34	0
86	OHX	6	2201	7/7	0.58	6.32	165,165,165,165	0
86	OHX	6	2175	7/7	0.34	6.32	118,118,118,118	0
85	MG	5	3705	1/1	0.16	6.31	43,43,43,43	0
86	OHX	5	4099	7/7	0.35	6.28	101,101,101,101	0
86	OHX	6	2150	7/7	0.29	6.27	157,157,157,157	0
85	MG	1	3686	1/1	0.22	6.26	89,89,89,89	0
86	OHX	2	2100	7/7	0.21	6.25	142,142,142,142	0
86	OHX	6	2122	7/7	0.33	6.25	136,136,136,136	0
85	MG	5	3604	1/1	0.30	6.22	20,20,20,20	0
86	OHX	4	230	7/7	0.26	6.21	104,104,104,104	0
86	OHX	1	3977	7/7	0.29	6.21	92,92,92,92	0
85	MG	5	3625	1/1	0.33	6.19	50,50,50,50	0
85	MG	s1	301	1/1	0.35	6.19	62,62,62,62	0
85	MG	1	3437	1/1	0.30	6.18	22,22,22,22	0
85	MG	1	3450	1/1	0.33	6.18	31,31,31,31	0
85	MG	6	2033	1/1	0.35	6.18	70,70,70,70	0
86	OHX	6	2196	7/7	0.33	6.17	136,136,136,136	0
85	MG	1	3702	1/1	0.27	6.17	29,29,29,29	0
85	MG	6	1978	1/1	0.20	6.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	n8	202	1/1	0.27	6.16	22,22,22,22	0
86	OHX	L3	403	7/7	0.28	6.16	117,117,117,117	0
85	MG	5	3690	1/1	0.23	6.15	35,35,35,35	0
85	MG	1	3653	1/1	0.34	6.15	31,31,31,31	0
85	MG	6	1923	1/1	0.41	6.14	64,64,64,64	0
85	MG	6	2023	1/1	0.32	6.12	55,55,55,55	0
85	MG	1	3417	1/1	0.36	6.12	34,34,34,34	0
85	MG	5	3598	1/1	0.28	6.11	31,31,31,31	0
85	MG	5	3533	1/1	0.26	6.10	42,42,42,42	0
86	OHX	5	4204	7/7	0.36	6.10	106,106,106,106	0
85	MG	5	3564	1/1	0.21	6.09	16,16,16,16	0
86	OHX	1	4031	7/7	0.29	6.09	108,108,108,108	0
85	MG	5	3740	1/1	0.26	6.06	29,29,29,29	0
85	MG	5	3829	1/1	0.33	6.06	27,27,27,27	0
85	MG	5	3495	1/1	0.31	6.04	16,16,16,16	0
85	MG	2	1965	1/1	0.57	6.04	36,36,36,36	0
85	MG	1	3577	1/1	0.38	6.04	14,14,14,14	0
86	OHX	5	4143	7/7	0.44	6.03	146,146,146,146	0
86	OHX	6	2121	7/7	0.31	6.02	106,106,106,106	0
85	MG	1	3439	1/1	0.47	6.01	17,17,17,17	0
85	MG	5	3462	1/1	0.25	6.00	35,35,35,35	0
86	OHX	1	4079	7/7	0.35	5.97	132,132,132,132	0
86	OHX	5	4218	7/7	0.35	5.95	147,147,147,147	0
86	OHX	5	4195	7/7	0.37	5.95	116,116,116,116	0
86	OHX	5	3977	7/7	0.26	5.94	95,95,95,95	0
85	MG	1	3598	1/1	0.28	5.92	30,30,30,30	0
85	MG	6	2031	1/1	0.31	5.92	42,42,42,42	0
85	MG	5	3612	1/1	0.23	5.92	23,23,23,23	0
86	OHX	2	2090	7/7	0.43	5.92	168,168,168,168	0
86	OHX	5	4160	7/7	0.37	5.91	128,128,128,128	0
86	OHX	5	4090	7/7	0.27	5.91	157,157,157,157	0
85	MG	C1	201	1/1	0.46	5.90	56,56,56,56	0
85	MG	2	2010	1/1	0.50	5.88	60,60,60,60	0
86	OHX	2	2073	7/7	0.27	5.88	110,110,110,110	0
85	MG	3	210	1/1	0.33	5.86	53,53,53,53	0
85	MG	5	3569	1/1	0.36	5.84	20,20,20,20	0
86	OHX	5	4134	7/7	0.29	5.81	121,121,121,121	0
86	OHX	5	4065	7/7	0.26	5.80	131,131,131,131	0
86	OHX	1	4182	7/7	0.32	5.79	141,141,141,141	0
85	MG	1	3613	1/1	0.22	5.78	24,24,24,24	0
86	OHX	5	4023	7/7	0.25	5.78	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3454	1/1	0.49	5.77	47,47,47,47	0
85	MG	6	2005	1/1	0.36	5.75	48,48,48,48	0
86	OHX	2	2162	7/7	0.30	5.75	171,171,171,171	0
85	MG	6	1930	1/1	0.35	5.73	42,42,42,42	0
86	OHX	2	2146	7/7	0.38	5.73	142,142,142,142	0
86	OHX	1	4206	7/7	0.42	5.72	119,119,119,119	0
86	OHX	1	4034	7/7	0.28	5.72	125,125,125,125	0
85	MG	17	301	1/1	0.29	5.71	26,26,26,26	0
86	OHX	5	4117	7/7	0.25	5.71	150,150,150,150	0
86	OHX	2	2160	7/7	0.58	5.71	130,130,130,130	0
85	MG	5	3623	1/1	0.32	5.70	27,27,27,27	0
86	OHX	2	2112	7/7	0.34	5.69	137,137,137,137	0
85	MG	5	3483	1/1	0.58	5.65	14,14,14,14	0
85	MG	5	3603	1/1	0.22	5.65	21,21,21,21	0
85	MG	1	3840	1/1	0.26	5.62	31,31,31,31	0
86	OHX	5	4139	7/7	0.28	5.62	115,115,115,115	0
85	MG	1	3670	1/1	0.28	5.62	29,29,29,29	0
86	OHX	1	4086	7/7	0.33	5.59	94,94,94,94	0
86	OHX	5	4234	7/7	0.28	5.57	181,181,181,181	0
85	MG	5	3660	1/1	0.21	5.57	42,42,42,42	0
85	MG	6	1962	1/1	0.31	5.55	36,36,36,36	0
86	OHX	6	2174	7/7	0.34	5.54	104,104,104,104	0
86	OHX	5	4217	7/7	0.42	5.53	118,118,118,118	0
86	OHX	1	4179	7/7	0.29	5.52	130,130,130,130	0
85	MG	5	3500	1/1	0.33	5.49	27,27,27,27	0
85	MG	5	3738	1/1	0.21	5.47	17,17,17,17	0
85	MG	5	3811	1/1	0.23	5.47	25,25,25,25	0
85	MG	5	3426	1/1	0.28	5.46	27,27,27,27	0
86	OHX	5	4226	7/7	0.23	5.45	169,169,169,169	0
85	MG	2	1904	1/1	0.49	5.45	63,63,63,63	0
85	MG	5	3593	1/1	0.39	5.44	31,31,31,31	0
85	MG	6	1997	1/1	0.23	5.42	51,51,51,51	0
85	MG	1	3616	1/1	0.42	5.42	54,54,54,54	0
85	MG	5	3882	1/1	0.23	5.40	33,33,33,33	0
85	MG	2	1948	1/1	0.43	5.40	44,44,44,44	0
85	MG	1	3699	1/1	0.27	5.40	31,31,31,31	0
85	MG	6	1957	1/1	0.86	5.39	33,33,33,33	0
86	OHX	5	3986	7/7	0.28	5.37	105,105,105,105	0
86	OHX	6	2186	7/7	0.38	5.36	143,143,143,143	0
85	MG	5	3755	1/1	0.29	5.34	48,48,48,48	0
85	MG	5	3776	1/1	0.46	5.33	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	2	2167	7/7	0.35	5.33	126,126,126,126	0
85	MG	6	1949	1/1	0.55	5.32	43,43,43,43	0
85	MG	1	3856	1/1	0.26	5.31	43,43,43,43	0
85	MG	2	1958	1/1	0.32	5.30	51,51,51,51	0
85	MG	1	3747	1/1	0.29	5.29	30,30,30,30	0
85	MG	5	3618	1/1	0.16	5.29	35,35,35,35	0
86	OHX	6	2167	7/7	0.29	5.29	161,161,161,161	0
85	MG	2	1982	1/1	0.28	5.28	47,47,47,47	0
86	OHX	1	4061	7/7	0.31	5.28	131,131,131,131	0
85	MG	5	3707	1/1	0.29	5.28	30,30,30,30	0
85	MG	5	3804	1/1	0.27	5.27	20,20,20,20	0
86	OHX	5	4242	7/7	0.32	5.27	127,127,127,127	0
86	OHX	1	4131	7/7	0.31	5.26	132,132,132,132	0
85	MG	1	3744	1/1	0.32	5.26	17,17,17,17	0
86	OHX	5	4155	7/7	0.32	5.26	116,116,116,116	0
86	OHX	2	2116	7/7	0.34	5.25	141,141,141,141	0
85	MG	5	3886	1/1	0.25	5.25	57,57,57,57	0
85	MG	6	1968	1/1	0.32	5.24	62,62,62,62	0
86	OHX	1	4195	7/7	0.33	5.22	125,125,125,125	0
85	MG	2	1954	1/1	0.19	5.22	50,50,50,50	0
86	OHX	1	4128	7/7	0.37	5.21	149,149,149,149	0
86	OHX	1	4181	7/7	0.34	5.20	138,138,138,138	0
85	MG	5	3651	1/1	0.24	5.19	20,20,20,20	0
86	OHX	5	4083	7/7	0.30	5.19	101,101,101,101	0
85	MG	1	3787	1/1	0.42	5.19	20,20,20,20	0
85	MG	6	2204	1/1	0.40	5.18	69,69,69,69	0
85	MG	1	3695	1/1	0.21	5.18	39,39,39,39	0
86	OHX	1	3986	7/7	0.20	5.18	109,109,109,109	0
85	MG	1	3760	1/1	0.22	5.17	28,28,28,28	0
86	OHX	2	2152	7/7	0.45	5.15	143,143,143,143	0
85	MG	1	3567	1/1	0.36	5.13	21,21,21,21	0
86	OHX	6	2101	7/7	0.29	5.13	120,120,120,120	0
85	MG	1	3721	1/1	0.29	5.12	16,16,16,16	0
85	MG	6	1985	1/1	0.23	5.08	32,32,32,32	0
86	OHX	6	2136	7/7	0.24	5.08	121,121,121,121	0
86	OHX	1	4156	7/7	0.36	5.07	145,145,145,145	0
86	OHX	1	4089	7/7	0.25	5.07	110,110,110,110	0
85	MG	2	1966	1/1	0.70	5.05	110,110,110,110	0
85	MG	1	3745	1/1	0.23	5.04	26,26,26,26	0
85	MG	N8	201	1/1	0.24	5.04	20,20,20,20	0
85	MG	5	3565	1/1	0.42	5.03	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	n8	204	1/1	0.29	5.03	29,29,29,29	0
85	MG	1	3602	1/1	0.25	5.03	26,26,26,26	0
85	MG	5	4248	1/1	0.49	5.03	32,32,32,32	0
86	OHX	2	2136	7/7	0.45	5.01	124,124,124,124	0
85	MG	2	1967	1/1	0.32	5.00	73,73,73,73	0
85	MG	6	1941	1/1	0.26	4.99	38,38,38,38	0
86	OHX	1	4014	7/7	0.29	4.99	112,112,112,112	0
85	MG	5	3891	1/1	0.22	4.98	27,27,27,27	0
86	OHX	2	2075	7/7	0.29	4.98	128,128,128,128	0
85	MG	1	3730	1/1	0.21	4.97	55,55,55,55	0
85	MG	5	3820	1/1	0.26	4.95	25,25,25,25	0
86	OHX	1	3954	7/7	0.24	4.95	103,103,103,103	0
85	MG	1	3641	1/1	0.25	4.95	36,36,36,36	0
85	MG	1	3621	1/1	0.20	4.94	31,31,31,31	0
85	MG	1	3629	1/1	0.30	4.94	25,25,25,25	0
85	MG	1	3606	1/1	0.27	4.93	45,45,45,45	0
85	MG	5	3543	1/1	0.23	4.93	24,24,24,24	0
86	OHX	5	4245	7/7	0.38	4.93	168,168,168,168	0
85	MG	1	3711	1/1	0.20	4.93	41,41,41,41	0
86	OHX	5	4130	7/7	0.43	4.91	128,128,128,128	0
86	OHX	1	4052	7/7	0.26	4.86	107,107,107,107	0
85	MG	1	3474	1/1	0.25	4.86	65,65,65,65	0
86	OHX	2	2080	7/7	0.20	4.86	134,134,134,134	0
86	OHX	5	4128	7/7	0.34	4.83	109,109,109,109	0
85	MG	5	3861	1/1	0.27	4.81	15,15,15,15	0
85	MG	1	3842	1/1	0.35	4.81	27,27,27,27	0
85	MG	2	1977	1/1	0.46	4.80	44,44,44,44	0
85	MG	1	3564	1/1	0.27	4.77	22,22,22,22	0
85	MG	5	3802	1/1	0.27	4.76	33,33,33,33	0
86	OHX	1	4036	7/7	0.28	4.75	114,114,114,114	0
85	MG	1	3625	1/1	0.31	4.75	24,24,24,24	0
86	OHX	5	4129	7/7	0.23	4.74	129,129,129,129	0
85	MG	5	3683	1/1	0.48	4.73	53,53,53,53	0
85	MG	5	3402	1/1	0.26	4.70	15,15,15,15	0
85	MG	2	1933	1/1	0.31	4.69	66,66,66,66	0
86	OHX	M7	205	7/7	0.32	4.67	138,138,138,138	0
85	MG	1	4213	1/1	0.26	4.66	21,21,21,21	0
86	OHX	1	4149	7/7	0.22	4.65	108,108,108,108	0
86	OHX	1	4066	7/7	0.25	4.65	126,126,126,126	0
85	MG	l3	403	1/1	0.34	4.65	24,24,24,24	0
85	MG	1	3471	1/1	0.26	4.63	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	1919	1/1	0.35	4.62	34,34,34,34	0
85	MG	5	3425	1/1	0.33	4.62	34,34,34,34	0
85	MG	6	1938	1/1	0.29	4.61	37,37,37,37	0
86	OHX	5	4182	7/7	0.41	4.61	157,157,157,157	0
