



wwPDB X-ray Structure Validation Summary Report i

Oct 9, 2014 – 10:00 PM BST

PDB ID : 4U55
Title : Crystal structure of Cryptopleurine bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.20 Å(reported)

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

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

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

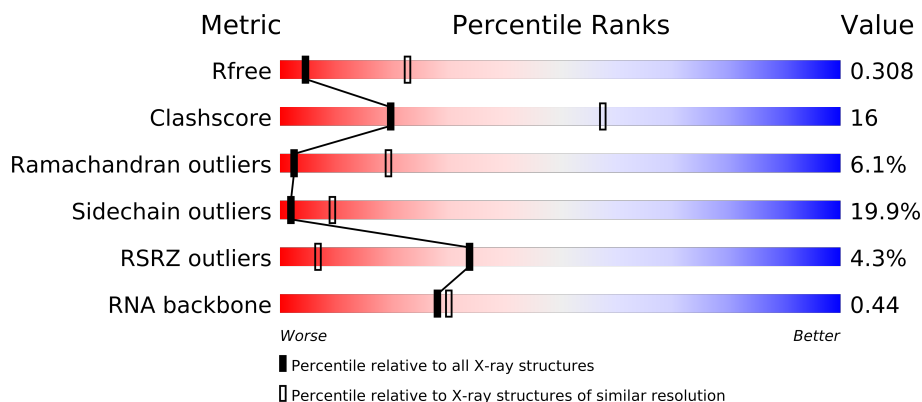
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.20 Å.

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



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

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

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

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

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

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

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Mol	Chain	Length	Quality of chain
70	o4	120	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	
81	p0	311	
82	m2	160	
83	p1	47	
84	p2	46	

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

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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3414	-	X
85	MG	1	3416	-	X
85	MG	1	3418	-	X
85	MG	1	3421	-	X
85	MG	1	3422	-	X
85	MG	1	3423	-	X
85	MG	1	3424	-	X
85	MG	1	3427	-	X
85	MG	1	3429	-	X
85	MG	1	3430	-	X
85	MG	1	3431	-	X
85	MG	1	3432	-	X
85	MG	1	3433	-	X
85	MG	1	3435	-	X
85	MG	1	3437	-	X
85	MG	1	3438	-	X
85	MG	1	3439	-	X
85	MG	1	3440	-	X
85	MG	1	3441	-	X
85	MG	1	3442	-	X
85	MG	1	3443	-	X
85	MG	1	3444	-	X
85	MG	1	3447	-	X
85	MG	1	3448	-	X
85	MG	1	3450	-	X
85	MG	1	3451	-	X
85	MG	1	3452	-	X
85	MG	1	3453	-	X
85	MG	1	3455	-	X
85	MG	1	3456	-	X
85	MG	1	3457	-	X
85	MG	1	3458	-	X
85	MG	1	3459	-	X
85	MG	1	3460	-	X
85	MG	1	3461	-	X
85	MG	1	3462	-	X
85	MG	1	3463	-	X
85	MG	1	3464	-	X
85	MG	1	3465	-	X
85	MG	1	3468	-	X
85	MG	1	3469	-	X
85	MG	1	3470	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3471	-	X
85	MG	1	3472	-	X
85	MG	1	3473	-	X
85	MG	1	3474	-	X
85	MG	1	3475	-	X
85	MG	1	3476	-	X
85	MG	1	3477	-	X
85	MG	1	3479	-	X
85	MG	1	3480	-	X
85	MG	1	3482	-	X
85	MG	1	3483	-	X
85	MG	1	3484	-	X
85	MG	1	3485	-	X
85	MG	1	3486	-	X
85	MG	1	3490	-	X
85	MG	1	3491	-	X
85	MG	1	3492	-	X
85	MG	1	3494	-	X
85	MG	1	3495	-	X
85	MG	1	3496	-	X
85	MG	1	3497	-	X
85	MG	1	3498	-	X
85	MG	1	3499	-	X
85	MG	1	3500	-	X
85	MG	1	3501	-	X
85	MG	1	3502	-	X
85	MG	1	3503	-	X
85	MG	1	3505	-	X
85	MG	1	3506	-	X
85	MG	1	3507	-	X
85	MG	1	3508	-	X
85	MG	1	3509	-	X
85	MG	1	3510	-	X
85	MG	1	3511	-	X
85	MG	1	3512	-	X
85	MG	1	3513	-	X
85	MG	1	3514	-	X
85	MG	1	3515	-	X
85	MG	1	3516	-	X
85	MG	1	3517	-	X
85	MG	1	3518	-	X
85	MG	1	3520	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3521	-	X
85	MG	1	3522	-	X
85	MG	1	3523	-	X
85	MG	1	3524	-	X
85	MG	1	3525	-	X
85	MG	1	3526	-	X
85	MG	1	3527	-	X
85	MG	1	3528	-	X
85	MG	1	3529	-	X
85	MG	1	3531	-	X
85	MG	1	3532	-	X
85	MG	1	3533	-	X
85	MG	1	3534	-	X
85	MG	1	3535	-	X
85	MG	1	3536	-	X
85	MG	1	3537	-	X
85	MG	1	3538	-	X
85	MG	1	3539	-	X
85	MG	1	3540	-	X
85	MG	1	3541	-	X
85	MG	1	3542	-	X
85	MG	1	3543	-	X
85	MG	1	3544	-	X
85	MG	1	3545	-	X
85	MG	1	3546	-	X
85	MG	1	3547	-	X
85	MG	1	3548	-	X
85	MG	1	3549	-	X
85	MG	1	3550	-	X
85	MG	1	3551	-	X
85	MG	1	3552	-	X
85	MG	1	3553	-	X
85	MG	1	3554	-	X
85	MG	1	3555	-	X
85	MG	1	3556	-	X
85	MG	1	3557	-	X
85	MG	1	3558	-	X
85	MG	1	3559	-	X
85	MG	1	3560	-	X
85	MG	1	3561	-	X
85	MG	1	3562	-	X
85	MG	1	3563	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3564	-	X
85	MG	1	3565	-	X
85	MG	1	3566	-	X
85	MG	1	3568	-	X
85	MG	1	3569	-	X
85	MG	1	3570	-	X
85	MG	1	3571	-	X
85	MG	1	3572	-	X
85	MG	1	3573	-	X
85	MG	1	3574	-	X
85	MG	1	3575	-	X
85	MG	1	3576	-	X
85	MG	1	3577	-	X
85	MG	1	3578	-	X
85	MG	1	3579	-	X
85	MG	1	3582	-	X
85	MG	1	3583	-	X
85	MG	1	3585	-	X
85	MG	1	3586	-	X
85	MG	1	3587	-	X
85	MG	1	3588	-	X
85	MG	1	3589	-	X
85	MG	1	3590	-	X
85	MG	1	3591	-	X
85	MG	1	3592	-	X
85	MG	1	3593	-	X
85	MG	1	3594	-	X
85	MG	1	3595	-	X
85	MG	1	3596	-	X
85	MG	1	3597	-	X
85	MG	1	3598	-	X
85	MG	1	3600	-	X
85	MG	1	3606	-	X
85	MG	1	3607	-	X
85	MG	1	3610	-	X
85	MG	1	3611	-	X
85	MG	1	3613	-	X
85	MG	1	3614	-	X
85	MG	1	3615	-	X
85	MG	1	3617	-	X
85	MG	1	3618	-	X
85	MG	1	3620	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3622	-	X
85	MG	1	3623	-	X
85	MG	1	3624	-	X
85	MG	1	3625	-	X
85	MG	1	3626	-	X
85	MG	1	3627	-	X
85	MG	1	3630	-	X
85	MG	1	3632	-	X
85	MG	1	3633	-	X
85	MG	1	3638	-	X
85	MG	1	3640	-	X
85	MG	1	3641	-	X
85	MG	1	3642	-	X
85	MG	1	3644	-	X
85	MG	1	3645	-	X
85	MG	1	3646	-	X
85	MG	1	3647	-	X
85	MG	1	3648	-	X
85	MG	1	3649	-	X
85	MG	1	3650	-	X
85	MG	1	3652	-	X
85	MG	1	3654	-	X
85	MG	1	3655	-	X
85	MG	1	3656	-	X
85	MG	1	3657	-	X
85	MG	1	3660	-	X
85	MG	1	3663	-	X
85	MG	1	3665	-	X
85	MG	1	3666	-	X
85	MG	1	3667	-	X
85	MG	1	3668	-	X
85	MG	1	3669	-	X
85	MG	1	3670	-	X
85	MG	1	3671	-	X
85	MG	1	3673	-	X
85	MG	1	3674	-	X
85	MG	1	3675	-	X
85	MG	1	3676	-	X
85	MG	1	3677	-	X
85	MG	1	3678	-	X
85	MG	1	3679	-	X
85	MG	1	3680	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3681	-	X
85	MG	1	3683	-	X
85	MG	1	3684	-	X
85	MG	1	3685	-	X
85	MG	1	3687	-	X
85	MG	1	3688	-	X
85	MG	1	3689	-	X
85	MG	1	3690	-	X
85	MG	1	3692	-	X
85	MG	1	3693	-	X
85	MG	1	3694	-	X
85	MG	1	3695	-	X
85	MG	1	3698	-	X
85	MG	1	3699	-	X
85	MG	1	3700	-	X
85	MG	1	3701	-	X
85	MG	1	3702	-	X
85	MG	1	3707	-	X
85	MG	1	3708	-	X
85	MG	1	3709	-	X
85	MG	1	3710	-	X
85	MG	1	3711	-	X
85	MG	1	3712	-	X
85	MG	1	3713	-	X
85	MG	1	3714	-	X
85	MG	1	3715	-	X
85	MG	1	3717	-	X
85	MG	1	3718	-	X
85	MG	1	3719	-	X
85	MG	1	3720	-	X
85	MG	1	3721	-	X
85	MG	1	3724	-	X
85	MG	1	3727	-	X
85	MG	1	3729	-	X
85	MG	1	3731	-	X
85	MG	1	3733	-	X
85	MG	1	3734	-	X
85	MG	1	3735	-	X
85	MG	1	3736	-	X
85	MG	1	3739	-	X
85	MG	1	3740	-	X
85	MG	1	3741	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3743	-	X
85	MG	1	3744	-	X
85	MG	1	3745	-	X
85	MG	1	3747	-	X
85	MG	1	3750	-	X
85	MG	1	3752	-	X
85	MG	1	3755	-	X
85	MG	1	3756	-	X
85	MG	1	3757	-	X
85	MG	1	3759	-	X
85	MG	1	3760	-	X
85	MG	1	3761	-	X
85	MG	1	3762	-	X
85	MG	1	3763	-	X
85	MG	1	3765	-	X
85	MG	1	3768	-	X
85	MG	1	3769	-	X
85	MG	1	3770	-	X
85	MG	1	3771	-	X
85	MG	1	3772	-	X
85	MG	1	3773	-	X
85	MG	1	3775	-	X
85	MG	1	3776	-	X
85	MG	1	3777	-	X
85	MG	1	3778	-	X
85	MG	1	3779	-	X
85	MG	1	3780	-	X
85	MG	1	3781	-	X
85	MG	1	3782	-	X
85	MG	1	3783	-	X
85	MG	1	3784	-	X
85	MG	1	3785	-	X
85	MG	1	3790	-	X
85	MG	1	3791	-	X
85	MG	1	3792	-	X
85	MG	1	3793	-	X
85	MG	1	3794	-	X
85	MG	1	3795	-	X
85	MG	1	3799	-	X
85	MG	1	3801	-	X
85	MG	1	3802	-	X
85	MG	1	3805	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3808	-	X
85	MG	1	3809	-	X
85	MG	1	3810	-	X
85	MG	1	3811	-	X
85	MG	1	3812	-	X
85	MG	1	3813	-	X
85	MG	1	3814	-	X
85	MG	1	3815	-	X
85	MG	1	3816	-	X
85	MG	1	3820	-	X
85	MG	1	3821	-	X
85	MG	1	3822	-	X
85	MG	1	3824	-	X
85	MG	1	3827	-	X
85	MG	1	3828	-	X
85	MG	1	3829	-	X
85	MG	1	3830	-	X
85	MG	1	3831	-	X
85	MG	1	3833	-	X
85	MG	1	3834	-	X
85	MG	1	3835	-	X
85	MG	1	3836	-	X
85	MG	1	3837	-	X
85	MG	1	3838	-	X
85	MG	1	3839	-	X
85	MG	1	3841	-	X
85	MG	1	3842	-	X
85	MG	1	3843	-	X
85	MG	1	3844	-	X
85	MG	1	3846	-	X
85	MG	1	3847	-	X
85	MG	1	3848	-	X
85	MG	1	3850	-	X
85	MG	1	3852	-	X
85	MG	1	3853	-	X
85	MG	1	3854	-	X
85	MG	1	3855	-	X
85	MG	1	3856	-	X
85	MG	1	3857	-	X
85	MG	1	3858	-	X
85	MG	1	3860	-	X
85	MG	1	4215	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	4216	-	X
85	MG	1	4217	-	X
85	MG	1	4218	-	X
85	MG	1	4219	-	X
85	MG	1	4220	-	X
85	MG	2	1902	-	X
85	MG	2	1903	-	X
85	MG	2	1905	-	X
85	MG	2	1906	-	X
85	MG	2	1907	-	X
85	MG	2	1908	-	X
85	MG	2	1909	-	X
85	MG	2	1910	-	X
85	MG	2	1911	-	X
85	MG	2	1913	-	X
85	MG	2	1914	-	X
85	MG	2	1915	-	X
85	MG	2	1916	-	X
85	MG	2	1917	-	X
85	MG	2	1918	-	X
85	MG	2	1919	-	X
85	MG	2	1920	-	X
85	MG	2	1921	-	X
85	MG	2	1923	-	X
85	MG	2	1924	-	X
85	MG	2	1925	-	X
85	MG	2	1926	-	X
85	MG	2	1927	-	X
85	MG	2	1928	-	X
85	MG	2	1930	-	X
85	MG	2	1931	-	X
85	MG	2	1932	-	X
85	MG	2	1934	-	X
85	MG	2	1935	-	X
85	MG	2	1936	-	X
85	MG	2	1937	-	X
85	MG	2	1938	-	X
85	MG	2	1939	-	X
85	MG	2	1940	-	X
85	MG	2	1942	-	X
85	MG	2	1943	-	X
85	MG	2	1944	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1945	-	X
85	MG	2	1946	-	X
85	MG	2	1947	-	X
85	MG	2	1949	-	X
85	MG	2	1950	-	X
85	MG	2	1952	-	X
85	MG	2	1954	-	X
85	MG	2	1955	-	X
85	MG	2	1956	-	X
85	MG	2	1957	-	X
85	MG	2	1958	-	X
85	MG	2	1959	-	X
85	MG	2	1960	-	X
85	MG	2	1961	-	X
85	MG	2	1962	-	X
85	MG	2	1963	-	X
85	MG	2	1965	-	X
85	MG	2	1966	-	X
85	MG	2	1968	-	X
85	MG	2	1970	-	X
85	MG	2	1971	-	X
85	MG	2	1972	-	X
85	MG	2	1973	-	X
85	MG	2	1974	-	X
85	MG	2	1975	-	X
85	MG	2	1976	-	X
85	MG	2	1979	-	X
85	MG	2	1981	-	X
85	MG	2	1982	-	X
85	MG	2	1983	-	X
85	MG	2	1984	-	X
85	MG	2	1985	-	X
85	MG	2	1988	-	X
85	MG	2	1989	-	X
85	MG	2	1990	-	X
85	MG	2	1991	-	X
85	MG	2	1992	-	X
85	MG	2	1993	-	X
85	MG	2	1994	-	X
85	MG	2	1995	-	X
85	MG	2	1996	-	X
85	MG	2	2000	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	2001	-	X
85	MG	2	2002	-	X
85	MG	2	2003	-	X
85	MG	2	2005	-	X
85	MG	2	2006	-	X
85	MG	2	2007	-	X
85	MG	2	2008	-	X
85	MG	2	2009	-	X
85	MG	2	2010	-	X
85	MG	2	2011	-	X
85	MG	2	2012	-	X
85	MG	2	2014	-	X
85	MG	2	2015	-	X
85	MG	2	2016	-	X
85	MG	2	2018	-	X
85	MG	2	2019	-	X
85	MG	2	2020	-	X
85	MG	2	2021	-	X
85	MG	2	2022	-	X
85	MG	3	201	-	X
85	MG	3	202	-	X
85	MG	3	203	-	X
85	MG	3	204	-	X
85	MG	3	205	-	X
85	MG	3	206	-	X
85	MG	3	207	-	X
85	MG	3	208	-	X
85	MG	3	209	-	X
85	MG	3	212	-	X
85	MG	3	213	-	X
85	MG	3	214	-	X
85	MG	4	201	-	X
85	MG	4	202	-	X
85	MG	4	203	-	X
85	MG	4	204	-	X
85	MG	4	205	-	X
85	MG	4	206	-	X
85	MG	4	207	-	X
85	MG	4	208	-	X
85	MG	4	210	-	X
85	MG	4	211	-	X
85	MG	4	212	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	4	213	-	X
85	MG	4	214	-	X
85	MG	4	215	-	X
85	MG	4	216	-	X
85	MG	4	217	-	X
85	MG	4	218	-	X
85	MG	4	219	-	X
85	MG	4	220	-	X
85	MG	5	3401	-	X
85	MG	5	3403	-	X
85	MG	5	3405	-	X
85	MG	5	3408	-	X
85	MG	5	3409	-	X
85	MG	5	3410	-	X
85	MG	5	3411	-	X
85	MG	5	3412	-	X
85	MG	5	3414	-	X
85	MG	5	3416	-	X
85	MG	5	3418	-	X
85	MG	5	3419	-	X
85	MG	5	3420	-	X
85	MG	5	3422	-	X
85	MG	5	3425	-	X
85	MG	5	3426	-	X
85	MG	5	3427	-	X
85	MG	5	3429	-	X
85	MG	5	3431	-	X
85	MG	5	3432	-	X
85	MG	5	3433	-	X
85	MG	5	3434	-	X
85	MG	5	3435	-	X
85	MG	5	3436	-	X
85	MG	5	3437	-	X
85	MG	5	3438	-	X
85	MG	5	3439	-	X
85	MG	5	3440	-	X
85	MG	5	3441	-	X
85	MG	5	3443	-	X
85	MG	5	3444	-	X
85	MG	5	3445	-	X
85	MG	5	3446	-	X
85	MG	5	3447	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3448	-	X
85	MG	5	3449	-	X
85	MG	5	3450	-	X
85	MG	5	3451	-	X
85	MG	5	3452	-	X
85	MG	5	3453	-	X
85	MG	5	3454	-	X
85	MG	5	3457	-	X
85	MG	5	3458	-	X
85	MG	5	3459	-	X
85	MG	5	3460	-	X
85	MG	5	3461	-	X
85	MG	5	3462	-	X
85	MG	5	3463	-	X
85	MG	5	3464	-	X
85	MG	5	3465	-	X
85	MG	5	3466	-	X
85	MG	5	3468	-	X
85	MG	5	3471	-	X
85	MG	5	3472	-	X
85	MG	5	3473	-	X
85	MG	5	3474	-	X
85	MG	5	3475	-	X
85	MG	5	3476	-	X
85	MG	5	3479	-	X
85	MG	5	3480	-	X
85	MG	5	3481	-	X
85	MG	5	3482	-	X
85	MG	5	3483	-	X
85	MG	5	3484	-	X
85	MG	5	3485	-	X
85	MG	5	3488	-	X
85	MG	5	3489	-	X
85	MG	5	3490	-	X
85	MG	5	3491	-	X
85	MG	5	3492	-	X
85	MG	5	3493	-	X
85	MG	5	3494	-	X
85	MG	5	3496	-	X
85	MG	5	3497	-	X
85	MG	5	3498	-	X
85	MG	5	3499	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3500	-	X
85	MG	5	3501	-	X
85	MG	5	3502	-	X
85	MG	5	3503	-	X
85	MG	5	3504	-	X
85	MG	5	3505	-	X
85	MG	5	3506	-	X
85	MG	5	3507	-	X
85	MG	5	3508	-	X
85	MG	5	3509	-	X
85	MG	5	3511	-	X
85	MG	5	3512	-	X
85	MG	5	3513	-	X
85	MG	5	3514	-	X
85	MG	5	3515	-	X
85	MG	5	3517	-	X
85	MG	5	3518	-	X
85	MG	5	3519	-	X
85	MG	5	3520	-	X
85	MG	5	3521	-	X
85	MG	5	3522	-	X
85	MG	5	3523	-	X
85	MG	5	3524	-	X
85	MG	5	3525	-	X
85	MG	5	3526	-	X
85	MG	5	3527	-	X
85	MG	5	3528	-	X
85	MG	5	3529	-	X
85	MG	5	3530	-	X
85	MG	5	3531	-	X
85	MG	5	3532	-	X
85	MG	5	3533	-	X
85	MG	5	3535	-	X
85	MG	5	3536	-	X
85	MG	5	3537	-	X
85	MG	5	3538	-	X
85	MG	5	3539	-	X
85	MG	5	3540	-	X
85	MG	5	3541	-	X
85	MG	5	3542	-	X
85	MG	5	3543	-	X
85	MG	5	3545	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3546	-	X
85	MG	5	3547	-	X
85	MG	5	3548	-	X
85	MG	5	3549	-	X
85	MG	5	3550	-	X
85	MG	5	3551	-	X
85	MG	5	3552	-	X
85	MG	5	3553	-	X
85	MG	5	3554	-	X
85	MG	5	3555	-	X
85	MG	5	3556	-	X
85	MG	5	3557	-	X
85	MG	5	3558	-	X
85	MG	5	3559	-	X
85	MG	5	3560	-	X
85	MG	5	3561	-	X
85	MG	5	3562	-	X
85	MG	5	3563	-	X
85	MG	5	3564	-	X
85	MG	5	3565	-	X
85	MG	5	3566	-	X
85	MG	5	3567	-	X
85	MG	5	3568	-	X
85	MG	5	3569	-	X
85	MG	5	3570	-	X
85	MG	5	3571	-	X
85	MG	5	3572	-	X
85	MG	5	3573	-	X
85	MG	5	3574	-	X
85	MG	5	3575	-	X
85	MG	5	3576	-	X
85	MG	5	3577	-	X
85	MG	5	3578	-	X
85	MG	5	3579	-	X
85	MG	5	3580	-	X
85	MG	5	3581	-	X
85	MG	5	3583	-	X
85	MG	5	3584	-	X
85	MG	5	3585	-	X
85	MG	5	3586	-	X
85	MG	5	3587	-	X
85	MG	5	3588	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3589	-	X
85	MG	5	3590	-	X
85	MG	5	3591	-	X
85	MG	5	3592	-	X
85	MG	5	3593	-	X
85	MG	5	3594	-	X
85	MG	5	3595	-	X
85	MG	5	3596	-	X
85	MG	5	3597	-	X
85	MG	5	3598	-	X
85	MG	5	3599	-	X
85	MG	5	3604	-	X
85	MG	5	3605	-	X
85	MG	5	3607	-	X
85	MG	5	3608	-	X
85	MG	5	3609	-	X
85	MG	5	3610	-	X
85	MG	5	3611	-	X
85	MG	5	3612	-	X
85	MG	5	3613	-	X
85	MG	5	3615	-	X
85	MG	5	3617	-	X
85	MG	5	3618	-	X
85	MG	5	3619	-	X
85	MG	5	3620	-	X
85	MG	5	3621	-	X
85	MG	5	3622	-	X
85	MG	5	3623	-	X
85	MG	5	3624	-	X
85	MG	5	3625	-	X
85	MG	5	3626	-	X
85	MG	5	3627	-	X
85	MG	5	3628	-	X
85	MG	5	3629	-	X
85	MG	5	3630	-	X
85	MG	5	3631	-	X
85	MG	5	3632	-	X
85	MG	5	3633	-	X
85	MG	5	3634	-	X
85	MG	5	3635	-	X
85	MG	5	3636	-	X
85	MG	5	3638	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3639	-	X
85	MG	5	3640	-	X
85	MG	5	3641	-	X
85	MG	5	3643	-	X
85	MG	5	3646	-	X
85	MG	5	3647	-	X
85	MG	5	3650	-	X
85	MG	5	3652	-	X
85	MG	5	3653	-	X
85	MG	5	3654	-	X
85	MG	5	3655	-	X
85	MG	5	3656	-	X
85	MG	5	3657	-	X
85	MG	5	3658	-	X
85	MG	5	3660	-	X
85	MG	5	3661	-	X
85	MG	5	3662	-	X
85	MG	5	3664	-	X
85	MG	5	3665	-	X
85	MG	5	3666	-	X
85	MG	5	3667	-	X
85	MG	5	3668	-	X
85	MG	5	3670	-	X
85	MG	5	3672	-	X
85	MG	5	3673	-	X
85	MG	5	3674	-	X
85	MG	5	3675	-	X
85	MG	5	3676	-	X
85	MG	5	3677	-	X
85	MG	5	3678	-	X
85	MG	5	3680	-	X
85	MG	5	3681	-	X
85	MG	5	3683	-	X
85	MG	5	3685	-	X
85	MG	5	3686	-	X
85	MG	5	3687	-	X
85	MG	5	3688	-	X
85	MG	5	3689	-	X
85	MG	5	3691	-	X
85	MG	5	3692	-	X
85	MG	5	3694	-	X
85	MG	5	3696	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3697	-	X
85	MG	5	3698	-	X
85	MG	5	3699	-	X
85	MG	5	3700	-	X
85	MG	5	3701	-	X
85	MG	5	3702	-	X
85	MG	5	3704	-	X
85	MG	5	3705	-	X
85	MG	5	3706	-	X
85	MG	5	3708	-	X
85	MG	5	3709	-	X
85	MG	5	3710	-	X
85	MG	5	3712	-	X
85	MG	5	3714	-	X
85	MG	5	3716	-	X
85	MG	5	3717	-	X
85	MG	5	3718	-	X
85	MG	5	3719	-	X
85	MG	5	3721	-	X
85	MG	5	3722	-	X
85	MG	5	3723	-	X
85	MG	5	3724	-	X
85	MG	5	3726	-	X
85	MG	5	3727	-	X
85	MG	5	3729	-	X
85	MG	5	3731	-	X
85	MG	5	3733	-	X
85	MG	5	3734	-	X
85	MG	5	3735	-	X
85	MG	5	3736	-	X
85	MG	5	3737	-	X
85	MG	5	3738	-	X
85	MG	5	3739	-	X
85	MG	5	3740	-	X
85	MG	5	3741	-	X
85	MG	5	3742	-	X
85	MG	5	3743	-	X
85	MG	5	3745	-	X
85	MG	5	3746	-	X
85	MG	5	3747	-	X
85	MG	5	3748	-	X
85	MG	5	3749	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3751	-	X
85	MG	5	3752	-	X
85	MG	5	3756	-	X
85	MG	5	3757	-	X
85	MG	5	3760	-	X
85	MG	5	3761	-	X
85	MG	5	3762	-	X
85	MG	5	3763	-	X
85	MG	5	3768	-	X
85	MG	5	3769	-	X
85	MG	5	3771	-	X
85	MG	5	3772	-	X
85	MG	5	3774	-	X
85	MG	5	3775	-	X
85	MG	5	3777	-	X
85	MG	5	3778	-	X
85	MG	5	3779	-	X
85	MG	5	3780	-	X
85	MG	5	3785	-	X
85	MG	5	3786	-	X
85	MG	5	3787	-	X
85	MG	5	3789	-	X
85	MG	5	3793	-	X
85	MG	5	3794	-	X
85	MG	5	3795	-	X
85	MG	5	3796	-	X
85	MG	5	3797	-	X
85	MG	5	3798	-	X
85	MG	5	3799	-	X
85	MG	5	3800	-	X
85	MG	5	3802	-	X
85	MG	5	3805	-	X
85	MG	5	3806	-	X
85	MG	5	3808	-	X
85	MG	5	3809	-	X
85	MG	5	3811	-	X
85	MG	5	3812	-	X
85	MG	5	3815	-	X
85	MG	5	3817	-	X
85	MG	5	3818	-	X
85	MG	5	3821	-	X
85	MG	5	3823	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3825	-	X
85	MG	5	3827	-	X
85	MG	5	3828	-	X
85	MG	5	3829	-	X
85	MG	5	3830	-	X
85	MG	5	3831	-	X
85	MG	5	3832	-	X
85	MG	5	3833	-	X
85	MG	5	3836	-	X
85	MG	5	3837	-	X
85	MG	5	3838	-	X
85	MG	5	3839	-	X
85	MG	5	3842	-	X
85	MG	5	3843	-	X
85	MG	5	3845	-	X
85	MG	5	3846	-	X
85	MG	5	3847	-	X
85	MG	5	3849	-	X
85	MG	5	3850	-	X
85	MG	5	3852	-	X
85	MG	5	3853	-	X
85	MG	5	3854	-	X
85	MG	5	3856	-	X
85	MG	5	3857	-	X
85	MG	5	3861	-	X
85	MG	5	3862	-	X
85	MG	5	3863	-	X
85	MG	5	3866	-	X
85	MG	5	3867	-	X
85	MG	5	3869	-	X
85	MG	5	3872	-	X
85	MG	5	3873	-	X
85	MG	5	3874	-	X
85	MG	5	3875	-	X
85	MG	5	3876	-	X
85	MG	5	3877	-	X
85	MG	5	3878	-	X
85	MG	5	3879	-	X
85	MG	5	3881	-	X
85	MG	5	3882	-	X
85	MG	5	3883	-	X
85	MG	5	3884	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3885	-	X
85	MG	5	3887	-	X
85	MG	5	3889	-	X
85	MG	5	3890	-	X
85	MG	5	3891	-	X
85	MG	5	3892	-	X
85	MG	5	3893	-	X
85	MG	5	3894	-	X
85	MG	5	3896	-	X
85	MG	5	3897	-	X
85	MG	5	3899	-	X
85	MG	5	4256	-	X
85	MG	5	4257	-	X
85	MG	5	4258	-	X
85	MG	5	4259	-	X
85	MG	6	1901	-	X
85	MG	6	1902	-	X
85	MG	6	1903	-	X
85	MG	6	1905	-	X
85	MG	6	1906	-	X
85	MG	6	1907	-	X
85	MG	6	1908	-	X
85	MG	6	1909	-	X
85	MG	6	1910	-	X
85	MG	6	1911	-	X
85	MG	6	1912	-	X
85	MG	6	1913	-	X
85	MG	6	1916	-	X
85	MG	6	1917	-	X
85	MG	6	1918	-	X
85	MG	6	1919	-	X
85	MG	6	1920	-	X
85	MG	6	1921	-	X
85	MG	6	1922	-	X
85	MG	6	1924	-	X
85	MG	6	1925	-	X
85	MG	6	1926	-	X
85	MG	6	1927	-	X
85	MG	6	1928	-	X
85	MG	6	1929	-	X
85	MG	6	1930	-	X
85	MG	6	1931	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1932	-	X
85	MG	6	1933	-	X
85	MG	6	1934	-	X
85	MG	6	1936	-	X
85	MG	6	1937	-	X
85	MG	6	1938	-	X
85	MG	6	1940	-	X
85	MG	6	1942	-	X
85	MG	6	1943	-	X
85	MG	6	1944	-	X
85	MG	6	1945	-	X
85	MG	6	1946	-	X
85	MG	6	1947	-	X
85	MG	6	1948	-	X
85	MG	6	1949	-	X
85	MG	6	1950	-	X
85	MG	6	1951	-	X
85	MG	6	1953	-	X
85	MG	6	1954	-	X
85	MG	6	1955	-	X
85	MG	6	1956	-	X
85	MG	6	1958	-	X
85	MG	6	1959	-	X
85	MG	6	1960	-	X
85	MG	6	1962	-	X
85	MG	6	1963	-	X
85	MG	6	1964	-	X
85	MG	6	1965	-	X
85	MG	6	1967	-	X
85	MG	6	1968	-	X
85	MG	6	1969	-	X
85	MG	6	1970	-	X
85	MG	6	1971	-	X
85	MG	6	1972	-	X
85	MG	6	1973	-	X
85	MG	6	1975	-	X
85	MG	6	1977	-	X
85	MG	6	1978	-	X
85	MG	6	1980	-	X
85	MG	6	1983	-	X
85	MG	6	1986	-	X
85	MG	6	1988	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1989	-	X
85	MG	6	1993	-	X
85	MG	6	1994	-	X
85	MG	6	1999	-	X
85	MG	6	2001	-	X
85	MG	6	2004	-	X
85	MG	6	2006	-	X
85	MG	6	2007	-	X
85	MG	6	2008	-	X
85	MG	6	2009	-	X
85	MG	6	2010	-	X
85	MG	6	2011	-	X
85	MG	6	2012	-	X
85	MG	6	2013	-	X
85	MG	6	2014	-	X
85	MG	6	2016	-	X
85	MG	6	2017	-	X
85	MG	6	2018	-	X
85	MG	6	2019	-	X
85	MG	6	2020	-	X
85	MG	6	2021	-	X
85	MG	6	2022	-	X
85	MG	6	2023	-	X
85	MG	6	2025	-	X
85	MG	6	2026	-	X
85	MG	6	2028	-	X
85	MG	6	2029	-	X
85	MG	6	2030	-	X
85	MG	6	2031	-	X
85	MG	6	2032	-	X
85	MG	6	2033	-	X
85	MG	6	2034	-	X
85	MG	6	2035	-	X
85	MG	6	2036	-	X
85	MG	6	2037	-	X
85	MG	6	2039	-	X
85	MG	6	2040	-	X
85	MG	6	2042	-	X
85	MG	6	2043	-	X
85	MG	6	2044	-	X
85	MG	7	201	-	X
85	MG	7	202	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	7	203	-	X
85	MG	7	204	-	X
85	MG	7	205	-	X
85	MG	7	206	-	X
85	MG	7	207	-	X
85	MG	7	208	-	X
85	MG	7	210	-	X
85	MG	7	211	-	X
85	MG	7	212	-	X
85	MG	7	214	-	X
85	MG	7	215	-	X
85	MG	7	216	-	X
85	MG	7	228	-	X
85	MG	8	202	-	X
85	MG	8	203	-	X
85	MG	8	204	-	X
85	MG	8	205	-	X
85	MG	8	206	-	X
85	MG	8	207	-	X
85	MG	8	208	-	X
85	MG	8	209	-	X
85	MG	8	210	-	X
85	MG	8	211	-	X
85	MG	8	212	-	X
85	MG	8	213	-	X
85	MG	D0	201	-	X
85	MG	L4	401	-	X
85	MG	L5	301	-	X
85	MG	L7	301	-	X
85	MG	L7	302	-	X
85	MG	L7	303	-	X
85	MG	L8	301	-	X
85	MG	M3	203	-	X
85	MG	M5	301	-	X
85	MG	M6	201	-	X
85	MG	M7	203	-	X
85	MG	M7	204	-	X
85	MG	M7	205	-	X
85	MG	N0	201	-	X
85	MG	N3	201	-	X
85	MG	N3	202	-	X
85	MG	N5	201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	N8	203	-	X
85	MG	N8	205	-	X
85	MG	O2	201	-	X
85	MG	O7	102	-	X
85	MG	O7	103	-	X
85	MG	O7	104	-	X
85	MG	S4	301	-	X
85	MG	S8	301	-	X
85	MG	SM	301	-	X
85	MG	c1	201	-	X
85	MG	c7	201	-	X
85	MG	d3	201	-	X
85	MG	d4	201	-	X
85	MG	l2	301	-	X
85	MG	l3	401	-	X
85	MG	l4	401	-	X
85	MG	l7	301	-	X
85	MG	l9	201	-	X
85	MG	m0	301	-	X
85	MG	m5	301	-	X
85	MG	m7	201	-	X
85	MG	m7	204	-	X
85	MG	m7	205	-	X
85	MG	n0	202	-	X
85	MG	n3	201	-	X
85	MG	n3	202	-	X
85	MG	n8	201	-	X
85	MG	n8	202	-	X
85	MG	n8	203	-	X
85	MG	n9	101	-	X
85	MG	o1	201	-	X
85	MG	o3	201	-	X
85	MG	o4	202	-	X
85	MG	o7	101	-	X
85	MG	s6	301	-	X
85	MG	s8	302	-	X
85	MG	sM	301	-	X
86	OHX	1	4042	-	X
86	OHX	1	4044	-	X
86	OHX	1	4060	-	X
86	OHX	1	4065	-	X
86	OHX	1	4068	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4071	-	X
86	OHX	1	4076	-	X
86	OHX	1	4080	-	X
86	OHX	1	4095	-	X
86	OHX	1	4106	-	X
86	OHX	1	4107	-	X
86	OHX	1	4111	-	X
86	OHX	1	4113	-	X
86	OHX	1	4114	-	X
86	OHX	1	4117	-	X
86	OHX	1	4118	-	X
86	OHX	1	4124	-	X
86	OHX	1	4125	-	X
86	OHX	1	4126	-	X
86	OHX	1	4131	-	X
86	OHX	1	4137	-	X
86	OHX	1	4138	-	X
86	OHX	1	4140	-	X
86	OHX	1	4141	-	X
86	OHX	1	4145	-	X
86	OHX	1	4151	-	X
86	OHX	1	4158	-	X
86	OHX	1	4159	-	X
86	OHX	1	4161	-	X
86	OHX	1	4162	-	X
86	OHX	1	4165	-	X
86	OHX	1	4166	-	X
86	OHX	1	4167	-	X
86	OHX	1	4168	-	X
86	OHX	1	4169	-	X
86	OHX	1	4172	-	X
86	OHX	1	4174	-	X
86	OHX	1	4175	-	X
86	OHX	1	4176	-	X
86	OHX	1	4179	-	X
86	OHX	1	4181	-	X
86	OHX	1	4183	-	X
86	OHX	1	4184	-	X
86	OHX	1	4186	-	X
86	OHX	1	4187	-	X
86	OHX	1	4190	-	X
86	OHX	1	4193	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4194	-	X
86	OHX	1	4195	-	X
86	OHX	1	4199	-	X
86	OHX	1	4200	-	X
86	OHX	1	4201	-	X
86	OHX	1	4202	-	X
86	OHX	1	4203	-	X
86	OHX	1	4204	-	X
86	OHX	1	4207	-	X
86	OHX	1	4208	-	X
86	OHX	1	4210	-	X
86	OHX	2	2102	-	X
86	OHX	2	2122	-	X
86	OHX	2	2131	-	X
86	OHX	2	2135	-	X
86	OHX	2	2136	-	X
86	OHX	2	2137	-	X
86	OHX	2	2140	-	X
86	OHX	2	2143	-	X
86	OHX	2	2147	-	X
86	OHX	2	2156	-	X
86	OHX	2	2158	-	X
86	OHX	2	2159	-	X
86	OHX	2	2161	-	X
86	OHX	2	2162	-	X
86	OHX	2	2163	-	X
86	OHX	2	2168	-	X
86	OHX	2	2174	-	X
86	OHX	2	2176	-	X
86	OHX	2	2177	-	X
86	OHX	4	232	-	X
86	OHX	4	235	-	X
86	OHX	5	3914	-	X
86	OHX	5	3925	-	X
86	OHX	5	4047	-	X
86	OHX	5	4053	-	X
86	OHX	5	4091	-	X
86	OHX	5	4099	-	X
86	OHX	5	4102	-	X
86	OHX	5	4108	-	X
86	OHX	5	4114	-	X
86	OHX	5	4116	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4123	-	X
86	OHX	5	4129	-	X
86	OHX	5	4141	-	X
86	OHX	5	4142	-	X
86	OHX	5	4143	-	X
86	OHX	5	4145	-	X
86	OHX	5	4151	-	X
86	OHX	5	4153	-	X
86	OHX	5	4155	-	X
86	OHX	5	4156	-	X
86	OHX	5	4158	-	X
86	OHX	5	4159	-	X
86	OHX	5	4160	-	X
86	OHX	5	4161	-	X
86	OHX	5	4162	-	X
86	OHX	5	4163	-	X
86	OHX	5	4164	-	X
86	OHX	5	4177	-	X
86	OHX	5	4180	-	X
86	OHX	5	4181	-	X
86	OHX	5	4183	-	X
86	OHX	5	4186	-	X
86	OHX	5	4187	-	X
86	OHX	5	4188	-	X
86	OHX	5	4189	-	X
86	OHX	5	4194	-	X
86	OHX	5	4197	-	X
86	OHX	5	4198	-	X
86	OHX	5	4204	-	X
86	OHX	5	4206	-	X
86	OHX	5	4208	-	X
86	OHX	5	4212	-	X
86	OHX	5	4218	-	X
86	OHX	5	4221	-	X
86	OHX	5	4222	-	X
86	OHX	5	4223	-	X
86	OHX	5	4224	-	X
86	OHX	5	4225	-	X
86	OHX	5	4226	-	X
86	OHX	5	4231	-	X
86	OHX	5	4233	-	X
86	OHX	5	4234	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4237	-	X
86	OHX	5	4238	-	X
86	OHX	5	4240	-	X
86	OHX	5	4242	-	X
86	OHX	5	4246	-	X
86	OHX	5	4249	-	X
86	OHX	5	4250	-	X
86	OHX	5	4251	-	X
86	OHX	5	4252	-	X
86	OHX	6	2048	-	X
86	OHX	6	2117	-	X
86	OHX	6	2121	-	X
86	OHX	6	2125	-	X
86	OHX	6	2137	-	X
86	OHX	6	2147	-	X
86	OHX	6	2156	-	X
86	OHX	6	2160	-	X
86	OHX	6	2169	-	X
86	OHX	6	2171	-	X
86	OHX	6	2174	-	X
86	OHX	6	2177	-	X
86	OHX	6	2178	-	X
86	OHX	6	2180	-	X
86	OHX	6	2181	-	X
86	OHX	6	2183	-	X
86	OHX	6	2186	-	X
86	OHX	6	2187	-	X
86	OHX	6	2189	-	X
86	OHX	6	2190	-	X
86	OHX	6	2195	-	X
86	OHX	6	2199	-	X
86	OHX	6	2203	-	X
86	OHX	6	2204	-	X
86	OHX	7	225	-	X
86	OHX	7	227	-	X
86	OHX	8	227	-	X
86	OHX	M7	206	-	X
86	OHX	M7	207	-	X
86	OHX	O9	101	-	X
86	OHX	l4	402	-	X
86	OHX	l4	403	-	X
88	ZN	d7	101	-	X

