



wwPDB X-ray Structure Validation Summary Report i

Oct 9, 2014 – 09:45 PM BST

PDB ID : 4U4O
Title : Crystal structure of Geneticin bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.60 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>

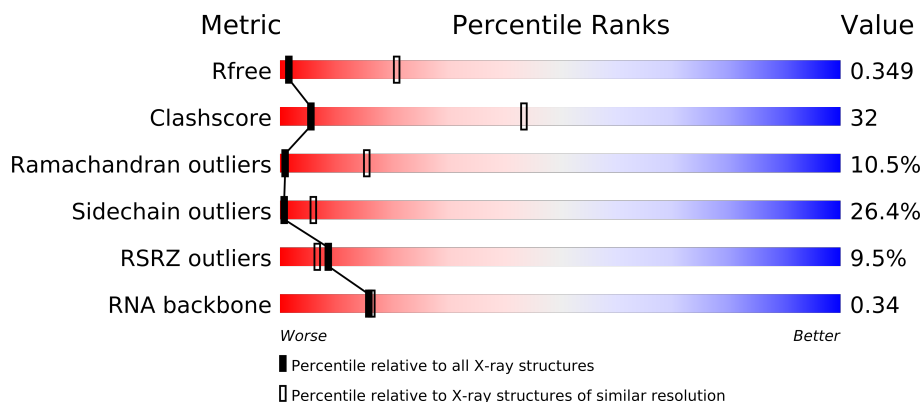
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.60 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	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)
RNA backbone	1838	1012 (4.40-2.76)

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	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	

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Mol	Chain	Length	Quality of chain
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	

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Mol	Chain	Length	Quality of chain
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	e1	76	
82	m2	160	
83	p0	311	
84	p1	47	
85	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
86	MG	1	3402	-	X
86	MG	1	3403	-	X
86	MG	1	3404	-	X
86	MG	1	3407	-	X
86	MG	1	3408	-	X
86	MG	1	3410	-	X
86	MG	1	3412	-	X
86	MG	1	3413	-	X
86	MG	1	3414	-	X
86	MG	1	3415	-	X
86	MG	1	3416	-	X
86	MG	1	3417	-	X
86	MG	1	3419	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3421	-	X
86	MG	1	3422	-	X
86	MG	1	3423	-	X
86	MG	1	3425	-	X
86	MG	1	3427	-	X
86	MG	1	3428	-	X
86	MG	1	3430	-	X
86	MG	1	3431	-	X
86	MG	1	3432	-	X
86	MG	1	3433	-	X
86	MG	1	3434	-	X
86	MG	1	3435	-	X
86	MG	1	3438	-	X
86	MG	1	3439	-	X
86	MG	1	3440	-	X
86	MG	1	3441	-	X
86	MG	1	3443	-	X
86	MG	1	3444	-	X
86	MG	1	3446	-	X
86	MG	1	3447	-	X
86	MG	1	3448	-	X
86	MG	1	3449	-	X
86	MG	1	3450	-	X
86	MG	1	3451	-	X
86	MG	1	3452	-	X
86	MG	1	3453	-	X
86	MG	1	3454	-	X
86	MG	1	3456	-	X
86	MG	1	3457	-	X
86	MG	1	3458	-	X
86	MG	1	3459	-	X
86	MG	1	3460	-	X
86	MG	1	3461	-	X
86	MG	1	3462	-	X
86	MG	1	3463	-	X
86	MG	1	3465	-	X
86	MG	1	3468	-	X
86	MG	1	3469	-	X
86	MG	1	3470	-	X
86	MG	1	3473	-	X
86	MG	1	3475	-	X
86	MG	1	3476	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3478	-	X
86	MG	1	3479	-	X
86	MG	1	3480	-	X
86	MG	1	3483	-	X
86	MG	1	3484	-	X
86	MG	1	3485	-	X
86	MG	1	3486	-	X
86	MG	1	3488	-	X
86	MG	1	3490	-	X
86	MG	1	3491	-	X
86	MG	1	3492	-	X
86	MG	1	3493	-	X
86	MG	1	3496	-	X
86	MG	1	3498	-	X
86	MG	1	3500	-	X
86	MG	1	3501	-	X
86	MG	1	3502	-	X
86	MG	1	3503	-	X
86	MG	1	3504	-	X
86	MG	1	3505	-	X
86	MG	1	3506	-	X
86	MG	1	3508	-	X
86	MG	1	3509	-	X
86	MG	1	3511	-	X
86	MG	1	3512	-	X
86	MG	1	3513	-	X
86	MG	1	3514	-	X
86	MG	1	3515	-	X
86	MG	1	3516	-	X
86	MG	1	3517	-	X
86	MG	1	3518	-	X
86	MG	1	3519	-	X
86	MG	1	3520	-	X
86	MG	1	3522	-	X
86	MG	1	3523	-	X
86	MG	1	3524	-	X
86	MG	1	3525	-	X
86	MG	1	3526	-	X
86	MG	1	3527	-	X
86	MG	1	3528	-	X
86	MG	1	3529	-	X
86	MG	1	3530	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3531	-	X
86	MG	1	3532	-	X
86	MG	1	3533	-	X
86	MG	1	3534	-	X
86	MG	1	3535	-	X
86	MG	1	3537	-	X
86	MG	1	3538	-	X
86	MG	1	3539	-	X
86	MG	1	3540	-	X
86	MG	1	3541	-	X
86	MG	1	3542	-	X
86	MG	1	3543	-	X
86	MG	1	3544	-	X
86	MG	1	3545	-	X
86	MG	1	3546	-	X
86	MG	1	3547	-	X
86	MG	1	3548	-	X
86	MG	1	3549	-	X
86	MG	1	3550	-	X
86	MG	1	3552	-	X
86	MG	1	3553	-	X
86	MG	1	3554	-	X
86	MG	1	3555	-	X
86	MG	1	3556	-	X
86	MG	1	3557	-	X
86	MG	1	3559	-	X
86	MG	1	3560	-	X
86	MG	1	3562	-	X
86	MG	1	3563	-	X
86	MG	1	3564	-	X
86	MG	1	3565	-	X
86	MG	1	3567	-	X
86	MG	1	3568	-	X
86	MG	1	3569	-	X
86	MG	1	3570	-	X
86	MG	1	3571	-	X
86	MG	1	3572	-	X
86	MG	1	3573	-	X
86	MG	1	3574	-	X
86	MG	1	3575	-	X
86	MG	1	3576	-	X
86	MG	1	3577	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3578	-	X
86	MG	1	3580	-	X
86	MG	1	3581	-	X
86	MG	1	3583	-	X
86	MG	1	3584	-	X
86	MG	1	3585	-	X
86	MG	1	3586	-	X
86	MG	1	3587	-	X
86	MG	1	3588	-	X
86	MG	1	3589	-	X
86	MG	1	3590	-	X
86	MG	1	3591	-	X
86	MG	1	3593	-	X
86	MG	1	3594	-	X
86	MG	1	3595	-	X
86	MG	1	3596	-	X
86	MG	1	3597	-	X
86	MG	1	3598	-	X
86	MG	1	3599	-	X
86	MG	1	3603	-	X
86	MG	1	3604	-	X
86	MG	1	3605	-	X
86	MG	1	3607	-	X
86	MG	1	3609	-	X
86	MG	1	3611	-	X
86	MG	1	3612	-	X
86	MG	1	3613	-	X
86	MG	1	3615	-	X
86	MG	1	3618	-	X
86	MG	1	3619	-	X
86	MG	1	3620	-	X
86	MG	1	3621	-	X
86	MG	1	3624	-	X
86	MG	1	3625	-	X
86	MG	1	3626	-	X
86	MG	1	3628	-	X
86	MG	1	3629	-	X
86	MG	1	3630	-	X
86	MG	1	3632	-	X
86	MG	1	3633	-	X
86	MG	1	3636	-	X
86	MG	1	3639	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3641	-	X
86	MG	1	3642	-	X
86	MG	1	3645	-	X
86	MG	1	3646	-	X
86	MG	1	3647	-	X
86	MG	1	3648	-	X
86	MG	1	3649	-	X
86	MG	1	3650	-	X
86	MG	1	3651	-	X
86	MG	1	3652	-	X
86	MG	1	3653	-	X
86	MG	1	3654	-	X
86	MG	1	3655	-	X
86	MG	1	3656	-	X
86	MG	1	3657	-	X
86	MG	1	3658	-	X
86	MG	1	3661	-	X
86	MG	1	3663	-	X
86	MG	1	3665	-	X
86	MG	1	3666	-	X
86	MG	1	3667	-	X
86	MG	1	3668	-	X
86	MG	1	3669	-	X
86	MG	1	3671	-	X
86	MG	1	3672	-	X
86	MG	1	3673	-	X
86	MG	1	3674	-	X
86	MG	1	3675	-	X
86	MG	1	3676	-	X
86	MG	1	3677	-	X
86	MG	1	3678	-	X
86	MG	1	3679	-	X
86	MG	1	3680	-	X
86	MG	1	3681	-	X
86	MG	1	3682	-	X
86	MG	1	3684	-	X
86	MG	1	3687	-	X
86	MG	1	3688	-	X
86	MG	1	3689	-	X
86	MG	1	3690	-	X
86	MG	1	3691	-	X
86	MG	1	3692	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3693	-	X
86	MG	1	3696	-	X
86	MG	1	3697	-	X
86	MG	1	3699	-	X
86	MG	1	3700	-	X
86	MG	1	3701	-	X
86	MG	1	3702	-	X
86	MG	1	3704	-	X
86	MG	1	3706	-	X
86	MG	1	3711	-	X
86	MG	1	3712	-	X
86	MG	1	3713	-	X
86	MG	1	3714	-	X
86	MG	1	3716	-	X
86	MG	1	3717	-	X
86	MG	1	3718	-	X
86	MG	1	3719	-	X
86	MG	1	3720	-	X
86	MG	1	3721	-	X
86	MG	1	3722	-	X
86	MG	1	3726	-	X
86	MG	1	3727	-	X
86	MG	1	3729	-	X
86	MG	1	3730	-	X
86	MG	1	3731	-	X
86	MG	1	3732	-	X
86	MG	1	3733	-	X
86	MG	1	3735	-	X
86	MG	1	3736	-	X
86	MG	1	3738	-	X
86	MG	1	3739	-	X
86	MG	1	3740	-	X
86	MG	1	3742	-	X
86	MG	1	3743	-	X
86	MG	1	3744	-	X
86	MG	1	3746	-	X
86	MG	1	3749	-	X
86	MG	1	3750	-	X
86	MG	1	3751	-	X
86	MG	1	3752	-	X
86	MG	1	3753	-	X
86	MG	1	3754	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3756	-	X
86	MG	1	3758	-	X
86	MG	1	3759	-	X
86	MG	1	3760	-	X
86	MG	1	3761	-	X
86	MG	1	3762	-	X
86	MG	1	3763	-	X
86	MG	1	3764	-	X
86	MG	1	3765	-	X
86	MG	1	3766	-	X
86	MG	1	3768	-	X
86	MG	1	3770	-	X
86	MG	1	3771	-	X
86	MG	1	3772	-	X
86	MG	1	3773	-	X
86	MG	1	3774	-	X
86	MG	1	3776	-	X
86	MG	1	3777	-	X
86	MG	1	3778	-	X
86	MG	1	3779	-	X
86	MG	1	3781	-	X
86	MG	1	3782	-	X
86	MG	1	3783	-	X
86	MG	1	3784	-	X
86	MG	1	3785	-	X
86	MG	1	3786	-	X
86	MG	1	3787	-	X
86	MG	1	3789	-	X
86	MG	1	3791	-	X
86	MG	1	3793	-	X
86	MG	1	3794	-	X
86	MG	1	3795	-	X
86	MG	1	3796	-	X
86	MG	1	3797	-	X
86	MG	1	3798	-	X
86	MG	1	3802	-	X
86	MG	1	3805	-	X
86	MG	1	3807	-	X
86	MG	1	3808	-	X
86	MG	1	3810	-	X
86	MG	1	3811	-	X
86	MG	1	3812	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3813	-	X
86	MG	1	3814	-	X
86	MG	1	3815	-	X
86	MG	1	3816	-	X
86	MG	1	3817	-	X
86	MG	1	3818	-	X
86	MG	1	3819	-	X
86	MG	1	3821	-	X
86	MG	1	3822	-	X
86	MG	1	3823	-	X
86	MG	1	3824	-	X
86	MG	1	3826	-	X
86	MG	1	3827	-	X
86	MG	1	3828	-	X
86	MG	1	3829	-	X
86	MG	1	3831	-	X
86	MG	1	3832	-	X
86	MG	1	3833	-	X
86	MG	1	3834	-	X
86	MG	1	3835	-	X
86	MG	1	3838	-	X
86	MG	1	3839	-	X
86	MG	1	3841	-	X
86	MG	1	3843	-	X
86	MG	1	3844	-	X
86	MG	1	3845	-	X
86	MG	1	3846	-	X
86	MG	1	3848	-	X
86	MG	1	3849	-	X
86	MG	1	3850	-	X
86	MG	1	3851	-	X
86	MG	1	3852	-	X
86	MG	1	3853	-	X
86	MG	1	3855	-	X
86	MG	1	3856	-	X
86	MG	1	3857	-	X
86	MG	1	3860	-	X
86	MG	1	3861	-	X
86	MG	1	3862	-	X
86	MG	1	3863	-	X
86	MG	1	3864	-	X
86	MG	1	3865	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	4213	-	X
86	MG	1	4214	-	X
86	MG	1	4215	-	X
86	MG	2	1902	-	X
86	MG	2	1903	-	X
86	MG	2	1904	-	X
86	MG	2	1905	-	X
86	MG	2	1908	-	X
86	MG	2	1910	-	X
86	MG	2	1912	-	X
86	MG	2	1913	-	X
86	MG	2	1914	-	X
86	MG	2	1916	-	X
86	MG	2	1917	-	X
86	MG	2	1918	-	X
86	MG	2	1919	-	X
86	MG	2	1921	-	X
86	MG	2	1922	-	X
86	MG	2	1923	-	X
86	MG	2	1926	-	X
86	MG	2	1927	-	X
86	MG	2	1928	-	X
86	MG	2	1930	-	X
86	MG	2	1933	-	X
86	MG	2	1935	-	X
86	MG	2	1937	-	X
86	MG	2	1939	-	X
86	MG	2	1941	-	X
86	MG	2	1942	-	X
86	MG	2	1943	-	X
86	MG	2	1944	-	X
86	MG	2	1945	-	X
86	MG	2	1946	-	X
86	MG	2	1947	-	X
86	MG	2	1956	-	X
86	MG	2	1957	-	X
86	MG	2	1958	-	X
86	MG	2	1960	-	X
86	MG	2	1962	-	X
86	MG	2	1966	-	X
86	MG	2	1967	-	X
86	MG	2	1969	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	2	1970	-	X
86	MG	2	1973	-	X
86	MG	2	1974	-	X
86	MG	2	1976	-	X
86	MG	2	1978	-	X
86	MG	2	1979	-	X
86	MG	2	1981	-	X
86	MG	2	1982	-	X
86	MG	2	1983	-	X
86	MG	2	1984	-	X
86	MG	2	1985	-	X
86	MG	2	1986	-	X
86	MG	2	1988	-	X
86	MG	2	1990	-	X
86	MG	2	1992	-	X
86	MG	2	1994	-	X
86	MG	2	1995	-	X
86	MG	2	1997	-	X
86	MG	2	1999	-	X
86	MG	2	2001	-	X
86	MG	2	2002	-	X
86	MG	2	2004	-	X
86	MG	2	2006	-	X
86	MG	2	2007	-	X
86	MG	2	2009	-	X
86	MG	2	2010	-	X
86	MG	2	2011	-	X
86	MG	2	2014	-	X
86	MG	2	2015	-	X
86	MG	2	2016	-	X
86	MG	2	2017	-	X
86	MG	2	2018	-	X
86	MG	2	2019	-	X
86	MG	2	2020	-	X
86	MG	2	2023	-	X
86	MG	3	202	-	X
86	MG	3	204	-	X
86	MG	3	205	-	X
86	MG	3	206	-	X
86	MG	3	208	-	X
86	MG	3	210	-	X
86	MG	3	212	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	4	201	-	X
86	MG	4	202	-	X
86	MG	4	203	-	X
86	MG	4	204	-	X
86	MG	4	206	-	X
86	MG	4	207	-	X
86	MG	4	208	-	X
86	MG	4	210	-	X
86	MG	4	211	-	X
86	MG	4	213	-	X
86	MG	4	214	-	X
86	MG	4	215	-	X
86	MG	4	217	-	X
86	MG	4	219	-	X
86	MG	4	220	-	X
86	MG	4	221	-	X
86	MG	4	222	-	X
86	MG	5	3403	-	X
86	MG	5	3404	-	X
86	MG	5	3405	-	X
86	MG	5	3406	-	X
86	MG	5	3407	-	X
86	MG	5	3408	-	X
86	MG	5	3409	-	X
86	MG	5	3410	-	X
86	MG	5	3411	-	X
86	MG	5	3412	-	X
86	MG	5	3414	-	X
86	MG	5	3416	-	X
86	MG	5	3418	-	X
86	MG	5	3420	-	X
86	MG	5	3424	-	X
86	MG	5	3425	-	X
86	MG	5	3426	-	X
86	MG	5	3427	-	X
86	MG	5	3428	-	X
86	MG	5	3430	-	X
86	MG	5	3431	-	X
86	MG	5	3432	-	X
86	MG	5	3433	-	X
86	MG	5	3434	-	X
86	MG	5	3435	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3439	-	X
86	MG	5	3440	-	X
86	MG	5	3441	-	X
86	MG	5	3442	-	X
86	MG	5	3443	-	X
86	MG	5	3444	-	X
86	MG	5	3445	-	X
86	MG	5	3447	-	X
86	MG	5	3449	-	X
86	MG	5	3450	-	X
86	MG	5	3451	-	X
86	MG	5	3452	-	X
86	MG	5	3454	-	X
86	MG	5	3455	-	X
86	MG	5	3457	-	X
86	MG	5	3458	-	X
86	MG	5	3459	-	X
86	MG	5	3461	-	X
86	MG	5	3464	-	X
86	MG	5	3465	-	X
86	MG	5	3467	-	X
86	MG	5	3468	-	X
86	MG	5	3469	-	X
86	MG	5	3470	-	X
86	MG	5	3471	-	X
86	MG	5	3473	-	X
86	MG	5	3474	-	X
86	MG	5	3475	-	X
86	MG	5	3476	-	X
86	MG	5	3481	-	X
86	MG	5	3482	-	X
86	MG	5	3484	-	X
86	MG	5	3485	-	X
86	MG	5	3486	-	X
86	MG	5	3487	-	X
86	MG	5	3488	-	X
86	MG	5	3489	-	X
86	MG	5	3491	-	X
86	MG	5	3493	-	X
86	MG	5	3494	-	X
86	MG	5	3495	-	X
86	MG	5	3496	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3497	-	X
86	MG	5	3498	-	X
86	MG	5	3499	-	X
86	MG	5	3500	-	X
86	MG	5	3501	-	X
86	MG	5	3503	-	X
86	MG	5	3504	-	X
86	MG	5	3505	-	X
86	MG	5	3506	-	X
86	MG	5	3507	-	X
86	MG	5	3509	-	X
86	MG	5	3510	-	X
86	MG	5	3511	-	X
86	MG	5	3513	-	X
86	MG	5	3514	-	X
86	MG	5	3515	-	X
86	MG	5	3516	-	X
86	MG	5	3517	-	X
86	MG	5	3518	-	X
86	MG	5	3519	-	X
86	MG	5	3520	-	X
86	MG	5	3521	-	X
86	MG	5	3522	-	X
86	MG	5	3523	-	X
86	MG	5	3524	-	X
86	MG	5	3525	-	X
86	MG	5	3526	-	X
86	MG	5	3528	-	X
86	MG	5	3529	-	X
86	MG	5	3530	-	X
86	MG	5	3531	-	X
86	MG	5	3532	-	X
86	MG	5	3534	-	X
86	MG	5	3535	-	X
86	MG	5	3536	-	X
86	MG	5	3537	-	X
86	MG	5	3538	-	X
86	MG	5	3539	-	X
86	MG	5	3540	-	X
86	MG	5	3541	-	X
86	MG	5	3544	-	X
86	MG	5	3545	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3546	-	X
86	MG	5	3547	-	X
86	MG	5	3548	-	X
86	MG	5	3549	-	X
86	MG	5	3551	-	X
86	MG	5	3552	-	X
86	MG	5	3553	-	X
86	MG	5	3554	-	X
86	MG	5	3555	-	X
86	MG	5	3557	-	X
86	MG	5	3559	-	X
86	MG	5	3560	-	X
86	MG	5	3561	-	X
86	MG	5	3562	-	X
86	MG	5	3563	-	X
86	MG	5	3564	-	X
86	MG	5	3565	-	X
86	MG	5	3566	-	X
86	MG	5	3567	-	X
86	MG	5	3568	-	X
86	MG	5	3569	-	X
86	MG	5	3570	-	X
86	MG	5	3571	-	X
86	MG	5	3572	-	X
86	MG	5	3573	-	X
86	MG	5	3574	-	X
86	MG	5	3575	-	X
86	MG	5	3576	-	X
86	MG	5	3578	-	X
86	MG	5	3580	-	X
86	MG	5	3581	-	X
86	MG	5	3582	-	X
86	MG	5	3583	-	X
86	MG	5	3584	-	X
86	MG	5	3585	-	X
86	MG	5	3586	-	X
86	MG	5	3587	-	X
86	MG	5	3588	-	X
86	MG	5	3589	-	X
86	MG	5	3590	-	X
86	MG	5	3593	-	X
86	MG	5	3594	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3595	-	X
86	MG	5	3597	-	X
86	MG	5	3598	-	X
86	MG	5	3600	-	X
86	MG	5	3601	-	X
86	MG	5	3602	-	X
86	MG	5	3603	-	X
86	MG	5	3604	-	X
86	MG	5	3605	-	X
86	MG	5	3606	-	X
86	MG	5	3608	-	X
86	MG	5	3610	-	X
86	MG	5	3614	-	X
86	MG	5	3616	-	X
86	MG	5	3617	-	X
86	MG	5	3619	-	X
86	MG	5	3621	-	X
86	MG	5	3622	-	X
86	MG	5	3623	-	X
86	MG	5	3624	-	X
86	MG	5	3625	-	X
86	MG	5	3626	-	X
86	MG	5	3627	-	X
86	MG	5	3628	-	X
86	MG	5	3629	-	X
86	MG	5	3634	-	X
86	MG	5	3635	-	X
86	MG	5	3636	-	X
86	MG	5	3637	-	X
86	MG	5	3639	-	X
86	MG	5	3640	-	X
86	MG	5	3641	-	X
86	MG	5	3642	-	X
86	MG	5	3643	-	X
86	MG	5	3644	-	X
86	MG	5	3645	-	X
86	MG	5	3646	-	X
86	MG	5	3647	-	X
86	MG	5	3648	-	X
86	MG	5	3649	-	X
86	MG	5	3650	-	X
86	MG	5	3651	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3653	-	X
86	MG	5	3654	-	X
86	MG	5	3655	-	X
86	MG	5	3656	-	X
86	MG	5	3657	-	X
86	MG	5	3658	-	X
86	MG	5	3659	-	X
86	MG	5	3660	-	X
86	MG	5	3661	-	X
86	MG	5	3664	-	X
86	MG	5	3665	-	X
86	MG	5	3666	-	X
86	MG	5	3667	-	X
86	MG	5	3669	-	X
86	MG	5	3670	-	X
86	MG	5	3671	-	X
86	MG	5	3672	-	X
86	MG	5	3673	-	X
86	MG	5	3674	-	X
86	MG	5	3675	-	X
86	MG	5	3676	-	X
86	MG	5	3677	-	X
86	MG	5	3678	-	X
86	MG	5	3679	-	X
86	MG	5	3680	-	X
86	MG	5	3683	-	X
86	MG	5	3684	-	X
86	MG	5	3685	-	X
86	MG	5	3687	-	X
86	MG	5	3688	-	X
86	MG	5	3689	-	X
86	MG	5	3690	-	X
86	MG	5	3691	-	X
86	MG	5	3694	-	X
86	MG	5	3695	-	X
86	MG	5	3697	-	X
86	MG	5	3699	-	X
86	MG	5	3701	-	X
86	MG	5	3702	-	X
86	MG	5	3703	-	X
86	MG	5	3704	-	X
86	MG	5	3705	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3707	-	X
86	MG	5	3708	-	X
86	MG	5	3709	-	X
86	MG	5	3711	-	X
86	MG	5	3712	-	X
86	MG	5	3713	-	X
86	MG	5	3714	-	X
86	MG	5	3717	-	X
86	MG	5	3718	-	X
86	MG	5	3720	-	X
86	MG	5	3723	-	X
86	MG	5	3724	-	X
86	MG	5	3725	-	X
86	MG	5	3726	-	X
86	MG	5	3727	-	X
86	MG	5	3728	-	X
86	MG	5	3729	-	X
86	MG	5	3730	-	X
86	MG	5	3731	-	X
86	MG	5	3733	-	X
86	MG	5	3734	-	X
86	MG	5	3735	-	X
86	MG	5	3736	-	X
86	MG	5	3737	-	X
86	MG	5	3739	-	X
86	MG	5	3741	-	X
86	MG	5	3742	-	X
86	MG	5	3745	-	X
86	MG	5	3746	-	X
86	MG	5	3748	-	X
86	MG	5	3749	-	X
86	MG	5	3750	-	X
86	MG	5	3752	-	X
86	MG	5	3753	-	X
86	MG	5	3754	-	X
86	MG	5	3755	-	X
86	MG	5	3756	-	X
86	MG	5	3757	-	X
86	MG	5	3759	-	X
86	MG	5	3760	-	X
86	MG	5	3762	-	X
86	MG	5	3764	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3765	-	X
86	MG	5	3767	-	X
86	MG	5	3771	-	X
86	MG	5	3772	-	X
86	MG	5	3773	-	X
86	MG	5	3774	-	X
86	MG	5	3775	-	X
86	MG	5	3777	-	X
86	MG	5	3779	-	X
86	MG	5	3780	-	X
86	MG	5	3783	-	X
86	MG	5	3784	-	X
86	MG	5	3785	-	X
86	MG	5	3786	-	X
86	MG	5	3787	-	X
86	MG	5	3790	-	X
86	MG	5	3792	-	X
86	MG	5	3793	-	X
86	MG	5	3794	-	X
86	MG	5	3797	-	X
86	MG	5	3798	-	X
86	MG	5	3799	-	X
86	MG	5	3800	-	X
86	MG	5	3801	-	X
86	MG	5	3802	-	X
86	MG	5	3803	-	X
86	MG	5	3805	-	X
86	MG	5	3806	-	X
86	MG	5	3807	-	X
86	MG	5	3808	-	X
86	MG	5	3809	-	X
86	MG	5	3812	-	X
86	MG	5	3814	-	X
86	MG	5	3816	-	X
86	MG	5	3817	-	X
86	MG	5	3818	-	X
86	MG	5	3819	-	X
86	MG	5	3821	-	X
86	MG	5	3822	-	X
86	MG	5	3823	-	X
86	MG	5	3824	-	X
86	MG	5	3828	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3829	-	X
86	MG	5	3830	-	X
86	MG	5	3831	-	X
86	MG	5	3832	-	X
86	MG	5	3833	-	X
86	MG	5	3835	-	X
86	MG	5	3837	-	X
86	MG	5	3840	-	X
86	MG	5	3841	-	X
86	MG	5	3842	-	X
86	MG	5	3843	-	X
86	MG	5	3845	-	X
86	MG	5	3847	-	X
86	MG	5	3848	-	X
86	MG	5	3850	-	X
86	MG	5	3853	-	X
86	MG	5	3854	-	X
86	MG	5	3856	-	X
86	MG	5	3857	-	X
86	MG	5	3858	-	X
86	MG	5	3859	-	X
86	MG	5	3860	-	X
86	MG	5	3862	-	X
86	MG	5	3863	-	X
86	MG	5	3864	-	X
86	MG	5	3865	-	X
86	MG	5	3866	-	X
86	MG	5	3867	-	X
86	MG	5	3868	-	X
86	MG	5	3869	-	X
86	MG	5	3870	-	X
86	MG	5	3871	-	X
86	MG	5	3873	-	X
86	MG	5	3874	-	X
86	MG	5	3875	-	X
86	MG	5	3876	-	X
86	MG	5	3877	-	X
86	MG	5	3878	-	X
86	MG	5	3879	-	X
86	MG	5	3880	-	X
86	MG	5	3881	-	X
86	MG	5	3882	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3883	-	X
86	MG	5	3885	-	X
86	MG	5	3886	-	X
86	MG	5	3893	-	X
86	MG	5	4247	-	X
86	MG	5	4248	-	X
86	MG	5	4249	-	X
86	MG	5	4250	-	X
86	MG	5	4252	-	X
86	MG	6	1901	-	X
86	MG	6	1903	-	X
86	MG	6	1905	-	X
86	MG	6	1908	-	X
86	MG	6	1911	-	X
86	MG	6	1912	-	X
86	MG	6	1913	-	X
86	MG	6	1914	-	X
86	MG	6	1916	-	X
86	MG	6	1917	-	X
86	MG	6	1918	-	X
86	MG	6	1921	-	X
86	MG	6	1922	-	X
86	MG	6	1923	-	X
86	MG	6	1926	-	X
86	MG	6	1927	-	X
86	MG	6	1929	-	X
86	MG	6	1930	-	X
86	MG	6	1932	-	X
86	MG	6	1934	-	X
86	MG	6	1937	-	X
86	MG	6	1938	-	X
86	MG	6	1939	-	X
86	MG	6	1941	-	X
86	MG	6	1942	-	X
86	MG	6	1943	-	X
86	MG	6	1944	-	X
86	MG	6	1945	-	X
86	MG	6	1946	-	X
86	MG	6	1948	-	X
86	MG	6	1949	-	X
86	MG	6	1950	-	X
86	MG	6	1951	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	6	1954	-	X
86	MG	6	1957	-	X
86	MG	6	1958	-	X
86	MG	6	1960	-	X
86	MG	6	1962	-	X
86	MG	6	1963	-	X
86	MG	6	1964	-	X
86	MG	6	1965	-	X
86	MG	6	1967	-	X
86	MG	6	1969	-	X
86	MG	6	1970	-	X
86	MG	6	1971	-	X
86	MG	6	1972	-	X
86	MG	6	1973	-	X
86	MG	6	1974	-	X
86	MG	6	1975	-	X
86	MG	6	1976	-	X
86	MG	6	1977	-	X
86	MG	6	1978	-	X
86	MG	6	1980	-	X
86	MG	6	1982	-	X
86	MG	6	1983	-	X
86	MG	6	1984	-	X
86	MG	6	1985	-	X
86	MG	6	1988	-	X
86	MG	6	1989	-	X
86	MG	6	1995	-	X
86	MG	6	1996	-	X
86	MG	6	1997	-	X
86	MG	6	1998	-	X
86	MG	6	2000	-	X
86	MG	6	2001	-	X
86	MG	6	2003	-	X
86	MG	6	2009	-	X
86	MG	6	2011	-	X
86	MG	6	2012	-	X
86	MG	6	2013	-	X
86	MG	6	2014	-	X
86	MG	6	2016	-	X
86	MG	6	2017	-	X
86	MG	6	2020	-	X
86	MG	6	2021	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	6	2022	-	X
86	MG	6	2024	-	X
86	MG	6	2025	-	X
86	MG	6	2027	-	X
86	MG	6	2029	-	X
86	MG	6	2031	-	X
86	MG	6	2032	-	X
86	MG	6	2033	-	X
86	MG	6	2034	-	X
86	MG	6	2035	-	X
86	MG	6	2036	-	X
86	MG	6	2037	-	X
86	MG	6	2038	-	X
86	MG	6	2039	-	X
86	MG	6	2040	-	X
86	MG	6	2043	-	X
86	MG	6	2044	-	X
86	MG	6	2045	-	X
86	MG	6	2046	-	X
86	MG	6	2049	-	X
86	MG	7	202	-	X
86	MG	7	203	-	X
86	MG	7	204	-	X
86	MG	7	205	-	X
86	MG	7	206	-	X
86	MG	7	207	-	X
86	MG	7	208	-	X
86	MG	7	210	-	X
86	MG	7	211	-	X
86	MG	7	212	-	X
86	MG	7	215	-	X
86	MG	8	202	-	X
86	MG	8	203	-	X
86	MG	8	204	-	X
86	MG	8	205	-	X
86	MG	8	206	-	X
86	MG	8	207	-	X
86	MG	8	209	-	X
86	MG	8	211	-	X
86	MG	8	212	-	X
86	MG	8	214	-	X
86	MG	8	215	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	8	216	-	X
86	MG	8	217	-	X
86	MG	D3	201	-	X
86	MG	D4	201	-	X
86	MG	L3	402	-	X
86	MG	L4	402	-	X
86	MG	L6	201	-	X
86	MG	L6	202	-	X
86	MG	L7	302	-	X
86	MG	L8	301	-	X
86	MG	M0	302	-	X
86	MG	M0	303	-	X
86	MG	M3	201	-	X
86	MG	M5	301	-	X
86	MG	M5	302	-	X
86	MG	M7	202	-	X
86	MG	M7	203	-	X
86	MG	M7	204	-	X
86	MG	N3	201	-	X
86	MG	N5	201	-	X
86	MG	N8	203	-	X
86	MG	N8	204	-	X
86	MG	N9	101	-	X
86	MG	O1	201	-	X
86	MG	O3	201	-	X
86	MG	O5	201	-	X
86	MG	O7	102	-	X
86	MG	SM	301	-	X
86	MG	l3	401	-	X
86	MG	l3	402	-	X
86	MG	l3	403	-	X
86	MG	l3	405	-	X
86	MG	l3	406	-	X
86	MG	l7	301	-	X
86	MG	m0	301	-	X
86	MG	m1	201	-	X
86	MG	m4	201	-	X
86	MG	m5	301	-	X
86	MG	m5	302	-	X
86	MG	m6	201	-	X
86	MG	m7	201	-	X
86	MG	m7	202	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	m7	203	-	X
86	MG	m7	204	-	X
86	MG	n3	201	-	X
86	MG	n4	201	-	X
86	MG	n8	201	-	X
86	MG	n8	202	-	X
86	MG	n9	101	-	X
86	MG	n9	102	-	X
86	MG	o1	201	-	X
86	MG	o2	201	-	X
86	MG	o3	201	-	X
86	MG	o3	202	-	X
86	MG	o4	201	-	X
86	MG	q0	203	-	X
86	MG	q1	101	-	X
86	MG	q3	503	-	X
86	MG	s8	302	-	X
87	OHX	1	3866	-	X
87	OHX	1	3872	-	X
87	OHX	1	3887	-	X
87	OHX	1	3891	-	X
87	OHX	1	3897	-	X
87	OHX	1	3946	-	X
87	OHX	1	4025	-	X
87	OHX	1	4056	-	X
87	OHX	1	4061	-	X
87	OHX	1	4092	-	X
87	OHX	1	4098	-	X
87	OHX	1	4112	-	X
87	OHX	1	4116	-	X
87	OHX	1	4123	-	X
87	OHX	1	4131	-	X
87	OHX	1	4136	-	X
87	OHX	1	4137	-	X
87	OHX	1	4138	-	X
87	OHX	1	4168	-	X
87	OHX	1	4169	-	X
87	OHX	1	4170	-	X
87	OHX	1	4175	-	X
87	OHX	1	4176	-	X
87	OHX	1	4178	-	X
87	OHX	1	4186	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	OHX	1	4189	-	X
87	OHX	1	4195	-	X
87	OHX	1	4199	-	X
87	OHX	1	4202	-	X
87	OHX	1	4203	-	X
87	OHX	1	4205	-	X
87	OHX	1	4206	-	X
87	OHX	1	4208	-	X
87	OHX	1	4209	-	X
87	OHX	1	4212	-	X
87	OHX	2	2108	-	X
87	OHX	2	2113	-	X
87	OHX	2	2149	-	X
87	OHX	2	2159	-	X
87	OHX	2	2160	-	X
87	OHX	2	2162	-	X
87	OHX	3	222	-	X
87	OHX	3	224	-	X
87	OHX	4	233	-	X
87	OHX	5	3895	-	X
87	OHX	5	3896	-	X
87	OHX	5	3899	-	X
87	OHX	5	3901	-	X
87	OHX	5	3905	-	X
87	OHX	5	3907	-	X
87	OHX	5	3939	-	X
87	OHX	5	3989	-	X
87	OHX	5	4068	-	X
87	OHX	5	4076	-	X
87	OHX	5	4091	-	X
87	OHX	5	4116	-	X
87	OHX	5	4123	-	X
87	OHX	5	4128	-	X
87	OHX	5	4134	-	X
87	OHX	5	4141	-	X
87	OHX	5	4144	-	X
87	OHX	5	4149	-	X
87	OHX	5	4151	-	X
87	OHX	5	4153	-	X
87	OHX	5	4173	-	X
87	OHX	5	4176	-	X
87	OHX	5	4178	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	OHX	5	4179	-	X
87	OHX	5	4182	-	X
87	OHX	5	4183	-	X
87	OHX	5	4188	-	X
87	OHX	5	4191	-	X
87	OHX	5	4196	-	X
87	OHX	5	4197	-	X
87	OHX	5	4198	-	X
87	OHX	5	4199	-	X
87	OHX	5	4216	-	X
87	OHX	5	4223	-	X
87	OHX	5	4224	-	X
87	OHX	5	4226	-	X
87	OHX	5	4229	-	X
87	OHX	5	4231	-	X
87	OHX	5	4244	-	X
87	OHX	6	2052	-	X
87	OHX	6	2057	-	X
87	OHX	6	2058	-	X
87	OHX	6	2113	-	X
87	OHX	6	2131	-	X
87	OHX	6	2170	-	X
87	OHX	6	2180	-	X
87	OHX	6	2183	-	X
87	OHX	6	2185	-	X
87	OHX	6	2193	-	X
87	OHX	6	2198	-	X
87	OHX	7	225	-	X
87	OHX	7	226	-	X
87	OHX	8	226	-	X
87	OHX	8	233	-	X
87	OHX	8	234	-	X
87	OHX	14	403	-	X
87	OHX	15	306	-	X
87	OHX	15	307	-	X

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411095 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	1791	Total	C	N	O	P	0	0	0
			38149	17055	6738	12565	1791			

- 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			

- 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
			679	402	140	137				

- Molecule 36 is a RNA chain called TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

- Molecule 37 is a RNA chain called TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

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

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	110	GLU	-	expression tag	UNP P87262

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Chain	Residue	Modelled	Actual	Comment	Reference
O4	111	ALA	-	expression tag	UNP P87262
O4	112	ALA	-	expression tag	UNP P87262
O4	113	LYS	-	expression tag	UNP P87262
O4	114	SER	-	expression tag	UNP P87262
O4	115	GLU	-	expression tag	UNP P87262
O4	116	LYS	-	expression tag	UNP P87262
O4	117	LYS	-	expression tag	UNP P87262
O4	118	ALA	-	expression tag	UNP P87262
O4	119	LYS	-	expression tag	UNP P87262
O4	120	LYS	-	expression tag	UNP P87262
o4	110	GLU	-	expression tag	UNP P87262
o4	111	ALA	-	expression tag	UNP P87262
o4	112	ALA	-	expression tag	UNP P87262
o4	113	LYS	-	expression tag	UNP P87262
o4	114	SER	-	expression tag	UNP P87262
o4	115	GLU	-	expression tag	UNP P87262
o4	116	LYS	-	expression tag	UNP P87262
o4	117	LYS	-	expression tag	UNP P87262
o4	118	ALA	-	expression tag	UNP P87262
o4	119	LYS	-	expression tag	UNP P87262
o4	120	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	S	0	0	0
			612	391	115	106				
74	o8	77	Total	C	N	O	S	0	0	0
			608	388	114	106				

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 Ubiquitin-40S ribosomal protein S31.

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

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

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

- Molecule 84 is a protein called unknown protein chain p1.

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

- Molecule 85 is a protein called unknown protein chain p2.

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

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	2	Total	Mg	0	0
			2	2		
86	N9	1	Total	Mg	0	0
			1	1		
86	n8	2	Total	Mg	0	0
			2	2		
86	o1	1	Total	Mg	0	0
			1	1		
86	N5	2	Total	Mg	0	0
			2	2		
86	6	150	Total	Mg	0	0
			150	150		
86	n4	1	Total	Mg	0	0
			1	1		
86	m5	2	Total	Mg	0	0
			2	2		
86	l3	6	Total	Mg	0	0
			6	6		
86	M1	1	Total	Mg	0	0
			1	1		
86	d6	1	Total	Mg	0	0
			1	1		
86	2	124	Total	Mg	0	0
			124	124		
86	O3	1	Total	Mg	0	0
			1	1		
86	L4	2	Total	Mg	0	0
			2	2		
86	l7	2	Total	Mg	0	0
			2	2		
86	M5	2	Total	Mg	0	0
			2	2		
86	o0	1	Total	Mg	0	0
			1	1		
86	S2	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L8	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	o4	1	Total 1	Mg 1	0	0
86	M9	1	Total 1	Mg 1	0	0
86	q0	2	Total 2	Mg 2	0	0
86	SM	1	Total 1	Mg 1	0	0
86	c8	1	Total 1	Mg 1	0	0
86	M0	3	Total 3	Mg 3	0	0
86	5	499	Total 499	Mg 499	0	0
86	L5	1	Total 1	Mg 1	0	0
86	O7	1	Total 1	Mg 1	0	0
86	l4	1	Total 1	Mg 1	0	0
86	n9	2	Total 2	Mg 2	0	0
86	1	468	Total 468	Mg 468	0	0
86	s2	1	Total 1	Mg 1	0	0
86	d3	1	Total 1	Mg 1	0	0
86	S8	1	Total 1	Mg 1	0	0
86	l2	1	Total 1	Mg 1	0	0
86	O2	1	Total 1	Mg 1	0	0
86	q3	2	Total 2	Mg 2	0	0
86	o3	2	Total 2	Mg 2	0	0

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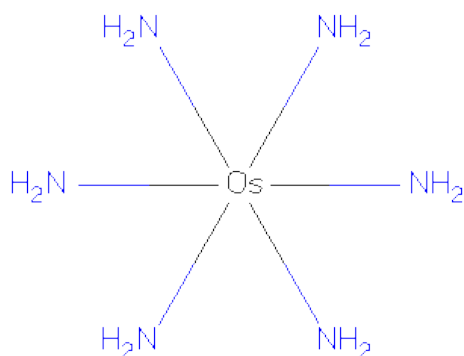
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	M3	2	Total 2	Mg 2	0	0
86	N3	2	Total 2	Mg 2	0	0
86	N8	4	Total 4	Mg 4	0	0
86	4	23	Total 23	Mg 23	0	0
86	D4	1	Total 1	Mg 1	0	0
86	L2	2	Total 2	Mg 2	0	0
86	m1	1	Total 1	Mg 1	0	0
86	l5	3	Total 3	Mg 3	0	0
86	m7	4	Total 4	Mg 4	0	0
86	M7	5	Total 5	Mg 5	0	0
86	m4	1	Total 1	Mg 1	0	0
86	L6	2	Total 2	Mg 2	0	0
86	s1	1	Total 1	Mg 1	0	0
86	l9	1	Total 1	Mg 1	0	0
86	O1	1	Total 1	Mg 1	0	0
86	s8	2	Total 2	Mg 2	0	0
86	o2	1	Total 1	Mg 1	0	0
86	c7	1	Total 1	Mg 1	0	0
86	7	15	Total 15	Mg 15	0	0
86	n3	1	Total 1	Mg 1	0	0
86	q1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L3	2	Total 2	Mg 2	0	0
86	O5	1	Total 1	Mg 1	0	0
86	m6	3	Total 3	Mg 3	0	0
86	N6	1	Total 1	Mg 1	0	0
86	8	17	Total 17	Mg 17	0	0
86	m0	1	Total 1	Mg 1	0	0
86	M6	1	Total 1	Mg 1	0	0
86	N0	1	Total 1	Mg 1	0	0
86	3	14	Total 14	Mg 14	0	0

- Molecule 87 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total 7	N 6	Os 1	0	0
87	2	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
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87	L4	1	Total	N	Os	0	0
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87	M0	1	Total	N	Os	0	0
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87	M5	1	Total	N	Os	0	0
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87	M6	1	Total	N	Os	0	0
			7	6	1		
87	M7	1	Total	N	Os	0	0
			7	6	1		
87	M9	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	N9	1	Total	N	Os	0	0
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87	O1	1	Total	N	Os	0	0
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87	O2	1	Total	N	Os	0	0
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87	O3	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
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87	Q2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		

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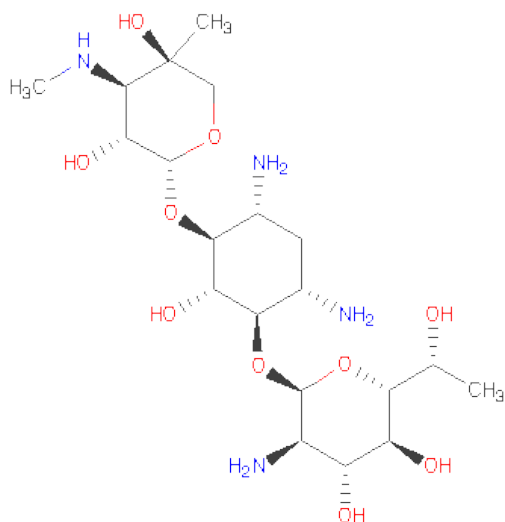
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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			7	6	1		
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			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		
87	15	1	Total	N	Os	0	0
			7	6	1		
87	15	1	Total	N	Os	0	0
			7	6	1		
87	15	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l9	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m1	1	Total	N	Os	0	0
			7	6	1		
87	m4	1	Total	N	Os	0	0
			7	6	1		
87	m5	1	Total	N	Os	0	0
			7	6	1		
87	m7	1	Total	N	Os	0	0
			7	6	1		
87	m9	1	Total	N	Os	0	0
			7	6	1		
87	n3	1	Total	N	Os	0	0
			7	6	1		
87	n9	1	Total	N	Os	0	0
			7	6	1		
87	o3	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o9	1	Total	N	Os	0	0
			7	6	1		
87	q1	1	Total	N	Os	0	0
			7	6	1		
87	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 88 is GENETICIN (three-letter code: GET) (formula: C₂₀H₄₀N₄O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	2	1	Total	C	N	O	0	0
			34	20	4	10		

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

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

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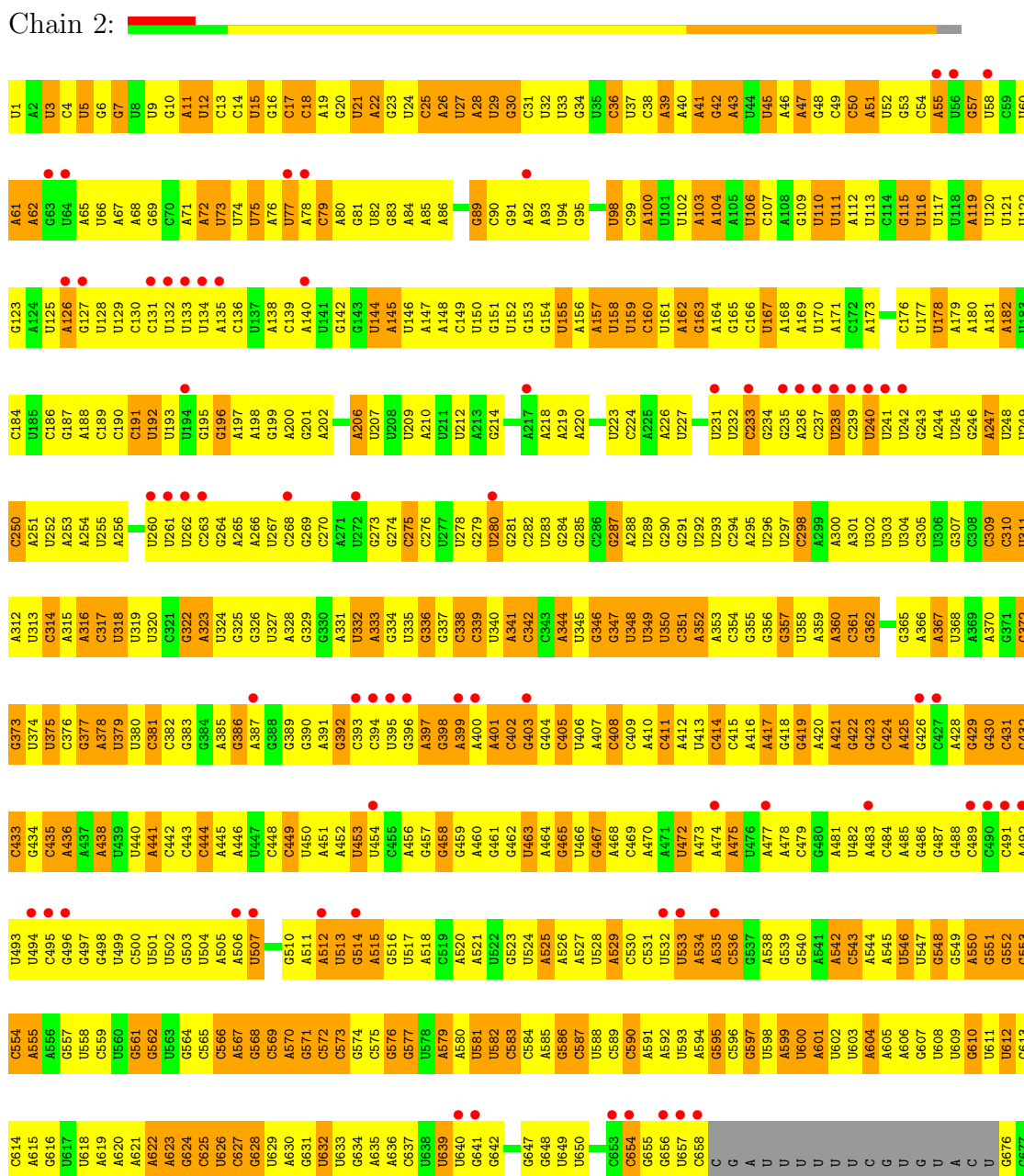
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	D7	1	Total 1	Zn 1	0	0
89	d6	1	Total 1	Zn 1	0	0
89	o7	1	Total 1	Zn 1	0	0
89	O7	1	Total 1	Zn 1	0	0
89	q2	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