85	MG	5	3741	1/1	0.26	4.60	36,36,36,36	0
86	OHX	1	4047	7/7	0.26	4.60	122,122,122,122	0
85	MG	5	3454	1/1	0.40	4.59	80,80,80,80	0
86	OHX	1	4009	7/7	0.23	4.59	131,131,131,131	0
85	MG	M3	203	1/1	0.29	4.57	18,18,18,18	0
85	MG	q0	202	1/1	0.25	4.57	36,36,36,36	0
85	MG	5	3553	1/1	0.41	4.56	23,23,23,23	0
85	MG	2	1974	1/1	0.27	4.56	47,47,47,47	0
85	MG	1	3618	1/1	0.28	4.54	60,60,60,60	0
85	MG	5	3640	1/1	0.20	4.54	25,25,25,25	0
85	MG	5	3473	1/1	0.23	4.54	47,47,47,47	0
86	OHX	6	2111	7/7	0.21	4.54	101,101,101,101	0
85	MG	5	3750	1/1	0.30	4.53	38,38,38,38	0
86	OHX	1	4013	7/7	0.26	4.51	127,127,127,127	0
86	OHX	5	4205	7/7	0.33	4.51	138,138,138,138	0
86	OHX	5	4126	7/7	0.33	4.50	116,116,116,116	0
86	OHX	1	4172	7/7	0.29	4.50	165,165,165,165	0
85	MG	4	214	1/1	0.27	4.45	36,36,36,36	0
85	MG	3	213	1/1	0.28	4.45	50,50,50,50	0
86	OHX	5	4216	7/7	0.36	4.44	144,144,144,144	0
85	MG	1	3824	1/1	0.22	4.43	35,35,35,35	0
85	MG	L3	401	1/1	0.26	4.41	25,25,25,25	0
86	OHX	5	4033	7/7	0.27	4.40	92,92,92,92	0
86	OHX	1	4112	7/7	0.27	4.39	118,118,118,118	0
85	MG	5	3753	1/1	0.24	4.39	29,29,29,29	0
85	MG	6	2021	1/1	0.41	4.39	60,60,60,60	0
86	OHX	1	4200	7/7	0.40	4.36	135,135,135,135	0
86	OHX	5	4066	7/7	0.27	4.36	113,113,113,113	0
85	MG	1	3789	1/1	0.30	4.36	77,77,77,77	0
85	MG	5	3840	1/1	0.24	4.35	22,22,22,22	0
86	OHX	2	2126	7/7	0.23	4.34	131,131,131,131	0
86	OHX	1	4002	7/7	0.19	4.32	104,104,104,104	0
85	MG	4	217	1/1	0.26	4.32	38,38,38,38	0
86	OHX	6	2198	7/7	0.26	4.31	150,150,150,150	0
86	OHX	5	4163	7/7	0.28	4.31	137,137,137,137	0
85	MG	5	3534	1/1	0.24	4.28	31,31,31,31	0
85	MG	1	3777	1/1	0.19	4.28	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	6	2132	7/7	0.27	4.26	134,134,134,134	0
86	OHX	6	2147	7/7	0.25	4.25	105,105,105,105	0
85	MG	5	3699	1/1	0.25	4.24	53,53,53,53	0
86	OHX	5	4101	7/7	0.34	4.23	127,127,127,127	0
86	OHX	6	2156	7/7	0.27	4.22	130,130,130,130	0
86	OHX	1	4074	7/7	0.19	4.21	133,133,133,133	0
85	MG	5	3720	1/1	0.33	4.20	39,39,39,39	0
85	MG	5	3449	1/1	0.29	4.20	49,49,49,49	0
85	MG	6	1973	1/1	0.28	4.15	39,39,39,39	0
86	OHX	1	3983	7/7	0.21	4.14	97,97,97,97	0
85	MG	7	209	1/1	0.32	4.14	38,38,38,38	0
85	MG	5	3634	1/1	0.42	4.13	38,38,38,38	0
85	MG	2	2003	1/1	0.39	4.13	51,51,51,51	0
85	MG	5	3785	1/1	0.25	4.12	12,12,12,12	0
85	MG	6	1983	1/1	0.31	4.10	68,68,68,68	0
85	MG	L2	301	1/1	0.34	4.10	24,24,24,24	0
86	OHX	1	4041	7/7	0.25	4.10	97,97,97,97	0
85	MG	5	3715	1/1	0.32	4.10	37,37,37,37	0
85	MG	6	1966	1/1	0.27	4.08	80,80,80,80	0
86	OHX	6	2115	7/7	0.41	4.08	143,143,143,143	0
85	MG	6	1950	1/1	0.29	4.08	33,33,33,33	0
86	OHX	5	4177	7/7	0.39	4.07	133,133,133,133	0
86	OHX	5	4154	7/7	0.41	4.06	147,147,147,147	0
85	MG	6	2203	1/1	0.41	4.03	52,52,52,52	0
86	OHX	2	2174	7/7	0.39	4.03	139,139,139,139	0
86	OHX	1	4130	7/7	0.26	4.03	115,115,115,115	0
85	MG	c1	201	1/1	0.36	4.01	39,39,39,39	0
85	MG	2	1930	1/1	0.30	4.01	53,53,53,53	0
86	OHX	5	3995	7/7	0.27	3.99	75,75,75,75	0
86	OHX	2	2145	7/7	0.31	3.97	141,141,141,141	0
85	MG	1	3643	1/1	0.28	3.97	57,57,57,57	0
85	MG	1	3430	1/1	0.44	3.96	39,39,39,39	0
86	OHX	5	4201	7/7	0.29	3.96	151,151,151,151	0
86	OHX	1	4113	7/7	0.27	3.96	117,117,117,117	0
85	MG	2	1999	1/1	0.22	3.95	71,71,71,71	0
86	OHX	1	4120	7/7	0.34	3.95	104,104,104,104	0
86	OHX	1	4073	7/7	0.28	3.95	116,116,116,116	0
85	MG	5	3698	1/1	0.24	3.95	28,28,28,28	0
85	MG	1	3696	1/1	0.24	3.95	37,37,37,37	0
86	OHX	5	4223	7/7	0.30	3.94	187,187,187,187	0
85	MG	1	3580	1/1	0.43	3.93	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	5	3695	1/1	0.28	3.93	45,45,45,45	0
86	OHX	1	4202	7/7	0.31	3.91	136,136,136,136	0
85	MG	6	1994	1/1	0.21	3.90	35,35,35,35	0
85	MG	1	3762	1/1	0.29	3.90	29,29,29,29	0
86	OHX	2	2137	7/7	0.25	3.89	158,158,158,158	0
85	MG	S4	301	1/1	0.29	3.87	60,60,60,60	0
85	MG	5	3460	1/1	0.27	3.86	34,34,34,34	0
86	OHX	6	2197	7/7	0.27	3.84	141,141,141,141	0
86	OHX	5	4105	7/7	0.23	3.84	127,127,127,127	0
85	MG	5	3605	1/1	0.20	3.81	27,27,27,27	0
86	OHX	5	4103	7/7	0.23	3.79	96,96,96,96	0
85	MG	1	3549	1/1	0.25	3.79	26,26,26,26	0
86	OHX	6	2137	7/7	0.22	3.79	129,129,129,129	0
86	OHX	1	4072	7/7	0.34	3.78	117,117,117,117	0
86	OHX	6	2173	7/7	0.23	3.77	147,147,147,147	0
85	MG	6	1991	1/1	0.29	3.76	51,51,51,51	0
85	MG	5	3773	1/1	0.25	3.76	73,73,73,73	0
85	MG	5	3633	1/1	0.24	3.75	42,42,42,42	0
85	MG	1	3495	1/1	0.24	3.72	36,36,36,36	0
85	MG	4	222	1/1	0.23	3.72	28,28,28,28	0
86	OHX	2	2115	7/7	0.42	3.71	152,152,152,152	0
85	MG	1	3772	1/1	0.40	3.71	41,41,41,41	0
85	MG	5	3478	1/1	0.23	3.71	49,49,49,49	0
86	OHX	5	4111	7/7	0.24	3.70	133,133,133,133	0
85	MG	1	3819	1/1	0.33	3.69	36,36,36,36	0
86	OHX	1	4064	7/7	0.43	3.68	111,111,111,111	0
86	OHX	5	4149	7/7	0.35	3.67	135,135,135,135	0
86	OHX	2	2078	7/7	0.24	3.66	117,117,117,117	0
86	OHX	5	4158	7/7	0.22	3.66	132,132,132,132	0
85	MG	5	3696	1/1	0.23	3.66	26,26,26,26	0
86	OHX	5	4112	7/7	0.30	3.64	115,115,115,115	0
85	MG	6	2001	1/1	0.22	3.63	48,48,48,48	0
85	MG	6	2040	1/1	0.44	3.63	81,81,81,81	0
85	MG	5	3745	1/1	0.27	3.63	38,38,38,38	0
86	OHX	2	2085	7/7	0.21	3.63	110,110,110,110	0
85	MG	L7	302	1/1	0.29	3.62	26,26,26,26	0
85	MG	5	3868	1/1	0.33	3.61	35,35,35,35	0
85	MG	1	3753	1/1	0.25	3.61	17,17,17,17	0
85	MG	1	3433	1/1	0.26	3.61	26,26,26,26	0
86	OHX	2	2169	7/7	0.41	3.61	142,142,142,142	0
86	OHX	5	4198	7/7	0.34	3.60	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	2015	1/1	0.43	3.57	49,49,49,49	0
85	MG	8	209	1/1	0.25	3.56	34,34,34,34	0
85	MG	6	2007	1/1	0.22	3.55	36,36,36,36	0
86	OHX	1	3972	7/7	0.22	3.55	113,113,113,113	0
86	OHX	2	2154	7/7	0.30	3.54	144,144,144,144	0
86	OHX	2	2131	7/7	0.34	3.51	128,128,128,128	0
85	MG	1	3732	1/1	0.28	3.51	45,45,45,45	0
85	MG	L7	303	1/1	0.20	3.50	32,32,32,32	0
85	MG	5	3854	1/1	0.24	3.50	53,53,53,53	0
85	MG	6	1953	1/1	0.37	3.49	50,50,50,50	0
85	MG	4	225	1/1	0.23	3.49	44,44,44,44	0
85	MG	2	1964	1/1	0.24	3.48	79,79,79,79	0
85	MG	1	3812	1/1	0.26	3.47	40,40,40,40	0
86	OHX	5	4070	7/7	0.37	3.46	127,127,127,127	0
85	MG	N6	201	1/1	0.33	3.46	34,34,34,34	0
85	MG	1	4220	1/1	0.30	3.44	23,23,23,23	0
86	OHX	1	4040	7/7	0.24	3.43	121,121,121,121	0
85	MG	5	3748	1/1	0.24	3.42	49,49,49,49	0
85	MG	1	3698	1/1	0.41	3.42	56,56,56,56	0
85	MG	1	3404	1/1	0.61	3.41	38,38,38,38	0
85	MG	1	3483	1/1	0.23	3.40	35,35,35,35	0
86	OHX	6	2171	7/7	0.33	3.40	146,146,146,146	0
86	OHX	5	4040	7/7	0.27	3.40	100,100,100,100	0
86	OHX	1	4147	7/7	0.31	3.40	134,134,134,134	0
86	OHX	5	4137	7/7	0.28	3.38	111,111,111,111	0
85	MG	4	215	1/1	0.24	3.38	28,28,28,28	0
86	OHX	1	4118	7/7	0.23	3.38	129,129,129,129	0
85	MG	5	3498	1/1	0.25	3.38	29,29,29,29	0
86	OHX	2	2057	7/7	0.21	3.37	110,110,110,110	0
85	MG	3	212	1/1	0.27	3.36	62,62,62,62	0
86	OHX	5	4127	7/7	0.23	3.35	127,127,127,127	0
85	MG	6	1989	1/1	0.35	3.34	60,60,60,60	0
85	MG	1	3642	1/1	0.30	3.34	31,31,31,31	0
85	MG	5	3578	1/1	0.24	3.33	21,21,21,21	0
86	OHX	5	4202	7/7	0.28	3.33	122,122,122,122	0
86	OHX	1	3952	7/7	0.18	3.33	98,98,98,98	0
85	MG	2	1971	1/1	0.26	3.32	61,61,61,61	0
85	MG	4	205	1/1	0.47	3.32	59,59,59,59	0
86	OHX	3	222	7/7	0.26	3.32	138,138,138,138	0
86	OHX	1	4093	7/7	0.26	3.31	146,146,146,146	0
86	OHX	5	4038	7/7	0.24	3.31	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2044	1/1	0.34	3.30	81,81,81,81	0
86	OHX	6	2177	7/7	0.24	3.30	145,145,145,145	0
85	MG	5	3827	1/1	0.17	3.29	28,28,28,28	0
85	MG	8	206	1/1	0.28	3.28	27,27,27,27	0
85	MG	1	3822	1/1	0.16	3.27	43,43,43,43	0
86	OHX	6	2168	7/7	0.38	3.26	153,153,153,153	0
85	MG	5	3821	1/1	0.36	3.26	22,22,22,22	0
85	MG	d3	201	1/1	0.26	3.25	40,40,40,40	0
85	MG	n6	201	1/1	0.40	3.25	32,32,32,32	0
86	OHX	2	2140	7/7	0.27	3.23	150,150,150,150	0
86	OHX	1	4203	7/7	0.36	3.22	143,143,143,143	0
85	MG	1	3716	1/1	0.24	3.20	29,29,29,29	0
86	OHX	5	4187	7/7	0.27	3.19	111,111,111,111	0
85	MG	5	3648	1/1	0.19	3.19	90,90,90,90	0
86	OHX	1	4178	7/7	0.48	3.18	134,134,134,134	0
86	OHX	1	3990	7/7	0.23	3.18	105,105,105,105	0
85	MG	M0	301	1/1	0.28	3.18	30,30,30,30	0
85	MG	5	3430	1/1	0.34	3.17	72,72,72,72	0
86	OHX	2	2134	7/7	0.24	3.17	138,138,138,138	0
85	MG	6	1964	1/1	0.20	3.17	53,53,53,53	0
86	OHX	1	4019	7/7	0.23	3.16	119,119,119,119	0
85	MG	5	3686	1/1	0.16	3.16	41,41,41,41	0
86	OHX	5	4063	7/7	0.25	3.16	142,142,142,142	0
86	OHX	5	4079	7/7	0.26	3.16	117,117,117,117	0
86	OHX	1	4209	7/7	0.30	3.15	160,160,160,160	0
86	OHX	2	2098	7/7	0.18	3.15	113,113,113,113	0
85	MG	1	3636	1/1	0.30	3.15	41,41,41,41	0
85	MG	1	3540	1/1	0.20	3.15	47,47,47,47	0