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411206 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called *Saccharomyces cerevisiae* chromosome XII cosmid 9634.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 82 is a protein called Unknown protein 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 Unknown protein chain p1.

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	3	Total	Mg	0	0
			3	3		
85	m6	1	Total	Mg	0	0
			1	1		
85	n8	4	Total	Mg	0	0
			4	4		
85	q3	1	Total	Mg	0	0
			1	1		
85	o1	1	Total	Mg	0	0
			1	1		
85	N5	1	Total	Mg	0	0
			1	1		
85	6	148	Total	Mg	0	0
			148	148		
85	sM	2	Total	Mg	0	0
			2	2		
85	O4	1	Total	Mg	0	0
			1	1		
85	m5	2	Total	Mg	0	0
			2	2		
85	l3	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	M1	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	125	Total 125	Mg 125	0	0
85	n0	2	Total 2	Mg 2	0	0
85	L4	1	Total 1	Mg 1	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	M0	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	505	Total 505	Mg 505	0	0
85	L5	2	Total 2	Mg 2	0	0
85	O7	3	Total 3	Mg 3	0	0
85	s6	1	Total 1	Mg 1	0	0

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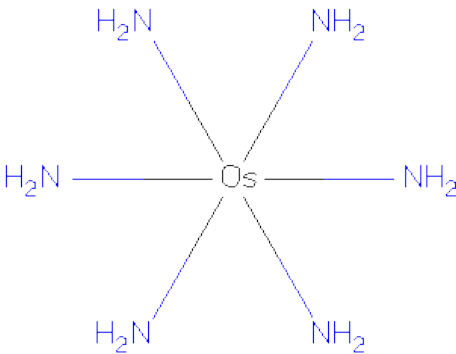
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	Q2	1	Total 1	Mg 1	0	0
85	d4	1	Total 1	Mg 1	0	0
85	n9	1	Total 1	Mg 1	0	0
85	1	469	Total 469	Mg 469	0	0
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	1	Total 1	Mg 1	0	0
85	O2	1	Total 1	Mg 1	0	0
85	o7	1	Total 1	Mg 1	0	0
85	o3	1	Total 1	Mg 1	0	0
85	d3	1	Total 1	Mg 1	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	2	Total 2	Mg 2	0	0
85	4	21	Total 21	Mg 21	0	0
85	n6	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	1	Total 1	Mg 1	0	0
85	m1	1	Total 1	Mg 1	0	0
85	l5	2	Total 2	Mg 2	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N8	5	Total 5	Mg 5	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	17	Total 17	Mg 17	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	3	Total 3	Mg 3	0	0
85	O5	1	Total 1	Mg 1	0	0
85	N6	2	Total 2	Mg 2	0	0
85	8	14	Total 14	Mg 14	0	0
85	l4	1	Total 1	Mg 1	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0
85	m0	1	Total 1	Mg 1	0	0
85	3	14	Total 14	Mg 14	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	C1	1	Total	N	Os	0	0
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86	C3	1	Total	N	Os	0	0
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86	C5	1	Total	N	Os	0	0
			7	6	1		
86	C8	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	L4	1	Total	N	Os	0	0
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86	M5	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M8	1	Total	N	Os	0	0
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86	M9	1	Total	N	Os	0	0
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86	N9	1	Total	N	Os	0	0
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86	O2	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
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86	s1	1	Total 7	N 6	Os 1	0	0
86	s4	1	Total 7	N 6	Os 1	0	0
86	s8	1	Total 7	N 6	Os 1	0	0
86	s9	1	Total 7	N 6	Os 1	0	0
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86	d9	1	Total 7	N 6	Os 1	0	0
86	sR	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	m9	1	Total	N	Os	0	0
			7	6	1		
86	n1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is (14aR)-2,3,6-trimethoxy-11,12,13,14,14a,15-hexahydro-9H-dibenzo[f,h]pyrido [1,2-b]isoquinoline (three-letter code: 3K8) (formula: C₂₄H₂₇NO₃).

Image
Not Available

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
87	2	1	Total	C	N	O	0	0
			28	24	1	3		
87	6	1	Total	C	N	O	0	0
			28	24	1	3		

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total	Zn	0	0
			1	1		
88	D6	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		

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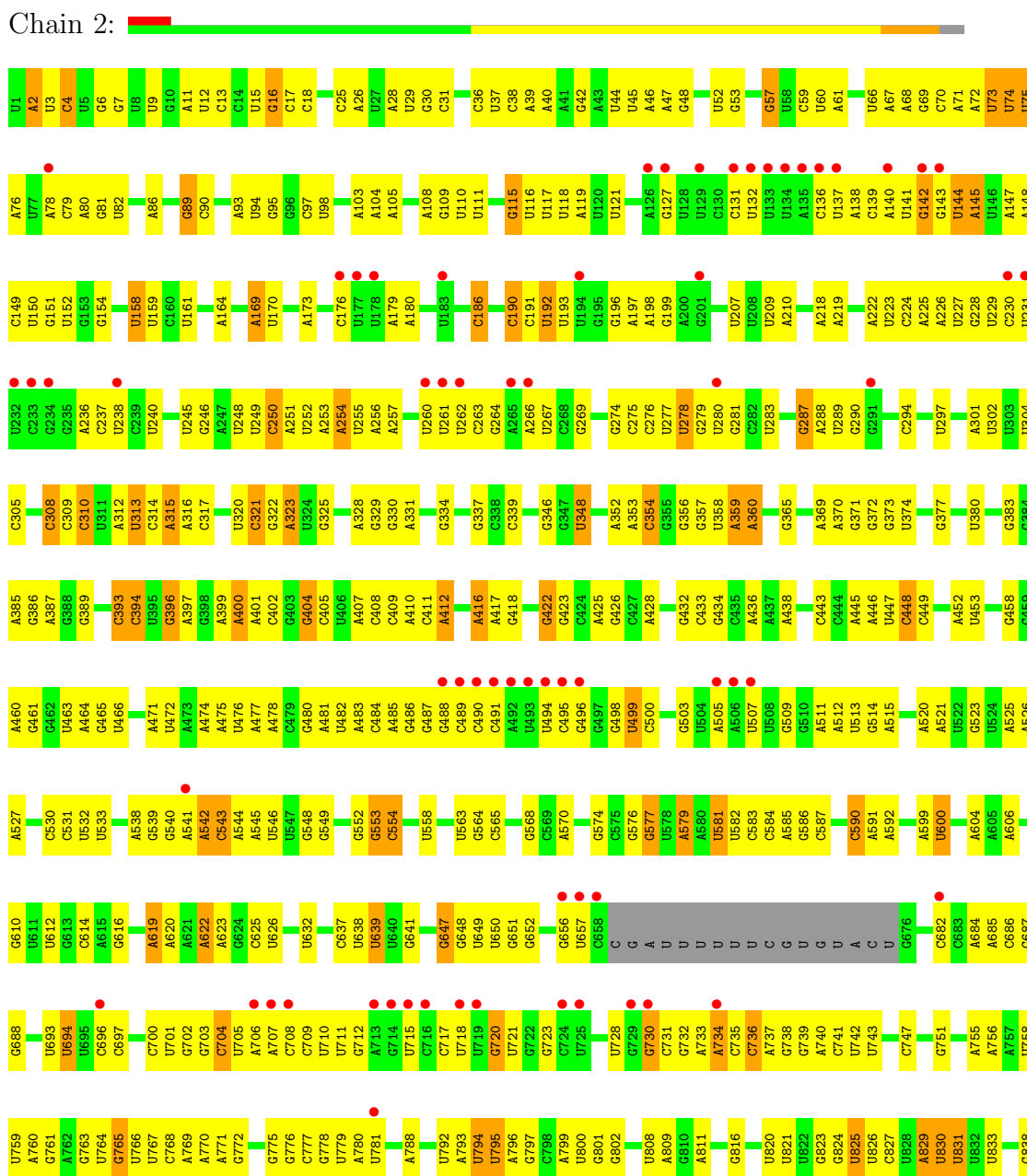
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	Q3	1	Total 1	Zn 1	0	0
88	D9	1	Total 1	Zn 1	0	0
88	E1	1	Total 1	Zn 1	0	0
88	Q0	1	Total 1	Zn 1	0	0
88	d7	1	Total 1	Zn 1	0	0
88	q3	1	Total 1	Zn 1	0	0
88	d9	1	Total 1	Zn 1	0	0
88	D7	1	Total 1	Zn 1	0	0
88	d6	1	Total 1	Zn 1	0	0
88	o7	1	Total 1	Zn 1	0	0
88	O7	1	Total 1	Zn 1	0	0
88	q2	1	Total 1	Zn 1	0	0

3 Residue-property plots

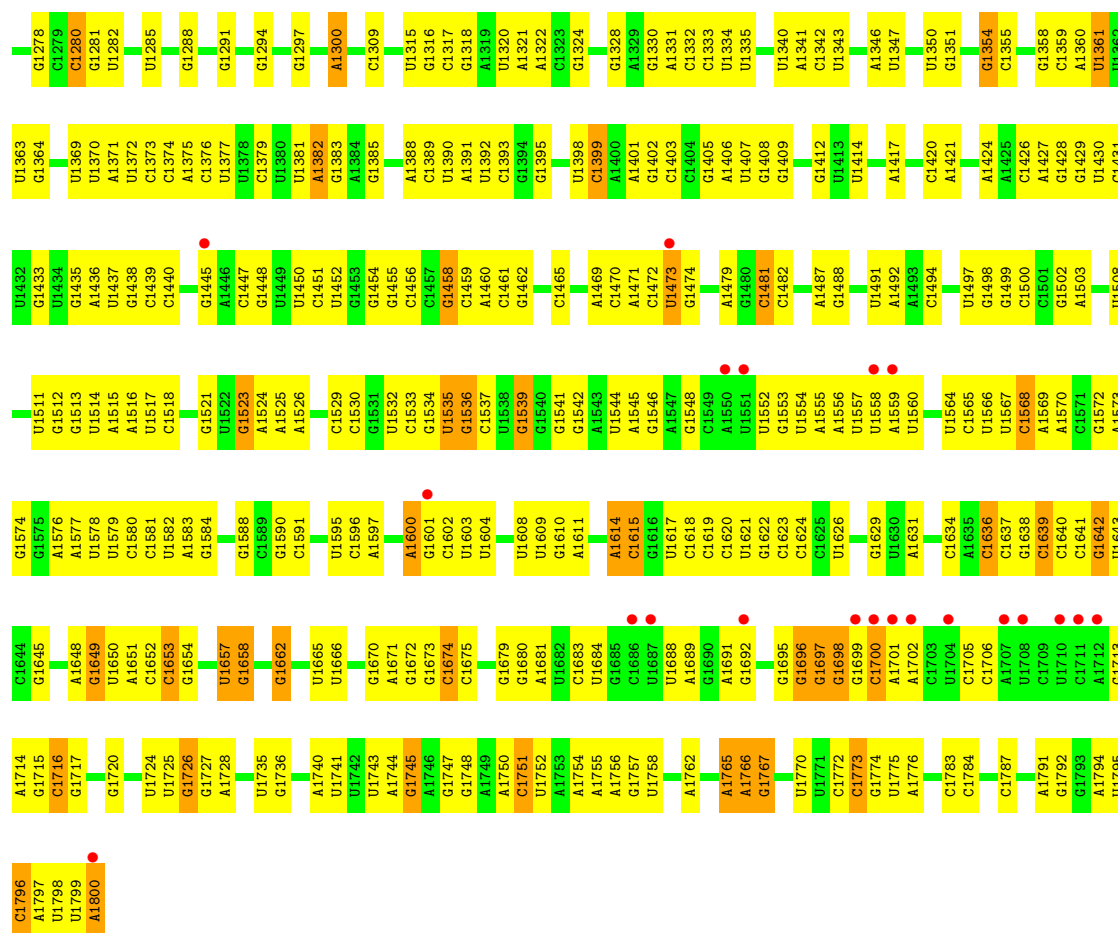
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



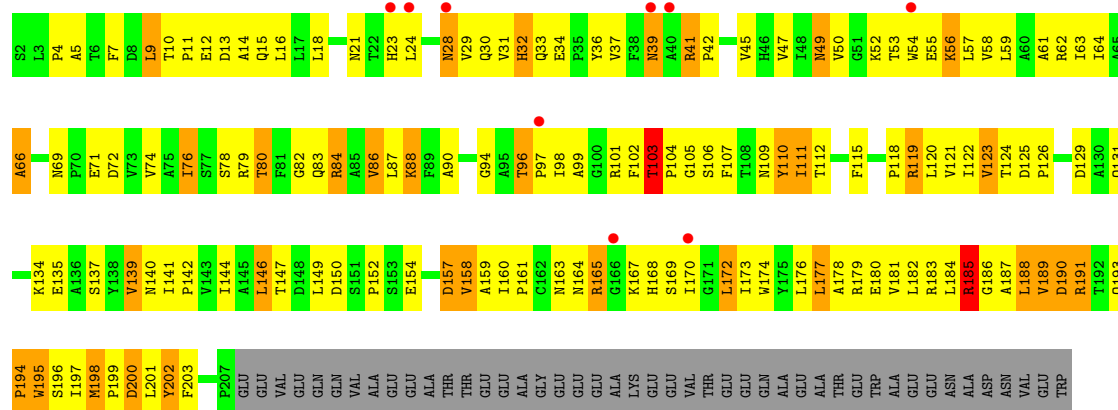






• Molecule 2: 40S ribosomal protein S0-A

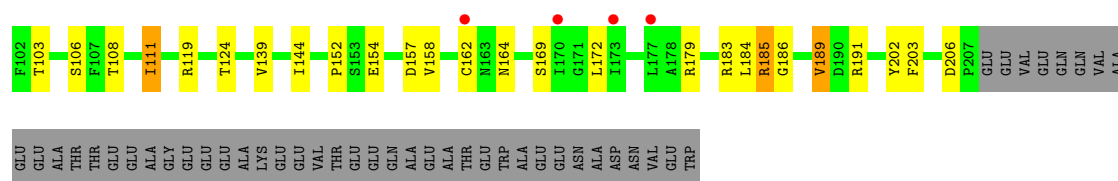
Chain S0:



• Molecule 2: 40S ribosomal protein S0-A

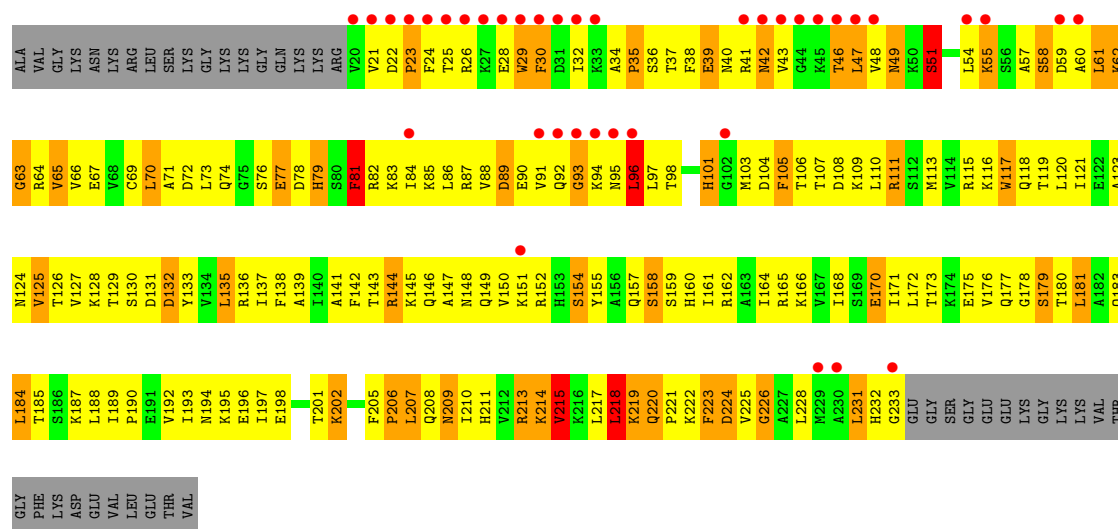
Chain s0:





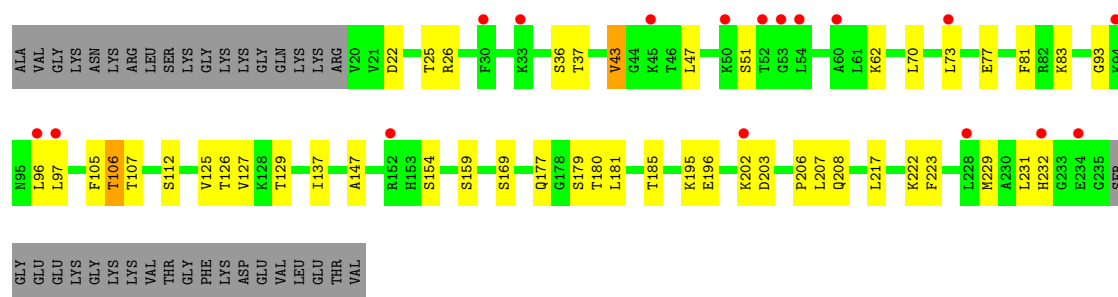
• Molecule 3: 40S ribosomal protein S1-A

Chain S1:



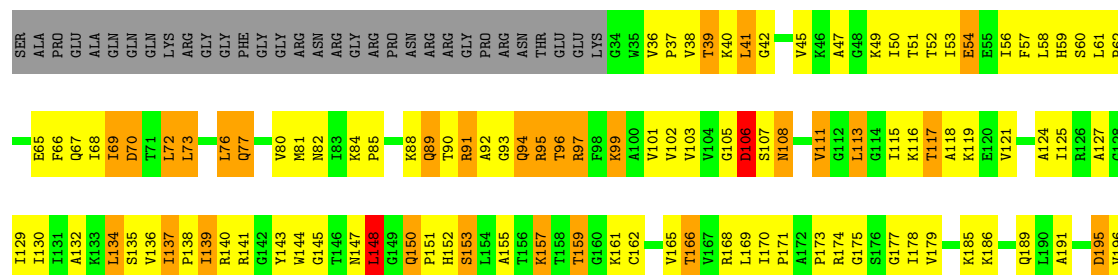
• Molecule 3: 40S ribosomal protein S1-A

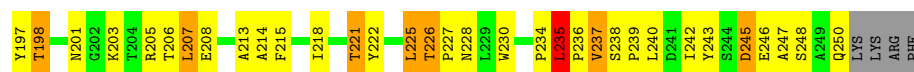
Chain s1:



• Molecule 4: 40S ribosomal protein S2

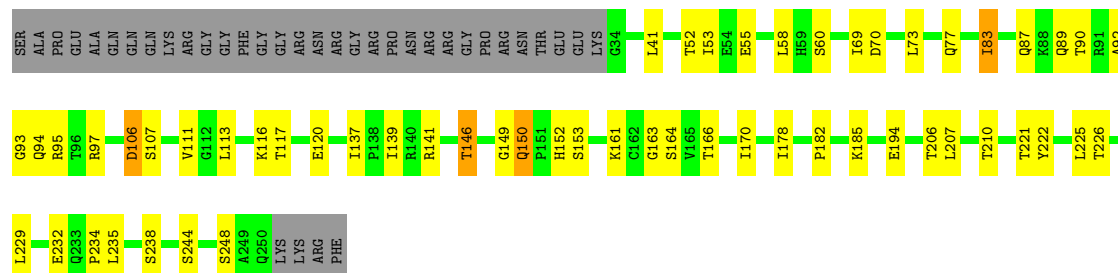
Chain S2:





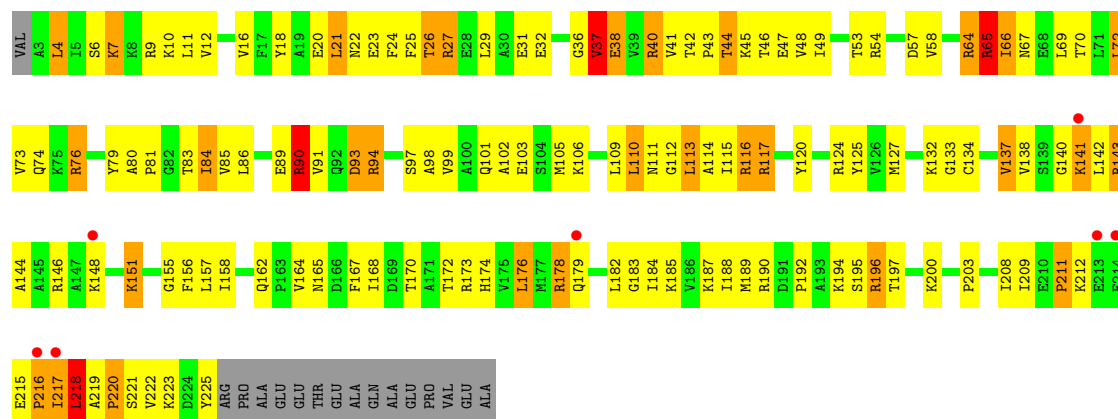
• Molecule 4: 40S ribosomal protein S2

Chain s2:



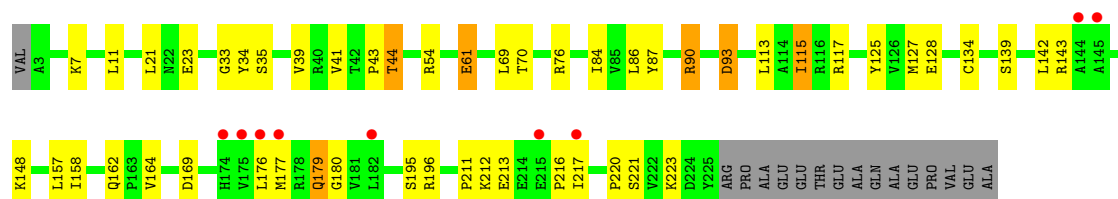
• Molecule 5: 40S ribosomal protein S3

Chain S3:



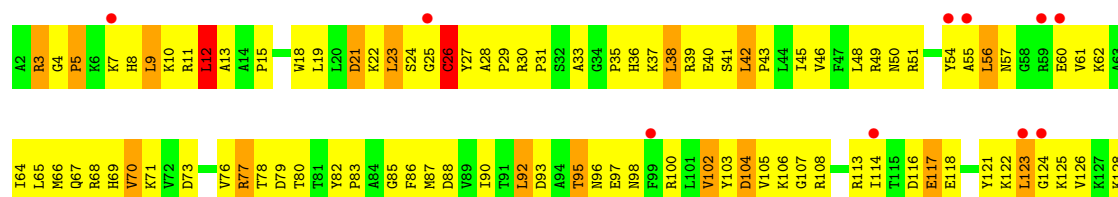
• Molecule 5: 40S ribosomal protein S3

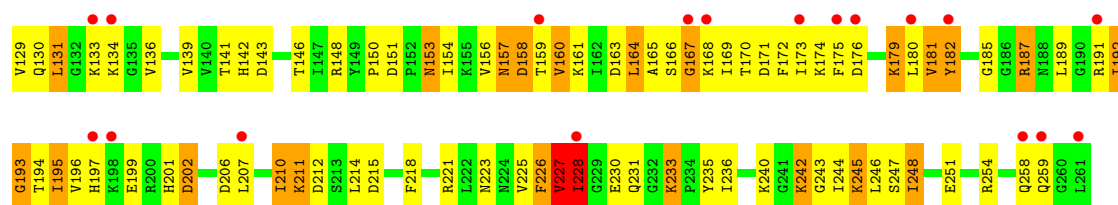
Chain s3:



• Molecule 6: 40S ribosomal protein S4-A

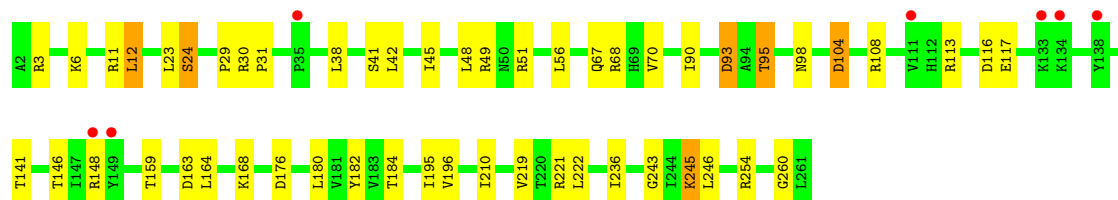
Chain S4:





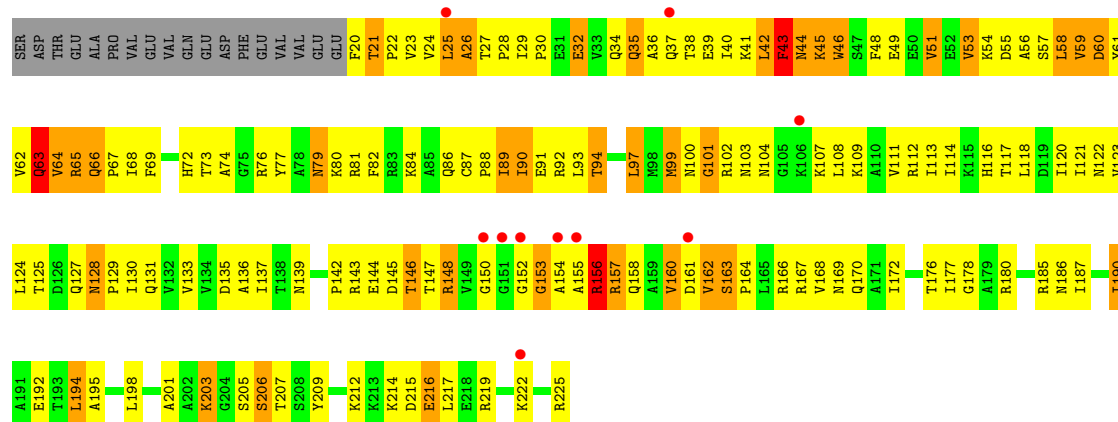
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



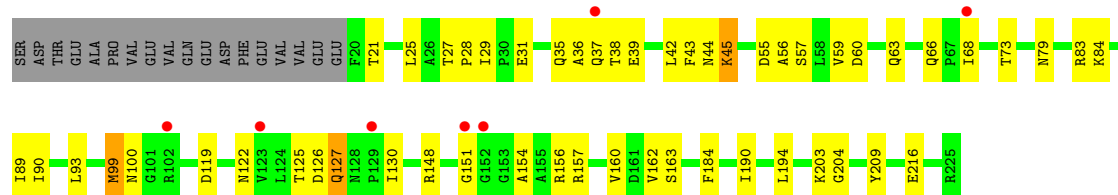
• Molecule 7: 40S ribosomal protein S5

Chain S5:



• Molecule 7: 40S ribosomal protein S5

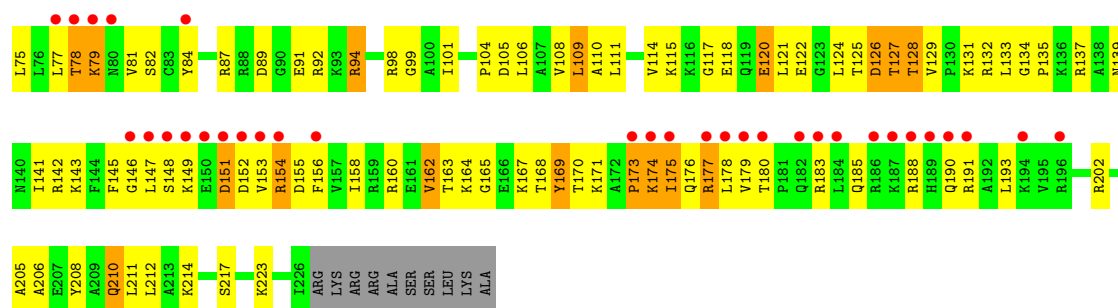
Chain s5:



• Molecule 8: 40S ribosomal protein S6-A

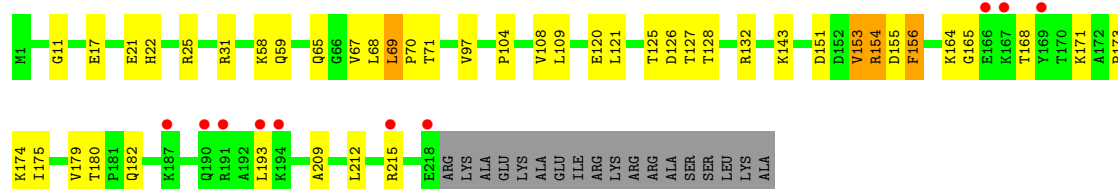
Chain S6:





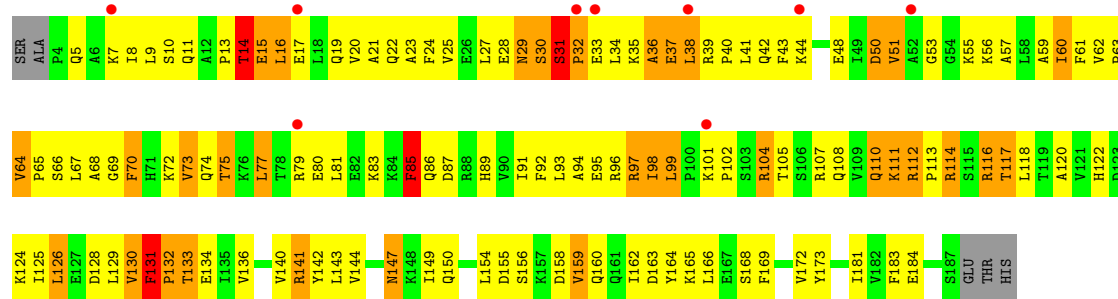
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