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

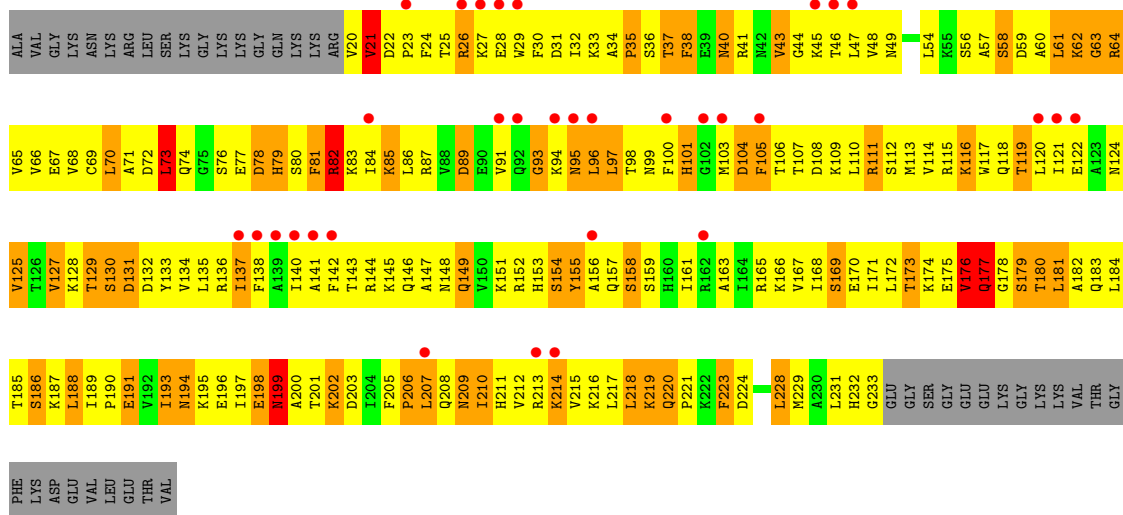


G1474	U1414	U1353	U1293	U1231	A1171	G1111	G1051	G987	C927	G866	A804	U743	A878
A1475	U1415	G1354	G1294	U1232	G1172	G1112	U1052	A988	U926	G867	U805	U744	U679
G1476	U1416	G1355	G1295	G1233	C1173	A1113	U1053	U989	A929	G868	A806	U745	U680
G1477	A1417	U1356	G1296	G1234	C1174	U1114	U1054	C990	A930	A869	A807	A746	U681
A1478	G1418	G1357	G1297	C1235	U1175	U1115	U1055	G991	U932	C870	U808	C747	C682
G1479	G1419	G1358	U1298	G1236	U1176	U1116	U1056	A992	U932	G871	A809	U748	C683
G1480	C1420	C1359	G1299	G1237	C1177	U1117	U1057	A993	A933	G872	G810	U749	A884
C1481	A1421	A1360	A1300	A1238	G1178	G1118	U1058	G994	C934	U873	A811	U750	A885
C1482	U1422	U1361	U1301	U1239	G1179	G1119	U1059	A995	U935	U873	A812	G751	C686
A1483	U1423	U1362	U1302	G1240	U1180	U1120	U1060	G996	C936	C874	A812	U751	G688
G1484	C1424	U1363	U1303	G1241	U1181	C1121	A1061	U996	C937	G875	A813	A752	A753
C1485	G1425	G1364	U1304	A1242	U1182	G1122	U1062	G997	U938	G876	G816	A754	G689
G1486	C1426	C1365	U1305		A1183	C1123	U1063		A939		A817	A755	
A1427	U1366	U1366	C1306	G1245	A1184	A1124	G1064	A1001	A940	G879	C818	A756	U694
G1488	G1428	G1367	U1307	C1246	U1185	A1125	A1065	A1002	A941	C880	C818	A757	U695
U1489	G1429	G1368	U1308	U1247	U1186	G1126	C1066	A1003	U820	U882	U820	U758	C696
C1490	U1430	U1369	C1309	U1248	U1187	G1127	C1067	U1004	C943	C883	U821	U759	C697
U1491	C1431	U1370	U1310	U1249	G1188	C1128	U1068	A884	A944	A884	U822	A760	U698
A1492	U1432	A1371	U1311	U1250	U1189	U1129	A1069	U1006	U945	G885	G823		
A1493	G1433	U1372	A1312	U1251	C1190	G1130	C1070	A1007	U946	U886	G824		G702
C1494	A1434	A1373	A1313	U1252	U1191	A1131	U1071	G1008	U947	A887	U825	U764	G703
C1495	G1435	C1374	U1314	U1253	C1192	A1132	C1072	U1009	U948	U888	U826	G765	C704
U1496	A1436	A1375	U1315	U1254	A1193	A1133	U1073	C1010	C949	U889	C827	U766	U705
U1497	U1437	C1376	G1316	G1255	A1194	C1134	G1074	G1011	C950	C890	U828	U767	A706
G1498	G1438	U1377	C1317	A1256	C1195	U1135	C1075	A891	A951	A891	C829	C768	A707
G1499	C1439		G1318	U1257	A1196	U1136	A1076	A892	A952	A892	U830	A769	C708
C1500	C1440	U1380	U1319	U1258	G1197	A1137	C1077	U893	G953	U893	U831	A770	C709
C1501	C1441	U1381	U1320	U1259	G1198	U1138	C1078	U894	U960	U894	U832	A771	U710
G1502	U1442	A1382	A1321	U1260	G1199	A1139	U1079	G895	A955	U895	U833	C772	U711
A1503	G1443	G1383	A1322		G1200	G1140	U1080	U1017	C956	U896		C773	G712
G1504	A1444	A1384	C1323	G1263	G1201	G1141	A1081	U1018	U957	C897	U836	A774	A713
A1505	G1445	G1385	G1324	G1264	A1202	A1142	C1082	A1019	U958	A898	G837	G775	G714
G1506	A1446	G1386	A1325	G1265	A1203	A1143	G1083		U959	G899	G838	G776	U715
G1507	C1447	G1387	A1326	G1267	C1205	U1145	A1084	C1022	U960	A901	U839	C777	C716
U1508	G1448	G1388	G1327	G1268	G1206	U1146	G1085		U961	G900	U840	G778	C717
	U1449	C1389	G1328	U1269	U1207	A1147	A1086	A1025	C962	G902	U841	U779	G902
U1511	U1450	U1390	A1329	G1270	C1207	A1147	A1087	A1026	U964	U903	U842	A780	U719
G1512	C1451	A1391	G1330	G1271	A1208	C1148	A1088	A1027	U965	G904	U843	U781	G720
G1513	U1452	U1392	C1331	G1272	C1209	G1149	U1089	C1028	A966	A905	A844	U782	U721
U1514	G1453	C1393	C1332	U1273	G1210	G1150	C1090	U1029	U967	A906	G845	G783	G722
A1515	G1454	G1394	C1333	C1273	A1211	A1151	A1091	A1030	U968	A907	G846	C784	G723
A1516	G1455	G1395	U1334	C1274	G1212	A1152	A1092	U1031	U969	U908	A847	U785	C724
U1517	C1456	U1396	U1335	A1275	G1213	G1153	A1093	G1032	C969	U909	C848	C786	U725
C1457	C1457	U1397	U1336	U1276	U1214	G1154	G1094	G1033	A970	C910	C849	C787	C726
G1458	U1398	U1398	A1337	G1277	C1215	G1155	U1095	C1034	A971	U911	A850	A788	U727
C1459	C1399	A1400	C1338	G1278	C1216	C1156	U1096	G1035	U972	U912	U851	A789	U728
A1460	A1401	A1401	C1339	C1279	A1217	A1157	U1097	A1036	A973	G912	C852	U790	G729
U1522	G1461	G1402	U1340	C1280	G1218	C1158	U1098	A1037	A974	G914	G853	A791	G730
G1523	C1462	G1403	A1341	G1281	A1219	U1159	U1099	U1038	C975	A915	U854	U792	C731
A1524	C1463	C1403	C1342	U1282	C1220	A1160	G1100	A1039	G976	U916	A855	A793	G732
A1525	G1464	G1404	U1343	U1283	A1221	C1161	G1101	A1040	A977	U917	A856	U794	A733
A1526	C1465	G1405	A1344	U1284	C1222	C1162	U1102	G1041	A978	U918	A857	U795	A734
C1527	G1466	A1406	A1345	U1285	A1223	U1163	U1103	A1042	A979	A919	G858	A796	C735
U1528	C1467	U1407	A1346	U1286	A1224	G1164	U1104	A1043	G980	U920	A859	G797	C736
C1529	U1468	G1408	U1347	A1287	U1225	G1165	C1105	U1044	U981	U921	U860	C798	A737
G1530	G1469	G1409	A1348	G1288	U1226	A1166	U1106	C1045	U982	G922	U861	G799	G738
G1531	C1470	A1410	G1349	U1289	A1227	G1167	G1107	G1046	A983	A923	A862	U800	G739
U1532	A1471	A1411	U1350	U1290	G1228	U1168	G1108		G984	A924	A863	G801	A740
C1533	C1472	G1412	G1229	G1291	G1229	U1169	G1109	U1049	G985	G925	U864	G802	C741
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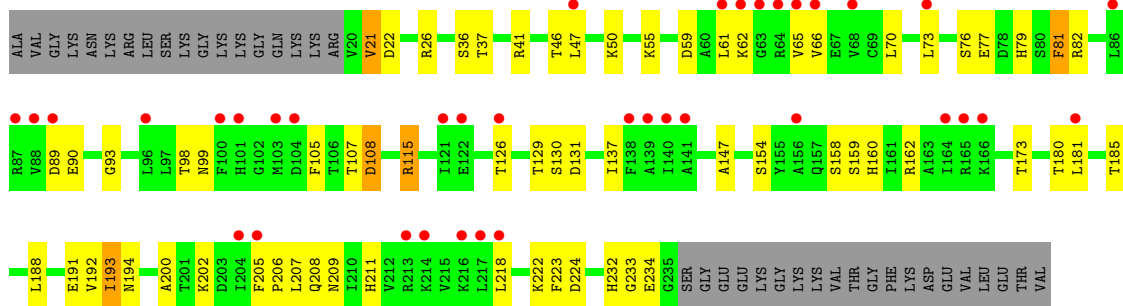
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C1403	U1343	U1282	A1221	C1161	G1101	G1040	G980	U920	U860	A796	C736	U675	U611	G551
G1404	A1344	U1283	C1222	C1162	G1102	G1041	U981	U921	U861	C798	A737	G676	U612	G552
A1405	A1345	C1284	A1223	A1163	U1103	G1042	U982	G922	G797	C798	G738	G677	G613	G553
A1406	U1346	U1285		G1164	U1104	A1043	A983	A923	A863	A799	G739	A678	C614	C554
U1407	U1347	U1286	A1226	G1165	C1105	U1044	G984	A924	U864	U800	A740	U679	A615	A555
G1408	A1348	A1287	A1227	A1166	U1106	C1045	G985	G925	A865	G801	C741	U680	G616	A556
A1409	G1349	G1288	G1228	A1167	G1107	G1046	G986	A926	G866	G802	U742	U681	G617	G557
G1410	U1350	U1289	G1229	U1168	G1108	G1047	G987	C927	G867	A803	U743	C882	U618	U558
A1411	G1351	U1290	A1230	G1169	G1109	U1048	A988	U928	G868	A804	U744	G683	A619	C559
G1412	G1352	G1291	U1231	G1170	G1110	U1049	U989	A929	A869	U805	U745	A684	A620	U560
U1413	U1353	U1292	G1232	A1171	G1111	G1050	C990	A930	C870		A746	A685	A621	G561
G1414	G1354	U1293	G1233	G1172	G1112	G1051	G991	C931	C871	U808	C747	C686	A622	G562
U1415	C1355	G1294	A1234	C1173	A1113	U1052	A992	U932	G872	A809	U748	C687	A623	U563
G1416	U1356	G1295	C1236	U1174	G1114	G1053	A993	A933	U873	G810	U749	G688	G624	G564
A1417	A1357	A1296	A1237	U1175	U1115	U1054	G994	C934	C874	A811	U750	C689	C625	C565
G1418	G1358	G1297	G1237	G1176	U1116	U1055	A995	U935	G875	A812	G751	C690	U626	C566
U1419	U1359	U1298	A1238	C1177	U1117	U1056	U996	G936	G876	U813	A752	C591	U627	A567
C1420	G1360	G1299	U1239	G1178	G1118	U1058	G997	C937	G877	A814	A753	C692	G628	G568
A1421	U1361	A1300	U1240	G1179	G1119	U1059	A998	G938	G878	G815	A754	U693	U629	C569
U1422	U1362	U1301	G1241	C1180	U1120	U1060	U999	A939	G879		U755	U694	A630	A570
U1423	G1363	U1302	A1242	U1181	C1121	A1061	U999	A940	C880	G816	A756	U695	A631	G571
A1424	G1364	U1303	G1243	A1182	G1122	A1062	A1001	A941	A881		A757	C696	U632	C572
A1425	C1365	G1304	A1244	A1183	C1123	U1063	G1002	G942	U882	U820	U758	C697	U633	C573
C1426	U1366	U1305	G1245	A1184	A1124	G1064	U1003	C943	C883	U821	U759	U698	G634	G574
A1427	G1367	C1306	C1246	U1185	A1125	A1065	U1004	A944	A884	U822	A760	U699	A635	C575
G1428	U1368	U1307	U1247	U1186	G1126	C1066	U1005	U945	G885	G823	G761	C700	A636	G576
G1429	U1369	G1308	C1248	U1187	G1127	C1067	C1006	U946	U886	G824	A762	U701	C637	G577
U1430	C1370	C1309	U1249	G1188	C1128	C1068	C1007	U947	U887	U825	G763	G702	U638	U578
A1431	U1371	U1310	U1250	A1189	G1129	A1069	G1008	G948	U888	U826	U764	G703	U639	A579
U1432	U1372	U1311	G1251	C1190	G1130	C1070	U1009	C949	U889	G827	G765	C704	U640	A580
G1433	C1373	A1312	C1252	U1191	A1131	U1071	G1010	C950	C900	U828	U766	U705	G641	U581
U1434	C1374	A1313	C1253	C1192	A1132	C1072	G1011	A951	A891	A829	U767	A706	G642	U582
G1435	U1375	U1314	U1254	A1193	G1133	G1073	U1012	A952	A892	U830	C768	A707	G643	C583
A1436	C1376	U1315	G1255	A1194	C1134	A1074	G953	G953	U893	U831	A769	C708	G644	C584
U1437	U1377	G1316	A1256	C1195	U1135	C1075	G1014	G954	U894	U832	A770	C709	G645	A585
G1438	U1378	C1317	U1257	A1196	U1136	A1076	U1015	A955	G895	U833	A771	U710	G646	G586
C1439	C1379	G1318	U1258	C1197	A1137	C1077	G1016	C956	U896	G834	G772	U711	G647	C587
C1440	U1380	A1319	U1259	G1198	A1138	C1078	U1017	G957	C897	U835	C773	G712	G648	U588
A1441	U1381	U1320	U1260	G1199	A1139	U1079	U1018	U958	A898	U836	A774	A713	U649	C589
U1442	A1382	A1321	G1261	G1200	G1140	U1080	A1019	U959	G899	U837	G775	G714	U650	C590
U1443	G1383	A1322	U1262	G1201	G1141	A1081	A1020	U960	A900	G838	G776	U715	G651	A591
A1444	C1384	C1323	G1263	A1202	A1142	G1082	C1021	U961	G901	U839	C777	C716	G652	A592
G1445	G1385	G1324	G1264	A1203	A1143	C1083	C1022	C962	G902	U841	C778	C717	C653	U593
A1446	U1386	A1325	G1265	A1204	U1144	A1084	A1023	A963	U903	C842	U779	U718	C654	A594
G1447	G1387	A1326	U1266	C1205	U1145	G1085	U1024	U964	G904	U843	A780	U719	G655	G595
G1448	A1388	U1267	G1267	U1206	G1146	A1086	A1025	U965	A905	A844	U781	G720	G656	C596
U1449	C1389	G1268	G1268	U1207	A1147	A1026	A966	A966	A906	G845	U782	U721	G657	C597
U1450	U1390	U1269	U1269	A1208	C1148	A1088	A1027	A967	A907	G846	G783	G722	A661	U598
C1451	A1391	C1209	G1270	C1210	G1149	U1089	C1028	U968	U908	A847	C784	G723	U652	A599
U1452	U1392	G1271	G1271	A1211	U1150	A1091	U1029	C969	C909	C848	U785	C724	U653	U600
C1453	C1393	U1272	A1212	G1212	A1151	A1092	A970	U970	C910	C849	G786	U725	U654	A601
G1454	U1394	G1273	G1273	A1152	A1152	A1093	U1031	A971	U911	A850	G787	C726	U655	U602
C1455	G1395	C1274	G1274	G1153	G1153	A1094	G972	G972	U912	U851	A788	U727	G656	U603
U1456	U1396	A1275	A1275	G1154	G1154	G1095	C1033	A973	G913	C852	U789	U728	G657	A604
G1457	U1397	U1276	U1276	C1215	G1155	U1096	C1034	A974	G914	C853	A790	G729	G658	A605
U1458	U1398	C1277	G1277	C1216	G1156	C1096	G1035	C975	A915	A856	A791	G730	U670	A606
C1459	U1399	C1339	G1278	A1217	C1157	U1097	A1036	C976	U916	A857	U792	C731	G	A607
A1460	A1400	U1279	C1279	G1218	A1157	U1098	C1037	A977	U917	U857	A793	U731	U	U608
C1461	A1401	A1341	C1280	A1219	C1159	U1099	U1038	A978	U918	G858	U794	A734	A673	U609



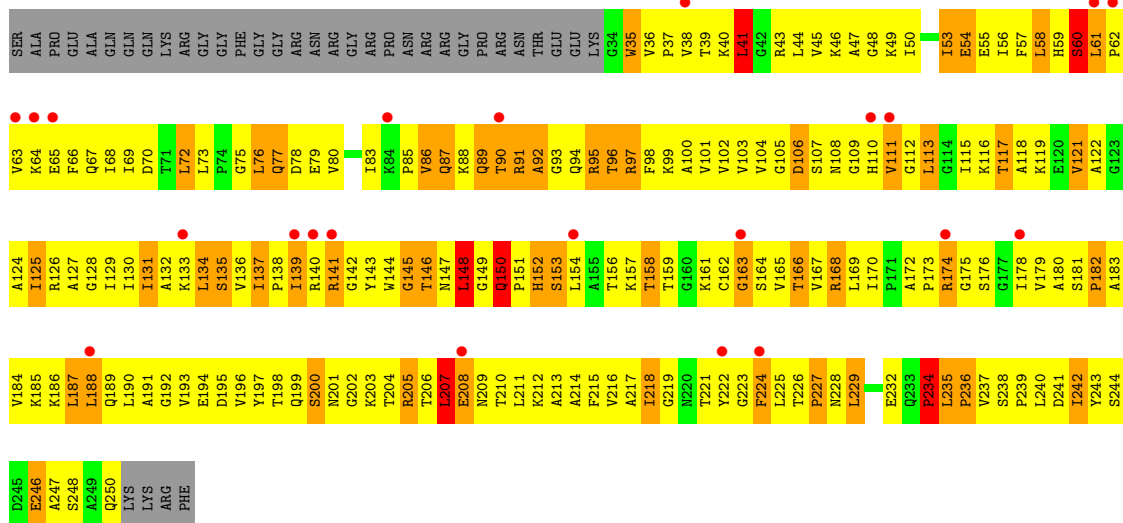
Chain S1:

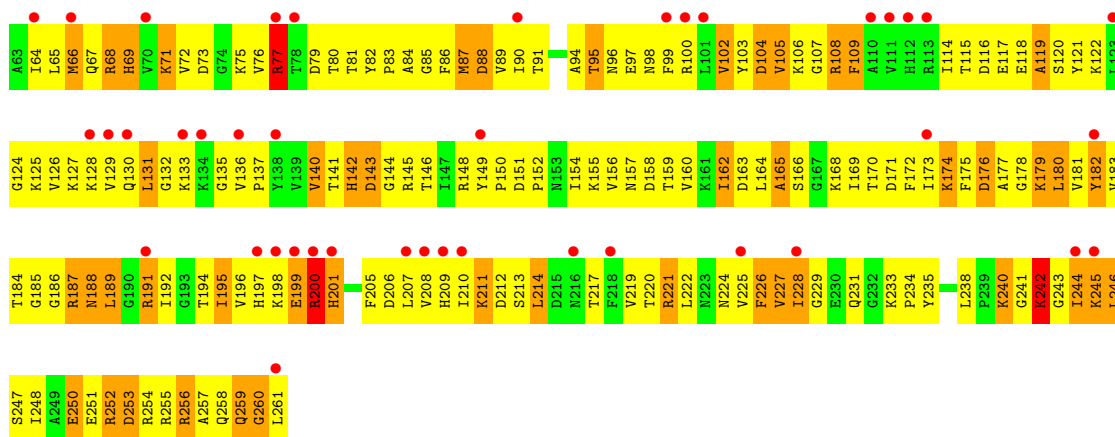


Chain s1: 



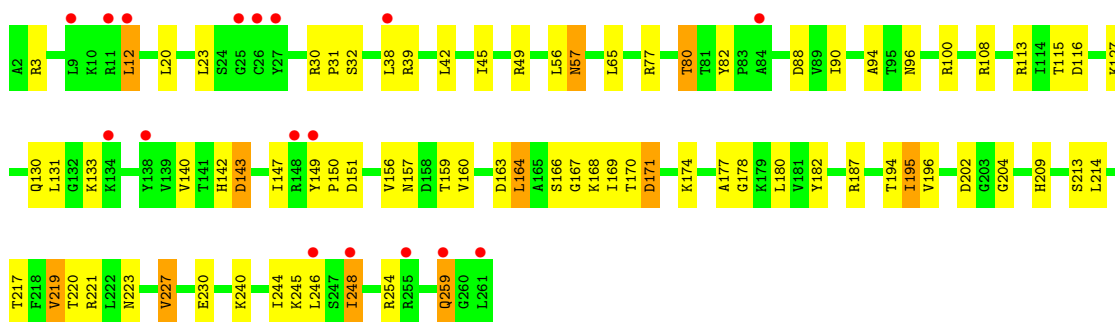
Chain S2:





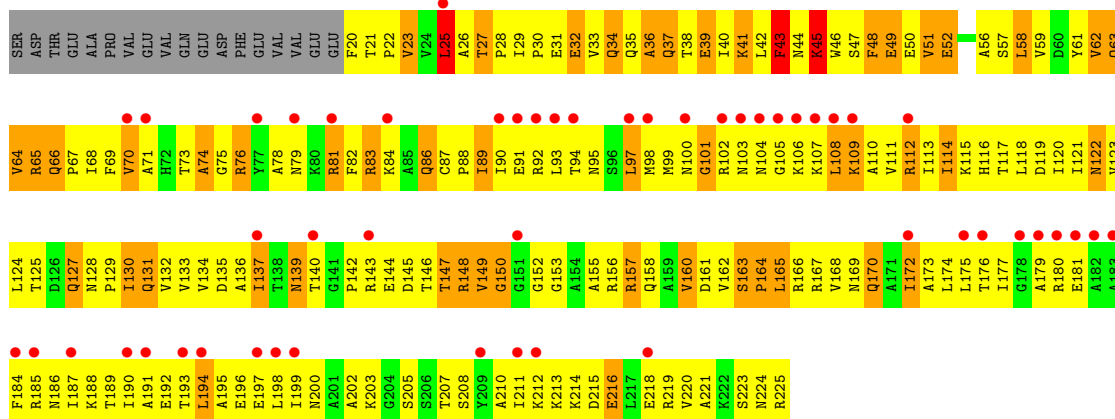
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



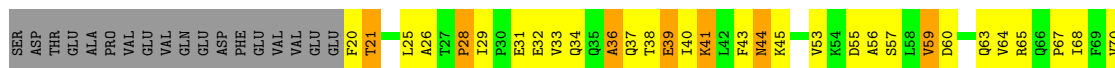
• Molecule 7: 40S ribosomal protein S5

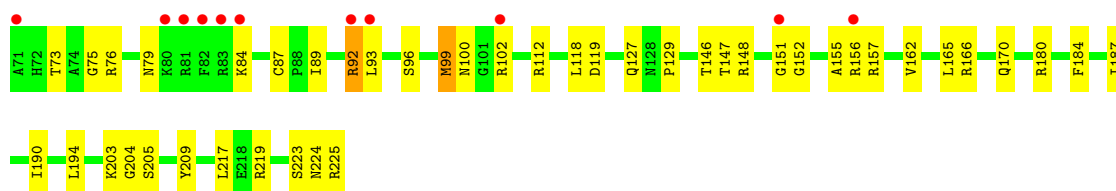
Chain S5:



• Molecule 7: 40S ribosomal protein S5

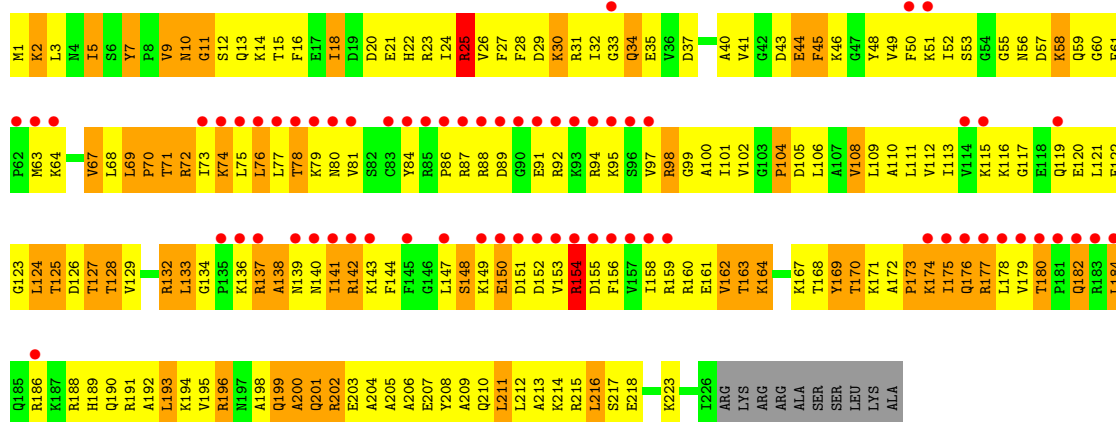
Chain s5:





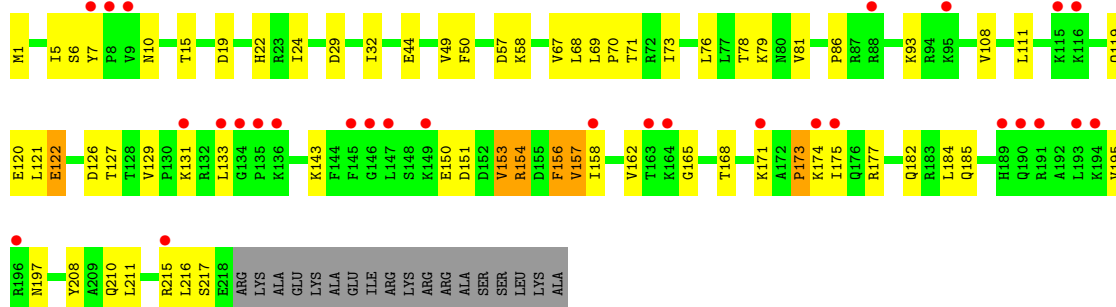
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



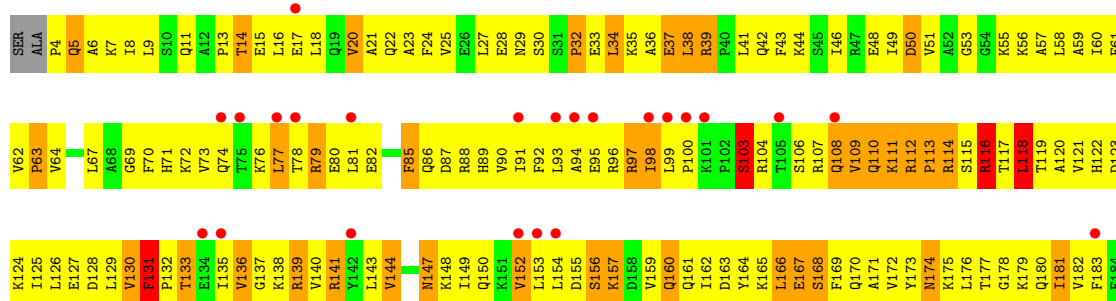
• Molecule 8: 40S ribosomal protein S6-A

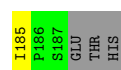
Chain s6:



• Molecule 9: 40S ribosomal protein S7-A

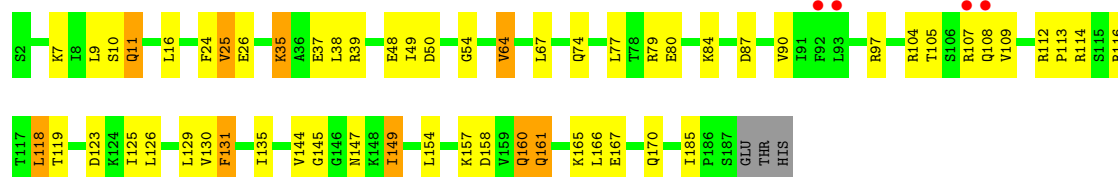
Chain S7:





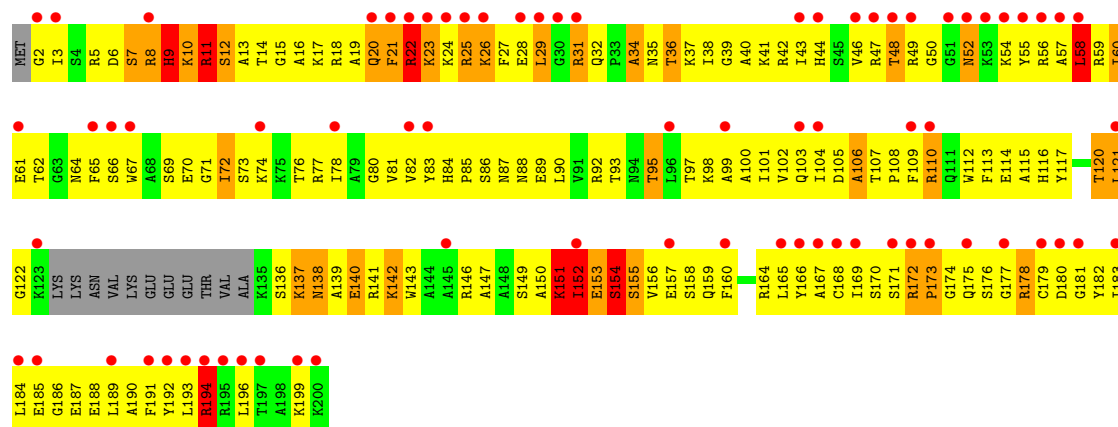
• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



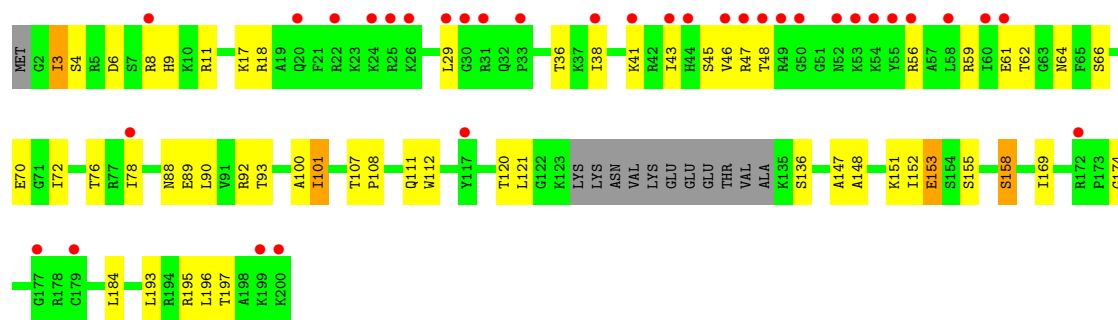
• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



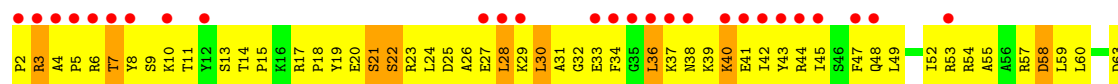
• Molecule 10: 40S ribosomal protein S8-A

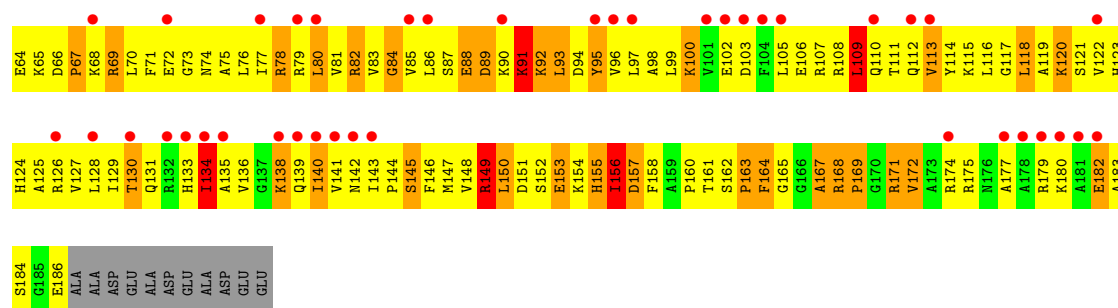
Chain s8:



• Molecule 11: 40S ribosomal protein S9-A

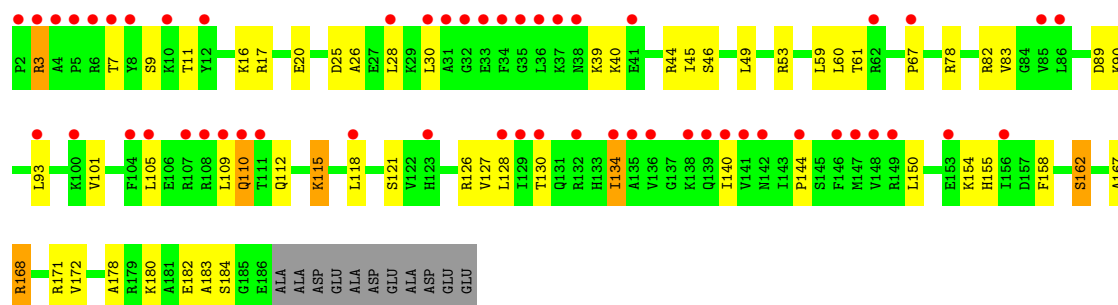
Chain S9:





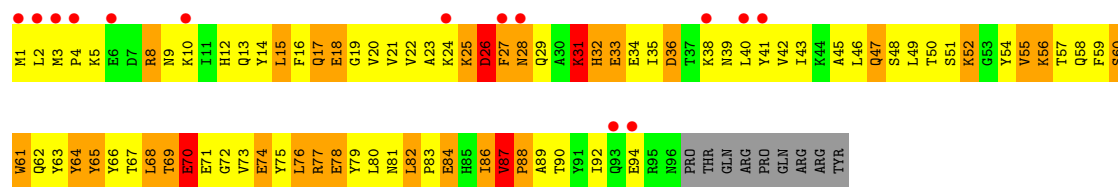
• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



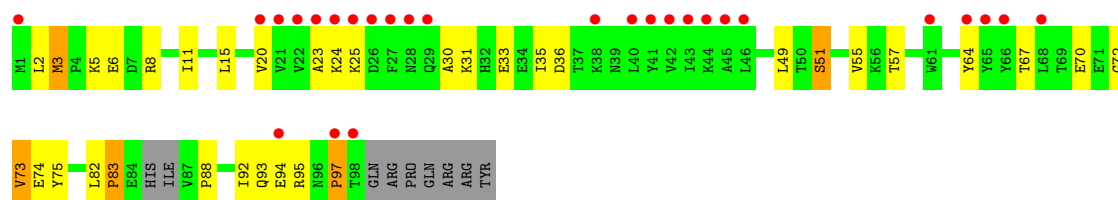
• Molecule 12: 40S ribosomal protein S10-A

Chain C0:



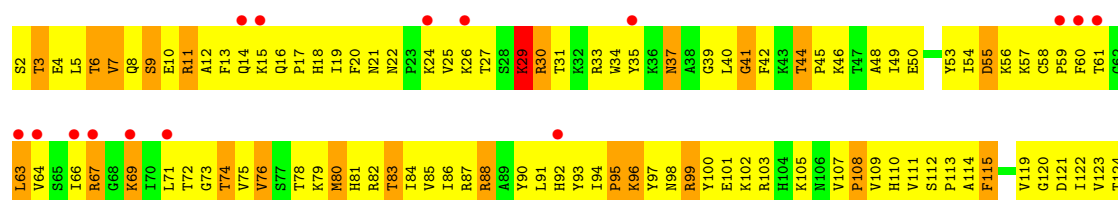
• Molecule 12: 40S ribosomal protein S10-A

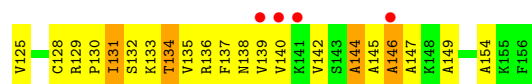
Chain c0:



• Molecule 13: 40S ribosomal protein S11-A

Chain C1:





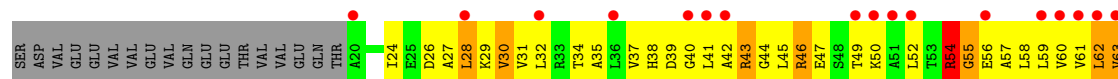
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



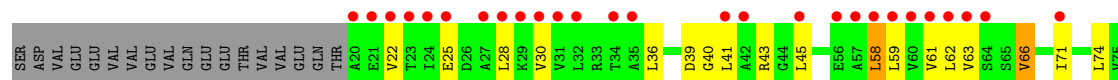
• Molecule 14: 40S ribosomal protein S12

Chain C2:



• Molecule 14: 40S ribosomal protein S12

Chain c2:



• Molecule 15: 40S ribosomal protein S13

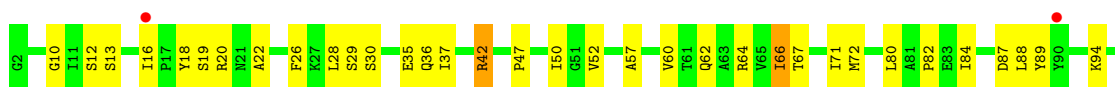
Chain C3:



• Molecule 15: 40S ribosomal protein S13

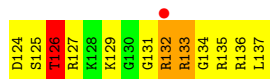
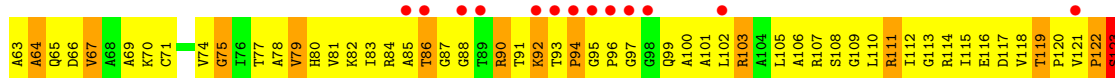
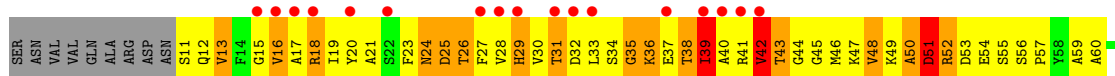


Chain c3:



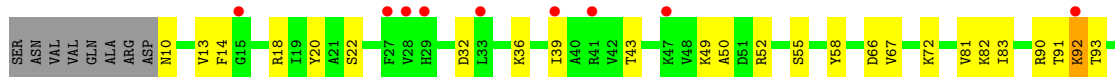
- Molecule 16: 40S ribosomal protein S14-A

Chain C4:



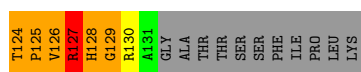
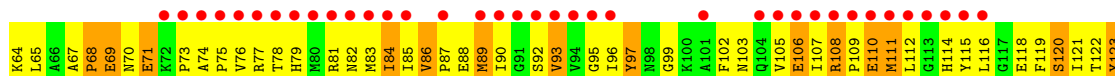
- Molecule 16: 40S ribosomal protein S14-A

Chain c4:



- Molecule 17: 40S ribosomal protein S15

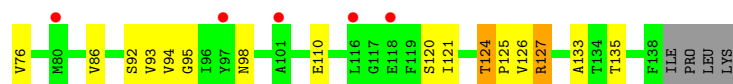
Chain C5:



- Molecule 17: 40S ribosomal protein S15

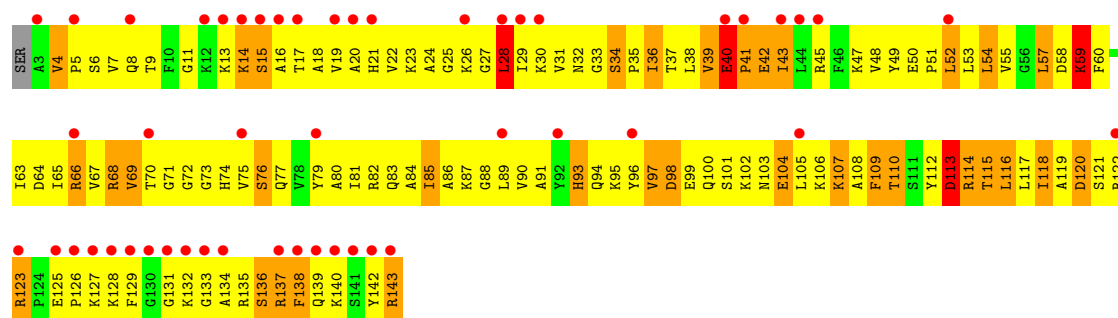
Chain c5:





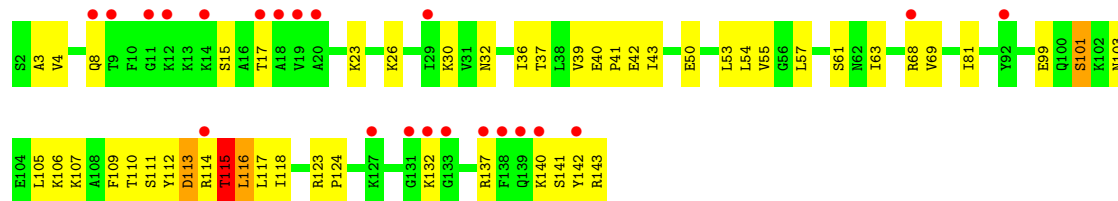
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:



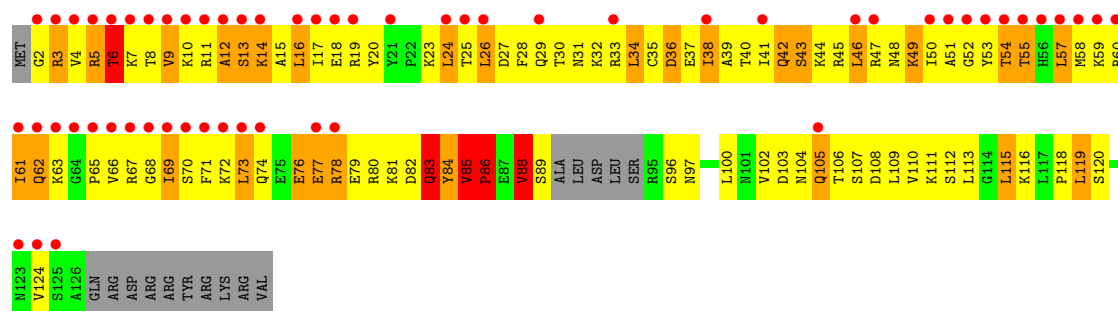
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:



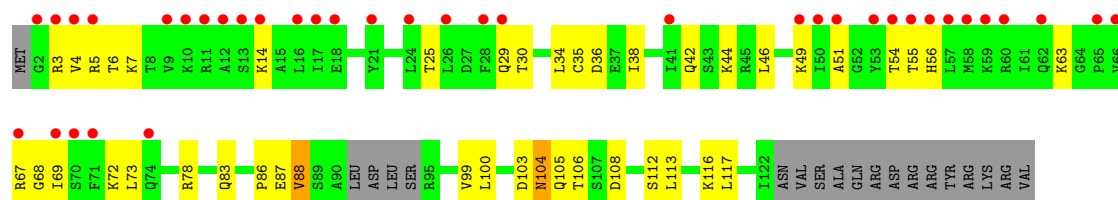
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:



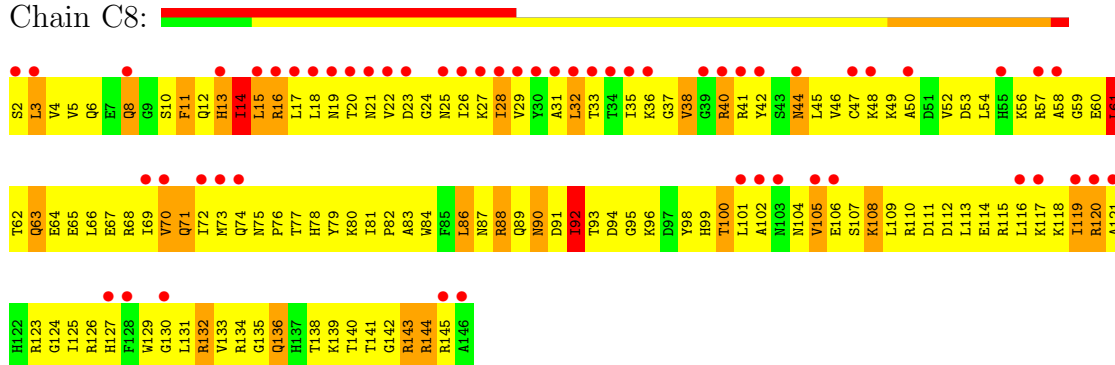
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:



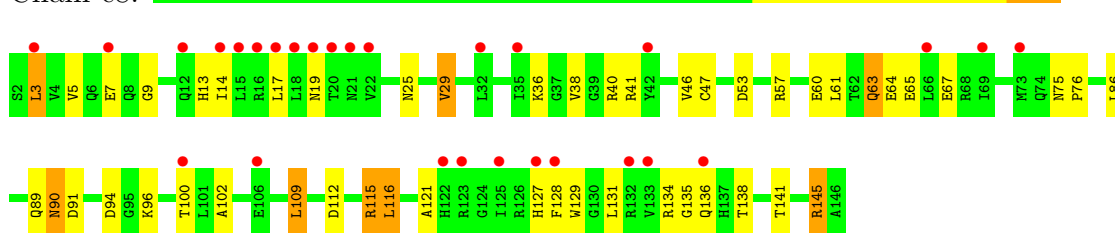
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:



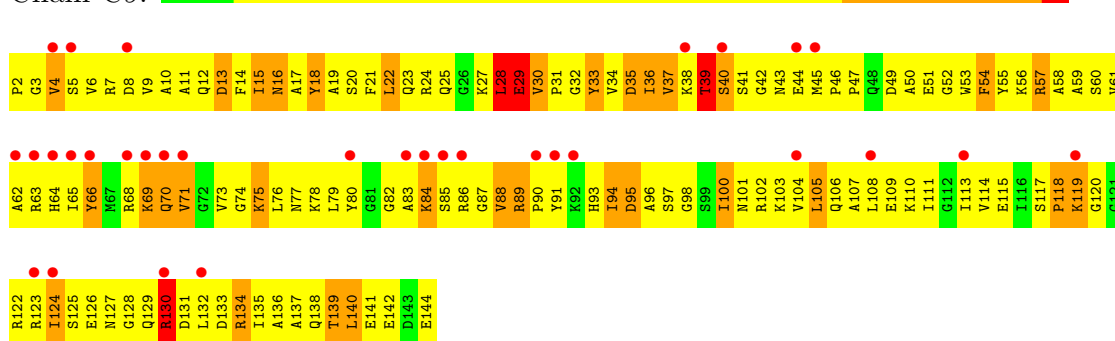
- Molecule 20: 40S ribosomal protein S18-A

Chain c8:



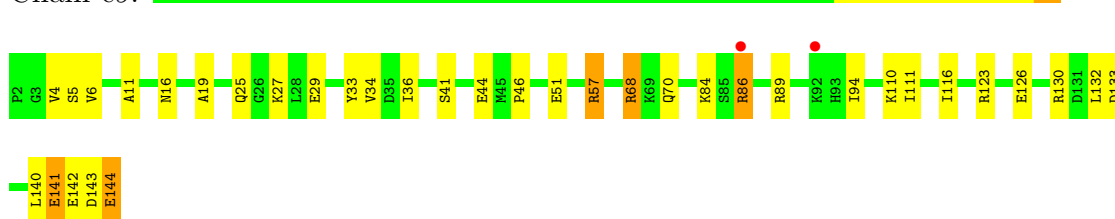
- Molecule 21: 40S ribosomal protein S19-A

Chain C9:



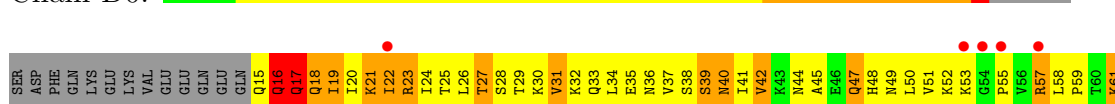
- Molecule 21: 40S ribosomal protein S19-A

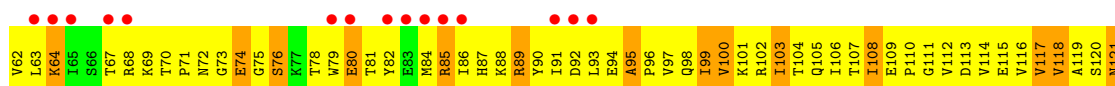
Chain c9:



- Molecule 22: 40S ribosomal protein S20

Chain D0:





- Molecule 22: 40S ribosomal protein S20

Chain d0:



- Molecule 23: 40S ribosomal protein S21-A

Chain D1:



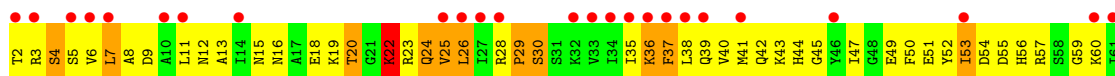
- Molecule 23: 40S ribosomal protein S21-A

Chain d1:



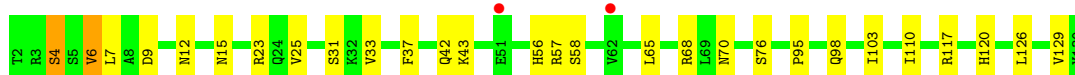
- Molecule 24: 40S ribosomal protein S22-A

Chain D2:



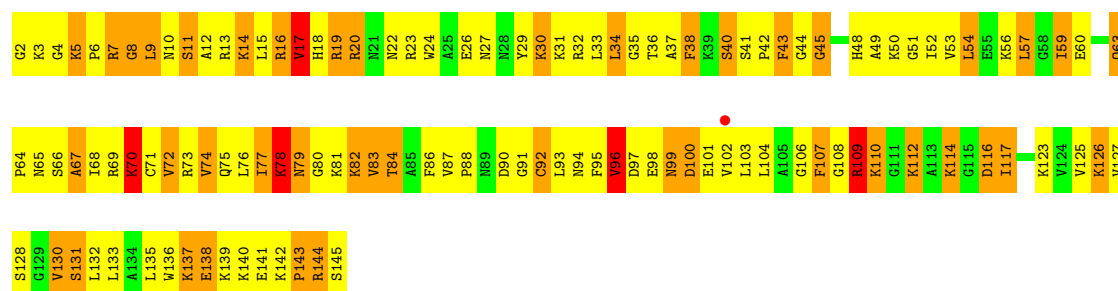
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:



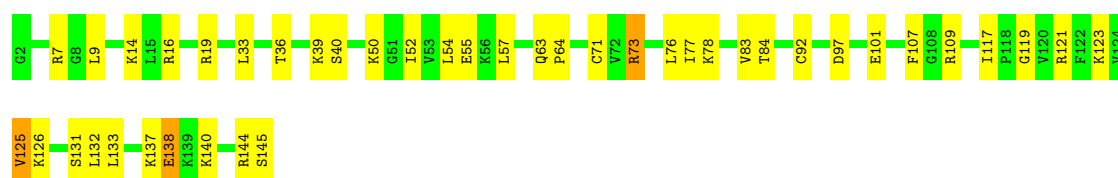
- Molecule 25: 40S ribosomal protein S23-A

Chain D3:



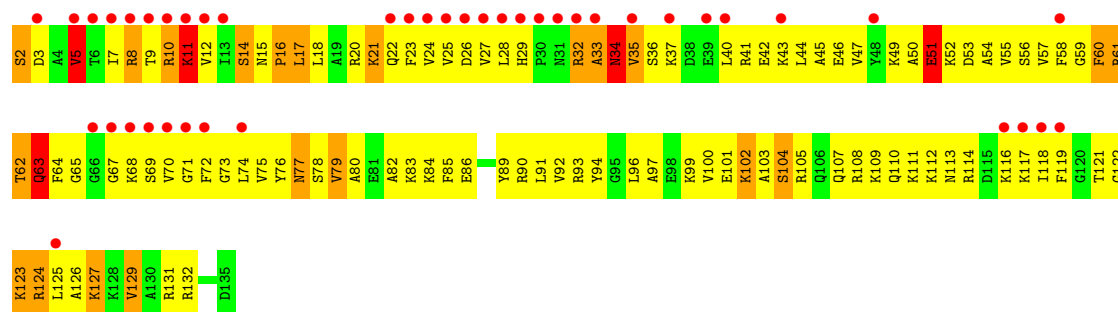
• Molecule 25: 40S ribosomal protein S23-A

Chain d3:



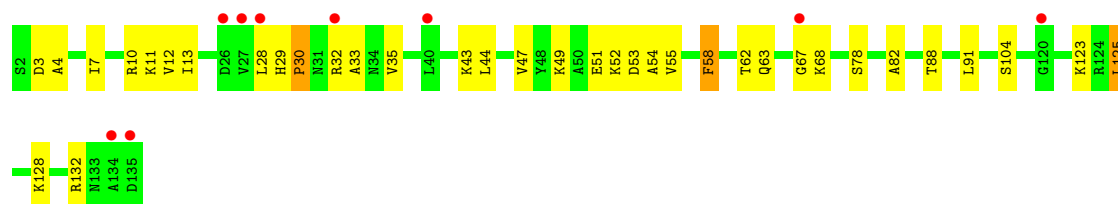
• Molecule 26: 40S ribosomal protein S24-A

Chain D4:



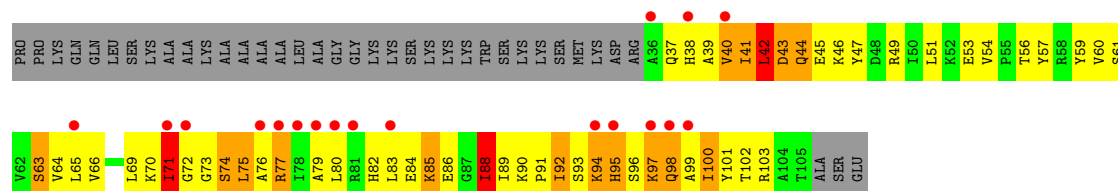
• Molecule 26: 40S ribosomal protein S24-A

Chain d4:



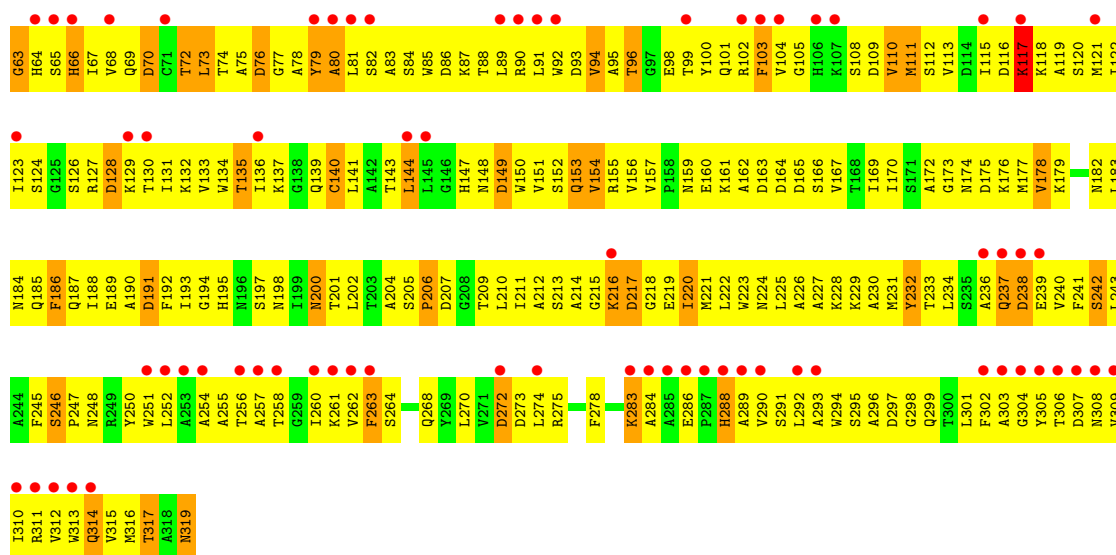
• Molecule 27: 40S ribosomal protein S25-A

Chain D5:



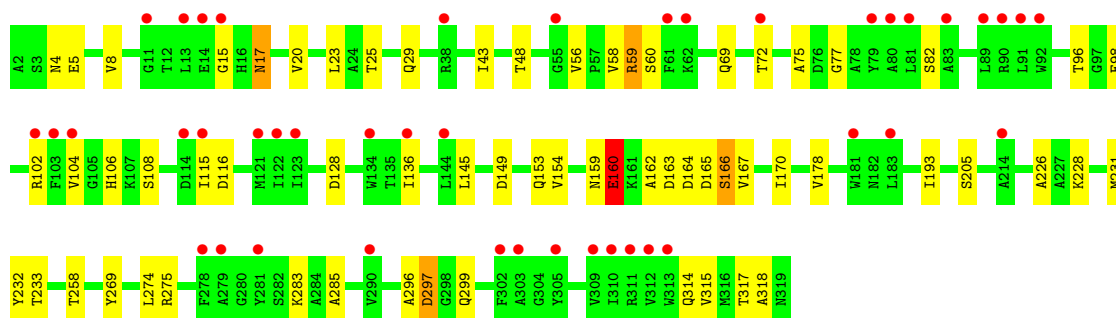
- Chain d5:

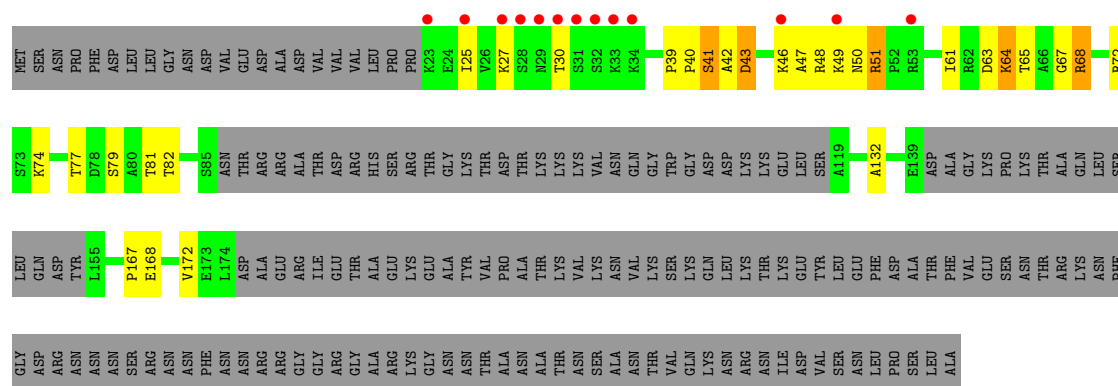




• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

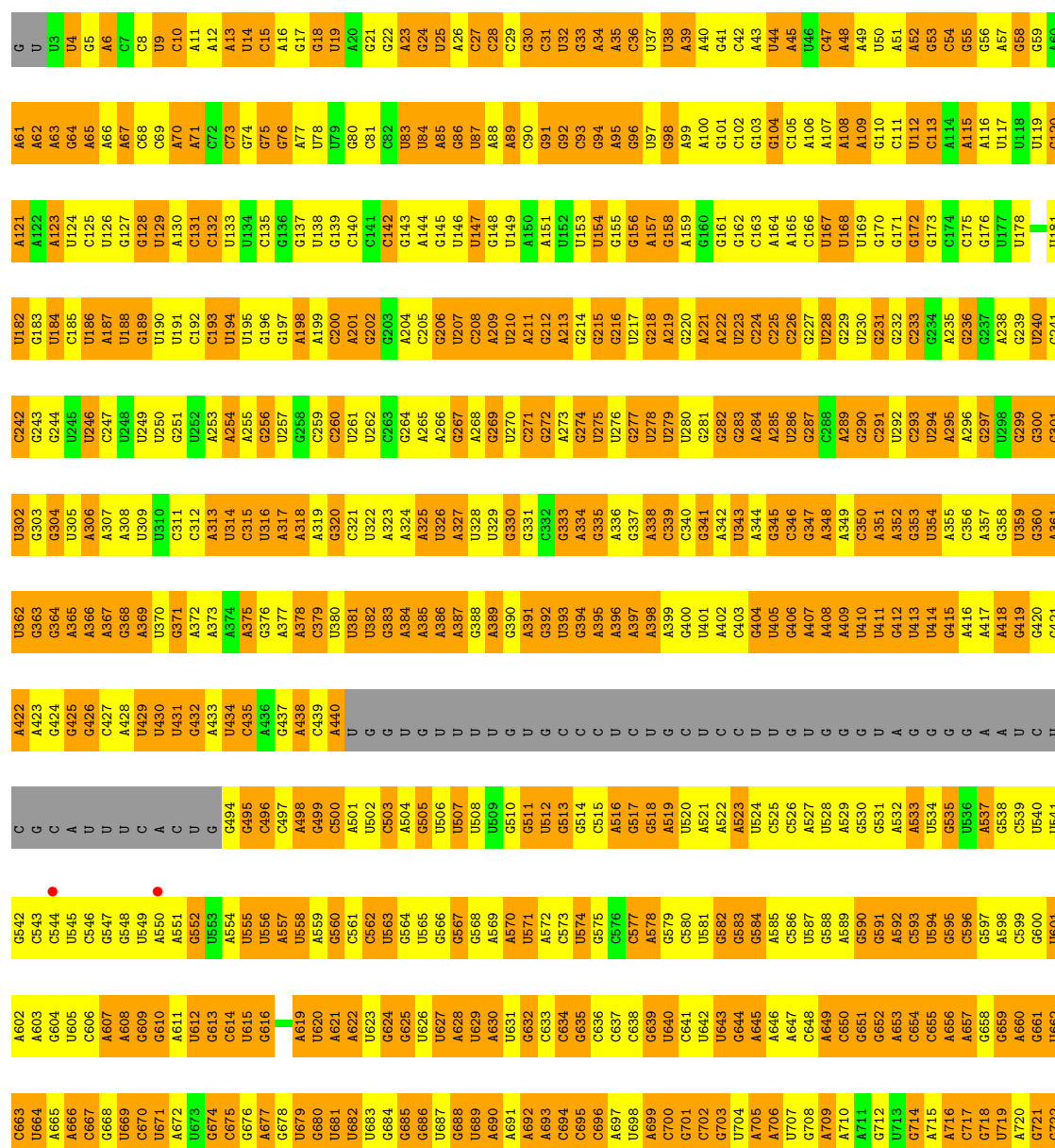
Chain sR:





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

Chain 1:



G1576	A1456	C1396	U1336	C1275	A1212	G1152	U1028	A967	G907	A847
G1577	U1457	C1397	A1337	U1276	G1213	A1153	G1029	C968	G908	A848
G1578	U1458	C1398	A1338	C1277	U1214	A1154	A1030	C969	G909	
G1579	A1459	C1399	A1339	U1278	U1215	C1155	U1096	A970	G910	C787
A1580	U1460	G1400	C1340	C1279	C1216	C1156	C1032	C971	G911	C788
G1581	A1461	A1401	U1341	C1280	A1217	G1157	U1033	A972	G912	C789
G1582	A1462	C1402	C1342	G1281		A1158	U1034	C973	G913	
G1583	U1463	C1403	A1343	U1282	U1220	A1159	G1035	A974	A914	C729
A1584	G1464	G1404	C1344	C1283	A1221	C1160	A1036	C975	G915	C730
G1585	U1465	U1405	G1345	G1284	G1222	G1161	G1101	C976	G916	C731
G1586	U1466	A1406	C1346	G1285	A1223	U1162	C1038	C977	A917	C732
G1587	U1467	A1407	U1347	G1286	C1224	A1163	U1039	C978	C918	C733
A1588	A1468	G1408	U1348	A1287	A1225	G1164	A1040	C979	C919	C734
A1589	U1469	G1409	A1349	U1288	G1226	A1165		A980	A920	A735
G1590	U1470	U1410	A1350	C1289	C1227	G1166	G1043	C981	G921	A736
G1591	C1531	U1471	U1351	U1352	G1228	U1167	U1044	C982	C922	G737
G1592	C1532	G1412	A1352	C1292	C1229	U1168	C1045	A983	G923	A738
U1593	U1533	G1413	U1353	U1293	G1230	A1169	A1046	C984	G924	G739
A1594	A1474	G1414	A1354	A1294	A1231	G1170	A1047	C985	G925	G740
U1595	U1535	U1415	A1355	G1295	C1232	G1171	A1048	A985	A926	
G1596	G1536	G1416	U1356	C1296	G1233	U1172	C1049	C986	C927	C742
U1597	A1477	G1417	G1357	C1297	G1234	G1173	G1113	U987	C928	C743
G1598	G1538	A1418	C1358	C1298	U1235	G1174	U1050	C988	C929	A744
A1599	U1479	A1419	C1359	U1299	G1236	C1175	U1051	A989	A929	C745
U1600	G1480	C1420	C1360	G1300	C1237	C1176	U1052	U990	U930	A746
G1601	A1481	G1421	U1361	A1301	C1238	G1177	A1053	C991	G931	A747
A1602	A1482	G1422	G1362	A1302	C1239	G1178	A1054	A992	U932	A748
G1603	G1483	C1423	A1363	C1303	U1240	A1179	U1056	C993	A933	C749
G1604	U1484	A1424	C1364	A1304	A1241	C1180	C1119	U994	G934	G750
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G1616	C1496	U1436	C1376	C1316		C1192	C1068	C1069	G947	G763
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	U3167	U3107	A3227	A3167	U2986	U3047	U2986	A2926	U2866	U2806	G2745	C2685	A2561
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	G3177	G3116	U3237	G3177	U2996	U3057	U2996	U2936	C2876	C2816	C2755	A2635	U2571
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	A3183	A3123	A3243	A3183	C3002	G3063	C3002	C2942	U2882	U2892	G2761	U2641	G2579
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	A3186	C3126	G3246	A3186	A3005	U3066	A3005	A2946	C2885	U2825	C2764	C2644	G2583
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	C3190	A3130	U3250	C3190	G3009	A3070	G3009	G2950	C2889	U2829	U2768	G2648	
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	G3192	C3132	G3252	G3192	A3011	C3072	A3011	G2952	U2891	G2831	G2770	U2650	A2590
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	G3197	C3137	C3257	G3197	A3016	A3077	A3016	G2957	A2896	C2836	U2775	U2655	A2595
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	A3199	A3139	G3259	A3199	C3018	U3079	C3018	A2959	G2898	U2838	G2777	A2657	U2597
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	C3201	A3141	U3261	C3201	U3020	C3081	U3020	G2960	C2900	C2840	A2779	G2659	U2599
	G3202	A3142	G3262	G3202	A3021	C3082	A3021	G2961	G2901	G2841	G2780	G2660	C2600
	U3203	C3143	G3263	U3203	G3022	G3083	G3022	U2962	A2902	U2842	U2781	G2661	A2601
	C3204	G3144	C3264	C3204	U3023	U3084	U3023	G2963	A2903	U2843	U2782	G2662	G2602
	G3205	C3145	G3265	G3205	A3024	G3085	A3024	U2964	U2904	C2844	U2783	G2663	G2603
	C3206	G3146	C3266	C3206	C3025	A3086	C3025	U2965	U2905	A2845	U2724	C2664	U2604
	U3207	G3147	U3267	U3207	G3026	A3087	G3026	G2966	C2906	A2846	U2725	U2665	G2605
	G3208	U3148	C3268	G3208	A3027	G3088	A3027	U2967	C2907	A2847	G2787	C2666	G2606
	A3209	G3149	U3269	A3209	G3028	C3089	G3028	G2968	G2908	G2848	C2788	A2667	G2607
	C3210	A3150	U3270	C3210	A3029	U3090	A3029	G2969	U2909	C2849	U2789	U2668	G2608
	U3211	U3151	G3271	U3211	G3030	A3091	G3030	C2970	U2910	G2850	U2729	G2669	A2609
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● Molecule 36: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

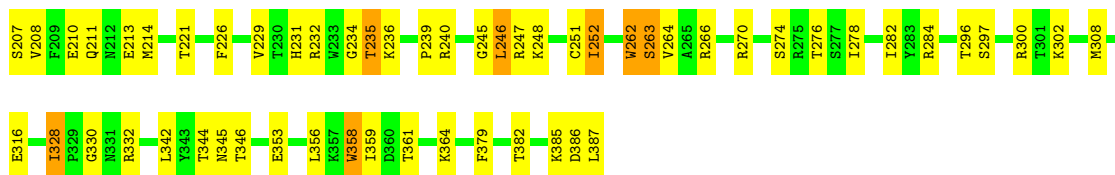
Chain 5:



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C8	A70	A254	U316	G376	A436	A498	A559	A619	G679	G739	A801		U922
A12	A71	A255	A317	A377	G437	C499	G560	U620	U680	G740	C802	C863	C923
A13	C72	G256	A318	A378	A438	G500	C561	A621	U681	U741	C803	G864	G924
C73	C73	U257	A319	A379	C439	C501	C562	A622	U682	G742	C804	U865	A925
U14	G74	G258	G320	U380	A440	A502	U563	U623	U683	C743	G805	A866	A926
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C16	G76	C260	U322	U382	G442	C503	U565	G625	G685	C745	A807	C868	C928
A16	A77	U261	U323	G383	G443	A504	G566	U626	G686	A746	A808	G869	A929
G17	A78	U262	A324	A384	U	G505	G567	U627	U687	A747	G809	G870	U930
U19	U79	C263	A325	A385	G	U506	G568	A628	G688	U748	A810	U871	C931
C20	G80	G264	U326	A386	U	U507	A569	U629	U689	C749	U811	U872	U932
A20	C81	A265	U327	A387	U	U508	A570	A630	A690	G750	G812	C873	A933
G21	C82	A266	U328	C388	U	U509	U571	U631	A691	A751	C813	U874	G934
C22	U83	A267	U329	A389	U	G510	A572	G632	A692	U752	U814	G875	U935
A23	U84	G268	G330	G390	U	G511	G573	C633	A693	C753	G815	A876	A936
G24	A85	U269	A331	A391	U	U512	U574	C634	C694	G754	A816	C877	G937
U25	G86	G270	G332	G392	G	G513	G575	G635	C695	A755	A817	U878	C938
A26	U87	C271	C333	U393	C	G514	C576	C636	C696	U756	C818	U879	U939
C27	A88	G272	A334	G394	C	C515	C577	C637	A697	C757	U819	G880	G940
C28	A89	A273	A335	A395	C	A516	A578	C638	U698		A820	C881	G941
C29	G90	G274	G336	A396	U	G517	G579	C639	A699	G760	U821	A882	U942
G30	G91	U275	G337	A397	C	U518	C580	U640	C700		G816	A883	U943
C31	G92	U276	A338	A398	U	A519	U581	C641	G701	G763	C817	A884	C944
U32	G93	G277	C339	A399	G	U520	G582	U642	C702	U764	C818	U885	C945
G33	G94	U278	G340	A400	C	A521	G583	U643	C703	C765	U825	C886	U946
A34	A95	G156	G341	U401	U	A522	G584	G644	A705	U766	G826	G887	U947
A35	A96	G157	G342	A402	C	A523	G585	A645	A706	U767	A827	A888	C948
U37	U97	A159	G343	C403	C	U524	C586	A646	C707	C768	U828	U889	C949
G38	G98	G160	A344	G404	U	C525	U587	A647	U707	G769	U829	C890	C950
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U38	A99	G162	C346	G406	G	A527	A589	A649	A709	A771	G831	U892	A952
A40	A100	C163	G347	A407	U	U528	G590	C650	A710	U772	G832	C893	G953
C41	G101	U167	U280	A408	U	A529	G591	G651	A711	G773	G833	G894	U954
C42	C102	A164	G281	A409	G	G530	A592	G652	G712	G774	U834	A895	U955
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U46	A108	G170	G290	U413	G	U534	C596	A656	A716	U778	G838	U899	C959
C47	A109	G171	C291	U414	U	G535	G597	A657	C717	G779	C839	G900	U960
A48	A110	G172	U292	G415	G	U536	A598	G658	G718	A780	C840	G901	C961
A49	C111	G173	C293	G416	G	U537	C599	G659	U719	G781	A841	G902	A962
U50	C111	C174	U294	A417	G	A538	G600	A660	A720	U782	G842	U903	G963
A51	U112	U181	A295	A418	A	G538	U601	G661	G721	A783	A843	A904	G964
A52	C113	U182	A296	G419	U	U541	A602	U662	G722	A784	G844	U905	A965
G53	A114	U177	C297	G420	C	G542	A603	G663	U723	G785	G845	A906	U966
C54	A115	U178	U298	G421	U	C543	G604	U664	U724	A786	A846	G907	A967
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A57	U118	U181	G301	G424	C	G546	A607	C667	G727	A789	C849	G910	U970
G58	U119	U182	U302	G425	A	G547	A608	G668	G728	U790	U850	C911	G971
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A60	A121	U184	G304	G427	U	U549	G610	C670	C730	G792	U852	A913	A973
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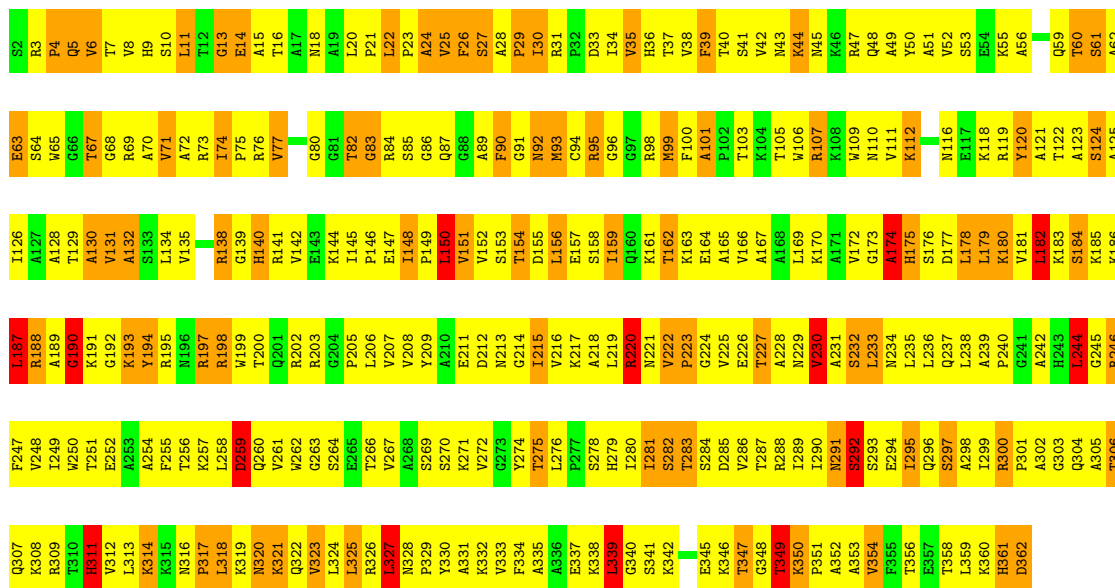
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G1766	A1704	C1644	C1583	G1523	C1402	C1342	G1282	U1220	C1160	U1100	A1040	A980
U1705	U1705	U1645	U1584	A1524	C1403	A1343	C1283	A1221	G1161	G1101	U1041	U981
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G1770	C1709	G1647	A1586	U1526	U1405	G1345	G1285	A1223	A1163	C1043	C1043	A983
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C1772	C1711	U1649	A1588	G1528	A1407	U1347	A1287	A1225	A1165	A1105	C1045	U985
C1773	G1712	G1650	A1589	U1529	G1408	U1348	U1288	G1226	G1166	G1106	A1046	U986
C1774	U1713	U1651	C1590	U1530	G1409	G1349	G1289	C1227	U1167	C1107	A1047	U987
G1775	G1713	G1652	U1591	C1531	U1410	A1350	A1290	G1228	U1168	U1108	A1048	U988
U1776	A1714	G1653	U1592	U1532	C1411	U1351	A1291	G1229	A1169	U1049	C1049	A989
U1777	A1715	A1654	G1593	U1533	G1412	A1352	C1292	G1230	C1170	U1110	U1050	U990
C1778	U1716	G1655	A1594	A1534	G1413	U1353	A1293	A1231	G1171	U1111	U1051	G991
G1779	U1717	A1656	U1595	A1535	G1414	G1354	A1294	C1232	G1172	A1112	U1052	A992
G1780	G1718	C1657	G1596	G1536	U1415	A1355	G1295	G1233	U1173	G1113	A1053	G993
C1781	G1719	G1658	A1597	A1537	C1416	U1356	C1296	G1234	G1174	U1114	A1054	G994
U1782	U1720	U1659	G1598	U1538	G1417	U1357	C1297	U1235	C1175	G1115	A1055	U995
G1783	U1721	C1660	G1599	A1539	A1418	C1358	U1298	G1236	C1176	G1116	U1056	A996
U1784	U1722	G1661	U1600	U1540	A1419	C1359	U1299	G1237	G1177	G1117	A1057	A997
U1785	A1723	G1662	U1601	G1541	C1420	U1360	G1300	G1238	C1178	C1118	U1058	A998
G1786	U1724	C1663	A1602	G1542	G1421	U1361	A1301	C1239	A1179	G1119	G1059	G999
A1787	C1725	G1664	A1603	G1543	G1422	G1362	A1302	A1240	A1180	A1120	U1060	C1000
G1788	C1726	C1665	G1604	G1544	C1423	A1363	A1303	U1241	A1181	U1121	A1061	G1001
G1789	G1727	G1666	A1605	A1545	C1424	C1364	A1304	G1242	G1182	U1122	A1062	A1002
G1790	G1728	A1667	U1606	A1546	U1425	G1365	G1305	U1243	C1183	U1123	G1063	A1003
C1791	A1729	G1668	U1607	G1547	C1426	A1366	G1306	A1244	A1184	U1124	A1064	U1004
G1792	G1730	C1669	C1608	G1548	U1427	G1367	G1307	A1245	C1185	U1125	A1065	G1005
G1793	A1731	C1670	C1609	U1549	A1428	U1368	A1308	G1246	C1186	G1126	G1066	A1006
G1794	U1732	C1671	G1610	C1550	G1429	A1369	U1309	U1247	U1187	U1067	U1067	U1007
U1795	G1733	U1672	A1611	C1551	U1430	G1370	G1310	C1248	C1188	U1128	C1068	U1008
G1796	C1734	G1673	A1612	G1552	G1431	C1371	C1311	G1249	C1189	A1129	C1069	A1009
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A1798	G1736	G1675	C1614	U1554	A1433	A1373	G1313	A1251	U1191	G1131	U1071	A1011
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C1802	C1738	G1677	U1616	C1556	A1435	G1375	U1315	U1253	A1193	A1133	U1073	G1013
C1803	U1739	G1678	C1617	A1557	U1436	C1376	C1316	G1256	G1194	G1134	U1074	U1014
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A1810	U1746	C1685	A1624	U1564	G1443	G1383	G1323	A1263	C1201	C1141	U1081	G1021
G1811	G1747	U1686	A1625	G1565	G1444	U1384	U1324	A1264	A1202	G1142	U1082	U1022
G1812	U1748	U1687	A1626	A1566	U1445	C1385	U1325	U1265	A1203	A1143	G1083	C1023
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A1814	U1750	U1689	U1629	U1568	G1447	C1387	C1327	U1267	A1205	G1145	A1085	A1025
U1815	G1751	C1690	U1630	A1569	U1448	U1388	C1328	G1268	G1206	C1146	C1086	A1026
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G1817	G1753	U1692	A1632	U1571	G1450	A1390	A1330	U1270	U1208	G1148	U1088	U1028
U1818	G1754	C1693	C1633	U1572	C1451	C1391	U1331	A1271	G1209	G1149	G1089	G1029
U1819	G1755	U1694	G1634	G1573	A1452	G1392	A1332	C1272	U1210	U1150	G1090	A1030
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U1821	A1757	A1696	U1636	A1575	A1454	A1394	U1334	G1274	A1212	G1152	C1092	C1032
C1822	U1760	C1698	A1638	G1577	A1456	C1396	U1336	U1276	G1213	A1153	A1093	U1033
												U1034

C2675	C2615	U2553	C	A2430	G2369	A2309	G2248	G2187	U2127	C	U	C1943	A1883	U1823
A2676	C2616	A2554	A	C2431	G2370	U2310	G2249	A2188	C2128	U	G	U1944	A1884	U1824
G2677	U2617	C2555	C	A2432	G2371	A2311	G2250	U2189	U2129	C	G	A1945	U1885	G1825
A2678	C2618	C2556	U	U2433	A2372	A2312	G2251	U2190	G2130	U	G	A1946	U1886	C1826
A2679	G2619	A2557	A	U2434	C2373	A2313	G2252	U2191	A2131	U	G	G1947	A1887	C1827
G2680	C2620	C	C	U2435	C2374	U2314	G2253	C2192	C2132	G	C	G1948	U1888	A1828
U2681	G2621	C2560	C	U2436	G2375	G2315	U2254	U2193	U2133	U	U	G1949	G1889	G1829
C2682	C2622	A2561	U	G2437	G2376	G2316	A2255	C2194	G2134	A	U	G1952	U1890	U1830
U2683	G2623	U2562	U	A2438	G2377	A2317	A2256	C2195	U2135	G	G	G1953	A1891	U1831
C2684	G2624	C2563	U	U2439	U2378	U2318	G2257	C2196	C2136	A	C	G	U1892	G1832
C2685	C2625	U2564	A	G2440	C2379	U2319	U2258	C2197	U2137	C	U	G	A1893	G1833
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G2687	C2627	C2566	A	G2442	G2381	A2321	U2260	G2199	A2139	G	U	A	A1895	A1835
U2688	A2628	C2567	G2503	A2443	G2382	C2322	G2261	U2200	U2140	U	G	A	A1896	C1836
G2689	U2629	C2568	U2504	C2444	C2383	G2323	A2262	G2201	U2141	C	U	G	G1897	U1837
C2690	C2630	U2505	A	A	A2384	A2324	C2263	C2202	A2142	C	U	G	G1898	G1838
A2691	U2631	U2506	U	U	G2385	G2325	U2264	U2203	A2143	C	A	G	A1899	A1839
A2692	G2632	C2507	C	A	A2386	A2326	G2265	C2204	A2144	U	G	G	A1900	U1940
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A2695	A2635	U2510	G	G	C2389	C2329	G2269	A2207	A2147	C	C	C	U1903	A1843
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G2699	G2639	U2513	G	U	G2393	C2333	G2273	U2211	C2151	A	U	G	C1907	A1847
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A2701	U2641	A2515	A	U	G2395	U2335	A2275	U2215	A2153	U	C	U	A1909	C1849
A2702	A2642	U2516	G	G	C2396	G2336	G2276	A2216	U2154	U	U	C	A1910	A1850
A2703	U2643	U2517	U	U	A2397	C2337	C2277	G2216	G2155	A	U	A	A1911	G1851
A2704	C2644	C2518	A	A	A2398	C2338	C2278	U2217	C2156	G	G	G	U1912	G1852
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G2706	U2646	U2520	U	A	G2400	U2340	A2280	A2219	A2158	U	G	C	G1914	U1854
C2707	A2647	U2521	A	U	A2401	A2341	A2281	A2220	U2159	U	U	G	A1915	U1855
C2708	C2648	G2522	G	U	A2402	U2342	U2282	G2221	G2160	C	C	C	U1916	C1856
C2709	U2649	A2523	U	G	G2403	C2343	G2283	A2222	C2161	C	A	U	C1917	C1857
C2710	U2650	A2524	G	U	A2404	U2344	C2284	A2223	U2162	C	G	C	C1918	A1858
C2711	G2651	G2525	G	G	C2405	A2345	C2285	A2224	C2163	U	C	G	G1919	A1859
U2712	U2652	U2526	G	U	G2406	C2346	U2286	U2225	A2164	U	G	G	U1920	G1860
G2713	C2653	G2527	A	G	C2407	U2347	C2287	U2226	G2165	G	G	G	A1921	G1861
G2714	C2654	A2593	G	U	U2408	A2348	G2288	G2227	A2166	U	U	C	A1922	U1862
A2715	U2655	C2531	C	U	G2409	U2349	U2289	A2228	A2167	C	U	C	C1923	G1863
U2716	A2656	U2532	U	C	U2410	C2350	C2290	A2229	A2168	G	U	C	U1924	A1864
U2717	A2657	G2533	U	U	U2411	U2351	A2291	C2230	C2169	U	U	U	U1925	A1865
U2718	G2658	G2534	C	C	G2412	A2352	U2292	C2231	U2170	A	G	C	C1926	C1866
U2719	U2659	A2535	G	U	A2413	G2353	C2293	A2232	G2171	G	G	C	G1927	A1867
G2720	G2660	A2536	G	U	C2414	C2354	U2294	G2233	A2172	A	A	U	G1928	G1868
A2721	C2661	U2537	C	G	C2415	G2355	A2295	G2234	U2173	C	U	U	C1929	G1869
U2722	G2662	G2538	C	U	U2416	A2356	A2296	C2235	G2174	G	G	G	A1930	C1870
U2723	G2663	G2602	G	U	U2417	A2357	U2297	G2236	U2175	C	U	U	U1931	U1871
U2724	C2664	U2541	C	U	G2418	A2358	U2298	C2237	U2176	C	G	G	A1932	C1872
U2725	U2665	U2542	A	U	A2419	C2359	A2299	G2238	G2177	C	G	G	A1933	U1873
G2726	C2666	U2543	G	U	C2420	C2360	G2300	G2239	A2178	U	A	G	G1934	A1874
A2727	A2667	G2607	U	U	U2421	A2361	U2301	G2240	C2179	U	U	C	G1935	G1875
G2728	U2668	C2546	G	U	C2422	C2362	G2302	U2241	G2180	A2120	U	U	A1936	U1876
U2729	G2669	A2547	A	A	U2423	A2363	A2303	A2242	G2181	G2121	C	G	U1937	U1877
G2730	G2670	C2548	A	U	A	G2364	C2304	A2243	A2182	G2122	U	C	U1938	G1878
U2731	A2671	U2611	A	U	C2365	G2305	A2244	A2245	A2183	C2123	A	U	G1839	A1879
G2732	U2672	U2612	U	U	C2366	C2306	C2245	C2246	U2184	G2124	G	U	G1940	U1880
A2733	C2673	U2613	U	C	U2427	C2307	G2246	G2247	A2185	A2125	G	G	C1941	A1881
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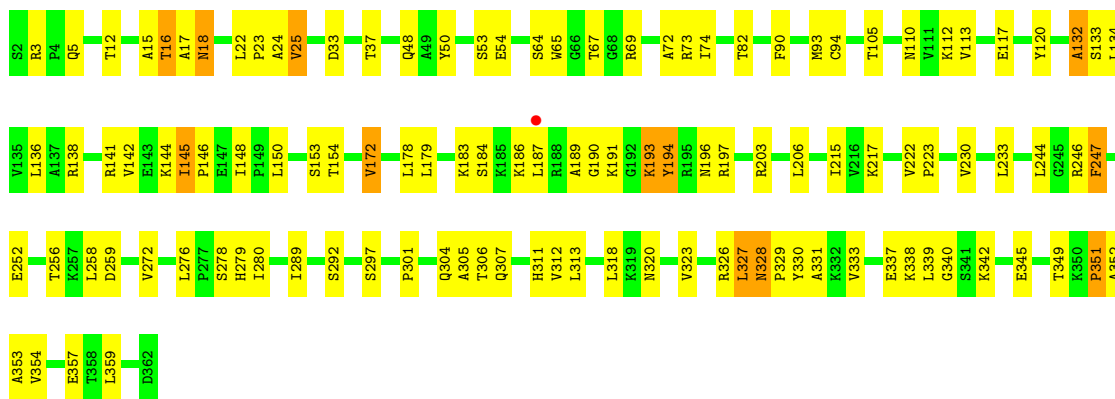
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



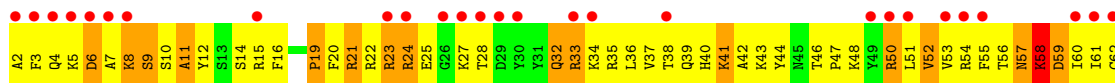
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:

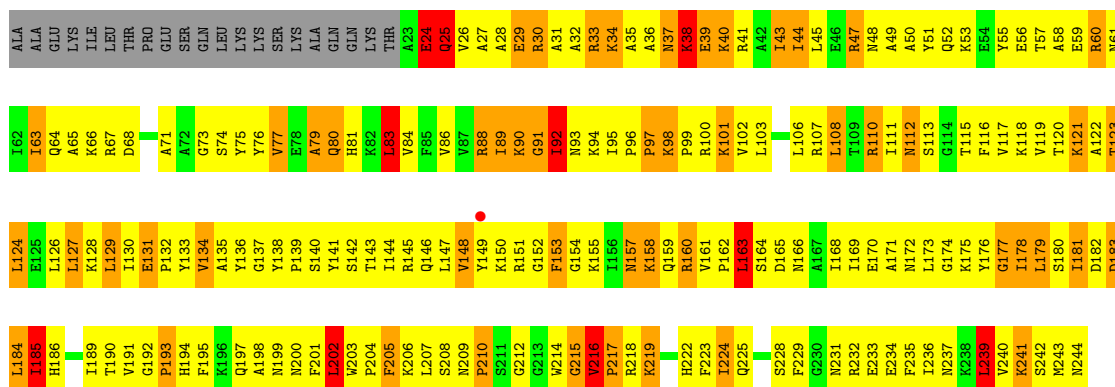


• Molecule 42: 60S ribosomal protein L5

Chain L5:

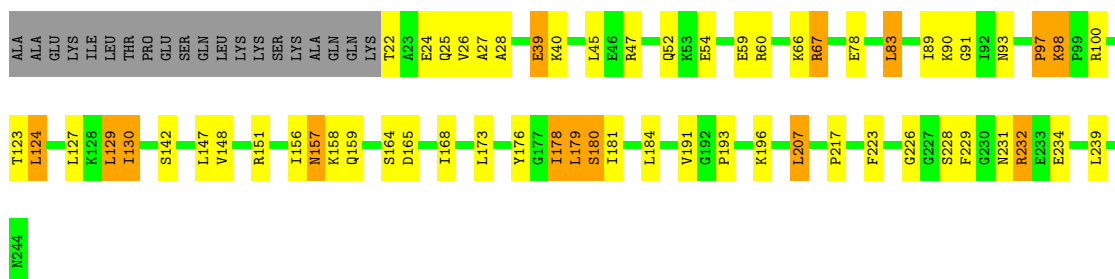


Chain L7:



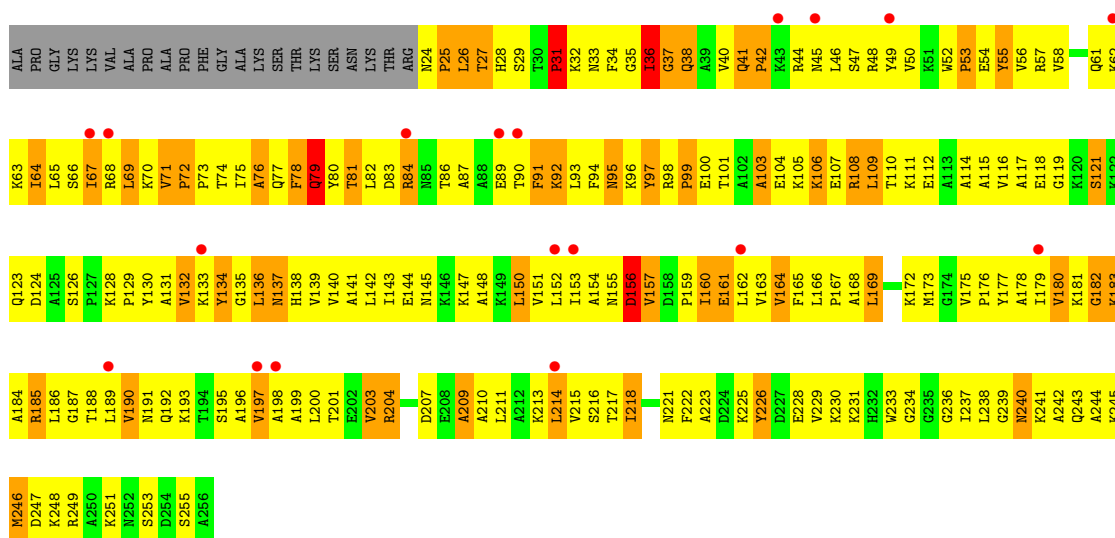
• Molecule 44: 60S ribosomal protein L7-A

Chain l7:



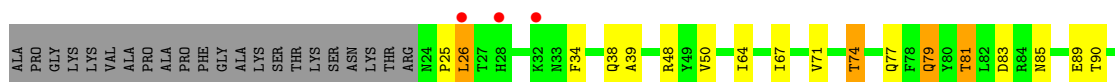
• Molecule 45: 60S ribosomal protein L8-A

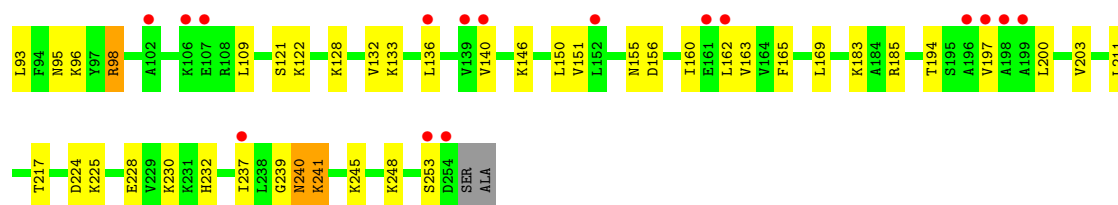
Chain L8:



• Molecule 45: 60S ribosomal protein L8-A

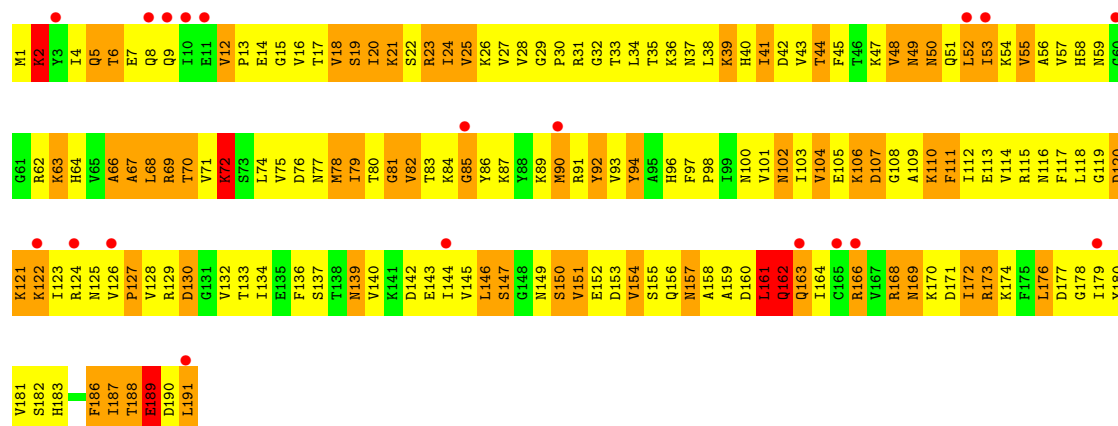
Chain l8:





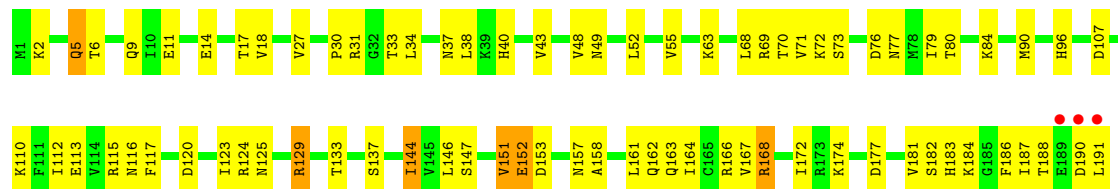
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



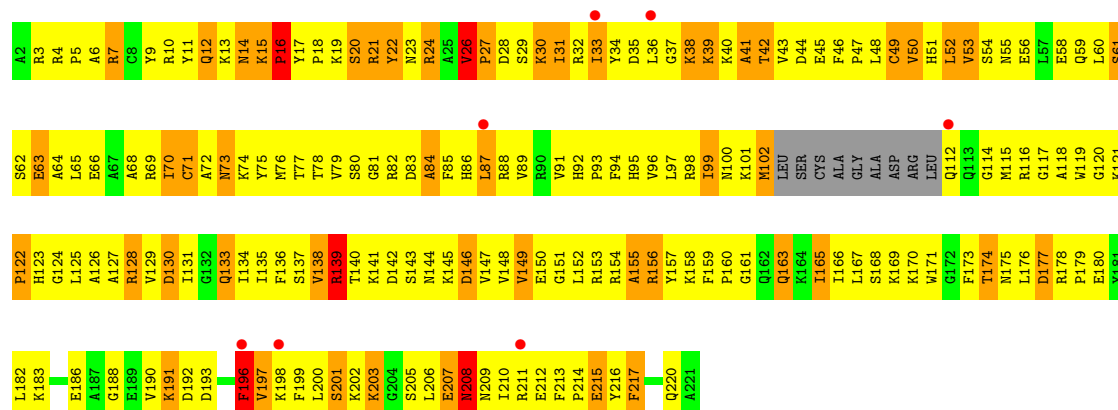
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



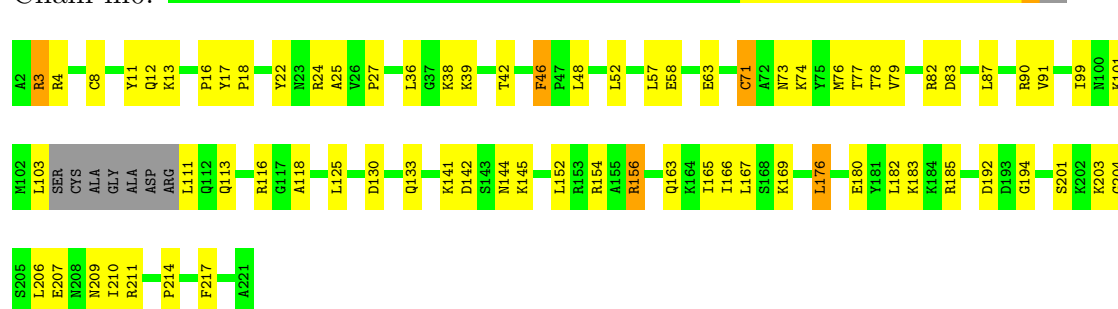
• Molecule 47: 60S ribosomal protein L10

Chain M0:



• Molecule 47: 60S ribosomal protein L10

Chain m0:



- Molecule 48: 60S ribosomal protein L11-B

Chain M1:



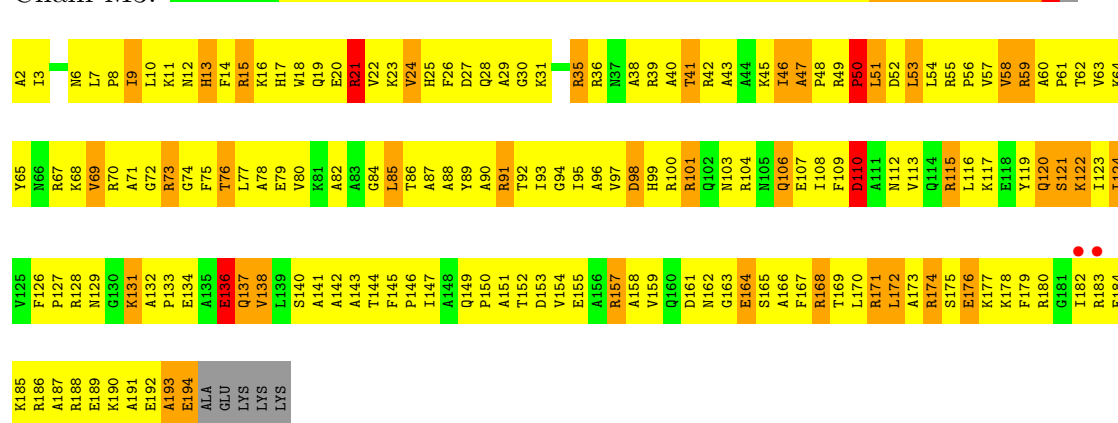
- Molecule 48: 60S ribosomal protein L11-B

Chain m1:



- Molecule 49: 60S ribosomal protein L13-A

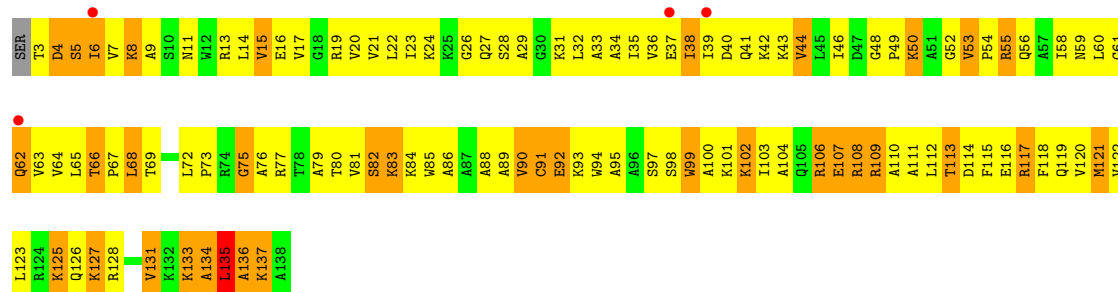
Chain M3:



- Molecule 49: 60S ribosomal protein L13-A

E199	R101	A2
A193	Q102	K5
E194	V113	L10
A195	K114	K11
GLU	R115	N12
LYS	L116	H13
LYS	I123	F14
LYS	I124	R15
	V125	K16
	N129	Q19
	G130	K23
	P133	V24
	E134	T41
	A135	R42
	V138	A43
	L139	A44
	S140	K45
	A141	L46
	T144	A47
	F145	P48
	A148	R49
	Q149	P50
	P150	L51
	A151	D52
	T152	L53
	D153	L54
	R157	V57
	A158	V58
	V159	R59
	Q160	A60
	D161	P61
	N162	T62
	G163	V63
	E164	K64
	R168	R67
	R171	K68
	R174	V69
	K177	T76
	R178	V80
	F179	G84
	R180	I93
	R183	G94
	E184	I95
	R186	A96
	A187	V97
	R189	R190

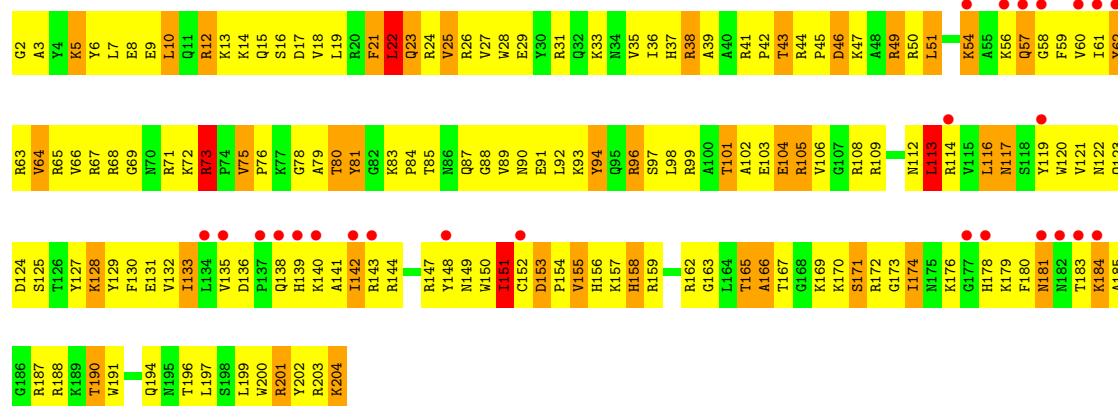
- Chain M4:



- Chain m4:

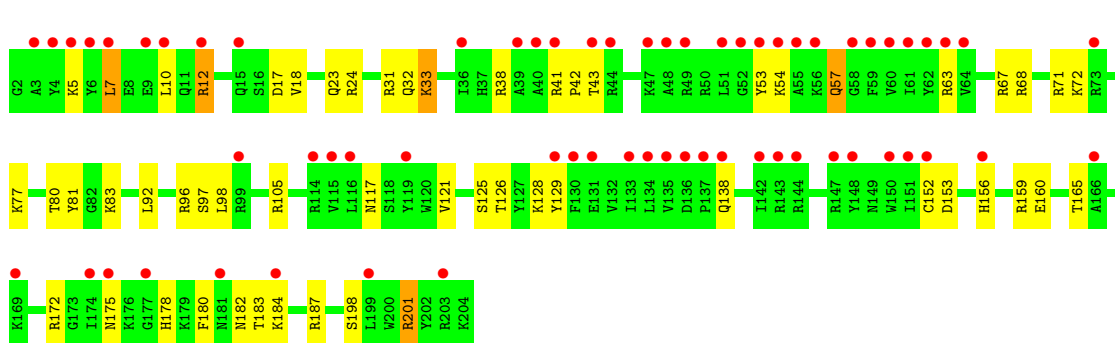


- Chain M5:



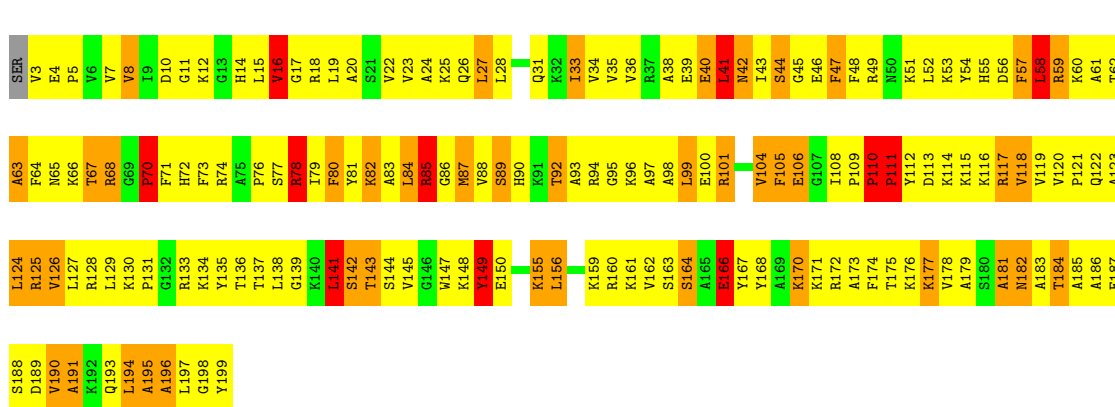
- WORLDWIDE
 **PDB**
PROTEIN DATA BANK

Chain m5:



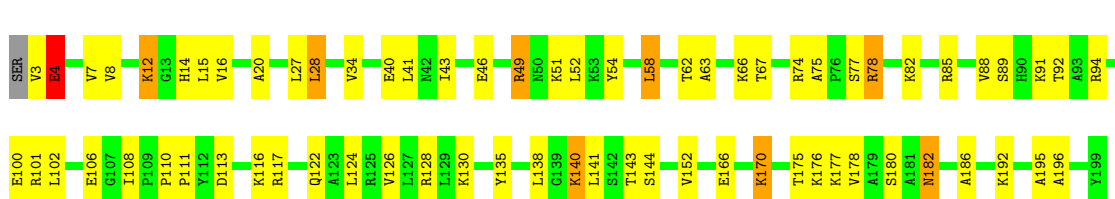
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:



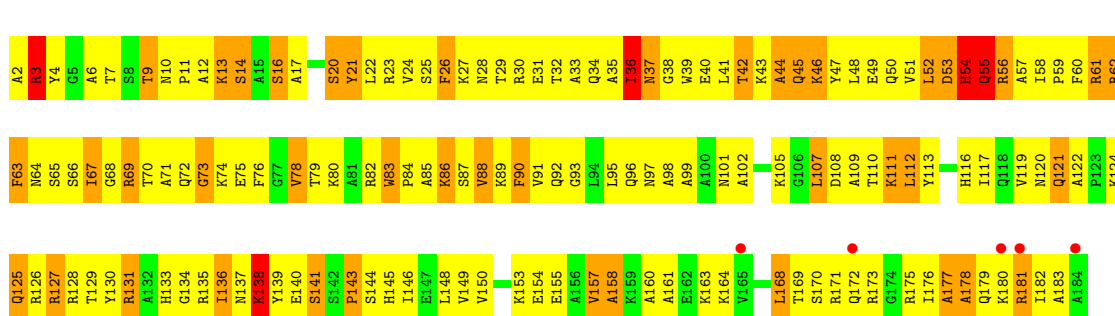
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:



- Molecule 53: 60S ribosomal protein L17-A

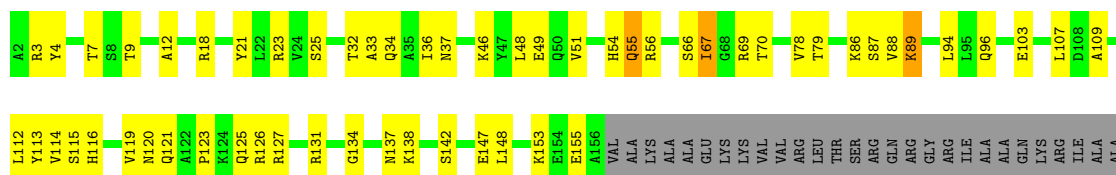
Chain M7:



- Molecule 53: 60S ribosomal protein L17-A

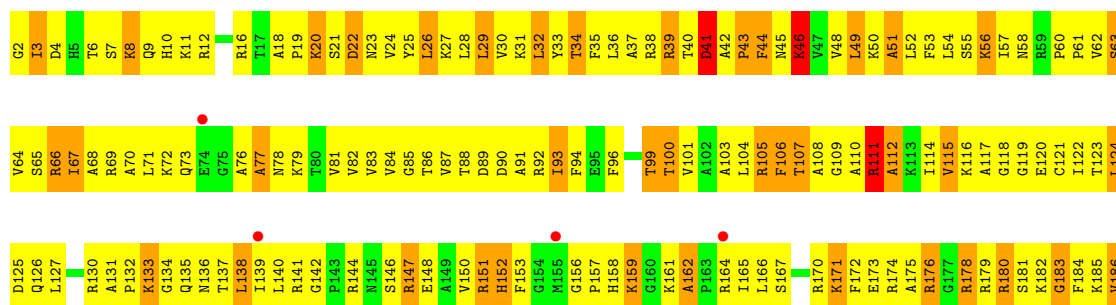
Chain m7:





• Molecule 54: 60S ribosomal protein L18-A

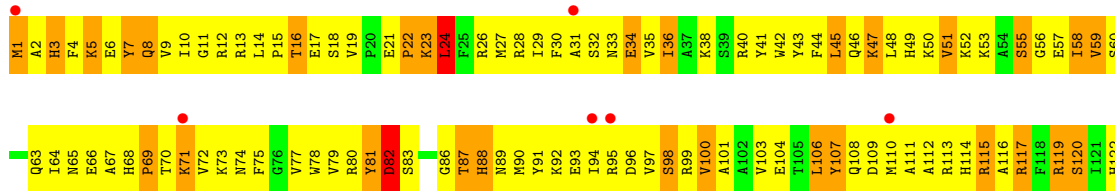
Chain M8:





- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



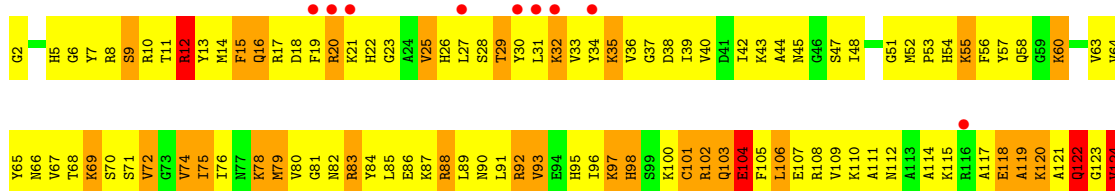
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:



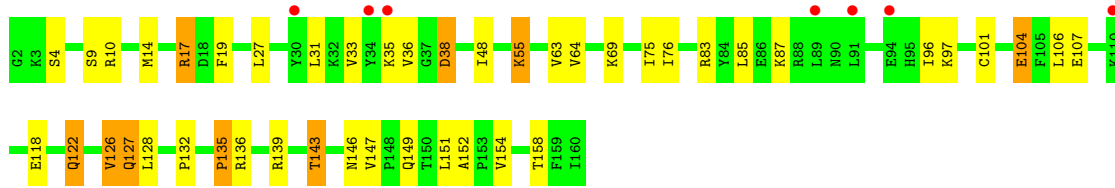
- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



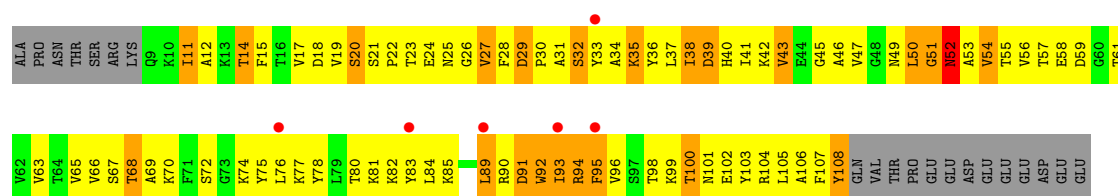
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:



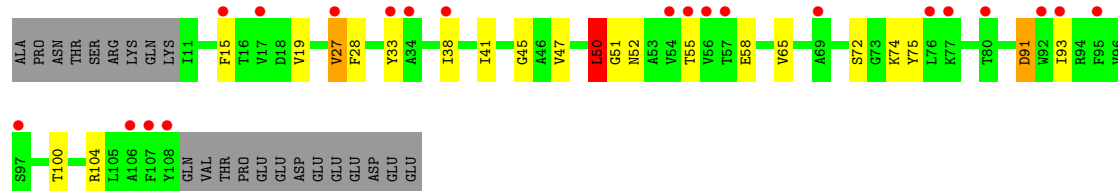
- Molecule 58: 60S ribosomal protein L22-A

Chain N2:



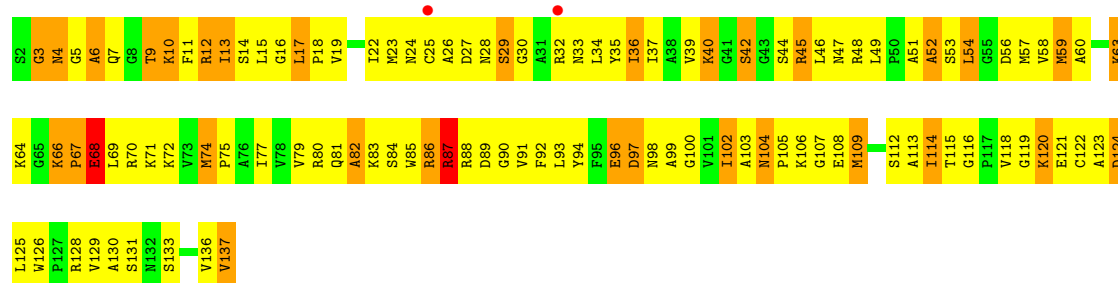
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



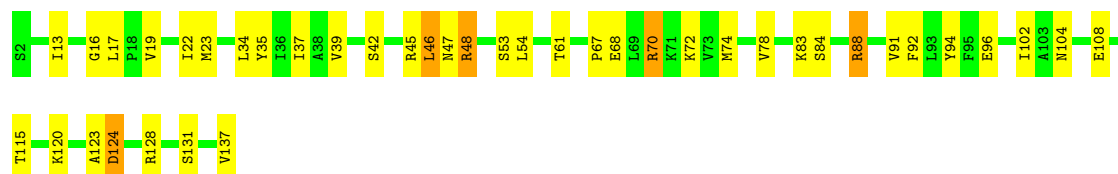
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



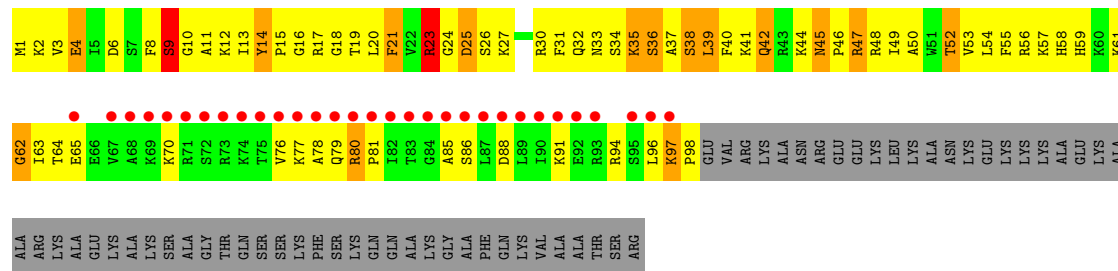
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



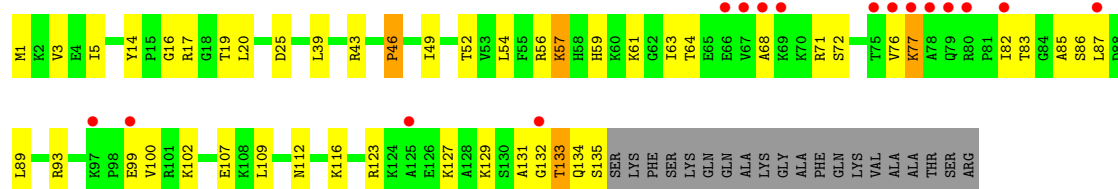
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



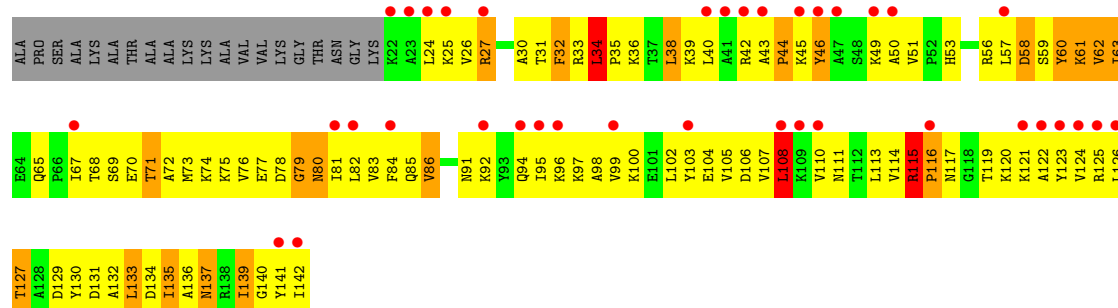
• Molecule 60: 60S ribosomal protein L24-A

Chain n4:



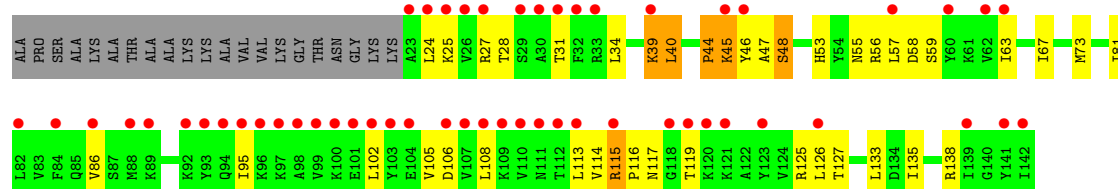
- Molecule 61: 60S ribosomal protein L25

Chain N5:



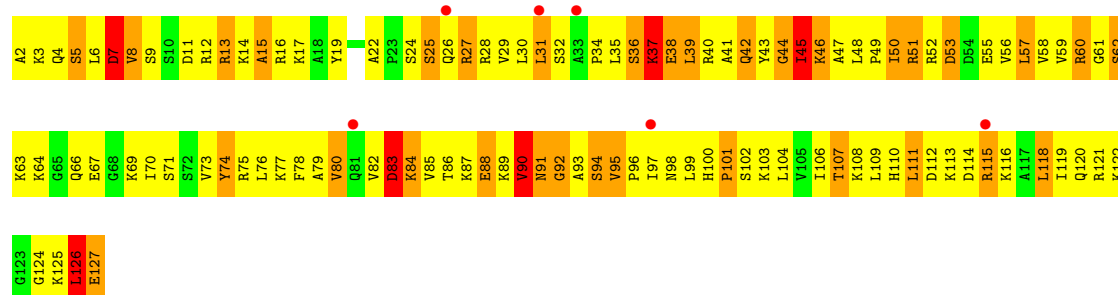
- Molecule 61: 60S ribosomal protein L25

Chain n5:



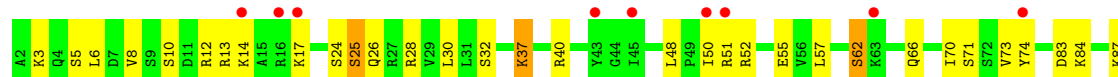
- Molecule 62: 60S ribosomal protein L26-A

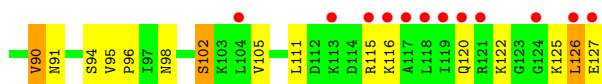
Chain N6:



- Molecule 62: 60S ribosomal protein L26-A

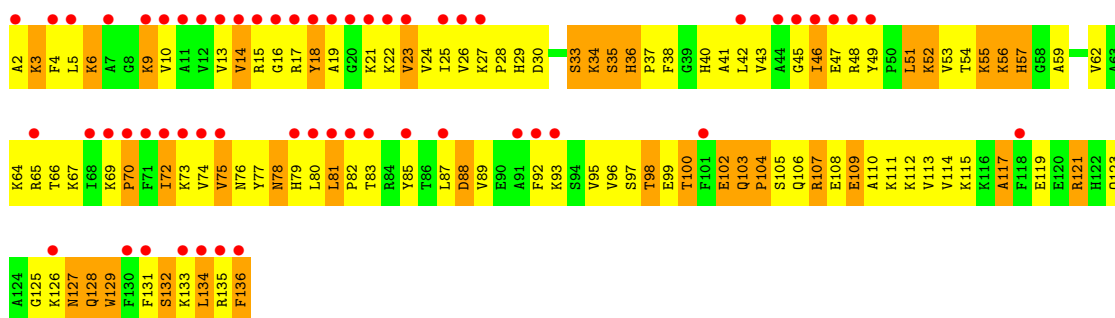
Chain n6:





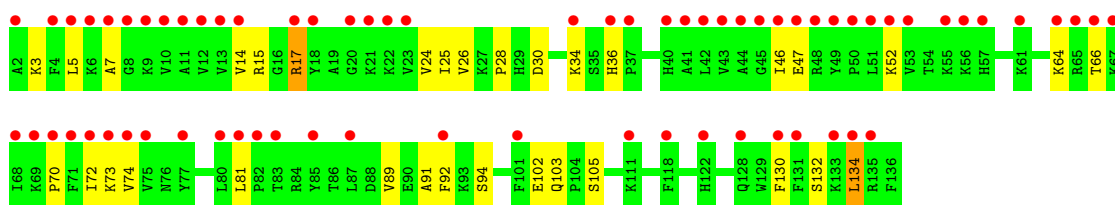
- Molecule 63: 60S ribosomal protein L27-A

Chain N7:



- Molecule 63: 60S ribosomal protein L27-A

Chain n7:

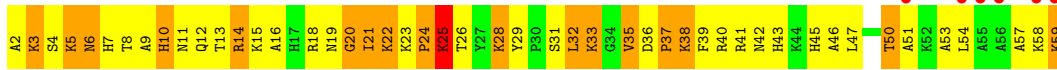


- Molecule 64: 60S ribosomal protein L28

Chain N8:

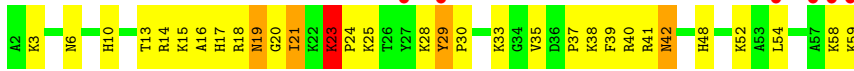


Chain N9: 



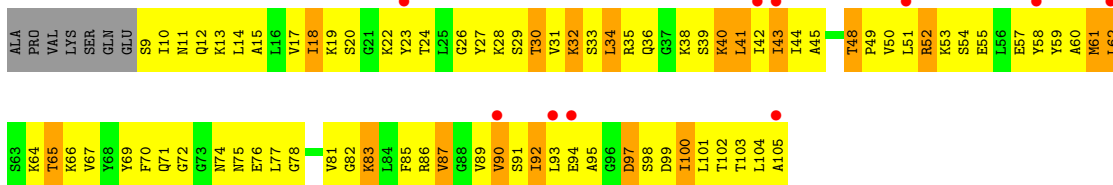
- Molecule 65: 60S ribosomal protein L29

Chain n9: 



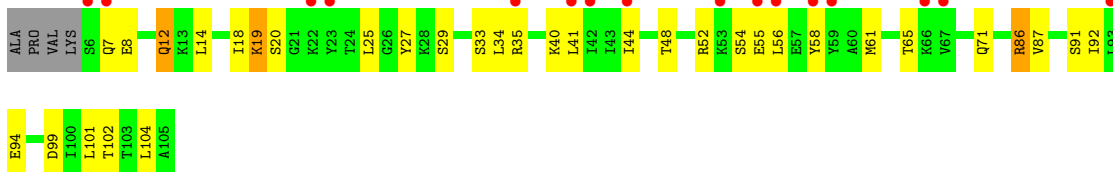
- Molecule 66: 60S ribosomal protein L30

Chain O0: 



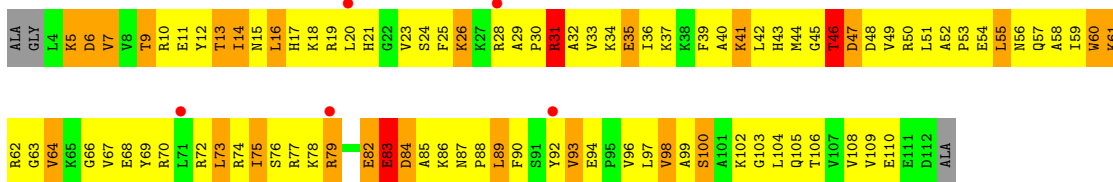
- Molecule 66: 60S ribosomal protein L30

Chain o0: 



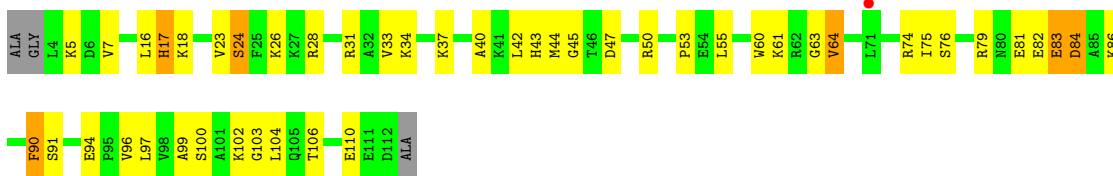
- Molecule 67: 60S ribosomal protein L31-A

Chain O1: 



- Molecule 67: 60S ribosomal protein L31-A

Chain o1: 



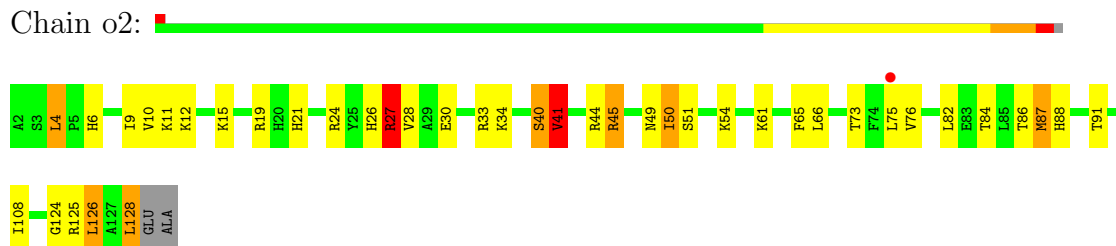
- Molecule 68: 60S ribosomal protein L32

Chain O2:



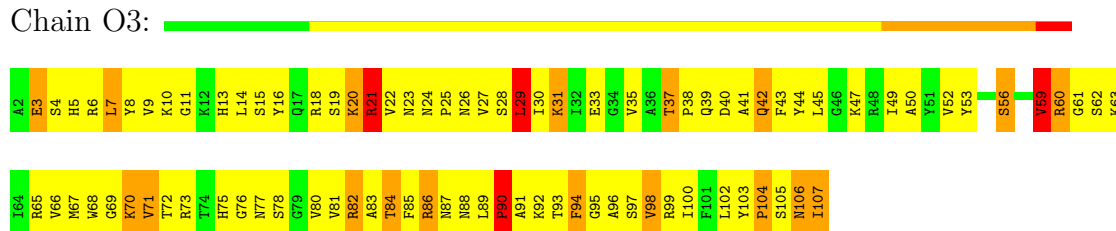
- Molecule 68: 60S ribosomal protein L32

Chain o2:



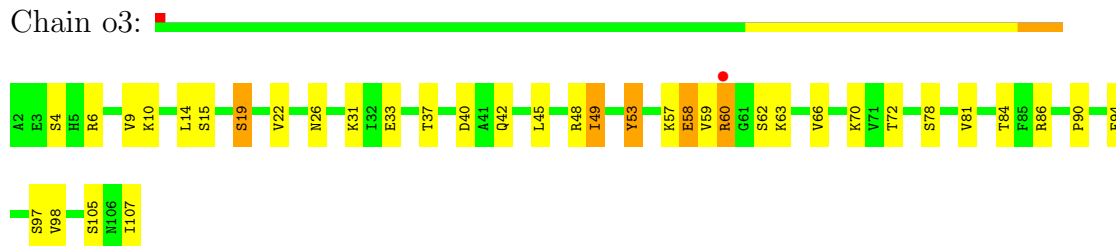
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



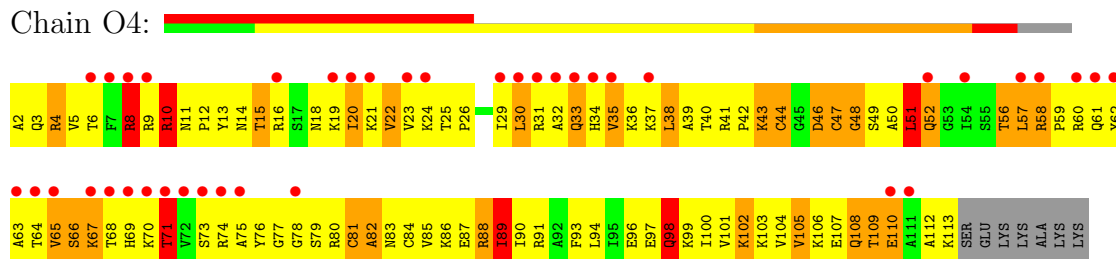
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



- Molecule 70: 60S ribosomal protein L34-A

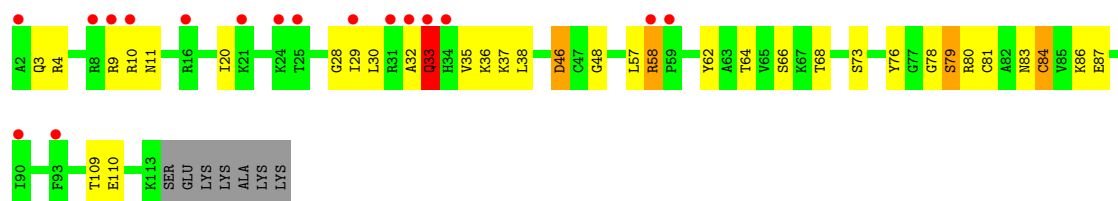
Chain O4:



- Molecule 70: 60S ribosomal protein L34-A

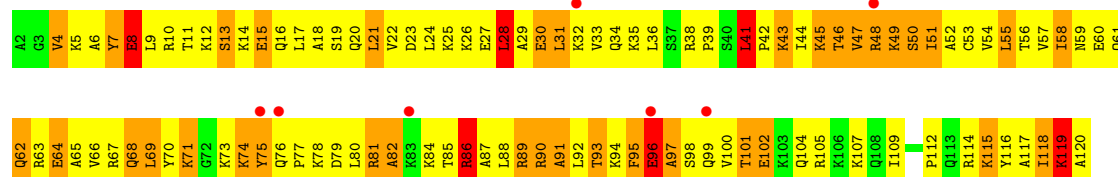
Chain o4:





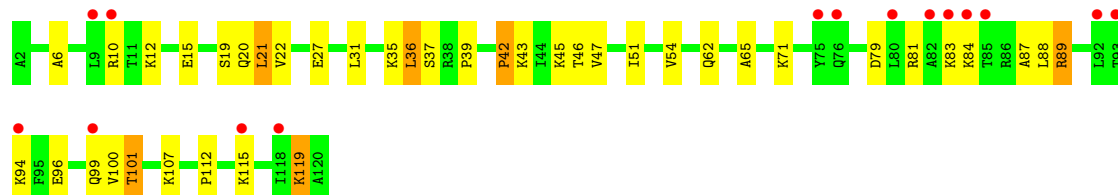
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



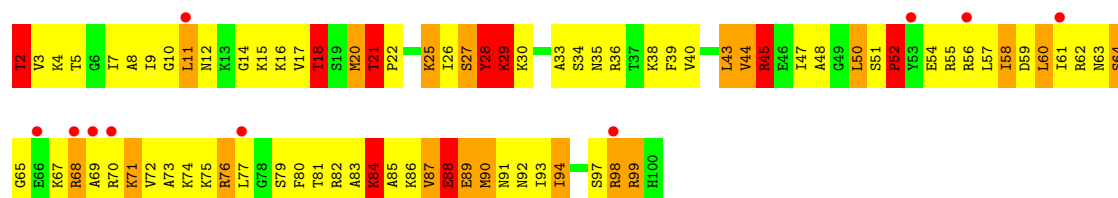
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:



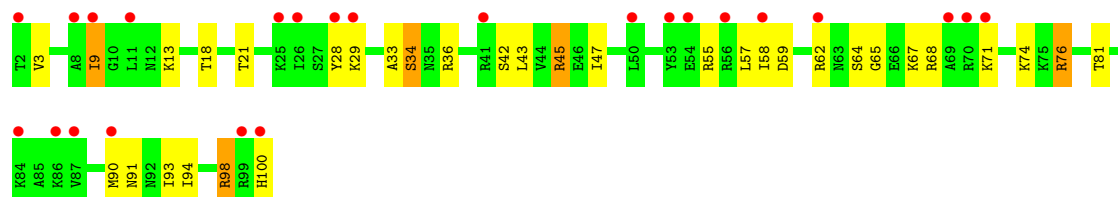
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:



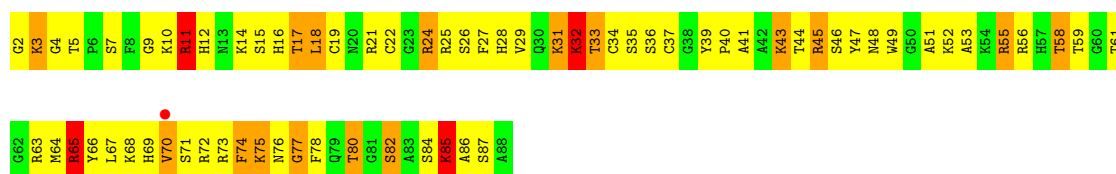
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



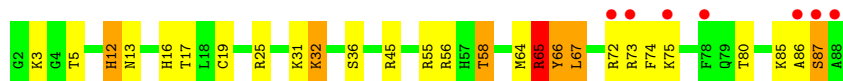
- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



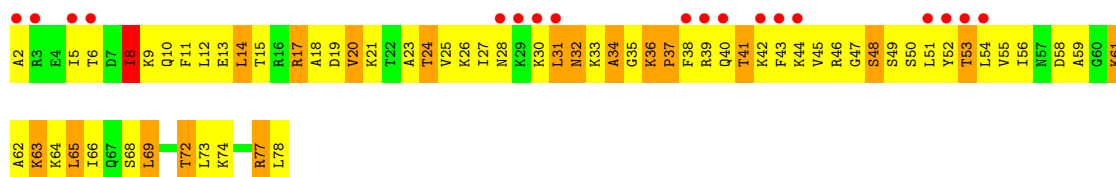
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



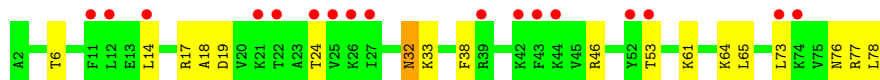
- Molecule 74: 60S ribosomal protein L38

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:



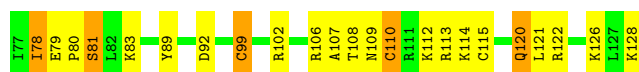
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



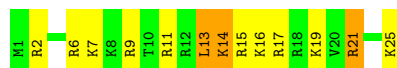
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



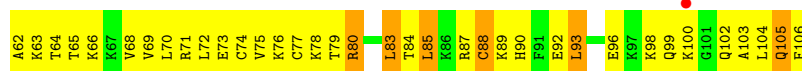
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:



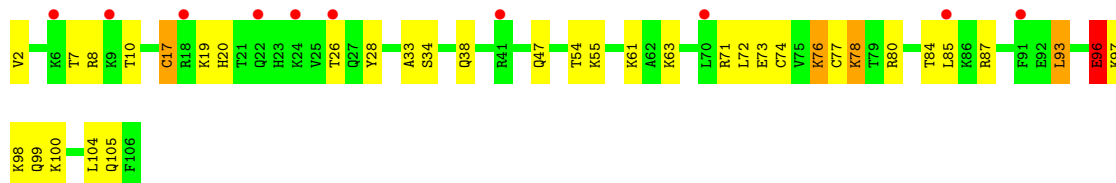
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



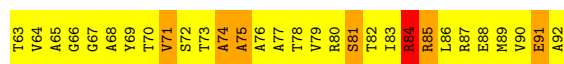
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:



- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



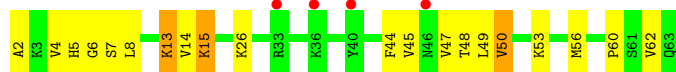
- Molecule 79: 60S ribosomal protein L43-A

Chain q3:



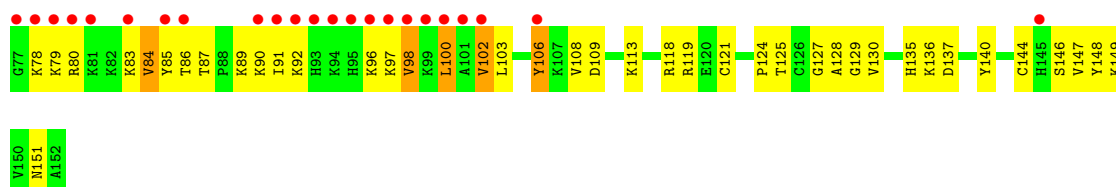
- Molecule 80: 40S ribosomal protein S30-A

Chain e0: 



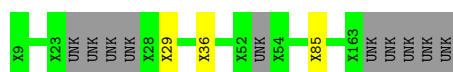
- Molecule 81: Ubiquitin-40S ribosomal protein S31

Chain e1: 



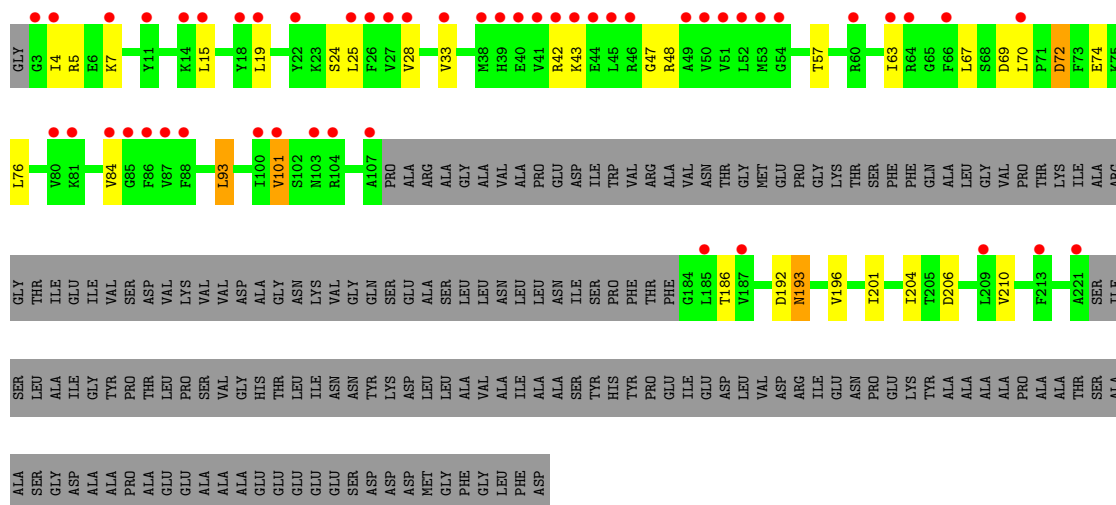
- Molecule 82: unknown protein chain m2

Chain m2: 



- Molecule 83: 60S acidic ribosomal protein P0

Chain p0: 



- Molecule 84: unknown protein chain p1

Chain p1: 

There are no outlier residues recorded for this chain.

- Molecule 85: unknown protein chain p2

Chain p2: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	437.00Å 286.75Å 305.18Å 90.00° 99.24° 90.00°	Depositor
Resolution (Å)	135.58 – 3.60 143.38 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (135.58-3.60) 99.9 (143.38-3.60)	Depositor EDS
R_{merge}	0.52	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.190 , 0.267 0.284 , 0.349	Depositor DCC
R_{free} test set	10648 reflections (1.25%)	DCC
Wilson B-factor (Å ²)	115.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 87.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 855155 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	411095	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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, GET

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	1.08	91/41698 (0.2%)	1.83	1528/64972 (2.4%)
1	6	1.44	367/42663 (0.9%)	2.19	2982/66472 (4.5%)
2	S0	0.60	0/1617	0.83	0/2215
2	s0	0.75	0/1623	0.92	1/2222 (0.0%)
3	S1	0.46	0/1735	0.74	0/2335
3	s1	0.67	0/1748	0.87	3/2352 (0.1%)
4	S2	0.74	2/1665 (0.1%)	0.90	2/2263 (0.1%)
4	s2	0.87	1/1665 (0.1%)	1.01	4/2263 (0.2%)
5	S3	0.72	0/1759	0.86	1/2368 (0.0%)
5	s3	0.72	0/1759	0.89	1/2368 (0.0%)
6	S4	0.65	0/2109	0.86	2/2839 (0.1%)
6	s4	0.77	0/2109	0.90	1/2839 (0.0%)
7	S5	0.54	0/1629	0.76	0/2202
7	s5	0.89	1/1629 (0.1%)	1.02	4/2202 (0.2%)
8	S6	0.64	0/1823	0.79	0/2439
8	s6	0.88	0/1779	0.99	2/2379 (0.1%)
9	S7	0.54	0/1506	0.75	0/2028
9	s7	0.68	0/1516	0.91	2/2043 (0.1%)
10	S8	0.79	0/1514	0.92	1/2021 (0.0%)
10	s8	0.86	0/1514	0.94	1/2021 (0.0%)
11	S9	0.65	0/1519	0.84	1/2035 (0.0%)
11	s9	0.79	0/1519	0.91	2/2035 (0.1%)
12	C0	0.66	0/790	0.86	2/1069 (0.2%)
12	c0	0.56	0/777	0.87	2/1049 (0.2%)
13	C1	0.82	0/1240	0.88	0/1675
13	c1	0.91	0/1194	1.00	2/1610 (0.1%)
14	C2	0.51	0/900	0.80	1/1224 (0.1%)
14	c2	0.46	0/900	0.69	1/1224 (0.1%)
15	C3	0.59	0/1215	0.76	0/1638
15	c3	0.80	0/1215	0.96	2/1638 (0.1%)
16	C4	0.50	0/901	0.79	0/1217
16	c4	0.76	0/960	0.91	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.69	0/998	0.81	0/1341
17	c5	0.89	0/1060	1.05	3/1426 (0.2%)
18	C6	0.60	0/1125	0.89	3/1510 (0.2%)
18	c6	0.93	0/1131	1.06	2/1518 (0.1%)
19	C7	0.59	0/935	0.87	3/1254 (0.2%)
19	c7	0.80	0/914	0.91	1/1224 (0.1%)
20	C8	0.61	0/1211	0.82	0/1628
20	c8	0.92	2/1211 (0.2%)	1.08	5/1628 (0.3%)
21	C9	0.61	0/1130	0.83	0/1517
21	c9	0.94	1/1130 (0.1%)	1.01	2/1517 (0.1%)
22	D0	0.65	0/865	0.83	0/1169
22	d0	0.79	0/892	0.97	1/1205 (0.1%)
23	D1	0.65	0/693	0.88	2/935 (0.2%)
23	d1	0.79	0/693	0.92	0/935
24	D2	0.63	0/1038	0.89	1/1395 (0.1%)
24	d2	0.88	0/1038	0.98	1/1395 (0.1%)
25	D3	0.90	1/1139 (0.1%)	1.04	1/1518 (0.1%)
25	d3	1.17	5/1139 (0.4%)	1.14	4/1518 (0.3%)
26	D4	0.66	0/1087	0.80	0/1449
26	d4	0.77	0/1087	0.92	0/1449
27	D5	0.61	0/571	0.84	0/768
27	d5	0.81	0/566	0.96	0/761
28	D6	0.66	0/782	0.84	0/1047
28	d6	0.81	0/782	0.92	1/1047 (0.1%)
29	D7	0.53	0/620	0.81	1/838 (0.1%)
29	d7	0.67	0/620	0.93	2/838 (0.2%)
30	D8	0.49	0/499	0.74	0/670
30	d8	0.76	0/499	0.97	1/670 (0.1%)
31	D9	0.75	0/452	0.86	0/600
31	d9	0.97	0/452	0.97	0/600
32	E0	0.69	0/483	0.87	0/643
33	E1	0.65	0/577	0.90	0/770
34	SR	0.54	0/2494	0.72	0/3393
34	sR	0.69	0/2495	0.85	2/3395 (0.1%)
35	SM	0.72	0/1113	0.91	2/1502 (0.1%)
35	sM	0.77	0/682	0.98	1/921 (0.1%)
36	1	1.76	1434/75394 (1.9%)	2.53	7929/117545 (6.7%)
36	5	1.87	1867/75414 (2.5%)	2.61	8463/117575 (7.2%)
37	3	1.50	28/2883 (1.0%)	2.28	214/4491 (4.8%)
37	7	2.04	91/2883 (3.2%)	2.85	410/4491 (9.1%)
38	4	1.54	29/3746 (0.8%)	2.42	331/5832 (5.7%)
38	8	1.43	34/3746 (0.9%)	2.16	250/5832 (4.3%)
39	L2	0.98	1/1948 (0.1%)	1.08	2/2617 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	l2	0.96	1/1946 (0.1%)	1.03	4/2614 (0.2%)
40	L3	1.12	3/3146 (0.1%)	1.12	11/4228 (0.3%)
40	l3	1.32	9/3146 (0.3%)	1.24	17/4228 (0.4%)
41	L4	1.03	0/2800	1.15	13/3790 (0.3%)
41	l4	1.02	1/2800 (0.0%)	1.11	5/3790 (0.1%)
42	L5	0.84	1/2425 (0.0%)	0.97	2/3271 (0.1%)
42	l5	1.16	2/2408 (0.1%)	1.08	3/3248 (0.1%)
43	L6	1.15	2/1260 (0.2%)	1.17	4/1694 (0.2%)
43	l6	1.18	2/1269 (0.2%)	1.15	3/1705 (0.2%)
44	L7	1.09	0/1821	1.13	9/2451 (0.4%)
44	l7	1.26	3/1828 (0.2%)	1.17	7/2461 (0.3%)
45	L8	0.74	0/1836	0.91	0/2481
45	l8	0.72	0/1795	0.86	1/2429 (0.0%)
46	L9	0.97	0/1539	1.07	1/2073 (0.0%)
46	l9	1.33	4/1539 (0.3%)	1.23	8/2073 (0.4%)
47	M0	1.02	4/1741 (0.2%)	1.04	1/2335 (0.0%)
47	m0	1.23	5/1758 (0.3%)	1.20	7/2358 (0.3%)
48	M1	0.80	1/1374 (0.1%)	0.93	3/1842 (0.2%)
48	m1	1.09	3/1374 (0.2%)	1.09	5/1842 (0.3%)
49	M3	0.96	2/1568 (0.1%)	1.09	4/2106 (0.2%)
49	m3	0.87	0/1573	1.02	0/2113
50	M4	1.10	0/1068	1.13	1/1438 (0.1%)
50	m4	1.30	1/1074 (0.1%)	1.15	3/1446 (0.2%)
51	M5	0.97	0/1757	1.04	5/2354 (0.2%)
51	m5	0.84	0/1757	0.93	2/2354 (0.1%)
52	M6	1.25	6/1585 (0.4%)	1.28	12/2128 (0.6%)
52	m6	1.54	9/1585 (0.6%)	1.38	14/2128 (0.7%)
53	M7	1.21	3/1443 (0.2%)	1.09	3/1944 (0.2%)
53	m7	1.18	1/1250 (0.1%)	1.19	2/1683 (0.1%)
54	M8	1.03	0/1465	1.12	5/1965 (0.3%)
54	m8	0.98	1/1465 (0.1%)	1.06	3/1965 (0.2%)
55	M9	0.84	0/1538	0.92	3/2050 (0.1%)
55	m9	0.88	1/1538 (0.1%)	0.92	2/2050 (0.1%)
56	N0	1.05	0/1481	1.10	5/1990 (0.3%)
56	n0	1.46	7/1481 (0.5%)	1.21	5/1990 (0.3%)
57	N1	1.09	1/1300 (0.1%)	1.10	4/1743 (0.2%)
57	n1	1.28	6/1300 (0.5%)	1.17	5/1743 (0.3%)
58	N2	0.73	1/812 (0.1%)	0.89	1/1099 (0.1%)
58	n2	0.73	0/794	0.84	1/1076 (0.1%)
59	N3	1.09	2/1018 (0.2%)	1.07	3/1369 (0.2%)
59	n3	1.35	7/1018 (0.7%)	1.28	7/1369 (0.5%)
60	N4	0.90	0/712	0.98	1/958 (0.1%)
60	n4	1.04	0/1052	1.04	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	N5	0.86	1/979 (0.1%)	1.00	4/1321 (0.3%)
61	n5	0.85	0/974	1.03	2/1314 (0.2%)
62	N6	0.92	0/1004	1.11	6/1341 (0.4%)
62	n6	0.89	0/1004	1.02	5/1341 (0.4%)
63	N7	0.68	0/1118	0.89	1/1497 (0.1%)
63	n7	0.67	0/1118	0.83	0/1497
64	N8	1.05	0/1204	1.10	5/1612 (0.3%)
64	n8	0.98	1/1204 (0.1%)	1.08	2/1612 (0.1%)
65	N9	0.98	0/473	1.07	1/629 (0.2%)
65	n9	1.12	1/473 (0.2%)	1.33	3/629 (0.5%)
66	O0	0.71	0/751	0.87	0/1008
66	o0	0.69	0/775	0.88	2/1040 (0.2%)
67	O1	0.90	0/890	1.00	1/1196 (0.1%)
67	o1	1.13	2/897 (0.2%)	1.20	3/1205 (0.2%)
68	O2	1.21	2/1041 (0.2%)	1.20	4/1394 (0.3%)
68	o2	1.15	2/1041 (0.2%)	1.13	5/1394 (0.4%)
69	O3	1.32	2/868 (0.2%)	1.23	3/1168 (0.3%)
69	o3	1.38	3/868 (0.3%)	1.19	2/1168 (0.2%)
70	O4	0.84	0/890	1.00	4/1189 (0.3%)
70	o4	0.83	1/890 (0.1%)	0.99	2/1189 (0.2%)
71	O5	0.98	2/978 (0.2%)	1.09	2/1301 (0.2%)
71	o5	0.82	0/974	0.89	1/1297 (0.1%)
72	O6	0.84	0/778	0.98	1/1034 (0.1%)
72	o6	0.79	0/777	0.98	1/1033 (0.1%)
73	O7	1.08	0/696	1.20	4/923 (0.4%)
73	o7	0.99	0/696	1.07	3/923 (0.3%)
74	O8	0.72	0/618	0.84	0/826
74	o8	0.66	0/614	0.90	0/822
75	O9	1.05	0/443	1.19	3/588 (0.5%)
75	o9	0.82	0/443	0.99	0/588
76	Q0	1.04	2/423 (0.5%)	1.14	1/562 (0.2%)
76	q0	1.58	3/423 (0.7%)	1.44	5/562 (0.9%)
77	Q1	0.76	0/234	1.11	2/300 (0.7%)
77	q1	1.03	0/234	1.30	3/300 (1.0%)
78	Q2	1.12	1/860 (0.1%)	1.07	2/1136 (0.2%)
78	q2	1.13	2/860 (0.2%)	1.09	2/1136 (0.2%)
79	Q3	1.04	0/701	1.10	3/934 (0.3%)
79	q3	1.07	1/701 (0.1%)	1.05	0/934
80	e0	0.81	0/499	0.95	0/665
81	e1	0.51	0/619	0.87	0/822
83	p0	0.75	0/1091	0.85	0/1472
All	All	1.39	4070/429970 (0.9%)	1.97	22469/631198 (3.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S0	0	2
2	s0	0	2
3	s1	0	3
5	S3	0	2
5	s3	0	2
6	s4	0	2
7	s5	0	3
9	s7	0	1
11	S9	0	2
11	s9	0	1
12	C0	0	2
15	c3	0	1
16	C4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	3
19	C7	0	1
19	c7	0	2
20	c8	0	1
21	c9	0	1
22	d0	0	1
23	D1	0	1
24	D2	0	1
24	d2	0	2
25	D3	0	2
26	D4	0	1
26	d4	0	2
27	D5	0	1
27	d5	0	1
28	D6	0	1
28	d6	0	1
33	E1	0	2
35	SM	0	1
39	l2	0	2
40	L3	0	3
40	l3	0	5
41	L4	0	5
41	l4	0	2
42	L5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	l5	0	3
43	L6	0	2
43	l6	0	1
44	L7	0	2
44	l7	0	3
45	l8	0	1
47	M0	0	2
47	m0	0	1
48	m1	0	1
49	m3	0	2
52	M6	0	2
52	m6	0	2
53	M7	0	1
53	m7	0	2
54	m8	0	1
56	n0	0	2
57	N1	0	1
57	n1	0	1
60	n4	0	1
61	n5	0	1
63	N7	0	2
64	N8	0	4
64	n8	0	2
65	N9	0	2
65	n9	0	1
67	o1	0	1
68	o2	0	2
69	O3	0	2
70	O4	0	2
70	o4	0	2
72	O6	0	1
76	q0	0	1
80	e0	0	2
81	e1	0	1
82	m2	0	3
83	p0	0	1
All	All	0	130

The worst 5 of 4070 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	15.17	2.08	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	806	A	N9-C4	-14.79	1.28	1.37
37	7	89	G	C6-O6	14.62	1.37	1.24
36	5	2397	A	N9-C4	-14.38	1.29	1.37
36	5	2875	U	N1-C2	13.97	1.51	1.38

The worst 5 of 22469 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-25.15	110.91	126.00
37	7	44	C	C6-N1-C2	24.27	130.01	120.30
36	5	648	C	N3-C4-C5	-23.62	112.45	121.90
36	5	884	A	N1-C6-N6	23.07	132.44	118.60
38	4	94	C	C6-N1-C2	22.99	129.50	120.30

There are no chirality outliers.

5 of 130 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S0	29	VAL	Peptide
2	S0	6	THR	Peptide
5	S3	144	ALA	Peptide
5	S3	42	THR	Peptide
11	S9	15	PRO	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	18756	1861	1
1	6	38149	0	19193	1847	0
2	S0	1577	0	1567	285	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	250	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	294	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	255	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	301	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	285	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	249	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	204	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	248	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	265	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	130	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	170	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	121	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	184	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	189	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	193	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	215	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	152	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	227	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	199	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	149	0
22	d0	882	0	939	0	1
23	D1	684	0	672	140	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	148	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	190	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	180	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	94	0
27	d5	558	0	598	0	0
28	D6	769	0	815	167	0
28	d6	769	0	814	0	0
29	D7	610	0	632	87	0
29	d7	610	0	632	0	0
30	D8	497	0	535	65	0
30	d8	497	0	535	0	0
31	D9	442	0	428	83	0
31	d9	442	0	428	0	0
32	E0	475	0	525	71	0
33	E1	566	0	601	93	0
34	SR	2441	0	2397	334	0
34	sR	2442	0	2392	0	2
35	SM	1104	0	996	156	0
35	sM	679	0	603	0	0
36	1	67355	0	33811	2977	1
36	5	67376	0	33824	2966	0
37	3	2579	0	1304	98	0
37	7	2579	0	1302	119	0
38	4	3353	0	1695	182	0
38	8	3353	0	1695	176	0
39	L2	1914	0	1981	336	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	507	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	484	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	406	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	196	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	321	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	278	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	271	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	322	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	221	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	268	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	190	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	279	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	285	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	228	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	236	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	258	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	224	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	232	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	104	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	144	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	90	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	145	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	174	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	166	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	231	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	81	0
65	n9	462	0	491	0	0
66	O0	743	0	797	113	0
66	o0	767	0	816	0	0
67	O1	876	0	912	142	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	157	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	o2	1020	0	1090	0	0
69	O3	850	0	880	153	0
69	o3	850	0	880	0	0
70	O4	880	0	945	171	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	177	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	155	0
72	o6	770	0	846	0	0
73	O7	681	0	684	117	0
73	o7	681	0	685	0	0
74	O8	612	0	682	93	0
74	o8	608	0	671	0	0
75	O9	436	0	475	86	0
75	o9	436	0	475	0	0
76	Q0	417	0	456	91	0
76	q0	417	0	456	0	0
77	Q1	233	0	284	44	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	135	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	134	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	e1	608	0	656	0	0
82	m2	750	0	175	0	0
83	p0	1076	0	1040	0	0
84	p1	235	0	51	0	0
85	p2	230	0	52	0	0
86	1	468	0	0	0	0
86	2	124	0	0	0	0
86	3	14	0	0	0	0
86	4	23	0	0	0	0
86	5	499	0	0	0	0
86	6	150	0	0	0	0
86	7	15	0	0	0	0
86	8	17	0	0	0	0
86	D3	1	0	0	0	0
86	D4	1	0	0	0	0
86	L2	2	0	0	0	0
86	L3	2	0	0	0	0
86	L4	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L5	1	0	0	0	0
86	L6	2	0	0	0	0
86	L7	2	0	0	0	0
86	L8	1	0	0	0	0
86	M0	3	0	0	0	0
86	M1	1	0	0	0	0
86	M3	2	0	0	0	0
86	M5	2	0	0	0	0
86	M6	1	0	0	0	0
86	M7	5	0	0	0	0
86	M9	1	0	0	0	0
86	N0	1	0	0	0	0
86	N3	2	0	0	0	0
86	N5	2	0	0	0	0
86	N6	1	0	0	0	0
86	N8	4	0	0	0	0
86	N9	1	0	0	0	0
86	O1	1	0	0	0	0
86	O2	1	0	0	0	0
86	O3	1	0	0	0	0
86	O5	1	0	0	0	0
86	O7	1	0	0	0	0
86	S2	2	0	0	0	0
86	S8	1	0	0	0	0
86	SM	1	0	0	0	0
86	c7	1	0	0	0	0
86	c8	1	0	0	0	0
86	d3	1	0	0	0	0
86	d6	1	0	0	0	0
86	l2	1	0	0	0	0
86	l3	6	0	0	0	0
86	l4	1	0	0	0	0
86	l5	3	0	0	0	0
86	l7	2	0	0	0	0
86	l9	1	0	0	0	0
86	m0	1	0	0	0	0
86	m1	1	0	0	0	0
86	m4	1	0	0	0	0
86	m5	2	0	0	0	0
86	m6	3	0	0	0	0
86	m7	4	0	0	0	0
86	n3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	n4	1	0	0	0	0
86	n8	2	0	0	0	0
86	n9	2	0	0	0	0
86	o0	1	0	0	0	0
86	o1	1	0	0	0	0
86	o2	1	0	0	0	0
86	o3	2	0	0	0	0
86	o4	1	0	0	0	0
86	q0	2	0	0	0	0
86	q1	1	0	0	0	0
86	q3	2	0	0	0	0
86	s1	1	0	0	0	0
86	s2	1	0	0	0	0
86	s8	2	0	0	0	0
87	1	2429	0	0	266	1
87	2	1099	0	0	117	0
87	3	77	0	0	5	0
87	4	119	0	0	10	0
87	5	2471	0	0	263	0
87	6	1134	0	0	132	0
87	7	77	0	0	4	0
87	8	126	0	0	13	0
87	C3	7	0	0	1	0
87	C5	7	0	0	5	0
87	C8	7	0	0	0	0
87	D3	7	0	0	0	0
87	D9	7	0	0	0	0
87	L3	21	0	0	1	0
87	L4	7	0	0	0	0
87	M0	7	0	0	0	0
87	M5	7	0	0	2	0
87	M6	7	0	0	0	0
87	M7	7	0	0	1	0
87	M9	14	0	0	2	0
87	N9	7	0	0	0	0
87	O1	7	0	0	6	0
87	O2	7	0	0	0	0
87	O3	7	0	0	1	0
87	O7	14	0	0	3	0
87	Q2	7	0	0	3	0
87	S8	7	0	0	1	0
87	SR	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	c3	7	0	0	0	0
87	c5	7	0	0	0	0
87	c8	7	0	0	0	0
87	d4	7	0	0	0	0
87	d9	7	0	0	0	0
87	l3	14	0	0	0	0
87	l4	14	0	0	0	0
87	l5	28	0	0	0	0
87	l9	7	0	0	0	0
87	m0	14	0	0	0	0
87	m1	7	0	0	0	0
87	m4	7	0	0	0	0
87	m5	7	0	0	0	0
87	m7	7	0	0	0	0
87	m9	7	0	0	0	0
87	n3	7	0	0	0	0
87	n9	7	0	0	0	0
87	o3	7	0	0	0	0
87	o7	7	0	0	0	0
87	o9	7	0	0	0	0
87	q1	7	0	0	0	0
87	q2	7	0	0	0	0
87	s1	7	0	0	0	0
87	s8	7	0	0	0	0
87	sR	7	0	0	0	0
88	2	34	0	40	9	0
89	D6	1	0	0	0	0
89	D7	1	0	0	0	0
89	D9	1	0	0	0	0
89	E1	1	0	0	0	0
89	O7	1	0	0	1	0
89	Q0	1	0	0	1	0
89	Q2	1	0	0	2	0
89	Q3	1	0	0	0	0
89	d6	1	0	0	0	0
89	d7	1	0	0	0	0
89	d9	1	0	0	0	0
89	e1	1	0	0	0	0
89	o7	1	0	0	0	0
89	q0	1	0	0	0	0
89	q2	1	0	0	0	0
89	q3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	411095	0	297211	21971	3

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 32.

The worst 5 of 21971 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:D3:63:GLN:CB	25:D3:63:GLN:CG	1.55	1.57
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	2.08	1.40
1:2:1754:A:HO2'	32:E0:2:ALA:N	1.52	1.08
78:Q2:17:CYS:SG	78:Q2:77:CYS:HB3	2.80	1.07
36:1:883:A:H5'	53:M7:133:HIS:HA	1.35	1.07

All (3) 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)
1:2:1491:U:O2'	22:d0:12:GLN:OE1[1_454]	2.02	0.18
36:1:3154:C:N4	34:sR:77:GLY:O[2_656]	2.15	0.05
34:sR:160:GLU:OE2	87:1:4023:OHX:N4[2_646]	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%)	137 (67%)	42 (21%)	25 (12%)	1	12
2	s0	204/251 (81%)	139 (68%)	31 (15%)	34 (17%)	0	6
3	S1	212/254 (84%)	142 (67%)	42 (20%)	28 (13%)	0	10
3	s1	214/254 (84%)	155 (72%)	39 (18%)	20 (9%)	1	20
4	S2	215/253 (85%)	148 (69%)	47 (22%)	20 (9%)	1	20
4	s2	215/253 (85%)	156 (73%)	30 (14%)	29 (14%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S3	221/239 (92%)	154 (70%)	48 (22%)	19 (9%)	1	22
5	s3	221/239 (92%)	147 (66%)	51 (23%)	23 (10%)	1	16
6	S4	258/260 (99%)	184 (71%)	44 (17%)	30 (12%)	1	13
6	s4	258/260 (99%)	175 (68%)	53 (20%)	30 (12%)	1	13
7	S5	204/224 (91%)	129 (63%)	46 (22%)	29 (14%)	0	9
7	s5	204/224 (91%)	124 (61%)	51 (25%)	29 (14%)	0	9
8	S6	224/236 (95%)	166 (74%)	37 (16%)	21 (9%)	1	20
8	s6	216/236 (92%)	165 (76%)	36 (17%)	15 (7%)	2	30
9	S7	182/189 (96%)	131 (72%)	35 (19%)	16 (9%)	1	22
9	s7	184/189 (97%)	126 (68%)	37 (20%)	21 (11%)	1	13
10	S8	184/200 (92%)	132 (72%)	32 (17%)	20 (11%)	1	14
10	s8	184/200 (92%)	144 (78%)	26 (14%)	14 (8%)	2	26
11	S9	183/196 (93%)	128 (70%)	36 (20%)	19 (10%)	1	16
11	s9	183/196 (93%)	122 (67%)	42 (23%)	19 (10%)	1	16
12	C0	94/105 (90%)	54 (57%)	21 (22%)	19 (20%)	0	3
12	c0	92/105 (88%)	56 (61%)	17 (18%)	19 (21%)	0	3
13	C1	153/155 (99%)	113 (74%)	22 (14%)	18 (12%)	1	13
13	c1	144/155 (93%)	108 (75%)	20 (14%)	16 (11%)	1	14
14	C2	122/142 (86%)	71 (58%)	22 (18%)	29 (24%)	0	1
14	c2	122/142 (86%)	65 (53%)	36 (30%)	21 (17%)	0	5
15	C3	148/150 (99%)	107 (72%)	29 (20%)	12 (8%)	1	24
15	c3	148/150 (99%)	95 (64%)	28 (19%)	25 (17%)	0	5
16	C4	125/136 (92%)	80 (64%)	25 (20%)	20 (16%)	0	6
16	c4	126/136 (93%)	90 (71%)	24 (19%)	12 (10%)	1	19
17	C5	122/141 (86%)	78 (64%)	26 (21%)	18 (15%)	0	7
17	c5	133/141 (94%)	75 (56%)	29 (22%)	29 (22%)	0	2
18	C6	139/142 (98%)	105 (76%)	22 (16%)	12 (9%)	1	22
18	c6	140/142 (99%)	97 (69%)	24 (17%)	19 (14%)	0	9
19	C7	116/136 (85%)	76 (66%)	22 (19%)	18 (16%)	0	6
19	c7	113/136 (83%)	73 (65%)	29 (26%)	11 (10%)	1	19
20	C8	143/145 (99%)	107 (75%)	27 (19%)	9 (6%)	2	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	c8	143/145 (99%)	98 (68%)	27 (19%)	18 (13%)	0	11
21	C9	141/143 (99%)	99 (70%)	31 (22%)	11 (8%)	1	25
21	c9	141/143 (99%)	98 (70%)	36 (26%)	7 (5%)	3	40
22	D0	105/120 (88%)	74 (70%)	22 (21%)	9 (9%)	1	22
22	d0	108/120 (90%)	75 (69%)	15 (14%)	18 (17%)	0	6
23	D1	85/87 (98%)	53 (62%)	18 (21%)	14 (16%)	0	6
23	d1	85/87 (98%)	64 (75%)	14 (16%)	7 (8%)	1	24
24	D2	127/129 (98%)	91 (72%)	28 (22%)	8 (6%)	2	33
24	d2	127/129 (98%)	105 (83%)	17 (13%)	5 (4%)	5	49
25	D3	142/144 (99%)	87 (61%)	29 (20%)	26 (18%)	0	4
25	d3	142/144 (99%)	119 (84%)	16 (11%)	7 (5%)	3	41
26	D4	132/134 (98%)	98 (74%)	25 (19%)	9 (7%)	2	30
26	d4	132/134 (98%)	101 (76%)	17 (13%)	14 (11%)	1	15
27	D5	68/107 (64%)	43 (63%)	16 (24%)	9 (13%)	0	10
27	d5	67/107 (63%)	45 (67%)	14 (21%)	8 (12%)	1	12
28	D6	95/97 (98%)	53 (56%)	18 (19%)	24 (25%)	0	1
28	d6	95/97 (98%)	71 (75%)	16 (17%)	8 (8%)	1	23
29	D7	79/81 (98%)	58 (73%)	14 (18%)	7 (9%)	1	21
29	d7	79/81 (98%)	61 (77%)	11 (14%)	7 (9%)	1	21
30	D8	61/66 (92%)	45 (74%)	11 (18%)	5 (8%)	1	24
30	d8	61/66 (92%)	39 (64%)	14 (23%)	8 (13%)	0	11
31	D9	51/55 (93%)	32 (63%)	11 (22%)	8 (16%)	0	6
31	d9	51/55 (93%)	35 (69%)	8 (16%)	8 (16%)	0	6
32	E0	58/60 (97%)	34 (59%)	16 (28%)	8 (14%)	0	9
33	E1	69/76 (91%)	39 (56%)	13 (19%)	17 (25%)	0	1
34	SR	316/318 (99%)	237 (75%)	56 (18%)	23 (7%)	2	28
34	sR	316/318 (99%)	251 (79%)	46 (15%)	19 (6%)	2	34
35	SM	155/273 (57%)	90 (58%)	40 (26%)	25 (16%)	0	6
35	sM	98/273 (36%)	59 (60%)	20 (20%)	19 (19%)	0	3
39	L2	250/253 (99%)	197 (79%)	31 (12%)	22 (9%)	1	22
39	l2	250/253 (99%)	192 (77%)	42 (17%)	16 (6%)	2	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	L3	384/386 (100%)	290 (76%)	63 (16%)	31 (8%)	1	24
40	l3	384/386 (100%)	299 (78%)	53 (14%)	32 (8%)	1	23
41	L4	359/361 (99%)	260 (72%)	62 (17%)	37 (10%)	1	16
41	l4	359/361 (99%)	251 (70%)	68 (19%)	40 (11%)	1	14
42	L5	294/296 (99%)	200 (68%)	58 (20%)	36 (12%)	1	12
42	l5	292/296 (99%)	221 (76%)	44 (15%)	27 (9%)	1	20
43	L6	152/175 (87%)	123 (81%)	17 (11%)	12 (8%)	1	25
43	l6	153/175 (87%)	107 (70%)	27 (18%)	19 (12%)	1	12
44	L7	220/243 (90%)	154 (70%)	45 (20%)	21 (10%)	1	19
44	l7	221/243 (91%)	165 (75%)	34 (15%)	22 (10%)	1	17
45	L8	231/255 (91%)	137 (59%)	65 (28%)	29 (13%)	0	11
45	l8	229/255 (90%)	155 (68%)	52 (23%)	22 (10%)	1	19
46	L9	189/191 (99%)	137 (72%)	30 (16%)	22 (12%)	1	13
46	l9	189/191 (99%)	142 (75%)	27 (14%)	20 (11%)	1	15
47	M0	207/220 (94%)	148 (72%)	38 (18%)	21 (10%)	1	17
47	m0	209/220 (95%)	149 (71%)	41 (20%)	19 (9%)	1	21
48	M1	167/173 (96%)	116 (70%)	27 (16%)	24 (14%)	0	8
48	m1	167/173 (96%)	120 (72%)	27 (16%)	20 (12%)	1	12
49	M3	191/198 (96%)	134 (70%)	46 (24%)	11 (6%)	3	35
49	m3	192/198 (97%)	126 (66%)	37 (19%)	29 (15%)	0	7
50	M4	134/137 (98%)	97 (72%)	25 (19%)	12 (9%)	1	21
50	m4	135/137 (98%)	92 (68%)	35 (26%)	8 (6%)	2	35
51	M5	201/203 (99%)	151 (75%)	38 (19%)	12 (6%)	2	34
51	m5	201/203 (99%)	151 (75%)	35 (17%)	15 (8%)	2	27
52	M6	195/198 (98%)	146 (75%)	36 (18%)	13 (7%)	2	31
52	m6	195/198 (98%)	151 (77%)	26 (13%)	18 (9%)	1	20
53	M7	181/183 (99%)	128 (71%)	34 (19%)	19 (10%)	1	15
53	m7	153/183 (84%)	111 (72%)	29 (19%)	13 (8%)	1	23
54	M8	183/185 (99%)	132 (72%)	36 (20%)	15 (8%)	1	24
54	m8	183/185 (99%)	134 (73%)	36 (20%)	13 (7%)	2	29
55	M9	186/188 (99%)	136 (73%)	33 (18%)	17 (9%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	m9	186/188 (99%)	125 (67%)	40 (22%)	21 (11%)	1	14
56	N0	170/172 (99%)	139 (82%)	21 (12%)	10 (6%)	2	35
56	n0	170/172 (99%)	145 (85%)	16 (9%)	9 (5%)	3	38
57	N1	157/159 (99%)	115 (73%)	28 (18%)	14 (9%)	1	21
57	n1	157/159 (99%)	121 (77%)	27 (17%)	9 (6%)	3	36
58	N2	98/120 (82%)	65 (66%)	26 (26%)	7 (7%)	2	29
58	n2	96/120 (80%)	64 (67%)	24 (25%)	8 (8%)	1	23
59	N3	134/136 (98%)	109 (81%)	16 (12%)	9 (7%)	2	31
59	n3	134/136 (98%)	113 (84%)	12 (9%)	9 (7%)	2	31
60	N4	96/155 (62%)	63 (66%)	16 (17%)	17 (18%)	0	4
60	n4	133/155 (86%)	88 (66%)	25 (19%)	20 (15%)	0	7
61	N5	119/141 (84%)	81 (68%)	30 (25%)	8 (7%)	2	31
61	n5	118/141 (84%)	91 (77%)	17 (14%)	10 (8%)	1	23
62	N6	124/126 (98%)	94 (76%)	18 (14%)	12 (10%)	1	19
62	n6	124/126 (98%)	92 (74%)	17 (14%)	15 (12%)	1	12
63	N7	133/135 (98%)	98 (74%)	19 (14%)	16 (12%)	1	12
63	n7	133/135 (98%)	94 (71%)	26 (20%)	13 (10%)	1	18
64	N8	146/148 (99%)	100 (68%)	30 (20%)	16 (11%)	1	14
64	n8	146/148 (99%)	104 (71%)	28 (19%)	14 (10%)	1	19
65	N9	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	21
65	n9	56/58 (97%)	33 (59%)	14 (25%)	9 (16%)	0	6
66	O0	95/104 (91%)	82 (86%)	10 (10%)	3 (3%)	6	55
66	o0	98/104 (94%)	75 (76%)	18 (18%)	5 (5%)	3	40
67	O1	107/112 (96%)	86 (80%)	12 (11%)	9 (8%)	1	23
67	o1	107/112 (96%)	73 (68%)	14 (13%)	20 (19%)	0	3
68	O2	125/129 (97%)	95 (76%)	20 (16%)	10 (8%)	1	25
68	o2	125/129 (97%)	89 (71%)	23 (18%)	13 (10%)	1	16
69	O3	104/106 (98%)	90 (86%)	7 (7%)	7 (7%)	2	31
69	o3	104/106 (98%)	82 (79%)	13 (12%)	9 (9%)	1	22
70	O4	110/119 (92%)	80 (73%)	19 (17%)	11 (10%)	1	17
70	o4	110/119 (92%)	75 (68%)	24 (22%)	11 (10%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	O5	117/119 (98%)	75 (64%)	28 (24%)	14 (12%)	1	12
71	o5	117/119 (98%)	80 (68%)	18 (15%)	19 (16%)	0	6
72	O6	97/99 (98%)	69 (71%)	16 (16%)	12 (12%)	1	12
72	o6	97/99 (98%)	67 (69%)	18 (19%)	12 (12%)	1	12
73	O7	85/87 (98%)	63 (74%)	16 (19%)	6 (7%)	2	29
73	o7	85/87 (98%)	60 (71%)	14 (16%)	11 (13%)	0	11
74	O8	75/77 (97%)	55 (73%)	12 (16%)	8 (11%)	1	15
74	o8	75/77 (97%)	53 (71%)	18 (24%)	4 (5%)	3	38
75	O9	48/50 (96%)	34 (71%)	10 (21%)	4 (8%)	1	23
75	o9	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	23
76	Q0	50/52 (96%)	32 (64%)	12 (24%)	6 (12%)	1	12
76	q0	50/52 (96%)	39 (78%)	6 (12%)	5 (10%)	1	17
77	Q1	23/25 (92%)	18 (78%)	3 (13%)	2 (9%)	1	22
77	q1	23/25 (92%)	16 (70%)	3 (13%)	4 (17%)	0	5
78	Q2	103/105 (98%)	75 (73%)	20 (19%)	8 (8%)	1	25
78	q2	103/105 (98%)	83 (81%)	14 (14%)	6 (6%)	3	35
79	Q3	89/91 (98%)	59 (66%)	16 (18%)	14 (16%)	0	6
79	q3	89/91 (98%)	71 (80%)	9 (10%)	9 (10%)	1	17
80	e0	60/62 (97%)	37 (62%)	14 (23%)	9 (15%)	0	7
81	e1	74/76 (97%)	28 (38%)	26 (35%)	20 (27%)	0	1
83	p0	139/311 (45%)	103 (74%)	27 (19%)	9 (6%)	2	32
All	All	22333/24141 (92%)	15914 (71%)	4073 (18%)	2346 (10%)	1	15

5 of 2346 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN
2	S0	39	ASN
2	S0	95	ALA
2	S0	132	ALA