85	MG	7	204	1/1	0.23	3.15	75,75,75,75	0
85	MG	1	3599	1/1	0.22	3.14	19,19,19,19	0
86	OHX	1	4163	7/7	0.35	3.14	127,127,127,127	0
86	OHX	5	4073	7/7	0.21	3.13	129,129,129,129	0
86	OHX	1	4049	7/7	0.20	3.13	135,135,135,135	0
85	MG	6	1992	1/1	0.29	3.12	49,49,49,49	0
86	OHX	5	4008	7/7	0.20	3.12	107,107,107,107	0
86	OHX	1	4024	7/7	0.22	3.11	131,131,131,131	0
85	MG	1	3660	1/1	0.26	3.10	23,23,23,23	0
86	OHX	1	4068	7/7	0.26	3.10	146,146,146,146	0
86	OHX	5	4238	7/7	0.39	3.09	139,139,139,139	0
85	MG	1	3742	1/1	0.25	3.07	32,32,32,32	0
85	MG	6	2002	1/1	0.33	3.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4006	7/7	0.19	3.06	105,105,105,105	0
86	OHX	5	4096	7/7	0.21	3.04	94,94,94,94	0
86	OHX	8	231	7/7	0.27	3.03	132,132,132,132	0
85	MG	6	1976	1/1	0.24	3.02	37,37,37,37	0
85	MG	1	3435	1/1	0.20	3.01	29,29,29,29	0
85	MG	1	3828	1/1	0.21	3.00	14,14,14,14	0
86	OHX	1	4065	7/7	0.26	2.99	132,132,132,132	0
85	MG	1	3668	1/1	0.16	2.98	65,65,65,65	0
86	OHX	L4	403	7/7	0.37	2.97	154,154,154,154	0
88	3L2	5	4246	36/36	0.23	2.97	20,20,20,20	0
86	OHX	1	4095	7/7	0.31	2.97	155,155,155,155	0
86	OHX	6	2194	7/7	0.31	2.97	183,183,183,183	0
86	OHX	1	4102	7/7	0.24	2.95	125,125,125,125	0
86	OHX	2	2149	7/7	0.25	2.93	166,166,166,166	0
85	MG	5	3452	1/1	0.18	2.92	22,22,22,22	0
86	OHX	6	2130	7/7	0.34	2.91	123,123,123,123	0
85	MG	1	3487	1/1	0.21	2.91	25,25,25,25	0
85	MG	1	3751	1/1	0.28	2.90	45,45,45,45	0
86	OHX	6	2164	7/7	0.29	2.90	143,143,143,143	0
85	MG	m7	203	1/1	0.29	2.90	37,37,37,37	0
86	OHX	1	4012	7/7	0.26	2.89	121,121,121,121	0
86	OHX	5	4053	7/7	0.24	2.88	111,111,111,111	0
86	OHX	2	2127	7/7	0.29	2.85	124,124,124,124	0
86	OHX	1	4003	7/7	0.20	2.85	120,120,120,120	0
85	MG	5	3764	1/1	0.25	2.84	33,33,33,33	0
86	OHX	5	4124	7/7	0.17	2.84	110,110,110,110	0
86	OHX	5	4138	7/7	0.24	2.81	129,129,129,129	0
86	OHX	6	2108	7/7	0.21	2.81	106,106,106,106	0
85	MG	5	3611	1/1	0.24	2.80	25,25,25,25	0
86	OHX	5	4170	7/7	0.30	2.80	133,133,133,133	0
86	OHX	1	3966	7/7	0.21	2.78	100,100,100,100	0
85	MG	7	214	1/1	0.25	2.77	27,27,27,27	0
85	MG	5	3678	1/1	0.18	2.76	25,25,25,25	0
85	MG	L4	402	1/1	0.22	2.76	19,19,19,19	0
86	OHX	14	403	7/7	0.32	2.74	168,168,168,168	0
85	MG	1	3719	1/1	0.34	2.74	34,34,34,34	0
86	OHX	2	2083	7/7	0.26	2.73	121,121,121,121	0
86	OHX	2	2105	7/7	0.24	2.72	129,129,129,129	0
86	OHX	5	4162	7/7	0.27	2.72	147,147,147,147	0
86	OHX	5	4041	7/7	0.25	2.72	130,130,130,130	0
86	OHX	2	2064	7/7	0.25	2.71	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3689	1/1	0.24	2.69	38,38,38,38	0
85	MG	5	3794	1/1	0.28	2.68	32,32,32,32	0
85	MG	1	3441	1/1	0.23	2.67	32,32,32,32	0
86	OHX	5	4004	7/7	0.20	2.66	104,104,104,104	0
85	MG	m1	201	1/1	0.30	2.65	46,46,46,46	0
85	MG	1	3406	1/1	0.45	2.62	120,120,120,120	0
85	MG	5	3769	1/1	0.21	2.60	23,23,23,23	0
85	MG	2	1961	1/1	0.36	2.60	134,134,134,134	0
86	OHX	2	2068	7/7	0.31	2.60	111,111,111,111	0
86	OHX	l3	405	7/7	0.23	2.59	112,112,112,112	0
86	OHX	O3	201	7/7	0.27	2.58	115,115,115,115	0
85	MG	1	3746	1/1	0.31	2.57	40,40,40,40	0
86	OHX	5	4184	7/7	0.38	2.56	137,137,137,137	0
86	OHX	2	2121	7/7	0.41	2.55	139,139,139,139	0
86	OHX	1	4185	7/7	0.56	2.55	180,180,180,180	0
85	MG	2	1947	1/1	0.24	2.55	42,42,42,42	0
86	OHX	1	4007	7/7	0.21	2.54	122,122,122,122	0
85	MG	1	3850	1/1	0.28	2.51	54,54,54,54	0
86	OHX	6	2191	7/7	0.36	2.51	183,183,183,183	0
85	MG	2	1950	1/1	0.38	2.51	91,91,91,91	0
85	MG	l2	303	1/1	0.30	2.51	34,34,34,34	0
86	OHX	1	4096	7/7	0.33	2.45	106,106,106,106	0
85	MG	5	3417	1/1	0.20	2.45	19,19,19,19	0
86	OHX	1	3999	7/7	0.33	2.45	108,108,108,108	0
85	MG	5	3680	1/1	0.18	2.45	22,22,22,22	0
85	MG	1	3705	1/1	0.19	2.43	56,56,56,56	0
85	MG	1	3481	1/1	0.23	2.43	23,23,23,23	0
86	OHX	5	4102	7/7	0.24	2.43	117,117,117,117	0
86	OHX	4	239	7/7	0.28	2.42	127,127,127,127	0
85	MG	5	3841	1/1	0.43	2.41	43,43,43,43	0
85	MG	1	3763	1/1	0.20	2.40	26,26,26,26	0
86	OHX	6	2104	7/7	0.25	2.40	117,117,117,117	0
86	OHX	5	4062	7/7	0.27	2.40	111,111,111,111	0
86	OHX	1	4155	7/7	0.26	2.40	111,111,111,111	0
85	MG	6	2012	1/1	0.23	2.39	59,59,59,59	0
85	MG	L2	302	1/1	0.28	2.38	26,26,26,26	0
86	OHX	1	4018	7/7	0.21	2.37	107,107,107,107	0
86	OHX	2	2150	7/7	0.38	2.37	160,160,160,160	0
85	MG	5	3800	1/1	0.21	2.37	28,28,28,28	0
85	MG	N5	202	1/1	0.25	2.36	55,55,55,55	0
86	OHX	4	238	7/7	0.26	2.36	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	6	1999	1/1	0.37	2.36	41,41,41,41	0
85	MG	5	3629	1/1	0.16	2.36	35,35,35,35	0
85	MG	8	212	1/1	0.36	2.35	33,33,33,33	0
85	MG	d6	102	1/1	0.30	2.35	45,45,45,45	0
86	OHX	5	4089	7/7	0.22	2.34	126,126,126,126	0
85	MG	1	3475	1/1	0.23	2.34	27,27,27,27	0
86	OHX	1	4145	7/7	0.43	2.34	135,135,135,135	0
86	OHX	5	4005	7/7	0.24	2.32	110,110,110,110	0
85	MG	1	3802	1/1	0.31	2.32	48,48,48,48	0
85	MG	5	3737	1/1	0.19	2.30	43,43,43,43	0
85	MG	m5	302	1/1	0.22	2.28	30,30,30,30	0
85	MG	6	2013	1/1	0.61	2.26	156,156,156,156	0
85	MG	1	3823	1/1	0.21	2.25	37,37,37,37	0
86	OHX	2	2147	7/7	0.26	2.24	166,166,166,166	0
86	OHX	1	4192	7/7	0.47	2.23	128,128,128,128	0
85	MG	5	3656	1/1	0.23	2.22	39,39,39,39	0
86	OHX	1	3921	7/7	0.20	2.22	104,104,104,104	0
86	OHX	1	4078	7/7	0.34	2.21	117,117,117,117	0
86	OHX	5	4193	7/7	0.19	2.20	111,111,111,111	0
85	MG	1	3669	1/1	0.30	2.20	36,36,36,36	0
85	MG	6	2000	1/1	0.19	2.20	90,90,90,90	0
85	MG	1	3688	1/1	0.22	2.19	26,26,26,26	0
85	MG	N6	202	1/1	0.25	2.19	35,35,35,35	0
85	MG	1	3609	1/1	0.29	2.18	33,33,33,33	0
85	MG	1	3740	1/1	0.23	2.17	34,34,34,34	0
86	OHX	5	4136	7/7	0.24	2.17	123,123,123,123	0
86	OHX	2	2086	7/7	0.24	2.16	122,122,122,122	0
86	OHX	2	2110	7/7	0.20	2.16	113,113,113,113	0
85	MG	4	207	1/1	0.32	2.14	22,22,22,22	0
86	OHX	D9	102	7/7	0.34	2.13	150,150,150,150	0
85	MG	5	3838	1/1	0.26	2.11	43,43,43,43	0
85	MG	1	3533	1/1	0.19	2.09	24,24,24,24	0
86	OHX	6	2126	7/7	0.35	2.08	164,164,164,164	0
86	OHX	m7	206	7/7	0.37	2.08	127,127,127,127	0
86	OHX	1	4104	7/7	0.29	2.07	116,116,116,116	0
86	OHX	1	4159	7/7	0.41	2.07	152,152,152,152	0
85	MG	1	3624	1/1	0.23	2.06	51,51,51,51	0
85	MG	5	3771	1/1	0.16	2.06	20,20,20,20	0
85	MG	S8	301	1/1	0.23	2.05	47,47,47,47	0
85	MG	5	3709	1/1	0.22	2.05	32,32,32,32	0
85	MG	5	3479	1/1	0.44	2.02	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	5	3708	1/1	0.18	2.02	79,79,79,79	0
85	MG	1	3620	1/1	0.23	2.02	32,32,32,32	0
85	MG	s8	301	1/1	0.25	2.01	39,39,39,39	0
85	MG	5	3702	1/1	0.26	2.00	31,31,31,31	0
85	MG	1	3707	1/1	0.19	2.00	29,29,29,29	0
85	MG	5	3489	1/1	0.20	1.99	20,20,20,20	0
85	MG	m1	202	1/1	0.20	1.99	42,42,42,42	0
85	MG	5	3781	1/1	0.20	1.98	25,25,25,25	0
86	OHX	5	4069	7/7	0.37	1.97	122,122,122,122	0
86	OHX	1	4189	7/7	0.20	1.96	147,147,147,147	0
85	MG	5	3600	1/1	0.20	1.95	36,36,36,36	0
85	MG	1	3845	1/1	0.22	1.95	33,33,33,33	0
86	OHX	M9	202	7/7	0.35	1.94	168,168,168,168	0
86	OHX	1	4142	7/7	0.19	1.94	115,115,115,115	0
85	MG	1	3749	1/1	0.20	1.94	47,47,47,47	0
85	MG	1	3627	1/1	0.27	1.93	50,50,50,50	0
86	OHX	5	4072	7/7	0.20	1.93	94,94,94,94	0
86	OHX	2	2117	7/7	0.29	1.93	151,151,151,151	0
85	MG	5	3826	1/1	0.31	1.92	61,61,61,61	0
85	MG	5	3410	1/1	0.17	1.91	49,49,49,49	0
85	MG	5	3883	1/1	0.22	1.90	25,25,25,25	0
86	OHX	2	2074	7/7	0.20	1.89	141,141,141,141	0
86	OHX	6	2193	7/7	0.38	1.88	157,157,157,157	0
85	MG	5	3719	1/1	0.25	1.88	26,26,26,26	0
86	OHX	5	4017	7/7	0.19	1.88	107,107,107,107	0
86	OHX	1	4027	7/7	0.20	1.88	124,124,124,124	0
86	OHX	1	3982	7/7	0.27	1.87	112,112,112,112	0
85	MG	5	3617	1/1	0.34	1.85	34,34,34,34	0
85	MG	q3	503	1/1	0.37	1.84	54,54,54,54	0
85	MG	2	1921	1/1	0.30	1.84	43,43,43,43	0
86	OHX	5	4244	7/7	0.35	1.83	149,149,149,149	0
85	MG	1	3714	1/1	0.18	1.83	25,25,25,25	0
86	OHX	1	4111	7/7	0.28	1.83	176,176,176,176	0
86	OHX	2	2114	7/7	0.29	1.82	120,120,120,120	0
86	OHX	2	2108	7/7	0.22	1.82	147,147,147,147	0
86	OHX	2	2087	7/7	0.27	1.81	128,128,128,128	0
86	OHX	5	4107	7/7	0.21	1.80	110,110,110,110	0
85	MG	5	4250	1/1	0.20	1.80	24,24,24,24	0
85	MG	5	3667	1/1	0.20	1.79	36,36,36,36	0
86	OHX	2	2053	7/7	0.23	1.77	138,138,138,138	0
86	OHX	2	2178	7/7	0.30	1.76	160,160,160,160	0
85	MG	3	211	1/1	0.21	1.76	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	n3	204	7/7	0.18	1.75	111,111,111,111	0
85	MG	5	3626	1/1	0.20	1.75	42,42,42,42	0
85	MG	5	3437	1/1	0.29	1.74	41,41,41,41	0
86	OHX	5	4183	7/7	0.35	1.73	127,127,127,127	0
85	MG	5	3818	1/1	0.21	1.73	34,34,34,34	0
86	OHX	5	4084	7/7	0.27	1.73	105,105,105,105	0
85	MG	6	1988	1/1	0.23	1.73	97,97,97,97	0
85	MG	1	3733	1/1	0.20	1.72	19,19,19,19	0