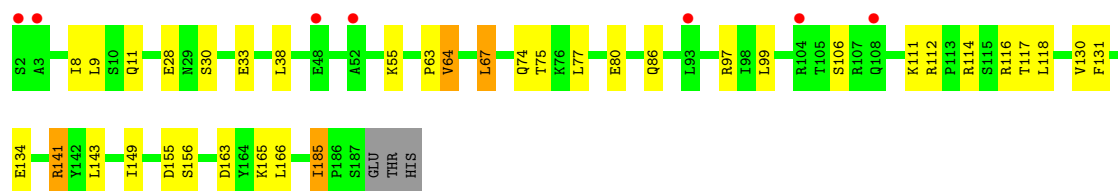
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



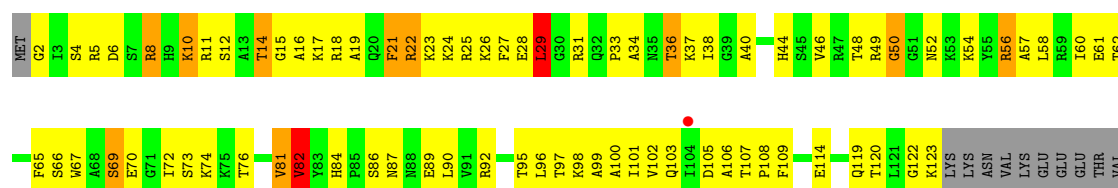
• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



• Molecule 10: 40S ribosomal protein S8-A

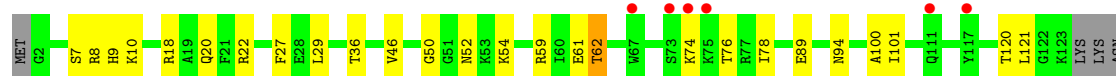
Chain S8:





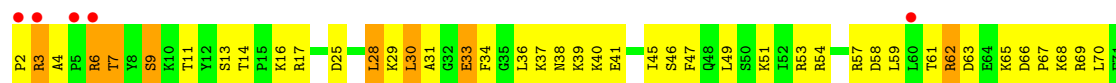
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



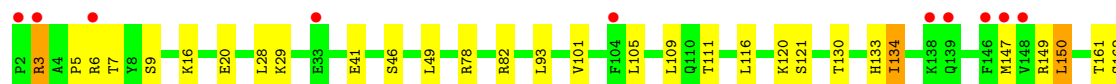
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



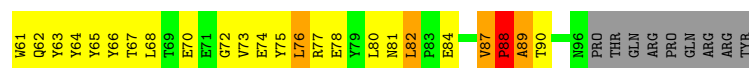
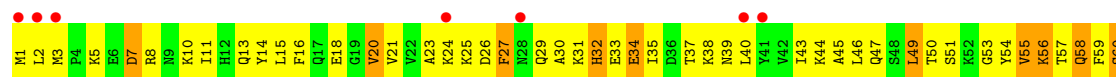
• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



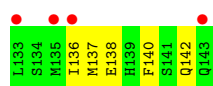
• Molecule 12: 40S ribosomal protein S10-A

Chain C0:



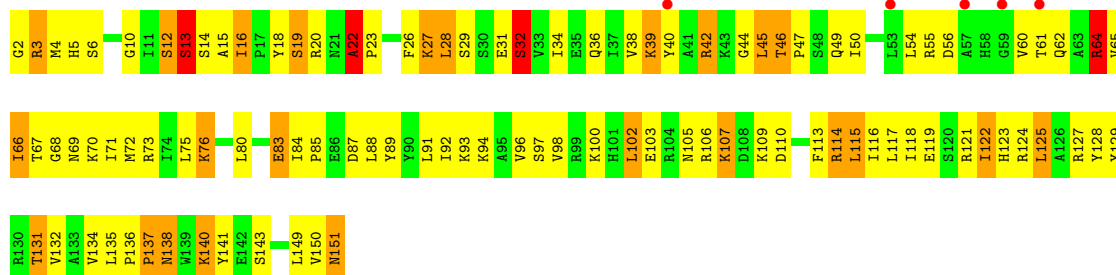
• Molecule 12: 40S ribosomal protein S10-A

Chain c0:



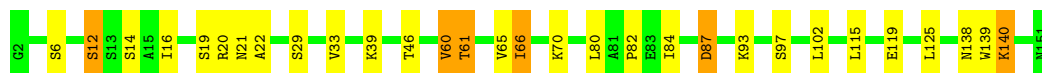
- Molecule 15: 40S ribosomal protein S13

Chain C3:



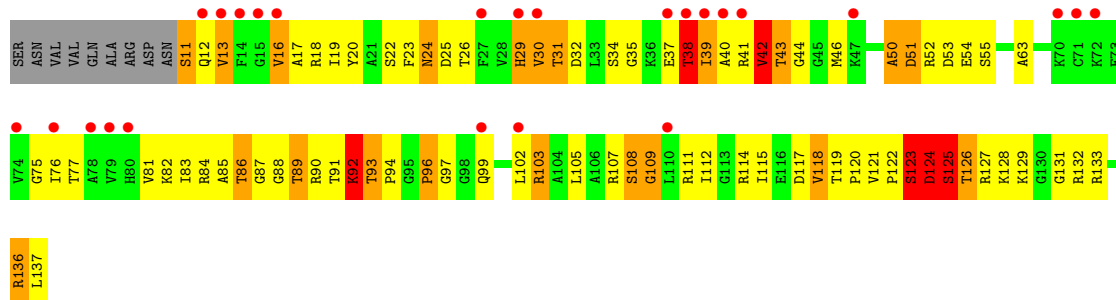
- Molecule 15: 40S ribosomal protein S13

Chain c3:



- Molecule 16: 40S ribosomal protein S14-A

Chain C4:



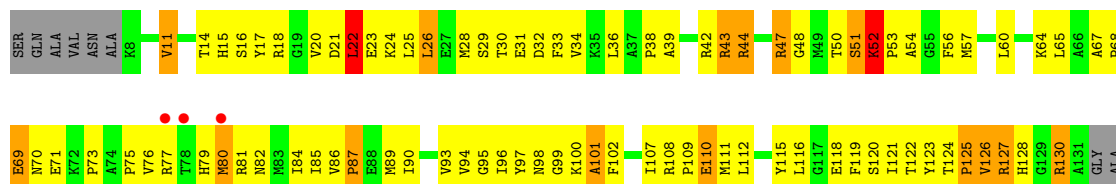
- Molecule 16: 40S ribosomal protein S14-A

Chain c4:



- Molecule 17: 40S ribosomal protein S15

Chain C5:



THR
THR
SER
SER
PHE
ILE
PRO
LEU
LYS

- Molecule 17: 40S ribosomal protein S15

Chain c5:

SER GLN A4 V5 N6 A7 K9 R10 V11 F12 K13 T14 Y17 K24 A28 V34 K35 L36 R40 K49 T50 S51 K52 P68 E69 N70 E71 K80 S92 N103 I107 E110 M111 G117 T122 Y123 T124 P125 V126 R127 T135 F138 ILE

PRO
LEU
LYS

- Molecule 18: 40S ribosomal protein S16-A

Chain C6:

SER A3 V4 P5 S6 V7 Q8 T9 F10 K12 G13 K14 S15 A16 T17 A18 V19 R20 H21 V22 K23 A24 K25 K26 C27 L28 T29 K30 V31 N32 C33 S34 P35 I36 T37 Q100 L38 V39 E40 P41 E42 I43 I44 R45 F46 K47 V48 Y49 E50 P51 L52 L53 L54 V55 V56 L57 D58 K59 F60

I63 D64 R66 R67 R68 V69 T70 G71 G72 G73 H74 Q77 V78 Y79 A80 I81 R82 R83 A84 I85 A86 K87 V90 Y92 H93 Q94 K95 Y96 V97 D98 E99 Q100 S101 K102 N103 E104 L105 K106 F109 T110 Y111 S111 Y112 D113 R114 T115 L116 L117 I118 A119 D120 S121 R122 R123 P126

K127 K128 F129 K132 G133 A134 R137 F138 Q139 K140 S141 Y142 R143

- Molecule 18: 40S ribosomal protein S16-A

Chain c6:

S2 A3 V4 Q8 T17 A18 V19 A20 H21 V22 K23 K26 G27 L28 S34 T37 L38 V39 E40 P41 E42 I43 K47 V48 L53 L54 L57 I63 R68 V69 I81 I85 A86 L89 V90 H93 Q94 V97 Q100 K106 T110

D113 R114 T115 L116 I117 I118 D120 K132 R137 F138 Q139 K140 S141 Y142 R143

- Molecule 19: 40S ribosomal protein S17-A

Chain C7:

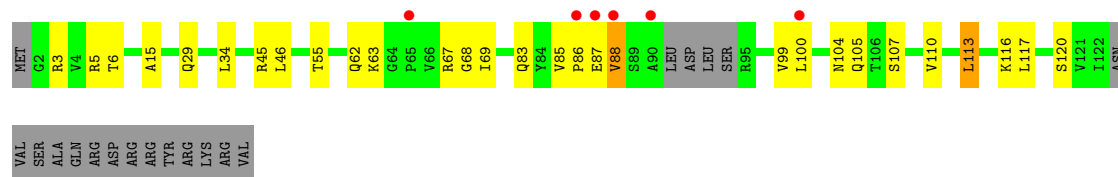
MET G2 R3 V4 T6 K7 T8 V9 K10 R11 K12 A13 S13 K14 L15 A16 I17 E18 R19 Y20 Y21 P22 K23 V24 T25 L26 D27 F28 Q29 T30 N31 K32 K33 L34 E37 I38 A39 T40 T41 K44 R45 L46 R47 N48 K49 T50 A51 G52 Y53 T54 T55 H56 L57 M58 K59 R60 Q62

K63 G64 P65 V66 R67 G68 I69 S70 F71 K72 L73 Q74 E77 R78 E79 R80 D82 Q83 Y84 P85 P86 E87 V88 S89 A89 L89 A89 S89 S96 N96 G98 V99 I100 N101 N104 Q105 T106 S107 D108 L109 V110 K111 S112 L113 G114 L115 K116 L117 P118 L119 S120 V124 S125 A126

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ASP
ARG
TYR
ARG
LYS
ARG
VAL

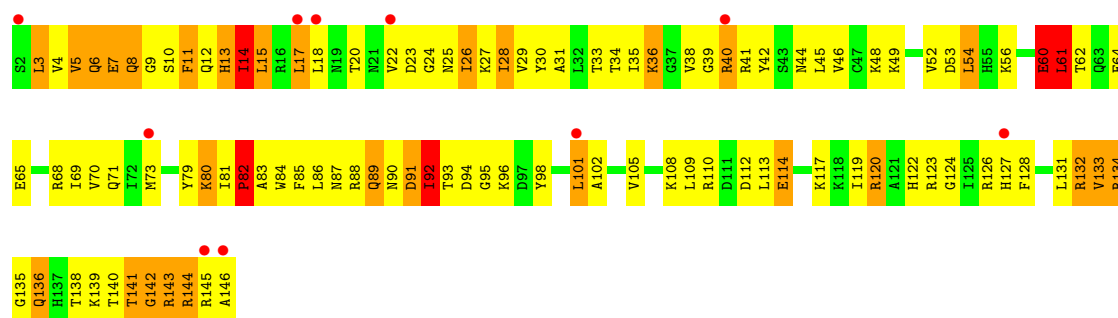
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:



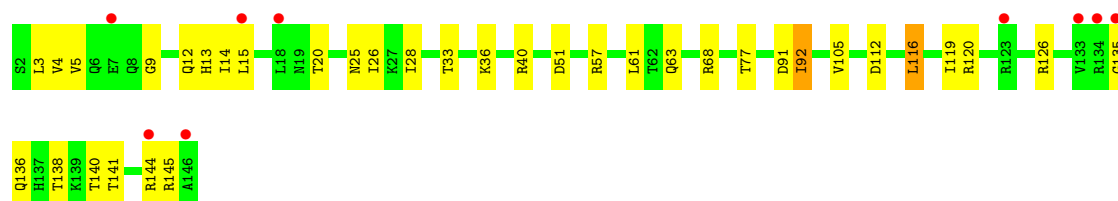
• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



• Molecule 20: 40S ribosomal protein S18-A

Chain c8:



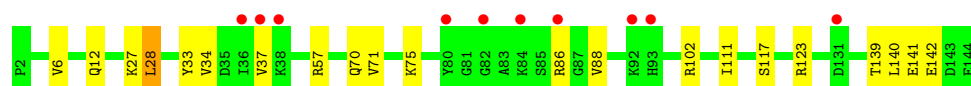
• Molecule 21: 40S ribosomal protein S19-A

Chain C9:

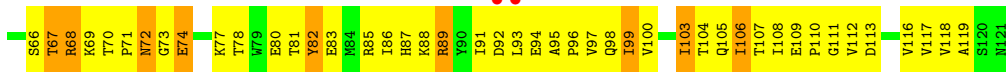


• Molecule 21: 40S ribosomal protein S19-A

Chain c9:



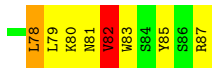
• Molecule 22: 40S ribosomal protein S20



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-
- | Age Group | Percentage |
|-----------|------------|
| 18-24 | 2% |
| 25-34 | 38% |
| 35-44 | 42% |
| 45-54 | 18% |

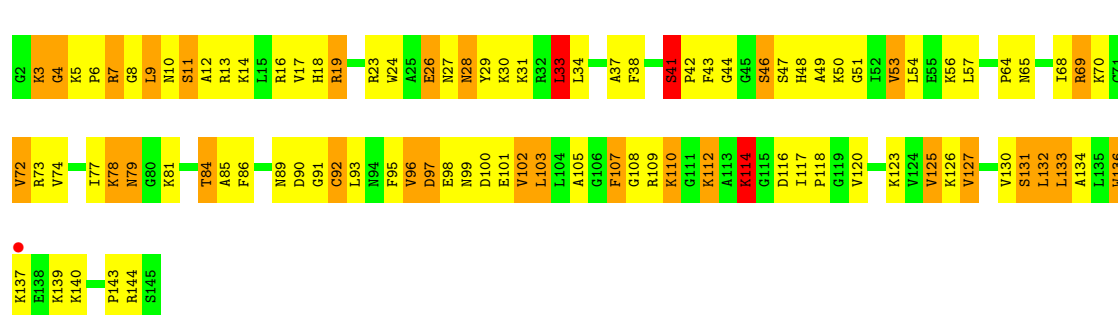


-
- | Age Group | Percentage |
|-----------|------------|
| 18-24 | 10% |
| 25-34 | 35% |
| 35-44 | 30% |
| 45-54 | 15% |
| 55-64 | 5% |
| 65-74 | 2% |
| 75-84 | 1% |
| 85+ | 1% |



- 

Chain D3:



- Molecule 25: 40S ribosomal protein S23-A

Chain d3:



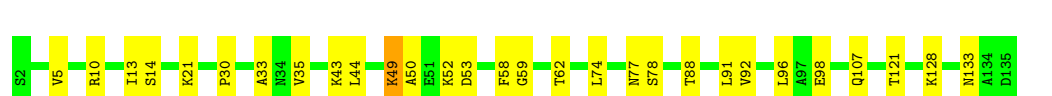
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:



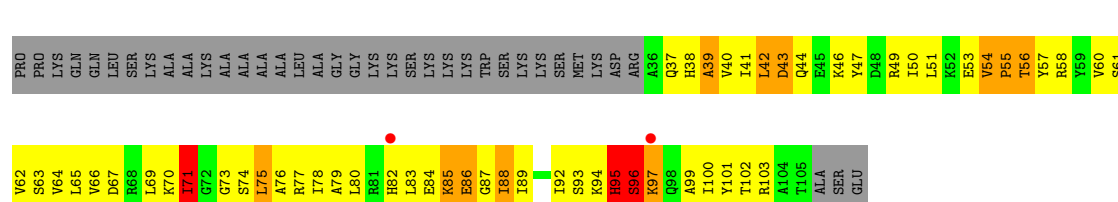
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:



- Molecule 27: 40S ribosomal protein S25-A

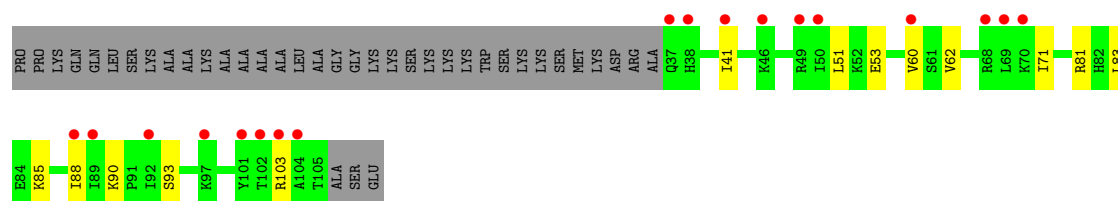
Chain D5:



- Molecule 27: 40S ribosomal protein S25-A

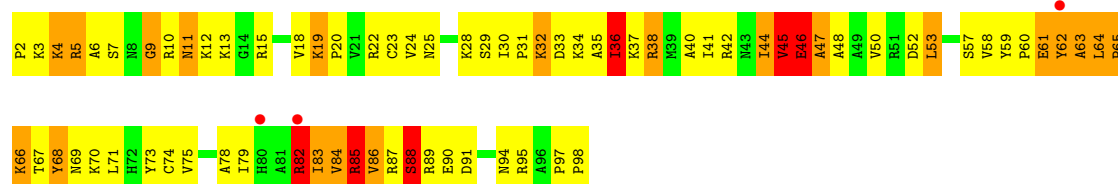
Chain d5:





- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



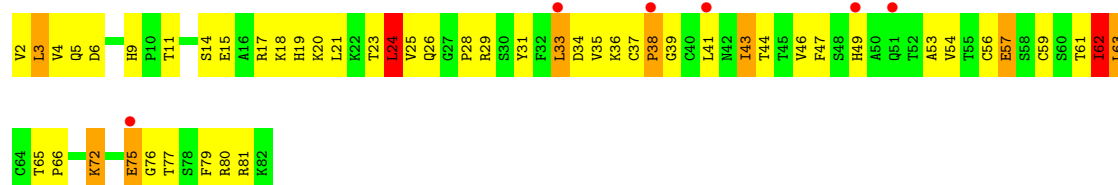
- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



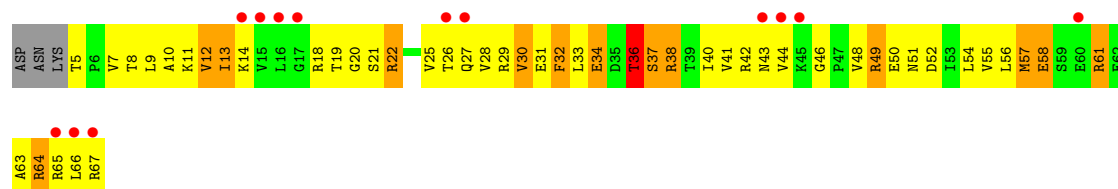
- Molecule 29: 40S ribosomal protein S27-A

Chain d7:



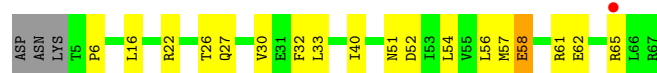
- Molecule 30: 40S ribosomal protein S28-A

Chain D8:



- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 



- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 



- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 



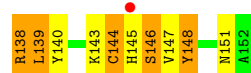
- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 



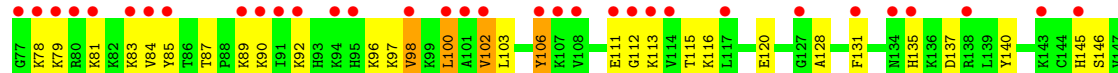
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 



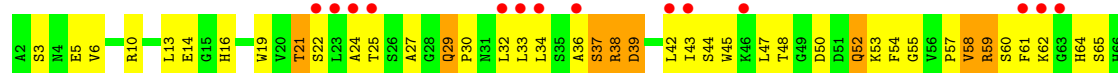
- Molecule 33: Ubiquitin-40S ribosomal protein S31

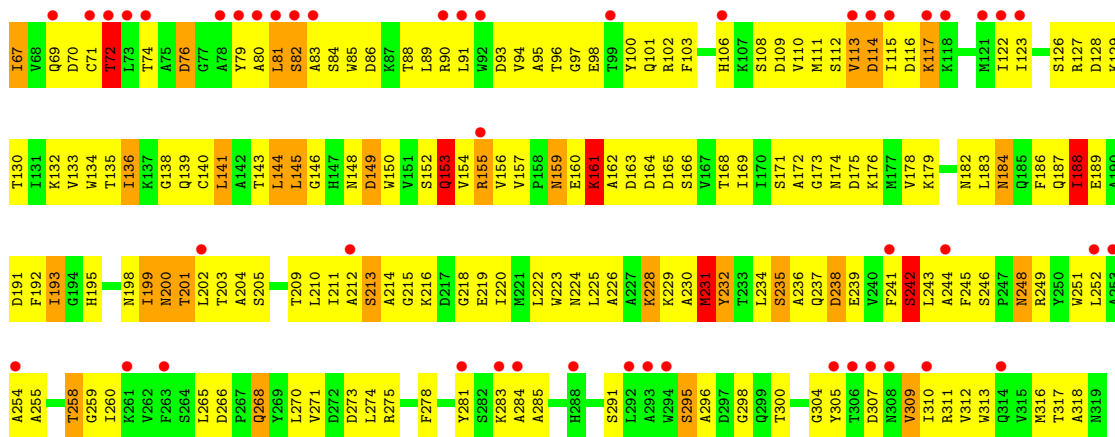
Chain e1: 



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

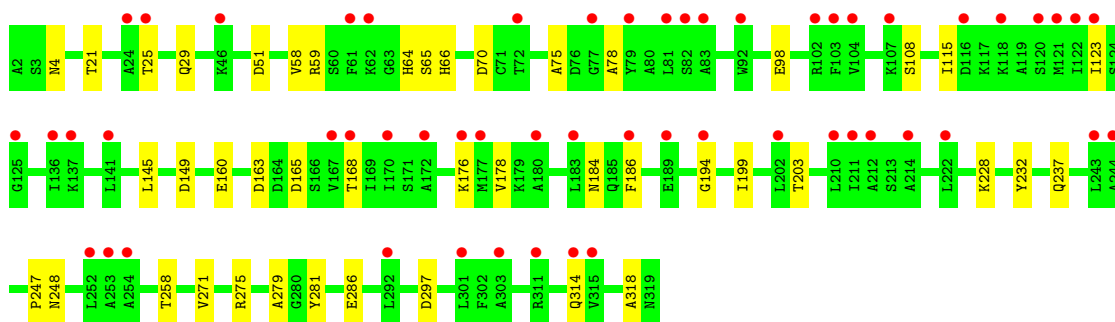
Chain SR: 





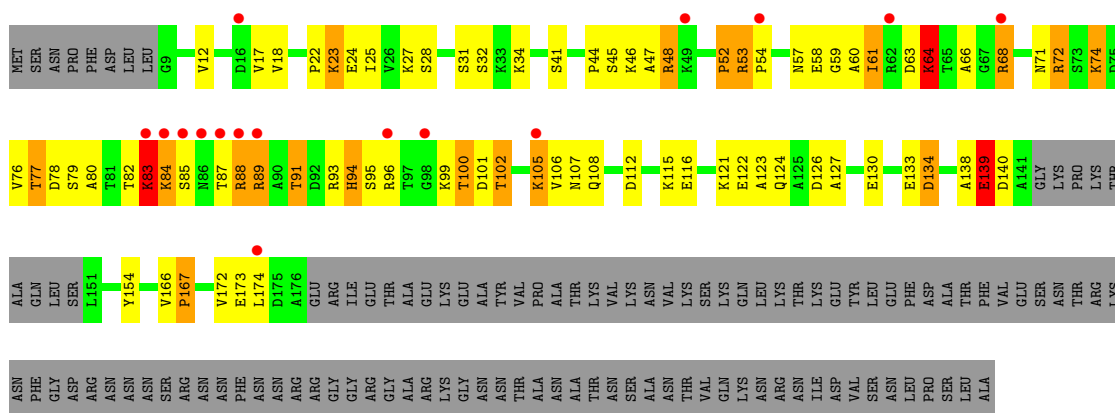
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



• Molecule 35: Suppressor protein STM1

Chain SM:



• Molecule 35: Suppressor protein STM1

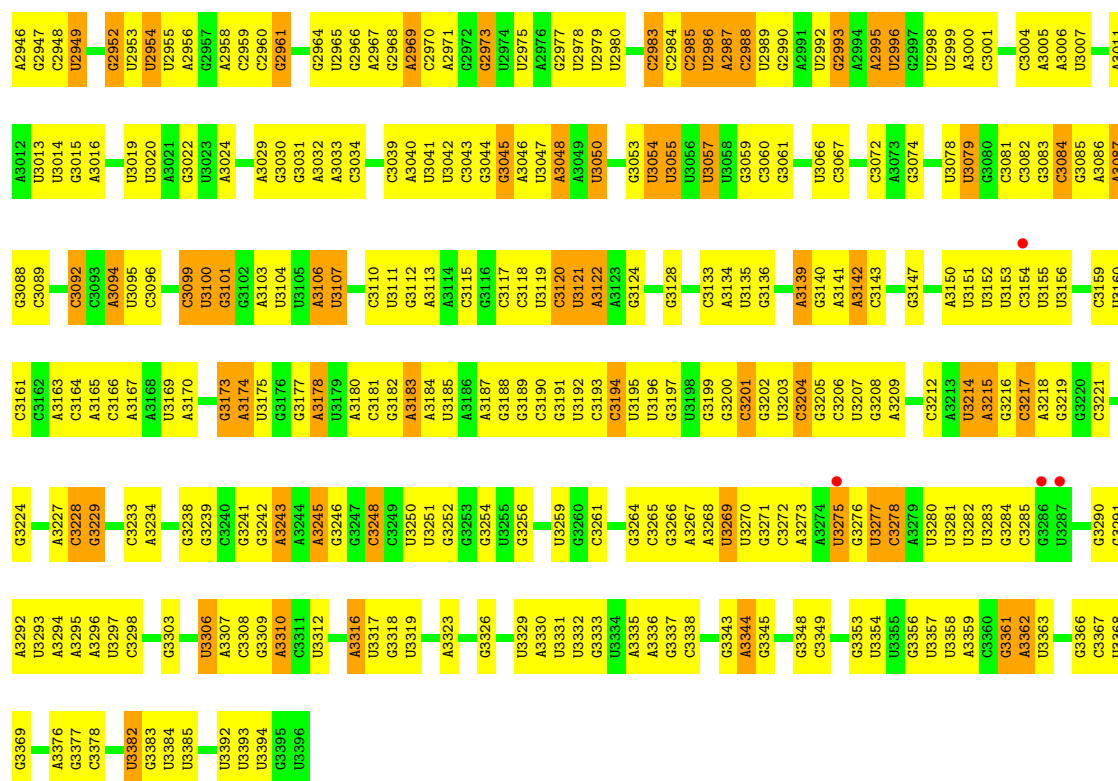
Chain sM:



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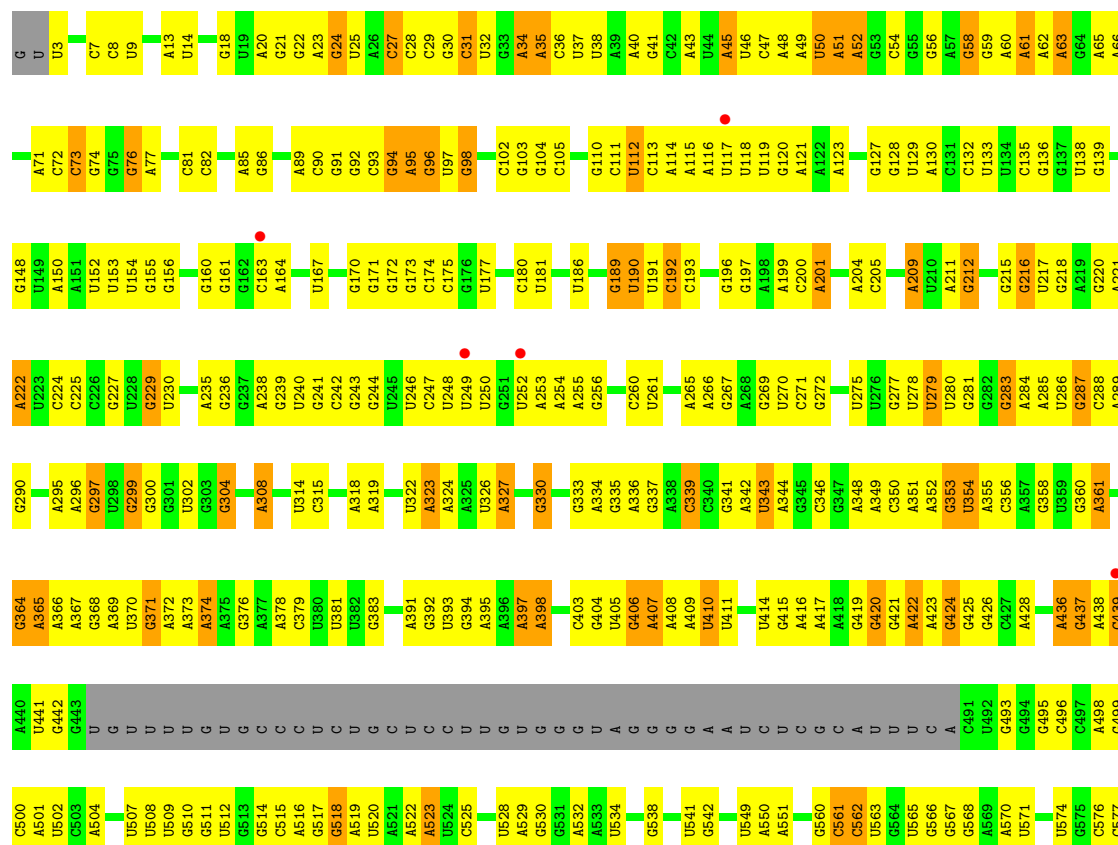


WORLD WIDE
PDB
PROTEIN DATA BANK



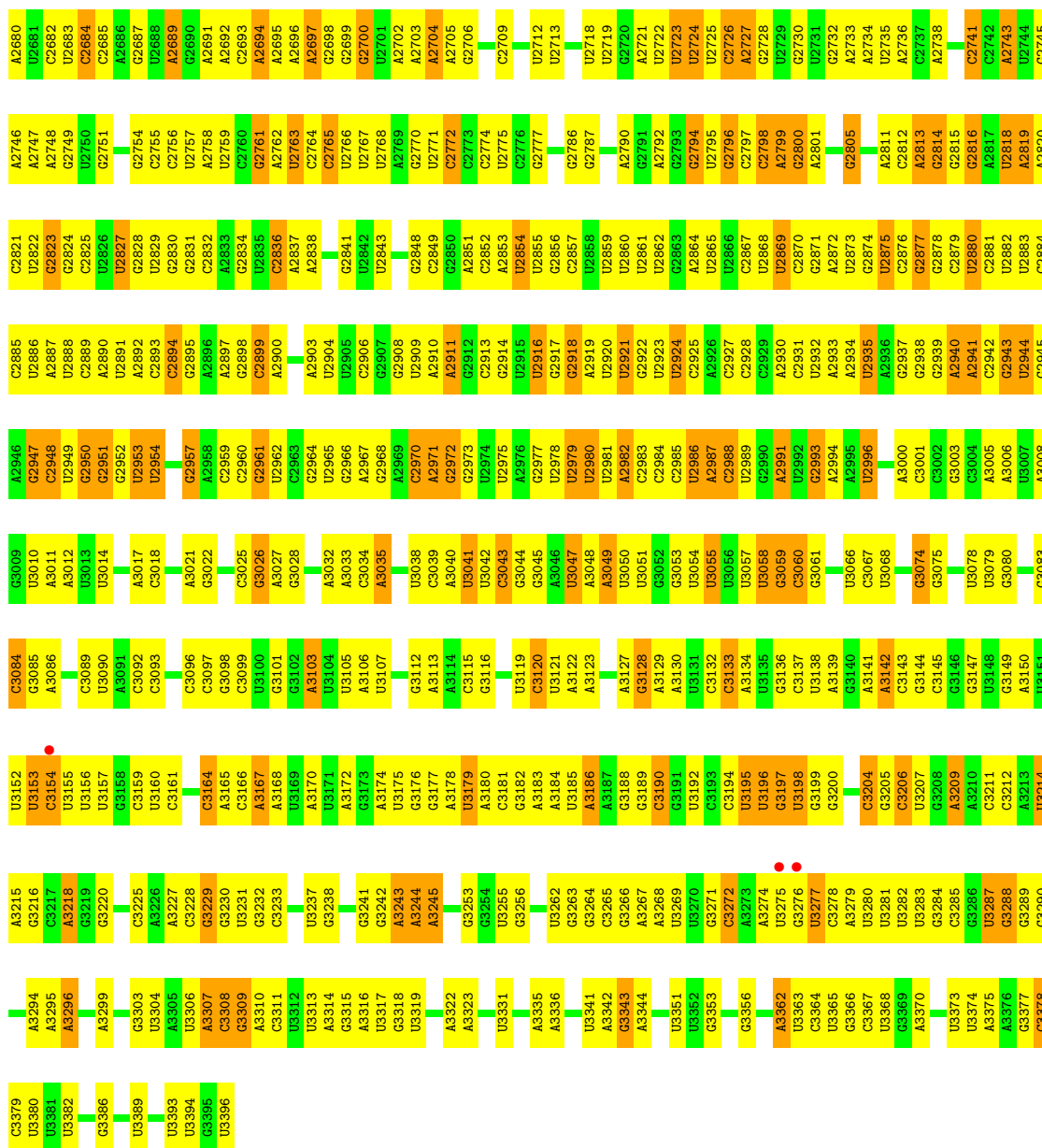
● Molecule 36: TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

Chain 5:



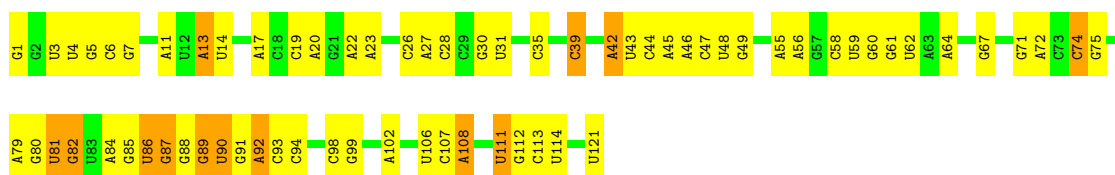
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U1566	A1489	G1421	A1350	G1281	A1195	C1132	G1066	G864	C787	U713	C650	
U1568	A1490	G1422	U1351	G1281	C1196	A1133		U865	C788	U714	G651	A585
U1569	G1493	C1423	A1352	A1197	A1198	G1134	C1069	G869	A789	A715	G652	C586
U1494	U1494	G1424	U1353	C1199	A1199	A1135	U1070	G870	U790	A716	C554	U587
U1495	U1495	U1425	G1354	A1286	A1200	G1137	G1072	U871	A791	C717	G588	G588
U1496	C1426	C1426	A1355	A1286	A1200	C1137		U872	G792	G718	C655	A589
C1497	C1497	U1427	U1356	U1356	A1201	G1142	U1073	U873	C793	U719	A656	G590
C1574	A1428	A1428	G1362	U1292	A1203	A1143	U1075	U874	G794	A720	G658	G591
A1498	G1429	G1429	A1363	U1294	A1205	U1144	U1078	G875	U796	G725	G659	A592
C1501	U1430	U1430	C1364	G1295	G1206	G1145	A1079	A876	A660	G726	A660	C593
C1502	G1431	G1431	C1365	C1296	G1207	C1146		C877	U594	G727	G661	G595
C1578	C1432	C1432	A1366	C1297	U1208	G1147	U1080	C878	U662	G727	U662	C596
C1579	A1433	A1433	A1367	U1298	G1209	G1148	U1081	U879	C663	C729	C663	
C1580	G1434	G1434	U1368	U1299	U1210	G1149	U1082	C803	U664	C730	U664	C599
C1581	U1435	U1435	A1369	A1301	U1211	A1150	G1083	C804	A665	U731	A665	G600
C1582	U1436	U1436	G1370	A1302	A1212	U1151	A1084	A882	A666	C732	A666	U601
C1583	C1437	C1437	G1371	A1303	G1213	G1152	A1085	A883	G687	G733	G687	A802
C1584	U1438	U1438	C1372	A1304	U1214	A1153		A884	G688	C734	G688	A803
C1585	U1439	U1439	A1373	A1305	A1221	U1154	G1090	U811	A670	A736	C670	G604
C1586	G1440	G1440	G1374	U1306	G1222	C1155	U1093	A888	U671	A737	A672	C506
C1587	U1441	U1441	G1375	G1307	G1222	G1156	A1094	U889	U673	G740	U673	A808
C1588	G1442	G1442	C1376	A1308	G1226	U1158	U1095	C890				
C1589	U1443	U1443	G1377	U1309		A1159	U1096	C891				
C1590	G1444	G1444	A1378	G1310	G1230	C1160	U1097	C893	G676	U741	G676	G609
C1591	U1445	U1445	G1379	A1311	A1231	G1161	A1098	U894	A611	C742	A611	G610
C1592	G1446	G1446	G1380	C1312	C1232	U1162	A1099	C988	A612	C743	A612	A611
C1593	U1447	U1447	A1381	G1313	G1233	U1163	U1100	U954	U679	A744	U679	U612
C1594	G1448	G1448	G1382	C1314	G1234	G1164	A1025	U955				G613
C1595	U1449	U1449	U1383	U1315	U1235	A1165	A1026	U956				
C1596	A1450	A1450	C1384	A1317	G1236	G1166	U1028	U957				
C1597	U1451	U1451	A1385	A1318	G1237	U1167	G1029	A965	G685	C749	G685	A619
C1598	G1452	G1452	A1386	G1319	C1238	U1168	U1032	U966	U687	C752	U687	U620
C1599	U1453	U1453	G1387	C1320	A1239	A1169	U1033	U967	G688	C753	G688	A622
C1600	U1454	U1454	U1388	C1321	U1241	A1170		U968	U689	U756	U689	U623
C1601	U1455	U1455	G1389	U1322	G1242	G1171	U1108	U969	A691	C757	A691	A628
C1602	U1456	U1456	A1390	G1323	G1243	U1172	U1109	A970	A692	C758	A692	U629
C1603	U1457	U1457	A1393	U1324	A1244	G1174	U1111	G971	C693	U759	C693	A630
C1604	G1464	G1464	C1397	U1325	A1245	G1175	A1112	A972	C694	U764	C694	U631
C1605	U1465	U1465	U1398	C1326	G1246	C1176	G1113	G973	G695		G695	G632
C1606	A1466	A1466	A1399	U1329	G1249	G1177	U1114	C975	C696	U767	C696	A628
C1607	U1467	U1467	G1400	A1330	U1250	A1178	G1115	U976	A697	C768	A697	A630
C1608	A1468	A1468	G1404	U1331	A1251	A1180	G1116	C977	C698	U769	C698	U629
C1609	C1469	C1469	G1404	U1332	A1252	U1181	G1117	G978	C699	G770	U699	G635
C1610	U1470	U1470	G1404	U1333	A1253	U1182	C1118	U979	C700	A771	C700	C636
C1611	A1471	A1471	G1404	U1334	U1254	A1183	C1119	A980	G701	U772	G701	C638
C1612	U1472	U1472	G1404	C1335	U1255	C1183	U1120	U981	C702	U776	C702	G639
C1613	A1473	A1473	U1407	U1336	A1256	A1184	A1121	C982	U703		U703	U640
C1614	U1474	U1474	G1408	A1337	U1257	C1185	U1122	A983	U704		U704	C641
C1615	C1475	C1475	U1409	C1338	G1261	G1186	U1123	G984	A705	G779	A705	U642
C1616	A1476	A1476	C1411	C1339	G1262	C1187	U1124	U985	U643	G780	A706	U643
C1617	U1477	U1477	C1412	G1340	A1263	U1188	U1125	G923	U644	G781	U707	G644
C1618	G1478	G1478	C1413	U1341	G1264	C1189	G1126	A925	A645	U782	U708	A645
C1619	U1479	U1479	U1414	U1344	U1270	A1190	U1127	A989	A646		A646	
C1620	A1480	A1480	U1415	G1344	A1271	U1191	A783	C927	A710		A710	A647
C1621	C1481	C1481	G1416	G1345		C1192		G991				
C1622	U1482	U1482										
C1623	A1483	A1483										
C1624	U1484	U1484										
C1625	C1485	C1485										
C1626	U1486	U1486										
C1627												
C1628												
C1629												
C1630												





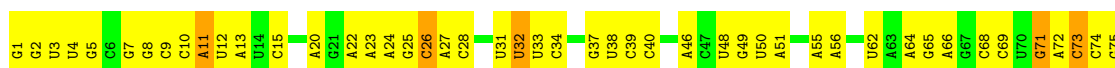
- Molecule 37: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

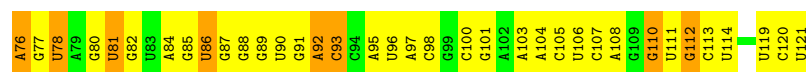
Chain 3:



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

Chain 7:





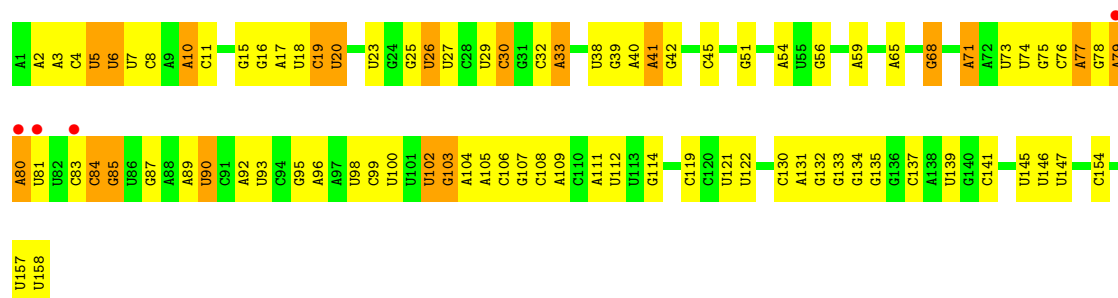
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 4:



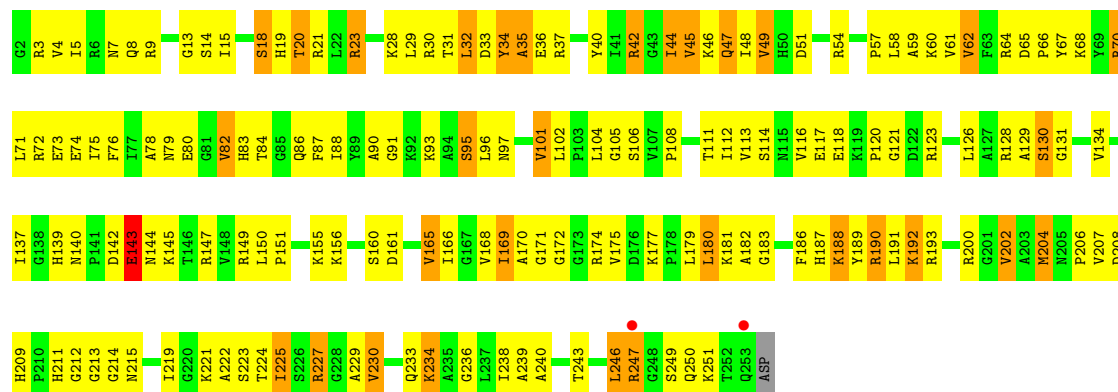
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 8:



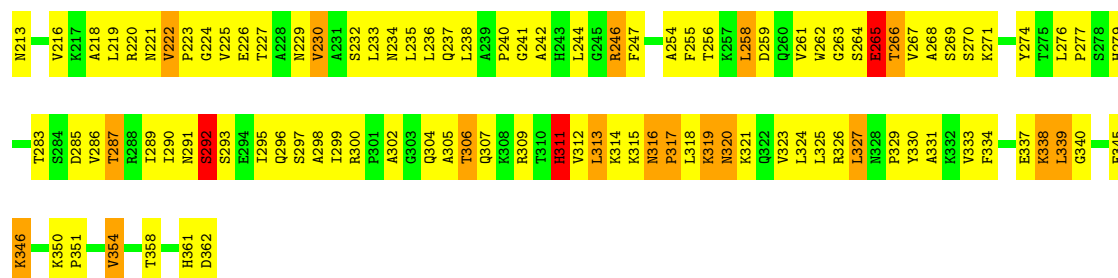
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



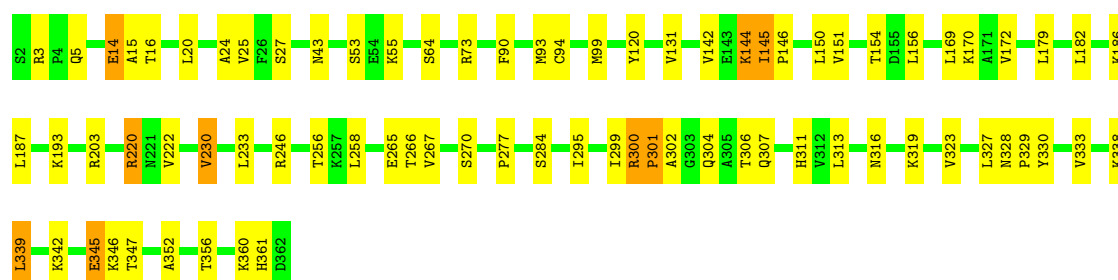
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



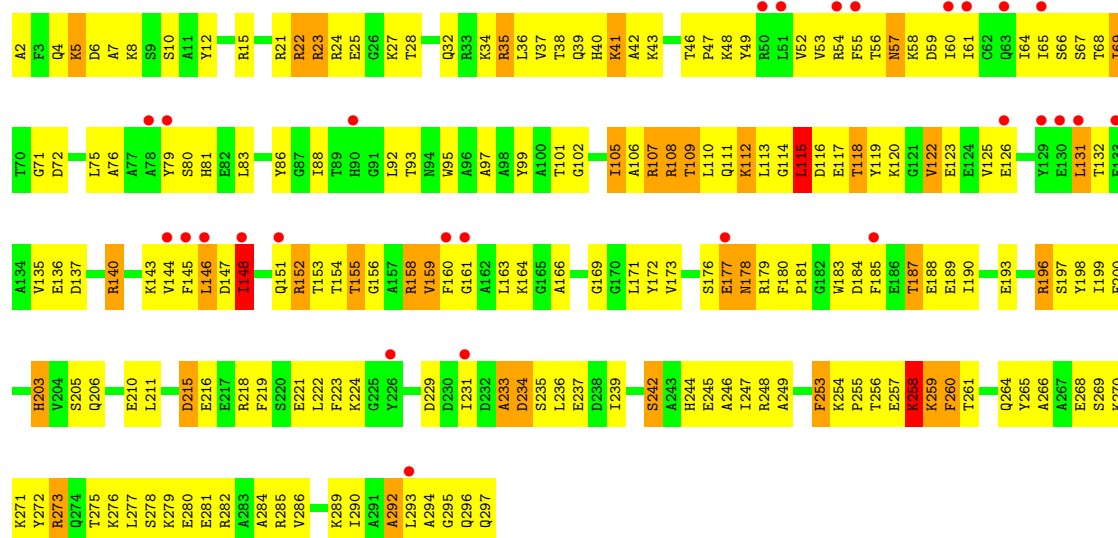
• Molecule 41: 60S ribosomal protein L4-A

Chain 14:



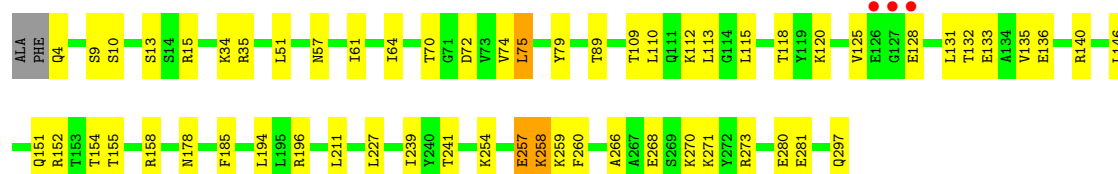
• Molecule 42: 60S ribosomal protein L5

Chain L5:

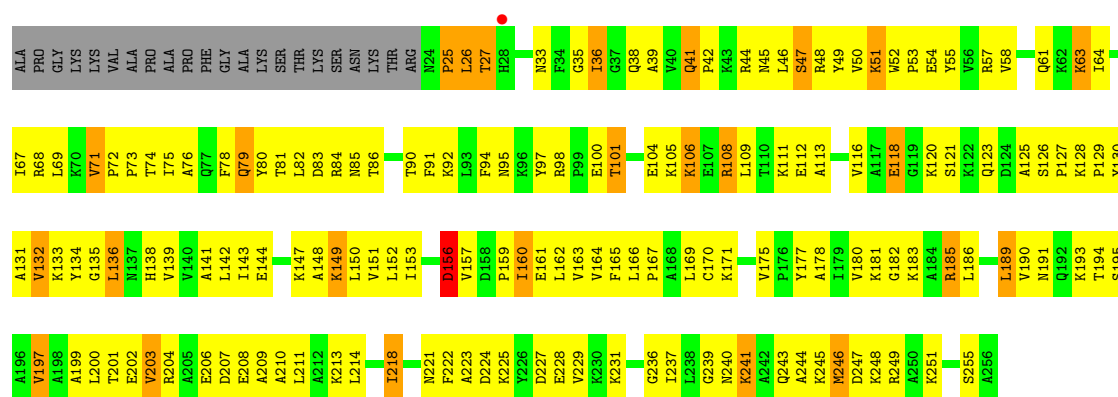


• Molecule 42: 60S ribosomal protein L5

Chain L5:

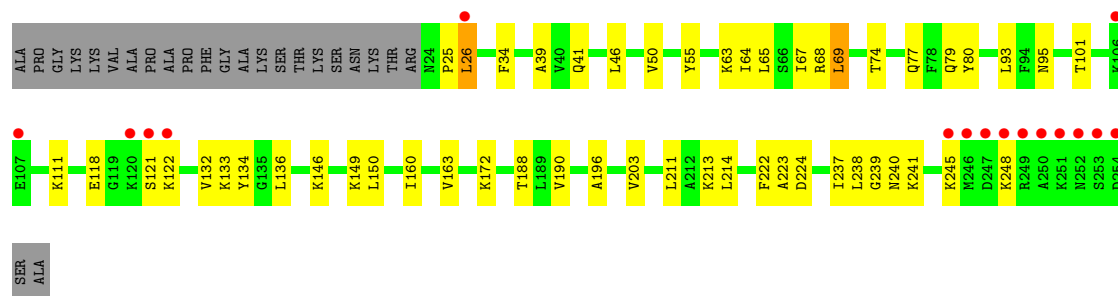






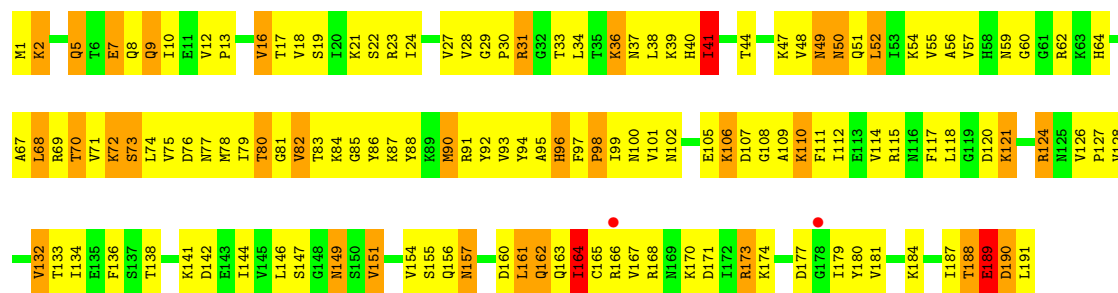
• Molecule 45: 60S ribosomal protein L8-A

Chain 18:



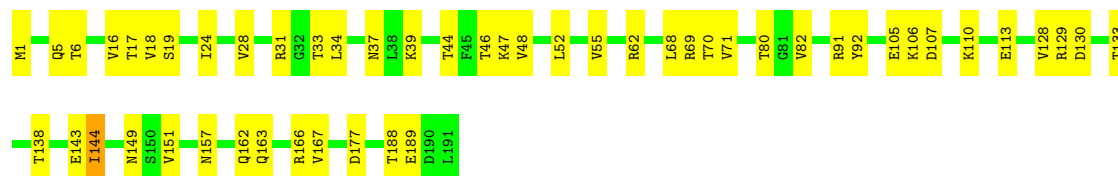
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



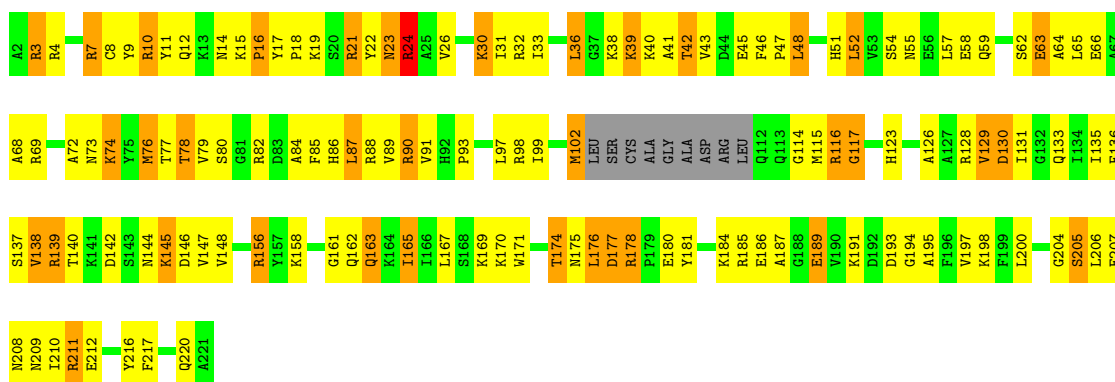
• Molecule 46: 60S ribosomal protein L9-A

Chain 19:



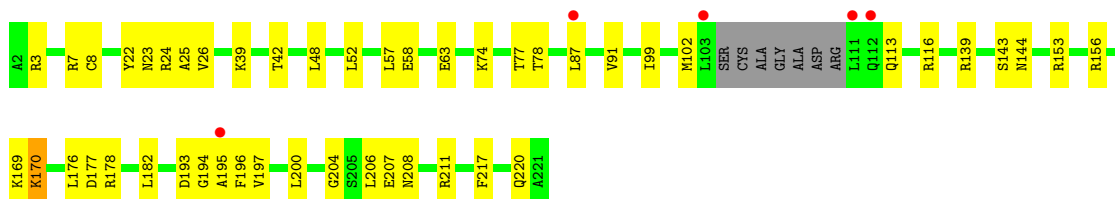
• Molecule 47: 60S ribosomal protein L10

Chain M0:



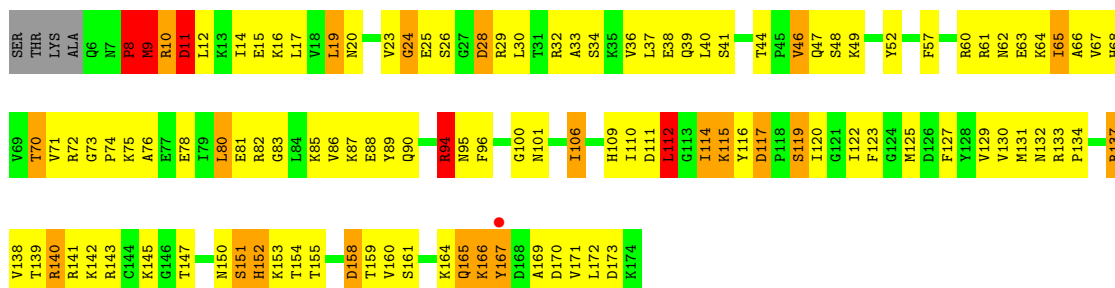
• Molecule 47: 60S ribosomal protein L10

Chain m0:



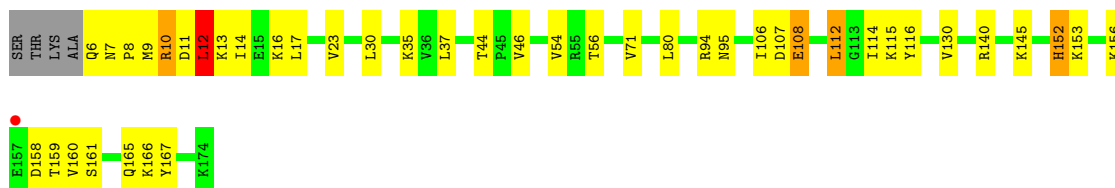
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



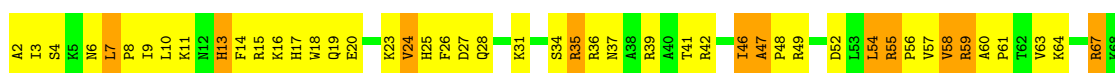
• Molecule 48: 60S ribosomal protein L11-B

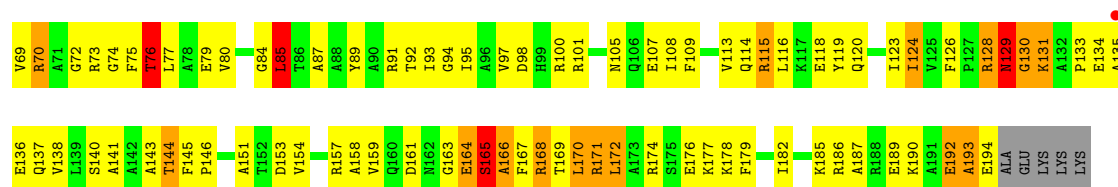
Chain m1:



• Molecule 49: 60S ribosomal protein L13-A

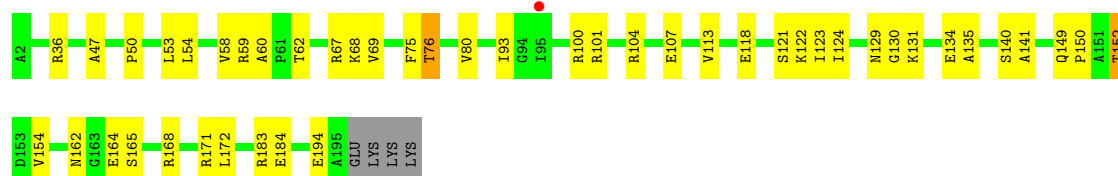
Chain M3:





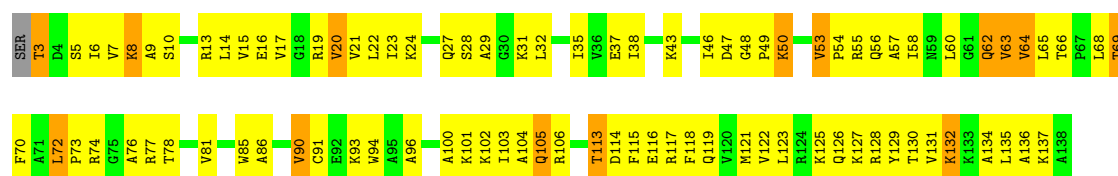
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



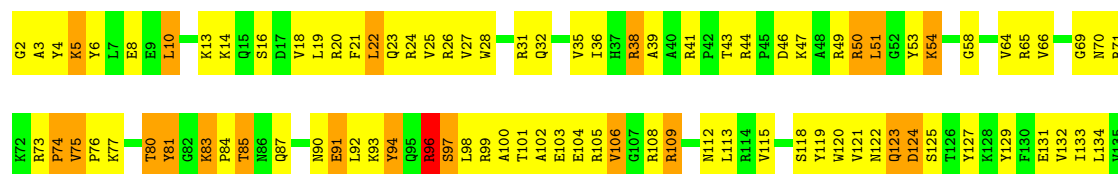
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



• Molecule 51: 60S ribosomal protein L15-A

Chain M5:



• Molecule 51: 60S ribosomal protein L15-A

Chain m5:





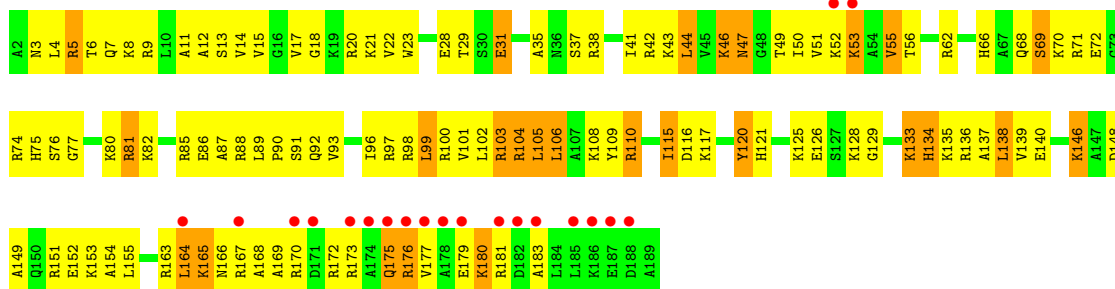


- Molecule 54: 60S ribosomal protein L18-A

Chain m8:

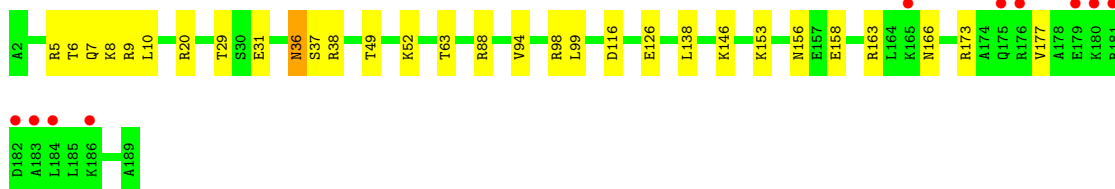
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:



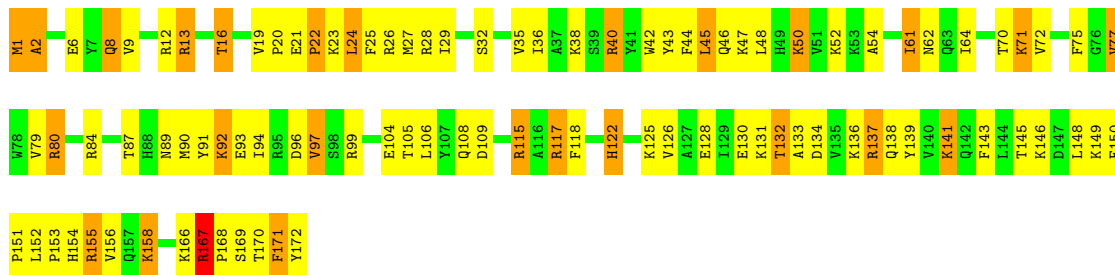
- Molecule 55: 60S ribosomal protein L19-A

Chain m9:



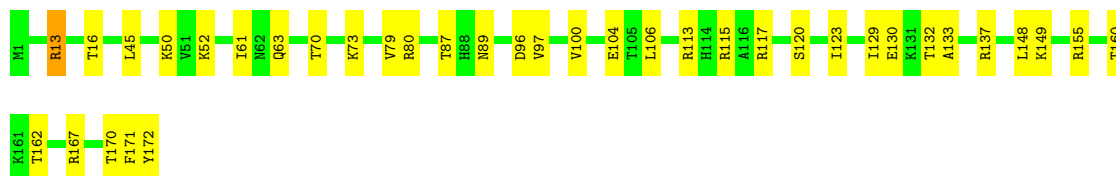
- Molecule 56: 60S ribosomal protein L20-A

Chain N0:

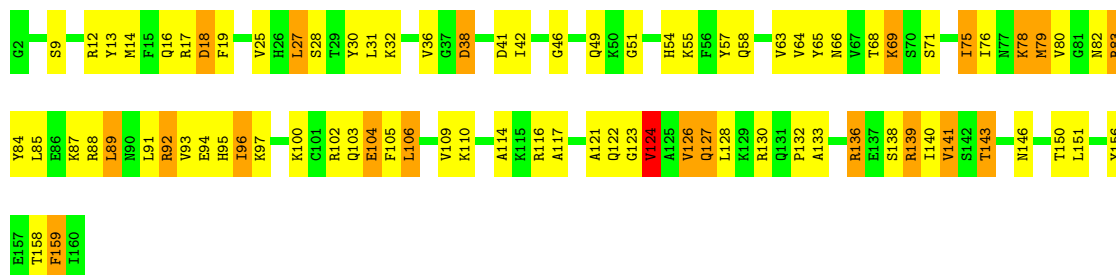


- Molecule 56: 60S ribosomal protein L20-A

Chain n0:




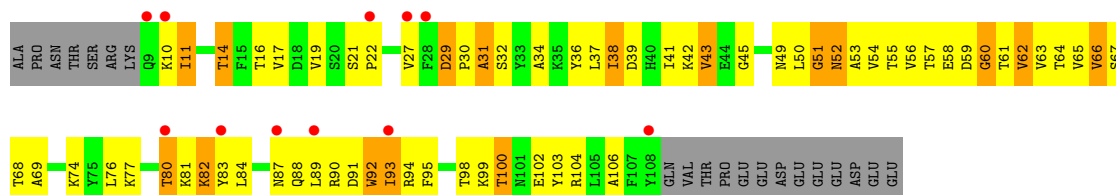
- Chain N1:



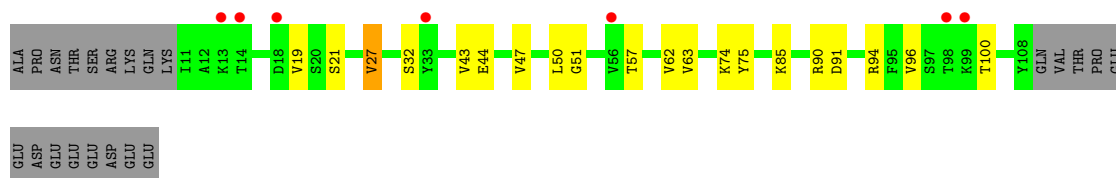
- Chain n1: 



- Chain N2: 



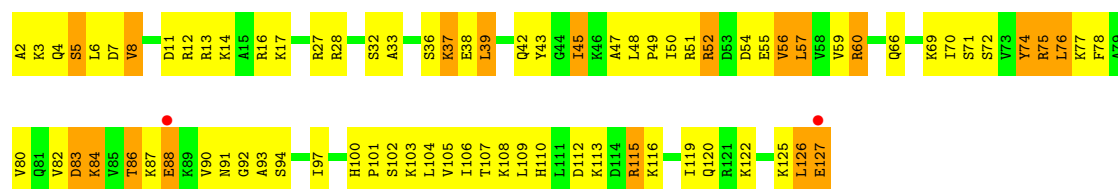
- Chain n2:



- Chain N3:

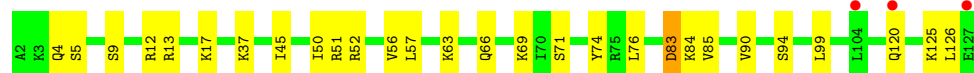


Chain N6: 



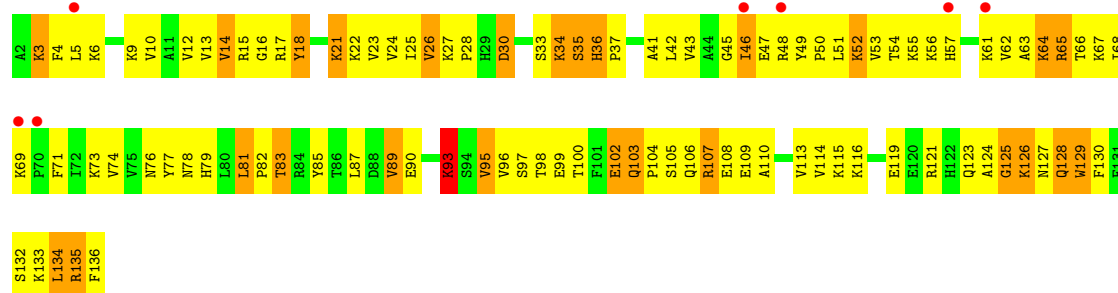
- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 



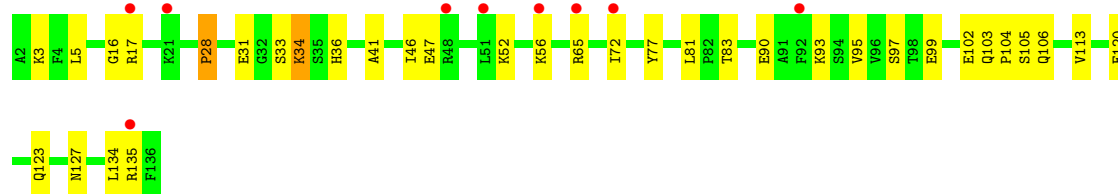
- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 



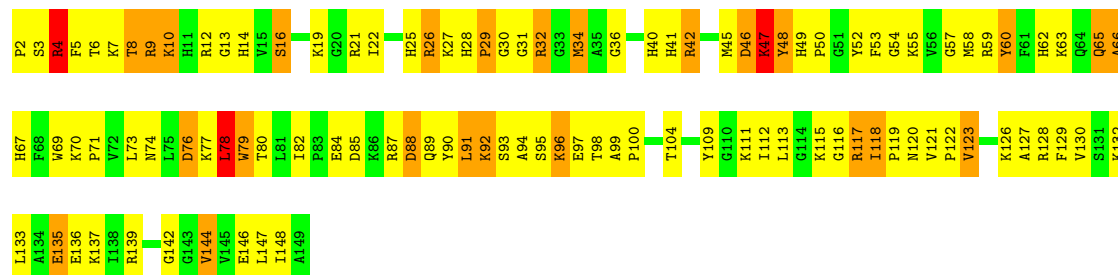
- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 

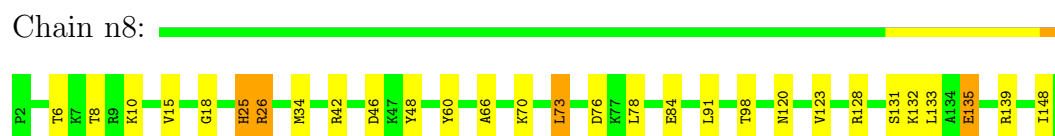


- Molecule 64: 60S ribosomal protein L28

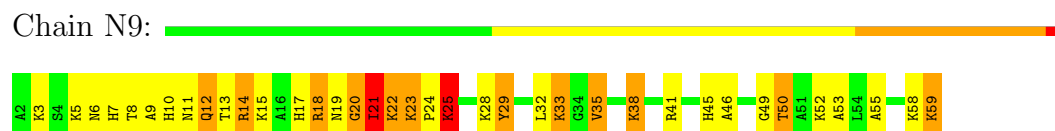
Chain N8: 



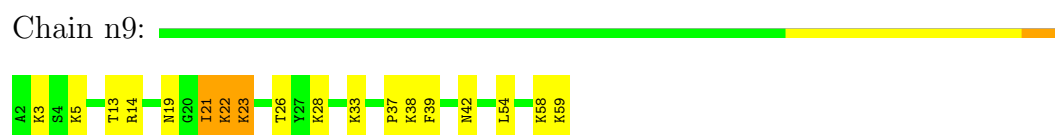
- Molecule 64: 60S ribosomal protein L28