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%)	117 (71%)	47 (29%)	0	4
2	s0	165/209 (79%)	123 (74%)	42 (26%)	1	7
3	S1	191/223 (86%)	139 (73%)	52 (27%)	0	5
3	s1	192/223 (86%)	147 (77%)	45 (23%)	1	8
4	S2	176/204 (86%)	126 (72%)	50 (28%)	0	4
4	s2	176/204 (86%)	119 (68%)	57 (32%)	0	3
5	S3	182/194 (94%)	133 (73%)	49 (27%)	1	5
5	s3	182/194 (94%)	131 (72%)	51 (28%)	0	5
6	S4	221/221 (100%)	170 (77%)	51 (23%)	1	8
6	s4	221/221 (100%)	165 (75%)	56 (25%)	1	7
7	S5	173/190 (91%)	136 (79%)	37 (21%)	1	10
7	s5	173/190 (91%)	125 (72%)	48 (28%)	0	5
8	S6	188/201 (94%)	139 (74%)	49 (26%)	1	6
8	s6	187/201 (93%)	132 (71%)	55 (29%)	0	4
9	S7	165/169 (98%)	127 (77%)	38 (23%)	1	8
9	s7	165/169 (98%)	122 (74%)	43 (26%)	1	6
10	S8	150/161 (93%)	118 (79%)	32 (21%)	1	10
10	s8	150/161 (93%)	106 (71%)	44 (29%)	0	4
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	8
11	s9	158/165 (96%)	116 (73%)	42 (27%)	1	6
12	C0	77/98 (79%)	58 (75%)	19 (25%)	1	7
12	c0	73/98 (74%)	54 (74%)	19 (26%)	1	6
13	C1	129/136 (95%)	111 (86%)	18 (14%)	5	30
13	c1	129/136 (95%)	98 (76%)	31 (24%)	1	7
14	C2	88/118 (75%)	66 (75%)	22 (25%)	1	7
14	c2	88/118 (75%)	62 (70%)	26 (30%)	0	4
15	C3	127/127 (100%)	101 (80%)	26 (20%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	c3	127/127 (100%)	96 (76%)	31 (24%)	1	7
16	C4	81/104 (78%)	58 (72%)	23 (28%)	0	4
16	c4	97/104 (93%)	67 (69%)	30 (31%)	0	4
17	C5	101/117 (86%)	72 (71%)	29 (29%)	0	4
17	c5	103/117 (88%)	73 (71%)	30 (29%)	0	4
18	C6	117/118 (99%)	83 (71%)	34 (29%)	0	4
18	c6	118/118 (100%)	87 (74%)	31 (26%)	1	6
19	C7	94/124 (76%)	65 (69%)	29 (31%)	0	4
19	c7	92/124 (74%)	61 (66%)	31 (34%)	0	3
20	C8	128/128 (100%)	101 (79%)	27 (21%)	1	10
20	c8	128/128 (100%)	96 (75%)	32 (25%)	1	7
21	C9	115/115 (100%)	83 (72%)	32 (28%)	0	5
21	c9	115/115 (100%)	85 (74%)	30 (26%)	1	6
22	D0	100/113 (88%)	74 (74%)	26 (26%)	1	6
22	d0	103/113 (91%)	67 (65%)	36 (35%)	0	2
23	D1	74/74 (100%)	59 (80%)	15 (20%)	2	11
23	d1	74/74 (100%)	52 (70%)	22 (30%)	0	4
24	D2	110/110 (100%)	81 (74%)	29 (26%)	1	6
24	d2	110/110 (100%)	88 (80%)	22 (20%)	2	12
25	D3	119/119 (100%)	79 (66%)	40 (34%)	0	3
25	d3	119/119 (100%)	89 (75%)	30 (25%)	1	7
26	D4	112/112 (100%)	88 (79%)	24 (21%)	1	10
26	d4	112/112 (100%)	89 (80%)	23 (20%)	2	11
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	8
27	d5	61/88 (69%)	47 (77%)	14 (23%)	1	8
28	D6	83/83 (100%)	60 (72%)	23 (28%)	0	5
28	d6	83/83 (100%)	51 (61%)	32 (39%)	0	1
29	D7	70/70 (100%)	57 (81%)	13 (19%)	2	15
29	d7	70/70 (100%)	54 (77%)	16 (23%)	1	8
30	D8	56/59 (95%)	39 (70%)	17 (30%)	0	4
30	d8	56/59 (95%)	42 (75%)	14 (25%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	D9	47/48 (98%)	34 (72%)	13 (28%)	0	5
31	d9	47/48 (98%)	32 (68%)	15 (32%)	0	3
32	E0	51/51 (100%)	35 (69%)	16 (31%)	0	4
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	7
34	SR	260/261 (100%)	216 (83%)	44 (17%)	3	20
34	sR	260/261 (100%)	213 (82%)	47 (18%)	2	16
35	SM	97/228 (42%)	68 (70%)	29 (30%)	0	4
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	5
39	L2	193/195 (99%)	138 (72%)	55 (28%)	0	4
39	l2	192/195 (98%)	137 (71%)	55 (29%)	0	4
40	L3	321/322 (100%)	229 (71%)	92 (29%)	0	4
40	l3	321/322 (100%)	235 (73%)	86 (27%)	1	5
41	L4	288/288 (100%)	212 (74%)	76 (26%)	1	6
41	l4	288/288 (100%)	208 (72%)	80 (28%)	0	5
42	L5	244/244 (100%)	195 (80%)	49 (20%)	2	12
42	l5	243/244 (100%)	176 (72%)	67 (28%)	0	5
43	L6	134/152 (88%)	110 (82%)	24 (18%)	2	17
43	l6	135/152 (89%)	105 (78%)	30 (22%)	1	9
44	L7	186/204 (91%)	138 (74%)	48 (26%)	1	6
44	l7	187/204 (92%)	146 (78%)	41 (22%)	1	9
45	L8	187/207 (90%)	144 (77%)	43 (23%)	1	8
45	l8	177/207 (86%)	134 (76%)	43 (24%)	1	7
46	L9	171/171 (100%)	110 (64%)	61 (36%)	0	2
46	l9	171/171 (100%)	119 (70%)	52 (30%)	0	4
47	M0	177/186 (95%)	135 (76%)	42 (24%)	1	7
47	m0	179/186 (96%)	131 (73%)	48 (27%)	1	5
48	M1	147/150 (98%)	111 (76%)	36 (24%)	1	7
48	m1	147/150 (98%)	91 (62%)	56 (38%)	0	1
49	M3	154/158 (98%)	114 (74%)	40 (26%)	1	6
49	m3	154/158 (98%)	102 (66%)	52 (34%)	0	3
50	M4	107/108 (99%)	78 (73%)	29 (27%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	m4	108/108 (100%)	81 (75%)	27 (25%)	1	7
51	M5	175/175 (100%)	143 (82%)	32 (18%)	2	16
51	m5	175/175 (100%)	132 (75%)	43 (25%)	1	7
52	M6	160/161 (99%)	120 (75%)	40 (25%)	1	7
52	m6	160/161 (99%)	119 (74%)	41 (26%)	1	7
53	M7	140/145 (97%)	98 (70%)	42 (30%)	0	4
53	m7	125/145 (86%)	83 (66%)	42 (34%)	0	3
54	M8	150/150 (100%)	115 (77%)	35 (23%)	1	8
54	m8	150/150 (100%)	104 (69%)	46 (31%)	0	4
55	M9	153/153 (100%)	112 (73%)	41 (27%)	1	5
55	m9	153/153 (100%)	113 (74%)	40 (26%)	1	6
56	N0	156/156 (100%)	108 (69%)	48 (31%)	0	4
56	n0	156/156 (100%)	114 (73%)	42 (27%)	1	5
57	N1	136/136 (100%)	100 (74%)	36 (26%)	1	6
57	n1	136/136 (100%)	100 (74%)	36 (26%)	1	6
58	N2	87/106 (82%)	68 (78%)	19 (22%)	1	9
58	n2	85/106 (80%)	68 (80%)	17 (20%)	2	12
59	N3	104/104 (100%)	79 (76%)	25 (24%)	1	7
59	n3	104/104 (100%)	78 (75%)	26 (25%)	1	7
60	N4	57/129 (44%)	45 (79%)	12 (21%)	1	10
60	n4	100/129 (78%)	69 (69%)	31 (31%)	0	4
61	N5	104/117 (89%)	83 (80%)	21 (20%)	2	12
61	n5	104/117 (89%)	70 (67%)	34 (33%)	0	3
62	N6	109/109 (100%)	80 (73%)	29 (27%)	1	6
62	n6	109/109 (100%)	75 (69%)	34 (31%)	0	4
63	N7	115/115 (100%)	92 (80%)	23 (20%)	2	12
63	n7	115/115 (100%)	93 (81%)	22 (19%)	2	14
64	N8	118/118 (100%)	95 (80%)	23 (20%)	2	13
64	n8	118/118 (100%)	85 (72%)	33 (28%)	0	5
65	N9	46/46 (100%)	30 (65%)	16 (35%)	0	2
65	n9	46/46 (100%)	23 (50%)	23 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1	8
66	o0	84/87 (97%)	54 (64%)	30 (36%)	0	2
67	O1	92/96 (96%)	67 (73%)	25 (27%)	0	5
67	o1	94/96 (98%)	67 (71%)	27 (29%)	0	4
68	O2	109/110 (99%)	73 (67%)	36 (33%)	0	3
68	o2	109/110 (99%)	78 (72%)	31 (28%)	0	4
69	O3	90/90 (100%)	71 (79%)	19 (21%)	1	10
69	o3	90/90 (100%)	62 (69%)	28 (31%)	0	4
70	O4	95/101 (94%)	66 (70%)	29 (30%)	0	4
70	o4	95/101 (94%)	70 (74%)	25 (26%)	1	6
71	O5	104/104 (100%)	69 (66%)	35 (34%)	0	3
71	o5	103/104 (99%)	77 (75%)	26 (25%)	1	7
72	O6	81/81 (100%)	56 (69%)	25 (31%)	0	4
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	4
73	O7	70/70 (100%)	51 (73%)	19 (27%)	1	5
73	o7	70/70 (100%)	48 (69%)	22 (31%)	0	4
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	9
74	o8	67/68 (98%)	52 (78%)	15 (22%)	1	9
75	O9	45/45 (100%)	35 (78%)	10 (22%)	1	9
75	o9	45/45 (100%)	34 (76%)	11 (24%)	1	7
76	Q0	47/47 (100%)	36 (77%)	11 (23%)	1	8
76	q0	47/47 (100%)	33 (70%)	14 (30%)	0	4
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	2
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	1
78	Q2	90/90 (100%)	65 (72%)	25 (28%)	0	5
78	q2	90/90 (100%)	58 (64%)	32 (36%)	0	2
79	Q3	71/71 (100%)	54 (76%)	17 (24%)	1	7
79	q3	71/71 (100%)	49 (69%)	22 (31%)	0	4
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	8
81	e1	66/66 (100%)	41 (62%)	25 (38%)	0	1
83	p0	105/253 (42%)	79 (75%)	26 (25%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	18730/20239 (92%)	13794 (74%)	4936 (26%)	1 6

5 of 4936 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
72	O6	59	ASP
10	s8	56	ARG
64	n8	102	ILE
76	Q0	127	LEU
5	s3	66	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
5	s3	74	GLN
13	c1	37	ASN
64	n8	25	HIS
5	s3	179	GLN
6	s4	224	ASN

5.3.3 RNA ⓘ

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

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2558 ligands modelled in this entry, 1426 are monoatomic - leaving 1132 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
87	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3891	-	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	$\# Z > 2$
87	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3934	-	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	$\# Z > 2$
87	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3977	-	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
87	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3996	36	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4020	-	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	$\# Z > 2$
87	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4063	-	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	$\# Z > 2$
87	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4106	-	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	$\# Z > 2$
87	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4149	-	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	$\# Z > 2$
87	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4192	-	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
87	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	GET	2	2181	-	36,36,36	0.45	0	55,55,55	1.78	13 (23%)
87	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	237	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	238	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	239	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	240	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3902	-	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	$\# Z > 2$
87	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3945	-	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	$\# Z > 2$
87	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3988	-	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	$\# Z > 2$
87	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4031	-	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	$\# Z > 2$
87	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4074	-	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	$\# Z > 2$
87	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4117	-	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	$\# Z > 2$
87	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4160	-	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	$\# Z > 2$
87	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4203	-	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
87	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4246	-	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
87	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	225	-	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
87	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	234	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	D3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M0	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M9	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	N9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O2	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	SR	401	-	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
87	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	407	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	408	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	307	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n9	103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	q1	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	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
87	OHX	1	3866	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3867	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3869	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3870	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3912	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3954	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3996	36	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4038	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4080	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4122	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4164	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4206	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2059	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2101	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2143	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
88	GET	2	2181	-	-	0/14/74/74	0/3/3/3
87	OHX	3	215	-	-	0/0/0/0	0/0/0/0
87	OHX	3	216	-	-	0/0/0/0	0/0/0/0
87	OHX	3	217	-	-	0/0/0/0	0/0/0/0
87	OHX	3	218	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	3	219	-	-	0/0/0/0	0/0/0/0
87	OHX	3	220	-	-	0/0/0/0	0/0/0/0
87	OHX	3	221	-	-	0/0/0/0	0/0/0/0
87	OHX	3	222	-	-	0/0/0/0	0/0/0/0
87	OHX	3	223	-	-	0/0/0/0	0/0/0/0
87	OHX	3	224	-	-	0/0/0/0	0/0/0/0
87	OHX	3	225	-	-	0/0/0/0	0/0/0/0
87	OHX	4	224	-	-	0/0/0/0	0/0/0/0
87	OHX	4	225	-	-	0/0/0/0	0/0/0/0
87	OHX	4	226	-	-	0/0/0/0	0/0/0/0
87	OHX	4	227	-	-	0/0/0/0	0/0/0/0
87	OHX	4	228	-	-	0/0/0/0	0/0/0/0
87	OHX	4	229	-	-	0/0/0/0	0/0/0/0
87	OHX	4	230	-	-	0/0/0/0	0/0/0/0
87	OHX	4	231	-	-	0/0/0/0	0/0/0/0
87	OHX	4	232	-	-	0/0/0/0	0/0/0/0
87	OHX	4	233	-	-	0/0/0/0	0/0/0/0
87	OHX	4	234	-	-	0/0/0/0	0/0/0/0
87	OHX	4	235	-	-	0/0/0/0	0/0/0/0
87	OHX	4	236	-	-	0/0/0/0	0/0/0/0
87	OHX	4	237	-	-	0/0/0/0	0/0/0/0
87	OHX	4	238	-	-	0/0/0/0	0/0/0/0
87	OHX	4	239	-	-	0/0/0/0	0/0/0/0
87	OHX	4	240	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3894	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3895	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3896	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3897	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3899	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3911	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3953	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3995	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4037	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4079	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4121	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4163	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4205	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2050	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2092	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2134	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2176	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2205	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2206	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2207	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2208	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2209	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2210	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2211	-	-	0/0/0/0	0/0/0/0
87	OHX	7	216	-	-	0/0/0/0	0/0/0/0
87	OHX	7	217	-	-	0/0/0/0	0/0/0/0
87	OHX	7	218	-	-	0/0/0/0	0/0/0/0
87	OHX	7	219	-	-	0/0/0/0	0/0/0/0
87	OHX	7	220	-	-	0/0/0/0	0/0/0/0
87	OHX	7	221	-	-	0/0/0/0	0/0/0/0
87	OHX	7	222	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	7	223	-	-	0/0/0/0	0/0/0/0
87	OHX	7	224	-	-	0/0/0/0	0/0/0/0
87	OHX	7	225	-	-	0/0/0/0	0/0/0/0
87	OHX	7	226	-	-	0/0/0/0	0/0/0/0
87	OHX	8	218	-	-	0/0/0/0	0/0/0/0
87	OHX	8	219	-	-	0/0/0/0	0/0/0/0
87	OHX	8	220	-	-	0/0/0/0	0/0/0/0
87	OHX	8	221	-	-	0/0/0/0	0/0/0/0
87	OHX	8	222	-	-	0/0/0/0	0/0/0/0
87	OHX	8	223	-	-	0/0/0/0	0/0/0/0
87	OHX	8	224	-	-	0/0/0/0	0/0/0/0
87	OHX	8	225	-	-	0/0/0/0	0/0/0/0
87	OHX	8	226	-	-	0/0/0/0	0/0/0/0
87	OHX	8	227	-	-	0/0/0/0	0/0/0/0
87	OHX	8	228	-	-	0/0/0/0	0/0/0/0
87	OHX	8	229	-	-	0/0/0/0	0/0/0/0
87	OHX	8	230	-	-	0/0/0/0	0/0/0/0
87	OHX	8	231	-	-	0/0/0/0	0/0/0/0
87	OHX	8	232	-	-	0/0/0/0	0/0/0/0
87	OHX	8	233	-	-	0/0/0/0	0/0/0/0
87	OHX	8	234	-	-	0/0/0/0	0/0/0/0
87	OHX	8	235	-	-	0/0/0/0	0/0/0/0
87	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	D3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
87	OHX	L4	403	-	-	0/0/0/0	0/0/0/0
87	OHX	M0	304	-	-	0/0/0/0	0/0/0/0
87	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	M6	202	-	-	0/0/0/0	0/0/0/0
87	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
87	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
87	OHX	M9	203	-	-	0/0/0/0	0/0/0/0
87	OHX	N9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	O1	202	-	-	0/0/0/0	0/0/0/0
87	OHX	O2	202	-	-	0/0/0/0	0/0/0/0
87	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	O7	103	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
87	OHX	Q2	502	-	-	0/0/0/0	0/0/0/0
87	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
87	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
87	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c8	202	-	-	0/0/0/0	0/0/0/0
87	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
87	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	407	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	408	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	307	-	-	0/0/0/0	0/0/0/0
87	OHX	l9	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	303	-	-	0/0/0/0	0/0/0/0
87	OHX	m1	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m4	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	m7	205	-	-	0/0/0/0	0/0/0/0
87	OHX	m9	201	-	-	0/0/0/0	0/0/0/0
87	OHX	n3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	n9	103	-	-	0/0/0/0	0/0/0/0
87	OHX	o3	203	-	-	0/0/0/0	0/0/0/0
87	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
87	OHX	o9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	q1	102	-	-	0/0/0/0	0/0/0/0
87	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
87	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
87	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
87	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	2	2181	GET	C23-C33-N33	-5.95	94.93	111.30
88	2	2181	GET	O11-C42-C32	-5.60	95.57	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	2	2181	GET	C43-C33-N33	-4.38	103.47	111.90
88	2	2181	GET	O62-C62-C12	-3.35	100.96	108.97
88	2	2181	GET	O11-C11-C21	-2.84	102.47	108.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.40	140 (8%) 12 8	77, 125, 214, 302	0
1	6	1791/1800 (99%)	0.29	98 (5%) 24 13	59, 93, 221, 311	0
2	S0	206/251 (82%)	0.89	31 (15%) 3 3	124, 145, 157, 186	0
2	s0	206/251 (82%)	0.35	2 (0%) 79 53	92, 111, 123, 133	0
3	S1	214/254 (84%)	0.83	32 (14%) 3 3	151, 183, 213, 218	0
3	s1	216/254 (85%)	0.97	37 (17%) 2 2	91, 109, 132, 145	0
4	S2	217/253 (85%)	0.75	22 (10%) 7 6	97, 113, 137, 142	0
4	s2	217/253 (85%)	0.94	31 (14%) 3 3	75, 91, 109, 127	0
5	S3	223/239 (93%)	0.62	22 (9%) 8 6	99, 118, 149, 159	0
5	s3	223/239 (93%)	0.25	7 (3%) 47 26	88, 119, 139, 151	0
6	S4	260/260 (100%)	1.29	65 (25%) 1 2	102, 125, 145, 175	0
6	s4	260/260 (100%)	0.45	17 (6%) 18 11	70, 104, 122, 149	0
7	S5	206/224 (91%)	1.27	51 (24%) 1 2	132, 156, 167, 176	0
7	s5	206/224 (91%)	0.29	11 (5%) 25 14	73, 91, 114, 132	0
8	S6	226/236 (95%)	1.43	66 (29%) 1 1	93, 134, 158, 174	0
8	s6	218/236 (92%)	0.74	29 (13%) 4 4	68, 98, 134, 150	0
9	S7	184/189 (97%)	0.76	23 (12%) 5 4	131, 163, 183, 187	0
9	s7	186/189 (98%)	0.32	4 (2%) 59 34	93, 130, 159, 170	0
10	S8	188/200 (94%)	1.68	74 (39%) 1 1	84, 100, 148, 163	0
10	s8	188/200 (94%)	1.03	34 (18%) 2 2	69, 90, 142, 159	0
11	S9	185/196 (94%)	1.73	67 (36%) 1 1	106, 135, 167, 180	0
11	s9	185/196 (94%)	1.39	54 (29%) 1 1	88, 112, 145, 169	0
12	C0	96/105 (91%)	0.77	14 (14%) 3 3	108, 134, 156, 178	0
12	c0	96/105 (91%)	1.24	27 (28%) 1 1	111, 149, 171, 188	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	0.94	19 (12%) 5 4	86, 103, 149, 153	0
13	c1	146/155 (94%)	0.20	2 (1%) 72 45	75, 89, 130, 157	0
14	C2	124/142 (87%)	1.53	38 (30%) 1 1	168, 179, 192, 201	0
14	c2	124/142 (87%)	2.06	58 (46%) 1 1	193, 214, 224, 226	0
15	C3	150/150 (100%)	0.93	26 (17%) 2 2	109, 137, 156, 161	0
15	c3	150/150 (100%)	0.32	3 (2%) 62 36	79, 102, 119, 138	0
16	C4	127/136 (93%)	1.17	31 (24%) 1 2	106, 177, 195, 198	0
16	c4	128/136 (94%)	0.76	9 (7%) 16 9	76, 102, 113, 128	0
17	C5	124/141 (87%)	1.52	43 (34%) 1 1	109, 126, 155, 173	0
17	c5	135/141 (95%)	0.45	7 (5%) 26 14	79, 99, 134, 149	0
18	C6	141/142 (99%)	1.68	49 (34%) 1 1	121, 143, 152, 155	0
18	c6	142/142 (100%)	0.97	22 (15%) 3 3	71, 84, 101, 132	0
19	C7	120/136 (88%)	2.03	58 (48%) 1 1	117, 140, 162, 165	0
19	c7	117/136 (86%)	1.33	38 (32%) 1 1	87, 102, 129, 133	0
20	C8	145/145 (100%)	1.74	56 (38%) 1 1	107, 139, 169, 176	0
20	c8	145/145 (100%)	1.11	28 (19%) 2 2	71, 90, 113, 125	0
21	C9	143/143 (100%)	1.17	32 (22%) 1 2	118, 140, 152, 169	0
21	c9	143/143 (100%)	0.29	2 (1%) 72 45	68, 76, 96, 112	0
22	D0	107/120 (89%)	1.12	20 (18%) 2 2	105, 139, 162, 172	0
22	d0	110/120 (91%)	1.53	34 (30%) 1 1	76, 111, 164, 179	0
23	D1	87/87 (100%)	0.61	5 (5%) 23 12	121, 137, 151, 161	0
23	d1	87/87 (100%)	0.34	0 100 100	91, 102, 125, 133	0
24	D2	129/129 (100%)	1.63	49 (37%) 1 1	101, 122, 134, 143	0
24	d2	129/129 (100%)	0.54	2 (1%) 68 41	76, 89, 99, 115	0
25	D3	144/144 (100%)	0.15	1 (0%) 84 63	82, 91, 103, 110	0
25	d3	144/144 (100%)	0.23	0 100 100	60, 68, 82, 103	0
26	D4	134/134 (100%)	1.37	42 (31%) 1 1	110, 138, 152, 156	0
26	d4	134/134 (100%)	0.52	9 (6%) 17 10	81, 110, 126, 147	0
27	D5	70/107 (65%)	1.19	18 (25%) 1 2	148, 169, 178, 180	0
27	d5	69/107 (64%)	0.49	6 (8%) 10 7	83, 103, 114, 122	0
28	D6	97/97 (100%)	0.87	14 (14%) 3 3	106, 128, 189, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.79	13 (13%) 4 4	79, 91, 117, 121	0
29	D7	81/81 (100%)	1.56	27 (33%) 1 1	131, 160, 192, 198	0
29	d7	81/81 (100%)	0.74	10 (12%) 5 4	95, 115, 148, 151	0
30	D8	63/66 (95%)	0.64	8 (12%) 4 4	142, 158, 173, 178	0
30	d8	63/66 (95%)	0.63	3 (4%) 29 16	89, 104, 120, 139	0
31	D9	53/55 (96%)	1.52	18 (33%) 1 1	103, 109, 132, 137	0
31	d9	53/55 (96%)	2.02	25 (47%) 1 1	80, 92, 132, 154	0
32	E0	60/60 (100%)	0.97	14 (23%) 1 2	93, 128, 170, 176	0
33	E1	71/76 (93%)	0.86	11 (15%) 3 3	129, 159, 171, 172	0
34	SR	318/318 (100%)	1.42	95 (29%) 1 1	83, 152, 174, 192	0
34	sR	318/318 (100%)	0.87	43 (13%) 4 4	99, 120, 141, 163	0
35	SM	159/273 (58%)	0.82	27 (16%) 2 3	76, 118, 176, 183	0
35	sM	104/273 (38%)	0.53	13 (12%) 5 4	89, 108, 202, 209	0
36	1	3149/3396 (92%)	0.15	67 (2%) 60 35	41, 75, 160, 278	0
36	5	3150/3396 (92%)	0.14	58 (1%) 65 39	38, 73, 149, 262	0
37	3	121/121 (100%)	0.24	2 (1%) 67 40	57, 94, 109, 117	0
37	7	121/121 (100%)	-0.11	0 100 100	44, 65, 80, 91	0
38	4	158/158 (100%)	0.06	2 (1%) 74 47	55, 84, 127, 172	0
38	8	158/158 (100%)	0.07	2 (1%) 74 47	60, 97, 140, 158	0
39	L2	252/253 (99%)	0.47	12 (4%) 29 16	53, 77, 99, 114	0
39	l2	252/253 (99%)	0.16	0 100 100	54, 80, 103, 116	0
40	L3	386/386 (100%)	0.01	1 (0%) 91 81	45, 68, 86, 121	0
40	l3	386/386 (100%)	0.00	0 100 100	39, 52, 69, 111	0
41	L4	361/361 (100%)	-0.08	0 100 100	49, 67, 86, 101	0
41	l4	361/361 (100%)	0.04	1 (0%) 91 81	55, 77, 102, 116	0
42	L5	296/296 (100%)	1.10	60 (20%) 1 2	74, 98, 116, 129	0
42	l5	294/296 (99%)	0.73	20 (6%) 17 10	51, 69, 100, 149	0
43	L6	156/175 (89%)	-0.00	1 (0%) 86 66	55, 65, 88, 112	0
43	l6	157/175 (89%)	0.07	1 (0%) 86 66	53, 66, 92, 109	0
44	L7	222/243 (91%)	0.22	1 (0%) 88 71	46, 59, 98, 136	0
44	l7	223/243 (91%)	0.12	0 100 100	42, 52, 99, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	L8	233/255 (91%)	0.52	18 (7%) 13 8	87, 105, 137, 148	0
45	l8	231/255 (90%)	0.77	19 (8%) 12 8	101, 120, 148, 155	0
46	L9	191/191 (100%)	0.84	19 (9%) 8 6	67, 80, 95, 109	0
46	l9	191/191 (100%)	0.15	3 (1%) 68 41	44, 52, 72, 84	0
47	M0	211/220 (95%)	0.38	7 (3%) 44 25	61, 79, 111, 128	0
47	m0	213/220 (96%)	-0.09	0 100 100	44, 65, 93, 123	0
48	M1	169/173 (97%)	1.54	54 (31%) 1 1	83, 105, 123, 133	0
48	m1	169/173 (97%)	0.59	8 (4%) 30 17	54, 72, 87, 96	0
49	M3	193/198 (97%)	0.26	2 (1%) 79 53	58, 83, 128, 153	0
49	m3	194/198 (97%)	0.58	8 (4%) 35 20	65, 94, 134, 149	0
50	M4	136/137 (99%)	0.28	4 (2%) 49 28	60, 70, 83, 96	0
50	m4	137/137 (100%)	-0.03	0 100 100	44, 56, 76, 93	0
51	M5	203/203 (100%)	0.92	25 (12%) 5 4	56, 78, 92, 97	0
51	m5	203/203 (100%)	1.53	64 (31%) 1 1	62, 88, 104, 112	0
52	M6	197/198 (99%)	0.02	0 100 100	46, 55, 78, 84	0
52	m6	197/198 (99%)	0.05	0 100 100	37, 43, 69, 74	0
53	M7	183/183 (100%)	0.24	5 (2%) 52 29	53, 61, 133, 149	0
53	m7	155/183 (84%)	0.19	0 100 100	50, 61, 74, 105	0
54	M8	185/185 (100%)	0.32	4 (2%) 59 34	52, 71, 92, 122	0
54	m8	185/185 (100%)	0.27	4 (2%) 59 34	56, 73, 82, 86	0
55	M9	188/188 (100%)	0.51	16 (8%) 11 7	77, 95, 187, 192	0
55	m9	188/188 (100%)	0.60	16 (8%) 11 7	74, 88, 154, 164	0
56	N0	172/172 (100%)	0.40	6 (3%) 42 23	56, 67, 83, 88	0
56	n0	172/172 (100%)	0.17	2 (1%) 75 49	40, 48, 62, 77	0
57	N1	159/159 (100%)	0.60	10 (6%) 19 11	56, 70, 119, 125	0
57	n1	159/159 (100%)	0.56	7 (4%) 33 18	45, 57, 106, 112	0
58	N2	100/120 (83%)	0.65	6 (6%) 21 12	104, 118, 132, 144	0
58	n2	98/120 (81%)	1.11	21 (21%) 1 2	98, 110, 124, 128	0
59	N3	136/136 (100%)	0.17	2 (1%) 70 43	57, 68, 83, 87	0
59	n3	136/136 (100%)	-0.02	0 100 100	40, 51, 66, 70	0
60	N4	98/155 (63%)	2.03	31 (31%) 1 1	66, 90, 209, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	n4	135/155 (87%)	0.69	16 (11%) 5 5	53, 110, 140, 151	0
61	N5	121/141 (85%)	1.56	37 (30%) 1 1	74, 90, 108, 150	0
61	n5	120/141 (85%)	1.83	53 (44%) 1 1	81, 97, 119, 132	0
62	N6	126/126 (100%)	0.68	6 (4%) 29 16	70, 82, 95, 108	0
62	n6	126/126 (100%)	1.05	21 (16%) 2 3	87, 95, 113, 123	0
63	N7	135/135 (100%)	1.71	57 (42%) 1 1	106, 118, 137, 149	0
63	n7	135/135 (100%)	2.26	69 (51%) 0 1	106, 124, 147, 158	0
64	N8	148/148 (100%)	0.37	2 (1%) 72 45	54, 72, 95, 105	0
64	n8	148/148 (100%)	0.40	6 (4%) 35 20	53, 76, 97, 102	0
65	N9	58/58 (100%)	0.69	6 (10%) 7 6	69, 80, 119, 127	0
65	n9	58/58 (100%)	0.82	6 (10%) 7 6	60, 72, 105, 119	0
66	O0	97/104 (93%)	0.62	10 (10%) 7 6	101, 109, 125, 128	0
66	o0	100/104 (96%)	0.98	16 (16%) 3 3	97, 108, 135, 143	0
67	O1	109/112 (97%)	0.75	5 (4%) 31 17	67, 78, 107, 132	0
67	o1	109/112 (97%)	0.33	1 (0%) 81 57	56, 68, 106, 127	0
68	O2	127/129 (98%)	0.03	1 (0%) 83 60	47, 60, 73, 92	0
68	o2	127/129 (98%)	0.25	1 (0%) 83 60	47, 73, 86, 99	0
69	O3	106/106 (100%)	0.08	0 100 100	48, 55, 78, 85	0
69	o3	106/106 (100%)	0.27	1 (0%) 81 57	44, 52, 82, 91	0
70	O4	112/119 (94%)	1.53	40 (35%) 1 1	77, 98, 130, 136	0
70	o4	112/119 (94%)	0.84	17 (15%) 3 3	74, 98, 130, 136	0
71	O5	119/119 (100%)	0.71	7 (5%) 22 12	77, 92, 107, 109	0
71	o5	119/119 (100%)	0.89	15 (12%) 4 4	95, 105, 129, 136	0
72	O6	99/99 (100%)	0.67	10 (10%) 7 6	79, 93, 126, 138	0
72	o6	99/99 (100%)	1.24	24 (24%) 1 2	84, 105, 125, 144	0
73	O7	87/87 (100%)	0.29	1 (1%) 77 50	55, 66, 97, 121	0
73	o7	87/87 (100%)	0.63	7 (8%) 12 8	62, 73, 116, 152	0
74	O8	77/77 (100%)	1.07	18 (23%) 1 2	107, 117, 133, 141	0
74	o8	77/77 (100%)	1.14	17 (22%) 1 2	107, 116, 124, 127	0
75	O9	50/50 (100%)	0.41	0 100 100	66, 73, 85, 92	0
75	o9	50/50 (100%)	0.95	8 (16%) 3 3	81, 84, 93, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	Q0	52/52 (100%)	0.50	4 (7%) 13 8	63, 70, 82, 91	0
76	q0	52/52 (100%)	0.05	0 100 100	42, 48, 57, 66	0
77	Q1	25/25 (100%)	0.91	2 (8%) 12 8	80, 85, 88, 96	0
77	q1	25/25 (100%)	0.25	0 100 100	65, 68, 82, 89	0
78	Q2	105/105 (100%)	0.48	2 (1%) 64 37	61, 78, 98, 131	0
78	q2	105/105 (100%)	0.76	10 (9%) 8 6	63, 74, 87, 123	0
79	Q3	91/91 (100%)	0.12	0 100 100	68, 80, 97, 104	0
79	q3	91/91 (100%)	0.02	0 100 100	61, 80, 96, 106	0
80	e0	62/62 (100%)	0.49	4 (6%) 18 11	73, 106, 134, 136	0
81	e1	76/76 (100%)	1.12	23 (30%) 1 1	162, 182, 192, 194	0
82	m2	0/160	-	-	-	-
83	p0	143/311 (45%)	1.71	51 (35%) 1 1	103, 123, 186, 190	0
84	p1	0/47	-	-	-	-
85	p2	0/46	-	-	-	-
All	All	33059/35344 (93%)	0.55	3149 (9%) 8 6	37, 92, 168, 311	0

The worst 5 of 3149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	75	THR	18.8
60	N4	74	LYS	13.4
60	N4	76	VAL	13.4
60	N4	77	LYS	12.0
1	2	718	U	11.7