88	3L2	1	4212	36/36	0.22	1.72	21,21,21,21	0
85	MG	1	3671	1/1	0.38	1.71	59,59,59,59	0
86	OHX	1	4186	7/7	0.31	1.70	137,137,137,137	0
85	MG	4	210	1/1	0.24	1.70	33,33,33,33	0
86	OHX	6	2123	7/7	0.29	1.68	145,145,145,145	0
86	OHX	6	2114	7/7	0.20	1.68	131,131,131,131	0
86	OHX	4	227	7/7	0.18	1.67	100,100,100,100	0
85	MG	5	3775	1/1	0.19	1.65	40,40,40,40	0
85	MG	2	1953	1/1	0.23	1.65	52,52,52,52	0
85	MG	1	3816	1/1	0.16	1.65	30,30,30,30	0
85	MG	O7	102	1/1	0.25	1.65	27,27,27,27	0
86	OHX	5	4167	7/7	0.20	1.64	91,91,91,91	0
85	MG	L5	301	1/1	0.51	1.62	61,61,61,61	0
86	OHX	2	2061	7/7	0.24	1.62	134,134,134,134	0
86	OHX	1	4029	7/7	0.20	1.62	132,132,132,132	0
85	MG	c7	201	1/1	0.24	1.62	72,72,72,72	0
86	OHX	2	2050	7/7	0.17	1.61	108,108,108,108	0
86	OHX	6	2151	7/7	0.24	1.60	137,137,137,137	0
86	OHX	5	4026	7/7	0.19	1.60	113,113,113,113	0
86	OHX	5	4046	7/7	0.22	1.60	95,95,95,95	0
86	OHX	1	4090	7/7	0.27	1.58	146,146,146,146	0
86	OHX	5	4031	7/7	0.21	1.58	112,112,112,112	0
86	OHX	5	4081	7/7	0.23	1.58	114,114,114,114	0
86	OHX	6	2160	7/7	0.30	1.57	119,119,119,119	0
85	MG	5	3493	1/1	0.19	1.56	33,33,33,33	0
86	OHX	2	2155	7/7	0.20	1.55	141,141,141,141	0
86	OHX	1	4045	7/7	0.19	1.54	119,119,119,119	0
86	OHX	5	4051	7/7	0.21	1.52	125,125,125,125	0
86	OHX	6	2161	7/7	0.24	1.52	129,129,129,129	0
85	MG	5	3825	1/1	0.23	1.52	37,37,37,37	0
85	MG	n8	205	1/1	0.21	1.50	27,27,27,27	0
85	MG	5	3732	1/1	0.20	1.50	29,29,29,29	0
86	OHX	1	4121	7/7	0.21	1.50	133,133,133,133	0
86	OHX	6	2146	7/7	0.22	1.49	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1946	1/1	0.36	1.49	80,80,80,80	0
86	OHX	1	4005	7/7	0.27	1.48	104,104,104,104	0
86	OHX	d9	102	7/7	0.54	1.48	184,184,184,184	0
85	MG	5	3793	1/1	0.20	1.47	29,29,29,29	0
85	MG	1	3709	1/1	0.17	1.45	41,41,41,41	0
86	OHX	6	2078	7/7	0.18	1.45	103,103,103,103	0
85	MG	5	3632	1/1	0.23	1.45	71,71,71,71	0
86	OHX	1	4082	7/7	0.22	1.42	124,124,124,124	0
85	MG	1	3608	1/1	0.17	1.39	32,32,32,32	0
86	OHX	2	2130	7/7	0.21	1.39	110,110,110,110	0
85	MG	5	3831	1/1	0.18	1.38	22,22,22,22	0
85	MG	1	3443	1/1	0.21	1.38	74,74,74,74	0
86	OHX	1	4091	7/7	0.20	1.38	144,144,144,144	0
85	MG	1	3658	1/1	0.27	1.37	23,23,23,23	0
85	MG	5	3797	1/1	0.14	1.37	33,33,33,33	0
85	MG	1	3797	1/1	0.26	1.37	38,38,38,38	0
86	OHX	1	4000	7/7	0.26	1.37	97,97,97,97	0
85	MG	5	3688	1/1	0.24	1.37	31,31,31,31	0
85	MG	1	3834	1/1	0.52	1.34	30,30,30,30	0
86	OHX	5	3976	7/7	0.20	1.34	98,98,98,98	0
86	OHX	2	2101	7/7	0.21	1.33	154,154,154,154	0
86	OHX	1	4160	7/7	0.25	1.33	133,133,133,133	0
85	MG	SM	301	1/1	0.23	1.32	46,46,46,46	0
85	MG	sM	302	1/1	0.27	1.32	35,35,35,35	0
85	MG	1	3470	1/1	0.16	1.32	27,27,27,27	0
86	OHX	1	4098	7/7	0.30	1.32	160,160,160,160	0
85	MG	5	3631	1/1	0.17	1.31	24,24,24,24	0
86	OHX	8	223	7/7	0.18	1.30	122,122,122,122	0
86	OHX	5	3994	7/7	0.29	1.30	101,101,101,101	0
86	OHX	2	2095	7/7	0.31	1.30	139,139,139,139	0
86	OHX	5	4164	7/7	0.25	1.29	190,190,190,190	0
85	MG	m7	204	1/1	0.23	1.28	27,27,27,27	0
86	OHX	6	2046	7/7	0.20	1.27	68,68,68,68	0
85	MG	1	3735	1/1	0.19	1.27	23,23,23,23	0
86	OHX	5	4021	7/7	0.19	1.27	104,104,104,104	0
85	MG	1	3766	1/1	0.21	1.27	50,50,50,50	0
86	OHX	1	4057	7/7	0.18	1.25	132,132,132,132	0
86	OHX	5	4013	7/7	0.23	1.25	120,120,120,120	0
86	OHX	6	2106	7/7	0.20	1.25	111,111,111,111	0
86	OHX	5	3902	7/7	0.17	1.23	56,56,56,56	0
86	OHX	1	4048	7/7	0.20	1.22	106,106,106,106	0
85	MG	1	3678	1/1	0.22	1.22	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4037	7/7	0.27	1.21	117,117,117,117	0
86	OHX	1	4100	7/7	0.17	1.20	142,142,142,142	0
85	MG	1	3416	1/1	0.31	1.20	41,41,41,41	0
85	MG	2	1968	1/1	0.27	1.19	56,56,56,56	0
86	OHX	6	2148	7/7	0.30	1.19	154,154,154,154	0
85	MG	1	3612	1/1	0.21	1.18	25,25,25,25	0
86	OHX	2	2165	7/7	0.26	1.17	150,150,150,150	0
85	MG	q1	101	1/1	0.26	1.17	32,32,32,32	0
85	MG	5	3860	1/1	0.21	1.17	18,18,18,18	0
86	OHX	5	3998	7/7	0.22	1.16	101,101,101,101	0
85	MG	5	3416	1/1	0.20	1.16	19,19,19,19	0
85	MG	1	3576	1/1	0.16	1.15	21,21,21,21	0
86	OHX	1	4180	7/7	0.23	1.15	103,103,103,103	0
85	MG	5	3609	1/1	0.19	1.15	24,24,24,24	0
86	OHX	1	4017	7/7	0.23	1.14	132,132,132,132	0
86	OHX	5	4100	7/7	0.29	1.14	116,116,116,116	0
85	MG	n3	202	1/1	0.32	1.13	35,35,35,35	0
86	OHX	m8	201	7/7	0.24	1.11	128,128,128,128	0
85	MG	7	213	1/1	0.17	1.10	58,58,58,58	0
85	MG	5	3875	1/1	0.26	1.09	84,84,84,84	0
86	OHX	1	4071	7/7	0.21	1.09	114,114,114,114	0
86	OHX	5	4194	7/7	0.23	1.08	117,117,117,117	0
85	MG	1	3422	1/1	0.17	1.07	24,24,24,24	0
86	OHX	1	4008	7/7	0.18	1.06	122,122,122,122	0
85	MG	1	4214	1/1	0.23	1.04	22,22,22,22	0
86	OHX	1	4051	7/7	0.21	1.02	124,124,124,124	0
85	MG	5	3850	1/1	0.30	1.02	34,34,34,34	0
86	OHX	2	2142	7/7	0.26	1.01	145,145,145,145	0
86	OHX	5	4016	7/7	0.18	1.00	113,113,113,113	0
86	OHX	6	2088	7/7	0.20	1.00	114,114,114,114	0
86	OHX	1	4148	7/7	0.32	1.00	151,151,151,151	0
86	OHX	5	4176	7/7	0.33	1.00	145,145,145,145	0
86	OHX	6	2105	7/7	0.36	0.99	159,159,159,159	0
86	OHX	1	3941	7/7	0.17	0.99	89,89,89,89	0
85	MG	n0	201	1/1	0.18	0.97	31,31,31,31	0
86	OHX	5	4034	7/7	0.17	0.97	124,124,124,124	0
86	OHX	1	4171	7/7	0.17	0.96	96,96,96,96	0
86	OHX	6	2170	7/7	0.27	0.96	143,143,143,143	0
86	OHX	5	3960	7/7	0.20	0.95	107,107,107,107	0
86	OHX	1	4081	7/7	0.24	0.95	145,145,145,145	0
86	OHX	2	2079	7/7	0.23	0.94	180,180,180,180	0
86	OHX	2	2071	7/7	0.25	0.94	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4221	7/7	0.29	0.94	156,156,156,156	0
86	OHX	1	4198	7/7	0.20	0.93	161,161,161,161	0
86	OHX	5	4115	7/7	0.31	0.93	133,133,133,133	0
86	OHX	6	2093	7/7	0.23	0.92	141,141,141,141	0
86	OHX	1	4028	7/7	0.23	0.92	103,103,103,103	0
86	OHX	5	4210	7/7	0.18	0.92	98,98,98,98	0
85	MG	1	3679	1/1	0.29	0.91	57,57,57,57	0
86	OHX	1	3997	7/7	0.19	0.91	104,104,104,104	0
86	OHX	1	3971	7/7	0.20	0.90	99,99,99,99	0
86	OHX	2	2111	7/7	0.35	0.89	159,159,159,159	0
85	MG	d3	203	1/1	0.20	0.89	37,37,37,37	0
86	OHX	s4	301	7/7	0.33	0.89	151,151,151,151	0
86	OHX	1	3968	7/7	0.17	0.88	101,101,101,101	0
86	OHX	2	2175	7/7	0.25	0.88	180,180,180,180	0
85	MG	6	1909	1/1	0.37	0.88	123,123,123,123	0
86	OHX	2	2129	7/7	0.26	0.87	204,204,204,204	0
86	OHX	6	2199	7/7	0.35	0.87	134,134,134,134	0
86	OHX	2	2099	7/7	0.28	0.87	150,150,150,150	0
85	MG	1	3482	1/1	0.27	0.86	38,38,38,38	0
85	MG	q3	502	1/1	0.26	0.86	54,54,54,54	0
85	MG	4	211	1/1	0.19	0.85	36,36,36,36	0
85	MG	6	1940	1/1	0.24	0.85	88,88,88,88	0
86	OHX	6	2135	7/7	0.34	0.85	125,125,125,125	0
85	MG	2	1927	1/1	0.27	0.82	46,46,46,46	0
85	MG	6	1982	1/1	0.20	0.82	47,47,47,47	0
87	ZN	D7	101	1/1	0.28	0.82	159,159,159,159	0
85	MG	m7	205	1/1	0.27	0.80	24,24,24,24	0
85	MG	m6	201	1/1	0.19	0.80	22,22,22,22	0
85	MG	1	3661	1/1	0.18	0.79	27,27,27,27	0
86	OHX	5	4227	7/7	0.24	0.79	100,100,100,100	0
86	OHX	5	4080	7/7	0.21	0.79	126,126,126,126	0
85	MG	5	3848	1/1	0.19	0.78	67,67,67,67	0
86	OHX	6	2190	7/7	0.27	0.77	159,159,159,159	0
85	MG	5	3528	1/1	0.18	0.76	16,16,16,16	0
85	MG	5	3649	1/1	0.25	0.75	66,66,66,66	0
86	OHX	5	4087	7/7	0.20	0.74	113,113,113,113	0
86	OHX	2	2123	7/7	0.30	0.74	131,131,131,131	0
86	OHX	8	219	7/7	0.25	0.73	113,113,113,113	0
85	MG	5	3768	1/1	0.29	0.73	61,61,61,61	0
85	MG	8	211	1/1	0.21	0.72	33,33,33,33	0
85	MG	2	1989	1/1	0.26	0.71	42,42,42,42	0
85	MG	1	3784	1/1	0.20	0.71	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	3632	1/1	0.29	0.71	55,55,55,55	0
86	OHX	5	4088	7/7	0.28	0.70	130,130,130,130	0
85	MG	5	3666	1/1	0.19	0.69	18,18,18,18	0
86	OHX	1	4087	7/7	0.17	0.69	128,128,128,128	0
85	MG	1	3752	1/1	0.16	0.68	28,28,28,28	0
85	MG	5	3484	1/1	0.23	0.68	61,61,61,61	0
86	OHX	5	4116	7/7	0.23	0.68	123,123,123,123	0
86	OHX	6	2183	7/7	0.27	0.67	188,188,188,188	0
85	MG	5	4247	1/1	0.18	0.65	25,25,25,25	0
85	MG	5	3754	1/1	0.16	0.64	48,48,48,48	0
86	OHX	2	2063	7/7	0.18	0.64	117,117,117,117	0
86	OHX	5	4148	7/7	0.19	0.64	112,112,112,112	0
86	OHX	S8	302	7/7	0.28	0.63	172,172,172,172	0
86	OHX	1	3869	7/7	0.15	0.62	48,48,48,48	0
86	OHX	6	2089	7/7	0.19	0.61	111,111,111,111	0
86	OHX	6	2165	7/7	0.26	0.61	194,194,194,194	0
85	MG	5	3542	1/1	0.26	0.60	57,57,57,57	0
86	OHX	5	4077	7/7	0.19	0.60	109,109,109,109	0
85	MG	1	3685	1/1	0.19	0.58	26,26,26,26	0
86	OHX	5	3987	7/7	0.28	0.57	132,132,132,132	0
85	MG	3	203	1/1	0.20	0.57	91,91,91,91	0
86	OHX	L3	405	7/7	0.45	0.54	154,154,154,154	0
85	MG	2	1976	1/1	0.20	0.54	78,78,78,78	0
85	MG	o4	201	1/1	0.30	0.54	45,45,45,45	0
85	MG	5	3599	1/1	0.16	0.54	34,34,34,34	0