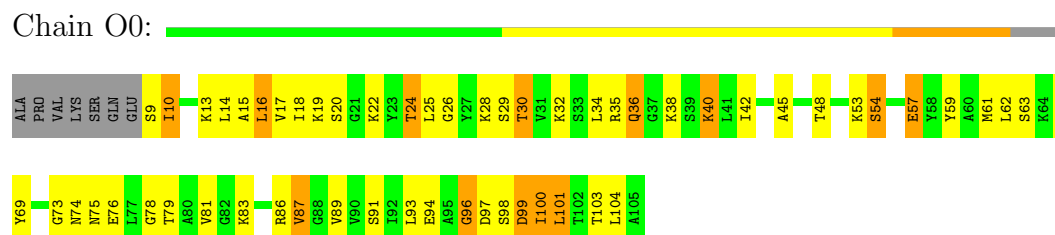
- Molecule 65: 60S ribosomal protein L29



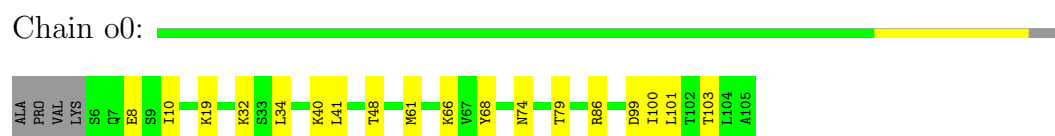
- Molecule 65: 60S ribosomal protein L29



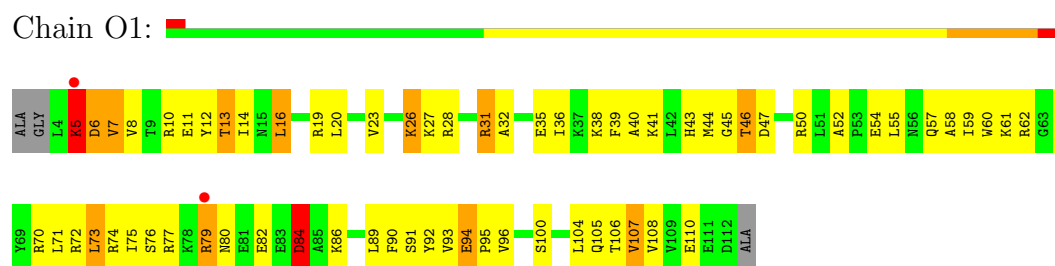
- Molecule 66: 60S ribosomal protein L30



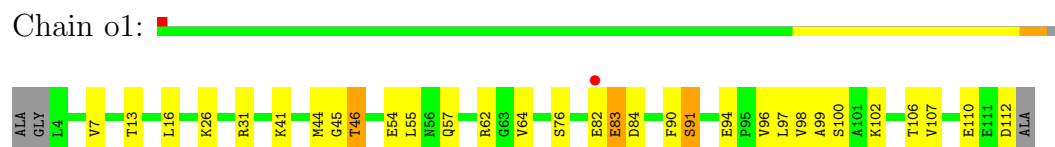
- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A



- Molecule 67: 60S ribosomal protein L31-A



- Molecule 68: 60S ribosomal protein L32

A2	S3	L4	K8	I9	K12	H13	T14	K15	K16	F17	K18	R19	H20	H21	R24	Y25	H26	R27	V28	N31	V32	R33	K34	Q35	K36	G37	S40	V41	V42	R43	R44	R45	F46	R47	G48	N49	S51	Q52	P53	K54	I55	G56	Y57	G58	S59	N60	K61	K62	T63	K64	F65	L66
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H71	K72	T73	F74	L75	V76	A77	N78	V79	K80	D81	L82	E83	T84	H88	T91	A97	I100	I101	A102	K103	H104	R105	V106	V107	I108	L109	A110	R111	L115	G116	I117	K118	V119	P122	K123	G124	R125	L126	A127	L128	G129	A130
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- Chain o2:

Amino Acid	Frequency (approx.)
A27	115
L28	115
A2	110
L4	105
P6	100
H6	95
F7	90
R8	85
T14	80
K15	75
K16	70
F17	65
H21	60
R24	55
R27	50
R33	45
K34	40
Q35	35
K36	30
V41	25
R47	20
S51	15
K62	10
T63	5
K64	5
H71	5
K72	5
I73	5
F74	5
L75	5
L82	5
H87	5
H88	5
T89	5
K90	5
T91	5
E95	5
S101	5
L109	5
A110	5
R111	5
K123	5
G124	5
I125	5
L126	5

- Chain 03: 

T72	T73	T74	T75	T76	T77		V80	V81	R82	A83		R86	N87	N88	L89	P90	A91	K92	T93	F94	G95	A96	S97	V98	R99	I100	F101	L102	Y103	P104	S105	N106	I107																									
A2	E3	S4	H5	R6	L7	Y8	V9	K10	G11	K12	H13	L14	S15	Y16		R21	N22	N23	N24	P25	N26	V27		K31	I32	E33	G34	V35		P38	Q39	D40	A41	Q42	F43	Y44	L45	G46	K47	R48	L49	A50	Y51	V52	Y53		S56	K57	E58	Y59	R60		V66	M67	W68	G69	K70	Y71

- Chain o3: 

Category	Count
A2	10
E3	10
S4	10
R18	10
S19	10
K31	10
Q42	10
I49	10
S56	10
K57	10
E58	10
V59	10
G61	10
S62	10
K63	10
K70	10
T74	10
V81	10
T84	10
P90	10
T93	10
V98	10
R99	10
I107	10

- Chain 04:

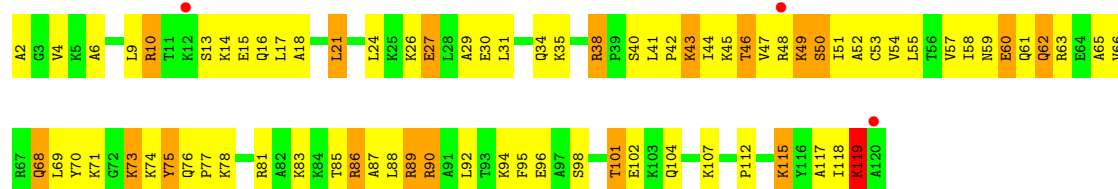
C81	C82	C83	C84	V85	K86	E87	R88	R89	I90	E91	L94	I95	E96	E97	Q98	E99	K99	I100	K102	K103	V104	V105	E107	Q108	T109	E110	K113	LYS	GLU	SLR	LYS	LYS	ALA	LYS	LYS	P59	R60	Q61	Y62	A63	V65	S66	K67	H68	H69	K70	T71	R74	A75	G78	S79	E80
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain 04: 

Category	Count
A2	1
V5	1
I20	1
K21	1
V22	1
V23	1
K24	1
Q33	1
H34	1
V35	1
K36	1
K37	1
T40	1
C47	1
L57	1
R58	1
P59	1
T71	1
S79	1
A82	1
N83	1
E87	1
R88	1
Q98	1
V104	1
K113	1
LYS	1
SER	1
GLU	1
LYS	1
LYS	1
ALA	1
LYS	1
LYS	1

- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



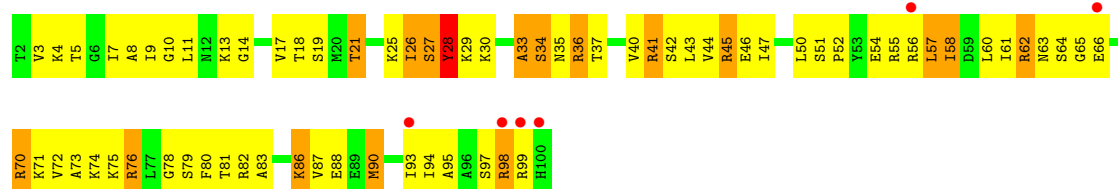
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:



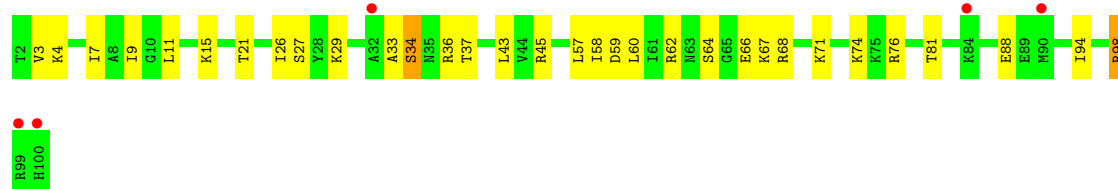
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:



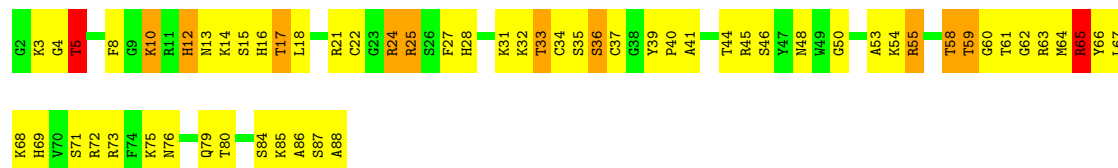
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



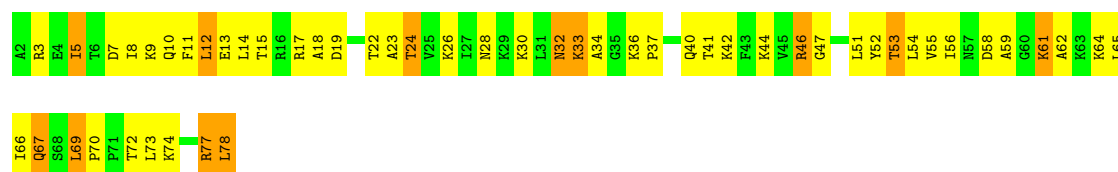
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



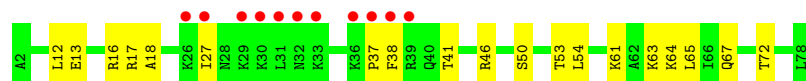
- Molecule 74: 60S ribosomal protein L38

Chain O8:



- Molecule 74: 60S ribosomal protein L38

Chain o8:



- Molecule 75: 60S ribosomal protein L39

Chain O9:



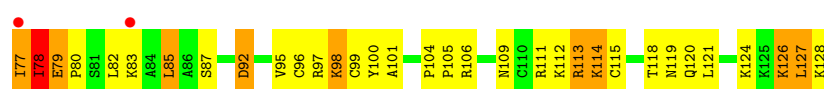
- Molecule 75: 60S ribosomal protein L39

Chain o9:



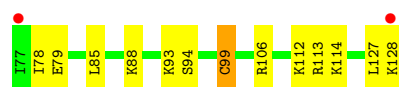
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



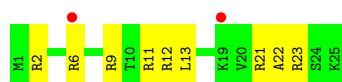
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



- Molecule 77: 60S ribosomal protein L41-A

Chain q1:



- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



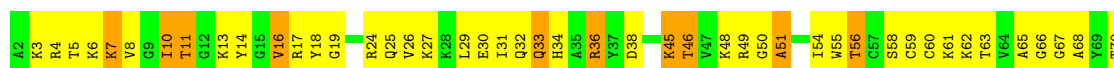
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:



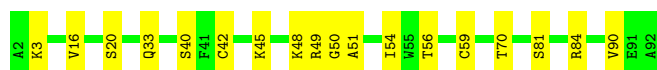
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



- Molecule 79: 60S ribosomal protein L43-A

Chain q3:



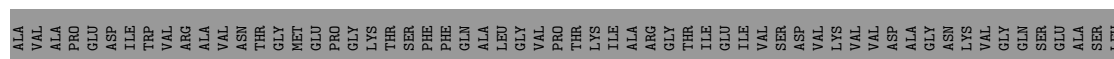
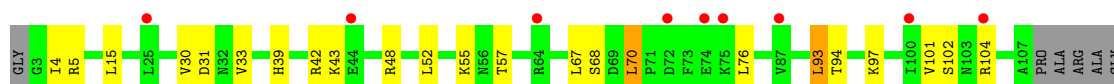
- Molecule 80: 40S ribosomal protein S30-A

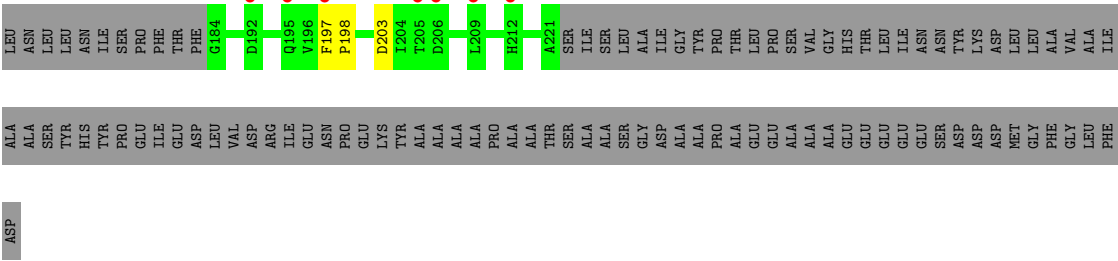
Chain e0:



- Molecule 81: 60S acidic ribosomal protein P0

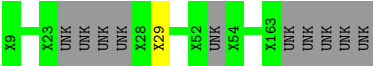
Chain p0:





- Molecule 82: Unknown protein chain m2

Chain m2:



- Molecule 83: Unknown protein chain p1

Chain p1:

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein chain p2

Chain p2:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.15Å 287.07Å 303.24Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	99.87 – 3.20 99.87 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.87-3.20) 99.9 (99.87-3.20)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.194 , 0.246 0.267 , 0.308	Depositor DCC
R_{free} test set	23915 reflections (1.98%)	DCC
Wilson B-factor (Å ²)	88.0	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 1206031 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	411206	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: MG, OHX, ZN, 3K8

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.79	5/41698 (0.0%)	1.34	378/64972 (0.6%)
1	6	0.90	17/42765 (0.0%)	1.39	452/66634 (0.7%)
2	S0	0.48	0/1617	0.67	0/2215
2	s0	0.47	0/1623	0.71	0/2222
3	S1	0.41	0/1735	0.68	2/2335 (0.1%)
3	s1	0.53	0/1748	0.70	0/2352
4	S2	0.52	0/1665	0.65	0/2263
4	s2	0.59	0/1665	0.74	0/2263
5	S3	0.50	0/1759	0.69	0/2368
5	s3	0.44	0/1759	0.59	0/2368
6	S4	0.51	0/2109	0.74	1/2839 (0.0%)
6	s4	0.55	0/2109	0.78	0/2839
7	S5	0.41	0/1629	0.62	0/2202
7	s5	0.46	0/1629	0.66	0/2202
8	S6	0.50	0/1823	0.67	0/2439
8	s6	0.59	0/1779	0.73	0/2379
9	S7	0.46	0/1506	0.69	0/2028
9	s7	0.47	0/1516	0.70	1/2043 (0.0%)
10	S8	0.59	0/1514	0.78	1/2021 (0.0%)
10	s8	0.64	0/1514	0.70	0/2021
11	S9	0.48	0/1519	0.69	0/2035
11	s9	0.57	0/1519	0.76	2/2035 (0.1%)
12	C0	0.44	0/790	0.67	1/1069 (0.1%)
12	c0	0.38	0/777	0.67	3/1049 (0.3%)
13	C1	0.62	0/1240	0.76	0/1675
13	c1	0.67	0/1194	0.77	0/1610
14	C2	0.37	0/900	0.64	0/1224
14	c2	0.29	0/900	0.56	0/1224
15	C3	0.51	0/1215	0.70	2/1638 (0.1%)
15	c3	0.61	0/1215	0.69	0/1638
16	C4	0.43	0/901	0.70	0/1217
16	c4	0.56	0/960	0.75	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.48	0/998	0.69	0/1341
17	c5	0.50	0/1060	0.69	0/1426
18	C6	0.46	0/1125	0.71	2/1510 (0.1%)
18	c6	0.49	0/1131	0.70	0/1518
19	C7	0.46	0/935	0.64	0/1254
19	c7	0.51	0/914	0.70	0/1224
20	C8	0.47	0/1211	0.65	1/1628 (0.1%)
20	c8	0.51	0/1211	0.73	2/1628 (0.1%)
21	C9	0.45	0/1130	0.66	0/1517
21	c9	0.52	0/1130	0.68	0/1517
22	D0	0.49	0/865	0.65	0/1169
22	d0	0.47	0/892	0.65	0/1205
23	D1	0.49	0/693	0.68	0/935
23	d1	0.52	0/693	0.69	0/935
24	D2	0.53	0/1038	0.74	2/1395 (0.1%)
24	d2	0.62	0/1038	0.78	1/1395 (0.1%)
25	D3	0.64	0/1139	0.80	2/1518 (0.1%)
25	d3	0.72	0/1139	0.85	2/1518 (0.1%)
26	D4	0.50	0/1087	0.64	0/1449
26	d4	0.54	0/1087	0.73	0/1449
27	D5	0.40	0/571	0.73	1/768 (0.1%)
27	d5	0.46	0/566	0.71	0/761
28	D6	0.51	0/782	0.69	0/1047
28	d6	0.56	0/782	0.69	0/1047
29	D7	0.47	0/620	0.66	0/838
29	d7	0.49	0/620	0.71	0/838
30	D8	0.37	0/499	0.58	0/670
30	d8	0.45	0/499	0.64	0/670
31	D9	0.56	0/452	0.73	1/600 (0.2%)
31	d9	0.51	0/452	0.68	0/600
32	E0	0.51	0/483	0.66	0/643
33	E1	0.47	0/577	0.81	0/770
33	e1	0.42	0/619	0.73	0/822
34	SR	0.41	0/2494	0.64	1/3393 (0.0%)
34	sR	0.38	0/2495	0.57	0/3395
35	SM	0.54	0/1113	0.75	2/1502 (0.1%)
35	sM	0.48	0/682	0.68	1/921 (0.1%)
36	1	1.25	247/75394 (0.3%)	1.73	2232/117545 (1.9%)
36	5	1.26	266/75414 (0.4%)	1.73	2109/117575 (1.8%)
37	3	1.02	0/2883	1.46	30/4491 (0.7%)
37	7	1.20	8/2883 (0.3%)	1.73	86/4491 (1.9%)
38	4	1.17	3/3746 (0.1%)	1.69	85/5832 (1.5%)
38	8	1.07	4/3746 (0.1%)	1.54	64/5832 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.81	0/1948	0.86	0/2617
39	l2	0.72	0/1946	0.88	3/2614 (0.1%)
40	L3	0.80	1/3146 (0.0%)	0.83	1/4228 (0.0%)
40	l3	0.90	1/3146 (0.0%)	0.89	2/4228 (0.0%)
41	L4	0.86	0/2800	0.94	7/3790 (0.2%)
41	l4	0.82	1/2800 (0.0%)	0.93	2/3790 (0.1%)
42	L5	0.58	0/2425	0.71	0/3271
42	l5	0.74	1/2408 (0.0%)	0.81	1/3248 (0.0%)
43	L6	0.82	0/1260	0.82	0/1694
43	l6	0.84	0/1269	0.88	1/1705 (0.1%)
44	L7	0.85	0/1821	0.92	3/2451 (0.1%)
44	l7	0.95	1/1828 (0.1%)	0.93	3/2461 (0.1%)
45	L8	0.60	0/1836	0.72	1/2481 (0.0%)
45	l8	0.54	0/1795	0.70	1/2429 (0.0%)
46	L9	0.73	0/1539	0.82	2/2073 (0.1%)
46	l9	0.84	0/1539	0.86	0/2073
47	M0	0.78	1/1741 (0.1%)	0.86	3/2335 (0.1%)
47	m0	0.80	1/1758 (0.1%)	0.88	0/2358
48	M1	0.53	0/1374	0.71	1/1842 (0.1%)
48	m1	0.69	0/1374	0.82	2/1842 (0.1%)
49	M3	0.81	0/1568	0.90	3/2106 (0.1%)
49	m3	0.73	0/1573	0.85	0/2113
50	M4	0.84	0/1068	0.86	0/1438
50	m4	0.92	0/1074	0.90	2/1446 (0.1%)
51	M5	0.83	1/1757 (0.1%)	0.89	2/2354 (0.1%)
51	m5	0.72	0/1757	0.86	4/2354 (0.2%)
52	M6	0.96	2/1585 (0.1%)	0.97	4/2128 (0.2%)
52	m6	1.04	2/1585 (0.1%)	0.96	4/2128 (0.2%)
53	M7	0.84	1/1443 (0.1%)	0.87	3/1944 (0.2%)
53	m7	0.97	1/1250 (0.1%)	0.93	1/1683 (0.1%)
54	M8	0.84	0/1465	0.88	0/1965
54	m8	0.78	0/1465	0.90	1/1965 (0.1%)
55	M9	0.61	0/1538	0.70	0/2050
55	m9	0.65	0/1538	0.71	0/2050
56	N0	0.86	0/1481	0.86	1/1990 (0.1%)
56	n0	0.93	0/1481	0.93	3/1990 (0.2%)
57	N1	0.84	0/1300	0.85	1/1743 (0.1%)
57	n1	0.93	3/1300 (0.2%)	0.85	1/1743 (0.1%)
58	N2	0.44	0/812	0.62	0/1099
58	n2	0.54	0/794	0.74	0/1076
59	N3	0.79	0/1018	0.87	0/1369
59	n3	0.90	0/1018	0.92	3/1369 (0.2%)
60	N4	0.64	0/712	0.74	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.69	0/1052	0.76	0/1398
61	N5	0.69	0/979	0.83	1/1321 (0.1%)
61	n5	0.68	0/974	0.79	2/1314 (0.2%)
62	N6	0.77	0/1004	0.89	1/1341 (0.1%)
62	n6	0.71	0/1004	0.89	1/1341 (0.1%)
63	N7	0.59	0/1118	0.71	0/1497
63	n7	0.53	0/1118	0.67	0/1497
64	N8	0.83	1/1204 (0.1%)	0.95	3/1612 (0.2%)
64	n8	0.78	0/1204	0.90	3/1612 (0.2%)
65	N9	0.74	0/473	0.88	1/629 (0.2%)
65	n9	0.85	0/473	1.01	1/629 (0.2%)
66	O0	0.55	0/751	0.68	0/1008
66	o0	0.53	0/775	0.69	0/1040
67	O1	0.70	0/890	0.78	1/1196 (0.1%)
67	o1	0.78	0/897	0.88	0/1205
68	O2	0.90	0/1041	0.91	3/1394 (0.2%)
68	o2	0.89	0/1041	0.94	2/1394 (0.1%)
69	O3	0.97	0/868	0.91	0/1168
69	o3	1.01	1/868 (0.1%)	0.94	2/1168 (0.2%)
70	O4	0.68	0/890	0.83	1/1189 (0.1%)
70	o4	0.63	0/890	0.78	0/1189
71	O5	0.78	0/978	0.85	0/1301
71	o5	0.61	0/974	0.75	0/1297
72	O6	0.67	0/778	0.86	0/1034
72	o6	0.63	0/777	0.77	0/1033
73	O7	0.90	0/696	1.01	3/923 (0.3%)
73	o7	0.75	0/696	0.86	2/923 (0.2%)
74	O8	0.59	0/618	0.70	0/826
74	o8	0.50	0/614	0.69	0/822
75	O9	0.81	0/443	0.93	0/588
75	o9	0.74	0/443	0.91	0/588
76	Q0	0.78	0/423	0.89	0/562
76	q0	0.93	1/423 (0.2%)	0.92	0/562
77	Q1	0.65	0/234	0.82	0/300
77	q1	0.81	0/234	1.10	1/300 (0.3%)
78	Q2	0.91	1/860 (0.1%)	0.84	0/1136
78	q2	0.89	2/860 (0.2%)	0.82	0/1136
79	Q3	0.80	0/701	0.83	0/934
79	q3	0.80	0/701	0.85	1/934 (0.1%)
80	e0	0.57	0/499	0.74	0/665
81	p0	0.46	0/1091	0.62	0/1472
All	All	0.96	573/430072 (0.1%)	1.35	5562/631360 (0.9%)

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	1
7	S5	0	1
7	s5	0	2
9	S7	0	2
9	s7	0	1
10	S8	0	1
16	C4	0	3
16	c4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	1
24	d2	0	1
26	d4	0	1
27	D5	0	3
28	D6	0	1
39	L2	0	1
39	l2	0	4
44	l7	0	2
46	L9	0	1
48	M1	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	1
56	n0	0	1
57	N1	0	1
59	n3	0	1
64	N8	0	2
64	n8	0	3
65	N9	0	1
67	O1	0	1
80	e0	0	1
82	m2	0	1
All	All	0	46

The worst 5 of 573 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	14.54	2.06	1.82

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	14.44	2.06	1.82
36	5	1152	G	N9-C4	-12.25	1.28	1.38
36	5	2971	A	N9-C4	9.75	1.43	1.37
36	5	1152	G	N9-C8	9.62	1.44	1.37

The worst 5 of 5562 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	28.50	142.85	128.60
36	5	1152	G	N3-C4-N9	-25.34	110.80	126.00
36	5	1152	G	C2-N3-C4	-23.17	100.31	111.90
36	5	424	G	C5-C6-O6	-17.79	117.92	128.60
36	5	1152	G	C5-N7-C8	-14.52	97.04	104.30

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	38	THR	Peptide
7	S5	44	ASN	Peptide
9	S7	131	PHE	Peptide
9	S7	31	SER	Peptide
10	S8	147	ALA	Peptide

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	996	1
1	6	38238	0	19241	944	0
2	S0	1577	0	1567	172	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	186	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	147	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	125	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	170	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	156	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1878	146	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	125	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	123	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	144	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	73	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	85	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	54	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	118	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	109	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	102	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	133	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	94	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	124	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	93	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	91	0
22	d0	882	0	939	0	0
23	D1	684	0	672	67	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	98	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	100	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	98	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	63	0
27	d5	558	0	598	0	0
28	D6	769	0	815	103	0
28	d6	769	0	814	0	0
29	D7	610	0	630	54	0
29	d7	610	0	631	0	0
30	D8	497	0	535	54	0
30	d8	497	0	535	0	0
31	D9	442	0	428	44	0
31	d9	442	0	428	0	0
32	E0	475	0	525	32	0
33	E1	566	0	603	60	0
33	e1	608	0	656	0	0
34	SR	2441	0	2397	197	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	72	0
35	sM	679	0	603	0	0
36	1	67355	0	33839	1388	0
36	5	67376	0	33855	1332	1
37	3	2579	0	1304	63	0
37	7	2579	0	1304	49	0
38	4	3353	0	1695	68	0
38	8	3353	0	1695	67	0
39	L2	1914	0	1981	157	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	280	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	253	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	211	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	90	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	150	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	152	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	144	0
46	l9	1518	0	1587	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	M0	1705	0	1735	141	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	110	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	158	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	94	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	143	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	127	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	112	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	107	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	121	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	108	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	108	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	55	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	90	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	26	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	86	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	80	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	92	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	137	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	41	0
65	n9	462	0	491	0	0
66	O0	743	0	797	59	0
66	o0	767	0	816	0	0
67	O1	876	0	912	63	0
67	o1	883	0	918	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	O2	1020	0	1090	85	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	66	0
69	o3	850	0	880	0	0
70	O4	880	0	945	69	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	89	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	74	0
72	o6	770	0	846	0	0
73	O7	681	0	682	60	0
73	o7	681	0	683	0	0
74	O8	612	0	682	46	0
74	o8	608	0	671	0	0
75	O9	436	0	475	49	0
75	o9	436	0	475	0	0
76	Q0	417	0	456	31	0
76	q0	417	0	456	0	0
77	Q1	233	0	284	29	0
77	q1	233	0	284	0	0
78	Q2	847	0	917	59	0
78	q2	847	0	918	0	0
79	Q3	694	0	734	58	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	p0	1076	0	1040	0	0
82	m2	750	0	170	0	0
83	p1	235	0	52	0	0
84	p2	230	0	51	0	0
85	1	469	0	0	0	0
85	2	125	0	0	0	0
85	3	14	0	0	0	0
85	4	21	0	0	0	0
85	5	505	0	0	0	0
85	6	148	0	0	0	0
85	7	17	0	0	0	0
85	8	14	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	L2	1	0	0	0	0
85	L3	3	0	0	0	0
85	L4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L5	2	0	0	0	0
85	L7	3	0	0	0	0
85	L8	1	0	0	0	0
85	M0	3	0	0	0	0
85	M1	1	0	0	0	0
85	M3	3	0	0	0	0
85	M5	1	0	0	0	0
85	M6	1	0	0	0	0
85	M7	5	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	2	0	0	0	0
85	N5	1	0	0	0	0
85	N6	2	0	0	0	0
85	N8	5	0	0	0	0
85	O2	1	0	0	0	0
85	O4	1	0	0	0	0
85	O5	1	0	0	0	0
85	O7	3	0	0	0	0
85	Q2	1	0	0	0	0
85	S4	1	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	1	0	0	0	0
85	c9	1	0	0	0	0
85	d3	1	0	0	0	0
85	d4	1	0	0	0	0
85	d6	1	0	0	0	0
85	l2	1	0	0	0	0
85	l3	1	0	0	0	0
85	l4	1	0	0	0	0
85	l5	2	0	0	0	0
85	l7	1	0	0	0	0
85	l9	1	0	0	0	0
85	m0	1	0	0	0	0
85	m1	1	0	0	0	0
85	m5	2	0	0	0	0
85	m6	1	0	0	0	0
85	m7	5	0	0	0	0
85	n0	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	n3	2	0	0	0	0
85	n6	1	0	0	0	0
85	n8	4	0	0	0	0
85	n9	1	0	0	0	0
85	o1	1	0	0	0	0
85	o3	1	0	0	0	0
85	o4	2	0	0	0	0
85	o7	1	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	1	0	0	0	0
85	s1	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2457	0	0	229	0
86	2	1092	0	0	109	0
86	3	77	0	0	5	0
86	4	98	0	0	7	0
86	5	2478	0	0	240	0
86	6	1106	0	0	107	0
86	7	77	0	0	10	0
86	8	119	0	0	18	0
86	C1	7	0	0	0	0
86	C3	7	0	0	1	0
86	C5	7	0	0	5	0
86	C8	7	0	0	0	0
86	D9	7	0	0	1	0
86	L3	21	0	0	2	0
86	L4	7	0	0	0	0
86	M0	7	0	0	1	0
86	M5	7	0	0	1	0
86	M7	14	0	0	2	0
86	M8	7	0	0	0	0
86	M9	7	0	0	0	0
86	N1	7	0	0	2	0
86	N9	7	0	0	0	0
86	O1	7	0	0	6	0
86	O2	7	0	0	0	0
86	O3	7	0	0	1	0
86	O7	14	0	0	6	0
86	O9	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	S8	7	0	0	0	0
86	SR	7	0	0	0	0
86	c3	7	0	0	0	0
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	21	0	0	0	0
86	l4	14	0	0	0	0
86	l5	21	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	0	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	m8	7	0	0	0	0
86	m9	7	0	0	0	0
86	n1	7	0	0	0	0
86	n3	7	0	0	0	0
86	n9	7	0	0	0	0
86	o3	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	0	0
86	sR	7	0	0	0	0
87	2	28	0	0	0	0
87	6	28	0	0	0	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	0	0
88	Q2	1	0	0	0	0
88	Q3	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
All	All	411206	0	297274	11062	1

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

The worst 5 of 11062 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.06	1.43
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.44	1.07
36:5:3274:A:H3'	36:5:3275:U:H5''	1.38	1.04
42:L5:111:GLN:HA	42:L5:116:ASP:HB3	3.45	1.02
1:2:992:A:H2	1:2:1012:U:H3	1.09	1.01