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
86	MG	8	211	1/1	1.13	1941.00	92,92,92,92	0
86	MG	1	3771	1/1	0.64	971.00	72,72,72,72	0
86	MG	5	3444	1/1	0.56	800.44	64,64,64,64	0
86	MG	1	3813	1/1	1.26	535.00	85,85,85,85	0
86	MG	5	3471	1/1	0.42	505.00	88,88,88,88	0
86	MG	5	3729	1/1	0.45	499.00	96,96,96,96	0
86	MG	8	217	1/1	0.73	388.33	96,96,96,96	0
86	MG	6	2035	1/1	0.35	343.00	90,90,90,90	0
86	MG	5	3718	1/1	0.56	326.00	67,67,67,67	0
86	MG	2	1973	1/1	0.91	282.50	94,94,94,94	0
86	MG	1	3502	1/1	1.11	202.37	55,55,55,55	0
86	MG	1	3759	1/1	0.38	201.00	78,78,78,78	0
86	MG	6	1989	1/1	1.23	188.64	80,80,80,80	0
86	MG	2	1958	1/1	0.65	185.00	108,108,108,108	0
86	MG	5	3410	1/1	0.60	183.00	98,98,98,98	0
86	MG	5	3830	1/1	1.08	174.72	64,64,64,64	0
86	MG	5	3734	1/1	0.47	156.00	65,65,65,65	0
86	MG	5	3775	1/1	0.80	155.00	100,100,100,100	0
86	MG	2	1957	1/1	0.61	151.00	97,97,97,97	0
86	MG	1	3538	1/1	0.76	147.89	58,58,58,58	0
86	MG	1	3738	1/1	0.71	145.00	58,58,58,58	0
86	MG	1	3439	1/1	0.87	143.44	60,60,60,60	0
86	MG	1	3463	1/1	0.62	142.33	38,38,38,38	0
86	MG	6	1916	1/1	1.08	132.28	73,73,73,73	0
86	MG	5	3754	1/1	0.40	129.00	62,62,62,62	0
86	MG	5	3875	1/1	0.62	128.67	44,44,44,44	0
86	MG	5	3771	1/1	0.79	124.43	48,48,48,48	0
86	MG	5	3799	1/1	0.55	124.33	72,72,72,72	0
86	MG	5	3404	1/1	0.79	123.10	82,82,82,82	0
86	MG	1	3562	1/1	0.42	120.02	50,50,50,50	0
86	MG	2	1995	1/1	1.54	114.08	113,113,113,113	0
86	MG	2	2009	1/1	2.45	111.85	83,83,83,83	0
86	MG	1	3704	1/1	0.71	109.60	69,69,69,69	0
86	MG	3	208	1/1	0.66	108.22	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3517	1/1	0.60	107.31	28,28,28,28	0
86	MG	1	3549	1/1	0.42	105.50	87,87,87,87	0
86	MG	1	3530	1/1	0.68	105.05	34,34,34,34	0
86	MG	5	3893	1/1	0.69	102.78	50,50,50,50	0
86	MG	1	3846	1/1	1.09	98.68	61,61,61,61	0
86	MG	1	3766	1/1	1.09	97.89	69,69,69,69	0
86	MG	1	3681	1/1	0.47	97.74	85,85,85,85	0
86	MG	2	1988	1/1	0.76	96.69	79,79,79,79	0
86	MG	2	1956	1/1	1.03	94.98	77,77,77,77	0
86	MG	5	3455	1/1	0.77	94.15	49,49,49,49	0
86	MG	1	3848	1/1	0.37	92.50	60,60,60,60	0
86	MG	5	3647	1/1	1.34	91.61	41,41,41,41	0
86	MG	5	3473	1/1	0.28	91.00	88,88,88,88	0
86	MG	5	3435	1/1	0.92	88.85	53,53,53,53	0
86	MG	5	3414	1/1	0.62	86.59	50,50,50,50	0
86	MG	1	3645	1/1	0.53	86.25	49,49,49,49	0
86	MG	1	3823	1/1	0.62	82.33	60,60,60,60	0
86	MG	2	1927	1/1	0.90	82.32	49,49,49,49	0
86	MG	5	3628	1/1	0.83	80.02	121,121,121,121	0
86	MG	5	3762	1/1	1.00	76.73	69,69,69,69	0
86	MG	1	3831	1/1	0.71	76.53	40,40,40,40	0
86	MG	1	3783	1/1	1.03	76.36	56,56,56,56	0
86	MG	5	3764	1/1	0.68	76.01	47,47,47,47	0
86	MG	1	3684	1/1	0.43	75.86	78,78,78,78	0
86	MG	1	3696	1/1	1.10	74.36	80,80,80,80	0
86	MG	5	3701	1/1	1.49	73.91	85,85,85,85	0
86	MG	5	3566	1/1	0.81	73.43	31,31,31,31	0
86	MG	6	2037	1/1	0.70	70.86	88,88,88,88	0
86	MG	5	3842	1/1	0.71	65.87	67,67,67,67	0
86	MG	1	3609	1/1	0.54	65.18	52,52,52,52	0
86	MG	1	3590	1/1	1.00	64.27	49,49,49,49	0
86	MG	1	3500	1/1	1.10	63.71	105,105,105,105	0
86	MG	1	3718	1/1	1.03	63.64	118,118,118,118	0
86	MG	5	3589	1/1	0.91	63.40	50,50,50,50	0
86	MG	8	212	1/1	0.94	62.53	95,95,95,95	0
86	MG	1	3402	1/1	0.92	62.01	61,61,61,61	0
86	MG	5	3546	1/1	0.52	60.77	61,61,61,61	0
86	MG	5	3731	1/1	0.54	60.29	105,105,105,105	0
86	MG	1	3656	1/1	0.92	60.22	50,50,50,50	0
86	MG	6	1983	1/1	1.13	60.21	99,99,99,99	0
86	MG	2	1935	1/1	0.53	59.53	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3785	1/1	0.89	58.37	66,66,66,66	0
86	MG	1	3852	1/1	0.76	57.88	89,89,89,89	0
86	MG	5	3645	1/1	0.81	57.02	83,83,83,83	0
86	MG	5	3869	1/1	0.85	56.33	64,64,64,64	0
86	MG	5	3841	1/1	1.05	55.91	63,63,63,63	0
86	MG	5	3854	1/1	0.76	54.36	88,88,88,88	0
86	MG	5	3856	1/1	0.50	54.24	58,58,58,58	0
86	MG	1	3675	1/1	0.59	54.23	87,87,87,87	0
86	MG	5	3845	1/1	0.57	54.22	100,100,100,100	0
87	OHX	1	4138	7/7	0.22	53.89	177,177,177,177	0
86	MG	5	3801	1/1	1.03	53.73	61,61,61,61	0
86	MG	1	3613	1/1	0.68	53.67	52,52,52,52	0
86	MG	5	3481	1/1	0.58	53.35	47,47,47,47	0
86	MG	1	3560	1/1	0.73	53.22	34,34,34,34	0
86	MG	1	3490	1/1	1.14	52.39	77,77,77,77	0
86	MG	2	1962	1/1	0.66	52.27	92,92,92,92	0
86	MG	1	3689	1/1	1.01	52.22	73,73,73,73	0
86	MG	2	1974	1/1	0.49	51.65	100,100,100,100	0
86	MG	1	3593	1/1	0.74	51.61	31,31,31,31	0
86	MG	5	3581	1/1	0.61	50.93	61,61,61,61	0
86	MG	1	3671	1/1	1.46	50.88	74,74,74,74	0
86	MG	1	3749	1/1	1.48	50.67	93,93,93,93	0
86	MG	5	3687	1/1	0.76	50.15	42,42,42,42	0
86	MG	1	3596	1/1	1.15	49.84	38,38,38,38	0
86	MG	6	2011	1/1	0.38	49.57	78,78,78,78	0
86	MG	1	3470	1/1	1.02	49.49	67,67,67,67	0
86	MG	1	3770	1/1	0.60	49.21	76,76,76,76	0
86	MG	5	3868	1/1	0.39	49.00	56,56,56,56	0
86	MG	5	3482	1/1	0.79	48.93	30,30,30,30	0
86	MG	1	3577	1/1	0.86	48.72	53,53,53,53	0
86	MG	5	3489	1/1	0.56	48.51	49,49,49,49	0
86	MG	5	3407	1/1	0.91	48.32	53,53,53,53	0
86	MG	6	2043	1/1	1.53	47.46	136,136,136,136	0
86	MG	1	3850	1/1	0.77	47.41	50,50,50,50	0
86	MG	1	3476	1/1	0.48	47.36	74,74,74,74	0
86	MG	2	1902	1/1	0.77	46.93	75,75,75,75	0
86	MG	5	3593	1/1	0.70	46.19	28,28,28,28	0
86	MG	1	3414	1/1	0.54	45.91	68,68,68,68	0
86	MG	6	2039	1/1	1.16	43.13	102,102,102,102	0
86	MG	1	3515	1/1	0.79	42.55	44,44,44,44	0
86	MG	5	3555	1/1	0.80	42.37	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3817	1/1	0.85	41.90	37,37,37,37	0
86	MG	5	3560	1/1	0.71	41.74	48,48,48,48	0
86	MG	5	3467	1/1	0.94	41.50	72,72,72,72	0
86	MG	1	3573	1/1	0.81	41.44	23,23,23,23	0
86	MG	1	3712	1/1	0.50	41.03	76,76,76,76	0
86	MG	1	3658	1/1	0.67	40.91	47,47,47,47	0
86	MG	5	3575	1/1	0.70	40.91	56,56,56,56	0
86	MG	2	1942	1/1	1.08	40.59	97,97,97,97	0
86	MG	1	3764	1/1	0.93	40.56	47,47,47,47	0
86	MG	5	3661	1/1	1.17	40.54	70,70,70,70	0
86	MG	1	3679	1/1	0.88	40.52	63,63,63,63	0
86	MG	5	3425	1/1	1.02	39.99	73,73,73,73	0
86	MG	5	3679	1/1	0.46	39.92	63,63,63,63	0
86	MG	1	3676	1/1	1.55	39.57	94,94,94,94	0
86	MG	5	3530	1/1	0.66	39.32	30,30,30,30	0
86	MG	5	3634	1/1	0.80	39.00	73,73,73,73	0
86	MG	4	217	1/1	1.59	38.92	100,100,100,100	0
86	MG	1	3541	1/1	0.73	38.40	64,64,64,64	0
86	MG	5	3879	1/1	0.73	38.27	51,51,51,51	0
86	MG	6	1941	1/1	0.24	38.20	96,96,96,96	0
86	MG	1	3550	1/1	0.92	38.16	49,49,49,49	0
86	MG	5	3624	1/1	0.58	37.71	74,74,74,74	0
86	MG	1	3843	1/1	1.18	37.67	81,81,81,81	0
86	MG	1	3832	1/1	0.70	37.65	44,44,44,44	0
86	MG	5	3772	1/1	0.38	37.46	110,110,110,110	0
86	MG	5	3576	1/1	0.47	37.40	36,36,36,36	0
86	MG	5	3614	1/1	0.61	37.39	48,48,48,48	0
86	MG	1	3786	1/1	0.64	37.34	57,57,57,57	0
86	MG	2	1904	1/1	0.43	36.85	110,110,110,110	0
86	MG	1	3648	1/1	0.67	36.39	51,51,51,51	0
86	MG	5	3656	1/1	0.65	36.26	59,59,59,59	0
86	MG	5	3635	1/1	1.24	35.99	60,60,60,60	0
86	MG	1	3661	1/1	0.69	35.51	62,62,62,62	0
86	MG	1	3459	1/1	0.89	35.50	46,46,46,46	0
86	MG	5	3583	1/1	0.75	35.40	28,28,28,28	0
86	MG	1	3468	1/1	0.36	35.36	75,75,75,75	0
86	MG	7	206	1/1	0.45	34.84	58,58,58,58	0
86	MG	5	3843	1/1	0.74	34.67	70,70,70,70	0
86	MG	1	3546	1/1	0.43	34.43	72,72,72,72	0
86	MG	5	3735	1/1	0.83	34.32	47,47,47,47	0
86	MG	5	3755	1/1	0.97	34.30	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3749	1/1	0.56	34.24	47,47,47,47	0
86	MG	1	3421	1/1	0.81	33.33	47,47,47,47	0
86	MG	1	3594	1/1	0.69	33.21	41,41,41,41	0
86	MG	1	3564	1/1	0.77	32.94	38,38,38,38	0
86	MG	5	3880	1/1	0.97	32.75	67,67,67,67	0
86	MG	1	3520	1/1	0.79	32.44	43,43,43,43	0
86	MG	2	1933	1/1	0.53	32.14	85,85,85,85	0
86	MG	6	1934	1/1	0.70	32.13	82,82,82,82	0
86	MG	1	3763	1/1	1.27	32.05	63,63,63,63	0
86	MG	5	3464	1/1	0.36	32.01	77,77,77,77	0
86	MG	1	3827	1/1	0.76	31.92	71,71,71,71	0
86	MG	1	3682	1/1	0.66	31.71	50,50,50,50	0
86	MG	1	3677	1/1	0.64	31.71	68,68,68,68	0
86	MG	5	3570	1/1	0.57	31.65	26,26,26,26	0
86	MG	1	3838	1/1	0.65	31.43	39,39,39,39	0
86	MG	5	3582	1/1	0.74	31.40	56,56,56,56	0
86	MG	1	3575	1/1	0.38	31.36	51,51,51,51	0
86	MG	5	3874	1/1	0.58	31.36	34,34,34,34	0
86	MG	1	3815	1/1	0.72	31.35	111,111,111,111	0
86	MG	1	3438	1/1	0.80	31.33	32,32,32,32	0
86	MG	5	3504	1/1	0.85	31.25	78,78,78,78	0
86	MG	1	3513	1/1	1.12	31.17	37,37,37,37	0
86	MG	5	3578	1/1	0.50	31.17	41,41,41,41	0
86	MG	5	3501	1/1	0.47	31.12	60,60,60,60	0
86	MG	5	3447	1/1	0.42	31.08	70,70,70,70	0
86	MG	1	3774	1/1	0.35	31.00	69,69,69,69	0
86	MG	1	3706	1/1	0.61	30.78	92,92,92,92	0
86	MG	2	1982	1/1	0.71	30.74	65,65,65,65	0
86	MG	D3	201	1/1	0.80	30.71	80,80,80,80	0
86	MG	5	3792	1/1	0.76	30.66	68,68,68,68	0
86	MG	5	3540	1/1	0.68	30.64	44,44,44,44	0
86	MG	1	3834	1/1	1.02	30.57	63,63,63,63	0
86	MG	1	3453	1/1	1.02	30.52	54,54,54,54	0
86	MG	5	3585	1/1	0.71	30.28	39,39,39,39	0
87	OHX	1	4205	7/7	0.51	30.20	192,192,192,192	0
86	MG	1	3452	1/1	0.51	30.05	47,47,47,47	0
86	MG	2	1918	1/1	0.95	29.91	61,61,61,61	0
86	MG	5	3864	1/1	1.01	29.90	41,41,41,41	0
86	MG	5	3551	1/1	0.69	29.56	35,35,35,35	0
86	MG	1	3865	1/1	0.55	29.46	103,103,103,103	0
86	MG	5	3748	1/1	0.85	29.33	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3428	1/1	1.08	29.30	55,55,55,55	0
86	MG	1	3811	1/1	0.44	29.29	64,64,64,64	0
86	MG	5	3779	1/1	0.42	29.12	45,45,45,45	0
86	MG	1	3410	1/1	0.78	28.74	35,35,35,35	0
86	MG	2	2007	1/1	0.66	28.72	107,107,107,107	0
86	MG	1	3583	1/1	0.64	28.62	68,68,68,68	0
86	MG	5	3871	1/1	0.50	28.60	57,57,57,57	0
86	MG	5	3445	1/1	0.51	28.37	40,40,40,40	0
87	OHX	5	4123	7/7	0.26	28.32	185,185,185,185	0
86	MG	1	3841	1/1	0.40	28.25	80,80,80,80	0
86	MG	5	3450	1/1	0.73	27.89	49,49,49,49	0
86	MG	4	213	1/1	0.51	27.78	89,89,89,89	0
86	MG	8	216	1/1	0.66	27.59	79,79,79,79	0
86	MG	6	2036	1/1	0.55	27.43	67,67,67,67	0
86	MG	1	3446	1/1	0.61	27.43	67,67,67,67	0
86	MG	2	1984	1/1	1.18	27.40	97,97,97,97	0
86	MG	6	2016	1/1	1.30	27.20	83,83,83,83	0
86	MG	5	3658	1/1	0.61	27.17	45,45,45,45	0
86	MG	1	3527	1/1	0.50	26.98	36,36,36,36	0
86	MG	2	1916	1/1	0.63	26.87	70,70,70,70	0
86	MG	5	3809	1/1	0.56	26.64	63,63,63,63	0
86	MG	5	3860	1/1	0.72	26.36	87,87,87,87	0
86	MG	5	3878	1/1	0.76	26.25	49,49,49,49	0
86	MG	5	3538	1/1	0.99	26.09	38,38,38,38	0
86	MG	5	3571	1/1	0.59	25.90	59,59,59,59	0
86	MG	6	1946	1/1	0.44	25.88	38,38,38,38	0
86	MG	5	3521	1/1	0.72	25.56	48,48,48,48	0
86	MG	5	3865	1/1	0.66	25.48	50,50,50,50	0
86	MG	1	3532	1/1	0.45	25.48	49,49,49,49	0
86	MG	1	3528	1/1	0.55	25.40	36,36,36,36	0
86	MG	1	3680	1/1	0.34	25.36	91,91,91,91	0
86	MG	6	1943	1/1	0.77	25.34	41,41,41,41	0
86	MG	5	3507	1/1	0.78	25.21	37,37,37,37	0
86	MG	5	3703	1/1	0.56	25.14	68,68,68,68	0
86	MG	1	3578	1/1	0.44	25.07	56,56,56,56	0
87	OHX	5	4224	7/7	0.15	25.00	204,204,204,204	0
86	MG	5	3774	1/1	1.06	24.98	60,60,60,60	0
86	MG	5	3553	1/1	0.90	24.97	63,63,63,63	0
86	MG	5	3649	1/1	0.75	24.94	80,80,80,80	0
86	MG	5	3814	1/1	0.45	24.81	83,83,83,83	0
86	MG	5	3683	1/1	0.67	24.69	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3621	1/1	0.57	24.63	57,57,57,57	0
86	MG	5	3532	1/1	0.43	24.57	44,44,44,44	0
86	MG	1	3512	1/1	0.78	24.50	55,55,55,55	0
86	MG	5	3806	1/1	0.37	24.50	43,43,43,43	0
86	MG	1	3496	1/1	0.70	24.49	38,38,38,38	0
86	MG	5	3506	1/1	0.97	24.46	39,39,39,39	0
86	MG	5	3742	1/1	0.45	24.37	71,71,71,71	0
86	MG	1	3758	1/1	0.69	24.31	46,46,46,46	0
86	MG	1	3542	1/1	0.52	23.86	45,45,45,45	0
86	MG	1	3523	1/1	0.67	23.81	44,44,44,44	0
86	MG	5	3723	1/1	0.55	23.76	53,53,53,53	0
86	MG	5	3654	1/1	0.32	23.69	56,56,56,56	0
86	MG	5	3636	1/1	0.68	23.68	53,53,53,53	0
86	MG	6	2049	1/1	0.55	23.63	123,123,123,123	0
86	MG	6	2029	1/1	1.08	23.56	88,88,88,88	0
86	MG	1	3690	1/1	0.52	23.24	52,52,52,52	0
86	MG	5	3433	1/1	0.57	23.17	44,44,44,44	0
86	MG	5	3442	1/1	0.42	23.04	40,40,40,40	0
86	MG	1	3835	1/1	0.60	22.93	64,64,64,64	0
86	MG	1	3531	1/1	0.70	22.83	79,79,79,79	0
86	MG	5	3639	1/1	0.48	22.63	51,51,51,51	0
87	OHX	5	3899	7/7	0.27	22.49	78,78,78,78	0
86	MG	1	3460	1/1	0.72	22.43	42,42,42,42	0
86	MG	1	3752	1/1	0.43	22.38	55,55,55,55	0
86	MG	1	3819	1/1	0.54	22.20	73,73,73,73	0
86	MG	5	3536	1/1	0.74	22.18	38,38,38,38	0
87	OHX	6	2113	7/7	0.34	22.09	184,184,184,184	0
86	MG	1	3678	1/1	0.44	22.01	64,64,64,64	0
86	MG	5	3673	1/1	0.71	21.94	72,72,72,72	0
86	MG	1	3864	1/1	0.68	21.83	74,74,74,74	0
86	MG	6	1929	1/1	0.51	21.80	81,81,81,81	0
86	MG	5	3803	1/1	0.85	21.70	61,61,61,61	0
86	MG	1	3475	1/1	0.39	21.70	52,52,52,52	0
86	MG	5	3594	1/1	0.52	21.69	49,49,49,49	0
86	MG	5	3676	1/1	0.71	21.66	98,98,98,98	0
86	MG	1	3652	1/1	0.33	21.61	57,57,57,57	0
86	MG	5	3784	1/1	0.81	21.44	86,86,86,86	0
86	MG	5	3574	1/1	0.66	21.41	30,30,30,30	0
86	MG	5	3882	1/1	0.75	21.29	113,113,113,113	0
86	MG	L3	402	1/1	0.48	21.25	77,77,77,77	0
86	MG	1	3849	1/1	0.58	21.23	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3537	1/1	0.56	21.03	54,54,54,54	0
86	MG	5	3619	1/1	0.35	21.00	90,90,90,90	0
86	MG	1	3563	1/1	0.68	20.92	52,52,52,52	0
86	MG	5	3535	1/1	0.92	20.82	37,37,37,37	0
86	MG	5	3524	1/1	0.55	20.63	40,40,40,40	0
86	MG	5	3603	1/1	0.75	20.53	60,60,60,60	0
86	MG	5	3418	1/1	0.85	20.52	40,40,40,40	0
86	MG	6	2012	1/1	0.51	20.48	77,77,77,77	0
86	MG	5	3697	1/1	0.58	20.42	62,62,62,62	0
86	MG	1	3673	1/1	0.41	20.22	75,75,75,75	0
86	MG	1	3526	1/1	0.45	20.21	44,44,44,44	0
86	MG	1	3539	1/1	0.43	20.13	64,64,64,64	0
86	MG	1	3544	1/1	0.56	20.12	47,47,47,47	0
86	MG	5	3883	1/1	0.58	20.06	78,78,78,78	0
86	MG	1	3692	1/1	0.87	20.06	67,67,67,67	0
86	MG	1	3587	1/1	0.58	20.04	58,58,58,58	0
86	MG	2	1985	1/1	1.07	20.04	77,77,77,77	0
86	MG	1	3443	1/1	0.67	20.01	83,83,83,83	0
86	MG	5	3561	1/1	0.87	19.97	34,34,34,34	0
86	MG	4	206	1/1	0.69	19.91	53,53,53,53	0
86	MG	2	1914	1/1	0.50	19.89	89,89,89,89	0
86	MG	6	1954	1/1	0.41	19.88	80,80,80,80	0
86	MG	5	3829	1/1	0.67	19.87	58,58,58,58	0
86	MG	1	3650	1/1	0.74	19.83	122,122,122,122	0
86	MG	2	2017	1/1	0.57	19.82	85,85,85,85	0
86	MG	1	3750	1/1	0.56	19.80	75,75,75,75	0
86	MG	5	3833	1/1	0.20	19.80	61,61,61,61	0
86	MG	6	1932	1/1	0.60	19.78	67,67,67,67	0
86	MG	5	3509	1/1	0.68	19.73	45,45,45,45	0
86	MG	5	3494	1/1	0.68	19.72	43,43,43,43	0
86	MG	1	3657	1/1	0.83	19.69	68,68,68,68	0
87	OHX	5	4216	7/7	0.41	19.54	217,217,217,217	0
86	MG	1	3533	1/1	0.57	19.49	51,51,51,51	0
86	MG	6	1988	1/1	0.67	19.44	91,91,91,91	0
86	MG	3	204	1/1	0.43	19.35	65,65,65,65	0
86	MG	5	3595	1/1	0.66	19.25	34,34,34,34	0
86	MG	6	2045	1/1	0.83	19.20	94,94,94,94	0
86	MG	5	3831	1/1	0.59	19.13	57,57,57,57	0
86	MG	1	3784	1/1	0.60	19.07	73,73,73,73	0
86	MG	6	1962	1/1	0.85	18.94	94,94,94,94	0
86	MG	1	3580	1/1	0.49	18.89	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3649	1/1	0.56	18.85	69,69,69,69	0
86	MG	5	3443	1/1	0.72	18.85	45,45,45,45	0
87	OHX	5	4116	7/7	0.31	18.64	197,197,197,197	0
86	MG	1	3572	1/1	0.48	18.63	51,51,51,51	0
86	MG	5	3730	1/1	0.31	18.56	46,46,46,46	0
86	MG	2	1923	1/1	0.62	18.56	88,88,88,88	0
86	MG	6	1918	1/1	0.54	18.50	80,80,80,80	0
86	MG	5	3807	1/1	0.70	18.45	109,109,109,109	0
86	MG	5	3565	1/1	0.45	18.39	67,67,67,67	0
86	MG	7	210	1/1	0.80	18.33	91,91,91,91	0
86	MG	1	3810	1/1	0.32	18.17	61,61,61,61	0
86	MG	5	3670	1/1	1.12	18.10	62,62,62,62	0
86	MG	1	3630	1/1	0.46	18.05	47,47,47,47	0
86	MG	1	3540	1/1	0.54	18.05	36,36,36,36	0
86	MG	5	3625	1/1	0.44	18.04	72,72,72,72	0
86	MG	5	3457	1/1	0.57	18.01	44,44,44,44	0
86	MG	5	3503	1/1	0.67	17.92	44,44,44,44	0
86	MG	5	3520	1/1	0.77	17.86	54,54,54,54	0
86	MG	1	3504	1/1	0.62	17.86	45,45,45,45	0
86	MG	1	3576	1/1	0.51	17.85	35,35,35,35	0
86	MG	5	3588	1/1	0.70	17.78	43,43,43,43	0
86	MG	1	3605	1/1	0.45	17.75	66,66,66,66	0
86	MG	6	2034	1/1	0.52	17.70	92,92,92,92	0
86	MG	5	3459	1/1	0.53	17.61	39,39,39,39	0
86	MG	5	3552	1/1	0.67	17.61	72,72,72,72	0
86	MG	1	3534	1/1	0.51	17.53	50,50,50,50	0
86	MG	5	3500	1/1	0.71	17.51	44,44,44,44	0
86	MG	1	3733	1/1	0.46	17.49	52,52,52,52	0
86	MG	1	3693	1/1	0.37	17.41	58,58,58,58	0
86	MG	5	3848	1/1	0.46	17.30	89,89,89,89	0
86	MG	6	1921	1/1	0.41	17.21	57,57,57,57	0
86	MG	5	3705	1/1	0.63	17.21	68,68,68,68	0
86	MG	6	2032	1/1	0.35	17.20	103,103,103,103	0
86	MG	1	3484	1/1	0.47	17.17	70,70,70,70	0
86	MG	5	3522	1/1	0.56	17.13	58,58,58,58	0
86	MG	5	3835	1/1	0.60	17.06	47,47,47,47	0
86	MG	1	3702	1/1	0.47	17.05	57,57,57,57	0
86	MG	2	1945	1/1	0.42	17.02	91,91,91,91	0
86	MG	5	3867	1/1	0.40	16.98	66,66,66,66	0
86	MG	5	3529	1/1	0.36	16.93	47,47,47,47	0
86	MG	5	3720	1/1	0.66	16.90	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3588	1/1	0.56	16.85	66,66,66,66	0
86	MG	7	202	1/1	0.61	16.70	9,9,9,9	0
86	MG	5	4247	1/1	0.43	16.68	64,64,64,64	0
86	MG	1	3615	1/1	1.67	16.68	108,108,108,108	0
86	MG	5	3733	1/1	0.35	16.66	54,54,54,54	0
86	MG	5	3737	1/1	0.70	16.63	50,50,50,50	0
86	MG	5	3573	1/1	0.61	16.56	53,53,53,53	0
86	MG	5	3870	1/1	0.40	16.52	42,42,42,42	0
86	MG	6	2022	1/1	0.55	16.52	64,64,64,64	0
86	MG	5	3760	1/1	1.10	16.51	49,49,49,49	0
86	MG	2	1966	1/1	0.46	16.44	126,126,126,126	0
86	MG	1	3498	1/1	0.36	16.44	53,53,53,53	0
86	MG	1	3440	1/1	0.61	16.44	59,59,59,59	0
86	MG	1	3451	1/1	0.42	16.42	51,51,51,51	0
86	MG	1	3765	1/1	0.43	16.34	68,68,68,68	0
86	MG	1	3620	1/1	0.95	16.34	63,63,63,63	0
86	MG	1	3473	1/1	0.54	16.33	33,33,33,33	0
86	MG	1	3853	1/1	0.24	16.31	95,95,95,95	0
86	MG	6	1917	1/1	0.37	16.30	58,58,58,58	0
86	MG	5	3759	1/1	0.25	16.27	94,94,94,94	0
86	MG	5	3873	1/1	0.48	16.25	47,47,47,47	0
86	MG	1	3552	1/1	0.55	16.07	56,56,56,56	0
86	MG	5	3461	1/1	0.60	16.03	46,46,46,46	0
86	MG	5	3797	1/1	0.35	16.00	58,58,58,58	0
86	MG	5	3405	1/1	0.58	16.00	72,72,72,72	0
86	MG	1	3571	1/1	0.69	15.98	40,40,40,40	0
86	MG	5	3518	1/1	0.46	15.86	31,31,31,31	0
86	MG	5	3712	1/1	0.53	15.86	57,57,57,57	0
86	MG	1	3559	1/1	0.36	15.85	56,56,56,56	0
86	MG	8	207	1/1	0.43	15.82	81,81,81,81	0
87	OHX	1	4056	7/7	0.31	15.81	147,147,147,147	0
86	MG	6	1944	1/1	0.44	15.79	53,53,53,53	0
86	MG	5	3667	1/1	0.42	15.72	63,63,63,63	0
86	MG	1	3519	1/1	0.58	15.66	40,40,40,40	0
86	MG	5	3409	1/1	0.62	15.64	53,53,53,53	0
86	MG	5	3526	1/1	0.53	15.63	46,46,46,46	0
86	MG	5	3610	1/1	0.62	15.61	44,44,44,44	0
86	MG	1	3719	1/1	0.55	15.60	55,55,55,55	0
86	MG	5	3629	1/1	0.64	15.49	49,49,49,49	0
86	MG	1	3514	1/1	0.55	15.44	36,36,36,36	0
86	MG	5	3491	1/1	0.39	15.41	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3653	1/1	0.91	15.39	62,62,62,62	0
86	MG	1	3721	1/1	0.35	15.32	45,45,45,45	0
86	MG	1	3826	1/1	0.52	15.31	50,50,50,50	0
86	MG	1	3581	1/1	0.72	15.18	65,65,65,65	0
86	MG	5	3745	1/1	0.60	15.16	51,51,51,51	0
86	MG	5	3627	1/1	0.54	15.13	58,58,58,58	0
86	MG	1	3506	1/1	0.61	15.07	59,59,59,59	0
86	MG	1	3833	1/1	0.90	15.06	55,55,55,55	0
86	MG	1	3829	1/1	0.48	14.91	43,43,43,43	0
86	MG	1	3486	1/1	0.58	14.86	54,54,54,54	0
86	MG	1	3458	1/1	0.59	14.81	82,82,82,82	0
86	MG	5	3812	1/1	0.28	14.80	51,51,51,51	0
86	MG	1	3517	1/1	0.76	14.77	50,50,50,50	0
86	MG	1	3697	1/1	1.87	14.73	96,96,96,96	0
86	MG	5	3657	1/1	0.43	14.69	38,38,38,38	0
86	MG	2	1919	1/1	0.58	14.68	67,67,67,67	0
86	MG	5	3885	1/1	0.51	14.65	53,53,53,53	0
86	MG	1	3441	1/1	0.53	14.54	42,42,42,42	0
86	MG	5	3616	1/1	0.33	14.47	68,68,68,68	0
86	MG	1	3570	1/1	0.74	14.47	39,39,39,39	0
86	MG	5	3617	1/1	0.52	14.44	52,52,52,52	0
86	MG	1	3672	1/1	1.17	14.42	73,73,73,73	0
86	MG	1	3503	1/1	0.58	14.37	45,45,45,45	0
86	MG	5	3704	1/1	0.72	14.35	63,63,63,63	0
86	MG	5	3750	1/1	0.45	14.32	63,63,63,63	0
86	MG	1	3595	1/1	0.65	14.30	47,47,47,47	0
86	MG	1	3603	1/1	0.99	14.28	89,89,89,89	0
86	MG	5	3642	1/1	0.37	14.24	50,50,50,50	0
86	MG	5	3470	1/1	0.42	14.22	60,60,60,60	0
86	MG	1	3805	1/1	0.56	14.22	54,54,54,54	0
86	MG	5	3431	1/1	0.42	14.22	45,45,45,45	0
86	MG	1	3791	1/1	0.67	14.19	53,53,53,53	0
86	MG	5	3699	1/1	0.41	14.18	58,58,58,58	0
86	MG	3	202	1/1	0.60	14.18	74,74,74,74	0
86	MG	6	1972	1/1	0.68	14.17	75,75,75,75	0
86	MG	1	3567	1/1	0.46	14.16	37,37,37,37	0
86	MG	5	3539	1/1	0.64	14.09	31,31,31,31	0
86	MG	1	3522	1/1	0.86	14.09	65,65,65,65	0
86	MG	5	3608	1/1	0.38	14.07	66,66,66,66	0
86	MG	5	3487	1/1	0.54	14.07	42,42,42,42	0
86	MG	6	1939	1/1	0.55	14.04	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	1923	1/1	0.42	14.00	88,88,88,88	0
86	MG	5	3428	1/1	0.38	14.00	43,43,43,43	0
86	MG	5	3523	1/1	0.60	14.00	63,63,63,63	0
86	MG	5	3655	1/1	0.45	13.99	53,53,53,53	0
86	MG	2	1978	1/1	0.43	13.97	86,86,86,86	0
86	MG	1	3423	1/1	0.48	13.95	57,57,57,57	0
86	MG	o2	201	1/1	0.44	13.93	47,47,47,47	0
86	MG	5	3531	1/1	0.67	13.91	53,53,53,53	0
86	MG	5	3458	1/1	0.39	13.88	63,63,63,63	0
86	MG	5	3432	1/1	0.42	13.82	89,89,89,89	0
86	MG	1	3509	1/1	0.61	13.76	35,35,35,35	0
86	MG	1	3789	1/1	0.34	13.74	117,117,117,117	0
86	MG	1	3818	1/1	0.46	13.71	71,71,71,71	0
86	MG	2	1905	1/1	0.63	13.69	74,74,74,74	0
86	MG	5	3690	1/1	0.49	13.68	60,60,60,60	0
86	MG	5	3685	1/1	0.32	13.67	56,56,56,56	0
86	MG	5	3430	1/1	0.39	13.61	51,51,51,51	0
86	MG	2	2002	1/1	0.51	13.57	133,133,133,133	0
86	MG	1	3798	1/1	0.53	13.55	58,58,58,58	0
86	MG	5	3590	1/1	0.64	13.48	41,41,41,41	0
86	MG	1	3761	1/1	0.68	13.44	56,56,56,56	0
86	MG	6	1930	1/1	0.35	13.44	76,76,76,76	0
86	MG	5	3497	1/1	0.27	13.39	52,52,52,52	0
86	MG	1	3665	1/1	0.51	13.34	53,53,53,53	0
86	MG	1	3535	1/1	0.45	13.29	41,41,41,41	0
86	MG	5	3756	1/1	0.41	13.28	70,70,70,70	0
86	MG	1	3407	1/1	0.44	13.28	63,63,63,63	0
86	MG	1	3687	1/1	0.44	13.20	58,58,58,58	0
87	OHX	5	4244	7/7	0.53	13.13	214,214,214,214	0
86	MG	5	3587	1/1	0.46	13.11	43,43,43,43	0
86	MG	6	2025	1/1	0.49	12.98	100,100,100,100	0
86	MG	1	3403	1/1	0.33	12.95	53,53,53,53	0
87	OHX	1	4206	7/7	0.79	12.93	225,225,225,225	0
86	MG	5	3643	1/1	0.65	12.91	65,65,65,65	0
86	MG	1	3753	1/1	0.31	12.91	44,44,44,44	0
86	MG	6	2024	1/1	0.47	12.89	144,144,144,144	0
86	MG	1	3655	1/1	0.58	12.85	64,64,64,64	0
86	MG	6	1908	1/1	0.45	12.83	58,58,58,58	0
86	MG	5	3454	1/1	0.40	12.80	38,38,38,38	0
86	MG	6	2014	1/1	0.52	12.79	69,69,69,69	0
86	MG	M3	201	1/1	0.72	12.78	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	2	1983	1/1	0.54	12.72	95,95,95,95	0
86	MG	5	3739	1/1	0.46	12.67	48,48,48,48	0
86	MG	6	2033	1/1	0.35	12.66	112,112,112,112	0
86	MG	1	3449	1/1	0.38	12.65	46,46,46,46	0
86	MG	5	3572	1/1	0.62	12.63	40,40,40,40	0
86	MG	1	3863	1/1	0.51	12.56	83,83,83,83	0
87	OHX	5	4182	7/7	0.48	12.56	149,149,149,149	0
86	MG	5	3876	1/1	0.45	12.47	57,57,57,57	0
86	MG	1	3618	1/1	0.30	12.44	60,60,60,60	0
86	MG	L8	301	1/1	0.52	12.33	104,104,104,104	0
86	MG	5	3513	1/1	0.58	12.31	36,36,36,36	0
86	MG	4	221	1/1	0.35	12.28	63,63,63,63	0
86	MG	5	3651	1/1	0.53	12.27	52,52,52,52	0
86	MG	5	3528	1/1	0.35	12.23	43,43,43,43	0
87	OHX	1	4199	7/7	0.34	12.20	159,159,159,159	0
86	MG	5	3650	1/1	0.51	12.18	48,48,48,48	0
86	MG	5	3641	1/1	0.73	12.18	64,64,64,64	0
86	MG	6	1963	1/1	0.65	12.17	68,68,68,68	0
86	MG	1	3768	1/1	0.50	12.13	48,48,48,48	0
86	MG	n4	201	1/1	0.52	12.08	60,60,60,60	0
86	MG	1	3862	1/1	0.41	12.05	117,117,117,117	0
86	MG	5	3886	1/1	0.46	12.02	42,42,42,42	0
86	MG	5	3866	1/1	0.50	11.96	41,41,41,41	0
86	MG	5	3476	1/1	0.31	11.96	79,79,79,79	0
86	MG	1	3628	1/1	0.49	11.89	58,58,58,58	0
86	MG	1	3812	1/1	0.55	11.85	64,64,64,64	0
86	MG	1	3485	1/1	0.39	11.83	62,62,62,62	0
86	MG	5	3465	1/1	0.30	11.73	47,47,47,47	0
86	MG	5	3541	1/1	0.34	11.55	40,40,40,40	0
86	MG	1	3545	1/1	0.50	11.55	62,62,62,62	0
86	MG	6	2013	1/1	0.70	11.54	66,66,66,66	0
86	MG	7	215	1/1	0.41	11.54	73,73,73,73	0
86	MG	5	3586	1/1	0.41	11.52	33,33,33,33	0
86	MG	5	3832	1/1	0.58	11.52	53,53,53,53	0
86	MG	5	4248	1/1	0.43	11.50	51,51,51,51	0
86	MG	6	2046	1/1	0.48	11.38	67,67,67,67	0
86	MG	1	3432	1/1	0.39	11.38	47,47,47,47	0
86	MG	1	3524	1/1	0.39	11.37	41,41,41,41	0
86	MG	1	3816	1/1	0.41	11.37	55,55,55,55	0
86	MG	1	3518	1/1	0.67	11.35	45,45,45,45	0
86	MG	1	3860	1/1	0.45	11.33	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	1	4209	7/7	0.38	11.33	160,160,160,160	0
86	MG	5	3753	1/1	0.24	11.30	66,66,66,66	0
86	MG	5	3567	1/1	0.47	11.26	34,34,34,34	0
86	MG	1	3448	1/1	0.78	11.25	59,59,59,59	0
86	MG	5	3680	1/1	0.66	11.24	104,104,104,104	0
86	MG	5	3441	1/1	0.51	11.18	53,53,53,53	0
86	MG	5	3554	1/1	0.46	11.17	51,51,51,51	0
86	MG	1	3589	1/1	0.52	11.17	57,57,57,57	0
86	MG	o3	202	1/1	0.46	11.14	49,49,49,49	0
86	MG	1	3543	1/1	0.47	11.13	36,36,36,36	0
86	MG	6	1948	1/1	0.54	11.12	62,62,62,62	0
86	MG	o1	201	1/1	1.04	11.10	116,116,116,116	0
86	MG	5	3600	1/1	0.42	11.05	56,56,56,56	0
86	MG	1	3857	1/1	0.40	11.04	52,52,52,52	0
86	MG	5	3790	1/1	0.79	11.04	69,69,69,69	0
86	MG	4	207	1/1	0.54	11.03	39,39,39,39	0
86	MG	1	3434	1/1	0.56	11.02	60,60,60,60	0
86	MG	1	3844	1/1	0.83	11.02	57,57,57,57	0
86	MG	2	1939	1/1	0.31	11.02	92,92,92,92	0
86	MG	5	3881	1/1	0.21	11.00	112,112,112,112	0
86	MG	1	3642	1/1	0.34	10.99	57,57,57,57	0
86	MG	1	3851	1/1	0.35	10.94	66,66,66,66	0
86	MG	1	3585	1/1	0.47	10.93	46,46,46,46	0
86	MG	5	3606	1/1	0.37	10.84	52,52,52,52	0
86	MG	5	3765	1/1	0.41	10.81	63,63,63,63	0
86	MG	2	1990	1/1	0.88	10.80	142,142,142,142	0
86	MG	m4	201	1/1	0.66	10.79	49,49,49,49	0
86	MG	6	1967	1/1	0.31	10.77	95,95,95,95	0
86	MG	2	1969	1/1	0.57	10.76	87,87,87,87	0
86	MG	5	3569	1/1	0.52	10.73	53,53,53,53	0
86	MG	1	3408	1/1	0.88	10.70	75,75,75,75	0
86	MG	1	3625	1/1	0.90	10.66	53,53,53,53	0
86	MG	1	3729	1/1	0.34	10.58	55,55,55,55	0
86	MG	1	3529	1/1	0.40	10.53	63,63,63,63	0
86	MG	5	3798	1/1	0.58	10.50	69,69,69,69	0
86	MG	5	3485	1/1	0.35	10.47	63,63,63,63	0
87	OHX	1	4202	7/7	0.32	10.46	166,166,166,166	0
86	MG	5	3821	1/1	0.37	10.41	49,49,49,49	0
86	MG	1	3794	1/1	0.43	10.39	44,44,44,44	0
86	MG	2	1917	1/1	0.72	10.36	83,83,83,83	0
86	MG	m0	301	1/1	0.56	10.35	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	1984	1/1	0.73	10.33	60,60,60,60	0
86	MG	1	3828	1/1	0.56	10.31	50,50,50,50	0
86	MG	5	3694	1/1	0.52	10.29	52,52,52,52	0
86	MG	5	4249	1/1	0.37	10.25	42,42,42,42	0
86	MG	5	3746	1/1	0.83	10.24	62,62,62,62	0
86	MG	4	215	1/1	0.57	10.19	64,64,64,64	0
86	MG	6	1937	1/1	0.38	10.19	97,97,97,97	0
86	MG	6	1901	1/1	0.43	10.14	65,65,65,65	0
86	MG	6	1997	1/1	0.46	10.11	72,72,72,72	0
86	MG	2	1910	1/1	0.55	10.10	75,75,75,75	0
86	MG	2	1947	1/1	0.42	10.10	87,87,87,87	0
86	MG	5	3427	1/1	0.51	10.09	67,67,67,67	0
86	MG	1	3781	1/1	0.38	9.98	80,80,80,80	0
86	MG	5	3434	1/1	0.32	9.97	42,42,42,42	0
87	OHX	2	2159	7/7	0.31	9.90	195,195,195,195	0
86	MG	1	3720	1/1	0.51	9.89	62,62,62,62	0
86	MG	5	3406	1/1	0.39	9.87	44,44,44,44	0
87	OHX	1	4203	7/7	0.28	9.84	182,182,182,182	0
86	MG	5	3707	1/1	0.47	9.84	55,55,55,55	0
86	MG	1	3480	1/1	0.60	9.82	62,62,62,62	0
86	MG	2	1946	1/1	0.40	9.81	111,111,111,111	0
86	MG	5	3562	1/1	0.78	9.78	26,26,26,26	0
86	MG	5	3828	1/1	0.34	9.77	49,49,49,49	0
86	MG	5	3469	1/1	0.41	9.76	66,66,66,66	0
86	MG	3	212	1/1	0.32	9.75	98,98,98,98	0
86	MG	1	3547	1/1	0.57	9.74	73,73,73,73	0
86	MG	6	1926	1/1	0.48	9.72	53,53,53,53	0
86	MG	6	1922	1/1	0.39	9.68	54,54,54,54	0
86	MG	6	1949	1/1	0.55	9.61	61,61,61,61	0
86	MG	5	3559	1/1	0.59	9.61	48,48,48,48	0
86	MG	8	204	1/1	0.51	9.61	63,63,63,63	0
86	MG	4	214	1/1	0.36	9.56	79,79,79,79	0
86	MG	1	3433	1/1	0.37	9.53	75,75,75,75	0
86	MG	5	3695	1/1	0.41	9.48	75,75,75,75	0
87	OHX	5	4199	7/7	0.32	9.41	187,187,187,187	0
86	MG	1	3778	1/1	0.45	9.35	68,68,68,68	0
86	MG	5	3557	1/1	0.55	9.33	40,40,40,40	0
86	MG	5	3689	1/1	0.37	9.32	82,82,82,82	0
86	MG	1	3732	1/1	1.03	9.28	86,86,86,86	0
86	MG	5	3548	1/1	0.33	9.27	84,84,84,84	0
86	MG	1	3824	1/1	0.49	9.27	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3461	1/1	0.45	9.26	42,42,42,42	0
86	MG	N9	101	1/1	0.35	9.26	46,46,46,46	0
86	MG	5	3678	1/1	0.32	9.20	72,72,72,72	0
86	MG	O1	201	1/1	0.55	9.15	76,76,76,76	0
87	OHX	5	4134	7/7	0.37	9.13	173,173,173,173	0
86	MG	5	3545	1/1	0.48	9.09	79,79,79,79	0
86	MG	1	3787	1/1	0.98	9.07	47,47,47,47	0
87	OHX	1	4169	7/7	0.40	9.01	233,233,233,233	0
86	MG	1	3415	1/1	0.61	8.96	46,46,46,46	0
86	MG	6	1927	1/1	0.42	8.94	63,63,63,63	0
87	OHX	8	233	7/7	0.32	8.93	189,189,189,189	0
86	MG	1	3555	1/1	0.45	8.92	26,26,26,26	0
86	MG	1	3861	1/1	0.54	8.92	86,86,86,86	0
86	MG	2	1908	1/1	0.26	8.92	97,97,97,97	0
86	MG	1	3762	1/1	0.32	8.92	77,77,77,77	0
86	MG	5	3564	1/1	0.40	8.91	37,37,37,37	0
86	MG	7	212	1/1	0.44	8.89	75,75,75,75	0
86	MG	5	3713	1/1	0.38	8.89	72,72,72,72	0
86	MG	3	206	1/1	0.45	8.88	46,46,46,46	0
86	MG	4	208	1/1	0.41	8.87	43,43,43,43	0
86	MG	5	3597	1/1	0.34	8.84	61,61,61,61	0
86	MG	5	3534	1/1	0.42	8.78	57,57,57,57	0
86	MG	5	3499	1/1	0.44	8.76	57,57,57,57	0
86	MG	1	3760	1/1	0.41	8.73	52,52,52,52	0
86	MG	l3	401	1/1	0.64	8.73	27,27,27,27	0
86	MG	5	3519	1/1	0.43	8.73	43,43,43,43	0
86	MG	5	3637	1/1	0.90	8.69	75,75,75,75	0
86	MG	5	3440	1/1	0.51	8.68	50,50,50,50	0
86	MG	1	3586	1/1	0.37	8.62	40,40,40,40	0
86	MG	1	3641	1/1	0.28	8.57	71,71,71,71	0
86	MG	4	204	1/1	0.51	8.54	72,72,72,72	0
86	MG	L6	202	1/1	0.38	8.52	64,64,64,64	0
86	MG	6	1964	1/1	0.67	8.52	75,75,75,75	0
86	MG	1	3668	1/1	0.37	8.44	55,55,55,55	0
86	MG	5	3859	1/1	0.25	8.43	78,78,78,78	0
86	MG	1	3699	1/1	0.42	8.42	68,68,68,68	0
86	MG	6	1903	1/1	0.42	8.42	51,51,51,51	0
87	OHX	1	4208	7/7	0.40	8.40	181,181,181,181	0
86	MG	5	3563	1/1	0.80	8.33	54,54,54,54	0
86	MG	5	3452	1/1	0.56	8.33	48,48,48,48	0
86	MG	5	3646	1/1	0.40	8.32	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	4196	7/7	0.51	8.28	162,162,162,162	0
86	MG	2	2018	1/1	0.76	8.26	116,116,116,116	0
86	MG	1	3701	1/1	0.42	8.24	52,52,52,52	0
86	MG	2	1986	1/1	0.96	8.22	95,95,95,95	0
86	MG	1	3431	1/1	0.38	8.21	55,55,55,55	0
86	MG	l3	405	1/1	0.52	8.21	44,44,44,44	0
86	MG	1	3674	1/1	0.36	8.17	44,44,44,44	0
86	MG	6	1971	1/1	0.39	8.11	63,63,63,63	0
86	MG	5	3475	1/1	0.39	8.10	40,40,40,40	0
86	MG	4	222	1/1	0.62	8.09	77,77,77,77	0
86	MG	1	3450	1/1	0.56	8.05	71,71,71,71	0
86	MG	6	1969	1/1	0.35	8.03	91,91,91,91	0
86	MG	5	3515	1/1	0.40	8.00	52,52,52,52	0
86	MG	L4	402	1/1	0.40	8.00	47,47,47,47	0
86	MG	7	205	1/1	0.49	7.99	35,35,35,35	0
87	OHX	6	2058	7/7	0.24	7.98	89,89,89,89	0
86	MG	1	3565	1/1	0.65	7.96	44,44,44,44	0
86	MG	5	3449	1/1	0.44	7.94	53,53,53,53	0
86	MG	5	3847	1/1	0.51	7.93	71,71,71,71	0
86	MG	6	2020	1/1	0.52	7.92	70,70,70,70	0
86	MG	6	2001	1/1	0.46	7.92	89,89,89,89	0
86	MG	5	3484	1/1	0.49	7.89	70,70,70,70	0
86	MG	1	3636	1/1	0.27	7.88	74,74,74,74	0
86	MG	5	3840	1/1	3.28	7.87	76,76,76,76	0
86	MG	5	3411	1/1	0.39	7.83	57,57,57,57	0
86	MG	6	1982	1/1	0.37	7.82	77,77,77,77	0
86	MG	1	3619	1/1	0.56	7.82	61,61,61,61	0
86	MG	5	3702	1/1	0.26	7.78	66,66,66,66	0
86	MG	5	3580	1/1	0.35	7.78	44,44,44,44	0
86	MG	1	3425	1/1	0.42	7.77	73,73,73,73	0
86	MG	q0	203	1/1	0.63	7.72	58,58,58,58	0
86	MG	5	3724	1/1	0.33	7.69	122,122,122,122	0
86	MG	8	206	1/1	0.29	7.68	82,82,82,82	0
86	MG	1	3556	1/1	0.48	7.67	56,56,56,56	0
86	MG	5	3671	1/1	0.49	7.66	43,43,43,43	0
86	MG	6	1976	1/1	0.40	7.60	69,69,69,69	0
86	MG	1	3730	1/1	0.56	7.59	42,42,42,42	0
86	MG	1	3591	1/1	0.59	7.57	50,50,50,50	0
86	MG	1	3744	1/1	0.34	7.54	44,44,44,44	0
86	MG	1	3711	1/1	0.34	7.51	76,76,76,76	0
86	MG	5	3604	1/1	0.36	7.50	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3493	1/1	0.41	7.47	68,68,68,68	0
86	MG	7	207	1/1	0.23	7.42	67,67,67,67	0
86	MG	1	3822	1/1	0.28	7.41	96,96,96,96	0
86	MG	4	211	1/1	0.35	7.40	79,79,79,79	0
86	MG	4	203	1/1	0.47	7.40	55,55,55,55	0
86	MG	5	3677	1/1	0.35	7.39	48,48,48,48	0
86	MG	2	2004	1/1	0.73	7.38	122,122,122,122	0
86	MG	5	3857	1/1	0.46	7.37	50,50,50,50	0
86	MG	1	3469	1/1	0.47	7.35	60,60,60,60	0
87	OHX	6	2193	7/7	0.32	7.34	202,202,202,202	0
86	MG	1	3465	1/1	0.52	7.33	89,89,89,89	0
86	MG	5	3468	1/1	0.41	7.32	58,58,58,58	0
86	MG	5	3439	1/1	0.71	7.27	56,56,56,56	0
86	MG	8	202	1/1	0.26	7.23	110,110,110,110	0
86	MG	6	1998	1/1	0.31	7.21	69,69,69,69	0
86	MG	1	3568	1/1	0.41	7.16	48,48,48,48	0
86	MG	5	3408	1/1	0.52	7.16	45,45,45,45	0
86	MG	3	210	1/1	2.97	7.15	95,95,95,95	0
86	MG	1	3629	1/1	0.41	7.09	48,48,48,48	0
86	MG	6	1973	1/1	0.35	7.04	78,78,78,78	0
86	MG	6	2009	1/1	1.55	7.04	96,96,96,96	0
86	MG	6	2040	1/1	0.40	7.03	88,88,88,88	0
86	MG	5	3783	1/1	0.42	7.00	48,48,48,48	0
86	MG	N8	203	1/1	0.37	6.96	66,66,66,66	0
86	MG	5	3741	1/1	0.39	6.96	56,56,56,56	0
86	MG	1	3736	1/1	0.54	6.95	61,61,61,61	0
86	MG	6	1912	1/1	0.34	6.94	96,96,96,96	0
86	MG	1	3462	1/1	0.43	6.94	36,36,36,36	0
86	MG	1	3491	1/1	0.36	6.93	42,42,42,42	0
86	MG	M0	302	1/1	0.41	6.93	63,63,63,63	0
86	MG	1	3624	1/1	0.37	6.89	49,49,49,49	0
86	MG	1	3726	1/1	0.35	6.87	66,66,66,66	0
86	MG	5	3648	1/1	0.60	6.85	93,93,93,93	0
86	MG	O7	102	1/1	0.60	6.84	61,61,61,61	0
86	MG	1	3727	1/1	0.43	6.82	90,90,90,90	0
86	MG	1	3511	1/1	0.43	6.81	44,44,44,44	0
86	MG	2	2010	1/1	0.38	6.80	107,107,107,107	0
86	MG	5	3516	1/1	0.26	6.80	61,61,61,61	0
86	MG	5	3666	1/1	0.34	6.78	37,37,37,37	0
86	MG	1	3479	1/1	0.30	6.77	77,77,77,77	0
86	MG	1	3548	1/1	0.38	6.76	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3508	1/1	0.35	6.75	51,51,51,51	0
86	MG	2	1941	1/1	0.32	6.74	94,94,94,94	0
86	MG	2	1928	1/1	0.51	6.65	131,131,131,131	0
86	MG	7	203	1/1	0.31	6.65	69,69,69,69	0
86	MG	5	3714	1/1	0.43	6.64	88,88,88,88	0
86	MG	1	3731	1/1	0.42	6.61	89,89,89,89	0
86	MG	5	3837	1/1	0.31	6.61	67,67,67,67	0
86	MG	n9	101	1/1	0.45	6.60	51,51,51,51	0
87	OHX	5	4229	7/7	0.35	6.59	202,202,202,202	0
86	MG	6	1980	1/1	0.37	6.59	64,64,64,64	0
87	OHX	8	234	7/7	0.31	6.55	165,165,165,165	0
86	MG	5	3584	1/1	0.53	6.53	39,39,39,39	0
86	MG	1	3457	1/1	0.44	6.52	64,64,64,64	0
86	MG	4	219	1/1	0.32	6.52	77,77,77,77	0
86	MG	1	3795	1/1	0.32	6.52	73,73,73,73	0
87	OHX	5	4223	7/7	0.28	6.52	156,156,156,156	0
86	MG	2	1992	1/1	0.44	6.47	80,80,80,80	0
86	MG	5	3412	1/1	0.35	6.44	46,46,46,46	0
87	OHX	5	4191	7/7	0.22	6.42	198,198,198,198	0
86	MG	1	3412	1/1	0.45	6.41	39,39,39,39	0
86	MG	5	3767	1/1	0.42	6.40	97,97,97,97	0
86	MG	1	3722	1/1	0.42	6.38	60,60,60,60	0
86	MG	5	3816	1/1	0.36	6.36	69,69,69,69	0
86	MG	5	3818	1/1	0.22	6.33	80,80,80,80	0
86	MG	1	3612	1/1	0.55	6.32	48,48,48,48	0
86	MG	5	3717	1/1	0.44	6.32	79,79,79,79	0
86	MG	1	3782	1/1	0.72	6.32	49,49,49,49	0
86	MG	5	3426	1/1	0.37	6.28	57,57,57,57	0
86	MG	N3	201	1/1	0.47	6.28	43,43,43,43	0
86	MG	5	3853	1/1	0.30	6.26	134,134,134,134	0
86	MG	1	3553	1/1	0.48	6.24	62,62,62,62	0
86	MG	1	3447	1/1	0.29	6.23	46,46,46,46	0
86	MG	5	3728	1/1	0.31	6.22	70,70,70,70	0
86	MG	1	3430	1/1	0.32	6.22	67,67,67,67	0
86	MG	1	3525	1/1	0.41	6.21	58,58,58,58	0
86	MG	6	1970	1/1	0.42	6.19	78,78,78,78	0
86	MG	o3	201	1/1	0.88	6.15	56,56,56,56	0
86	MG	2	2023	1/1	0.65	6.11	129,129,129,129	0
86	MG	5	3780	1/1	0.40	6.11	41,41,41,41	0
86	MG	1	3717	1/1	0.71	6.10	58,58,58,58	0
86	MG	5	3709	1/1	0.36	6.08	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	2	1903	1/1	0.30	6.08	73,73,73,73	0
86	MG	1	3569	1/1	0.48	6.05	76,76,76,76	0
86	MG	6	1913	1/1	0.48	6.05	52,52,52,52	0
87	OHX	5	4231	7/7	0.23	6.03	202,202,202,202	0
86	MG	2	2019	1/1	0.37	6.00	106,106,106,106	0
86	MG	1	3793	1/1	0.60	5.99	67,67,67,67	0
86	MG	1	3735	1/1	0.31	5.99	58,58,58,58	0
86	MG	2	2014	1/1	0.44	5.95	98,98,98,98	0
86	MG	2	1944	1/1	0.66	5.95	93,93,93,93	0
86	MG	5	3451	1/1	0.29	5.94	52,52,52,52	0
86	MG	5	3793	1/1	0.31	5.90	55,55,55,55	0
86	MG	5	3514	1/1	0.34	5.88	60,60,60,60	0
86	MG	6	2017	1/1	0.57	5.85	86,86,86,86	0
86	MG	n3	201	1/1	0.46	5.85	33,33,33,33	0
87	OHX	5	4173	7/7	0.32	5.83	142,142,142,142	0
86	MG	5	3605	1/1	0.26	5.82	48,48,48,48	0
86	MG	1	4215	1/1	0.53	5.74	65,65,65,65	0
86	MG	1	3839	1/1	0.24	5.72	94,94,94,94	0
86	MG	5	3858	1/1	0.40	5.71	56,56,56,56	0
86	MG	8	214	1/1	0.59	5.68	71,71,71,71	0
86	MG	1	3654	1/1	0.30	5.68	54,54,54,54	0
86	MG	1	3714	1/1	0.32	5.67	101,101,101,101	0
86	MG	5	3877	1/1	0.40	5.66	116,116,116,116	0
86	MG	6	1945	1/1	0.29	5.66	65,65,65,65	0
86	MG	8	209	1/1	0.32	5.64	97,97,97,97	0
86	MG	1	3493	1/1	0.30	5.63	106,106,106,106	0
86	MG	l3	402	1/1	0.51	5.63	45,45,45,45	0
86	MG	5	3674	1/1	0.23	5.62	63,63,63,63	0
86	MG	5	3621	1/1	0.41	5.61	66,66,66,66	0
87	OHX	1	4189	7/7	0.36	5.60	181,181,181,181	0
86	MG	5	3684	1/1	0.37	5.59	106,106,106,106	0
87	OHX	5	4153	7/7	0.26	5.59	168,168,168,168	0
86	MG	8	203	1/1	0.56	5.56	62,62,62,62	0
86	MG	1	3688	1/1	0.27	5.50	58,58,58,58	0
86	MG	5	3623	1/1	0.33	5.48	79,79,79,79	0
86	MG	n9	102	1/1	0.46	5.47	51,51,51,51	0
86	MG	5	3688	1/1	0.39	5.45	42,42,42,42	0
86	MG	6	1977	1/1	0.32	5.43	80,80,80,80	0
86	MG	5	4250	1/1	0.34	5.40	54,54,54,54	0
87	OHX	5	4197	7/7	0.22	5.39	175,175,175,175	0
86	MG	M7	203	1/1	0.51	5.38	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3727	1/1	0.20	5.35	71,71,71,71	0
86	MG	5	3525	1/1	0.27	5.31	73,73,73,73	0
86	MG	N5	201	1/1	1.12	5.31	71,71,71,71	0
86	MG	1	3456	1/1	0.35	5.29	47,47,47,47	0
86	MG	5	3598	1/1	0.28	5.27	53,53,53,53	0
86	MG	1	3808	1/1	0.36	5.26	61,61,61,61	0
86	MG	6	2031	1/1	0.34	5.23	94,94,94,94	0
86	MG	4	220	1/1	0.32	5.21	64,64,64,64	0
86	MG	1	3663	1/1	0.64	5.18	83,83,83,83	0
86	MG	5	3725	1/1	0.33	5.16	37,37,37,37	0
86	MG	1	3492	1/1	0.28	5.13	70,70,70,70	0
86	MG	L7	302	1/1	0.82	5.13	53,53,53,53	0
86	MG	5	3711	1/1	0.26	5.13	61,61,61,61	0
86	MG	1	3666	1/1	0.32	5.10	116,116,116,116	0
86	MG	5	3568	1/1	0.65	5.08	52,52,52,52	0
86	MG	4	210	1/1	0.49	5.02	64,64,64,64	0
87	OHX	5	4091	7/7	0.33	4.99	205,205,205,205	0
86	MG	3	205	1/1	0.42	4.98	43,43,43,43	0
86	MG	6	1978	1/1	0.53	4.97	74,74,74,74	0
86	MG	1	3483	1/1	0.33	4.93	64,64,64,64	0
87	OHX	5	4149	7/7	0.36	4.90	142,142,142,142	0
87	OHX	6	2131	7/7	0.37	4.88	128,128,128,128	0
86	MG	2	1922	1/1	0.29	4.84	97,97,97,97	0
86	MG	5	3808	1/1	0.50	4.81	76,76,76,76	0
86	MG	1	4214	1/1	0.29	4.80	41,41,41,41	0
86	MG	5	3665	1/1	0.40	4.78	48,48,48,48	0
86	MG	1	3651	1/1	0.38	4.76	92,92,92,92	0
87	OHX	5	3895	7/7	0.28	4.75	58,58,58,58	0
87	OHX	1	4116	7/7	0.28	4.74	164,164,164,164	0
87	OHX	5	4076	7/7	0.27	4.73	142,142,142,142	0
86	MG	6	2044	1/1	0.29	4.72	70,70,70,70	0
86	MG	2	1979	1/1	0.25	4.70	129,129,129,129	0
86	MG	1	3856	1/1	0.31	4.66	86,86,86,86	0
86	MG	1	3700	1/1	0.53	4.63	144,144,144,144	0
86	MG	1	3772	1/1	0.35	4.59	73,73,73,73	0
86	MG	5	3496	1/1	0.30	4.58	62,62,62,62	0
86	MG	4	201	1/1	0.38	4.57	62,62,62,62	0
86	MG	O5	201	1/1	1.04	4.55	70,70,70,70	0
86	MG	m6	201	1/1	0.33	4.53	46,46,46,46	0
87	OHX	1	3887	7/7	0.23	4.53	87,87,87,87	0
86	MG	1	3814	1/1	0.41	4.53	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	2	2015	1/1	0.57	4.53	71,71,71,71	0
87	OHX	1	4176	7/7	0.37	4.47	190,190,190,190	0
86	MG	1	3427	1/1	0.45	4.47	67,67,67,67	0
86	MG	5	3511	1/1	0.31	4.44	54,54,54,54	0
86	MG	5	3549	1/1	0.39	4.42	73,73,73,73	0
86	MG	5	3420	1/1	0.22	4.41	128,128,128,128	0
86	MG	5	3424	1/1	0.37	4.41	46,46,46,46	0
86	MG	D4	201	1/1	1.26	4.39	115,115,115,115	0
86	MG	6	1960	1/1	0.42	4.39	81,81,81,81	0
86	MG	5	3822	1/1	0.33	4.37	39,39,39,39	0
86	MG	2	1960	1/1	0.46	4.36	89,89,89,89	0
86	MG	5	3824	1/1	0.32	4.35	101,101,101,101	0
86	MG	1	3639	1/1	0.39	4.32	61,61,61,61	0
86	MG	6	1942	1/1	0.31	4.31	71,71,71,71	0
86	MG	6	1974	1/1	0.24	4.31	77,77,77,77	0
86	MG	5	3850	1/1	0.32	4.30	78,78,78,78	0
86	MG	l3	406	1/1	0.56	4.29	47,47,47,47	0
86	MG	2	2001	1/1	0.29	4.22	109,109,109,109	0
86	MG	1	3779	1/1	0.35	4.20	71,71,71,71	0
86	MG	5	3786	1/1	0.33	4.20	48,48,48,48	0
86	MG	5	4252	1/1	0.42	4.15	60,60,60,60	0
86	MG	1	3584	1/1	0.41	4.15	55,55,55,55	0
86	MG	1	3777	1/1	0.40	4.15	59,59,59,59	0
86	MG	5	3819	1/1	0.47	4.14	47,47,47,47	0
86	MG	7	208	1/1	0.62	4.12	60,60,60,60	0
86	MG	1	3626	1/1	0.31	4.11	78,78,78,78	0
86	MG	5	3805	1/1	0.34	4.11	51,51,51,51	0
86	MG	m7	203	1/1	0.59	4.11	52,52,52,52	0
86	MG	5	3403	1/1	1.90	4.10	65,65,65,65	0
86	MG	2	1970	1/1	0.54	4.08	105,105,105,105	0
86	MG	1	3669	1/1	0.21	4.08	105,105,105,105	0
86	MG	2	1943	1/1	0.47	4.07	117,117,117,117	0
86	MG	2	1912	1/1	0.41	4.07	91,91,91,91	0