85	MG	1	3701	1/1	0.19	0.53	34,34,34,34	0
85	MG	5	3691	1/1	0.17	0.52	28,28,28,28	0
86	OHX	1	4016	7/7	0.22	0.52	112,112,112,112	0
85	MG	1	3581	1/1	0.29	0.51	20,20,20,20	0
86	OHX	1	4038	7/7	0.20	0.51	113,113,113,113	0
86	OHX	4	234	7/7	0.18	0.51	125,125,125,125	0
85	MG	M6	201	1/1	0.23	0.50	25,25,25,25	0
86	OHX	6	2141	7/7	0.28	0.49	143,143,143,143	0
86	OHX	sR	401	7/7	0.25	0.49	159,159,159,159	0
85	MG	1	3425	1/1	0.21	0.48	17,17,17,17	0
85	MG	O2	201	1/1	0.21	0.47	19,19,19,19	0
86	OHX	2	2084	7/7	0.26	0.47	142,142,142,142	0
85	MG	2	2000	1/1	0.35	0.47	56,56,56,56	0
85	MG	1	3488	1/1	0.31	0.47	37,37,37,37	0
85	MG	5	3722	1/1	0.21	0.46	25,25,25,25	0
86	OHX	d4	202	7/7	0.28	0.46	182,182,182,182	0
86	OHX	1	3970	7/7	0.26	0.46	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	O7	104	7/7	0.20	0.45	97,97,97,97	0
86	OHX	5	4165	7/7	0.29	0.45	160,160,160,160	0
86	OHX	6	2180	7/7	0.38	0.44	126,126,126,126	0
85	MG	1	3717	1/1	0.18	0.44	62,62,62,62	0
85	MG	5	3746	1/1	0.18	0.43	38,38,38,38	0
85	MG	5	3643	1/1	0.20	0.43	40,40,40,40	0
86	OHX	6	2140	7/7	0.29	0.43	125,125,125,125	0
86	OHX	2	2056	7/7	0.21	0.42	149,149,149,149	0
86	OHX	1	4099	7/7	0.28	0.41	139,139,139,139	0
85	MG	2	1997	1/1	0.32	0.41	60,60,60,60	0
85	MG	M9	201	1/1	0.29	0.40	43,43,43,43	0
85	MG	1	3775	1/1	0.27	0.40	47,47,47,47	0
85	MG	5	3810	1/1	0.15	0.39	31,31,31,31	0
85	MG	6	2019	1/1	0.18	0.38	108,108,108,108	0
86	OHX	S6	301	7/7	0.39	0.38	150,150,150,150	0
86	OHX	1	4164	7/7	0.35	0.38	226,226,226,226	0
85	MG	Q2	502	1/1	0.26	0.37	54,54,54,54	0
86	OHX	1	4101	7/7	0.23	0.36	113,113,113,113	0
86	OHX	5	4219	7/7	0.32	0.35	143,143,143,143	0
86	OHX	6	2103	7/7	0.17	0.35	119,119,119,119	0
85	MG	1	3782	1/1	0.22	0.34	52,52,52,52	0
86	OHX	2	2133	7/7	0.22	0.34	151,151,151,151	0
86	OHX	2	2151	7/7	0.27	0.34	193,193,193,193	0
86	OHX	2	2144	7/7	0.43	0.34	174,174,174,174	0
86	OHX	1	3988	7/7	0.19	0.33	95,95,95,95	0
86	OHX	5	4012	7/7	0.17	0.31	98,98,98,98	0
85	MG	1	3436	1/1	0.19	0.31	33,33,33,33	0
85	MG	l4	401	1/1	0.22	0.31	23,23,23,23	0
86	OHX	m5	304	7/7	0.22	0.30	123,123,123,123	0
86	OHX	2	2113	7/7	0.18	0.30	161,161,161,161	0
85	MG	1	3725	1/1	0.17	0.30	51,51,51,51	0
86	OHX	6	2153	7/7	0.17	0.29	110,110,110,110	0
85	MG	6	1969	1/1	0.18	0.29	48,48,48,48	0
86	OHX	l9	600	7/7	0.23	0.28	117,117,117,117	0
86	OHX	5	4110	7/7	0.24	0.28	95,95,95,95	0
86	OHX	o3	202	7/7	0.19	0.27	105,105,105,105	0
86	OHX	6	2066	7/7	0.17	0.27	100,100,100,100	0
86	OHX	5	4029	7/7	0.18	0.27	123,123,123,123	0
85	MG	s8	302	1/1	0.20	0.26	37,37,37,37	0
85	MG	5	3465	1/1	0.22	0.26	80,80,80,80	0
87	ZN	d7	101	1/1	0.37	0.26	155,155,155,155	0
85	MG	5	3616	1/1	0.17	0.25	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	2	2081	7/7	0.20	0.25	160,160,160,160	0
86	OHX	1	3888	7/7	0.15	0.24	72,72,72,72	0
86	OHX	2	2120	7/7	0.23	0.24	145,145,145,145	0
86	OHX	1	3867	7/7	0.20	0.23	50,50,50,50	0
85	MG	6	1981	1/1	0.27	0.23	41,41,41,41	0
86	OHX	1	3965	7/7	0.18	0.23	117,117,117,117	0
85	MG	M7	203	1/1	0.27	0.22	27,27,27,27	0
85	MG	2	1942	1/1	0.18	0.22	58,58,58,58	0
86	OHX	1	4143	7/7	0.26	0.22	156,156,156,156	0
85	MG	1	3659	1/1	0.22	0.22	52,52,52,52	0
86	OHX	5	4014	7/7	0.18	0.22	98,98,98,98	0
86	OHX	2	2164	7/7	0.21	0.21	175,175,175,175	0
86	OHX	l3	406	7/7	0.30	0.21	133,133,133,133	0
85	MG	N8	203	1/1	0.22	0.20	34,34,34,34	0
86	OHX	5	4059	7/7	0.17	0.20	112,112,112,112	0
86	OHX	1	4050	7/7	0.26	0.20	146,146,146,146	0
86	OHX	6	2107	7/7	0.17	0.18	114,114,114,114	0
86	OHX	1	3908	7/7	0.20	0.17	82,82,82,82	0
86	OHX	5	3948	7/7	0.20	0.17	91,91,91,91	0
86	OHX	1	4129	7/7	0.32	0.17	156,156,156,156	0
85	MG	1	3638	1/1	0.16	0.17	57,57,57,57	0
86	OHX	8	228	7/7	0.23	0.16	137,137,137,137	0
85	MG	l5	301	1/1	0.14	0.16	48,48,48,48	0
86	OHX	M5	302	7/7	0.21	0.15	112,112,112,112	0
85	MG	5	3467	1/1	0.17	0.14	24,24,24,24	0
85	MG	6	2025	1/1	0.19	0.14	90,90,90,90	0
86	OHX	2	2054	7/7	0.19	0.13	109,109,109,109	0
86	OHX	1	4056	7/7	0.22	0.13	181,181,181,181	0
86	OHX	1	4035	7/7	0.14	0.12	139,139,139,139	0
86	OHX	n3	203	7/7	0.17	0.12	103,103,103,103	0
86	OHX	1	4115	7/7	0.18	0.11	127,127,127,127	0
86	OHX	5	4118	7/7	0.26	0.10	149,149,149,149	0
86	OHX	5	4232	7/7	0.19	0.10	143,143,143,143	0
86	OHX	1	4033	7/7	0.22	0.09	96,96,96,96	0
86	OHX	l5	303	7/7	0.29	0.05	145,145,145,145	0
86	OHX	s8	303	7/7	0.36	0.04	171,171,171,171	0
86	OHX	3	221	7/7	0.18	0.04	122,122,122,122	0
85	MG	m7	202	1/1	0.20	0.03	25,25,25,25	0
86	OHX	6	2127	7/7	0.19	0.02	140,140,140,140	0
86	OHX	1	3976	7/7	0.17	0.02	94,94,94,94	0
86	OHX	o7	502	7/7	0.15	0.01	104,104,104,104	0
86	OHX	1	4042	7/7	0.22	0.00	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3806	1/1	0.18	0.00	47,47,47,47	0
86	OHX	1	3956	7/7	0.18	-0.00	97,97,97,97	0
86	OHX	5	4030	7/7	0.19	-0.03	126,126,126,126	0
85	MG	1	3692	1/1	0.18	-0.03	34,34,34,34	0
85	MG	1	3603	1/1	0.15	-0.03	31,31,31,31	0
86	OHX	m0	302	7/7	0.31	-0.04	118,118,118,118	0
86	OHX	6	2084	7/7	0.18	-0.04	117,117,117,117	0
86	OHX	2	2138	7/7	0.18	-0.06	135,135,135,135	0
85	MG	5	3512	1/1	0.15	-0.06	24,24,24,24	0
85	MG	N3	203	1/1	0.20	-0.07	42,42,42,42	0
85	MG	5	3434	1/1	0.17	-0.09	21,21,21,21	0
86	OHX	2	2124	7/7	0.25	-0.09	145,145,145,145	0
86	OHX	m1	203	7/7	0.37	-0.11	147,147,147,147	0
86	OHX	1	4046	7/7	0.19	-0.12	141,141,141,141	0
86	OHX	1	4088	7/7	0.22	-0.12	142,142,142,142	0
85	MG	5	3890	1/1	0.17	-0.13	57,57,57,57	0
85	MG	1	3623	1/1	0.19	-0.14	37,37,37,37	0
86	OHX	1	4010	7/7	0.19	-0.14	130,130,130,130	0
85	MG	5	3704	1/1	0.15	-0.14	35,35,35,35	0
85	MG	5	3808	1/1	0.15	-0.15	53,53,53,53	0
86	OHX	2	2088	7/7	0.20	-0.16	108,108,108,108	0
85	MG	1	3445	1/1	0.18	-0.16	36,36,36,36	0
85	MG	5	3429	1/1	0.18	-0.17	18,18,18,18	0
86	OHX	4	229	7/7	0.17	-0.17	118,118,118,118	0
86	OHX	5	4192	7/7	0.18	-0.18	88,88,88,88	0
86	OHX	2	2062	7/7	0.15	-0.19	130,130,130,130	0
85	MG	5	3681	1/1	0.18	-0.19	25,25,25,25	0
85	MG	1	3804	1/1	0.15	-0.19	25,25,25,25	0
85	MG	2	1994	1/1	0.17	-0.21	83,83,83,83	0
86	OHX	6	2144	7/7	0.21	-0.22	124,124,124,124	0
86	OHX	5	4019	7/7	0.17	-0.23	108,108,108,108	0
85	MG	s6	301	1/1	0.24	-0.23	70,70,70,70	0
86	OHX	2	2024	7/7	0.17	-0.23	80,80,80,80	0
85	MG	M3	202	1/1	0.36	-0.23	93,93,93,93	0
86	OHX	5	4097	7/7	0.17	-0.24	151,151,151,151	0
85	MG	1	3813	1/1	0.12	-0.25	42,42,42,42	0
86	OHX	5	4075	7/7	0.17	-0.25	105,105,105,105	0
86	OHX	5	3919	7/7	0.15	-0.25	66,66,66,66	0
86	OHX	5	3997	7/7	0.15	-0.26	104,104,104,104	0
86	OHX	5	4057	7/7	0.16	-0.27	122,122,122,122	0
86	OHX	15	302	7/7	0.15	-0.28	132,132,132,132	0
86	OHX	6	2152	7/7	0.18	-0.29	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3778	1/1	0.13	-0.29	29,29,29,29	0
85	MG	1	3815	1/1	0.27	-0.29	111,111,111,111	0
85	MG	6	1963	1/1	0.23	-0.30	107,107,107,107	0
85	MG	5	3830	1/1	0.16	-0.32	54,54,54,54	0
86	OHX	2	2094	7/7	0.19	-0.35	145,145,145,145	0
85	MG	1	3833	1/1	0.14	-0.37	29,29,29,29	0
86	OHX	c5	201	7/7	0.31	-0.39	171,171,171,171	0
85	MG	5	3866	1/1	0.14	-0.40	30,30,30,30	0
85	MG	5	3751	1/1	0.18	-0.40	35,35,35,35	0
85	MG	1	3825	1/1	0.15	-0.40	49,49,49,49	0
86	OHX	2	2092	7/7	0.19	-0.41	145,145,145,145	0
86	OHX	1	3987	7/7	0.15	-0.42	119,119,119,119	0
86	OHX	5	4054	7/7	0.15	-0.42	138,138,138,138	0
85	MG	1	3426	1/1	0.17	-0.42	52,52,52,52	0
85	MG	5	3806	1/1	0.14	-0.44	79,79,79,79	0
86	OHX	3	219	7/7	0.16	-0.45	115,115,115,115	0
85	MG	1	3465	1/1	0.17	-0.45	42,42,42,42	0
86	OHX	8	225	7/7	0.21	-0.46	124,124,124,124	0
86	OHX	1	4023	7/7	0.17	-0.47	104,104,104,104	0
86	OHX	1	4022	7/7	0.19	-0.47	146,146,146,146	0
86	OHX	5	4236	7/7	0.17	-0.48	86,86,86,86	0
86	OHX	2	2066	7/7	0.14	-0.49	134,134,134,134	0
85	MG	2	1985	1/1	0.20	-0.51	64,64,64,64	0
85	MG	5	3765	1/1	0.15	-0.51	45,45,45,45	0
86	OHX	5	3958	7/7	0.14	-0.52	89,89,89,89	0
86	OHX	5	4074	7/7	0.16	-0.52	118,118,118,118	0
86	OHX	1	3946	7/7	0.14	-0.52	113,113,113,113	0
86	OHX	5	3973	7/7	0.16	-0.53	108,108,108,108	0
86	OHX	n6	202	7/7	0.19	-0.54	137,137,137,137	0
86	OHX	7	223	7/7	0.15	-0.55	104,104,104,104	0
85	MG	5	3685	1/1	0.14	-0.55	30,30,30,30	0
86	OHX	6	2102	7/7	0.15	-0.56	116,116,116,116	0
86	OHX	5	4009	7/7	0.14	-0.56	99,99,99,99	0
86	OHX	5	3975	7/7	0.15	-0.56	88,88,88,88	0
86	OHX	2	2106	7/7	0.14	-0.56	110,110,110,110	0
85	MG	1	3635	1/1	0.22	-0.57	72,72,72,72	0
86	OHX	1	3957	7/7	0.17	-0.58	78,78,78,78	0
86	OHX	1	3885	7/7	0.16	-0.58	56,56,56,56	0
86	OHX	1	4021	7/7	0.12	-0.59	144,144,144,144	0
85	MG	5	3447	1/1	0.14	-0.59	35,35,35,35	0
86	OHX	5	4098	7/7	0.19	-0.60	133,133,133,133	0