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:1353:U:O2'	36:5:3165:A:OP1[2_546]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	148 (72%)	39 (19%)	17 (8%)	1	9
2	s0	204/251 (81%)	148 (72%)	32 (16%)	24 (12%)	1	4
3	S1	212/254 (84%)	149 (70%)	34 (16%)	29 (14%)	0	2
3	s1	214/254 (84%)	178 (83%)	23 (11%)	13 (6%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S2	215/253 (85%)	178 (83%)	26 (12%)	11 (5%)	3	25
4	s2	215/253 (85%)	169 (79%)	30 (14%)	16 (7%)	2	12
5	S3	221/239 (92%)	173 (78%)	28 (13%)	20 (9%)	1	8
5	s3	221/239 (92%)	176 (80%)	29 (13%)	16 (7%)	2	13
6	S4	258/260 (99%)	203 (79%)	38 (15%)	17 (7%)	2	16
6	s4	258/260 (99%)	209 (81%)	29 (11%)	20 (8%)	1	11
7	S5	204/224 (91%)	155 (76%)	28 (14%)	21 (10%)	1	6
7	s5	204/224 (91%)	156 (76%)	26 (13%)	22 (11%)	1	5
8	S6	224/236 (95%)	191 (85%)	22 (10%)	11 (5%)	3	26
8	s6	216/236 (92%)	179 (83%)	22 (10%)	15 (7%)	2	14
9	S7	182/189 (96%)	137 (75%)	25 (14%)	20 (11%)	1	5
9	s7	184/189 (97%)	140 (76%)	28 (15%)	16 (9%)	1	8
10	S8	184/200 (92%)	154 (84%)	21 (11%)	9 (5%)	3	26
10	s8	184/200 (92%)	161 (88%)	12 (6%)	11 (6%)	2	20
11	S9	183/196 (93%)	147 (80%)	24 (13%)	12 (7%)	2	16
11	s9	183/196 (93%)	149 (81%)	26 (14%)	8 (4%)	4	29
12	C0	94/105 (90%)	70 (74%)	18 (19%)	6 (6%)	2	17
12	c0	92/105 (88%)	66 (72%)	11 (12%)	15 (16%)	0	1
13	C1	153/155 (99%)	118 (77%)	17 (11%)	18 (12%)	1	4
13	c1	144/155 (93%)	114 (79%)	24 (17%)	6 (4%)	4	31
14	C2	122/142 (86%)	75 (62%)	21 (17%)	26 (21%)	0	0
14	c2	122/142 (86%)	71 (58%)	31 (25%)	20 (16%)	0	1
15	C3	148/150 (99%)	123 (83%)	12 (8%)	13 (9%)	1	8
15	c3	148/150 (99%)	115 (78%)	22 (15%)	11 (7%)	2	12
16	C4	125/136 (92%)	95 (76%)	15 (12%)	15 (12%)	1	4
16	c4	126/136 (93%)	104 (82%)	16 (13%)	6 (5%)	4	27
17	C5	122/141 (86%)	81 (66%)	28 (23%)	13 (11%)	1	5
17	c5	133/141 (94%)	90 (68%)	26 (20%)	17 (13%)	0	3
18	C6	139/142 (98%)	109 (78%)	20 (14%)	10 (7%)	2	13
18	c6	140/142 (99%)	112 (80%)	16 (11%)	12 (9%)	1	8
19	C7	116/136 (85%)	82 (71%)	25 (22%)	9 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	c7	113/136 (83%)	87 (77%)	14 (12%)	12 (11%)	1	5
20	C8	143/145 (99%)	115 (80%)	15 (10%)	13 (9%)	1	8
20	c8	143/145 (99%)	117 (82%)	20 (14%)	6 (4%)	4	31
21	C9	141/143 (99%)	115 (82%)	20 (14%)	6 (4%)	4	30
21	c9	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	8	44
22	D0	105/120 (88%)	82 (78%)	20 (19%)	3 (3%)	7	43
22	d0	108/120 (90%)	84 (78%)	14 (13%)	10 (9%)	1	8
23	D1	85/87 (98%)	64 (75%)	15 (18%)	6 (7%)	2	13
23	d1	85/87 (98%)	70 (82%)	8 (9%)	7 (8%)	1	10
24	D2	127/129 (98%)	105 (83%)	20 (16%)	2 (2%)	14	63
24	d2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	27	77
25	D3	142/144 (99%)	115 (81%)	14 (10%)	13 (9%)	1	8
25	d3	142/144 (99%)	123 (87%)	13 (9%)	6 (4%)	4	31
26	D4	132/134 (98%)	107 (81%)	19 (14%)	6 (4%)	4	29
26	d4	132/134 (98%)	100 (76%)	21 (16%)	11 (8%)	1	9
27	D5	68/107 (64%)	45 (66%)	13 (19%)	10 (15%)	0	2
27	d5	67/107 (63%)	52 (78%)	12 (18%)	3 (4%)	4	29
28	D6	95/97 (98%)	61 (64%)	17 (18%)	17 (18%)	0	1
28	d6	95/97 (98%)	71 (75%)	16 (17%)	8 (8%)	1	9
29	D7	79/81 (98%)	62 (78%)	11 (14%)	6 (8%)	2	12
29	d7	79/81 (98%)	59 (75%)	15 (19%)	5 (6%)	2	18
30	D8	61/66 (92%)	45 (74%)	11 (18%)	5 (8%)	1	10
30	d8	61/66 (92%)	46 (75%)	10 (16%)	5 (8%)	1	10
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	2	20
31	d9	51/55 (93%)	37 (72%)	8 (16%)	6 (12%)	1	4
32	E0	58/60 (97%)	42 (72%)	12 (21%)	4 (7%)	2	14
33	E1	69/76 (91%)	34 (49%)	11 (16%)	24 (35%)	0	0
33	e1	74/76 (97%)	34 (46%)	22 (30%)	18 (24%)	0	0
34	SR	316/318 (99%)	238 (75%)	56 (18%)	22 (7%)	2	13
34	sR	316/318 (99%)	261 (83%)	39 (12%)	16 (5%)	3	25
35	SM	155/273 (57%)	109 (70%)	26 (17%)	20 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	sM	98/273 (36%)	61 (62%)	23 (24%)	14 (14%)	0	2
39	L2	250/253 (99%)	218 (87%)	22 (9%)	10 (4%)	5	32
39	l2	250/253 (99%)	209 (84%)	26 (10%)	15 (6%)	2	20
40	L3	384/386 (100%)	333 (87%)	34 (9%)	17 (4%)	4	29
40	l3	384/386 (100%)	339 (88%)	32 (8%)	13 (3%)	6	38
41	L4	359/361 (99%)	302 (84%)	40 (11%)	17 (5%)	4	27
41	l4	359/361 (99%)	293 (82%)	40 (11%)	26 (7%)	2	13
42	L5	294/296 (99%)	239 (81%)	34 (12%)	21 (7%)	2	13
42	l5	292/296 (99%)	252 (86%)	32 (11%)	8 (3%)	8	46
43	L6	152/175 (87%)	134 (88%)	16 (10%)	2 (1%)	18	68
43	l6	153/175 (87%)	127 (83%)	23 (15%)	3 (2%)	11	56
44	L7	220/243 (90%)	195 (89%)	19 (9%)	6 (3%)	8	46
44	l7	221/243 (91%)	193 (87%)	23 (10%)	5 (2%)	10	52
45	L8	231/255 (91%)	188 (81%)	36 (16%)	7 (3%)	7	42
45	l8	229/255 (90%)	181 (79%)	31 (14%)	17 (7%)	2	12
46	L9	189/191 (99%)	156 (82%)	25 (13%)	8 (4%)	4	31
46	l9	189/191 (99%)	162 (86%)	23 (12%)	4 (2%)	11	55
47	M0	207/220 (94%)	172 (83%)	21 (10%)	14 (7%)	2	15
47	m0	209/220 (95%)	165 (79%)	30 (14%)	14 (7%)	2	16
48	M1	167/173 (96%)	127 (76%)	24 (14%)	16 (10%)	1	7
48	m1	167/173 (96%)	142 (85%)	10 (6%)	15 (9%)	1	8
49	M3	191/198 (96%)	156 (82%)	23 (12%)	12 (6%)	2	18
49	m3	192/198 (97%)	149 (78%)	25 (13%)	18 (9%)	1	7
50	M4	134/137 (98%)	115 (86%)	12 (9%)	7 (5%)	3	25
50	m4	135/137 (98%)	120 (89%)	13 (10%)	2 (2%)	15	64
51	M5	201/203 (99%)	179 (89%)	17 (8%)	5 (2%)	9	49
51	m5	201/203 (99%)	175 (87%)	17 (8%)	9 (4%)	4	29
52	M6	195/198 (98%)	176 (90%)	14 (7%)	5 (3%)	8	47
52	m6	195/198 (98%)	170 (87%)	18 (9%)	7 (4%)	5	36
53	M7	181/183 (99%)	150 (83%)	22 (12%)	9 (5%)	3	26
53	m7	153/183 (84%)	136 (89%)	12 (8%)	5 (3%)	6	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	M8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	6	38
54	m8	183/185 (99%)	158 (86%)	23 (13%)	2 (1%)	21	72
55	M9	186/188 (99%)	158 (85%)	23 (12%)	5 (3%)	8	46
55	m9	186/188 (99%)	165 (89%)	20 (11%)	1 (0%)	38	85
56	N0	170/172 (99%)	150 (88%)	17 (10%)	3 (2%)	13	60
56	n0	170/172 (99%)	154 (91%)	15 (9%)	1 (1%)	33	83
57	N1	157/159 (99%)	132 (84%)	19 (12%)	6 (4%)	5	34
57	n1	157/159 (99%)	143 (91%)	13 (8%)	1 (1%)	33	83
58	N2	98/120 (82%)	77 (79%)	17 (17%)	4 (4%)	4	32
58	n2	96/120 (80%)	76 (79%)	14 (15%)	6 (6%)	2	18
59	N3	134/136 (98%)	120 (90%)	12 (9%)	2 (2%)	15	64
59	n3	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	10	53
60	N4	96/155 (62%)	69 (72%)	17 (18%)	10 (10%)	1	5
60	n4	133/155 (86%)	106 (80%)	17 (13%)	10 (8%)	2	12
61	N5	119/141 (84%)	103 (87%)	10 (8%)	6 (5%)	3	26
61	n5	118/141 (84%)	94 (80%)	15 (13%)	9 (8%)	2	12
62	N6	124/126 (98%)	110 (89%)	11 (9%)	3 (2%)	9	51
62	n6	124/126 (98%)	112 (90%)	7 (6%)	5 (4%)	5	32
63	N7	133/135 (98%)	108 (81%)	12 (9%)	13 (10%)	1	7
63	n7	133/135 (98%)	101 (76%)	21 (16%)	11 (8%)	1	9
64	N8	146/148 (99%)	120 (82%)	19 (13%)	7 (5%)	4	27
64	n8	146/148 (99%)	117 (80%)	21 (14%)	8 (6%)	3	23
65	N9	56/58 (97%)	47 (84%)	5 (9%)	4 (7%)	2	13
65	n9	56/58 (97%)	37 (66%)	13 (23%)	6 (11%)	1	5
66	O0	95/104 (91%)	86 (90%)	8 (8%)	1 (1%)	21	72
66	o0	98/104 (94%)	88 (90%)	9 (9%)	1 (1%)	22	74
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	3	23
67	o1	107/112 (96%)	84 (78%)	15 (14%)	8 (8%)	2	12
68	O2	125/129 (97%)	106 (85%)	14 (11%)	5 (4%)	5	32
68	o2	125/129 (97%)	105 (84%)	15 (12%)	5 (4%)	5	32
69	O3	104/106 (98%)	94 (90%)	6 (6%)	4 (4%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	o3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	7	43
70	O4	110/120 (92%)	90 (82%)	19 (17%)	1 (1%)	25	76
70	o4	110/120 (92%)	97 (88%)	10 (9%)	3 (3%)	8	46
71	O5	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	8	47
71	o5	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	8	47
72	O6	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	1	10
72	o6	97/99 (98%)	81 (84%)	11 (11%)	5 (5%)	3	25
73	O7	85/87 (98%)	72 (85%)	12 (14%)	1 (1%)	19	70
73	o7	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	2	20
74	O8	75/77 (97%)	61 (81%)	12 (16%)	2 (3%)	8	46
74	o8	75/77 (97%)	64 (85%)	8 (11%)	3 (4%)	5	32
75	O9	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	11	55
75	o9	48/50 (96%)	40 (83%)	8 (17%)	0	100	100
76	Q0	50/52 (96%)	44 (88%)	4 (8%)	2 (4%)	5	32
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	11	56
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	4	30
78	Q2	103/105 (98%)	76 (74%)	19 (18%)	8 (8%)	1	11
78	q2	103/105 (98%)	86 (84%)	14 (14%)	3 (3%)	7	43
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	6	38
79	q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	21	72
80	e0	60/62 (97%)	44 (73%)	8 (13%)	8 (13%)	0	2
81	p0	139/311 (45%)	110 (79%)	21 (15%)	8 (6%)	3	21
All	All	22333/24143 (92%)	18176 (81%)	2788 (12%)	1369 (6%)	2	19

5 of 1369 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	66	ALA
2	S0	139	VAL
2	S0	158	VAL

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	135 (82%)	29 (18%)	3	13
2	s0	165/209 (79%)	134 (81%)	31 (19%)	2	11
3	S1	191/223 (86%)	154 (81%)	37 (19%)	2	10
3	s1	192/223 (86%)	155 (81%)	37 (19%)	2	10
4	S2	176/204 (86%)	138 (78%)	38 (22%)	1	7
4	s2	176/204 (86%)	131 (74%)	45 (26%)	1	2
5	S3	182/194 (94%)	145 (80%)	37 (20%)	2	9
5	s3	182/194 (94%)	141 (78%)	41 (22%)	1	6
6	S4	221/221 (100%)	170 (77%)	51 (23%)	1	5
6	s4	221/221 (100%)	183 (83%)	38 (17%)	3	14
7	S5	173/190 (91%)	137 (79%)	36 (21%)	2	8
7	s5	173/190 (91%)	141 (82%)	32 (18%)	2	11
8	S6	188/201 (94%)	154 (82%)	34 (18%)	2	12
8	s6	187/201 (93%)	153 (82%)	34 (18%)	2	12
9	S7	165/169 (98%)	136 (82%)	29 (18%)	3	13
9	s7	165/169 (98%)	142 (86%)	23 (14%)	5	24
10	S8	150/161 (93%)	129 (86%)	21 (14%)	5	23
10	s8	150/161 (93%)	124 (83%)	26 (17%)	3	13
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	5
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	11
12	C0	77/98 (79%)	66 (86%)	11 (14%)	5	22
12	c0	73/98 (74%)	58 (80%)	15 (20%)	2	8
13	C1	129/136 (95%)	111 (86%)	18 (14%)	5	23
13	c1	129/136 (95%)	99 (77%)	30 (23%)	1	5
14	C2	88/118 (75%)	69 (78%)	19 (22%)	1	7
14	c2	88/118 (75%)	62 (70%)	26 (30%)	0	1
15	C3	127/127 (100%)	101 (80%)	26 (20%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	c3	127/127 (100%)	102 (80%)	25 (20%)	2	10
16	C4	81/104 (78%)	58 (72%)	23 (28%)	0	2
16	c4	97/104 (93%)	77 (79%)	20 (21%)	2	8
17	C5	101/117 (86%)	87 (86%)	14 (14%)	5	24
17	c5	103/117 (88%)	85 (82%)	18 (18%)	3	13
18	C6	117/118 (99%)	92 (79%)	25 (21%)	1	7
18	c6	118/118 (100%)	95 (80%)	23 (20%)	2	10
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1	6
19	c7	92/124 (74%)	73 (79%)	19 (21%)	2	8
20	C8	128/128 (100%)	97 (76%)	31 (24%)	1	4
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	5
21	C9	115/115 (100%)	87 (76%)	28 (24%)	1	3
21	c9	115/115 (100%)	97 (84%)	18 (16%)	4	17
22	D0	100/113 (88%)	80 (80%)	20 (20%)	2	9
22	d0	103/113 (91%)	77 (75%)	26 (25%)	1	3
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	7
23	d1	74/74 (100%)	55 (74%)	19 (26%)	1	2
24	D2	110/110 (100%)	89 (81%)	21 (19%)	2	11
24	d2	110/110 (100%)	95 (86%)	15 (14%)	5	25
25	D3	119/119 (100%)	95 (80%)	24 (20%)	2	9
25	d3	119/119 (100%)	97 (82%)	22 (18%)	2	11
26	D4	112/112 (100%)	95 (85%)	17 (15%)	4	19
26	d4	112/112 (100%)	94 (84%)	18 (16%)	3	16
27	D5	61/88 (69%)	49 (80%)	12 (20%)	2	10
27	d5	61/88 (69%)	51 (84%)	10 (16%)	3	15
28	D6	83/83 (100%)	65 (78%)	18 (22%)	1	7
28	d6	83/83 (100%)	73 (88%)	10 (12%)	7	32
29	D7	70/70 (100%)	59 (84%)	11 (16%)	4	17
29	d7	70/70 (100%)	60 (86%)	10 (14%)	5	22
30	D8	56/59 (95%)	41 (73%)	15 (27%)	1	2
30	d8	56/59 (95%)	42 (75%)	14 (25%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	D9	47/48 (98%)	38 (81%)	9 (19%)	2	11
31	d9	47/48 (98%)	36 (77%)	11 (23%)	1	5
32	E0	51/51 (100%)	43 (84%)	8 (16%)	4	17
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	4
33	e1	66/66 (100%)	47 (71%)	19 (29%)	0	1
34	SR	260/261 (100%)	213 (82%)	47 (18%)	2	12
34	sR	260/261 (100%)	232 (89%)	28 (11%)	9	37
35	SM	97/228 (42%)	69 (71%)	28 (29%)	0	1
35	sM	54/228 (24%)	40 (74%)	14 (26%)	1	2
39	L2	193/195 (99%)	153 (79%)	40 (21%)	2	8
39	l2	192/195 (98%)	149 (78%)	43 (22%)	1	6
40	L3	320/322 (99%)	251 (78%)	69 (22%)	1	7
40	l3	320/322 (99%)	258 (81%)	62 (19%)	2	10
41	L4	288/288 (100%)	225 (78%)	63 (22%)	1	7
41	l4	288/288 (100%)	230 (80%)	58 (20%)	2	9
42	L5	244/244 (100%)	197 (81%)	47 (19%)	2	10
42	l5	243/244 (100%)	191 (79%)	52 (21%)	1	7
43	L6	134/152 (88%)	118 (88%)	16 (12%)	8	33
43	l6	135/152 (89%)	112 (83%)	23 (17%)	3	14
44	L7	186/204 (91%)	165 (89%)	21 (11%)	9	36
44	l7	187/204 (92%)	158 (84%)	29 (16%)	4	17
45	L8	187/207 (90%)	151 (81%)	36 (19%)	2	10
45	l8	177/207 (86%)	141 (80%)	36 (20%)	2	9
46	L9	171/171 (100%)	137 (80%)	34 (20%)	2	9
46	l9	171/171 (100%)	123 (72%)	48 (28%)	0	2
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	7
47	m0	179/186 (96%)	145 (81%)	34 (19%)	2	11
48	M1	147/150 (98%)	123 (84%)	24 (16%)	3	15
48	m1	147/150 (98%)	115 (78%)	32 (22%)	1	7
49	M3	154/158 (98%)	123 (80%)	31 (20%)	2	9
49	m3	154/158 (98%)	124 (80%)	30 (20%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	M4	107/108 (99%)	87 (81%)	20 (19%)	2	11
50	m4	108/108 (100%)	81 (75%)	27 (25%)	1	3
51	M5	175/175 (100%)	143 (82%)	32 (18%)	2	12
51	m5	175/175 (100%)	142 (81%)	33 (19%)	2	11
52	M6	160/161 (99%)	141 (88%)	19 (12%)	8	33
52	m6	160/161 (99%)	130 (81%)	30 (19%)	2	11
53	M7	140/145 (97%)	107 (76%)	33 (24%)	1	4
53	m7	125/145 (86%)	100 (80%)	25 (20%)	2	9
54	M8	150/150 (100%)	126 (84%)	24 (16%)	3	16
54	m8	150/150 (100%)	122 (81%)	28 (19%)	2	11
55	M9	153/153 (100%)	121 (79%)	32 (21%)	1	8
55	m9	153/153 (100%)	123 (80%)	30 (20%)	2	10
56	N0	156/156 (100%)	127 (81%)	29 (19%)	2	11
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1	7
57	N1	136/136 (100%)	111 (82%)	25 (18%)	2	11
57	n1	136/136 (100%)	108 (79%)	28 (21%)	2	8
58	N2	87/106 (82%)	70 (80%)	17 (20%)	2	10
58	n2	85/106 (80%)	70 (82%)	15 (18%)	3	13
59	N3	104/104 (100%)	87 (84%)	17 (16%)	3	15
59	n3	104/104 (100%)	89 (86%)	15 (14%)	5	22
60	N4	57/129 (44%)	51 (90%)	6 (10%)	10	39
60	n4	100/129 (78%)	82 (82%)	18 (18%)	2	12
61	N5	104/117 (89%)	84 (81%)	20 (19%)	2	10
61	n5	104/117 (89%)	82 (79%)	22 (21%)	1	8
62	N6	109/109 (100%)	85 (78%)	24 (22%)	1	7
62	n6	109/109 (100%)	86 (79%)	23 (21%)	1	8
63	N7	115/115 (100%)	93 (81%)	22 (19%)	2	11
63	n7	115/115 (100%)	89 (77%)	26 (23%)	1	6
64	N8	118/118 (100%)	95 (80%)	23 (20%)	2	10
64	n8	118/118 (100%)	99 (84%)	19 (16%)	3	16
65	N9	46/46 (100%)	33 (72%)	13 (28%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0	1
66	O0	81/87 (93%)	64 (79%)	17 (21%)	1	8
66	o0	84/87 (97%)	67 (80%)	17 (20%)	2	9
67	O1	92/96 (96%)	74 (80%)	18 (20%)	2	10
67	o1	94/96 (98%)	68 (72%)	26 (28%)	0	2
68	O2	109/110 (99%)	88 (81%)	21 (19%)	2	10
68	o2	109/110 (99%)	81 (74%)	28 (26%)	1	2
69	O3	90/90 (100%)	75 (83%)	15 (17%)	3	14
69	o3	90/90 (100%)	75 (83%)	15 (17%)	3	14
70	O4	95/102 (93%)	74 (78%)	21 (22%)	1	7
70	o4	95/102 (93%)	77 (81%)	18 (19%)	2	11
71	O5	104/104 (100%)	81 (78%)	23 (22%)	1	7
71	o5	103/104 (99%)	78 (76%)	25 (24%)	1	3
72	O6	81/81 (100%)	59 (73%)	22 (27%)	0	2
72	o6	80/81 (99%)	51 (64%)	29 (36%)	0	0
73	O7	70/70 (100%)	52 (74%)	18 (26%)	1	2
73	o7	70/70 (100%)	57 (81%)	13 (19%)	2	11
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	5
74	o8	67/68 (98%)	51 (76%)	16 (24%)	1	4
75	O9	45/45 (100%)	38 (84%)	7 (16%)	4	17
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	13
76	Q0	47/47 (100%)	36 (77%)	11 (23%)	1	5
76	q0	47/47 (100%)	35 (74%)	12 (26%)	1	3
77	Q1	23/23 (100%)	18 (78%)	5 (22%)	1	7
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	69 (77%)	21 (23%)	1	5
78	q2	90/90 (100%)	74 (82%)	16 (18%)	2	13
79	Q3	71/71 (100%)	55 (78%)	16 (22%)	1	6
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	6
80	e0	53/53 (100%)	40 (76%)	13 (24%)	1	3
81	p0	105/253 (42%)	85 (81%)	20 (19%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	18728/20241 (92%)	15006 (80%)	3722 (20%)	2 9

5 of 3722 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	O4	71	THR
8	s6	175	ILE
64	n8	135	GLU
72	O6	81	THR
3	s1	185	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
53	M7	179	GLN
70	O4	3	GLN
62	n6	4	GLN
62	N6	120	GLN
75	O9	50	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 2559 ligands modelled in this entry, 1426 are monoatomic - leaving 1133 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	3861	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3862	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3863	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	3K8	2	2179	-	32,32,32	0.77	1 (3%)	47,47,47	0.96	2 (4%)
86	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4252	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4253	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4254	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	3K8	6	2205	-	32,32,32	0.54	0	47,47,47	0.78	1 (2%)
86	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O2	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	c8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3861	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3862	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3863	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3864	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3865	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3866	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3867	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3869	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3906	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3948	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3990	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4032	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4074	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4116	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4158	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4200	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2053	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2095	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2137	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
87	3K8	2	2179	-	-	0/6/25/25	0/5/5/5

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3959	-	-	0/0/0/0	0/0/0/0

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4252	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4253	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4254	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2087	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2129	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2171	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
87	3K8	6	2205	-	-	0/6/25/25	0/5/5/5
86	OHX	7	217	-	-	0/0/0/0	0/0/0/0
86	OHX	7	218	-	-	0/0/0/0	0/0/0/0
86	OHX	7	219	-	-	0/0/0/0	0/0/0/0
86	OHX	7	220	-	-	0/0/0/0	0/0/0/0
86	OHX	7	221	-	-	0/0/0/0	0/0/0/0
86	OHX	7	222	-	-	0/0/0/0	0/0/0/0
86	OHX	7	223	-	-	0/0/0/0	0/0/0/0
86	OHX	7	224	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	7	225	-	-	0/0/0/0	0/0/0/0
86	OHX	7	226	-	-	0/0/0/0	0/0/0/0
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	215	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	-	-	0/0/0/0	0/0/0/0
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0
86	OHX	8	219	-	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	-	-	0/0/0/0	0/0/0/0
86	OHX	8	222	-	-	0/0/0/0	0/0/0/0
86	OHX	8	223	-	-	0/0/0/0	0/0/0/0
86	OHX	8	224	-	-	0/0/0/0	0/0/0/0
86	OHX	8	225	-	-	0/0/0/0	0/0/0/0
86	OHX	8	226	-	-	0/0/0/0	0/0/0/0
86	OHX	8	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	229	-	-	0/0/0/0	0/0/0/0
86	OHX	8	230	-	-	0/0/0/0	0/0/0/0
86	OHX	8	231	-	-	0/0/0/0	0/0/0/0
86	OHX	C1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	406	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	304	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	302	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O2	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	105	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	106	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	202	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	202	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	m6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	2	2179	3K8	C8-C7	3.45	1.42	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	2	2179	3K8	C15-C7-C4	-4.12	116.14	120.39
87	6	2205	3K8	C11-C10-N	2.46	118.55	110.85
87	2	2179	3K8	C11-C10-N	2.44	118.48	110.85

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%)	0.21	81 (4%) 31 6	55, 90, 172, 265	0
1	6	1795/1800 (99%)	0.27	105 (5%) 22 5	44, 80, 191, 285	0
2	S0	206/251 (82%)	0.68	9 (4%) 33 7	94, 111, 124, 153	0
2	s0	206/251 (82%)	0.54	15 (7%) 15 3	78, 99, 115, 126	0
3	S1	214/254 (84%)	1.01	38 (17%) 2 1	94, 126, 153, 157	0
3	s1	216/254 (85%)	0.45	17 (7%) 13 3	69, 86, 109, 122	0
4	S2	217/253 (85%)	-0.20	0 100 100	72, 88, 108, 126	0
4	s2	217/253 (85%)	-0.18	0 100 100	58, 76, 97, 109	0
5	S3	223/239 (93%)	0.02	7 (3%) 47 10	79, 94, 128, 148	0
5	s3	223/239 (93%)	0.16	9 (4%) 36 7	80, 114, 137, 146	0
6	S4	260/260 (100%)	0.81	28 (10%) 6 2	63, 89, 102, 129	0
6	s4	260/260 (100%)	0.46	7 (2%) 52 11	57, 79, 97, 125	0
7	S5	206/224 (91%)	0.31	10 (4%) 28 6	98, 119, 139, 154	0
7	s5	206/224 (91%)	0.23	7 (3%) 43 9	71, 97, 123, 147	0
8	S6	226/236 (95%)	0.71	34 (15%) 3 1	65, 101, 120, 153	0
8	s6	218/236 (92%)	0.32	10 (4%) 31 6	56, 83, 111, 135	0
9	S7	184/189 (97%)	0.61	9 (4%) 28 6	86, 118, 146, 158	0
9	s7	186/189 (98%)	0.49	7 (3%) 38 7	75, 109, 141, 156	0
10	S8	188/200 (94%)	0.24	2 (1%) 77 27	56, 73, 113, 131	0
10	s8	188/200 (94%)	0.41	7 (3%) 39 8	48, 70, 116, 134	0
11	S9	185/196 (94%)	0.66	11 (5%) 22 5	83, 99, 134, 164	0
11	s9	185/196 (94%)	0.52	10 (5%) 25 5	69, 84, 121, 158	0
12	C0	96/105 (91%)	0.30	7 (7%) 15 3	83, 106, 146, 165	0
12	c0	96/105 (91%)	0.94	18 (18%) 2 1	107, 139, 160, 189	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	0.03	7 (4%) 32 6	59, 71, 129, 137	0
13	c1	146/155 (94%)	0.19	3 (2%) 60 15	51, 68, 104, 128	0
14	C2	124/142 (87%)	1.11	20 (16%) 2 1	134, 149, 164, 175	0
14	c2	124/142 (87%)	2.66	84 (67%) 0 0	186, 202, 221, 224	0
15	C3	150/150 (100%)	0.30	5 (3%) 44 9	67, 88, 106, 111	0
15	c3	150/150 (100%)	0.02	0 100 100	58, 76, 96, 114	0
16	C4	127/136 (93%)	0.99	25 (19%) 2 1	70, 116, 138, 148	0
16	c4	128/136 (94%)	0.30	1 (0%) 83 35	58, 81, 92, 101	0
17	C5	124/141 (87%)	0.39	3 (2%) 56 13	80, 96, 134, 149	0
17	c5	135/141 (95%)	0.61	9 (6%) 17 4	83, 108, 136, 172	0
18	C6	141/142 (99%)	0.97	23 (16%) 2 1	83, 109, 118, 122	0
18	c6	142/142 (100%)	0.90	18 (12%) 4 1	70, 90, 110, 137	0
19	C7	120/136 (88%)	0.55	8 (6%) 17 4	94, 112, 137, 140	0
19	c7	117/136 (86%)	0.48	6 (5%) 27 5	81, 100, 125, 130	0
20	C8	145/145 (100%)	0.69	10 (6%) 17 4	81, 109, 133, 143	0
20	c8	145/145 (100%)	0.69	9 (6%) 20 4	75, 92, 117, 136	0
21	C9	143/143 (100%)	1.26	35 (24%) 1 1	92, 107, 125, 139	0
21	c9	143/143 (100%)	0.83	10 (6%) 16 4	69, 84, 108, 127	0
22	D0	107/120 (89%)	0.45	4 (3%) 39 8	75, 115, 152, 155	0
22	d0	110/120 (91%)	0.48	7 (6%) 19 4	74, 113, 155, 187	0
23	D1	87/87 (100%)	0.40	4 (4%) 31 6	89, 98, 117, 132	0
23	d1	87/87 (100%)	0.04	1 (1%) 77 27	73, 83, 106, 121	0
24	D2	129/129 (100%)	0.35	1 (0%) 83 35	70, 81, 90, 103	0
24	d2	129/129 (100%)	0.07	1 (0%) 83 35	55, 68, 76, 91	0
25	D3	144/144 (100%)	0.30	1 (0%) 84 38	59, 65, 78, 97	0
25	d3	144/144 (100%)	0.12	0 100 100	48, 55, 67, 83	0
26	D4	134/134 (100%)	0.83	13 (9%) 8 2	76, 103, 121, 130	0
26	d4	134/134 (100%)	0.17	0 100 100	61, 88, 103, 137	0
27	D5	70/107 (65%)	0.50	2 (2%) 49 10	113, 131, 143, 147	0
27	d5	69/107 (64%)	1.45	18 (26%) 1 1	84, 114, 131, 139	0
28	D6	97/97 (100%)	0.49	3 (3%) 47 10	74, 94, 142, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.24	2 (2%) 60 15	60, 76, 98, 108	0
29	D7	81/81 (100%)	0.92	6 (7%) 14 3	83, 101, 140, 146	0
29	d7	81/81 (100%)	0.70	3 (3%) 39 8	72, 88, 134, 143	0
30	D8	63/66 (95%)	1.10	13 (20%) 1 1	113, 131, 148, 162	0
30	d8	63/66 (95%)	0.37	1 (1%) 68 20	90, 108, 127, 147	0
31	D9	53/55 (96%)	0.69	4 (7%) 14 3	77, 83, 105, 118	0
31	d9	53/55 (96%)	1.45	14 (26%) 1 1	77, 90, 134, 149	0
32	E0	60/60 (100%)	0.92	6 (10%) 8 2	70, 96, 145, 151	0
33	E1	71/76 (93%)	1.47	19 (26%) 1 1	109, 129, 150, 157	0
33	e1	76/76 (100%)	2.16	33 (43%) 1 0	132, 173, 186, 188	0
34	SR	318/318 (100%)	1.24	61 (19%) 2 1	69, 121, 144, 166	0
34	sR	318/318 (100%)	1.02	54 (16%) 2 1	102, 124, 143, 162	0
35	SM	159/273 (58%)	0.53	16 (10%) 7 2	65, 93, 144, 146	0
35	sM	104/273 (38%)	0.32	8 (7%) 13 3	67, 106, 192, 201	0
36	1	3149/3396 (92%)	0.02	68 (2%) 59 14	28, 52, 140, 267	0
36	5	3150/3396 (92%)	0.01	58 (1%) 65 18	28, 52, 127, 268	0
37	3	121/121 (100%)	-0.20	0 100 100	42, 71, 88, 93	0
37	7	121/121 (100%)	-0.35	0 100 100	34, 56, 69, 79	0
38	4	158/158 (100%)	-0.13	2 (1%) 74 24	35, 53, 93, 136	0
38	8	158/158 (100%)	-0.04	4 (2%) 54 12	39, 60, 105, 132	0
39	L2	252/253 (99%)	0.05	2 (0%) 83 35	35, 49, 65, 77	0
39	l2	252/253 (99%)	0.04	0 100 100	36, 55, 77, 88	0
40	L3	386/386 (100%)	0.22	2 (0%) 88 46	35, 55, 71, 106	0
40	l3	386/386 (100%)	-0.06	0 100 100	29, 43, 59, 97	0
41	L4	361/361 (100%)	-0.20	0 100 100	29, 44, 64, 71	0
41	l4	361/361 (100%)	-0.01	0 100 100	35, 50, 70, 83	0
42	L5	296/296 (100%)	0.69	28 (9%) 8 2	54, 79, 99, 128	0
42	l5	294/296 (99%)	0.26	3 (1%) 79 29	43, 60, 87, 137	0
43	L6	156/175 (89%)	0.02	1 (0%) 86 41	40, 49, 71, 101	0
43	l6	157/175 (89%)	0.21	2 (1%) 74 24	42, 50, 73, 88	0
44	L7	222/243 (91%)	0.05	0 100 100	34, 42, 78, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	-0.08	0 100 100	31, 39, 84, 129	0
45	L8	233/255 (91%)	0.14	1 (0%) 90 51	55, 71, 108, 122	0
45	l8	231/255 (90%)	0.47	16 (6%) 17 4	70, 83, 115, 124	0
46	L9	191/191 (100%)	0.18	2 (1%) 79 29	48, 62, 80, 95	0
46	l9	191/191 (100%)	-0.12	0 100 100	39, 47, 72, 101	0
47	M0	211/220 (95%)	0.32	0 100 100	41, 54, 94, 134	0
47	m0	213/220 (96%)	0.38	5 (2%) 57 13	35, 58, 87, 102	0
48	M1	169/173 (97%)	0.25	1 (0%) 86 41	62, 86, 100, 111	0
48	m1	169/173 (97%)	0.09	1 (0%) 86 41	44, 65, 81, 93	0
49	M3	193/198 (97%)	0.09	1 (0%) 88 46	36, 55, 104, 132	0
49	m3	194/198 (97%)	0.05	1 (0%) 88 46	45, 64, 109, 142	0
50	M4	136/137 (99%)	-0.06	0 100 100	44, 50, 64, 76	0
50	m4	137/137 (100%)	-0.21	0 100 100	36, 43, 66, 82	0
51	M5	203/203 (100%)	-0.03	0 100 100	33, 47, 58, 61	0
51	m5	203/203 (100%)	-0.01	1 (0%) 88 46	41, 57, 70, 75	0
52	M6	197/198 (99%)	-0.17	0 100 100	34, 40, 61, 67	0
52	m6	197/198 (99%)	-0.20	0 100 100	28, 34, 62, 68	0
53	M7	183/183 (100%)	0.35	18 (9%) 8 2	38, 46, 132, 154	0
53	m7	155/183 (84%)	-0.01	0 100 100	30, 42, 53, 84	0
54	M8	185/185 (100%)	-0.18	0 100 100	37, 45, 61, 79	0
54	m8	185/185 (100%)	-0.06	0 100 100	38, 51, 61, 65	0
55	M9	188/188 (100%)	0.53	20 (10%) 7 2	51, 68, 166, 175	0
55	m9	188/188 (100%)	0.31	10 (5%) 25 5	49, 63, 150, 163	0
56	N0	172/172 (100%)	-0.21	0 100 100	40, 48, 64, 73	0
56	n0	172/172 (100%)	-0.22	0 100 100	33, 40, 52, 67	0
57	N1	159/159 (100%)	0.02	0 100 100	40, 50, 96, 104	0
57	n1	159/159 (100%)	0.05	0 100 100	38, 44, 82, 88	0
58	N2	100/120 (83%)	0.82	11 (11%) 6 2	80, 100, 118, 137	0
58	n2	98/120 (81%)	0.81	7 (7%) 16 4	73, 90, 102, 106	0
59	N3	136/136 (100%)	0.12	0 100 100	40, 51, 66, 77	0
59	n3	136/136 (100%)	0.03	1 (0%) 84 38	31, 41, 59, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	1.32	20 (20%) 1 1	51, 65, 162, 173	0
60	n4	135/155 (87%)	0.32	6 (4%) 33 7	43, 90, 133, 148	0
61	N5	121/141 (85%)	-0.13	0 100 100	46, 59, 85, 123	0
61	n5	120/141 (85%)	0.23	1 (0%) 83 35	50, 65, 89, 96	0
62	N6	126/126 (100%)	0.44	2 (1%) 68 20	44, 56, 67, 81	0
62	n6	126/126 (100%)	0.43	3 (2%) 56 13	48, 60, 78, 88	0
63	N7	135/135 (100%)	0.65	7 (5%) 26 5	68, 83, 98, 106	0
63	n7	135/135 (100%)	0.70	9 (6%) 17 4	78, 94, 115, 128	0
64	N8	148/148 (100%)	0.12	0 100 100	30, 45, 72, 86	0
64	n8	148/148 (100%)	-0.07	0 100 100	37, 51, 74, 76	0
65	N9	58/58 (100%)	0.14	0 100 100	41, 55, 107, 125	0
65	n9	58/58 (100%)	-0.19	0 100 100	36, 54, 87, 101	0
66	O0	97/104 (93%)	-0.10	0 100 100	67, 78, 105, 117	0
66	o0	100/104 (96%)	-0.29	0 100 100	74, 85, 115, 127	0
67	O1	109/112 (97%)	0.23	2 (1%) 65 18	45, 62, 105, 123	0
67	o1	109/112 (97%)	0.24	1 (0%) 81 32	40, 54, 98, 119	0
68	O2	127/129 (98%)	0.22	2 (1%) 68 20	28, 43, 56, 74	0
68	o2	127/129 (98%)	0.36	3 (2%) 56 13	29, 48, 62, 89	0
69	O3	106/106 (100%)	-0.09	0 100 100	35, 41, 69, 84	0
69	o3	106/106 (100%)	0.18	1 (0%) 81 32	32, 39, 70, 85	0
70	O4	112/120 (93%)	0.42	5 (4%) 32 6	46, 64, 113, 130	0
70	o4	112/120 (93%)	0.24	0 100 100	48, 68, 118, 127	0
71	O5	119/119 (100%)	0.28	3 (2%) 54 12	45, 63, 72, 74	0
71	o5	119/119 (100%)	0.14	1 (0%) 83 35	52, 68, 84, 91	0
72	O6	99/99 (100%)	0.66	6 (6%) 21 4	52, 64, 98, 122	0
72	o6	99/99 (100%)	0.81	5 (5%) 27 5	59, 72, 95, 115	0
73	O7	87/87 (100%)	-0.04	0 100 100	35, 42, 71, 99	0
73	o7	87/87 (100%)	0.09	3 (3%) 43 9	40, 45, 84, 120	0
74	O8	77/77 (100%)	0.68	0 100 100	71, 84, 112, 123	0
74	o8	77/77 (100%)	0.92	11 (14%) 3 1	74, 89, 104, 110	0
75	O9	50/50 (100%)	-0.26	0 100 100	43, 49, 56, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	-0.20	0 100 100	49, 53, 64, 75	0
76	Q0	52/52 (100%)	0.42	2 (3%) 38 7	44, 52, 79, 91	0
76	q0	52/52 (100%)	0.13	2 (3%) 38 7	34, 40, 54, 63	0
77	Q1	25/25 (100%)	0.83	3 (12%) 5 1	54, 58, 62, 67	0
77	q1	25/25 (100%)	0.99	2 (8%) 12 3	48, 51, 65, 71	0
78	Q2	105/105 (100%)	0.12	1 (0%) 79 29	43, 58, 85, 128	0
78	q2	105/105 (100%)	0.29	0 100 100	45, 58, 85, 117	0
79	Q3	91/91 (100%)	-0.15	0 100 100	43, 52, 70, 88	0
79	q3	91/91 (100%)	-0.19	0 100 100	41, 57, 73, 84	0
80	e0	62/62 (100%)	0.69	4 (6%) 18 4	62, 85, 126, 146	0
81	p0	143/311 (45%)	0.94	16 (11%) 6 2	87, 109, 183, 194	0
82	m2	0/160	-	-	-	-
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35346 (93%)	0.26	1406 (4%) 34 7	28, 70, 137, 285	0