86	MG	5	3601	1/1	0.28	4.07	44,44,44,44	0
87	OHX	l5	307	7/7	0.42	4.06	177,177,177,177	0
86	MG	1	3554	1/1	0.48	4.02	50,50,50,50	0
86	MG	1	3419	1/1	0.30	4.01	83,83,83,83	0
86	MG	1	3604	1/1	0.87	4.00	65,65,65,65	0
86	MG	6	1914	1/1	0.35	3.99	55,55,55,55	0
86	MG	5	3752	1/1	0.30	3.98	67,67,67,67	0
86	MG	1	3667	1/1	0.34	3.97	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	4144	7/7	0.35	3.97	167,167,167,167	0
86	MG	5	3659	1/1	0.35	3.94	48,48,48,48	0
86	MG	5	3777	1/1	0.33	3.92	112,112,112,112	0
86	MG	q3	503	1/1	0.41	3.92	89,89,89,89	0
87	OHX	5	3901	7/7	0.25	3.92	73,73,73,73	0
86	MG	1	3713	1/1	1.04	3.91	75,75,75,75	0
86	MG	6	1965	1/1	0.26	3.90	103,103,103,103	0
86	MG	5	3785	1/1	0.45	3.88	86,86,86,86	0
86	MG	6	1950	1/1	0.66	3.86	64,64,64,64	0
86	MG	1	3435	1/1	0.36	3.85	63,63,63,63	0
86	MG	1	3607	1/1	0.26	3.81	73,73,73,73	0
86	MG	5	3675	1/1	0.42	3.80	54,54,54,54	0
86	MG	1	3855	1/1	0.32	3.78	38,38,38,38	0
86	MG	6	1996	1/1	0.43	3.78	72,72,72,72	0
86	MG	6	2038	1/1	1.18	3.75	93,93,93,93	0
86	MG	6	2027	1/1	0.20	3.74	74,74,74,74	0
87	OHX	1	4123	7/7	0.32	3.74	146,146,146,146	0
86	MG	1	3647	1/1	0.36	3.74	67,67,67,67	0
86	MG	1	3797	1/1	0.57	3.74	56,56,56,56	0
86	MG	1	3751	1/1	0.25	3.71	69,69,69,69	0
86	MG	2	1994	1/1	0.40	3.68	116,116,116,116	0
87	OHX	1	3891	7/7	0.18	3.67	112,112,112,112	0
87	OHX	5	3905	7/7	0.22	3.66	102,102,102,102	0
86	MG	1	3422	1/1	0.42	3.63	51,51,51,51	0
86	MG	5	3800	1/1	0.37	3.62	188,188,188,188	0
86	MG	1	3739	1/1	0.47	3.62	83,83,83,83	0
86	MG	6	1975	1/1	0.32	3.61	59,59,59,59	0
86	MG	5	3736	1/1	0.25	3.61	108,108,108,108	0
86	MG	m7	201	1/1	0.55	3.61	46,46,46,46	0
86	MG	1	3632	1/1	0.36	3.57	83,83,83,83	0
86	MG	5	3498	1/1	0.33	3.56	50,50,50,50	0
86	MG	1	3845	1/1	0.34	3.55	68,68,68,68	0
86	MG	1	3598	1/1	0.34	3.55	52,52,52,52	0
86	MG	1	3537	1/1	0.30	3.54	71,71,71,71	0
86	MG	2	1921	1/1	0.43	3.53	79,79,79,79	0
86	MG	1	3742	1/1	0.34	3.52	75,75,75,75	0
86	MG	1	3633	1/1	0.82	3.51	65,65,65,65	0
86	MG	l3	403	1/1	0.48	3.51	44,44,44,44	0
86	MG	5	3802	1/1	0.37	3.50	102,102,102,102	0
86	MG	4	202	1/1	0.41	3.50	91,91,91,91	0
86	MG	n8	201	1/1	0.41	3.49	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3626	1/1	0.63	3.44	65,65,65,65	0
87	OHX	5	4198	7/7	0.30	3.43	162,162,162,162	0
86	MG	O3	201	1/1	0.55	3.42	67,67,67,67	0
87	OHX	1	4195	7/7	0.15	3.42	192,192,192,192	0
86	MG	1	3740	1/1	0.31	3.42	66,66,66,66	0
87	OHX	1	4168	7/7	0.28	3.38	192,192,192,192	0
86	MG	2	2020	1/1	0.70	3.37	100,100,100,100	0
86	MG	6	1958	1/1	0.54	3.37	49,49,49,49	0
87	OHX	14	403	7/7	0.36	3.36	185,185,185,185	0
87	OHX	5	3896	7/7	0.27	3.35	70,70,70,70	0
86	MG	1	3796	1/1	0.34	3.33	53,53,53,53	0
86	MG	1	3646	1/1	0.33	3.32	55,55,55,55	0
86	MG	5	3823	1/1	0.30	3.31	65,65,65,65	0
86	MG	17	301	1/1	0.31	3.28	52,52,52,52	0
86	MG	5	3622	1/1	0.29	3.27	53,53,53,53	0
86	MG	7	204	1/1	0.27	3.27	95,95,95,95	0
86	MG	1	3611	1/1	0.36	3.27	57,57,57,57	0
86	MG	1	3716	1/1	0.31	3.26	54,54,54,54	0
86	MG	1	3501	1/1	0.63	3.26	47,47,47,47	0
86	MG	5	3664	1/1	0.44	3.26	72,72,72,72	0
86	MG	5	3757	1/1	0.22	3.26	54,54,54,54	0
86	MG	SM	301	1/1	0.91	3.25	75,75,75,75	0
86	MG	2	1930	1/1	0.27	3.25	99,99,99,99	0
86	MG	5	3495	1/1	0.26	3.19	56,56,56,56	0
87	OHX	8	226	7/7	0.22	3.18	183,183,183,183	0
87	OHX	2	2108	7/7	0.42	3.18	188,188,188,188	0
86	MG	6	1951	1/1	0.31	3.17	60,60,60,60	0
86	MG	1	4213	1/1	0.28	3.17	95,95,95,95	0
86	MG	2	1926	1/1	0.42	3.14	110,110,110,110	0
86	MG	L6	201	1/1	0.23	3.12	67,67,67,67	0
86	MG	6	1938	1/1	0.30	3.12	59,59,59,59	0
86	MG	1	3746	1/1	0.41	3.12	61,61,61,61	0
86	MG	1	3557	1/1	0.36	3.11	72,72,72,72	0
86	MG	q1	101	1/1	0.43	3.10	58,58,58,58	0
86	MG	5	3787	1/1	0.34	3.10	68,68,68,68	0
86	MG	1	3416	1/1	0.85	3.10	78,78,78,78	0
87	OHX	5	4183	7/7	0.29	3.08	202,202,202,202	0
86	MG	M0	303	1/1	0.51	3.06	67,67,67,67	0
86	MG	5	3653	1/1	0.50	3.06	73,73,73,73	0
86	MG	5	3544	1/1	0.26	3.05	57,57,57,57	0
86	MG	1	3574	1/1	0.45	2.99	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	6	2052	7/7	0.26	2.99	90,90,90,90	0
86	MG	5	3863	1/1	0.32	2.95	46,46,46,46	0
87	OHX	6	2183	7/7	0.31	2.95	142,142,142,142	0
87	OHX	2	2162	7/7	0.37	2.95	219,219,219,219	0
86	MG	1	3597	1/1	0.25	2.94	59,59,59,59	0
86	MG	5	3862	1/1	0.35	2.93	51,51,51,51	0
87	OHX	1	4098	7/7	0.25	2.93	206,206,206,206	0
87	OHX	5	4178	7/7	0.22	2.93	182,182,182,182	0
87	OHX	6	2180	7/7	0.28	2.90	165,165,165,165	0
86	MG	1	3743	1/1	1.07	2.88	88,88,88,88	0
86	MG	5	3547	1/1	0.43	2.85	70,70,70,70	0
86	MG	1	3756	1/1	0.48	2.85	41,41,41,41	0
86	MG	5	3505	1/1	0.32	2.83	38,38,38,38	0
86	MG	1	3404	1/1	0.70	2.81	76,76,76,76	0
86	MG	5	3660	1/1	0.30	2.80	69,69,69,69	0
86	MG	8	215	1/1	0.49	2.77	82,82,82,82	0
86	MG	7	211	1/1	0.33	2.76	54,54,54,54	0
86	MG	1	3454	1/1	1.30	2.76	88,88,88,88	0
87	OHX	5	4179	7/7	0.22	2.75	158,158,158,158	0
86	MG	5	3488	1/1	0.23	2.73	47,47,47,47	0
87	OHX	1	3897	7/7	0.23	2.72	95,95,95,95	0
86	MG	6	1957	1/1	0.55	2.71	51,51,51,51	0
87	OHX	7	225	7/7	0.24	2.70	149,149,149,149	0
87	OHX	3	222	7/7	0.43	2.69	151,151,151,151	0
86	MG	5	3510	1/1	0.38	2.67	34,34,34,34	0
86	MG	m7	202	1/1	0.33	2.66	65,65,65,65	0
87	OHX	5	4141	7/7	0.23	2.66	152,152,152,152	0
86	MG	1	3802	1/1	0.52	2.66	75,75,75,75	0
86	MG	5	3672	1/1	0.23	2.65	75,75,75,75	0
87	OHX	2	2113	7/7	0.25	2.64	168,168,168,168	0
87	OHX	1	4186	7/7	0.27	2.62	204,204,204,204	0
87	OHX	3	224	7/7	0.21	2.61	165,165,165,165	0
86	MG	6	1911	1/1	0.25	2.60	75,75,75,75	0
87	OHX	1	4137	7/7	0.28	2.59	135,135,135,135	0
86	MG	1	3505	1/1	0.30	2.58	45,45,45,45	0
86	MG	1	3821	1/1	0.27	2.58	60,60,60,60	0
87	OHX	5	3939	7/7	0.21	2.58	119,119,119,119	0
86	MG	1	3773	1/1	0.28	2.57	78,78,78,78	0
86	MG	8	205	1/1	0.52	2.57	54,54,54,54	0
87	OHX	6	2170	7/7	0.52	2.54	172,172,172,172	0
86	MG	1	3478	1/1	0.39	2.53	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3754	1/1	0.25	2.53	111,111,111,111	0
86	MG	1	3413	1/1	0.29	2.53	57,57,57,57	0
86	MG	1	3807	1/1	0.34	2.52	72,72,72,72	0
86	MG	5	3794	1/1	0.32	2.52	55,55,55,55	0
87	OHX	1	4092	7/7	0.23	2.51	171,171,171,171	0
86	MG	5	3416	1/1	0.40	2.51	49,49,49,49	0
86	MG	6	1995	1/1	0.35	2.51	75,75,75,75	0
87	OHX	1	4131	7/7	0.29	2.51	171,171,171,171	0
86	MG	1	3488	1/1	0.58	2.50	79,79,79,79	0
87	OHX	5	4068	7/7	0.20	2.50	144,144,144,144	0
87	OHX	1	3866	7/7	0.26	2.50	55,55,55,55	0
86	MG	m5	301	1/1	0.60	2.49	74,74,74,74	0
86	MG	o4	201	1/1	0.61	2.48	81,81,81,81	0
87	OHX	7	226	7/7	0.35	2.46	171,171,171,171	0
87	OHX	6	2198	7/7	0.40	2.44	187,187,187,187	0
86	MG	2	1997	1/1	0.64	2.44	140,140,140,140	0
86	MG	1	3516	1/1	0.30	2.43	58,58,58,58	0
86	MG	5	3644	1/1	0.23	2.43	44,44,44,44	0
86	MG	5	3486	1/1	0.27	2.43	80,80,80,80	0
86	MG	m7	204	1/1	0.40	2.42	62,62,62,62	0
87	OHX	1	4175	7/7	0.25	2.41	145,145,145,145	0
87	OHX	4	233	7/7	0.24	2.38	144,144,144,144	0
86	MG	6	2003	1/1	0.28	2.36	69,69,69,69	0
86	MG	5	3474	1/1	0.32	2.35	58,58,58,58	0
86	MG	M7	202	1/1	0.83	2.34	100,100,100,100	0
86	MG	1	3691	1/1	0.29	2.34	55,55,55,55	0
86	MG	6	2000	1/1	0.25	2.34	77,77,77,77	0
87	OHX	1	4136	7/7	0.43	2.33	183,183,183,183	0
87	OHX	1	4025	7/7	0.24	2.33	175,175,175,175	0
86	MG	5	3708	1/1	0.18	2.32	128,128,128,128	0
87	OHX	1	4112	7/7	0.40	2.32	155,155,155,155	0
86	MG	M5	302	1/1	0.40	2.32	75,75,75,75	0
86	MG	2	2006	1/1	0.28	2.29	92,92,92,92	0
86	MG	M7	204	1/1	0.37	2.28	45,45,45,45	0
86	MG	n8	202	1/1	0.32	2.28	64,64,64,64	0
86	MG	6	2021	1/1	0.45	2.27	62,62,62,62	0
87	OHX	2	2149	7/7	0.22	2.27	229,229,229,229	0
86	MG	2	1976	1/1	0.33	2.26	87,87,87,87	0
87	OHX	5	3989	7/7	0.22	2.26	143,143,143,143	0
87	OHX	5	3907	7/7	0.29	2.24	68,68,68,68	0
86	MG	2	1937	1/1	0.32	2.24	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3776	1/1	0.27	2.23	96,96,96,96	0
86	MG	2	1981	1/1	0.24	2.22	96,96,96,96	0
86	MG	6	1905	1/1	0.49	2.22	69,69,69,69	0
86	MG	1	3599	1/1	0.33	2.22	50,50,50,50	0
86	MG	5	3691	1/1	0.29	2.18	47,47,47,47	0
87	OHX	5	4226	7/7	0.29	2.18	150,150,150,150	0
87	OHX	5	4188	7/7	0.26	2.17	157,157,157,157	0
87	OHX	5	4151	7/7	0.40	2.17	177,177,177,177	0
87	OHX	5	4176	7/7	0.20	2.16	177,177,177,177	0
86	MG	5	3669	1/1	0.41	2.16	41,41,41,41	0
87	OHX	5	4128	7/7	0.34	2.14	175,175,175,175	0
86	MG	2	1999	1/1	0.46	2.13	97,97,97,97	0
87	OHX	1	4170	7/7	0.31	2.12	169,169,169,169	0
86	MG	5	3817	1/1	0.35	2.12	141,141,141,141	0
86	MG	2	1913	1/1	0.32	2.11	118,118,118,118	0
87	OHX	6	2185	7/7	0.33	2.11	169,169,169,169	0
86	MG	5	3602	1/1	0.19	2.11	42,42,42,42	0
86	MG	m1	201	1/1	0.56	2.09	68,68,68,68	0
87	OHX	1	4061	7/7	0.25	2.07	159,159,159,159	0
86	MG	1	3417	1/1	0.29	2.06	52,52,52,52	0
87	OHX	1	3946	7/7	0.22	2.05	134,134,134,134	0
86	MG	5	3640	1/1	0.92	2.02	63,63,63,63	0
87	OHX	1	4212	7/7	0.29	2.02	194,194,194,194	0
86	MG	2	2016	1/1	0.64	2.02	82,82,82,82	0
87	OHX	1	3872	7/7	0.20	2.01	89,89,89,89	0
87	OHX	6	2057	7/7	0.25	2.01	97,97,97,97	0
86	MG	1	3769	1/1	0.25	2.00	95,95,95,95	0
87	OHX	6	2174	7/7	0.41	1.99	149,149,149,149	0
86	MG	M3	202	1/1	0.30	1.99	39,39,39,39	0
86	MG	5	3891	1/1	0.27	1.98	83,83,83,83	0
86	MG	1	3747	1/1	0.44	1.97	60,60,60,60	0
86	MG	5	3820	1/1	0.31	1.97	71,71,71,71	0
86	MG	5	3417	1/1	0.23	1.97	44,44,44,44	0
87	OHX	5	4170	7/7	0.25	1.97	184,184,184,184	0
87	OHX	8	227	7/7	0.23	1.97	143,143,143,143	0
86	MG	l5	302	1/1	0.32	1.96	77,77,77,77	0
87	OHX	1	3906	7/7	0.18	1.96	107,107,107,107	0
87	OHX	5	3934	7/7	0.21	1.96	104,104,104,104	0
86	MG	1	3445	1/1	0.34	1.93	75,75,75,75	0
86	MG	1	3640	1/1	0.49	1.92	49,49,49,49	0
86	MG	1	3803	1/1	0.45	1.91	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	2	2175	7/7	0.38	1.91	188,188,188,188	0
86	MG	5	3448	1/1	0.25	1.91	72,72,72,72	0
87	OHX	2	2143	7/7	0.33	1.90	163,163,163,163	0
87	OHX	4	232	7/7	0.28	1.89	170,170,170,170	0
87	OHX	5	4214	7/7	0.33	1.89	220,220,220,220	0
86	MG	1	3592	1/1	0.45	1.88	42,42,42,42	0
87	OHX	4	237	7/7	0.21	1.88	194,194,194,194	0
86	MG	6	1952	1/1	0.32	1.88	79,79,79,79	0
87	OHX	3	223	7/7	0.29	1.88	216,216,216,216	0
87	OHX	6	2171	7/7	0.40	1.88	202,202,202,202	0
86	MG	5	3782	1/1	0.31	1.88	61,61,61,61	0
86	MG	6	1985	1/1	0.98	1.87	67,67,67,67	0
86	MG	7	213	1/1	0.20	1.86	87,87,87,87	0
86	MG	1	3487	1/1	0.29	1.86	50,50,50,50	0
87	OHX	6	2125	7/7	0.23	1.85	141,141,141,141	0
86	MG	6	1919	1/1	0.29	1.83	82,82,82,82	0
87	OHX	2	2026	7/7	0.23	1.83	112,112,112,112	0
86	MG	5	3550	1/1	0.37	1.83	86,86,86,86	0
86	MG	2	2011	1/1	0.65	1.83	77,77,77,77	0
87	OHX	1	4110	7/7	0.28	1.83	133,133,133,133	0
86	MG	2	1938	1/1	0.24	1.81	90,90,90,90	0
86	MG	19	201	1/1	0.33	1.81	44,44,44,44	0
87	OHX	6	2211	7/7	0.24	1.81	189,189,189,189	0
86	MG	5	3743	1/1	0.28	1.81	71,71,71,71	0
87	OHX	m7	205	7/7	0.46	1.80	172,172,172,172	0
86	MG	1	3536	1/1	0.24	1.79	70,70,70,70	0
86	MG	6	1991	1/1	0.24	1.79	65,65,65,65	0
86	MG	6	1920	1/1	0.45	1.79	56,56,56,56	0
86	MG	1	3705	1/1	0.31	1.78	72,72,72,72	0
87	OHX	5	4121	7/7	0.16	1.78	174,174,174,174	0
87	OHX	5	3919	7/7	0.25	1.76	95,95,95,95	0
86	MG	1	3709	1/1	0.26	1.75	74,74,74,74	0
86	MG	2	1934	1/1	0.29	1.73	103,103,103,103	0
86	MG	5	3726	1/1	0.67	1.73	113,113,113,113	0
86	MG	1	3429	1/1	0.29	1.72	71,71,71,71	0
87	OHX	6	2207	7/7	0.27	1.69	202,202,202,202	0
86	MG	5	3825	1/1	0.36	1.69	59,59,59,59	0
87	OHX	8	218	7/7	0.22	1.68	80,80,80,80	0
86	MG	1	3436	1/1	0.31	1.68	53,53,53,53	0
86	MG	1	3734	1/1	0.44	1.67	98,98,98,98	0
87	OHX	5	4190	7/7	0.21	1.66	152,152,152,152	0
86	MG	7	201	1/1	0.32	1.64	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3446	1/1	0.20	1.64	56,56,56,56	0
86	MG	L7	301	1/1	0.46	1.63	57,57,57,57	0
86	MG	1	3809	1/1	0.31	1.62	54,54,54,54	0
87	OHX	1	4211	7/7	0.36	1.61	164,164,164,164	0
86	MG	N8	204	1/1	0.55	1.61	59,59,59,59	0
87	OHX	5	4222	7/7	0.47	1.60	209,209,209,209	0
86	MG	5	3437	1/1	0.21	1.60	74,74,74,74	0
87	OHX	1	4161	7/7	0.27	1.59	195,195,195,195	0
87	OHX	6	2145	7/7	0.17	1.58	182,182,182,182	0
87	OHX	1	4015	7/7	0.34	1.57	156,156,156,156	0
87	OHX	1	4000	7/7	0.26	1.56	145,145,145,145	0
86	MG	l2	301	1/1	0.39	1.56	52,52,52,52	0
86	MG	1	3600	1/1	0.24	1.55	61,61,61,61	0
86	MG	8	210	1/1	0.36	1.54	77,77,77,77	0
86	MG	5	3732	1/1	0.46	1.54	61,61,61,61	0
86	MG	4	212	1/1	0.46	1.54	78,78,78,78	0
86	MG	1	3579	1/1	0.40	1.53	63,63,63,63	0
87	OHX	5	4108	7/7	0.25	1.52	132,132,132,132	0
87	OHX	5	3930	7/7	0.21	1.52	96,96,96,96	0
87	OHX	5	4087	7/7	0.21	1.52	141,141,141,141	0
86	MG	2	1975	1/1	0.47	1.51	102,102,102,102	0
86	MG	5	3402	1/1	0.25	1.50	38,38,38,38	0
87	OHX	5	4094	7/7	0.26	1.49	157,157,157,157	0
88	GET	2	2181	34/34	0.30	1.48	91,91,91,91	0
86	MG	1	3694	1/1	0.38	1.47	62,62,62,62	0
86	MG	m5	302	1/1	1.10	1.47	107,107,107,107	0
86	MG	5	3770	1/1	0.27	1.47	47,47,47,47	0
87	OHX	m9	201	7/7	0.45	1.47	173,173,173,173	0
87	OHX	2	2174	7/7	0.25	1.46	209,209,209,209	0
86	MG	2	2021	1/1	0.31	1.45	123,123,123,123	0
86	MG	5	3492	1/1	0.37	1.45	72,72,72,72	0
87	OHX	6	2202	7/7	0.22	1.44	209,209,209,209	0
86	MG	1	3847	1/1	0.23	1.44	67,67,67,67	0
86	MG	5	3421	1/1	0.27	1.44	59,59,59,59	0
87	OHX	1	4102	7/7	0.26	1.42	164,164,164,164	0
87	OHX	M7	206	7/7	0.27	1.42	151,151,151,151	0
86	MG	5	3618	1/1	0.25	1.42	49,49,49,49	0
87	OHX	4	236	7/7	0.32	1.41	164,164,164,164	0
86	MG	6	1981	1/1	0.28	1.41	102,102,102,102	0
86	MG	5	3761	1/1	0.24	1.38	59,59,59,59	0
87	OHX	2	2084	7/7	0.27	1.38	169,169,169,169	0
86	MG	1	3442	1/1	0.32	1.38	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	MG	2	1971	1/1	0.25	1.36	116,116,116,116	0
87	OHX	2	2117	7/7	0.48	1.35	182,182,182,182	0
87	OHX	N9	102	7/7	0.21	1.35	84,84,84,84	0
87	OHX	6	2165	7/7	0.29	1.35	168,168,168,168	0
86	MG	1	3608	1/1	0.36	1.34	68,68,68,68	0
86	MG	6	1961	1/1	0.38	1.33	51,51,51,51	0
86	MG	5	3401	1/1	0.32	1.32	76,76,76,76	0
87	OHX	5	4100	7/7	0.37	1.32	136,136,136,136	0
87	OHX	1	3985	7/7	0.30	1.31	149,149,149,149	0
87	OHX	5	4230	7/7	0.24	1.31	159,159,159,159	0
86	MG	M7	205	1/1	0.34	1.30	52,52,52,52	0
86	MG	6	2006	1/1	0.38	1.29	84,84,84,84	0
86	MG	2	1955	1/1	0.23	1.29	95,95,95,95	0
86	MG	o0	201	1/1	0.45	1.29	95,95,95,95	0
86	MG	S2	302	1/1	0.38	1.28	96,96,96,96	0
87	OHX	2	2122	7/7	0.30	1.28	201,201,201,201	0
87	OHX	2	2169	7/7	0.28	1.28	207,207,207,207	0
86	MG	5	3849	1/1	0.41	1.27	60,60,60,60	0
86	MG	s8	302	1/1	0.67	1.26	65,65,65,65	0
86	MG	5	3778	1/1	0.17	1.23	92,92,92,92	0
86	MG	5	3836	1/1	0.32	1.22	70,70,70,70	0
86	MG	M5	301	1/1	0.74	1.22	74,74,74,74	0
86	MG	1	3437	1/1	0.34	1.22	71,71,71,71	0
86	MG	1	3409	1/1	0.30	1.21	48,48,48,48	0
86	MG	N0	201	1/1	0.30	1.21	66,66,66,66	0
87	OHX	1	3931	7/7	0.25	1.21	92,92,92,92	0
86	MG	6	1955	1/1	0.27	1.21	80,80,80,80	0
86	MG	l4	401	1/1	0.46	1.20	63,63,63,63	0
86	MG	2	1965	1/1	0.34	1.20	85,85,85,85	0
86	MG	m6	203	1/1	0.43	1.20	41,41,41,41	0
87	OHX	5	4106	7/7	0.34	1.19	178,178,178,178	0
86	MG	m6	202	1/1	0.30	1.19	78,78,78,78	0
87	OHX	5	3922	7/7	0.23	1.19	92,92,92,92	0
86	MG	1	3820	1/1	0.26	1.19	81,81,81,81	0
87	OHX	2	2072	7/7	0.28	1.18	176,176,176,176	0
86	MG	6	1993	1/1	0.35	1.16	91,91,91,91	0
86	MG	2	1925	1/1	0.33	1.15	92,92,92,92	0
86	MG	5	3715	1/1	0.31	1.14	62,62,62,62	0
87	OHX	2	2176	7/7	0.24	1.14	176,176,176,176	0
87	OHX	2	2179	7/7	0.33	1.14	183,183,183,183	0
86	MG	1	3499	1/1	0.29	1.13	101,101,101,101	0
86	MG	5	3508	1/1	0.33	1.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2128	7/7	0.19	1.13	200,200,200,200	0
86	MG	6	1959	1/1	0.34	1.13	76,76,76,76	0
87	OHX	1	3951	7/7	0.18	1.13	160,160,160,160	0
86	MG	1	3617	1/1	0.27	1.12	112,112,112,112	0
87	OHX	6	2075	7/7	0.15	1.10	141,141,141,141	0
87	OHX	6	2112	7/7	0.29	1.10	151,151,151,151	0
87	OHX	6	2059	7/7	0.24	1.09	96,96,96,96	0
87	OHX	6	2121	7/7	0.40	1.09	166,166,166,166	0
86	MG	5	3462	1/1	0.26	1.09	80,80,80,80	0
87	OHX	2	2152	7/7	0.22	1.08	192,192,192,192	0
87	OHX	5	4213	7/7	0.31	1.07	180,180,180,180	0
86	MG	1	3521	1/1	0.29	1.05	52,52,52,52	0
87	OHX	1	3918	7/7	0.17	1.05	124,124,124,124	0
87	OHX	5	4185	7/7	0.23	1.04	169,169,169,169	0
87	OHX	6	2053	7/7	0.19	1.03	92,92,92,92	0
86	MG	1	3780	1/1	0.40	1.03	55,55,55,55	0
86	MG	5	3788	1/1	0.25	1.02	49,49,49,49	0
86	MG	S8	301	1/1	0.36	1.02	85,85,85,85	0
87	OHX	6	2142	7/7	0.38	0.99	144,144,144,144	0
87	OHX	1	4140	7/7	0.29	0.99	163,163,163,163	0
86	MG	5	3744	1/1	0.20	0.99	97,97,97,97	0
86	MG	1	3455	1/1	0.35	0.99	90,90,90,90	0
87	OHX	2	2027	7/7	0.23	0.99	102,102,102,102	0
86	MG	6	1909	1/1	0.24	0.98	114,114,114,114	0
87	OHX	1	4183	7/7	0.26	0.97	133,133,133,133	0
86	MG	5	3615	1/1	0.38	0.97	65,65,65,65	0
86	MG	5	3502	1/1	0.24	0.94	66,66,66,66	0
86	MG	1	3631	1/1	0.40	0.94	111,111,111,111	0
87	OHX	1	4066	7/7	0.36	0.93	175,175,175,175	0
87	OHX	3	225	7/7	0.23	0.93	167,167,167,167	0
86	MG	5	3527	1/1	0.41	0.92	93,93,93,93	0
87	OHX	5	4132	7/7	0.43	0.91	169,169,169,169	0
86	MG	2	1906	1/1	0.43	0.91	80,80,80,80	0
86	MG	6	2028	1/1	0.46	0.89	58,58,58,58	0
86	MG	5	3827	1/1	0.24	0.89	59,59,59,59	0
87	OHX	4	225	7/7	0.22	0.89	79,79,79,79	0
86	MG	8	213	1/1	0.26	0.89	111,111,111,111	0
87	OHX	1	3868	7/7	0.26	0.89	70,70,70,70	0
86	MG	6	1925	1/1	0.31	0.88	133,133,133,133	0
87	OHX	5	3910	7/7	0.20	0.88	92,92,92,92	0
86	MG	5	3700	1/1	0.28	0.88	65,65,65,65	0
87	OHX	6	2179	7/7	0.41	0.88	170,170,170,170	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3838	1/1	0.37	0.88	64,64,64,64	0
87	OHX	5	4064	7/7	0.15	0.88	179,179,179,179	0
87	OHX	1	4078	7/7	0.39	0.87	165,165,165,165	0
87	OHX	5	4008	7/7	0.14	0.87	163,163,163,163	0
86	MG	4	216	1/1	0.30	0.86	89,89,89,89	0
87	OHX	1	3869	7/7	0.26	0.86	76,76,76,76	0
86	MG	5	3773	1/1	0.89	0.85	92,92,92,92	0
87	OHX	6	2055	7/7	0.23	0.85	95,95,95,95	0
87	OHX	1	3867	7/7	0.21	0.84	70,70,70,70	0
86	MG	1	3715	1/1	0.28	0.82	62,62,62,62	0
87	OHX	1	3944	7/7	0.17	0.81	137,137,137,137	0
87	OHX	5	4245	7/7	0.20	0.79	183,183,183,183	0
86	MG	15	301	1/1	0.29	0.79	71,71,71,71	0
86	MG	2	1980	1/1	0.37	0.78	95,95,95,95	0
87	OHX	5	4161	7/7	0.23	0.78	182,182,182,182	0
87	OHX	2	2172	7/7	0.26	0.77	191,191,191,191	0
86	MG	6	1953	1/1	0.28	0.76	64,64,64,64	0
87	OHX	6	2163	7/7	0.21	0.76	198,198,198,198	0
86	MG	6	2008	1/1	0.18	0.76	120,120,120,120	0
86	MG	5	3577	1/1	0.50	0.76	66,66,66,66	0
86	MG	5	3722	1/1	0.37	0.74	87,87,87,87	0
86	MG	5	3890	1/1	0.23	0.74	78,78,78,78	0
87	OHX	5	3928	7/7	0.19	0.74	128,128,128,128	0
87	OHX	1	4014	7/7	0.50	0.74	179,179,179,179	0
86	MG	1	3507	1/1	0.46	0.73	57,57,57,57	0
87	OHX	1	4113	7/7	0.18	0.73	166,166,166,166	0
86	MG	1	3755	1/1	0.21	0.72	60,60,60,60	0
87	OHX	6	2162	7/7	0.31	0.71	162,162,162,162	0
86	MG	5	3696	1/1	0.22	0.70	48,48,48,48	0
86	MG	5	3662	1/1	0.25	0.70	72,72,72,72	0
87	OHX	6	2105	7/7	0.14	0.69	200,200,200,200	0
87	OHX	6	2210	7/7	0.37	0.69	166,166,166,166	0
86	MG	5	3480	1/1	0.48	0.69	92,92,92,92	0
87	OHX	5	3935	7/7	0.19	0.68	94,94,94,94	0
86	MG	5	3834	1/1	0.30	0.68	81,81,81,81	0
86	MG	2	1967	1/1	0.53	0.67	108,108,108,108	0
86	MG	5	3415	1/1	0.22	0.67	73,73,73,73	0
87	OHX	5	4130	7/7	0.23	0.66	154,154,154,154	0
86	MG	5	3693	1/1	0.22	0.66	99,99,99,99	0
86	MG	1	3775	1/1	0.29	0.64	54,54,54,54	0
87	OHX	5	4240	7/7	0.24	0.63	188,188,188,188	0
87	OHX	4	227	7/7	0.19	0.62	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3471	1/1	0.30	0.61	56,56,56,56	0
86	MG	6	1915	1/1	0.46	0.61	85,85,85,85	0
87	OHX	6	2056	7/7	0.16	0.61	113,113,113,113	0
87	OHX	1	3904	7/7	0.22	0.61	96,96,96,96	0
87	OHX	5	4157	7/7	0.19	0.61	146,146,146,146	0
86	MG	5	3413	1/1	0.49	0.59	45,45,45,45	0
87	OHX	1	3894	7/7	0.19	0.59	95,95,95,95	0
87	OHX	2	2040	7/7	0.18	0.58	128,128,128,128	0
87	OHX	6	2208	7/7	0.47	0.58	182,182,182,182	0
87	OHX	5	4220	7/7	0.19	0.58	187,187,187,187	0
86	MG	2	1953	1/1	0.34	0.55	179,179,179,179	0
87	OHX	5	3898	7/7	0.25	0.55	77,77,77,77	0
87	OHX	5	4095	7/7	0.14	0.55	175,175,175,175	0
87	OHX	6	2203	7/7	0.18	0.55	205,205,205,205	0
86	MG	1	3710	1/1	0.26	0.54	47,47,47,47	0
86	MG	5	3512	1/1	0.29	0.54	79,79,79,79	0
87	OHX	2	2136	7/7	0.21	0.54	203,203,203,203	0
87	OHX	5	3917	7/7	0.20	0.53	93,93,93,93	0
86	MG	5	3721	1/1	0.34	0.52	41,41,41,41	0
86	MG	2	1920	1/1	0.45	0.52	86,86,86,86	0
86	MG	1	3635	1/1	0.38	0.52	86,86,86,86	0
87	OHX	5	4115	7/7	0.17	0.51	153,153,153,153	0
86	MG	5	3740	1/1	0.20	0.51	60,60,60,60	0
87	OHX	2	2160	7/7	0.52	0.51	176,176,176,176	0
86	MG	5	3556	1/1	0.30	0.50	35,35,35,35	0
86	MG	6	2005	1/1	0.22	0.50	66,66,66,66	0
87	OHX	5	4225	7/7	0.22	0.49	180,180,180,180	0
87	OHX	1	4197	7/7	0.23	0.48	149,149,149,149	0
86	MG	5	3810	1/1	0.32	0.48	55,55,55,55	0
87	OHX	5	4201	7/7	0.28	0.48	181,181,181,181	0
87	OHX	5	4065	7/7	0.36	0.48	149,149,149,149	0
86	MG	5	3591	1/1	0.27	0.47	58,58,58,58	0
86	MG	c7	201	1/1	0.31	0.47	62,62,62,62	0
86	MG	5	3751	1/1	0.32	0.46	77,77,77,77	0
87	OHX	1	4178	7/7	0.63	0.45	184,184,184,184	0
86	MG	5	3668	1/1	0.24	0.45	68,68,68,68	0
87	OHX	6	2176	7/7	0.31	0.45	190,190,190,190	0
87	OHX	6	2173	7/7	0.20	0.45	200,200,200,200	0
87	OHX	1	3929	7/7	0.17	0.44	143,143,143,143	0
86	MG	2	1911	1/1	0.40	0.42	89,89,89,89	0
87	OHX	1	4084	7/7	0.22	0.42	174,174,174,174	0
87	OHX	5	3972	7/7	0.21	0.42	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	2	1959	1/1	0.20	0.42	143,143,143,143	0
86	MG	2	1909	1/1	0.24	0.42	121,121,121,121	0
87	OHX	8	230	7/7	0.18	0.42	178,178,178,178	0
86	MG	2	2000	1/1	0.46	0.41	134,134,134,134	0
86	MG	1	3725	1/1	0.16	0.39	69,69,69,69	0
86	MG	N6	201	1/1	0.37	0.38	72,72,72,72	0
86	MG	1	3622	1/1	0.27	0.38	72,72,72,72	0
87	OHX	2	2178	7/7	0.28	0.37	211,211,211,211	0
86	MG	d3	201	1/1	0.43	0.36	76,76,76,76	0
86	MG	1	3685	1/1	0.28	0.36	58,58,58,58	0
87	OHX	5	4099	7/7	0.22	0.36	161,161,161,161	0
87	OHX	1	4173	7/7	0.16	0.35	184,184,184,184	0
86	MG	5	3429	1/1	0.20	0.34	81,81,81,81	0
86	MG	6	2007	1/1	0.24	0.34	93,93,93,93	0
87	OHX	6	2186	7/7	0.20	0.33	187,187,187,187	0
87	OHX	5	3960	7/7	0.20	0.33	130,130,130,130	0
86	MG	5	3892	1/1	0.44	0.33	93,93,93,93	0
87	OHX	6	2201	7/7	0.18	0.32	195,195,195,195	0
87	OHX	2	2173	7/7	0.28	0.32	199,199,199,199	0
86	MG	5	3758	1/1	0.27	0.32	66,66,66,66	0
86	MG	5	3846	1/1	0.45	0.32	75,75,75,75	0
86	MG	6	2010	1/1	0.29	0.31	80,80,80,80	0
86	MG	6	1999	1/1	0.26	0.31	102,102,102,102	0
86	MG	8	208	1/1	0.32	0.31	70,70,70,70	0
86	MG	6	1936	1/1	0.37	0.30	66,66,66,66	0
87	OHX	6	2120	7/7	0.25	0.30	145,145,145,145	0
87	OHX	5	3951	7/7	0.23	0.29	118,118,118,118	0
87	OHX	5	3970	7/7	0.24	0.29	107,107,107,107	0
87	OHX	2	2165	7/7	0.16	0.29	235,235,235,235	0
87	OHX	1	4200	7/7	0.19	0.27	174,174,174,174	0
87	OHX	1	3980	7/7	0.24	0.27	139,139,139,139	0
86	MG	q3	502	1/1	0.41	0.27	83,83,83,83	0
87	OHX	6	2147	7/7	0.32	0.26	164,164,164,164	0
86	MG	1	3566	1/1	0.26	0.25	43,43,43,43	0
86	MG	5	3460	1/1	0.26	0.25	43,43,43,43	0
87	OHX	1	4145	7/7	0.21	0.25	168,168,168,168	0
87	OHX	1	4104	7/7	0.22	0.25	153,153,153,153	0
86	MG	5	3811	1/1	0.27	0.24	54,54,54,54	0
87	OHX	2	2157	7/7	0.23	0.24	152,152,152,152	0
87	OHX	2	2164	7/7	0.24	0.24	173,173,173,173	0
86	MG	5	3781	1/1	0.17	0.23	60,60,60,60	0
86	MG	1	3601	1/1	0.23	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3842	1/1	0.23	0.22	58,58,58,58	0
87	OHX	5	3947	7/7	0.15	0.22	142,142,142,142	0
87	OHX	1	4207	7/7	0.23	0.22	151,151,151,151	0
87	OHX	5	4086	7/7	0.22	0.22	134,134,134,134	0
87	OHX	2	2137	7/7	0.28	0.22	216,216,216,216	0
86	MG	5	3692	1/1	0.20	0.22	61,61,61,61	0
86	MG	5	3453	1/1	0.20	0.21	63,63,63,63	0
87	OHX	1	4062	7/7	0.18	0.20	154,154,154,154	0
87	OHX	5	4239	7/7	0.36	0.19	179,179,179,179	0
86	MG	1	3708	1/1	0.22	0.19	76,76,76,76	0
86	MG	5	3663	1/1	0.29	0.19	52,52,52,52	0
87	OHX	6	2070	7/7	0.18	0.18	152,152,152,152	0
87	OHX	2	2096	7/7	0.35	0.18	189,189,189,189	0
87	OHX	2	2054	7/7	0.26	0.17	192,192,192,192	0
86	MG	N3	202	1/1	0.38	0.16	62,62,62,62	0
87	OHX	1	3889	7/7	0.22	0.15	99,99,99,99	0
87	OHX	2	2041	7/7	0.18	0.15	164,164,164,164	0
87	OHX	1	4194	7/7	0.35	0.15	172,172,172,172	0
87	OHX	5	4177	7/7	0.17	0.14	181,181,181,181	0
86	MG	5	3747	1/1	0.24	0.14	57,57,57,57	0
87	OHX	5	3915	7/7	0.18	0.14	101,101,101,101	0
86	MG	3	201	1/1	0.20	0.13	95,95,95,95	0
87	OHX	5	4206	7/7	0.17	0.13	172,172,172,172	0
87	OHX	1	4165	7/7	0.23	0.13	134,134,134,134	0
87	OHX	1	4088	7/7	0.12	0.12	197,197,197,197	0
87	OHX	2	2151	7/7	0.17	0.11	236,236,236,236	0
87	OHX	D9	102	7/7	0.38	0.11	184,184,184,184	0
87	OHX	5	3996	7/7	0.20	0.11	130,130,130,130	0
87	OHX	1	3938	7/7	0.22	0.11	123,123,123,123	0
87	OHX	5	4001	7/7	0.20	0.11	126,126,126,126	0
86	MG	1	3420	1/1	0.47	0.10	113,113,113,113	0
86	MG	1	3748	1/1	0.22	0.10	62,62,62,62	0
86	MG	8	201	1/1	0.27	0.10	69,69,69,69	0
86	MG	2	1949	1/1	0.21	0.10	86,86,86,86	0
87	OHX	1	3881	7/7	0.19	0.09	91,91,91,91	0
87	OHX	5	4164	7/7	0.23	0.09	165,165,165,165	0
86	MG	4	218	1/1	0.25	0.09	84,84,84,84	0
86	MG	4	209	1/1	0.23	0.08	56,56,56,56	0
87	OHX	1	4128	7/7	0.17	0.08	194,194,194,194	0
87	OHX	1	4119	7/7	0.29	0.08	197,197,197,197	0
87	OHX	1	4157	7/7	0.23	0.08	165,165,165,165	0
87	OHX	5	4042	7/7	0.41	0.07	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	4184	7/7	0.40	0.07	166,166,166,166	0
86	MG	1	3757	1/1	0.16	0.06	72,72,72,72	0
86	MG	5	3768	1/1	0.22	0.04	45,45,45,45	0
87	OHX	1	4162	7/7	0.14	0.04	190,190,190,190	0
86	MG	2	1996	1/1	0.25	0.04	123,123,123,123	0
87	OHX	2	2134	7/7	0.31	0.03	192,192,192,192	0
87	OHX	1	4179	7/7	0.24	0.03	174,174,174,174	0
87	OHX	1	4181	7/7	0.40	0.03	166,166,166,166	0
86	MG	1	3444	1/1	0.53	0.02	66,66,66,66	0
87	OHX	5	4114	7/7	0.24	0.02	148,148,148,148	0
86	MG	c8	201	1/1	0.35	0.02	53,53,53,53	0
87	OHX	1	4079	7/7	0.27	0.01	157,157,157,157	0
86	MG	1	3830	1/1	0.19	0.01	54,54,54,54	0
87	OHX	2	2115	7/7	0.27	0.00	161,161,161,161	0
87	OHX	1	3874	7/7	0.21	0.00	78,78,78,78	0
87	OHX	1	4111	7/7	0.22	0.00	213,213,213,213	0
87	OHX	1	4172	7/7	0.12	-0.02	213,213,213,213	0
87	OHX	5	3900	7/7	0.20	-0.02	80,80,80,80	0
87	OHX	5	4003	7/7	0.21	-0.02	91,91,91,91	0
86	MG	5	3632	1/1	0.33	-0.03	62,62,62,62	0
87	OHX	5	4234	7/7	0.20	-0.03	217,217,217,217	0
86	MG	L2	302	1/1	0.25	-0.03	62,62,62,62	0
86	MG	1	3627	1/1	0.22	-0.03	77,77,77,77	0
86	MG	5	3579	1/1	0.21	-0.03	40,40,40,40	0
87	OHX	6	2177	7/7	0.22	-0.04	141,141,141,141	0
87	OHX	1	3921	7/7	0.13	-0.04	135,135,135,135	0
86	MG	1	3662	1/1	0.36	-0.04	92,92,92,92	0
87	OHX	5	4246	7/7	0.35	-0.05	205,205,205,205	0
87	OHX	2	2071	7/7	0.40	-0.05	184,184,184,184	0
87	OHX	2	2150	7/7	0.22	-0.05	213,213,213,213	0
87	OHX	D3	202	7/7	0.31	-0.05	210,210,210,210	0
86	MG	6	1956	1/1	0.33	-0.07	48,48,48,48	0
87	OHX	2	2075	7/7	0.19	-0.07	186,186,186,186	0
86	MG	2	2012	1/1	0.33	-0.07	88,88,88,88	0
87	OHX	5	3902	7/7	0.21	-0.07	91,91,91,91	0
86	MG	5	3851	1/1	0.34	-0.08	71,71,71,71	0
86	MG	5	3738	1/1	0.19	-0.11	67,67,67,67	0
87	OHX	2	2180	7/7	0.23	-0.11	205,205,205,205	0
86	MG	M1	201	1/1	0.30	-0.11	104,104,104,104	0
87	OHX	5	4111	7/7	0.14	-0.11	230,230,230,230	0
87	OHX	5	3942	7/7	0.20	-0.12	116,116,116,116	0
87	OHX	5	4186	7/7	0.23	-0.13	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2135	7/7	0.19	-0.13	182,182,182,182	0
87	OHX	1	4069	7/7	0.31	-0.13	163,163,163,163	0
89	ZN	d7	101	1/1	0.24	-0.14	156,156,156,156	0
87	OHX	6	2199	7/7	0.15	-0.14	188,188,188,188	0
87	OHX	1	3940	7/7	0.19	-0.14	123,123,123,123	0
86	MG	l3	404	1/1	0.24	-0.14	58,58,58,58	0
87	OHX	l5	306	7/7	0.52	-0.14	175,175,175,175	0
87	OHX	7	220	7/7	0.21	-0.15	137,137,137,137	0
87	OHX	5	3969	7/7	0.17	-0.15	133,133,133,133	0
87	OHX	7	218	7/7	0.17	-0.15	106,106,106,106	0
87	OHX	6	2129	7/7	0.17	-0.16	156,156,156,156	0
86	MG	1	3707	1/1	0.21	-0.16	64,64,64,64	0
87	OHX	1	3886	7/7	0.18	-0.16	105,105,105,105	0
86	MG	1	3670	1/1	0.23	-0.16	61,61,61,61	0
87	OHX	2	2139	7/7	0.37	-0.17	213,213,213,213	0
87	OHX	1	4002	7/7	0.12	-0.17	147,147,147,147	0
87	OHX	1	4144	7/7	0.20	-0.17	182,182,182,182	0
86	MG	6	2023	1/1	0.26	-0.17	67,67,67,67	0
87	OHX	6	2184	7/7	0.30	-0.19	164,164,164,164	0
87	OHX	5	3909	7/7	0.21	-0.19	92,92,92,92	0
87	OHX	1	4135	7/7	0.24	-0.20	159,159,159,159	0
86	MG	5	3438	1/1	0.20	-0.20	41,41,41,41	0
86	MG	N8	202	1/1	0.29	-0.20	64,64,64,64	0
87	OHX	5	4180	7/7	0.16	-0.20	152,152,152,152	0
87	OHX	5	4217	7/7	0.18	-0.20	192,192,192,192	0
86	MG	1	3634	1/1	0.26	-0.21	95,95,95,95	0
87	OHX	7	224	7/7	0.16	-0.21	188,188,188,188	0
87	OHX	1	4184	7/7	0.21	-0.22	166,166,166,166	0
87	OHX	5	4204	7/7	0.20	-0.23	175,175,175,175	0
86	MG	1	3606	1/1	0.29	-0.23	96,96,96,96	0
86	MG	2	1915	1/1	0.22	-0.24	96,96,96,96	0
86	MG	5	3789	1/1	0.22	-0.24	67,67,67,67	0
87	OHX	2	2146	7/7	0.15	-0.25	167,167,167,167	0
87	OHX	2	2144	7/7	0.19	-0.25	223,223,223,223	0
86	MG	1	3790	1/1	0.14	-0.25	78,78,78,78	0
86	MG	5	3795	1/1	0.18	-0.25	100,100,100,100	0
87	OHX	6	2205	7/7	0.22	-0.25	204,204,204,204	0
87	OHX	1	4177	7/7	0.17	-0.25	280,280,280,280	0
87	OHX	1	3879	7/7	0.15	-0.26	92,92,92,92	0
86	MG	O2	201	1/1	0.26	-0.26	46,46,46,46	0
86	MG	5	3472	1/1	0.39	-0.27	72,72,72,72	0
86	MG	2	1929	1/1	0.24	-0.27	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2116	7/7	0.23	-0.28	188,188,188,188	0
86	MG	6	2041	1/1	0.32	-0.28	81,81,81,81	0
87	OHX	1	4158	7/7	0.14	-0.28	199,199,199,199	0
87	OHX	1	3994	7/7	0.19	-0.29	195,195,195,195	0
87	OHX	5	4227	7/7	0.12	-0.29	207,207,207,207	0
87	OHX	1	4038	7/7	0.19	-0.30	152,152,152,152	0
86	MG	5	3543	1/1	0.19	-0.30	97,97,97,97	0
87	OHX	1	4151	7/7	0.19	-0.30	172,172,172,172	0
87	OHX	1	4153	7/7	0.23	-0.31	177,177,177,177	0
86	MG	M9	201	1/1	0.34	-0.34	92,92,92,92	0
87	OHX	1	4046	7/7	0.20	-0.34	156,156,156,156	0
87	OHX	6	2158	7/7	0.18	-0.34	176,176,176,176	0
87	OHX	5	4063	7/7	0.26	-0.34	145,145,145,145	0
87	OHX	1	4164	7/7	0.25	-0.34	247,247,247,247	0
87	OHX	1	4068	7/7	0.20	-0.35	143,143,143,143	0
87	OHX	4	230	7/7	0.18	-0.36	171,171,171,171	0
87	OHX	1	4037	7/7	0.18	-0.36	138,138,138,138	0
87	OHX	2	2030	7/7	0.18	-0.36	163,163,163,163	0
87	OHX	d4	201	7/7	0.26	-0.36	187,187,187,187	0
86	MG	s8	301	1/1	0.33	-0.37	71,71,71,71	0
87	OHX	6	2089	7/7	0.14	-0.37	128,128,128,128	0
86	MG	1	3489	1/1	0.23	-0.37	51,51,51,51	0
87	OHX	1	4103	7/7	0.13	-0.38	185,185,185,185	0
87	OHX	2	2098	7/7	0.16	-0.38	206,206,206,206	0
87	OHX	5	4145	7/7	0.21	-0.39	182,182,182,182	0
87	OHX	5	4066	7/7	0.20	-0.39	170,170,170,170	0
87	OHX	2	2102	7/7	0.22	-0.39	182,182,182,182	0
86	MG	5	3791	1/1	0.19	-0.39	88,88,88,88	0
87	OHX	6	2141	7/7	0.29	-0.40	165,165,165,165	0
86	MG	1	3806	1/1	0.20	-0.40	224,224,224,224	0
87	OHX	1	3924	7/7	0.24	-0.40	113,113,113,113	0
87	OHX	1	3878	7/7	0.24	-0.40	80,80,80,80	0
86	MG	L5	301	1/1	0.43	-0.40	81,81,81,81	0
87	OHX	2	2109	7/7	0.20	-0.41	205,205,205,205	0
87	OHX	1	3983	7/7	0.18	-0.42	159,159,159,159	0
87	OHX	1	4085	7/7	0.24	-0.42	151,151,151,151	0
87	OHX	1	4182	7/7	0.15	-0.42	188,188,188,188	0
86	MG	2	1931	1/1	0.35	-0.42	96,96,96,96	0
86	MG	5	3477	1/1	0.23	-0.43	90,90,90,90	0
86	MG	6	1904	1/1	0.19	-0.43	75,75,75,75	0
86	MG	1	3614	1/1	0.13	-0.43	94,94,94,94	0
86	MG	5	3558	1/1	0.26	-0.43	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2101	7/7	0.18	-0.44	195,195,195,195	0
87	OHX	7	216	7/7	0.17	-0.45	108,108,108,108	0
87	OHX	2	2090	7/7	0.18	-0.45	172,172,172,172	0
86	MG	5	3612	1/1	0.22	-0.45	61,61,61,61	0
86	MG	2	2022	1/1	0.16	-0.45	115,115,115,115	0
87	OHX	6	2195	7/7	0.22	-0.45	183,183,183,183	0
87	OHX	2	2035	7/7	0.20	-0.45	136,136,136,136	0
87	OHX	1	4156	7/7	0.17	-0.46	192,192,192,192	0
86	MG	5	3710	1/1	0.22	-0.46	73,73,73,73	0
86	MG	2	2005	1/1	0.21	-0.46	100,100,100,100	0
87	OHX	1	4005	7/7	0.18	-0.46	151,151,151,151	0
87	OHX	1	3936	7/7	0.15	-0.46	119,119,119,119	0
87	OHX	c8	202	7/7	0.14	-0.47	177,177,177,177	0
86	MG	2	1901	1/1	0.20	-0.47	117,117,117,117	0
87	OHX	5	4135	7/7	0.14	-0.47	172,172,172,172	0
86	MG	3	207	1/1	0.16	-0.47	86,86,86,86	0
86	MG	6	1928	1/1	0.18	-0.47	65,65,65,65	0
87	OHX	2	2047	7/7	0.14	-0.47	162,162,162,162	0
87	OHX	1	3907	7/7	0.20	-0.48	104,104,104,104	0
87	OHX	5	3943	7/7	0.30	-0.48	104,104,104,104	0
87	OHX	6	2078	7/7	0.15	-0.48	170,170,170,170	0
87	OHX	6	2133	7/7	0.27	-0.48	173,173,173,173	0
87	OHX	1	3885	7/7	0.20	-0.49	98,98,98,98	0
86	MG	5	3592	1/1	0.25	-0.49	42,42,42,42	0
87	OHX	6	2187	7/7	0.18	-0.50	164,164,164,164	0
87	OHX	2	2124	7/7	0.17	-0.50	207,207,207,207	0
87	OHX	6	2196	7/7	0.15	-0.50	176,176,176,176	0
87	OHX	2	2062	7/7	0.22	-0.50	161,161,161,161	0
86	MG	7	214	1/1	0.13	-0.50	47,47,47,47	0
87	OHX	1	4201	7/7	0.20	-0.50	164,164,164,164	0
87	OHX	2	2161	7/7	0.38	-0.51	199,199,199,199	0
87	OHX	1	4139	7/7	0.19	-0.51	167,167,167,167	0
87	OHX	2	2076	7/7	0.20	-0.51	176,176,176,176	0
86	MG	1	3800	1/1	0.20	-0.52	80,80,80,80	0
87	OHX	5	4089	7/7	0.18	-0.52	171,171,171,171	0
87	OHX	1	3914	7/7	0.25	-0.53	101,101,101,101	0
87	OHX	1	4075	7/7	0.19	-0.53	188,188,188,188	0
86	MG	5	3607	1/1	0.21	-0.53	55,55,55,55	0
87	OHX	3	221	7/7	0.15	-0.53	173,173,173,173	0
87	OHX	1	4133	7/7	0.21	-0.53	146,146,146,146	0
87	OHX	5	3932	7/7	0.15	-0.53	101,101,101,101	0
86	MG	2	1987	1/1	0.16	-0.53	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3463	1/1	0.22	-0.53	113,113,113,113	0
87	OHX	M6	202	7/7	0.22	-0.53	182,182,182,182	0
86	MG	2	1993	1/1	0.21	-0.54	96,96,96,96	0
87	OHX	1	3888	7/7	0.15	-0.54	115,115,115,115	0
87	OHX	2	2140	7/7	0.15	-0.54	200,200,200,200	0
87	OHX	6	2178	7/7	0.22	-0.54	182,182,182,182	0
87	OHX	8	235	7/7	0.18	-0.54	175,175,175,175	0
86	MG	6	1966	1/1	0.18	-0.56	83,83,83,83	0
87	OHX	1	4054	7/7	0.13	-0.56	178,178,178,178	0
87	OHX	3	216	7/7	0.21	-0.56	155,155,155,155	0
87	OHX	1	3877	7/7	0.19	-0.57	86,86,86,86	0
87	OHX	2	2131	7/7	0.22	-0.57	168,168,168,168	0
87	OHX	1	3934	7/7	0.32	-0.57	126,126,126,126	0
87	OHX	5	4210	7/7	0.19	-0.57	165,165,165,165	0
87	OHX	2	2053	7/7	0.09	-0.58	177,177,177,177	0
87	OHX	6	2111	7/7	0.19	-0.58	155,155,155,155	0
87	OHX	5	3926	7/7	0.19	-0.58	93,93,93,93	0
87	OHX	1	3911	7/7	0.20	-0.59	118,118,118,118	0
86	MG	1	3411	1/1	0.19	-0.60	79,79,79,79	0
86	MG	1	3551	1/1	0.22	-0.60	68,68,68,68	0
87	OHX	M9	202	7/7	0.17	-0.60	169,169,169,169	0
87	OHX	5	4219	7/7	0.32	-0.60	178,178,178,178	0
87	OHX	5	3908	7/7	0.15	-0.60	92,92,92,92	0
86	MG	5	3611	1/1	0.14	-0.61	72,72,72,72	0
87	OHX	d9	102	7/7	0.32	-0.61	189,189,189,189	0
86	MG	5	3706	1/1	0.17	-0.62	120,120,120,120	0
87	OHX	C8	201	7/7	0.14	-0.62	158,158,158,158	0
87	OHX	5	4232	7/7	0.12	-0.62	173,173,173,173	0
87	OHX	1	3970	7/7	0.18	-0.63	160,160,160,160	0
87	OHX	1	4196	7/7	0.15	-0.64	186,186,186,186	0
87	OHX	2	2094	7/7	0.15	-0.64	216,216,216,216	0
86	MG	5	3698	1/1	0.20	-0.64	89,89,89,89	0
87	OHX	O7	104	7/7	0.21	-0.65	144,144,144,144	0
87	OHX	1	3871	7/7	0.18	-0.65	77,77,77,77	0
87	OHX	5	3913	7/7	0.17	-0.65	69,69,69,69	0
87	OHX	6	2087	7/7	0.12	-0.66	157,157,157,157	0
87	OHX	8	223	7/7	0.08	-0.66	180,180,180,180	0
87	OHX	1	3989	7/7	0.19	-0.66	146,146,146,146	0
87	OHX	6	2181	7/7	0.12	-0.66	189,189,189,189	0
86	MG	1	3859	1/1	0.19	-0.67	71,71,71,71	0
87	OHX	5	4102	7/7	0.18	-0.67	152,152,152,152	0
87	OHX	2	2121	7/7	0.23	-0.67	201,201,201,201	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	4156	7/7	0.14	-0.69	145,145,145,145	0
87	OHX	2	2085	7/7	0.22	-0.69	180,180,180,180	0
87	OHX	6	2137	7/7	0.24	-0.69	158,158,158,158	0
87	OHX	2	2100	7/7	0.24	-0.69	188,188,188,188	0
87	OHX	s1	302	7/7	0.33	-0.69	194,194,194,194	0
87	OHX	5	4200	7/7	0.19	-0.70	174,174,174,174	0
87	OHX	2	2147	7/7	0.16	-0.70	240,240,240,240	0
86	MG	5	3766	1/1	0.16	-0.70	73,73,73,73	0
87	OHX	2	2154	7/7	0.24	-0.71	185,185,185,185	0
86	MG	1	3482	1/1	0.18	-0.71	82,82,82,82	0
87	OHX	2	2081	7/7	0.17	-0.72	194,194,194,194	0
87	OHX	6	2068	7/7	0.16	-0.72	113,113,113,113	0
87	OHX	1	4159	7/7	0.15	-0.72	194,194,194,194	0
86	MG	s2	301	1/1	0.16	-0.73	97,97,97,97	0
87	OHX	1	4035	7/7	0.20	-0.73	158,158,158,158	0
87	OHX	8	229	7/7	0.19	-0.73	168,168,168,168	0
87	OHX	6	2189	7/7	0.16	-0.74	147,147,147,147	0
87	OHX	6	2073	7/7	0.10	-0.74	114,114,114,114	0
87	OHX	1	4027	7/7	0.19	-0.74	135,135,135,135	0
87	OHX	2	2107	7/7	0.14	-0.74	144,144,144,144	0
87	OHX	5	4243	7/7	0.19	-0.75	187,187,187,187	0
86	MG	1	3724	1/1	0.12	-0.76	67,67,67,67	0
87	OHX	1	3982	7/7	0.10	-0.77	135,135,135,135	0
86	MG	5	3852	1/1	0.14	-0.77	108,108,108,108	0
86	MG	6	1987	1/1	0.15	-0.77	104,104,104,104	0
86	MG	2	2182	1/1	0.28	-0.77	103,103,103,103	0
86	MG	5	3419	1/1	0.20	-0.78	55,55,55,55	0
87	OHX	1	4210	7/7	0.13	-0.78	217,217,217,217	0
87	OHX	1	4023	7/7	0.14	-0.78	172,172,172,172	0
86	MG	6	1992	1/1	0.12	-0.79	98,98,98,98	0
87	OHX	1	3969	7/7	0.16	-0.80	162,162,162,162	0
87	OHX	6	2160	7/7	0.15	-0.80	146,146,146,146	0
86	MG	1	3467	1/1	0.14	-0.80	64,64,64,64	0
86	MG	6	1902	1/1	0.19	-0.81	75,75,75,75	0
87	OHX	2	2057	7/7	0.14	-0.81	180,180,180,180	0
87	OHX	1	4204	7/7	0.16	-0.81	182,182,182,182	0
87	OHX	5	4189	7/7	0.29	-0.81	218,218,218,218	0
86	MG	6	1935	1/1	0.14	-0.81	77,77,77,77	0
87	OHX	2	2126	7/7	0.23	-0.81	194,194,194,194	0
86	MG	M6	201	1/1	0.17	-0.82	55,55,55,55	0
86	MG	2	1936	1/1	0.27	-0.83	81,81,81,81	0
87	OHX	5	4124	7/7	0.13	-0.83	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	M0	304	7/7	0.18	-0.83	154,154,154,154	0
87	OHX	5	3949	7/7	0.17	-0.84	112,112,112,112	0
87	OHX	1	3927	7/7	0.09	-0.84	173,173,173,173	0
87	OHX	2	2037	7/7	0.12	-0.84	162,162,162,162	0
87	OHX	6	2130	7/7	0.14	-0.85	176,176,176,176	0
87	OHX	2	2074	7/7	0.19	-0.85	166,166,166,166	0
87	OHX	o7	502	7/7	0.14	-0.85	153,153,153,153	0
87	OHX	2	2156	7/7	0.17	-0.85	295,295,295,295	0
87	OHX	5	4069	7/7	0.17	-0.86	157,157,157,157	0
86	MG	5	3620	1/1	0.17	-0.86	73,73,73,73	0
87	OHX	5	4012	7/7	0.15	-0.86	177,177,177,177	0
89	ZN	O7	101	1/1	0.12	-0.86	68,68,68,68	0
87	OHX	2	2087	7/7	0.17	-0.87	182,182,182,182	0
87	OHX	2	2048	7/7	0.14	-0.87	146,146,146,146	0
87	OHX	5	3950	7/7	0.16	-0.87	126,126,126,126	0
87	OHX	1	3937	7/7	0.18	-0.87	118,118,118,118	0
86	MG	5	3638	1/1	0.17	-0.88	83,83,83,83	0
86	MG	2	1989	1/1	0.32	-0.88	83,83,83,83	0
87	OHX	2	2024	7/7	0.18	-0.90	120,120,120,120	0
86	MG	1	3703	1/1	0.20	-0.91	62,62,62,62	0
86	MG	6	1907	1/1	0.20	-0.92	82,82,82,82	0
87	OHX	6	2154	7/7	0.18	-0.92	139,139,139,139	0
86	MG	2	1940	1/1	0.12	-0.92	104,104,104,104	0
87	OHX	1	3963	7/7	0.09	-0.92	170,170,170,170	0
87	OHX	6	2101	7/7	0.11	-0.92	163,163,163,163	0
86	MG	2	1977	1/1	0.15	-0.93	122,122,122,122	0
86	MG	5	3681	1/1	0.20	-0.93	44,44,44,44	0
87	OHX	4	239	7/7	0.15	-0.93	165,165,165,165	0
86	MG	5	3609	1/1	0.21	-0.93	51,51,51,51	0
87	OHX	5	3990	7/7	0.14	-0.94	171,171,171,171	0
86	MG	d6	102	1/1	0.27	-0.94	70,70,70,70	0
86	MG	1	3401	1/1	0.14	-0.94	61,61,61,61	0
87	OHX	L3	405	7/7	0.19	-0.95	187,187,187,187	0
87	OHX	5	4041	7/7	0.14	-0.95	119,119,119,119	0
87	OHX	1	4106	7/7	0.13	-0.95	154,154,154,154	0
87	OHX	1	3882	7/7	0.20	-0.95	86,86,86,86	0
87	OHX	6	2200	7/7	0.14	-0.96	211,211,211,211	0
87	OHX	1	3892	7/7	0.14	-0.96	87,87,87,87	0
87	OHX	6	2126	7/7	0.10	-0.96	167,167,167,167	0
87	OHX	2	2067	7/7	0.14	-0.97	180,180,180,180	0
87	OHX	5	3921	7/7	0.20	-0.97	73,73,73,73	0
89	ZN	q3	501	1/1	0.15	-0.97	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	6	2172	7/7	0.12	-0.97	237,237,237,237	0
86	MG	5	3490	1/1	0.22	-0.98	70,70,70,70	0
87	OHX	5	3977	7/7	0.22	-0.98	101,101,101,101	0
86	MG	6	2212	1/1	0.17	-0.98	82,82,82,82	0
87	OHX	6	2050	7/7	0.17	-0.98	106,106,106,106	0
87	OHX	5	4140	7/7	0.13	-0.99	167,167,167,167	0
87	OHX	5	3984	7/7	0.14	-0.99	165,165,165,165	0
87	OHX	5	3976	7/7	0.13	-0.99	141,141,141,141	0
87	OHX	2	2129	7/7	0.10	-1.00	250,250,250,250	0
87	OHX	2	2163	7/7	0.17	-1.00	236,236,236,236	0
86	MG	1	3728	1/1	0.16	-1.00	56,56,56,56	0