86	OHX	5	4058	7/7	0.15	-0.60	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	o2	201	7/7	0.18	-0.61	92,92,92,92	0
85	MG	2	1998	1/1	0.19	-0.61	76,76,76,76	0
85	MG	1	3428	1/1	0.17	-0.61	44,44,44,44	0
85	MG	5	3674	1/1	0.13	-0.62	28,28,28,28	0
86	OHX	8	220	7/7	0.11	-0.63	124,124,124,124	0
85	MG	1	3478	1/1	0.16	-0.63	80,80,80,80	0
85	MG	2	2179	1/1	0.19	-0.64	96,96,96,96	0
86	OHX	1	4053	7/7	0.20	-0.64	144,144,144,144	0
86	OHX	5	3892	7/7	0.16	-0.66	38,38,38,38	0
86	OHX	7	222	7/7	0.13	-0.66	104,104,104,104	0
86	OHX	6	2117	7/7	0.25	-0.67	122,122,122,122	0
86	OHX	2	2132	7/7	0.15	-0.67	152,152,152,152	0
86	OHX	1	3989	7/7	0.17	-0.67	104,104,104,104	0
86	OHX	5	4068	7/7	0.17	-0.67	113,113,113,113	0
86	OHX	1	3978	7/7	0.15	-0.68	99,99,99,99	0
86	OHX	5	4007	7/7	0.15	-0.68	93,93,93,93	0
86	OHX	5	3967	7/7	0.10	-0.68	102,102,102,102	0
86	OHX	6	2116	7/7	0.18	-0.69	147,147,147,147	0
86	OHX	6	2157	7/7	0.15	-0.69	105,105,105,105	0
86	OHX	1	3878	7/7	0.14	-0.69	59,59,59,59	0
86	OHX	5	4052	7/7	0.16	-0.70	137,137,137,137	0
86	OHX	c3	201	7/7	0.26	-0.70	158,158,158,158	0
86	OHX	5	4188	7/7	0.25	-0.70	169,169,169,169	0
85	MG	1	3466	1/1	0.14	-0.71	36,36,36,36	0
85	MG	1	3809	1/1	0.15	-0.71	40,40,40,40	0
85	MG	6	2024	1/1	0.12	-0.71	69,69,69,69	0
86	OHX	2	2097	7/7	0.11	-0.71	152,152,152,152	0
85	MG	1	3767	1/1	0.16	-0.71	86,86,86,86	0
86	OHX	1	3985	7/7	0.19	-0.72	113,113,113,113	0
85	MG	7	208	1/1	0.14	-0.73	51,51,51,51	0
86	OHX	5	3989	7/7	0.18	-0.74	97,97,97,97	0
86	OHX	4	233	7/7	0.13	-0.75	137,137,137,137	0
85	MG	sM	301	1/1	0.17	-0.77	35,35,35,35	0
86	OHX	1	4011	7/7	0.14	-0.78	130,130,130,130	0
86	OHX	1	4122	7/7	0.14	-0.79	143,143,143,143	0
85	MG	5	3710	1/1	0.15	-0.79	55,55,55,55	0
86	OHX	2	2141	7/7	0.22	-0.80	176,176,176,176	0
86	OHX	5	3968	7/7	0.13	-0.80	95,95,95,95	0
86	OHX	5	3899	7/7	0.13	-0.82	54,54,54,54	0
86	OHX	5	4060	7/7	0.14	-0.82	112,112,112,112	0
87	ZN	q3	501	1/1	0.10	-0.83	50,50,50,50	0
85	MG	1	3727	1/1	0.15	-0.83	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3900	7/7	0.14	-0.83	50,50,50,50	0
86	OHX	1	3930	7/7	0.13	-0.84	109,109,109,109	0
86	OHX	L3	404	7/7	0.15	-0.84	109,109,109,109	0
87	ZN	q2	501	1/1	0.13	-0.84	71,71,71,71	0
87	ZN	D6	500	1/1	0.09	-0.85	65,65,65,65	0
86	OHX	5	3992	7/7	0.11	-0.85	109,109,109,109	0
85	MG	1	3420	1/1	0.23	-0.86	71,71,71,71	0
86	OHX	1	3964	7/7	0.16	-0.86	104,104,104,104	0
86	OHX	1	4103	7/7	0.15	-0.86	135,135,135,135	0
86	OHX	5	4025	7/7	0.14	-0.88	136,136,136,136	0
86	OHX	1	3945	7/7	0.13	-0.89	89,89,89,89	0
86	OHX	7	224	7/7	0.13	-0.89	136,136,136,136	0
86	OHX	5	3925	7/7	0.13	-0.90	84,84,84,84	0
86	OHX	1	4134	7/7	0.15	-0.90	100,100,100,100	0
86	OHX	2	2166	7/7	0.14	-0.90	151,151,151,151	0
86	OHX	5	4027	7/7	0.15	-0.91	99,99,99,99	0
85	MG	5	3816	1/1	0.22	-0.92	89,89,89,89	0
86	OHX	1	4032	7/7	0.12	-0.93	153,153,153,153	0
87	ZN	Q2	501	1/1	0.16	-0.93	73,73,73,73	0
86	OHX	5	3985	7/7	0.15	-0.94	103,103,103,103	0
86	OHX	3	216	7/7	0.14	-0.94	116,116,116,116	0
86	OHX	1	3894	7/7	0.15	-0.94	67,67,67,67	0
86	OHX	C5	201	7/7	0.20	-0.96	169,169,169,169	0
86	OHX	6	2091	7/7	0.17	-0.97	107,107,107,107	0
85	MG	1	3538	1/1	0.13	-0.98	30,30,30,30	0
85	MG	5	3601	1/1	0.12	-0.98	50,50,50,50	0
86	OHX	5	3962	7/7	0.11	-0.98	101,101,101,101	0
86	OHX	5	3896	7/7	0.14	-0.99	47,47,47,47	0
86	OHX	5	3978	7/7	0.15	-1.00	81,81,81,81	0
85	MG	5	3836	1/1	0.14	-1.00	39,39,39,39	0
85	MG	6	2016	1/1	0.17	-1.02	26,26,26,26	0
86	OHX	1	4030	7/7	0.11	-1.02	95,95,95,95	0
85	MG	5	3778	1/1	0.14	-1.03	69,69,69,69	0
86	OHX	5	4092	7/7	0.13	-1.03	126,126,126,126	0
85	MG	L8	301	1/1	0.28	-1.05	50,50,50,50	0
86	OHX	1	3920	7/7	0.07	-1.05	93,93,93,93	0
86	OHX	6	2062	7/7	0.13	-1.06	93,93,93,93	0
86	OHX	1	4039	7/7	0.15	-1.07	123,123,123,123	0
86	OHX	6	2119	7/7	0.11	-1.07	144,144,144,144	0
86	OHX	1	3906	7/7	0.11	-1.07	86,86,86,86	0
86	OHX	5	4024	7/7	0.12	-1.07	116,116,116,116	0
85	MG	5	3697	1/1	0.16	-1.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2072	7/7	0.18	-1.07	146,146,146,146	0
85	MG	6	1995	1/1	0.14	-1.07	64,64,64,64	0
85	MG	c9	201	1/1	0.24	-1.08	59,59,59,59	0
85	MG	M0	302	1/1	0.16	-1.09	32,32,32,32	0
85	MG	5	3795	1/1	0.16	-1.10	63,63,63,63	0
85	MG	M7	202	1/1	0.15	-1.10	29,29,29,29	0
85	MG	1	3615	1/1	0.11	-1.11	55,55,55,55	0
85	MG	5	3885	1/1	0.14	-1.12	70,70,70,70	0
86	OHX	2	2047	7/7	0.13	-1.12	115,115,115,115	0
85	MG	5	3757	1/1	0.17	-1.14	41,41,41,41	0
85	MG	1	3489	1/1	0.16	-1.14	24,24,24,24	0
85	MG	5	3684	1/1	0.14	-1.14	68,68,68,68	0
86	OHX	5	4123	7/7	0.11	-1.14	134,134,134,134	0
85	MG	1	3736	1/1	0.14	-1.16	48,48,48,48	0
86	OHX	1	3998	7/7	0.14	-1.16	89,89,89,89	0
86	OHX	5	4174	7/7	0.22	-1.17	148,148,148,148	0
86	OHX	6	2086	7/7	0.15	-1.17	127,127,127,127	0
85	MG	M3	201	1/1	0.14	-1.18	32,32,32,32	0
86	OHX	7	218	7/7	0.14	-1.19	93,93,93,93	0
86	OHX	8	218	7/7	0.07	-1.19	113,113,113,113	0
85	MG	1	3706	1/1	0.15	-1.19	62,62,62,62	0
86	OHX	6	2192	7/7	0.36	-1.19	200,200,200,200	0
86	OHX	6	2080	7/7	0.10	-1.19	107,107,107,107	0
86	OHX	1	3933	7/7	0.12	-1.20	97,97,97,97	0
86	OHX	C3	201	7/7	0.17	-1.20	155,155,155,155	0
86	OHX	1	3871	7/7	0.12	-1.22	56,56,56,56	0
86	OHX	1	3937	7/7	0.07	-1.22	108,108,108,108	0
85	MG	5	3801	1/1	0.18	-1.22	89,89,89,89	0
87	ZN	Q0	500	1/1	0.11	-1.22	37,37,37,37	0
86	OHX	M0	303	7/7	0.16	-1.23	119,119,119,119	0
86	OHX	2	2109	7/7	0.10	-1.24	120,120,120,120	0
86	OHX	6	2143	7/7	0.15	-1.25	132,132,132,132	0
86	OHX	6	2065	7/7	0.10	-1.27	88,88,88,88	0
86	OHX	1	3886	7/7	0.14	-1.27	70,70,70,70	0
86	OHX	1	3891	7/7	0.12	-1.27	66,66,66,66	0
86	OHX	n9	102	7/7	0.11	-1.28	64,64,64,64	0
86	OHX	5	4010	7/7	0.16	-1.28	140,140,140,140	0
86	OHX	6	2200	7/7	0.32	-1.28	202,202,202,202	0
85	MG	5	3812	1/1	0.11	-1.28	56,56,56,56	0
86	OHX	1	3940	7/7	0.15	-1.29	103,103,103,103	0
86	OHX	O7	103	7/7	0.09	-1.29	101,101,101,101	0
86	OHX	5	3916	7/7	0.14	-1.29	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4235	7/7	0.38	-1.30	241,241,241,241	0
86	OHX	6	2133	7/7	0.14	-1.30	136,136,136,136	0
85	MG	5	3851	1/1	0.14	-1.32	73,73,73,73	0
85	MG	5	3613	1/1	0.14	-1.32	42,42,42,42	0
86	OHX	N9	101	7/7	0.12	-1.32	60,60,60,60	0
86	OHX	Q2	503	7/7	0.11	-1.32	75,75,75,75	0
85	MG	5	3419	1/1	0.14	-1.34	25,25,25,25	0
87	ZN	Q3	501	1/1	0.06	-1.34	49,49,49,49	0
87	ZN	e1	501	1/1	0.20	-1.35	199,199,199,199	0
85	MG	5	3404	1/1	0.14	-1.36	38,38,38,38	0
86	OHX	c8	202	7/7	0.13	-1.36	167,167,167,167	0
86	OHX	6	2052	7/7	0.16	-1.36	73,73,73,73	0
87	ZN	E1	501	1/1	0.08	-1.37	118,118,118,118	0
86	OHX	5	4061	7/7	0.13	-1.39	118,118,118,118	0
86	OHX	2	2051	7/7	0.14	-1.39	110,110,110,110	0
86	OHX	1	3868	7/7	0.11	-1.40	40,40,40,40	0
86	OHX	2	2034	7/7	0.14	-1.40	94,94,94,94	0
85	MG	6	2006	1/1	0.11	-1.40	42,42,42,42	0
86	OHX	2	2093	7/7	0.07	-1.41	143,143,143,143	0
85	MG	5	3401	1/1	0.14	-1.43	52,52,52,52	0
86	OHX	6	2162	7/7	0.27	-1.43	197,197,197,197	0
85	MG	6	1984	1/1	0.18	-1.43	97,97,97,97	0
87	ZN	O7	101	1/1	0.10	-1.43	28,28,28,28	0
86	OHX	2	2035	7/7	0.07	-1.44	86,86,86,86	0
86	OHX	6	2092	7/7	0.10	-1.45	138,138,138,138	0
87	ZN	d6	101	1/1	0.13	-1.46	50,50,50,50	0
85	MG	6	2015	1/1	0.13	-1.46	67,67,67,67	0
86	OHX	1	3935	7/7	0.14	-1.47	94,94,94,94	0
86	OHX	5	4168	7/7	0.16	-1.48	111,111,111,111	0
86	OHX	6	2047	7/7	0.13	-1.48	58,58,58,58	0
86	OHX	2	2059	7/7	0.12	-1.49	99,99,99,99	0
85	MG	5	3723	1/1	0.10	-1.50	50,50,50,50	0
86	OHX	7	217	7/7	0.10	-1.51	87,87,87,87	0
86	OHX	2	2039	7/7	0.13	-1.52	96,96,96,96	0
86	OHX	5	3893	7/7	0.14	-1.52	35,35,35,35	0
86	OHX	1	4058	7/7	0.10	-1.52	143,143,143,143	0
86	OHX	2	2067	7/7	0.14	-1.53	159,159,159,159	0
86	OHX	l3	404	7/7	0.14	-1.53	98,98,98,98	0
86	OHX	5	4095	7/7	0.18	-1.54	140,140,140,140	0
86	OHX	1	3866	7/7	0.11	-1.55	44,44,44,44	0
86	OHX	6	2071	7/7	0.13	-1.55	152,152,152,152	0
86	OHX	1	3881	7/7	0.14	-1.55	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	4217	1/1	0.12	-1.55	36,36,36,36	0
86	OHX	2	2032	7/7	0.11	-1.57	105,105,105,105	0
86	OHX	1	3949	7/7	0.11	-1.57	117,117,117,117	0
86	OHX	1	3974	7/7	0.12	-1.58	103,103,103,103	0
86	OHX	6	2109	7/7	0.13	-1.58	127,127,127,127	0
87	ZN	D9	101	1/1	0.10	-1.60	67,67,67,67	0
86	OHX	5	4035	7/7	0.07	-1.61	151,151,151,151	0
87	ZN	d9	101	1/1	0.07	-1.61	93,93,93,93	0
86	OHX	5	3950	7/7	0.09	-1.61	83,83,83,83	0
86	OHX	1	3991	7/7	0.14	-1.62	130,130,130,130	0
85	MG	5	3799	1/1	0.16	-1.62	163,163,163,163	0
86	OHX	6	2053	7/7	0.14	-1.62	85,85,85,85	0