The worst 5 of 1406 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	c2	20	ALA	14.0
31	d9	4	GLU	11.8
14	C2	20	ALA	9.9
60	N4	76	VAL	9.4
33	e1	145	HIS	9.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	5	3777	1/1	0.68	1011.00	105,105,105,105	0
85	MG	5	3853	1/1	0.51	737.00	57,57,57,57	0
85	MG	1	3499	1/1	0.81	647.00	76,76,76,76	0
85	MG	1	3620	1/1	0.47	607.00	49,49,49,49	0
85	MG	1	3557	1/1	0.77	392.33	49,49,49,49	0
85	MG	5	3867	1/1	0.54	392.00	48,48,48,48	0
85	MG	6	1933	1/1	1.11	294.17	70,70,70,70	0
85	MG	5	3452	1/1	0.60	267.67	38,38,38,38	0
85	MG	1	3701	1/1	0.70	255.00	48,48,48,48	0
85	MG	1	3835	1/1	0.92	246.00	57,57,57,57	0
85	MG	2	2015	1/1	1.14	229.03	63,63,63,63	0
85	MG	4	202	1/1	0.70	217.80	50,50,50,50	0
85	MG	6	1924	1/1	0.54	209.67	106,106,106,106	0
85	MG	2	1903	1/1	0.81	187.69	45,45,45,45	0
85	MG	2	1996	1/1	0.48	165.67	97,97,97,97	0
85	MG	5	3540	1/1	0.59	150.60	24,24,24,24	0
85	MG	5	3622	1/1	0.72	141.38	52,52,52,52	0
85	MG	1	3582	1/1	0.67	141.29	29,29,29,29	0
85	MG	1	3740	1/1	0.30	141.00	53,53,53,53	0
85	MG	5	3584	1/1	0.58	133.25	41,41,41,41	0
85	MG	5	3646	1/1	0.74	127.76	44,44,44,44	0
85	MG	2	2010	1/1	0.91	126.36	76,76,76,76	0
85	MG	5	3861	1/1	0.54	120.14	70,70,70,70	0
85	MG	5	3862	1/1	1.37	119.62	87,87,87,87	0
85	MG	1	3841	1/1	0.96	119.26	63,63,63,63	0
85	MG	5	3899	1/1	0.48	117.09	97,97,97,97	0
85	MG	5	3852	1/1	0.62	115.15	47,47,47,47	0
85	MG	5	3877	1/1	0.51	112.00	40,40,40,40	0
85	MG	6	2018	1/1	0.89	111.50	54,54,54,54	0
85	MG	2	1958	1/1	1.26	108.52	97,97,97,97	0
85	MG	5	3482	1/1	0.97	106.54	68,68,68,68	0
85	MG	1	3587	1/1	0.76	105.87	27,27,27,27	0
85	MG	5	3440	1/1	0.81	99.73	41,41,41,41	0
85	MG	5	3499	1/1	0.53	98.78	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3687	1/1	1.07	96.54	54,54,54,54	0
85	MG	6	1928	1/1	0.82	95.57	79,79,79,79	0
85	MG	1	3546	1/1	0.23	92.74	67,67,67,67	0
85	MG	5	3522	1/1	1.15	92.70	36,36,36,36	0
85	MG	2	1984	1/1	0.57	91.00	77,77,77,77	0
85	MG	5	3674	1/1	0.51	87.28	54,54,54,54	0
85	MG	5	3496	1/1	0.62	85.26	42,42,42,42	0
85	MG	5	3668	1/1	0.93	84.52	46,46,46,46	0
85	MG	1	3846	1/1	1.15	78.25	58,58,58,58	0
85	MG	5	3592	1/1	0.80	76.28	48,48,48,48	0
85	MG	4	210	1/1	0.33	75.93	56,56,56,56	0
85	MG	1	3772	1/1	0.73	75.71	57,57,57,57	0
85	MG	5	3789	1/1	1.13	72.71	86,86,86,86	0
85	MG	7	203	1/1	0.48	68.80	27,27,27,27	0
85	MG	2	1923	1/1	0.89	68.29	67,67,67,67	0
85	MG	5	3488	1/1	0.64	68.14	58,58,58,58	0
85	MG	1	3842	1/1	0.77	67.98	51,51,51,51	0
85	MG	5	3885	1/1	0.51	67.91	85,85,85,85	0
85	MG	5	3471	1/1	0.98	64.11	46,46,46,46	0
85	MG	8	213	1/1	0.60	63.86	47,47,47,47	0
85	MG	1	3531	1/1	0.58	63.38	27,27,27,27	0
85	MG	5	3771	1/1	1.15	63.00	38,38,38,38	0
85	MG	2	2020	1/1	1.20	62.31	77,77,77,77	0
85	MG	1	3473	1/1	0.60	60.80	24,24,24,24	0
85	MG	6	1980	1/1	1.13	60.75	64,64,64,64	0
85	MG	1	3673	1/1	0.63	60.63	63,63,63,63	0
85	MG	2	1973	1/1	1.11	59.96	74,74,74,74	0
85	MG	5	3414	1/1	0.72	58.20	36,36,36,36	0
85	MG	1	3402	1/1	0.91	58.15	50,50,50,50	0
85	MG	5	3568	1/1	0.69	58.02	27,27,27,27	0
85	MG	5	3585	1/1	0.46	57.74	30,30,30,30	0
85	MG	5	3735	1/1	0.51	57.17	67,67,67,67	0
85	MG	4	205	1/1	0.76	56.79	51,51,51,51	0
85	MG	1	3596	1/1	0.65	56.54	27,27,27,27	0
85	MG	5	3878	1/1	0.48	56.01	42,42,42,42	0
85	MG	1	3510	1/1	0.86	55.70	48,48,48,48	0
85	MG	5	3453	1/1	0.88	55.62	42,42,42,42	0
85	MG	1	3809	1/1	0.24	55.51	51,51,51,51	0
85	MG	8	210	1/1	0.76	54.23	59,59,59,59	0
85	MG	1	3598	1/1	0.63	54.23	14,14,14,14	0
85	MG	1	3458	1/1	1.19	54.14	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3538	1/1	0.45	53.76	42,42,42,42	0
85	MG	1	3827	1/1	0.62	52.94	37,37,37,37	0
85	MG	5	3520	1/1	0.56	52.89	25,25,25,25	0
85	MG	5	3554	1/1	0.89	52.48	38,38,38,38	0
85	MG	1	3412	1/1	0.84	52.22	46,46,46,46	0
85	MG	6	1948	1/1	0.56	52.17	43,43,43,43	0
85	MG	5	3627	1/1	0.57	52.14	32,32,32,32	0
85	MG	5	3618	1/1	0.40	52.11	32,32,32,32	0
85	MG	6	1942	1/1	0.28	51.99	36,36,36,36	0
85	MG	8	204	1/1	0.92	51.32	54,54,54,54	0
85	MG	1	3505	1/1	0.83	51.16	34,34,34,34	0
85	MG	1	3595	1/1	0.71	51.12	25,25,25,25	0
85	MG	1	3860	1/1	0.69	50.80	64,64,64,64	0
85	MG	5	3667	1/1	0.85	50.45	64,64,64,64	0
85	MG	1	3498	1/1	0.89	50.06	62,62,62,62	0
85	MG	1	3756	1/1	0.31	49.93	54,54,54,54	0
85	MG	5	3590	1/1	0.78	49.72	27,27,27,27	0
85	MG	6	1903	1/1	0.58	49.66	43,43,43,43	0
85	MG	1	3555	1/1	0.67	49.53	38,38,38,38	0
85	MG	1	3717	1/1	0.47	49.34	56,56,56,56	0
85	MG	2	1950	1/1	0.56	48.20	81,81,81,81	0
85	MG	2	2014	1/1	0.95	47.77	65,65,65,65	0
85	MG	5	3650	1/1	0.92	47.44	48,48,48,48	0
85	MG	5	3492	1/1	0.48	46.69	55,55,55,55	0
85	MG	1	3440	1/1	0.80	46.46	39,39,39,39	0
85	MG	5	3881	1/1	0.68	46.32	28,28,28,28	0
85	MG	1	3795	1/1	0.58	46.31	56,56,56,56	0
85	MG	1	3578	1/1	0.55	46.25	36,36,36,36	0
85	MG	6	1921	1/1	0.44	45.80	50,50,50,50	0
85	MG	6	2009	1/1	0.72	45.80	63,63,63,63	0
85	MG	5	3480	1/1	0.57	45.78	70,70,70,70	0
85	MG	1	3570	1/1	0.85	45.56	41,41,41,41	0
85	MG	1	3736	1/1	0.51	45.17	48,48,48,48	0
85	MG	7	208	1/1	0.49	45.14	62,62,62,62	0
85	MG	1	3479	1/1	0.74	45.06	66,66,66,66	0
85	MG	1	3588	1/1	0.50	44.85	28,28,28,28	0
85	MG	1	3459	1/1	0.57	44.48	36,36,36,36	0
85	MG	1	3614	1/1	0.85	44.42	44,44,44,44	0
85	MG	6	2012	1/1	0.62	44.39	50,50,50,50	0
85	MG	5	4259	1/1	0.66	44.29	37,37,37,37	0
85	MG	1	3858	1/1	0.77	44.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	1965	1/1	0.51	43.94	72,72,72,72	0
85	MG	m5	301	1/1	0.53	43.94	54,54,54,54	0
85	MG	5	3884	1/1	0.65	43.36	56,56,56,56	0
85	MG	6	2043	1/1	0.52	43.13	54,54,54,54	0
85	MG	1	3404	1/1	0.86	42.93	75,75,75,75	0
85	MG	7	205	1/1	0.69	42.48	64,64,64,64	0
85	MG	6	2034	1/1	0.72	42.46	63,63,63,63	0
85	MG	2	1989	1/1	0.53	42.44	89,89,89,89	0
85	MG	5	3692	1/1	0.41	42.20	61,61,61,61	0
85	MG	2	1991	1/1	0.79	41.97	98,98,98,98	0
85	MG	5	3532	1/1	0.58	41.90	45,45,45,45	0
85	MG	6	1901	1/1	0.72	41.57	46,46,46,46	0
85	MG	5	3629	1/1	0.43	41.53	51,51,51,51	0
85	MG	1	3670	1/1	0.33	41.34	49,49,49,49	0
85	MG	1	3834	1/1	0.74	40.85	39,39,39,39	0
85	MG	1	3495	1/1	0.41	40.45	40,40,40,40	0
85	MG	1	3413	1/1	1.01	40.40	59,59,59,59	0
85	MG	5	3640	1/1	1.02	40.06	63,63,63,63	0
85	MG	5	3723	1/1	0.69	39.64	51,51,51,51	0
85	MG	2	1974	1/1	0.50	39.26	75,75,75,75	0
85	MG	1	3452	1/1	0.55	39.22	52,52,52,52	0
85	MG	5	3572	1/1	0.71	39.19	24,24,24,24	0
85	MG	1	3522	1/1	0.94	39.10	75,75,75,75	0
85	MG	5	3799	1/1	0.88	38.87	81,81,81,81	0
85	MG	5	3426	1/1	0.30	38.80	45,45,45,45	0
85	MG	2	1957	1/1	0.78	38.68	69,69,69,69	0
85	MG	1	3460	1/1	0.59	38.51	25,25,25,25	0
85	MG	1	3694	1/1	0.42	38.50	50,50,50,50	0
85	MG	2	2022	1/1	0.71	38.45	120,120,120,120	0
85	MG	2	1975	1/1	1.14	38.39	82,82,82,82	0
85	MG	5	3484	1/1	0.40	38.33	54,54,54,54	0
85	MG	1	3527	1/1	0.80	38.25	35,35,35,35	0
85	MG	2	2001	1/1	0.50	38.16	105,105,105,105	0
85	MG	1	3724	1/1	0.92	38.12	41,41,41,41	0
85	MG	1	3627	1/1	0.69	38.05	57,57,57,57	0
85	MG	5	3812	1/1	0.72	37.87	43,43,43,43	0
85	MG	3	205	1/1	0.74	37.80	42,42,42,42	0
85	MG	5	3677	1/1	0.72	37.76	56,56,56,56	0
85	MG	5	3705	1/1	0.91	37.52	59,59,59,59	0
85	MG	1	3597	1/1	0.83	37.48	43,43,43,43	0
85	MG	5	3437	1/1	0.60	37.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3554	1/1	0.78	36.75	28,28,28,28	0
85	MG	1	3821	1/1	0.78	36.67	48,48,48,48	0
85	MG	1	3655	1/1	0.58	36.53	38,38,38,38	0
85	MG	5	3445	1/1	0.49	36.53	45,45,45,45	0
85	MG	1	3529	1/1	0.52	36.38	34,34,34,34	0
85	MG	5	3761	1/1	0.34	36.33	44,44,44,44	0
85	MG	5	3717	1/1	0.45	36.31	51,51,51,51	0
85	MG	6	2021	1/1	0.44	36.15	96,96,96,96	0
85	MG	2	1917	1/1	0.69	35.83	59,59,59,59	0
85	MG	2	1947	1/1	0.95	35.83	59,59,59,59	0
85	MG	5	3519	1/1	0.68	35.68	22,22,22,22	0
85	MG	1	3418	1/1	0.69	35.59	42,42,42,42	0
85	MG	O7	103	1/1	1.51	35.54	65,65,65,65	0
85	MG	5	3531	1/1	0.76	35.45	21,21,21,21	0
85	MG	1	3560	1/1	0.79	35.27	38,38,38,38	0
85	MG	1	3679	1/1	0.36	35.21	46,46,46,46	0
85	MG	6	1970	1/1	0.49	34.89	69,69,69,69	0
85	MG	1	3692	1/1	0.57	34.81	34,34,34,34	0
85	MG	1	3698	1/1	0.56	34.66	43,43,43,43	0
85	MG	1	3657	1/1	0.97	34.65	54,54,54,54	0
85	MG	1	3563	1/1	0.64	34.63	41,41,41,41	0
85	MG	5	3528	1/1	0.93	34.58	29,29,29,29	0
85	MG	1	3512	1/1	0.65	34.53	25,25,25,25	0
85	MG	2	1936	1/1	0.74	34.45	57,57,57,57	0
85	MG	1	3783	1/1	0.37	34.32	44,44,44,44	0
85	MG	1	3683	1/1	0.53	34.32	39,39,39,39	0
85	MG	2	1905	1/1	0.67	34.16	68,68,68,68	0
85	MG	2	1981	1/1	0.80	34.11	58,58,58,58	0
85	MG	3	202	1/1	0.50	34.07	50,50,50,50	0
85	MG	4	215	1/1	0.45	33.92	74,74,74,74	0
85	MG	1	3507	1/1	0.55	33.72	25,25,25,25	0
85	MG	2	1945	1/1	0.51	33.68	80,80,80,80	0
85	MG	5	3681	1/1	0.20	33.67	42,42,42,42	0
85	MG	1	3442	1/1	0.61	33.66	26,26,26,26	0
85	MG	1	3607	1/1	0.80	33.61	74,74,74,74	0
85	MG	2	1928	1/1	0.60	33.54	76,76,76,76	0
85	MG	5	3887	1/1	0.67	33.43	53,53,53,53	0
85	MG	2	1919	1/1	0.47	33.06	63,63,63,63	0
85	MG	5	3897	1/1	0.53	32.96	57,57,57,57	0
85	MG	1	3486	1/1	0.51	32.73	42,42,42,42	0
85	MG	5	3579	1/1	0.73	32.69	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3557	1/1	0.79	32.54	37,37,37,37	0
85	MG	M7	203	1/1	0.81	32.38	37,37,37,37	0
85	MG	5	3489	1/1	0.52	32.33	54,54,54,54	0
85	MG	6	1944	1/1	0.62	32.10	71,71,71,71	0
85	MG	5	3431	1/1	0.33	32.01	83,83,83,83	0
85	MG	6	1910	1/1	0.49	31.99	56,56,56,56	0
85	MG	1	3468	1/1	0.64	31.76	56,56,56,56	0
85	MG	6	1958	1/1	0.55	31.72	51,51,51,51	0
85	MG	5	3882	1/1	0.54	31.66	33,33,33,33	0
85	MG	5	3817	1/1	0.36	31.65	59,59,59,59	0
85	MG	5	3550	1/1	0.70	31.22	47,47,47,47	0
85	MG	6	1922	1/1	0.59	31.02	61,61,61,61	0
85	MG	5	3849	1/1	0.38	30.95	40,40,40,40	0
85	MG	5	3436	1/1	0.36	30.92	35,35,35,35	0
85	MG	5	3857	1/1	0.78	30.74	52,52,52,52	0
85	MG	5	3553	1/1	0.63	30.71	44,44,44,44	0
85	MG	1	3833	1/1	0.65	30.60	37,37,37,37	0
85	MG	1	3762	1/1	0.52	30.57	55,55,55,55	0
85	MG	5	3533	1/1	0.39	30.53	35,35,35,35	0
85	MG	1	3574	1/1	0.66	30.51	22,22,22,22	0
85	MG	1	3707	1/1	0.66	30.48	33,33,33,33	0
85	MG	1	3611	1/1	0.54	30.47	45,45,45,45	0
85	MG	1	3407	1/1	0.57	30.41	42,42,42,42	0
85	MG	5	3780	1/1	0.54	30.31	74,74,74,74	0
85	MG	1	3656	1/1	0.75	30.27	43,43,43,43	0
85	MG	4	204	1/1	0.77	30.26	44,44,44,44	0
85	MG	1	3576	1/1	0.54	30.10	31,31,31,31	0
85	MG	5	3806	1/1	0.63	30.10	73,73,73,73	0
85	MG	1	3771	1/1	0.53	30.07	63,63,63,63	0
85	MG	5	3518	1/1	0.32	30.05	39,39,39,39	0
85	MG	1	3839	1/1	0.97	29.93	58,58,58,58	0
85	MG	1	3593	1/1	0.65	29.89	29,29,29,29	0
85	MG	1	3838	1/1	0.61	29.86	48,48,48,48	0
85	MG	1	3520	1/1	0.62	29.81	75,75,75,75	0
85	MG	5	3869	1/1	0.56	29.80	42,42,42,42	0
85	MG	6	1943	1/1	0.58	29.72	45,45,45,45	0
85	MG	3	207	1/1	0.48	29.70	61,61,61,61	0
85	MG	5	3641	1/1	0.83	29.56	45,45,45,45	0
85	MG	2	1925	1/1	0.85	29.23	64,64,64,64	0
85	MG	1	3462	1/1	0.61	29.06	28,28,28,28	0
85	MG	5	3656	1/1	0.50	28.97	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3778	1/1	0.60	28.86	38,38,38,38	0
85	MG	2	1982	1/1	0.90	28.78	67,67,67,67	0
85	MG	5	3462	1/1	0.57	28.71	47,47,47,47	0
85	MG	5	3619	1/1	0.29	28.50	51,51,51,51	0
85	MG	5	3546	1/1	0.92	28.25	48,48,48,48	0
85	MG	1	3618	1/1	0.64	28.20	73,73,73,73	0
85	MG	1	3680	1/1	0.47	28.20	43,43,43,43	0
85	MG	5	3837	1/1	0.70	28.11	38,38,38,38	0
85	MG	5	3620	1/1	0.61	28.09	44,44,44,44	0
85	MG	5	3563	1/1	0.60	27.94	27,27,27,27	0
85	MG	5	3508	1/1	0.83	27.75	40,40,40,40	0
85	MG	5	3543	1/1	0.40	27.75	30,30,30,30	0
85	MG	5	3617	1/1	0.87	27.70	48,48,48,48	0
85	MG	7	206	1/1	0.65	27.68	25,25,25,25	0
85	MG	1	3793	1/1	0.57	27.55	41,41,41,41	0
85	MG	6	1925	1/1	0.67	27.47	42,42,42,42	0
85	MG	6	1955	1/1	0.59	27.42	40,40,40,40	0
85	MG	1	3647	1/1	0.73	27.35	49,49,49,49	0
85	MG	5	3597	1/1	0.54	27.31	18,18,18,18	0
85	MG	2	1965	1/1	1.00	27.21	64,64,64,64	0
85	MG	5	3439	1/1	0.57	27.04	29,29,29,29	0
85	MG	1	3747	1/1	0.57	26.97	51,51,51,51	0
85	MG	S4	301	1/1	1.07	26.95	79,79,79,79	0
85	MG	1	3854	1/1	0.51	26.93	53,53,53,53	0
85	MG	5	3538	1/1	0.80	26.86	33,33,33,33	0
85	MG	1	3435	1/1	0.56	26.84	44,44,44,44	0
85	MG	2	1909	1/1	0.47	26.55	70,70,70,70	0
85	MG	1	3476	1/1	0.84	26.34	46,46,46,46	0
85	MG	8	203	1/1	1.01	26.18	56,56,56,56	0
85	MG	5	3873	1/1	0.89	26.10	43,43,43,43	0
85	MG	6	1926	1/1	0.66	26.09	52,52,52,52	0
85	MG	1	3502	1/1	0.49	25.90	33,33,33,33	0
85	MG	5	3418	1/1	0.78	25.89	24,24,24,24	0
85	MG	6	1950	1/1	0.48	25.87	49,49,49,49	0
85	MG	2	1924	1/1	0.85	25.84	86,86,86,86	0
85	MG	1	3469	1/1	0.49	25.80	46,46,46,46	0
85	MG	1	3513	1/1	0.40	25.73	34,34,34,34	0
85	MG	2	1918	1/1	0.65	25.72	54,54,54,54	0
85	MG	1	3561	1/1	0.69	25.72	27,27,27,27	0
85	MG	5	3573	1/1	0.53	25.71	42,42,42,42	0
85	MG	6	1953	1/1	0.65	25.71	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3521	1/1	0.64	25.68	33,33,33,33	0
85	MG	2	1902	1/1	0.69	25.44	38,38,38,38	0
85	MG	5	3587	1/1	0.78	25.40	24,24,24,24	0
85	MG	6	1927	1/1	0.47	25.35	53,53,53,53	0
85	MG	2	1994	1/1	0.67	25.32	122,122,122,122	0
85	MG	1	3734	1/1	0.40	25.26	63,63,63,63	0
85	MG	5	3828	1/1	0.43	25.10	47,47,47,47	0
85	MG	5	3458	1/1	0.37	25.02	38,38,38,38	0
85	MG	1	3431	1/1	0.56	25.00	46,46,46,46	0
85	MG	5	3509	1/1	0.69	24.93	29,29,29,29	0
85	MG	1	3461	1/1	0.59	24.89	27,27,27,27	0
85	MG	1	3688	1/1	0.56	24.86	41,41,41,41	0
85	MG	1	3429	1/1	0.66	24.82	46,46,46,46	0
85	MG	5	3726	1/1	0.52	24.72	50,50,50,50	0
85	MG	5	3580	1/1	0.54	24.49	25,25,25,25	0
85	MG	6	2010	1/1	0.50	24.41	52,52,52,52	0
85	MG	5	3422	1/1	0.51	24.37	40,40,40,40	0
85	MG	5	3552	1/1	0.61	24.24	36,36,36,36	0
85	MG	6	1919	1/1	0.65	24.21	46,46,46,46	0
85	MG	5	3512	1/1	0.66	24.19	27,27,27,27	0
85	MG	1	3537	1/1	0.73	24.19	35,35,35,35	0
85	MG	1	3829	1/1	0.72	24.16	55,55,55,55	0
85	MG	5	3607	1/1	0.31	24.09	34,34,34,34	0
85	MG	1	3665	1/1	0.54	24.06	53,53,53,53	0
85	MG	5	3524	1/1	0.44	23.80	40,40,40,40	0
85	MG	1	3590	1/1	0.53	23.71	34,34,34,34	0
85	MG	5	3562	1/1	0.75	23.70	25,25,25,25	0
85	MG	1	3534	1/1	0.71	23.69	31,31,31,31	0
85	MG	1	3594	1/1	0.70	23.63	24,24,24,24	0
85	MG	5	4257	1/1	0.99	23.49	30,30,30,30	0
85	MG	5	3610	1/1	0.46	23.44	30,30,30,30	0
85	MG	5	3460	1/1	0.74	23.33	31,31,31,31	0
85	MG	8	211	1/1	0.64	22.98	51,51,51,51	0
85	MG	5	3449	1/1	0.60	22.93	65,65,65,65	0
85	MG	5	3490	1/1	0.82	22.90	32,32,32,32	0
85	MG	2	1971	1/1	0.54	22.89	70,70,70,70	0
85	MG	5	3639	1/1	0.48	22.87	52,52,52,52	0
85	MG	2	2008	1/1	0.89	22.86	51,51,51,51	0
85	MG	5	3593	1/1	0.67	22.83	24,24,24,24	0
85	MG	5	3599	1/1	0.59	22.79	31,31,31,31	0
85	MG	6	2004	1/1	0.75	22.78	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3537	1/1	0.46	22.75	40,40,40,40	0
85	MG	1	3674	1/1	0.46	22.71	39,39,39,39	0
85	MG	1	3484	1/1	0.33	22.67	46,46,46,46	0
85	MG	6	1945	1/1	0.45	22.63	42,42,42,42	0
85	MG	1	3551	1/1	0.51	22.62	36,36,36,36	0
85	MG	4	216	1/1	0.20	22.60	57,57,57,57	0
85	MG	1	3568	1/1	0.57	22.56	27,27,27,27	0
85	MG	1	3676	1/1	0.42	22.49	40,40,40,40	0
85	MG	5	3696	1/1	0.60	22.42	54,54,54,54	0
85	MG	5	3535	1/1	0.59	22.38	36,36,36,36	0
85	MG	1	3828	1/1	0.51	22.33	25,25,25,25	0
85	MG	1	3501	1/1	0.55	22.29	42,42,42,42	0
85	MG	5	3556	1/1	0.73	22.20	39,39,39,39	0
86	OHX	5	4181	7/7	0.37	22.17	156,156,156,156	0
85	MG	1	3464	1/1	0.44	22.17	54,54,54,54	0
85	MG	2	2021	1/1	1.31	22.15	99,99,99,99	0
85	MG	1	3496	1/1	0.47	22.14	42,42,42,42	0
85	MG	5	3461	1/1	0.67	22.13	35,35,35,35	0
85	MG	2	2016	1/1	0.74	21.89	94,94,94,94	0
85	MG	5	3465	1/1	0.62	21.86	40,40,40,40	0
85	MG	5	3662	1/1	0.52	21.69	30,30,30,30	0
85	MG	5	3737	1/1	0.44	21.67	77,77,77,77	0
85	MG	1	3539	1/1	0.49	21.59	24,24,24,24	0
85	MG	m7	201	1/1	0.80	21.51	34,34,34,34	0
85	MG	1	3649	1/1	0.64	21.47	65,65,65,65	0
85	MG	1	3430	1/1	0.69	21.46	46,46,46,46	0
85	MG	1	3463	1/1	0.37	21.43	44,44,44,44	0
85	MG	1	3524	1/1	0.39	21.40	43,43,43,43	0
85	MG	5	3719	1/1	0.74	21.38	62,62,62,62	0
85	MG	1	3509	1/1	0.59	21.36	28,28,28,28	0
85	MG	1	3586	1/1	0.60	21.34	38,38,38,38	0
85	MG	5	3574	1/1	0.46	21.32	32,32,32,32	0
85	MG	5	3473	1/1	0.38	21.24	56,56,56,56	0
85	MG	2	1995	1/1	0.55	21.24	57,57,57,57	0
85	MG	6	1913	1/1	0.55	21.17	39,39,39,39	0
85	MG	4	211	1/1	0.51	21.13	58,58,58,58	0
85	MG	5	3558	1/1	0.64	21.07	31,31,31,31	0
85	MG	3	204	1/1	0.44	21.05	63,63,63,63	0
85	MG	5	3666	1/1	0.93	21.03	59,59,59,59	0
85	MG	5	3576	1/1	0.40	21.02	27,27,27,27	0
85	MG	5	3757	1/1	0.55	20.98	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3660	1/1	0.39	20.91	55,55,55,55	0
85	MG	6	1956	1/1	0.63	20.85	48,48,48,48	0
85	MG	5	3545	1/1	0.55	20.84	35,35,35,35	0
85	MG	6	1959	1/1	0.46	20.77	58,58,58,58	0
85	MG	1	3573	1/1	0.46	20.75	39,39,39,39	0
85	MG	5	3483	1/1	0.49	20.71	41,41,41,41	0
85	MG	5	3741	1/1	0.42	20.66	47,47,47,47	0
85	MG	5	3774	1/1	0.87	20.45	105,105,105,105	0
85	MG	1	3850	1/1	0.62	20.40	28,28,28,28	0
85	MG	6	1968	1/1	0.56	20.38	76,76,76,76	0
85	MG	1	3685	1/1	0.48	20.35	51,51,51,51	0
85	MG	1	3536	1/1	0.61	20.33	43,43,43,43	0
85	MG	1	3592	1/1	0.69	20.19	62,62,62,62	0
85	MG	4	219	1/1	0.72	20.14	49,49,49,49	0
85	MG	5	3523	1/1	0.47	20.03	34,34,34,34	0
85	MG	5	3694	1/1	0.54	19.98	43,43,43,43	0
85	MG	1	3781	1/1	0.26	19.95	40,40,40,40	0
85	MG	1	3432	1/1	0.57	19.93	41,41,41,41	0
85	MG	5	3526	1/1	0.47	19.85	31,31,31,31	0
85	MG	5	3795	1/1	0.53	19.83	46,46,46,46	0
85	MG	1	3450	1/1	0.65	19.80	44,44,44,44	0
86	OHX	6	2174	7/7	0.34	19.79	141,141,141,141	0
85	MG	5	3525	1/1	0.57	19.74	37,37,37,37	0
85	MG	1	3640	1/1	0.54	19.72	35,35,35,35	0
85	MG	5	3429	1/1	0.43	19.66	28,28,28,28	0
85	MG	1	3847	1/1	0.45	19.64	45,45,45,45	0
85	MG	5	3463	1/1	0.62	19.62	35,35,35,35	0
85	MG	5	3839	1/1	0.57	19.56	43,43,43,43	0
85	MG	1	3645	1/1	0.35	19.54	40,40,40,40	0
85	MG	1	3433	1/1	0.47	19.46	36,36,36,36	0
85	MG	6	1975	1/1	0.52	19.37	67,67,67,67	0
85	MG	7	201	1/1	0.44	19.28	40,40,40,40	0
85	MG	5	3530	1/1	0.47	19.27	32,32,32,32	0
85	MG	5	3583	1/1	0.72	19.25	37,37,37,37	0
85	MG	d3	201	1/1	1.22	19.23	56,56,56,56	0
85	MG	5	3796	1/1	0.61	19.17	101,101,101,101	0
85	MG	5	3448	1/1	0.67	19.15	58,58,58,58	0
85	MG	6	1907	1/1	0.52	19.00	76,76,76,76	0
85	MG	7	216	1/1	0.39	19.00	55,55,55,55	0
85	MG	5	3570	1/1	0.50	18.95	36,36,36,36	0
85	MG	1	3424	1/1	0.33	18.89	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3632	1/1	0.64	18.69	52,52,52,52	0
85	MG	2	1926	1/1	0.70	18.66	97,97,97,97	0
85	MG	5	3712	1/1	0.42	18.65	47,47,47,47	0
85	MG	1	3808	1/1	0.57	18.57	45,45,45,45	0
85	MG	5	3565	1/1	0.55	18.56	33,33,33,33	0
85	MG	5	3564	1/1	0.92	18.52	35,35,35,35	0
85	MG	5	3457	1/1	0.42	18.43	29,29,29,29	0
85	MG	1	3837	1/1	0.54	18.43	62,62,62,62	0
85	MG	N3	202	1/1	0.41	18.38	59,59,59,59	0
85	MG	6	1967	1/1	0.37	18.35	89,89,89,89	0
85	MG	1	3630	1/1	0.34	18.35	36,36,36,36	0
85	MG	5	3756	1/1	0.48	18.29	49,49,49,49	0
85	MG	6	1937	1/1	0.44	18.26	42,42,42,42	0
85	MG	6	2011	1/1	0.58	18.25	56,56,56,56	0
85	MG	6	2029	1/1	0.69	18.23	92,92,92,92	0
85	MG	1	3447	1/1	0.39	18.22	29,29,29,29	0
85	MG	3	212	1/1	0.54	18.15	78,78,78,78	0
85	MG	6	1954	1/1	0.53	18.12	51,51,51,51	0
85	MG	1	3755	1/1	0.49	17.85	41,41,41,41	0
85	MG	5	3787	1/1	0.38	17.85	30,30,30,30	0
85	MG	5	3427	1/1	0.53	17.80	39,39,39,39	0
85	MG	1	3558	1/1	0.42	17.70	27,27,27,27	0
85	MG	5	3850	1/1	1.01	17.67	36,36,36,36	0
85	MG	3	206	1/1	0.59	17.64	32,32,32,32	0
85	MG	5	3798	1/1	0.54	17.63	48,48,48,48	0
85	MG	5	3710	1/1	0.31	17.60	53,53,53,53	0
85	MG	1	3690	1/1	0.46	17.57	50,50,50,50	0
85	MG	5	3505	1/1	0.62	17.54	31,31,31,31	0
85	MG	1	3511	1/1	0.64	17.51	31,31,31,31	0
85	MG	6	2040	1/1	0.66	17.37	97,97,97,97	0
85	MG	1	3497	1/1	0.42	17.35	36,36,36,36	0
85	MG	1	3801	1/1	0.42	17.33	43,43,43,43	0
85	MG	1	3443	1/1	0.36	17.26	67,67,67,67	0
85	MG	N8	203	1/1	0.64	17.25	34,34,34,34	0
85	MG	1	3523	1/1	0.75	17.20	25,25,25,25	0
85	MG	1	3813	1/1	0.90	17.19	127,127,127,127	0
85	MG	1	3506	1/1	0.72	17.13	32,32,32,32	0
85	MG	1	3615	1/1	0.69	17.12	39,39,39,39	0
85	MG	5	3571	1/1	0.64	17.02	33,33,33,33	0
85	MG	2	2012	1/1	0.49	17.02	68,68,68,68	0
85	MG	2	1970	1/1	0.42	17.01	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3876	1/1	0.54	16.97	41,41,41,41	0
85	MG	1	3549	1/1	0.48	16.95	38,38,38,38	0
85	MG	5	3733	1/1	0.22	16.94	57,57,57,57	0
85	MG	6	1920	1/1	0.83	16.92	56,56,56,56	0
85	MG	2	1944	1/1	0.42	16.90	68,68,68,68	0
85	MG	1	3503	1/1	0.36	16.82	45,45,45,45	0
85	MG	2	1911	1/1	0.58	16.82	55,55,55,55	0
85	MG	1	4216	1/1	0.48	16.81	37,37,37,37	0
85	MG	6	1994	1/1	0.45	16.76	62,62,62,62	0