87	OHX	5	4202	7/7	0.18	-1.00	187,187,187,187	0
87	OHX	2	2042	7/7	0.07	-1.00	134,134,134,134	0
89	ZN	d6	101	1/1	0.14	-1.00	88,88,88,88	0
87	OHX	5	4166	7/7	0.16	-1.01	192,192,192,192	0
87	OHX	8	232	7/7	0.15	-1.01	179,179,179,179	0
87	OHX	5	3965	7/7	0.11	-1.01	132,132,132,132	0
87	OHX	1	3971	7/7	0.17	-1.01	142,142,142,142	0
87	OHX	6	2088	7/7	0.10	-1.01	145,145,145,145	0
87	OHX	n9	103	7/7	0.16	-1.02	89,89,89,89	0
87	OHX	1	4147	7/7	0.11	-1.02	188,188,188,188	0
87	OHX	6	2110	7/7	0.12	-1.02	142,142,142,142	0
87	OHX	1	4187	7/7	0.12	-1.02	167,167,167,167	0
87	OHX	1	4090	7/7	0.14	-1.02	215,215,215,215	0
87	OHX	1	3913	7/7	0.18	-1.03	103,103,103,103	0
87	OHX	6	2062	7/7	0.14	-1.03	123,123,123,123	0
87	OHX	2	2130	7/7	0.16	-1.03	150,150,150,150	0
87	OHX	5	4036	7/7	0.09	-1.03	202,202,202,202	0
87	OHX	5	3906	7/7	0.17	-1.04	63,63,63,63	0
86	MG	5	3542	1/1	0.18	-1.04	52,52,52,52	0
87	OHX	6	2148	7/7	0.12	-1.04	158,158,158,158	0
87	OHX	6	2051	7/7	0.19	-1.04	82,82,82,82	0
86	MG	2	1907	1/1	0.25	-1.05	78,78,78,78	0
86	MG	5	3889	1/1	0.17	-1.05	161,161,161,161	0
87	OHX	6	2175	7/7	0.16	-1.05	204,204,204,204	0
87	OHX	5	3953	7/7	0.14	-1.05	109,109,109,109	0
87	OHX	5	4019	7/7	0.12	-1.05	142,142,142,142	0
87	OHX	1	4122	7/7	0.17	-1.06	186,186,186,186	0
87	OHX	5	4110	7/7	0.17	-1.06	147,147,147,147	0
87	OHX	5	4007	7/7	0.21	-1.06	148,148,148,148	0
86	MG	2	1948	1/1	0.21	-1.06	122,122,122,122	0
86	MG	2	2008	1/1	0.26	-1.06	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	1	4047	7/7	0.08	-1.06	175,175,175,175	0
87	OHX	8	220	7/7	0.07	-1.07	154,154,154,154	0
87	OHX	1	3917	7/7	0.16	-1.08	125,125,125,125	0
87	OHX	1	4107	7/7	0.16	-1.08	187,187,187,187	0
86	MG	5	3436	1/1	0.15	-1.09	77,77,77,77	0
87	OHX	2	2099	7/7	0.12	-1.09	152,152,152,152	0
86	MG	6	1947	1/1	0.19	-1.09	77,77,77,77	0
87	OHX	1	4148	7/7	0.14	-1.09	170,170,170,170	0
86	MG	5	3633	1/1	0.16	-1.09	79,79,79,79	0
86	MG	2	1968	1/1	0.22	-1.10	160,160,160,160	0
86	MG	6	2026	1/1	0.16	-1.10	87,87,87,87	0
87	OHX	6	2064	7/7	0.16	-1.10	105,105,105,105	0
86	MG	5	3533	1/1	0.15	-1.11	78,78,78,78	0
87	OHX	5	3974	7/7	0.15	-1.11	124,124,124,124	0
87	OHX	1	3898	7/7	0.15	-1.11	112,112,112,112	0
87	OHX	5	4000	7/7	0.14	-1.12	125,125,125,125	0
86	MG	1	3723	1/1	0.17	-1.12	80,80,80,80	0
87	OHX	5	4056	7/7	0.15	-1.12	140,140,140,140	0
87	OHX	1	4074	7/7	0.11	-1.12	142,142,142,142	0
87	OHX	5	4155	7/7	0.20	-1.12	161,161,161,161	0
86	MG	5	3686	1/1	0.15	-1.12	73,73,73,73	0
87	OHX	6	2091	7/7	0.19	-1.13	142,142,142,142	0
87	OHX	5	4083	7/7	0.22	-1.13	133,133,133,133	0
87	OHX	l3	408	7/7	0.17	-1.13	180,180,180,180	0
87	OHX	1	4100	7/7	0.16	-1.14	160,160,160,160	0
87	OHX	6	2134	7/7	0.16	-1.14	180,180,180,180	0
89	ZN	Q3	501	1/1	0.08	-1.14	96,96,96,96	0
87	OHX	5	4236	7/7	0.12	-1.15	157,157,157,157	0
86	MG	5	3483	1/1	0.11	-1.16	98,98,98,98	0
86	MG	1	3801	1/1	0.19	-1.16	84,84,84,84	0
87	OHX	o9	101	7/7	0.16	-1.16	155,155,155,155	0
87	OHX	6	2100	7/7	0.08	-1.17	159,159,159,159	0
87	OHX	5	4203	7/7	0.10	-1.17	205,205,205,205	0
86	MG	1	3698	1/1	0.15	-1.18	113,113,113,113	0
86	MG	L2	301	1/1	0.17	-1.18	50,50,50,50	0
87	OHX	1	4030	7/7	0.17	-1.18	147,147,147,147	0
86	MG	5	3630	1/1	0.13	-1.19	111,111,111,111	0
87	OHX	5	4071	7/7	0.10	-1.19	220,220,220,220	0
87	OHX	1	3995	7/7	0.20	-1.19	133,133,133,133	0
87	OHX	O1	202	7/7	0.08	-1.19	151,151,151,151	0
87	OHX	5	4074	7/7	0.12	-1.19	154,154,154,154	0
87	OHX	1	3972	7/7	0.12	-1.19	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	2	2043	7/7	0.14	-1.19	147,147,147,147	0
86	MG	2	1951	1/1	0.15	-1.20	121,121,121,121	0
87	OHX	1	4142	7/7	0.19	-1.20	137,137,137,137	0
87	OHX	3	218	7/7	0.07	-1.20	151,151,151,151	0
87	OHX	6	2150	7/7	0.12	-1.21	160,160,160,160	0
87	OHX	1	4017	7/7	0.16	-1.21	132,132,132,132	0
87	OHX	S8	302	7/7	0.29	-1.21	191,191,191,191	0
87	OHX	6	2188	7/7	0.18	-1.21	186,186,186,186	0
87	OHX	1	3996	7/7	0.06	-1.21	196,196,196,196	0
87	OHX	5	4175	7/7	0.23	-1.22	207,207,207,207	0
87	OHX	2	2033	7/7	0.14	-1.22	175,175,175,175	0
89	ZN	D7	101	1/1	0.15	-1.22	208,208,208,208	0
87	OHX	1	4108	7/7	0.16	-1.22	134,134,134,134	0
87	OHX	5	4137	7/7	0.14	-1.23	187,187,187,187	0
86	MG	1	3582	1/1	0.14	-1.24	74,74,74,74	0
87	OHX	6	2209	7/7	0.08	-1.25	235,235,235,235	0
86	MG	M7	201	1/1	0.24	-1.25	47,47,47,47	0
87	OHX	6	2103	7/7	0.11	-1.25	212,212,212,212	0
87	OHX	2	2177	7/7	0.14	-1.25	210,210,210,210	0
86	MG	3	209	1/1	0.10	-1.26	75,75,75,75	0
87	OHX	m1	202	7/7	0.10	-1.26	178,178,178,178	0
87	OHX	M9	203	7/7	0.12	-1.27	213,213,213,213	0
87	OHX	4	228	7/7	0.12	-1.27	139,139,139,139	0
86	MG	4	205	1/1	0.09	-1.28	108,108,108,108	0
87	OHX	1	4012	7/7	0.11	-1.28	181,181,181,181	0
87	OHX	1	4011	7/7	0.19	-1.28	173,173,173,173	0
86	MG	6	2015	1/1	0.14	-1.28	83,83,83,83	0
87	OHX	5	4242	7/7	0.16	-1.28	177,177,177,177	0
89	ZN	Q0	500	1/1	0.12	-1.28	68,68,68,68	0
86	MG	2	1964	1/1	0.19	-1.28	141,141,141,141	0
86	MG	1	3466	1/1	0.11	-1.29	70,70,70,70	0
86	MG	7	209	1/1	0.14	-1.30	42,42,42,42	0
87	OHX	5	3933	7/7	0.14	-1.30	111,111,111,111	0
87	OHX	1	4057	7/7	0.07	-1.30	210,210,210,210	0
87	OHX	1	4032	7/7	0.12	-1.30	127,127,127,127	0
87	OHX	5	3931	7/7	0.18	-1.30	108,108,108,108	0
87	OHX	1	3910	7/7	0.16	-1.30	101,101,101,101	0
87	OHX	6	2152	7/7	0.14	-1.31	141,141,141,141	0
87	OHX	2	2032	7/7	0.11	-1.31	157,157,157,157	0
86	MG	6	1940	1/1	0.16	-1.31	70,70,70,70	0
87	OHX	1	3945	7/7	0.11	-1.31	135,135,135,135	0
87	OHX	1	3902	7/7	0.16	-1.32	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4163	7/7	0.16	-1.32	154,154,154,154	0
87	OHX	C5	201	7/7	0.09	-1.33	201,201,201,201	0
87	OHX	1	4006	7/7	0.14	-1.33	129,129,129,129	0
87	OHX	8	221	7/7	0.15	-1.33	156,156,156,156	0
86	MG	N8	201	1/1	0.18	-1.33	57,57,57,57	0
86	MG	q0	202	1/1	0.15	-1.33	73,73,73,73	0
87	OHX	1	4141	7/7	0.16	-1.33	179,179,179,179	0
87	OHX	2	2110	7/7	0.06	-1.33	167,167,167,167	0
87	OHX	1	3953	7/7	0.15	-1.33	136,136,136,136	0
87	OHX	1	3920	7/7	0.13	-1.34	118,118,118,118	0
87	OHX	1	4082	7/7	0.11	-1.34	179,179,179,179	0
86	MG	3	213	1/1	0.15	-1.34	78,78,78,78	0
87	OHX	2	2025	7/7	0.16	-1.34	122,122,122,122	0
87	OHX	5	4238	7/7	0.10	-1.34	200,200,200,200	0
87	OHX	1	4029	7/7	0.07	-1.35	183,183,183,183	0
87	OHX	6	2136	7/7	0.12	-1.35	177,177,177,177	0
87	OHX	1	3880	7/7	0.16	-1.35	90,90,90,90	0
87	OHX	O7	103	7/7	0.09	-1.35	129,129,129,129	0
87	OHX	1	4070	7/7	0.15	-1.36	174,174,174,174	0
87	OHX	5	3956	7/7	0.12	-1.36	128,128,128,128	0
87	OHX	1	3895	7/7	0.18	-1.37	99,99,99,99	0
87	OHX	1	4024	7/7	0.20	-1.38	140,140,140,140	0
86	MG	6	1986	1/1	0.20	-1.38	91,91,91,91	0
87	OHX	6	2099	7/7	0.15	-1.38	168,168,168,168	0
86	MG	5	3813	1/1	0.16	-1.39	87,87,87,87	0
87	OHX	SR	401	7/7	0.10	-1.40	223,223,223,223	0
87	OHX	5	4006	7/7	0.10	-1.40	150,150,150,150	0
87	OHX	1	4192	7/7	0.14	-1.40	193,193,193,193	0
87	OHX	1	4008	7/7	0.16	-1.41	159,159,159,159	0
87	OHX	Q2	502	7/7	0.14	-1.41	114,114,114,114	0
87	OHX	6	2192	7/7	0.12	-1.41	220,220,220,220	0
87	OHX	1	4166	7/7	0.14	-1.41	151,151,151,151	0
87	OHX	1	4191	7/7	0.14	-1.42	177,177,177,177	0
87	OHX	1	4040	7/7	0.07	-1.42	165,165,165,165	0
87	OHX	5	3957	7/7	0.16	-1.43	116,116,116,116	0
89	ZN	D6	500	1/1	0.10	-1.43	120,120,120,120	0
87	OHX	m0	303	7/7	0.13	-1.43	153,153,153,153	0
87	OHX	6	2066	7/7	0.11	-1.43	117,117,117,117	0
87	OHX	2	2036	7/7	0.16	-1.44	110,110,110,110	0
87	OHX	1	4185	7/7	0.15	-1.44	188,188,188,188	0
87	OHX	6	2115	7/7	0.13	-1.44	151,151,151,151	0
87	OHX	5	3894	7/7	0.17	-1.44	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	6	2077	7/7	0.12	-1.45	150,150,150,150	0
87	OHX	O3	202	7/7	0.12	-1.45	145,145,145,145	0
87	OHX	5	3991	7/7	0.16	-1.45	134,134,134,134	0
87	OHX	1	4099	7/7	0.13	-1.46	189,189,189,189	0
87	OHX	5	4032	7/7	0.17	-1.46	153,153,153,153	0
87	OHX	4	224	7/7	0.18	-1.46	71,71,71,71	0
87	OHX	3	219	7/7	0.15	-1.46	155,155,155,155	0
87	OHX	6	2169	7/7	0.11	-1.46	243,243,243,243	0
86	MG	L3	401	1/1	0.20	-1.46	46,46,46,46	0
87	OHX	1	3919	7/7	0.07	-1.46	156,156,156,156	0
86	MG	2	1924	1/1	0.20	-1.47	108,108,108,108	0
87	OHX	6	2108	7/7	0.15	-1.47	134,134,134,134	0
87	OHX	1	3960	7/7	0.12	-1.48	135,135,135,135	0
87	OHX	6	2123	7/7	0.17	-1.48	173,173,173,173	0
86	MG	6	1979	1/1	0.17	-1.49	68,68,68,68	0
86	MG	6	1931	1/1	0.15	-1.49	65,65,65,65	0
87	OHX	5	3941	7/7	0.26	-1.49	89,89,89,89	0
87	OHX	6	2116	7/7	0.16	-1.50	179,179,179,179	0
87	OHX	5	3954	7/7	0.16	-1.50	97,97,97,97	0
87	OHX	1	4042	7/7	0.14	-1.50	143,143,143,143	0
87	OHX	5	4037	7/7	0.16	-1.50	182,182,182,182	0
87	OHX	1	3933	7/7	0.10	-1.50	137,137,137,137	0
87	OHX	6	2191	7/7	0.19	-1.50	152,152,152,152	0
87	OHX	8	231	7/7	0.12	-1.51	183,183,183,183	0
87	OHX	l3	407	7/7	0.12	-1.51	153,153,153,153	0
86	MG	5	3826	1/1	0.14	-1.51	94,94,94,94	0
87	OHX	4	234	7/7	0.07	-1.52	185,185,185,185	0
87	OHX	2	2132	7/7	0.08	-1.52	198,198,198,198	0
87	OHX	6	2071	7/7	0.11	-1.52	106,106,106,106	0
87	OHX	2	2092	7/7	0.14	-1.52	148,148,148,148	0
87	OHX	5	3993	7/7	0.10	-1.53	130,130,130,130	0
89	ZN	D9	101	1/1	0.07	-1.55	111,111,111,111	0
89	ZN	d9	101	1/1	0.07	-1.55	95,95,95,95	0
87	OHX	5	3918	7/7	0.14	-1.55	109,109,109,109	0
87	OHX	1	4093	7/7	0.18	-1.55	193,193,193,193	0
86	MG	3	214	1/1	0.14	-1.55	91,91,91,91	0
87	OHX	5	4078	7/7	0.11	-1.56	192,192,192,192	0
87	OHX	1	3997	7/7	0.08	-1.56	189,189,189,189	0
87	OHX	7	222	7/7	0.07	-1.56	122,122,122,122	0
87	OHX	6	2069	7/7	0.12	-1.56	128,128,128,128	0
87	OHX	6	2079	7/7	0.09	-1.56	124,124,124,124	0
87	OHX	2	2093	7/7	0.09	-1.56	194,194,194,194	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3870	7/7	0.14	-1.56	78,78,78,78	0
87	OHX	5	4038	7/7	0.19	-1.56	139,139,139,139	0
89	ZN	q0	201	1/1	0.14	-1.56	47,47,47,47	0
87	OHX	2	2158	7/7	0.12	-1.57	285,285,285,285	0
87	OHX	c5	201	7/7	0.08	-1.57	181,181,181,181	0
87	OHX	5	4150	7/7	0.12	-1.59	138,138,138,138	0
87	OHX	1	4031	7/7	0.12	-1.59	189,189,189,189	0
87	OHX	1	3883	7/7	0.18	-1.59	87,87,87,87	0
86	MG	2	1998	1/1	0.15	-1.59	125,125,125,125	0
87	OHX	2	2142	7/7	0.12	-1.60	166,166,166,166	0
87	OHX	5	4088	7/7	0.13	-1.60	149,149,149,149	0
87	OHX	5	4120	7/7	0.09	-1.60	170,170,170,170	0
86	MG	2	1954	1/1	0.22	-1.60	133,133,133,133	0
87	OHX	1	4146	7/7	0.17	-1.60	177,177,177,177	0
89	ZN	e1	501	1/1	0.06	-1.61	189,189,189,189	0
87	OHX	6	2127	7/7	0.13	-1.61	184,184,184,184	0
87	OHX	1	3988	7/7	0.12	-1.61	129,129,129,129	0
87	OHX	2	2055	7/7	0.14	-1.62	152,152,152,152	0
87	OHX	6	2060	7/7	0.13	-1.62	119,119,119,119	0
86	MG	1	3659	1/1	0.19	-1.63	100,100,100,100	0
87	OHX	2	2068	7/7	0.12	-1.63	201,201,201,201	0
87	OHX	1	4129	7/7	0.12	-1.64	173,173,173,173	0
86	MG	1	3424	1/1	0.16	-1.64	78,78,78,78	0
87	OHX	c3	201	7/7	0.11	-1.64	187,187,187,187	0
87	OHX	6	2107	7/7	0.21	-1.64	154,154,154,154	0
87	OHX	5	3897	7/7	0.17	-1.64	60,60,60,60	0
87	OHX	6	2061	7/7	0.10	-1.64	108,108,108,108	0
87	OHX	6	2197	7/7	0.16	-1.65	175,175,175,175	0
87	OHX	2	2058	7/7	0.13	-1.66	165,165,165,165	0
87	OHX	5	4096	7/7	0.10	-1.66	170,170,170,170	0
87	OHX	2	2044	7/7	0.12	-1.67	121,121,121,121	0
87	OHX	1	3943	7/7	0.14	-1.69	126,126,126,126	0
87	OHX	5	4055	7/7	0.10	-1.69	180,180,180,180	0
87	OHX	1	4149	7/7	0.13	-1.69	144,144,144,144	0
87	OHX	5	3952	7/7	0.10	-1.69	120,120,120,120	0
87	OHX	5	4165	7/7	0.20	-1.69	217,217,217,217	0
87	OHX	6	2206	7/7	0.17	-1.70	189,189,189,189	0
87	OHX	2	2170	7/7	0.11	-1.70	152,152,152,152	0
86	MG	1	3561	1/1	0.20	-1.70	72,72,72,72	0
87	OHX	5	4060	7/7	0.15	-1.70	145,145,145,145	0
87	OHX	5	3955	7/7	0.21	-1.70	88,88,88,88	0
87	OHX	5	3914	7/7	0.12	-1.70	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	4129	7/7	0.12	-1.71	192,192,192,192	0
87	OHX	1	4101	7/7	0.14	-1.71	165,165,165,165	0
87	OHX	2	2066	7/7	0.06	-1.71	180,180,180,180	0
87	OHX	2	2167	7/7	0.11	-1.71	203,203,203,203	0
87	OHX	5	3994	7/7	0.12	-1.72	122,122,122,122	0
87	OHX	15	305	7/7	0.13	-1.72	164,164,164,164	0
87	OHX	2	2083	7/7	0.17	-1.72	167,167,167,167	0
87	OHX	5	3998	7/7	0.10	-1.72	140,140,140,140	0
86	MG	1	3477	1/1	0.19	-1.73	64,64,64,64	0
86	MG	1	3602	1/1	0.10	-1.73	66,66,66,66	0
87	OHX	3	220	7/7	0.11	-1.73	160,160,160,160	0
87	OHX	5	4117	7/7	0.07	-1.73	170,170,170,170	0
87	OHX	6	2128	7/7	0.16	-1.73	178,178,178,178	0
87	OHX	5	3963	7/7	0.09	-1.74	148,148,148,148	0
87	OHX	1	4143	7/7	0.12	-1.74	180,180,180,180	0
87	OHX	6	2139	7/7	0.13	-1.75	171,171,171,171	0
86	MG	1	3558	1/1	0.17	-1.75	53,53,53,53	0
87	OHX	19	202	7/7	0.09	-1.75	140,140,140,140	0
87	OHX	5	4062	7/7	0.09	-1.76	150,150,150,150	0
87	OHX	6	2086	7/7	0.15	-1.76	146,146,146,146	0
89	ZN	o7	501	1/1	0.11	-1.76	72,72,72,72	0
87	OHX	1	4127	7/7	0.12	-1.76	193,193,193,193	0
87	OHX	2	2141	7/7	0.07	-1.76	201,201,201,201	0
87	OHX	2	2070	7/7	0.08	-1.77	170,170,170,170	0
86	MG	6	1910	1/1	0.10	-1.78	76,76,76,76	0
87	OHX	2	2069	7/7	0.17	-1.78	146,146,146,146	0
86	MG	1	3481	1/1	0.14	-1.78	56,56,56,56	0
87	OHX	5	3944	7/7	0.13	-1.79	108,108,108,108	0
87	OHX	6	2144	7/7	0.15	-1.79	165,165,165,165	0
87	OHX	1	4063	7/7	0.13	-1.79	126,126,126,126	0
86	MG	M0	301	1/1	0.15	-1.80	65,65,65,65	0
87	OHX	2	2133	7/7	0.12	-1.80	200,200,200,200	0
87	OHX	1	3993	7/7	0.12	-1.80	112,112,112,112	0
87	OHX	5	4112	7/7	0.20	-1.81	99,99,99,99	0
87	OHX	2	2138	7/7	0.09	-1.81	174,174,174,174	0
87	OHX	2	2078	7/7	0.13	-1.81	183,183,183,183	0
87	OHX	5	4058	7/7	0.09	-1.81	160,160,160,160	0
87	OHX	2	2112	7/7	0.13	-1.82	213,213,213,213	0
87	OHX	7	217	7/7	0.11	-1.83	113,113,113,113	0
87	OHX	1	3948	7/7	0.09	-1.83	149,149,149,149	0
87	OHX	5	4103	7/7	0.14	-1.83	146,146,146,146	0
87	OHX	1	4095	7/7	0.07	-1.84	184,184,184,184	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4059	7/7	0.10	-1.84	195,195,195,195	0
87	OHX	2	2049	7/7	0.08	-1.84	160,160,160,160	0
87	OHX	1	3925	7/7	0.15	-1.84	110,110,110,110	0
87	OHX	6	2143	7/7	0.13	-1.85	173,173,173,173	0
87	OHX	1	3950	7/7	0.09	-1.86	143,143,143,143	0
86	MG	2	1932	1/1	0.15	-1.86	89,89,89,89	0
87	OHX	5	4033	7/7	0.06	-1.86	182,182,182,182	0
87	OHX	5	4002	7/7	0.07	-1.86	150,150,150,150	0
87	OHX	C3	201	7/7	0.10	-1.86	208,208,208,208	0
87	OHX	5	4098	7/7	0.10	-1.86	169,169,169,169	0
86	MG	5	3844	1/1	0.19	-1.86	73,73,73,73	0
86	MG	2	1972	1/1	0.08	-1.87	117,117,117,117	0
87	OHX	m0	302	7/7	0.12	-1.87	139,139,139,139	0
89	ZN	E1	501	1/1	0.07	-1.88	155,155,155,155	0
87	OHX	1	4155	7/7	0.07	-1.88	149,149,149,149	0
87	OHX	6	2138	7/7	0.14	-1.90	194,194,194,194	0
87	OHX	1	4171	7/7	0.13	-1.90	144,144,144,144	0
86	MG	5	3479	1/1	0.17	-1.91	66,66,66,66	0
87	OHX	1	3890	7/7	0.13	-1.91	82,82,82,82	0
87	OHX	q2	502	7/7	0.09	-1.91	115,115,115,115	0
87	OHX	1	4167	7/7	0.14	-1.91	143,143,143,143	0
87	OHX	1	4077	7/7	0.17	-1.91	171,171,171,171	0
87	OHX	2	2088	7/7	0.12	-1.91	179,179,179,179	0
87	OHX	5	4026	7/7	0.09	-1.92	196,196,196,196	0
86	MG	2	1991	1/1	0.13	-1.92	136,136,136,136	0
87	OHX	2	2123	7/7	0.13	-1.94	182,182,182,182	0
87	OHX	1	3923	7/7	0.14	-1.95	144,144,144,144	0
87	OHX	1	3916	7/7	0.08	-1.95	141,141,141,141	0
87	OHX	6	2106	7/7	0.08	-1.95	147,147,147,147	0
87	OHX	2	2104	7/7	0.08	-1.96	257,257,257,257	0
87	OHX	6	2124	7/7	0.11	-1.96	166,166,166,166	0
86	MG	6	1994	1/1	0.09	-1.96	88,88,88,88	0
87	OHX	5	4142	7/7	0.14	-1.96	151,151,151,151	0
86	MG	1	3854	1/1	0.09	-1.96	63,63,63,63	0
87	OHX	2	2039	7/7	0.13	-1.96	126,126,126,126	0
87	OHX	1	3930	7/7	0.18	-1.98	131,131,131,131	0
87	OHX	5	3927	7/7	0.15	-1.98	95,95,95,95	0
87	OHX	5	3911	7/7	0.17	-1.98	93,93,93,93	0
87	OHX	6	2092	7/7	0.11	-1.99	154,154,154,154	0
87	OHX	5	3968	7/7	0.15	-1.99	120,120,120,120	0
87	OHX	1	4041	7/7	0.19	-2.00	162,162,162,162	0
87	OHX	1	4193	7/7	0.07	-2.00	206,206,206,206	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3745	1/1	0.12	-2.00	62,62,62,62	0
86	MG	5	3682	1/1	0.22	-2.00	54,54,54,54	0
86	MG	1	3495	1/1	0.15	-2.02	74,74,74,74	0
87	OHX	7	221	7/7	0.09	-2.03	124,124,124,124	0
87	OHX	6	2096	7/7	0.11	-2.03	149,149,149,149	0
87	OHX	5	4049	7/7	0.20	-2.03	136,136,136,136	0
87	OHX	5	4154	7/7	0.13	-2.04	134,134,134,134	0
86	MG	6	1924	1/1	0.10	-2.04	85,85,85,85	0
87	OHX	5	4146	7/7	0.18	-2.04	145,145,145,145	0
87	OHX	5	4013	7/7	0.10	-2.05	173,173,173,173	0
86	MG	6	1968	1/1	0.09	-2.05	113,113,113,113	0
86	MG	1	3406	1/1	0.27	-2.05	158,158,158,158	0
87	OHX	5	4160	7/7	0.13	-2.05	194,194,194,194	0
87	OHX	6	2074	7/7	0.13	-2.06	127,127,127,127	0
86	MG	1	3474	1/1	0.14	-2.08	114,114,114,114	0
87	OHX	5	4127	7/7	0.08	-2.08	225,225,225,225	0
87	OHX	5	3903	7/7	0.15	-2.09	70,70,70,70	0
86	MG	1	3664	1/1	0.17	-2.10	79,79,79,79	0
87	OHX	5	3983	7/7	0.09	-2.11	154,154,154,154	0
87	OHX	8	225	7/7	0.13	-2.11	150,150,150,150	0
87	OHX	6	2153	7/7	0.15	-2.11	175,175,175,175	0
86	MG	2	1952	1/1	0.07	-2.11	140,140,140,140	0
87	OHX	5	4171	7/7	0.10	-2.11	167,167,167,167	0
86	MG	6	1933	1/1	0.15	-2.13	63,63,63,63	0
87	OHX	1	4016	7/7	0.13	-2.14	190,190,190,190	0
89	ZN	q2	501	1/1	0.06	-2.14	97,97,97,97	0
87	OHX	L4	403	7/7	0.15	-2.15	166,166,166,166	0
87	OHX	5	4045	7/7	0.10	-2.15	174,174,174,174	0
86	MG	5	3466	1/1	0.10	-2.15	134,134,134,134	0
87	OHX	1	4045	7/7	0.17	-2.16	145,145,145,145	0
87	OHX	6	2122	7/7	0.11	-2.17	139,139,139,139	0
87	OHX	5	4159	7/7	0.11	-2.17	173,173,173,173	0
87	OHX	6	2054	7/7	0.15	-2.18	110,110,110,110	0
86	MG	2	1961	1/1	0.11	-2.19	85,85,85,85	0
86	MG	1	3643	1/1	0.10	-2.20	92,92,92,92	0
87	OHX	2	2045	7/7	0.13	-2.20	136,136,136,136	0
87	OHX	1	3926	7/7	0.17	-2.21	103,103,103,103	0
87	OHX	1	4115	7/7	0.13	-2.21	176,176,176,176	0
87	OHX	5	4205	7/7	0.17	-2.22	129,129,129,129	0
86	MG	1	3637	1/1	0.12	-2.22	91,91,91,91	0
87	OHX	2	2056	7/7	0.09	-2.25	178,178,178,178	0
87	OHX	1	3952	7/7	0.09	-2.26	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	6	2104	7/7	0.19	-2.27	251,251,251,251	0
87	OHX	1	3915	7/7	0.14	-2.27	120,120,120,120	0
87	OHX	s8	303	7/7	0.11	-2.28	199,199,199,199	0
87	OHX	1	4048	7/7	0.18	-2.29	146,146,146,146	0
87	OHX	2	2089	7/7	0.14	-2.29	146,146,146,146	0
87	OHX	2	2111	7/7	0.13	-2.29	150,150,150,150	0
87	OHX	1	4036	7/7	0.07	-2.30	177,177,177,177	0
87	OHX	1	3967	7/7	0.10	-2.30	156,156,156,156	0
87	OHX	4	229	7/7	0.09	-2.30	150,150,150,150	0
87	OHX	1	4034	7/7	0.08	-2.31	197,197,197,197	0
87	OHX	5	3964	7/7	0.11	-2.32	147,147,147,147	0
86	MG	5	3423	1/1	0.14	-2.33	96,96,96,96	0
87	OHX	L3	404	7/7	0.13	-2.33	158,158,158,158	0
87	OHX	o3	203	7/7	0.08	-2.33	129,129,129,129	0
87	OHX	2	2148	7/7	0.16	-2.33	147,147,147,147	0
87	OHX	5	4172	7/7	0.09	-2.34	174,174,174,174	0
86	MG	1	3825	1/1	0.10	-2.34	73,73,73,73	0
87	OHX	1	3873	7/7	0.12	-2.34	80,80,80,80	0
87	OHX	1	4180	7/7	0.13	-2.34	119,119,119,119	0
87	OHX	5	3916	7/7	0.16	-2.35	88,88,88,88	0
87	OHX	5	4081	7/7	0.10	-2.35	153,153,153,153	0
87	OHX	1	4152	7/7	0.16	-2.35	162,162,162,162	0
87	OHX	1	3875	7/7	0.17	-2.35	90,90,90,90	0
87	OHX	1	4087	7/7	0.08	-2.36	163,163,163,163	0
87	OHX	1	3968	7/7	0.10	-2.37	118,118,118,118	0
87	OHX	1	4120	7/7	0.13	-2.37	135,135,135,135	0
87	OHX	1	4051	7/7	0.10	-2.39	191,191,191,191	0
87	OHX	5	4125	7/7	0.05	-2.39	189,189,189,189	0
87	OHX	1	4114	7/7	0.10	-2.40	148,148,148,148	0
87	OHX	4	238	7/7	0.11	-2.40	174,174,174,174	0
87	OHX	1	3974	7/7	0.08	-2.41	162,162,162,162	0
87	OHX	5	4054	7/7	0.16	-2.41	116,116,116,116	0
87	OHX	2	2106	7/7	0.13	-2.41	180,180,180,180	0
87	OHX	m5	303	7/7	0.14	-2.41	168,168,168,168	0
87	OHX	6	2065	7/7	0.15	-2.42	168,168,168,168	0
86	MG	l5	303	1/1	0.11	-2.42	60,60,60,60	0
87	OHX	8	219	7/7	0.14	-2.42	109,109,109,109	0
86	MG	1	3660	1/1	0.17	-2.43	54,54,54,54	0
87	OHX	5	4143	7/7	0.09	-2.43	151,151,151,151	0
87	OHX	l4	402	7/7	0.12	-2.44	181,181,181,181	0
89	ZN	Q2	501	1/1	0.03	-2.45	109,109,109,109	0
87	OHX	6	2072	7/7	0.11	-2.45	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	3936	7/7	0.15	-2.46	104,104,104,104	0
87	OHX	1	3956	7/7	0.15	-2.46	150,150,150,150	0
87	OHX	1	4134	7/7	0.17	-2.46	130,130,130,130	0
87	OHX	1	3959	7/7	0.11	-2.48	100,100,100,100	0
87	OHX	3	215	7/7	0.12	-2.49	137,137,137,137	0
87	OHX	sR	401	7/7	0.13	-2.50	180,180,180,180	0
87	OHX	2	2073	7/7	0.12	-2.50	183,183,183,183	0
86	MG	6	1990	1/1	0.09	-2.50	77,77,77,77	0
87	OHX	5	4133	7/7	0.13	-2.50	167,167,167,167	0
87	OHX	5	4047	7/7	0.09	-2.51	112,112,112,112	0
87	OHX	1	4117	7/7	0.16	-2.52	141,141,141,141	0
87	OHX	2	2034	7/7	0.11	-2.52	139,139,139,139	0
87	OHX	6	2140	7/7	0.08	-2.52	170,170,170,170	0
87	OHX	8	228	7/7	0.09	-2.52	195,195,195,195	0
86	MG	3	203	1/1	0.15	-2.53	114,114,114,114	0
87	OHX	1	4124	7/7	0.14	-2.53	180,180,180,180	0
87	OHX	1	4073	7/7	0.09	-2.53	150,150,150,150	0
87	OHX	5	3975	7/7	0.15	-2.54	131,131,131,131	0
86	MG	3	211	1/1	0.10	-2.54	100,100,100,100	0
87	OHX	5	3971	7/7	0.17	-2.54	129,129,129,129	0
87	OHX	2	2082	7/7	0.07	-2.55	199,199,199,199	0
87	OHX	5	4119	7/7	0.11	-2.55	174,174,174,174	0
86	MG	5	3631	1/1	0.16	-2.56	74,74,74,74	0
87	OHX	2	2166	7/7	0.07	-2.56	198,198,198,198	0
87	OHX	5	4207	7/7	0.12	-2.56	185,185,185,185	0
87	OHX	5	3946	7/7	0.14	-2.56	123,123,123,123	0
87	OHX	4	235	7/7	0.05	-2.57	171,171,171,171	0
87	OHX	5	4093	7/7	0.11	-2.59	172,172,172,172	0
87	OHX	5	4050	7/7	0.07	-2.59	125,125,125,125	0
87	OHX	6	2146	7/7	0.09	-2.59	207,207,207,207	0
87	OHX	6	2151	7/7	0.12	-2.59	157,157,157,157	0
86	MG	5	3456	1/1	0.17	-2.60	97,97,97,97	0
87	OHX	1	3991	7/7	0.08	-2.60	183,183,183,183	0
87	OHX	5	3923	7/7	0.16	-2.61	122,122,122,122	0
87	OHX	1	4126	7/7	0.07	-2.62	152,152,152,152	0
87	OHX	2	2079	7/7	0.14	-2.62	152,152,152,152	0
87	OHX	1	3986	7/7	0.11	-2.62	143,143,143,143	0
87	OHX	5	4022	7/7	0.13	-2.63	134,134,134,134	0
87	OHX	5	4004	7/7	0.10	-2.63	110,110,110,110	0
87	OHX	2	2029	7/7	0.11	-2.65	137,137,137,137	0
87	OHX	5	4073	7/7	0.17	-2.65	194,194,194,194	0
87	OHX	2	2168	7/7	0.08	-2.65	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4001	7/7	0.12	-2.66	122,122,122,122	0
87	OHX	6	2159	7/7	0.13	-2.66	153,153,153,153	0
87	OHX	2	2145	7/7	0.10	-2.67	190,190,190,190	0
87	OHX	6	2117	7/7	0.17	-2.67	140,140,140,140	0
87	OHX	5	4048	7/7	0.13	-2.67	133,133,133,133	0
87	OHX	6	2182	7/7	0.15	-2.68	144,144,144,144	0
87	OHX	1	3928	7/7	0.09	-2.68	122,122,122,122	0
87	OHX	5	3945	7/7	0.14	-2.69	107,107,107,107	0
87	OHX	1	3947	7/7	0.17	-2.69	103,103,103,103	0
87	OHX	1	4132	7/7	0.15	-2.70	143,143,143,143	0
87	OHX	1	4003	7/7	0.09	-2.71	119,119,119,119	0
86	MG	s1	301	1/1	0.11	-2.71	104,104,104,104	0
87	OHX	6	2093	7/7	0.09	-2.72	153,153,153,153	0
87	OHX	5	4035	7/7	0.14	-2.72	160,160,160,160	0
87	OHX	1	3939	7/7	0.13	-2.73	122,122,122,122	0
87	OHX	1	3900	7/7	0.11	-2.74	114,114,114,114	0
87	OHX	5	4046	7/7	0.11	-2.75	127,127,127,127	0
87	OHX	1	3876	7/7	0.13	-2.75	107,107,107,107	0
87	OHX	1	3978	7/7	0.15	-2.75	120,120,120,120	0
86	MG	5	3887	1/1	0.15	-2.76	89,89,89,89	0
87	OHX	M5	303	7/7	0.16	-2.78	155,155,155,155	0
87	OHX	1	4039	7/7	0.13	-2.79	137,137,137,137	0
87	OHX	1	3984	7/7	0.13	-2.79	116,116,116,116	0
87	OHX	1	4076	7/7	0.19	-2.80	154,154,154,154	0
87	OHX	5	4152	7/7	0.11	-2.81	162,162,162,162	0
87	OHX	5	3961	7/7	0.09	-2.81	152,152,152,152	0
86	MG	1	3510	1/1	0.11	-2.83	75,75,75,75	0
87	OHX	5	4139	7/7	0.11	-2.83	131,131,131,131	0
87	OHX	O2	202	7/7	0.13	-2.83	119,119,119,119	0
87	OHX	1	3949	7/7	0.12	-2.83	139,139,139,139	0
87	OHX	5	3995	7/7	0.09	-2.84	149,149,149,149	0
87	OHX	1	3999	7/7	0.10	-2.85	130,130,130,130	0
87	OHX	4	240	7/7	0.17	-2.86	172,172,172,172	0
87	OHX	1	3903	7/7	0.12	-2.86	122,122,122,122	0
87	OHX	5	4080	7/7	0.12	-2.87	147,147,147,147	0
87	OHX	2	2077	7/7	0.11	-2.88	149,149,149,149	0
87	OHX	3	217	7/7	0.12	-2.88	132,132,132,132	0
87	OHX	m4	202	7/7	0.18	-2.88	241,241,241,241	0
87	OHX	2	2063	7/7	0.07	-2.91	187,187,187,187	0
87	OHX	6	2168	7/7	0.13	-2.91	171,171,171,171	0
87	OHX	1	4130	7/7	0.14	-2.93	150,150,150,150	0
87	OHX	6	2063	7/7	0.12	-2.94	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2031	7/7	0.08	-2.96	149,149,149,149	0
86	MG	6	1906	1/1	0.14	-2.98	64,64,64,64	0
87	OHX	5	4212	7/7	0.12	-2.98	176,176,176,176	0
87	OHX	5	4017	7/7	0.16	-2.99	167,167,167,167	0
87	OHX	2	2095	7/7	0.10	-2.99	189,189,189,189	0
87	OHX	5	4059	7/7	0.08	-2.99	189,189,189,189	0
87	OHX	1	4052	7/7	0.08	-3.00	174,174,174,174	0
87	OHX	1	3955	7/7	0.14	-3.01	127,127,127,127	0
87	OHX	1	3899	7/7	0.12	-3.03	129,129,129,129	0
87	OHX	2	2119	7/7	0.10	-3.03	193,193,193,193	0
87	OHX	6	2155	7/7	0.07	-3.04	176,176,176,176	0
87	OHX	5	3981	7/7	0.13	-3.05	103,103,103,103	0
87	OHX	5	4118	7/7	0.17	-3.07	152,152,152,152	0
87	OHX	2	2120	7/7	0.13	-3.07	184,184,184,184	0
87	OHX	15	304	7/7	0.07	-3.08	173,173,173,173	0
87	OHX	6	2082	7/7	0.16	-3.08	113,113,113,113	0
87	OHX	5	4237	7/7	0.08	-3.09	121,121,121,121	0
87	OHX	2	2114	7/7	0.13	-3.09	183,183,183,183	0
87	OHX	5	4148	7/7	0.18	-3.10	142,142,142,142	0
86	MG	6	2030	1/1	0.07	-3.11	95,95,95,95	0
87	OHX	2	2051	7/7	0.12	-3.12	169,169,169,169	0
87	OHX	1	4118	7/7	0.13	-3.12	172,172,172,172	0
87	OHX	1	4026	7/7	0.13	-3.14	157,157,157,157	0
87	OHX	1	4020	7/7	0.13	-3.16	140,140,140,140	0
86	MG	1	3741	1/1	0.12	-3.17	64,64,64,64	0
87	OHX	5	4136	7/7	0.12	-3.17	177,177,177,177	0
87	OHX	1	3954	7/7	0.13	-3.18	121,121,121,121	0
86	MG	5	3804	1/1	0.17	-3.19	88,88,88,88	0
87	OHX	5	4181	7/7	0.12	-3.19	160,160,160,160	0
87	OHX	2	2060	7/7	0.10	-3.22	142,142,142,142	0
87	OHX	1	4065	7/7	0.09	-3.22	137,137,137,137	0
87	OHX	1	4071	7/7	0.15	-3.23	124,124,124,124	0
87	OHX	1	4094	7/7	0.07	-3.23	176,176,176,176	0
87	OHX	2	2097	7/7	0.07	-3.24	225,225,225,225	0
87	OHX	q1	102	7/7	0.13	-3.25	114,114,114,114	0
87	OHX	5	4113	7/7	0.11	-3.26	150,150,150,150	0
87	OHX	6	2081	7/7	0.13	-3.27	130,130,130,130	0
87	OHX	5	4053	7/7	0.10	-3.28	180,180,180,180	0
87	OHX	6	2094	7/7	0.08	-3.29	138,138,138,138	0
86	MG	5	3422	1/1	0.10	-3.30	55,55,55,55	0
87	OHX	1	3987	7/7	0.07	-3.31	150,150,150,150	0
87	OHX	5	4040	7/7	0.14	-3.32	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4150	7/7	0.08	-3.32	154,154,154,154	0
87	OHX	1	4018	7/7	0.09	-3.32	155,155,155,155	0
87	OHX	5	4241	7/7	0.14	-3.33	171,171,171,171	0
87	OHX	1	3981	7/7	0.14	-3.33	106,106,106,106	0
87	OHX	1	4053	7/7	0.14	-3.33	134,134,134,134	0
87	OHX	4	226	7/7	0.16	-3.38	107,107,107,107	0
87	OHX	5	3958	7/7	0.14	-3.38	117,117,117,117	0
87	OHX	5	4028	7/7	0.08	-3.38	123,123,123,123	0
86	MG	1	3737	1/1	0.10	-3.39	81,81,81,81	0
87	OHX	1	3976	7/7	0.08	-3.39	133,133,133,133	0
87	OHX	1	4050	7/7	0.04	-3.41	171,171,171,171	0
87	OHX	1	3901	7/7	0.10	-3.41	117,117,117,117	0
87	OHX	2	2061	7/7	0.07	-3.41	160,160,160,160	0
87	OHX	1	4009	7/7	0.15	-3.42	142,142,142,142	0
87	OHX	1	4058	7/7	0.07	-3.44	152,152,152,152	0
87	OHX	5	3912	7/7	0.15	-3.45	89,89,89,89	0
87	OHX	7	223	7/7	0.09	-3.45	156,156,156,156	0
86	MG	1	3644	1/1	0.08	-3.45	81,81,81,81	0
87	OHX	2	2153	7/7	0.20	-3.45	207,207,207,207	0
87	OHX	5	4092	7/7	0.11	-3.47	155,155,155,155	0
87	OHX	1	4007	7/7	0.11	-3.48	148,148,148,148	0
87	OHX	5	3986	7/7	0.09	-3.49	136,136,136,136	0
87	OHX	1	4125	7/7	0.16	-3.49	190,190,190,190	0
87	OHX	2	2080	7/7	0.04	-3.49	219,219,219,219	0
87	OHX	5	4085	7/7	0.13	-3.50	123,123,123,123	0
87	OHX	1	4021	7/7	0.13	-3.50	173,173,173,173	0
87	OHX	5	4233	7/7	0.17	-3.51	169,169,169,169	0
87	OHX	6	2194	7/7	0.15	-3.53	167,167,167,167	0
87	OHX	2	2038	7/7	0.08	-3.53	142,142,142,142	0
86	MG	1	3472	1/1	0.16	-3.54	51,51,51,51	0
86	MG	1	3418	1/1	0.13	-3.54	68,68,68,68	0
87	OHX	5	4101	7/7	0.09	-3.55	133,133,133,133	0
87	OHX	1	4004	7/7	0.06	-3.55	137,137,137,137	0
87	OHX	L3	403	7/7	0.10	-3.56	143,143,143,143	0
87	OHX	5	3987	7/7	0.10	-3.56	134,134,134,134	0
87	OHX	5	3924	7/7	0.12	-3.57	113,113,113,113	0
87	OHX	6	2157	7/7	0.14	-3.57	200,200,200,200	0
87	OHX	n3	202	7/7	0.08	-3.58	132,132,132,132	0
87	OHX	1	4188	7/7	0.13	-3.59	148,148,148,148	0
87	OHX	5	3962	7/7	0.15	-3.60	123,123,123,123	0
87	OHX	5	4084	7/7	0.09	-3.60	116,116,116,116	0
87	OHX	1	3975	7/7	0.11	-3.61	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	5	4218	7/7	0.18	-3.61	139,139,139,139	0
87	OHX	5	3929	7/7	0.14	-3.62	112,112,112,112	0
87	OHX	8	224	7/7	0.08	-3.62	165,165,165,165	0
87	OHX	6	2156	7/7	0.13	-3.62	145,145,145,145	0
86	MG	1	3497	1/1	0.16	-3.62	67,67,67,67	0
87	OHX	6	2067	7/7	0.14	-3.63	151,151,151,151	0
87	OHX	6	2164	7/7	0.10	-3.63	134,134,134,134	0
87	OHX	2	2091	7/7	0.14	-3.65	174,174,174,174	0
87	OHX	5	4077	7/7	0.12	-3.66	151,151,151,151	0
87	OHX	5	4228	7/7	0.10	-3.70	144,144,144,144	0
87	OHX	6	2118	7/7	0.10	-3.71	163,163,163,163	0
87	OHX	1	3932	7/7	0.12	-3.73	104,104,104,104	0
87	OHX	5	4009	7/7	0.11	-3.73	115,115,115,115	0
87	OHX	5	4195	7/7	0.10	-3.74	166,166,166,166	0
87	OHX	5	4030	7/7	0.08	-3.77	156,156,156,156	0
87	OHX	5	3940	7/7	0.17	-3.78	101,101,101,101	0
87	OHX	5	4052	7/7	0.09	-3.78	162,162,162,162	0
87	OHX	5	4024	7/7	0.09	-3.79	118,118,118,118	0
87	OHX	6	2097	7/7	0.12	-3.80	135,135,135,135	0
87	OHX	6	2135	7/7	0.18	-3.80	130,130,130,130	0
87	OHX	5	4107	7/7	0.12	-3.82	140,140,140,140	0
86	MG	5	3596	1/1	0.13	-3.83	71,71,71,71	0
87	OHX	5	3997	7/7	0.12	-3.84	95,95,95,95	0
86	MG	5	3599	1/1	0.16	-3.84	51,51,51,51	0
87	OHX	6	2190	7/7	0.20	-3.84	197,197,197,197	0
87	OHX	6	2119	7/7	0.09	-3.86	155,155,155,155	0
87	OHX	5	4168	7/7	0.13	-3.87	120,120,120,120	0
87	OHX	1	4154	7/7	0.08	-3.89	132,132,132,132	0
87	OHX	5	4122	7/7	0.10	-3.89	134,134,134,134	0
87	OHX	6	2083	7/7	0.09	-3.91	121,121,121,121	0
87	OHX	5	4187	7/7	0.13	-3.92	147,147,147,147	0
87	OHX	5	4167	7/7	0.12	-3.93	119,119,119,119	0
87	OHX	1	4013	7/7	0.15	-3.93	166,166,166,166	0
87	OHX	5	3938	7/7	0.11	-3.99	125,125,125,125	0
87	OHX	2	2028	7/7	0.12	-4.02	133,133,133,133	0
87	OHX	1	4081	7/7	0.15	-4.03	203,203,203,203	0
87	OHX	1	3893	7/7	0.12	-4.06	98,98,98,98	0
87	OHX	1	3935	7/7	0.12	-4.09	110,110,110,110	0
86	MG	5	4251	1/1	0.14	-4.10	44,44,44,44	0
87	OHX	6	2102	7/7	0.07	-4.11	153,153,153,153	0
87	OHX	6	2090	7/7	0.10	-4.11	147,147,147,147	0
87	OHX	6	2167	7/7	0.14	-4.12	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	1	4083	7/7	0.08	-4.16	215,215,215,215	0
87	OHX	5	3937	7/7	0.08	-4.17	136,136,136,136	0
87	OHX	5	4005	7/7	0.08	-4.20	131,131,131,131	0
87	OHX	1	4096	7/7	0.13	-4.25	119,119,119,119	0
87	OHX	5	3985	7/7	0.10	-4.26	105,105,105,105	0
87	OHX	1	3958	7/7	0.11	-4.27	123,123,123,123	0
87	OHX	5	3948	7/7	0.12	-4.28	110,110,110,110	0
87	OHX	1	3965	7/7	0.12	-4.29	94,94,94,94	0
87	OHX	5	3959	7/7	0.16	-4.35	110,110,110,110	0
87	OHX	1	3909	7/7	0.13	-4.36	119,119,119,119	0
87	OHX	5	4193	7/7	0.14	-4.37	116,116,116,116	0
87	OHX	1	3961	7/7	0.10	-4.39	151,151,151,151	0
87	OHX	5	4209	7/7	0.05	-4.40	224,224,224,224	0
87	OHX	2	2046	7/7	0.10	-4.40	161,161,161,161	0
87	OHX	5	4082	7/7	0.10	-4.41	143,143,143,143	0
87	OHX	5	4097	7/7	0.11	-4.41	123,123,123,123	0
87	OHX	1	4067	7/7	0.09	-4.42	144,144,144,144	0
87	OHX	1	3992	7/7	0.10	-4.42	163,163,163,163	0
87	OHX	1	4089	7/7	0.10	-4.45	134,134,134,134	0
87	OHX	2	2065	7/7	0.07	-4.50	134,134,134,134	0
87	OHX	1	4043	7/7	0.08	-4.53	129,129,129,129	0
87	OHX	2	2064	7/7	0.11	-4.54	149,149,149,149	0
87	OHX	5	4057	7/7	0.13	-4.56	154,154,154,154	0
87	OHX	1	3896	7/7	0.15	-4.57	111,111,111,111	0
87	OHX	1	4049	7/7	0.12	-4.58	152,152,152,152	0
87	OHX	1	4121	7/7	0.08	-4.63	172,172,172,172	0
87	OHX	5	4031	7/7	0.11	-4.67	167,167,167,167	0
87	OHX	5	4061	7/7	0.04	-4.67	154,154,154,154	0
87	OHX	5	4075	7/7	0.08	-4.68	133,133,133,133	0
87	OHX	5	4235	7/7	0.09	-4.68	251,251,251,251	0
87	OHX	1	3922	7/7	0.12	-4.69	120,120,120,120	0
87	OHX	1	3964	7/7	0.11	-4.69	117,117,117,117	0
87	OHX	5	3925	7/7	0.18	-4.69	113,113,113,113	0
87	OHX	4	231	7/7	0.07	-4.70	135,135,135,135	0
87	OHX	8	222	7/7	0.07	-4.71	143,143,143,143	0
86	MG	1	3767	1/1	0.16	-4.71	110,110,110,110	0
87	OHX	6	2132	7/7	0.13	-4.72	145,145,145,145	0
87	OHX	1	3977	7/7	0.10	-4.73	107,107,107,107	0
87	OHX	2	2125	7/7	0.11	-4.76	167,167,167,167	0
86	MG	1	3426	1/1	0.12	-4.76	64,64,64,64	0
87	OHX	5	4090	7/7	0.09	-4.78	155,155,155,155	0
87	OHX	1	4097	7/7	0.09	-4.78	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	4015	7/7	0.10	-4.78	141,141,141,141	0
87	OHX	6	2114	7/7	0.08	-4.80	149,149,149,149	0
87	OHX	5	4072	7/7	0.14	-4.83	133,133,133,133	0
87	OHX	5	4105	7/7	0.10	-4.86	113,113,113,113	0
87	OHX	6	2166	7/7	0.11	-4.86	155,155,155,155	0
87	OHX	5	3967	7/7	0.11	-4.88	108,108,108,108	0
87	OHX	6	2149	7/7	0.17	-4.89	157,157,157,157	0
87	OHX	5	3920	7/7	0.09	-4.90	106,106,106,106	0
87	OHX	6	2098	7/7	0.06	-4.96	173,173,173,173	0
86	MG	1	3858	1/1	0.16	-4.98	70,70,70,70	0
87	OHX	5	4039	7/7	0.10	-4.98	126,126,126,126	0
87	OHX	5	3988	7/7	0.11	-5.04	141,141,141,141	0
87	OHX	2	2052	7/7	0.13	-5.05	178,178,178,178	0
87	OHX	6	2076	7/7	0.11	-5.06	118,118,118,118	0
87	OHX	5	4029	7/7	0.09	-5.15	141,141,141,141	0
87	OHX	5	4192	7/7	0.09	-5.15	150,150,150,150	0
87	OHX	5	4051	7/7	0.11	-5.17	140,140,140,140	0
87	OHX	5	4174	7/7	0.12	-5.19	162,162,162,162	0
87	OHX	5	4147	7/7	0.09	-5.20	161,161,161,161	0
87	OHX	5	4169	7/7	0.09	-5.21	155,155,155,155	0
87	OHX	6	2204	7/7	0.08	-5.22	168,168,168,168	0
87	OHX	5	4034	7/7	0.16	-5.22	129,129,129,129	0
87	OHX	5	3979	7/7	0.09	-5.25	124,124,124,124	0
87	OHX	6	2085	7/7	0.08	-5.26	146,146,146,146	0
87	OHX	5	4025	7/7	0.11	-5.28	142,142,142,142	0
87	OHX	5	3973	7/7	0.13	-5.31	97,97,97,97	0
87	OHX	5	4109	7/7	0.08	-5.44	139,139,139,139	0
87	OHX	1	3973	7/7	0.05	-5.44	136,136,136,136	0
87	OHX	2	2118	7/7	0.19	-5.44	191,191,191,191	0
87	OHX	5	4027	7/7	0.12	-5.56	136,136,136,136	0
87	OHX	5	4020	7/7	0.09	-5.59	129,129,129,129	0
87	OHX	5	4221	7/7	0.14	-5.60	166,166,166,166	0
87	OHX	2	2059	7/7	0.09	-5.62	153,153,153,153	0
87	OHX	1	4160	7/7	0.15	-5.63	170,170,170,170	0
87	OHX	2	2105	7/7	0.10	-5.71	151,151,151,151	0
87	OHX	1	4105	7/7	0.15	-5.71	174,174,174,174	0
87	OHX	5	4011	7/7	0.10	-5.72	140,140,140,140	0
87	OHX	1	3979	7/7	0.10	-5.74	140,140,140,140	0
87	OHX	1	4060	7/7	0.10	-5.80	170,170,170,170	0
87	OHX	1	3966	7/7	0.09	-5.81	128,128,128,128	0
87	OHX	1	3905	7/7	0.09	-5.81	106,106,106,106	0
87	OHX	6	2109	7/7	0.15	-5.88	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4010	7/7	0.07	-5.90	154,154,154,154	0
87	OHX	5	3999	7/7	0.15	-5.90	160,160,160,160	0
87	OHX	5	3966	7/7	0.10	-5.93	135,135,135,135	0
87	OHX	5	4126	7/7	0.07	-5.93	129,129,129,129	0
87	OHX	1	4086	7/7	0.10	-5.97	104,104,104,104	0
87	OHX	5	3980	7/7	0.14	-5.97	124,124,124,124	0
87	OHX	1	3998	7/7	0.10	-6.05	133,133,133,133	0
87	OHX	5	4010	7/7	0.09	-6.05	150,150,150,150	0
87	OHX	2	2171	7/7	0.13	-6.13	169,169,169,169	0
86	MG	1	3494	1/1	0.08	-6.16	74,74,74,74	0
87	OHX	1	3908	7/7	0.14	-6.19	111,111,111,111	0
87	OHX	6	2095	7/7	0.07	-6.24	141,141,141,141	0
86	MG	1	3804	1/1	0.13	-6.26	59,59,59,59	0
87	OHX	5	4018	7/7	0.12	-6.27	142,142,142,142	0
87	OHX	1	4064	7/7	0.09	-6.35	191,191,191,191	0
87	OHX	6	2084	7/7	0.13	-6.35	151,151,151,151	0
87	OHX	2	2155	7/7	0.09	-6.36	173,173,173,173	0
87	OHX	5	4070	7/7	0.15	-6.42	145,145,145,145	0
87	OHX	1	4198	7/7	0.09	-6.52	153,153,153,153	0
87	OHX	5	4162	7/7	0.13	-6.63	186,186,186,186	0
87	OHX	5	4023	7/7	0.11	-6.67	110,110,110,110	0
87	OHX	1	3957	7/7	0.11	-6.72	168,168,168,168	0
87	OHX	1	4055	7/7	0.12	-6.86	117,117,117,117	0
86	MG	1	3638	1/1	0.09	-6.95	85,85,85,85	0
87	OHX	1	3884	7/7	0.09	-6.97	92,92,92,92	0
87	OHX	2	2086	7/7	0.10	-7.03	141,141,141,141	0
87	OHX	1	3912	7/7	0.10	-7.09	141,141,141,141	0
87	OHX	5	4194	7/7	0.08	-7.42	135,135,135,135	0
87	OHX	2	2103	7/7	0.08	-7.44	172,172,172,172	0
87	OHX	5	4079	7/7	0.09	-7.50	137,137,137,137	0
87	OHX	1	3990	7/7	0.14	-7.50	137,137,137,137	0
87	OHX	1	4019	7/7	0.08	-7.50	134,134,134,134	0
87	OHX	5	4163	7/7	0.08	-7.63	177,177,177,177	0
87	OHX	1	4044	7/7	0.09	-7.77	134,134,134,134	0
87	OHX	5	3978	7/7	0.09	-7.94	112,112,112,112	0
87	OHX	1	3942	7/7	0.08	-7.99	136,136,136,136	0
87	OHX	1	4091	7/7	0.06	-8.09	168,168,168,168	0
87	OHX	2	2050	7/7	0.12	-8.37	170,170,170,170	0
87	OHX	5	4016	7/7	0.07	-8.52	112,112,112,112	0
87	OHX	1	4080	7/7	0.19	-8.56	183,183,183,183	0
87	OHX	1	3941	7/7	0.06	-8.62	145,145,145,145	0
87	OHX	7	219	7/7	0.11	-8.64	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	4211	7/7	0.10	-8.68	130,130,130,130	0
87	OHX	5	4021	7/7	0.08	-8.71	123,123,123,123	0
87	OHX	1	4174	7/7	0.14	-9.00	180,180,180,180	0
87	OHX	5	3992	7/7	0.10	-9.01	122,122,122,122	0
87	OHX	1	4190	7/7	0.12	-9.14	174,174,174,174	0
87	OHX	1	4072	7/7	0.09	-9.24	152,152,152,152	0
87	OHX	5	4215	7/7	0.16	-9.44	167,167,167,167	0
87	OHX	5	4044	7/7	0.09	-9.45	143,143,143,143	0
87	OHX	5	4158	7/7	0.08	-9.74	126,126,126,126	0
86	MG	1	3686	1/1	0.13	-9.86	118,118,118,118	0
87	OHX	5	4138	7/7	0.09	-9.88	168,168,168,168	0
87	OHX	1	3962	7/7	0.13	-9.96	138,138,138,138	0
87	OHX	5	3904	7/7	0.12	-10.08	74,74,74,74	0
87	OHX	1	4022	7/7	0.08	-10.13	173,173,173,173	0
86	MG	5	3763	1/1	0.10	-10.17	74,74,74,74	0
87	OHX	5	4104	7/7	0.14	-10.29	137,137,137,137	0
87	OHX	5	4208	7/7	0.14	-10.53	136,136,136,136	0
87	OHX	1	4033	7/7	0.13	-10.57	139,139,139,139	0
86	MG	5	3855	1/1	0.16	-10.60	83,83,83,83	0
86	MG	1	3623	1/1	0.08	-10.68	92,92,92,92	0
86	MG	N5	202	1/1	0.12	-10.68	83,83,83,83	0
87	OHX	1	4028	7/7	0.06	-10.85	153,153,153,153	0
87	OHX	5	4131	7/7	0.07	-11.02	173,173,173,173	0
87	OHX	5	4014	7/7	0.13	-12.20	126,126,126,126	0
87	OHX	6	2080	7/7	0.10	-12.49	157,157,157,157	0
87	OHX	6	2161	7/7	0.10	-15.29	212,212,212,212	0
86	MG	5	3839	1/1	0.15	-15.35	50,50,50,50	0
86	MG	5	3815	1/1	0.10	-16.35	87,87,87,87	0
87	OHX	5	4067	7/7	0.15	-17.28	161,161,161,161	0
87	OHX	5	3982	7/7	0.12	-20.25	114,114,114,114	0
87	OHX	2	2127	7/7	0.13	-23.70	174,174,174,174	0
87	OHX	5	4043	7/7	0.08	-31.82	139,139,139,139	0
87	OHX	1	4109	7/7	0.13	-32.20	216,216,216,216	0
86	MG	1	3695	1/1	0.58	-	66,66,66,66	0
86	MG	17	302	1/1	0.60	-	55,55,55,55	0
86	MG	1	3837	1/1	0.69	-	43,43,43,43	0
86	MG	5	3776	1/1	0.30	-	108,108,108,108	0
86	MG	5	3872	1/1	1.19	-	66,66,66,66	0
86	MG	4	223	1/1	0.46	-	113,113,113,113	0
86	MG	1	3792	1/1	0.61	-	77,77,77,77	0
86	MG	2	1950	1/1	0.53	-	137,137,137,137	0
86	MG	2	2003	1/1	0.56	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3799	1/1	0.15	-	107,107,107,107	0
86	MG	5	3478	1/1	0.88	-	77,77,77,77	0
86	MG	5	3716	1/1	0.29	-	53,53,53,53	0
86	MG	5	3613	1/1	0.63	-	36,36,36,36	0
86	MG	6	2018	1/1	0.33	-	166,166,166,166	0
86	MG	1	3788	1/1	0.14	-	92,92,92,92	0
86	MG	6	2002	1/1	0.13	-	133,133,133,133	0
86	MG	6	2042	1/1	0.33	-	90,90,90,90	0
86	MG	1	3464	1/1	1.44	-	94,94,94,94	0
86	MG	5	3861	1/1	0.32	-	47,47,47,47	0
86	MG	1	3610	1/1	0.24	-	81,81,81,81	0
86	MG	5	3719	1/1	0.35	-	70,70,70,70	0
86	MG	5	3769	1/1	0.34	-	103,103,103,103	0
86	MG	1	3683	1/1	0.43	-	53,53,53,53	0
86	MG	5	3796	1/1	1.37	-	63,63,63,63	0
86	MG	1	3836	1/1	0.98	-	53,53,53,53	0
86	MG	1	3616	1/1	0.59	-	49,49,49,49	0
86	MG	5	3888	1/1	0.14	-	75,75,75,75	0
86	MG	6	2048	1/1	1.11	-	123,123,123,123	0
86	MG	L4	401	1/1	1.10	-	67,67,67,67	0
86	MG	1	3840	1/1	0.46	-	63,63,63,63	0
86	MG	S2	301	1/1	0.56	-	89,89,89,89	0
86	MG	2	1963	1/1	0.90	-	110,110,110,110	0
86	MG	6	2047	1/1	0.89	-	77,77,77,77	0
86	MG	6	2019	1/1	1.47	-	79,79,79,79	0
86	MG	5	3652	1/1	1.21	-	73,73,73,73	0
86	MG	5	3884	1/1	0.97	-	30,30,30,30	0
86	MG	6	2004	1/1	0.17	-	122,122,122,122	0
86	MG	1	3405	1/1	0.20	-	73,73,73,73	0
86	MG	2	2013	1/1	0.92	-	93,93,93,93	0

6.5 Other polymers ⓘ

There are no such residues in this entry.