85	MG	5	3752	1/1	0.12	-1.62	42,42,42,42	0
86	OHX	2	2045	7/7	0.10	-1.65	120,120,120,120	0
85	MG	5	3743	1/1	0.13	-1.65	55,55,55,55	0
86	OHX	2	2036	7/7	0.10	-1.66	126,126,126,126	0
86	OHX	q2	502	7/7	0.10	-1.66	76,76,76,76	0
86	OHX	6	2120	7/7	0.14	-1.66	135,135,135,135	0
85	MG	1	3434	1/1	0.11	-1.66	36,36,36,36	0
86	OHX	6	2098	7/7	0.19	-1.68	194,194,194,194	0
86	OHX	2	2052	7/7	0.14	-1.68	131,131,131,131	0
86	OHX	1	3918	7/7	0.12	-1.68	112,112,112,112	0
86	OHX	6	2096	7/7	0.11	-1.71	117,117,117,117	0
86	OHX	6	2050	7/7	0.12	-1.72	63,63,63,63	0
86	OHX	2	2156	7/7	0.38	-1.73	251,251,251,251	0
86	OHX	7	219	7/7	0.11	-1.73	95,95,95,95	0
86	OHX	5	4011	7/7	0.08	-1.73	121,121,121,121	0
86	OHX	6	2068	7/7	0.14	-1.74	92,92,92,92	0
86	OHX	1	3864	7/7	0.12	-1.74	39,39,39,39	0
86	OHX	3	220	7/7	0.14	-1.75	118,118,118,118	0
85	MG	6	1996	1/1	0.10	-1.77	49,49,49,49	0
85	MG	5	3412	1/1	0.14	-1.77	20,20,20,20	0
85	MG	5	3408	1/1	0.10	-1.77	21,21,21,21	0
86	OHX	5	4032	7/7	0.14	-1.77	123,123,123,123	0
86	OHX	5	3897	7/7	0.12	-1.78	46,46,46,46	0
86	OHX	1	3993	7/7	0.09	-1.79	126,126,126,126	0
86	OHX	6	2087	7/7	0.06	-1.79	124,124,124,124	0
86	OHX	5	3983	7/7	0.12	-1.80	93,93,93,93	0
86	OHX	5	4047	7/7	0.13	-1.80	96,96,96,96	0
86	OHX	6	2099	7/7	0.06	-1.81	168,168,168,168	0
86	OHX	5	4000	7/7	0.12	-1.81	115,115,115,115	0
86	OHX	C8	201	7/7	0.06	-1.81	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4002	7/7	0.14	-1.83	94,94,94,94	0
86	OHX	6	2073	7/7	0.09	-1.83	84,84,84,84	0
86	OHX	6	2051	7/7	0.12	-1.83	74,74,74,74	0
86	OHX	6	2090	7/7	0.11	-1.84	117,117,117,117	0
86	OHX	1	3922	7/7	0.11	-1.84	85,85,85,85	0
87	ZN	q0	201	1/1	0.11	-1.86	23,23,23,23	0
86	OHX	1	4154	7/7	0.12	-1.87	98,98,98,98	0
86	OHX	1	3895	7/7	0.11	-1.87	70,70,70,70	0
86	OHX	2	2082	7/7	0.12	-1.87	124,124,124,124	0
86	OHX	6	2094	7/7	0.09	-1.89	127,127,127,127	0
86	OHX	1	4191	7/7	0.09	-1.89	167,167,167,167	0
86	OHX	1	3872	7/7	0.11	-1.91	58,58,58,58	0
86	OHX	2	2028	7/7	0.11	-1.91	103,103,103,103	0
86	OHX	2	2042	7/7	0.09	-1.91	106,106,106,106	0
86	OHX	2	2026	7/7	0.11	-1.93	69,69,69,69	0
86	OHX	1	3903	7/7	0.06	-1.93	83,83,83,83	0
86	OHX	1	3914	7/7	0.10	-1.94	90,90,90,90	0
86	OHX	2	2070	7/7	0.14	-1.94	121,121,121,121	0
85	MG	5	3725	1/1	0.13	-1.94	93,93,93,93	0
86	OHX	1	3948	7/7	0.10	-1.94	119,119,119,119	0
85	MG	5	3432	1/1	0.15	-1.95	36,36,36,36	0
86	OHX	5	3906	7/7	0.12	-1.96	60,60,60,60	0
86	OHX	6	2095	7/7	0.14	-1.96	169,169,169,169	0
85	MG	5	3407	1/1	0.11	-1.97	30,30,30,30	0
86	OHX	1	3877	7/7	0.09	-1.97	56,56,56,56	0
86	OHX	7	221	7/7	0.14	-1.99	99,99,99,99	0
85	MG	1	3855	1/1	0.17	-2.00	54,54,54,54	0
86	OHX	6	2129	7/7	0.18	-2.01	146,146,146,146	0
86	OHX	1	4020	7/7	0.11	-2.01	110,110,110,110	0
86	OHX	m0	301	7/7	0.07	-2.02	120,120,120,120	0
86	OHX	1	3938	7/7	0.11	-2.02	93,93,93,93	0
86	OHX	5	3980	7/7	0.08	-2.03	96,96,96,96	0
86	OHX	1	3962	7/7	0.14	-2.04	94,94,94,94	0
86	OHX	5	3953	7/7	0.10	-2.05	74,74,74,74	0
86	OHX	2	2033	7/7	0.11	-2.05	94,94,94,94	0
87	ZN	o7	501	1/1	0.11	-2.07	36,36,36,36	0
86	OHX	6	2075	7/7	0.12	-2.08	107,107,107,107	0
86	OHX	5	3935	7/7	0.12	-2.08	88,88,88,88	0
86	OHX	1	3863	7/7	0.13	-2.08	35,35,35,35	0
86	OHX	2	2055	7/7	0.12	-2.09	125,125,125,125	0
85	MG	5	3843	1/1	0.12	-2.10	53,53,53,53	0
86	OHX	1	4015	7/7	0.11	-2.10	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	3	218	7/7	0.13	-2.11	95,95,95,95	0
86	OHX	5	3932	7/7	0.10	-2.15	82,82,82,82	0
86	OHX	6	2045	7/7	0.12	-2.15	48,48,48,48	0
85	MG	1	3748	1/1	0.13	-2.15	34,34,34,34	0
85	MG	1	3683	1/1	0.15	-2.15	35,35,35,35	0
85	MG	5	3694	1/1	0.12	-2.16	26,26,26,26	0
86	OHX	s1	302	7/7	0.12	-2.19	81,81,81,81	0
86	OHX	2	2046	7/7	0.09	-2.19	124,124,124,124	0
86	OHX	SR	401	7/7	0.13	-2.20	159,159,159,159	0
86	OHX	1	3898	7/7	0.09	-2.21	83,83,83,83	0
86	OHX	5	3963	7/7	0.08	-2.21	103,103,103,103	0
86	OHX	2	2158	7/7	0.18	-2.22	260,260,260,260	0
86	OHX	1	4025	7/7	0.14	-2.23	117,117,117,117	0
86	OHX	2	2023	7/7	0.09	-2.23	73,73,73,73	0
86	OHX	5	3914	7/7	0.10	-2.23	58,58,58,58	0
86	OHX	6	2067	7/7	0.07	-2.23	96,96,96,96	0
86	OHX	4	228	7/7	0.09	-2.24	113,113,113,113	0
86	OHX	5	4071	7/7	0.06	-2.24	152,152,152,152	0
86	OHX	6	2100	7/7	0.17	-2.24	118,118,118,118	0
86	OHX	8	217	7/7	0.12	-2.25	47,47,47,47	0
86	OHX	6	2054	7/7	0.11	-2.25	70,70,70,70	0
86	OHX	5	3931	7/7	0.11	-2.26	69,69,69,69	0
86	OHX	1	3902	7/7	0.12	-2.27	81,81,81,81	0
86	OHX	6	2079	7/7	0.12	-2.28	105,105,105,105	0
86	OHX	2	2096	7/7	0.10	-2.29	176,176,176,176	0
86	OHX	6	2128	7/7	0.14	-2.29	121,121,121,121	0
85	MG	1	3715	1/1	0.14	-2.29	31,31,31,31	0
86	OHX	1	3926	7/7	0.11	-2.30	94,94,94,94	0
86	OHX	1	3944	7/7	0.10	-2.30	102,102,102,102	0
86	OHX	5	3996	7/7	0.10	-2.31	104,104,104,104	0
85	MG	1	3448	1/1	0.10	-2.31	26,26,26,26	0
86	OHX	6	2057	7/7	0.10	-2.31	90,90,90,90	0
85	MG	5	3783	1/1	0.09	-2.32	30,30,30,30	0
85	MG	1	3674	1/1	0.07	-2.33	62,62,62,62	0
86	OHX	5	3905	7/7	0.10	-2.33	57,57,57,57	0
86	OHX	1	4083	7/7	0.17	-2.34	196,196,196,196	0
86	OHX	5	3933	7/7	0.11	-2.35	86,86,86,86	0
86	OHX	1	3910	7/7	0.07	-2.35	80,80,80,80	0
85	MG	5	3784	1/1	0.08	-2.36	43,43,43,43	0
86	OHX	3	215	7/7	0.09	-2.37	94,94,94,94	0
85	MG	5	3675	1/1	0.10	-2.37	88,88,88,88	0
86	OHX	5	3949	7/7	0.09	-2.39	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2030	7/7	0.10	-2.41	103,103,103,103	0
86	OHX	2	2038	7/7	0.10	-2.41	93,93,93,93	0
86	OHX	1	4001	7/7	0.10	-2.43	114,114,114,114	0
86	OHX	5	3923	7/7	0.11	-2.45	60,60,60,60	0
86	OHX	1	3947	7/7	0.12	-2.45	111,111,111,111	0
86	OHX	1	3913	7/7	0.07	-2.45	102,102,102,102	0
86	OHX	1	3905	7/7	0.11	-2.46	81,81,81,81	0
85	MG	1	3821	1/1	0.14	-2.47	28,28,28,28	0
86	OHX	5	3904	7/7	0.12	-2.47	51,51,51,51	0
86	OHX	5	3972	7/7	0.09	-2.48	88,88,88,88	0
86	OHX	1	3873	7/7	0.11	-2.49	47,47,47,47	0
86	OHX	5	4044	7/7	0.09	-2.49	125,125,125,125	0
86	OHX	2	2076	7/7	0.11	-2.50	112,112,112,112	0
86	OHX	5	3988	7/7	0.12	-2.50	110,110,110,110	0
86	OHX	5	3907	7/7	0.11	-2.53	50,50,50,50	0
85	MG	5	3646	1/1	0.13	-2.54	33,33,33,33	0
86	OHX	6	2083	7/7	0.08	-2.54	122,122,122,122	0
86	OHX	5	4018	7/7	0.10	-2.54	112,112,112,112	0
86	OHX	1	3994	7/7	0.14	-2.55	93,93,93,93	0
86	OHX	1	3969	7/7	0.10	-2.55	106,106,106,106	0
85	MG	5	3468	1/1	0.13	-2.56	97,97,97,97	0
86	OHX	1	3943	7/7	0.10	-2.59	93,93,93,93	0
86	OHX	1	3975	7/7	0.11	-2.59	97,97,97,97	0
86	OHX	1	3931	7/7	0.07	-2.60	95,95,95,95	0
85	MG	5	3422	1/1	0.13	-2.62	32,32,32,32	0
86	OHX	2	2044	7/7	0.08	-2.62	99,99,99,99	0
86	OHX	5	4078	7/7	0.13	-2.63	134,134,134,134	0
86	OHX	5	4037	7/7	0.13	-2.65	105,105,105,105	0
86	OHX	5	3965	7/7	0.13	-2.65	89,89,89,89	0
86	OHX	1	3936	7/7	0.09	-2.66	91,91,91,91	0
86	OHX	1	4177	7/7	0.22	-2.66	252,252,252,252	0
86	OHX	1	3900	7/7	0.07	-2.67	78,78,78,78	0
86	OHX	2	2031	7/7	0.09	-2.68	96,96,96,96	0
86	OHX	5	3959	7/7	0.10	-2.69	101,101,101,101	0
86	OHX	1	3911	7/7	0.06	-2.69	78,78,78,78	0
86	OHX	5	3942	7/7	0.07	-2.69	98,98,98,98	0
85	MG	5	3700	1/1	0.13	-2.70	43,43,43,43	0
85	MG	5	3824	1/1	0.09	-2.71	64,64,64,64	0
86	OHX	6	2097	7/7	0.15	-2.72	181,181,181,181	0
86	OHX	6	2060	7/7	0.09	-2.75	90,90,90,90	0
86	OHX	1	3992	7/7	0.11	-2.76	125,125,125,125	0
85	MG	7	207	1/1	0.10	-2.77	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	3910	7/7	0.08	-2.78	59,59,59,59	0
86	OHX	8	221	7/7	0.08	-2.79	114,114,114,114	0
86	OHX	1	3880	7/7	0.11	-2.79	52,52,52,52	0
86	OHX	1	3967	7/7	0.11	-2.80	117,117,117,117	0
85	MG	5	3817	1/1	0.10	-2.80	57,57,57,57	0
86	OHX	5	4015	7/7	0.09	-2.82	109,109,109,109	0
86	OHX	6	2112	7/7	0.12	-2.82	129,129,129,129	0
86	OHX	2	2029	7/7	0.11	-2.83	86,86,86,86	0
86	OHX	2	2065	7/7	0.08	-2.83	125,125,125,125	0
85	MG	1	3631	1/1	0.13	-2.85	21,21,21,21	0
86	OHX	2	2103	7/7	0.23	-2.88	196,196,196,196	0
86	OHX	5	3894	7/7	0.11	-2.91	65,65,65,65	0
86	OHX	5	3930	7/7	0.10	-2.92	78,78,78,78	0
86	OHX	4	226	7/7	0.11	-2.92	44,44,44,44	0
86	OHX	6	2074	7/7	0.11	-2.94	110,110,110,110	0
86	OHX	N1	201	7/7	0.09	-2.95	58,58,58,58	0
86	OHX	1	3884	7/7	0.10	-2.95	62,62,62,62	0
85	MG	1	3820	1/1	0.12	-2.95	44,44,44,44	0
86	OHX	1	4150	7/7	0.12	-2.95	117,117,117,117	0
85	MG	1	3800	1/1	0.15	-2.96	44,44,44,44	0
86	OHX	2	2022	7/7	0.11	-2.96	63,63,63,63	0
86	OHX	1	3927	7/7	0.11	-2.97	98,98,98,98	0
86	OHX	5	3951	7/7	0.09	-2.98	87,87,87,87	0
86	OHX	2	2058	7/7	0.09	-3.01	114,114,114,114	0
85	MG	1	3520	1/1	0.09	-3.01	23,23,23,23	0
86	OHX	1	3939	7/7	0.10	-3.01	99,99,99,99	0
86	OHX	5	3955	7/7	0.06	-3.04	88,88,88,88	0
86	OHX	1	3924	7/7	0.09	-3.08	110,110,110,110	0
86	OHX	6	2085	7/7	0.10	-3.09	101,101,101,101	0
86	OHX	5	3993	7/7	0.08	-3.09	104,104,104,104	0
86	OHX	5	3991	7/7	0.08	-3.09	104,104,104,104	0
86	OHX	1	3874	7/7	0.10	-3.09	56,56,56,56	0
86	OHX	5	3941	7/7	0.07	-3.10	83,83,83,83	0
86	OHX	1	3979	7/7	0.11	-3.12	100,100,100,100	0
86	OHX	1	4063	7/7	0.10	-3.13	150,150,150,150	0
86	OHX	5	3981	7/7	0.09	-3.14	119,119,119,119	0
86	OHX	5	3954	7/7	0.06	-3.14	91,91,91,91	0
86	OHX	6	2048	7/7	0.10	-3.14	70,70,70,70	0
85	MG	5	3849	1/1	0.04	-3.14	49,49,49,49	0
86	OHX	5	3944	7/7	0.13	-3.17	97,97,97,97	0
86	OHX	5	3940	7/7	0.09	-3.17	87,87,87,87	0
86	OHX	5	3929	7/7	0.05	-3.18	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	6	2055	7/7	0.07	-3.19	86,86,86,86	0
86	OHX	8	224	7/7	0.11	-3.20	139,139,139,139	0
86	OHX	6	2056	7/7	0.09	-3.21	90,90,90,90	0
86	OHX	5	3924	7/7	0.12	-3.22	69,69,69,69	0
86	OHX	1	3942	7/7	0.07	-3.24	96,96,96,96	0
86	OHX	1	3996	7/7	0.10	-3.31	150,150,150,150	0
85	MG	1	3601	1/1	0.13	-3.36	26,26,26,26	0
86	OHX	2	2037	7/7	0.08	-3.36	97,97,97,97	0
86	OHX	5	3971	7/7	0.10	-3.37	79,79,79,79	0
86	OHX	3	217	7/7	0.08	-3.37	106,106,106,106	0
86	OHX	1	3995	7/7	0.09	-3.38	157,157,157,157	0
86	OHX	6	2064	7/7	0.11	-3.42	122,122,122,122	0
85	MG	1	3805	1/1	0.26	-3.43	195,195,195,195	0
86	OHX	5	3926	7/7	0.11	-3.49	68,68,68,68	0
86	OHX	1	3925	7/7	0.07	-3.49	81,81,81,81	0
86	OHX	1	3875	7/7	0.10	-3.49	54,54,54,54	0
86	OHX	5	3970	7/7	0.09	-3.54	93,93,93,93	0
86	OHX	5	3961	7/7	0.09	-3.55	90,90,90,90	0
85	MG	1	4215	1/1	0.10	-3.60	60,60,60,60	0
86	OHX	1	3981	7/7	0.07	-3.60	110,110,110,110	0
86	OHX	5	3908	7/7	0.09	-3.61	66,66,66,66	0
86	OHX	2	2077	7/7	0.12	-3.63	119,119,119,119	0
86	OHX	6	2110	7/7	0.12	-3.63	117,117,117,117	0
85	MG	5	3647	1/1	0.09	-3.64	15,15,15,15	0
86	OHX	8	216	7/7	0.08	-3.66	49,49,49,49	0
86	OHX	1	3897	7/7	0.14	-3.67	89,89,89,89	0
86	OHX	1	3951	7/7	0.11	-3.67	108,108,108,108	0
86	OHX	6	2072	7/7	0.08	-3.67	151,151,151,151	0
86	OHX	5	3898	7/7	0.15	-3.68	47,47,47,47	0
86	OHX	2	2027	7/7	0.12	-3.68	92,92,92,92	0
86	OHX	1	3907	7/7	0.11	-3.70	69,69,69,69	0
85	MG	1	3808	1/1	0.07	-3.72	24,24,24,24	0
86	OHX	1	3961	7/7	0.08	-3.76	117,117,117,117	0
86	OHX	1	3865	7/7	0.10	-3.78	56,56,56,56	0
86	OHX	1	3916	7/7	0.06	-3.78	98,98,98,98	0
86	OHX	5	4006	7/7	0.06	-3.80	144,144,144,144	0
86	OHX	5	3952	7/7	0.12	-3.80	65,65,65,65	0
86	OHX	2	2025	7/7	0.09	-3.81	83,83,83,83	0
86	OHX	2	2049	7/7	0.10	-3.83	114,114,114,114	0
86	OHX	5	4208	7/7	0.16	-3.84	195,195,195,195	0
86	OHX	1	3901	7/7	0.11	-3.87	79,79,79,79	0
86	OHX	1	3932	7/7	0.07	-3.94	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	3934	7/7	0.09	-3.97	83,83,83,83	0
86	OHX	6	2061	7/7	0.07	-4.01	82,82,82,82	0
86	OHX	1	3896	7/7	0.08	-4.05	78,78,78,78	0
86	OHX	1	3915	7/7	0.09	-4.05	89,89,89,89	0
86	OHX	5	4049	7/7	0.08	-4.06	98,98,98,98	0
86	OHX	6	2049	7/7	0.13	-4.06	72,72,72,72	0
86	OHX	5	3903	7/7	0.10	-4.09	46,46,46,46	0
86	OHX	5	4125	7/7	0.17	-4.10	187,187,187,187	0
86	OHX	1	3919	7/7	0.13	-4.11	99,99,99,99	0
86	OHX	6	2063	7/7	0.07	-4.18	109,109,109,109	0
86	OHX	6	2076	7/7	0.11	-4.18	93,93,93,93	0
86	OHX	6	2069	7/7	0.09	-4.19	98,98,98,98	0
86	OHX	5	3928	7/7	0.09	-4.21	74,74,74,74	0
86	OHX	1	3889	7/7	0.10	-4.21	61,61,61,61	0
86	OHX	6	2081	7/7	0.10	-4.23	119,119,119,119	0
86	OHX	5	4003	7/7	0.08	-4.25	100,100,100,100	0
86	OHX	5	3990	7/7	0.05	-4.25	116,116,116,116	0
86	OHX	6	2077	7/7	0.07	-4.28	100,100,100,100	0
86	OHX	5	3964	7/7	0.14	-4.29	100,100,100,100	0
86	OHX	1	3883	7/7	0.07	-4.31	66,66,66,66	0
86	OHX	5	3956	7/7	0.11	-4.32	91,91,91,91	0
86	OHX	5	4028	7/7	0.09	-4.32	103,103,103,103	0
86	OHX	m6	202	7/7	0.09	-4.35	96,96,96,96	0
86	OHX	5	3999	7/7	0.11	-4.37	103,103,103,103	0
86	OHX	5	3943	7/7	0.09	-4.45	78,78,78,78	0
86	OHX	1	3959	7/7	0.08	-4.46	108,108,108,108	0
86	OHX	5	4001	7/7	0.09	-4.46	63,63,63,63	0
86	OHX	6	2058	7/7	0.06	-4.49	84,84,84,84	0
86	OHX	1	3923	7/7	0.07	-4.49	84,84,84,84	0
86	OHX	5	3979	7/7	0.08	-4.50	83,83,83,83	0
86	OHX	5	3915	7/7	0.08	-4.50	66,66,66,66	0
86	OHX	2	2048	7/7	0.06	-4.51	119,119,119,119	0
86	OHX	5	3895	7/7	0.08	-4.56	50,50,50,50	0
86	OHX	2	2069	7/7	0.07	-4.66	119,119,119,119	0
86	OHX	5	4022	7/7	0.09	-4.66	81,81,81,81	0
86	OHX	2	2041	7/7	0.06	-4.67	101,101,101,101	0
86	OHX	1	3963	7/7	0.07	-4.69	66,66,66,66	0
85	MG	5	3756	1/1	0.07	-4.72	34,34,34,34	0
86	OHX	1	3909	7/7	0.07	-4.80	96,96,96,96	0
86	OHX	5	3936	7/7	0.08	-4.80	85,85,85,85	0
86	OHX	5	3912	7/7	0.10	-4.82	57,57,57,57	0
85	MG	1	3769	1/1	0.12	-4.82	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	7	220	7/7	0.08	-4.84	86,86,86,86	0
86	OHX	1	3950	7/7	0.10	-4.85	91,91,91,91	0
86	OHX	1	3953	7/7	0.10	-4.88	91,91,91,91	0
86	OHX	5	3969	7/7	0.11	-4.94	99,99,99,99	0
86	OHX	5	3921	7/7	0.07	-4.96	83,83,83,83	0
86	OHX	5	3947	7/7	0.09	-4.98	89,89,89,89	0
85	MG	1	3463	1/1	0.09	-5.00	27,27,27,27	0
86	OHX	1	3973	7/7	0.09	-5.04	118,118,118,118	0
86	OHX	5	3901	7/7	0.07	-5.06	52,52,52,52	0
86	OHX	1	3960	7/7	0.09	-5.14	94,94,94,94	0
85	MG	5	3845	1/1	0.07	-5.14	42,42,42,42	0
85	MG	1	3712	1/1	0.13	-5.14	42,42,42,42	0
86	OHX	1	3876	7/7	0.07	-5.17	52,52,52,52	0
86	OHX	5	3938	7/7	0.07	-5.25	79,79,79,79	0
86	OHX	5	3984	7/7	0.07	-5.27	91,91,91,91	0
86	OHX	5	3939	7/7	0.07	-5.27	67,67,67,67	0
86	OHX	5	3945	7/7	0.09	-5.32	99,99,99,99	0
85	MG	5	3835	1/1	0.11	-5.37	24,24,24,24	0
86	OHX	1	3934	7/7	0.08	-5.37	91,91,91,91	0
86	OHX	1	3870	7/7	0.07	-5.40	60,60,60,60	0
86	OHX	1	3899	7/7	0.07	-5.49	62,62,62,62	0
86	OHX	1	3929	7/7	0.07	-5.52	89,89,89,89	0
86	OHX	5	3918	7/7	0.10	-5.58	56,56,56,56	0
85	MG	5	3834	1/1	0.07	-5.58	57,57,57,57	0
86	OHX	1	3958	7/7	0.13	-5.68	103,103,103,103	0
86	OHX	1	3904	7/7	0.08	-5.89	87,87,87,87	0
86	OHX	1	3890	7/7	0.06	-6.13	61,61,61,61	0
86	OHX	2	2043	7/7	0.07	-6.21	100,100,100,100	0
86	OHX	1	3893	7/7	0.10	-6.26	74,74,74,74	0
86	OHX	2	2040	7/7	0.05	-6.34	92,92,92,92	0
86	OHX	6	2082	7/7	0.08	-6.39	115,115,115,115	0
86	OHX	5	3909	7/7	0.06	-6.40	58,58,58,58	0
86	OHX	2	2060	7/7	0.09	-6.46	122,122,122,122	0
86	OHX	5	3922	7/7	0.10	-6.65	79,79,79,79	0
86	OHX	5	3982	7/7	0.05	-6.70	76,76,76,76	0
86	OHX	1	3955	7/7	0.11	-6.82	104,104,104,104	0
86	OHX	1	3879	7/7	0.07	-6.85	63,63,63,63	0
86	OHX	5	3927	7/7	0.08	-6.92	80,80,80,80	0
86	OHX	6	2059	7/7	0.07	-7.01	83,83,83,83	0
86	OHX	1	3917	7/7	0.08	-7.02	87,87,87,87	0
86	OHX	1	3980	7/7	0.07	-7.03	75,75,75,75	0
85	MG	1	3604	1/1	0.07	-7.45	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	5	3913	7/7	0.07	-7.64	72,72,72,72	0
85	MG	2	1995	1/1	0.10	-8.27	70,70,70,70	0
86	OHX	1	3912	7/7	0.07	-8.41	83,83,83,83	0
86	OHX	1	3892	7/7	0.05	-8.82	69,69,69,69	0
86	OHX	1	3887	7/7	0.08	-9.24	67,67,67,67	0
86	OHX	5	3974	7/7	0.09	-9.39	86,86,86,86	0
85	MG	1	3801	1/1	0.07	-9.63	50,50,50,50	0
86	OHX	5	3917	7/7	0.05	-10.36	68,68,68,68	0
86	OHX	5	3957	7/7	0.08	-11.35	85,85,85,85	0
85	MG	5	3762	1/1	0.08	-11.62	51,51,51,51	0
86	OHX	1	3928	7/7	0.06	-11.90	85,85,85,85	0
86	OHX	1	3882	7/7	0.06	-15.66	58,58,58,58	0
86	OHX	5	3937	7/7	0.10	-16.38	84,84,84,84	0
86	OHX	5	3920	7/7	0.06	-20.60	76,76,76,76	0
86	OHX	5	3911	7/7	0.08	-29.80	69,69,69,69	0
85	MG	5	3833	1/1	0.07	-69.00	42,42,42,42	0
85	MG	6	2030	1/1	0.34	-	50,50,50,50	0
85	MG	1	3611	1/1	0.22	-	48,48,48,48	0
85	MG	1	3799	1/1	0.11	-	87,87,87,87	0
85	MG	1	3788	1/1	0.19	-	58,58,58,58	0
85	MG	1	3792	1/1	0.20	-	47,47,47,47	0
85	MG	2	1951	1/1	0.45	-	88,88,88,88	0
85	MG	o1	201	1/1	0.41	-	86,86,86,86	0
85	MG	1	3754	1/1	0.20	-	74,74,74,74	0
85	MG	L3	402	1/1	0.61	-	35,35,35,35	0
85	MG	1	3836	1/1	0.30	-	28,28,28,28	0
85	MG	1	3837	1/1	0.78	-	38,38,38,38	0
85	MG	5	3729	1/1	0.52	-	65,65,65,65	0
85	MG	5	3803	1/1	0.12	-	62,62,62,62	0
85	MG	6	2036	1/1	0.37	-	42,42,42,42	0
85	MG	2	1996	1/1	0.24	-	104,104,104,104	0
85	MG	5	3870	1/1	0.45	-	42,42,42,42	0
85	MG	6	1998	1/1	0.48	-	95,95,95,95	0
85	MG	5	3796	1/1	0.20	-	30,30,30,30	0
85	MG	8	201	1/1	0.29	-	62,62,62,62	0
85	MG	6	2039	1/1	0.28	-	40,40,40,40	0
85	MG	6	1924	1/1	0.95	-	117,117,117,117	0
85	MG	1	3847	1/1	0.53	-	35,35,35,35	0
85	MG	5	3615	1/1	0.44	-	27,27,27,27	0
85	MG	6	2026	1/1	0.34	-	56,56,56,56	0
85	MG	6	2037	1/1	0.32	-	72,72,72,72	0
85	MG	5	3676	1/1	0.15	-	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	1	3734	1/1	0.40	-	53,53,53,53	0
85	MG	5	3791	1/1	0.47	-	71,71,71,71	0

6.5 Other polymers ⓘ

There are no such residues in this entry.