85	MG	6	2017	1/1	0.39	16.68	46,46,46,46	0
85	MG	O7	104	1/1	0.62	16.67	34,34,34,34	0
85	MG	5	3605	1/1	0.46	16.62	35,35,35,35	0
85	MG	1	3564	1/1	0.46	16.62	35,35,35,35	0
85	MG	5	3613	1/1	0.46	16.58	47,47,47,47	0
85	MG	L4	401	1/1	0.42	16.58	34,34,34,34	0
85	MG	5	3893	1/1	0.56	16.53	29,29,29,29	0
85	MG	5	3843	1/1	0.20	16.50	57,57,57,57	0
85	MG	2	2011	1/1	0.89	16.43	63,63,63,63	0
85	MG	5	3609	1/1	0.48	16.40	33,33,33,33	0
85	MG	5	3654	1/1	0.83	16.35	77,77,77,77	0
85	MG	6	1946	1/1	0.53	16.30	73,73,73,73	0
85	MG	1	3572	1/1	0.62	16.28	23,23,23,23	0
85	MG	5	3631	1/1	0.50	16.22	44,44,44,44	0
85	MG	6	1932	1/1	0.46	16.21	48,48,48,48	0
85	MG	6	1940	1/1	0.53	16.17	97,97,97,97	0
85	MG	4	212	1/1	0.67	16.16	36,36,36,36	0
85	MG	1	3508	1/1	0.42	16.15	45,45,45,45	0
85	MG	4	214	1/1	0.41	16.15	52,52,52,52	0
85	MG	5	3665	1/1	0.48	16.13	51,51,51,51	0
85	MG	1	3456	1/1	0.39	16.11	31,31,31,31	0
85	MG	5	3479	1/1	0.53	16.09	31,31,31,31	0
85	MG	6	2044	1/1	0.37	16.08	51,51,51,51	0
85	MG	5	3561	1/1	0.46	16.01	36,36,36,36	0
85	MG	1	3470	1/1	0.49	16.00	42,42,42,42	0
85	MG	5	3626	1/1	0.43	15.99	41,41,41,41	0
85	MG	2	2000	1/1	0.38	15.95	85,85,85,85	0
85	MG	5	3749	1/1	0.27	15.90	63,63,63,63	0
85	MG	5	3736	1/1	0.34	15.89	44,44,44,44	0
85	MG	6	1917	1/1	0.40	15.78	63,63,63,63	0
85	MG	1	3852	1/1	0.39	15.70	45,45,45,45	0
85	MG	1	3422	1/1	0.58	15.69	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3515	1/1	0.62	15.61	28,28,28,28	0
85	MG	5	3432	1/1	0.43	15.52	35,35,35,35	0
85	MG	1	3474	1/1	0.37	15.46	74,74,74,74	0
85	MG	2	1966	1/1	0.36	15.44	85,85,85,85	0
85	MG	4	208	1/1	0.90	15.41	47,47,47,47	0
85	MG	o7	101	1/1	0.56	15.37	47,47,47,47	0
85	MG	2	1927	1/1	0.60	15.36	51,51,51,51	0
85	MG	5	3742	1/1	0.36	15.34	59,59,59,59	0
85	MG	5	3830	1/1	0.65	15.25	38,38,38,38	0
85	MG	1	3414	1/1	0.51	15.18	38,38,38,38	0
85	MG	5	3670	1/1	0.50	15.17	35,35,35,35	0
85	MG	6	2019	1/1	0.61	15.13	52,52,52,52	0
85	MG	1	3465	1/1	0.43	15.08	51,51,51,51	0
85	MG	4	203	1/1	0.55	15.05	53,53,53,53	0
85	MG	5	3704	1/1	0.45	15.05	38,38,38,38	0
85	MG	1	3541	1/1	0.43	15.03	29,29,29,29	0
85	MG	1	3526	1/1	0.46	15.01	26,26,26,26	0
85	MG	17	301	1/1	0.42	14.94	39,39,39,39	0
86	OHX	5	4177	7/7	0.41	14.89	150,150,150,150	0
85	MG	1	3455	1/1	0.55	14.87	57,57,57,57	0
85	MG	6	1908	1/1	0.35	14.86	49,49,49,49	0
85	MG	5	3586	1/1	0.66	14.85	30,30,30,30	0
85	MG	5	3875	1/1	0.54	14.84	50,50,50,50	0
85	MG	1	3517	1/1	0.61	14.84	33,33,33,33	0
86	OHX	1	4175	7/7	0.37	14.84	131,131,131,131	0
85	MG	6	1999	1/1	0.52	14.84	59,59,59,59	0
85	MG	2	1961	1/1	0.58	14.75	61,61,61,61	0
85	MG	5	3825	1/1	0.51	14.74	48,48,48,48	0
86	OHX	1	4186	7/7	0.32	14.71	137,137,137,137	0
85	MG	5	3548	1/1	0.63	14.69	47,47,47,47	0
85	MG	5	3608	1/1	0.38	14.67	56,56,56,56	0
85	MG	2	1913	1/1	0.37	14.64	88,88,88,88	0
85	MG	1	3471	1/1	0.40	14.61	43,43,43,43	0
85	MG	5	3815	1/1	0.50	14.60	39,39,39,39	0
85	MG	5	3578	1/1	0.48	14.59	38,38,38,38	0
85	MG	1	3669	1/1	0.67	14.58	60,60,60,60	0
85	MG	5	3541	1/1	0.77	14.54	29,29,29,29	0
85	MG	1	3622	1/1	0.32	14.50	47,47,47,47	0
85	MG	2	2005	1/1	0.61	14.49	67,67,67,67	0
85	MG	1	3518	1/1	0.66	14.43	41,41,41,41	0
85	MG	5	3612	1/1	0.43	14.43	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3409	1/1	0.36	14.41	23,23,23,23	0
85	MG	1	3548	1/1	0.48	14.40	48,48,48,48	0
85	MG	1	3480	1/1	0.53	14.39	44,44,44,44	0
85	MG	1	3610	1/1	0.26	14.30	44,44,44,44	0
85	MG	6	2030	1/1	0.46	14.21	105,105,105,105	0
85	MG	1	3773	1/1	0.48	14.18	31,31,31,31	0
85	MG	6	2042	1/1	0.79	14.12	76,76,76,76	0
85	MG	5	3701	1/1	0.42	14.10	41,41,41,41	0
85	MG	1	3626	1/1	0.91	14.09	37,37,37,37	0
85	MG	6	2007	1/1	0.71	14.06	65,65,65,65	0
85	MG	2	1908	1/1	0.35	14.04	74,74,74,74	0
85	MG	12	301	1/1	0.46	14.03	42,42,42,42	0
85	MG	6	2014	1/1	0.47	14.02	171,171,171,171	0
85	MG	4	220	1/1	0.49	14.00	81,81,81,81	0
85	MG	2	1959	1/1	0.51	13.98	98,98,98,98	0
85	MG	D0	201	1/1	0.71	13.93	79,79,79,79	0
85	MG	2	2003	1/1	0.59	13.89	90,90,90,90	0
85	MG	6	1929	1/1	0.53	13.86	58,58,58,58	0
85	MG	6	2023	1/1	0.53	13.71	61,61,61,61	0
85	MG	1	3824	1/1	0.36	13.67	30,30,30,30	0
86	OHX	6	2181	7/7	0.31	13.56	147,147,147,147	0
85	MG	5	3624	1/1	0.48	13.50	74,74,74,74	0
85	MG	1	3642	1/1	0.39	13.48	49,49,49,49	0
85	MG	5	3621	1/1	0.27	13.38	46,46,46,46	0
85	MG	5	3709	1/1	0.41	13.37	49,49,49,49	0
85	MG	1	3405	1/1	0.44	13.34	93,93,93,93	0
85	MG	5	3636	1/1	0.41	13.33	88,88,88,88	0
85	MG	1	3777	1/1	0.44	13.25	48,48,48,48	0
85	MG	14	401	1/1	0.73	13.21	41,41,41,41	0
85	MG	1	3768	1/1	0.42	13.20	54,54,54,54	0
85	MG	1	3739	1/1	0.36	13.18	52,52,52,52	0
85	MG	5	3425	1/1	0.36	13.15	36,36,36,36	0
85	MG	5	3468	1/1	0.30	13.11	41,41,41,41	0
85	MG	1	3812	1/1	0.41	12.99	53,53,53,53	0
85	MG	1	3641	1/1	0.44	12.99	44,44,44,44	0
85	MG	6	2037	1/1	0.63	12.97	72,72,72,72	0
85	MG	1	3729	1/1	0.36	12.92	86,86,86,86	0
85	MG	5	3661	1/1	0.34	12.91	49,49,49,49	0
85	MG	6	2032	1/1	0.53	12.88	55,55,55,55	0
85	MG	7	211	1/1	0.28	12.87	79,79,79,79	0
85	MG	1	3791	1/1	0.35	12.83	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1940	1/1	0.38	12.78	63,63,63,63	0
85	MG	1	3457	1/1	0.43	12.77	44,44,44,44	0
85	MG	5	3891	1/1	0.37	12.76	43,43,43,43	0
85	MG	5	3658	1/1	0.42	12.75	58,58,58,58	0
85	MG	8	202	1/1	0.44	12.75	39,39,39,39	0
85	MG	5	3577	1/1	0.37	12.65	41,41,41,41	0
86	OHX	5	4223	7/7	0.36	12.62	148,148,148,148	0
85	MG	5	3405	1/1	0.46	12.60	31,31,31,31	0
85	MG	5	3466	1/1	0.30	12.54	61,61,61,61	0
85	MG	5	3746	1/1	0.39	12.54	35,35,35,35	0
85	MG	5	3517	1/1	0.48	12.50	28,28,28,28	0
85	MG	5	3874	1/1	0.58	12.46	37,37,37,37	0
85	MG	1	3644	1/1	0.38	12.45	68,68,68,68	0
85	MG	1	3441	1/1	0.60	12.45	46,46,46,46	0
85	MG	5	3698	1/1	0.41	12.42	72,72,72,72	0
86	OHX	1	4187	7/7	0.43	12.32	151,151,151,151	0
85	MG	1	3411	1/1	0.45	12.29	33,33,33,33	0
86	OHX	5	4189	7/7	0.52	12.27	124,124,124,124	0
85	MG	1	3565	1/1	0.45	12.24	34,34,34,34	0
85	MG	1	3633	1/1	0.34	12.23	69,69,69,69	0
85	MG	1	3545	1/1	0.48	12.20	55,55,55,55	0
85	MG	1	3532	1/1	0.41	12.16	35,35,35,35	0
85	MG	6	2013	1/1	0.40	12.14	76,76,76,76	0
85	MG	5	3729	1/1	0.27	12.08	38,38,38,38	0
85	MG	1	3712	1/1	0.40	12.04	46,46,46,46	0
85	MG	5	3854	1/1	0.40	12.04	55,55,55,55	0
85	MG	M3	203	1/1	0.61	12.02	36,36,36,36	0
85	MG	1	3654	1/1	0.32	12.00	34,34,34,34	0
85	MG	5	3675	1/1	0.56	11.97	34,34,34,34	0
85	MG	1	3668	1/1	0.52	11.93	47,47,47,47	0
85	MG	1	3421	1/1	0.65	11.90	36,36,36,36	0
85	MG	5	3604	1/1	0.53	11.89	43,43,43,43	0
85	MG	1	3743	1/1	0.41	11.89	56,56,56,56	0
85	MG	S8	301	1/1	0.36	11.85	62,62,62,62	0
85	MG	6	1960	1/1	0.51	11.81	44,44,44,44	0
85	MG	6	1947	1/1	0.53	11.77	57,57,57,57	0
86	OHX	1	4166	7/7	0.24	11.76	128,128,128,128	0
85	MG	1	3477	1/1	0.43	11.71	42,42,42,42	0
85	MG	1	3408	1/1	0.57	11.62	37,37,37,37	0
85	MG	2	1938	1/1	0.50	11.61	69,69,69,69	0
85	MG	1	3472	1/1	0.31	11.57	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2025	1/1	0.42	11.57	69,69,69,69	0
85	MG	5	3625	1/1	0.44	11.57	44,44,44,44	0
85	MG	2	2018	1/1	0.48	11.56	79,79,79,79	0
85	MG	1	3552	1/1	0.54	11.52	33,33,33,33	0
85	MG	1	3760	1/1	0.34	11.51	46,46,46,46	0
85	MG	1	3535	1/1	0.51	11.43	53,53,53,53	0
85	MG	6	1906	1/1	0.51	11.42	48,48,48,48	0
85	MG	5	3412	1/1	0.35	11.42	35,35,35,35	0
85	MG	1	3423	1/1	0.43	11.41	47,47,47,47	0
85	MG	5	3866	1/1	0.28	11.38	52,52,52,52	0
85	MG	5	3598	1/1	0.48	11.36	37,37,37,37	0
85	MG	5	3763	1/1	0.37	11.26	65,65,65,65	0
85	MG	5	3547	1/1	0.49	11.25	48,48,48,48	0
85	MG	2	1937	1/1	0.41	11.22	61,61,61,61	0
85	MG	6	1918	1/1	0.53	11.21	71,71,71,71	0
85	MG	1	3623	1/1	0.38	11.20	54,54,54,54	0
86	OHX	6	2190	7/7	0.31	11.12	157,157,157,157	0
85	MG	5	3569	1/1	0.46	11.09	24,24,24,24	0
86	OHX	5	4183	7/7	0.35	11.09	144,144,144,144	0
85	MG	o3	201	1/1	0.47	11.09	37,37,37,37	0
86	OHX	5	4047	7/7	0.23	11.08	132,132,132,132	0
85	MG	1	4220	1/1	0.44	11.07	43,43,43,43	0
85	MG	1	3482	1/1	0.46	11.07	51,51,51,51	0
85	MG	5	3769	1/1	0.45	11.05	42,42,42,42	0
85	MG	1	3444	1/1	0.60	11.03	42,42,42,42	0
85	MG	L7	303	1/1	0.55	10.96	47,47,47,47	0
85	MG	1	3720	1/1	0.28	10.93	54,54,54,54	0
85	MG	2	1921	1/1	0.53	10.91	52,52,52,52	0
85	MG	5	3863	1/1	0.36	10.87	64,64,64,64	0
85	MG	1	3693	1/1	0.30	10.84	48,48,48,48	0
85	MG	5	3408	1/1	0.44	10.75	32,32,32,32	0
85	MG	1	3403	1/1	0.42	10.73	37,37,37,37	0
85	MG	2	1916	1/1	0.44	10.73	53,53,53,53	0
86	OHX	1	4169	7/7	0.31	10.73	168,168,168,168	0
85	MG	6	2028	1/1	0.53	10.72	66,66,66,66	0
86	OHX	1	4106	7/7	0.23	10.72	139,139,139,139	0
85	MG	5	3818	1/1	0.29	10.66	70,70,70,70	0
85	MG	5	3594	1/1	0.66	10.60	29,29,29,29	0
85	MG	5	3786	1/1	0.46	10.59	61,61,61,61	0
85	MG	5	3883	1/1	0.38	10.58	35,35,35,35	0
85	MG	8	205	1/1	0.38	10.56	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2183	7/7	0.55	10.55	148,148,148,148	0
85	MG	o4	202	1/1	0.98	10.52	63,63,63,63	0
86	OHX	1	4095	7/7	0.14	10.49	152,152,152,152	0
85	MG	1	3577	1/1	0.39	10.48	27,27,27,27	0
85	MG	2	1942	1/1	0.34	10.47	70,70,70,70	0
86	OHX	2	2143	7/7	0.50	10.47	137,137,137,137	0
85	MG	5	3734	1/1	0.25	10.45	39,39,39,39	0
86	OHX	1	4071	7/7	0.35	10.45	116,116,116,116	0
85	MG	5	3823	1/1	0.43	10.30	69,69,69,69	0
85	MG	6	1911	1/1	0.33	10.26	94,94,94,94	0
85	MG	m0	301	1/1	0.77	10.24	37,37,37,37	0
85	MG	2	1935	1/1	0.50	10.21	52,52,52,52	0
85	MG	5	3410	1/1	0.31	10.19	49,49,49,49	0
85	MG	1	3713	1/1	0.32	10.19	41,41,41,41	0
86	OHX	1	4195	7/7	0.33	10.14	139,139,139,139	0
85	MG	2	1914	1/1	0.47	10.14	71,71,71,71	0
85	MG	4	213	1/1	0.29	10.13	61,61,61,61	0
85	MG	1	3483	1/1	0.37	10.08	52,52,52,52	0
85	MG	5	3438	1/1	0.43	10.01	55,55,55,55	0
85	MG	2	1910	1/1	0.41	9.95	57,57,57,57	0
85	MG	1	3515	1/1	0.55	9.93	41,41,41,41	0
85	MG	5	3724	1/1	0.38	9.91	39,39,39,39	0
85	MG	1	3856	1/1	0.77	9.89	68,68,68,68	0
85	MG	2	1962	1/1	0.49	9.85	81,81,81,81	0
85	MG	1	3844	1/1	0.32	9.84	52,52,52,52	0
85	MG	5	3443	1/1	0.37	9.81	28,28,28,28	0
85	MG	1	3625	1/1	0.33	9.79	39,39,39,39	0
85	MG	1	4219	1/1	0.71	9.78	31,31,31,31	0
85	MG	1	3741	1/1	0.39	9.75	31,31,31,31	0
85	MG	1	3695	1/1	0.30	9.73	54,54,54,54	0
85	MG	5	4258	1/1	0.71	9.72	41,41,41,41	0
85	MG	1	3702	1/1	0.56	9.72	62,62,62,62	0
85	MG	4	217	1/1	0.44	9.71	43,43,43,43	0
85	MG	1	3805	1/1	0.36	9.66	44,44,44,44	0
85	MG	1	3589	1/1	0.40	9.62	43,43,43,43	0
85	MG	7	207	1/1	0.29	9.62	36,36,36,36	0
85	MG	1	3525	1/1	0.38	9.62	27,27,27,27	0
85	MG	5	3475	1/1	0.38	9.61	61,61,61,61	0
85	MG	5	3856	1/1	0.32	9.57	63,63,63,63	0
85	MG	7	204	1/1	0.37	9.53	55,55,55,55	0
85	MG	l3	401	1/1	0.53	9.53	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3847	1/1	0.34	9.52	46,46,46,46	0
85	MG	3	208	1/1	0.43	9.52	49,49,49,49	0
85	MG	1	3406	1/1	0.48	9.51	41,41,41,41	0
86	OHX	5	4231	7/7	0.33	9.50	135,135,135,135	0
85	MG	1	3542	1/1	0.42	9.45	33,33,33,33	0
85	MG	1	3830	1/1	0.41	9.43	29,29,29,29	0
85	MG	1	3544	1/1	0.32	9.43	38,38,38,38	0
85	MG	1	3547	1/1	0.43	9.43	44,44,44,44	0
85	MG	1	3490	1/1	0.34	9.39	33,33,33,33	0
85	MG	5	3501	1/1	0.47	9.39	40,40,40,40	0
85	MG	N0	201	1/1	0.48	9.38	48,48,48,48	0
85	MG	5	3685	1/1	0.34	9.36	33,33,33,33	0
86	OHX	5	4242	7/7	0.38	9.29	156,156,156,156	0
86	OHX	5	4162	7/7	0.32	9.29	137,137,137,137	0
85	MG	5	3778	1/1	0.35	9.28	36,36,36,36	0
85	MG	6	2008	1/1	0.27	9.27	61,61,61,61	0
85	MG	6	1902	1/1	0.50	9.21	59,59,59,59	0
85	MG	8	209	1/1	0.26	9.19	65,65,65,65	0
85	MG	5	3846	1/1	0.48	9.19	56,56,56,56	0
85	MG	5	3420	1/1	0.41	9.18	71,71,71,71	0
85	MG	1	3855	1/1	0.53	9.16	75,75,75,75	0
85	MG	1	3843	1/1	0.29	9.13	46,46,46,46	0
85	MG	6	1973	1/1	0.44	9.13	57,57,57,57	0
85	MG	5	3743	1/1	0.31	9.10	36,36,36,36	0
85	MG	5	3441	1/1	0.43	9.08	31,31,31,31	0
85	MG	5	3779	1/1	0.35	9.05	31,31,31,31	0
86	OHX	5	3925	7/7	0.24	9.02	75,75,75,75	0
85	MG	5	3889	1/1	0.37	9.00	63,63,63,63	0
85	MG	1	3543	1/1	0.48	8.98	38,38,38,38	0
85	MG	1	3780	1/1	0.63	8.96	38,38,38,38	0
86	OHX	1	4179	7/7	0.23	8.95	141,141,141,141	0
86	OHX	1	4065	7/7	0.29	8.95	124,124,124,124	0
86	OHX	6	2204	7/7	0.32	8.89	156,156,156,156	0
85	MG	7	212	1/1	0.34	8.87	68,68,68,68	0
86	OHX	1	4204	7/7	0.34	8.85	135,135,135,135	0
85	MG	5	3664	1/1	0.41	8.85	37,37,37,37	0
85	MG	6	1936	1/1	0.51	8.82	84,84,84,84	0
85	MG	5	3485	1/1	0.70	8.82	28,28,28,28	0
85	MG	1	3765	1/1	0.41	8.80	43,43,43,43	0
85	MG	6	2031	1/1	0.38	8.80	77,77,77,77	0
85	MG	m7	204	1/1	0.39	8.80	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	L7	302	1/1	0.69	8.80	46,46,46,46	0
85	MG	5	3434	1/1	0.41	8.80	86,86,86,86	0
85	MG	5	3506	1/1	0.40	8.79	53,53,53,53	0
85	MG	1	3652	1/1	0.33	8.75	49,49,49,49	0
85	MG	5	3403	1/1	0.56	8.74	61,61,61,61	0
86	OHX	1	4199	7/7	0.27	8.73	150,150,150,150	0
85	MG	1	3745	1/1	0.38	8.72	47,47,47,47	0
85	MG	2	1932	1/1	0.29	8.71	65,65,65,65	0
85	MG	1	3735	1/1	0.43	8.71	56,56,56,56	0
85	MG	5	3802	1/1	0.48	8.67	49,49,49,49	0
86	OHX	5	4249	7/7	0.27	8.63	152,152,152,152	0
85	MG	1	3836	1/1	0.33	8.62	31,31,31,31	0
85	MG	5	3591	1/1	0.33	8.61	34,34,34,34	0
85	MG	5	3502	1/1	0.33	8.61	32,32,32,32	0
85	MG	5	3683	1/1	0.35	8.60	42,42,42,42	0
85	MG	5	3714	1/1	0.41	8.60	44,44,44,44	0
85	MG	5	3838	1/1	0.39	8.58	38,38,38,38	0
85	MG	2	1983	1/1	0.30	8.57	78,78,78,78	0
85	MG	1	3600	1/1	0.46	8.56	28,28,28,28	0
85	MG	1	3775	1/1	0.49	8.54	45,45,45,45	0
85	MG	2	1943	1/1	0.49	8.52	69,69,69,69	0
85	MG	6	1988	1/1	0.27	8.45	70,70,70,70	0
85	MG	1	3650	1/1	0.59	8.42	101,101,101,101	0
85	MG	5	3450	1/1	0.37	8.37	32,32,32,32	0
85	MG	5	3716	1/1	0.31	8.32	45,45,45,45	0
85	MG	5	3829	1/1	0.38	8.32	36,36,36,36	0
85	MG	5	3539	1/1	0.43	8.31	39,39,39,39	0
85	MG	2	2006	1/1	0.50	8.31	81,81,81,81	0
85	MG	5	3511	1/1	0.48	8.29	33,33,33,33	0
85	MG	1	3559	1/1	0.39	8.28	40,40,40,40	0
85	MG	1	3453	1/1	0.34	8.27	38,38,38,38	0
85	MG	M5	301	1/1	0.38	8.24	51,51,51,51	0
85	MG	1	3514	1/1	0.51	8.23	39,39,39,39	0
86	OHX	5	4091	7/7	0.40	8.22	118,118,118,118	0
86	OHX	14	403	7/7	0.41	8.19	184,184,184,184	0
85	MG	5	3416	1/1	0.38	8.16	36,36,36,36	0
85	MG	5	3879	1/1	0.29	8.13	47,47,47,47	0
85	MG	5	3507	1/1	0.44	8.10	33,33,33,33	0
86	OHX	5	4197	7/7	0.35	8.10	144,144,144,144	0
85	MG	5	3472	1/1	0.44	8.09	38,38,38,38	0
85	MG	5	3676	1/1	0.27	8.08	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3675	1/1	0.35	8.08	47,47,47,47	0
85	MG	5	3555	1/1	0.56	8.08	37,37,37,37	0
85	MG	5	3740	1/1	0.27	8.07	51,51,51,51	0
85	MG	5	3411	1/1	0.44	8.03	41,41,41,41	0
85	MG	5	3762	1/1	0.17	8.00	56,56,56,56	0
85	MG	5	3811	1/1	0.34	8.00	38,38,38,38	0
86	OHX	4	235	7/7	0.43	7.97	143,143,143,143	0
86	OHX	1	4184	7/7	0.43	7.94	195,195,195,195	0
86	OHX	2	2163	7/7	0.29	7.93	150,150,150,150	0
85	MG	5	3444	1/1	0.32	7.90	35,35,35,35	0
85	MG	3	213	1/1	0.33	7.90	59,59,59,59	0
85	MG	5	3451	1/1	0.40	7.89	41,41,41,41	0
85	MG	c1	201	1/1	0.51	7.88	46,46,46,46	0
85	MG	2	1915	1/1	0.41	7.84	75,75,75,75	0
85	MG	5	3481	1/1	0.49	7.84	62,62,62,62	0
85	MG	2	1972	1/1	0.46	7.83	88,88,88,88	0
85	MG	O2	201	1/1	0.38	7.81	35,35,35,35	0
85	MG	1	3646	1/1	0.29	7.79	47,47,47,47	0
86	OHX	1	4181	7/7	0.36	7.75	149,149,149,149	0
85	MG	5	3560	1/1	0.39	7.75	36,36,36,36	0
85	MG	5	3513	1/1	0.44	7.73	33,33,33,33	0
85	MG	5	3476	1/1	0.60	7.73	52,52,52,52	0
85	MG	1	3492	1/1	0.26	7.67	83,83,83,83	0
85	MG	5	3634	1/1	0.41	7.67	43,43,43,43	0
85	MG	1	3575	1/1	0.49	7.66	32,32,32,32	0
86	OHX	1	4140	7/7	0.36	7.66	150,150,150,150	0
85	MG	1	3491	1/1	0.47	7.65	61,61,61,61	0
85	MG	1	3583	1/1	0.42	7.64	45,45,45,45	0
85	MG	6	1930	1/1	0.42	7.64	59,59,59,59	0
85	MG	4	218	1/1	0.29	7.64	38,38,38,38	0
86	OHX	5	4221	7/7	0.33	7.63	143,143,143,143	0
85	MG	1	3792	1/1	0.32	7.62	51,51,51,51	0
85	MG	5	3493	1/1	0.38	7.62	55,55,55,55	0
86	OHX	1	4138	7/7	0.42	7.62	120,120,120,120	0
85	MG	6	1993	1/1	0.26	7.59	59,59,59,59	0
85	MG	1	3410	1/1	0.33	7.59	44,44,44,44	0
85	MG	n3	202	1/1	0.90	7.57	54,54,54,54	0
85	MG	1	3810	1/1	0.35	7.56	50,50,50,50	0
86	OHX	5	4222	7/7	0.31	7.53	177,177,177,177	0
85	MG	1	3820	1/1	0.27	7.53	64,64,64,64	0
85	MG	5	3805	1/1	0.24	7.51	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3624	1/1	0.48	7.48	89,89,89,89	0
85	MG	5	4256	1/1	0.37	7.48	47,47,47,47	0
85	MG	5	3521	1/1	0.36	7.46	35,35,35,35	0
85	MG	2	1963	1/1	0.32	7.43	150,150,150,150	0
85	MG	8	206	1/1	0.49	7.42	46,46,46,46	0
85	MG	6	1989	1/1	0.27	7.42	52,52,52,52	0
86	OHX	1	4124	7/7	0.31	7.34	127,127,127,127	0
85	MG	2	1976	1/1	0.35	7.30	60,60,60,60	0
85	MG	5	3680	1/1	0.33	7.29	96,96,96,96	0
86	OHX	6	2156	7/7	0.48	7.28	196,196,196,196	0
85	MG	6	2039	1/1	0.67	7.26	88,88,88,88	0
85	MG	d4	201	1/1	0.64	7.25	66,66,66,66	0
86	OHX	1	4168	7/7	0.31	7.25	162,162,162,162	0
85	MG	5	3542	1/1	0.41	7.22	33,33,33,33	0
85	MG	1	3666	1/1	0.35	7.20	44,44,44,44	0
85	MG	5	3794	1/1	0.29	7.20	58,58,58,58	0
85	MG	5	3497	1/1	0.45	7.19	29,29,29,29	0
85	MG	5	3721	1/1	0.38	7.18	62,62,62,62	0
85	MG	5	3872	1/1	0.66	7.17	49,49,49,49	0
86	OHX	2	2135	7/7	0.29	7.17	137,137,137,137	0
85	MG	6	2001	1/1	0.36	7.14	59,59,59,59	0
85	MG	5	3433	1/1	0.26	7.13	50,50,50,50	0
85	MG	1	3533	1/1	0.28	7.06	40,40,40,40	0
85	MG	1	4218	1/1	0.43	7.03	35,35,35,35	0
86	OHX	5	4141	7/7	0.18	7.02	131,131,131,131	0
85	MG	n8	202	1/1	0.34	7.01	50,50,50,50	0
86	OHX	1	4068	7/7	0.30	6.97	126,126,126,126	0
85	MG	2	1906	1/1	0.53	6.96	58,58,58,58	0
85	MG	5	3722	1/1	0.39	6.95	66,66,66,66	0
85	MG	5	3739	1/1	0.34	6.94	41,41,41,41	0
85	MG	5	3657	1/1	0.33	6.92	70,70,70,70	0
85	MG	5	3589	1/1	0.54	6.91	52,52,52,52	0
85	MG	1	3677	1/1	0.60	6.87	64,64,64,64	0
86	OHX	5	4180	7/7	0.37	6.84	122,122,122,122	0
85	MG	5	3808	1/1	0.26	6.82	161,161,161,161	0
85	MG	5	3503	1/1	0.31	6.82	44,44,44,44	0
86	OHX	2	2176	7/7	0.35	6.80	185,185,185,185	0
85	MG	1	3553	1/1	0.38	6.79	36,36,36,36	0
85	MG	1	3784	1/1	0.37	6.72	38,38,38,38	0
85	MG	1	3770	1/1	0.29	6.71	69,69,69,69	0
85	MG	1	3727	1/1	0.38	6.70	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1930	1/1	0.30	6.68	67,67,67,67	0
85	MG	1	3667	1/1	0.33	6.68	78,78,78,78	0
85	MG	6	1912	1/1	0.61	6.66	52,52,52,52	0
85	MG	1	3451	1/1	0.35	6.66	38,38,38,38	0
86	OHX	2	2147	7/7	0.27	6.65	125,125,125,125	0
85	MG	1	3613	1/1	0.31	6.64	32,32,32,32	0
85	MG	N5	201	1/1	0.29	6.64	71,71,71,71	0
85	MG	1	3710	1/1	0.33	6.63	78,78,78,78	0
86	OHX	5	4160	7/7	0.27	6.61	144,144,144,144	0
85	MG	1	3718	1/1	0.34	6.59	45,45,45,45	0
85	MG	6	1977	1/1	0.33	6.56	48,48,48,48	0
85	MG	5	3655	1/1	0.33	6.55	34,34,34,34	0
85	MG	5	3678	1/1	0.35	6.53	49,49,49,49	0
85	MG	2	1952	1/1	0.37	6.49	100,100,100,100	0
85	MG	4	201	1/1	0.30	6.48	46,46,46,46	0
85	MG	1	3437	1/1	0.36	6.48	35,35,35,35	0
85	MG	1	3750	1/1	0.33	6.45	30,30,30,30	0
85	MG	6	1969	1/1	0.38	6.44	65,65,65,65	0
85	MG	5	3748	1/1	0.33	6.38	48,48,48,48	0
86	OHX	2	2158	7/7	0.31	6.38	159,159,159,159	0
86	OHX	2	2137	7/7	0.26	6.36	174,174,174,174	0
86	OHX	5	4204	7/7	0.23	6.33	144,144,144,144	0
85	MG	5	3474	1/1	0.36	6.32	37,37,37,37	0
86	OHX	1	4174	7/7	0.26	6.27	161,161,161,161	0
86	OHX	5	4156	7/7	0.42	6.26	131,131,131,131	0
85	MG	1	3550	1/1	0.44	6.23	42,42,42,42	0
85	MG	2	1946	1/1	0.41	6.23	65,65,65,65	0
86	OHX	5	4161	7/7	0.23	6.19	120,120,120,120	0
85	MG	2	2002	1/1	0.33	6.15	126,126,126,126	0
85	MG	4	206	1/1	0.38	6.13	39,39,39,39	0
86	OHX	5	4164	7/7	0.36	6.13	125,125,125,125	0
85	MG	2	1931	1/1	0.49	6.12	57,57,57,57	0
86	OHX	5	4151	7/7	0.27	6.11	136,136,136,136	0
85	MG	5	3588	1/1	0.33	6.10	28,28,28,28	0
85	MG	1	3562	1/1	0.37	6.06	49,49,49,49	0
85	MG	5	3491	1/1	0.32	6.06	30,30,30,30	0
85	MG	1	3799	1/1	0.43	6.05	59,59,59,59	0
85	MG	1	3494	1/1	0.34	6.05	47,47,47,47	0
85	MG	6	1931	1/1	0.48	6.04	68,68,68,68	0
86	OHX	1	4145	7/7	0.31	6.03	140,140,140,140	0
86	OHX	5	4155	7/7	0.32	6.02	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3827	1/1	0.21	5.99	65,65,65,65	0
86	OHX	2	2174	7/7	0.25	5.98	145,145,145,145	0
85	MG	1	3427	1/1	0.33	5.97	40,40,40,40	0
85	MG	2	2019	1/1	0.35	5.94	78,78,78,78	0
85	MG	5	3688	1/1	0.42	5.94	67,67,67,67	0
85	MG	1	3816	1/1	0.38	5.93	59,59,59,59	0
86	OHX	1	4176	7/7	0.32	5.83	161,161,161,161	0
86	OHX	8	227	7/7	0.21	5.83	137,137,137,137	0
85	MG	1	3822	1/1	0.22	5.83	49,49,49,49	0
85	MG	5	3623	1/1	0.29	5.82	45,45,45,45	0
85	MG	1	3606	1/1	0.41	5.78	50,50,50,50	0
86	OHX	1	4126	7/7	0.42	5.78	153,153,153,153	0
86	OHX	5	4145	7/7	0.30	5.73	143,143,143,143	0
85	MG	s8	302	1/1	0.30	5.70	46,46,46,46	0
85	MG	2	1979	1/1	0.55	5.69	60,60,60,60	0
86	OHX	4	232	7/7	0.26	5.68	154,154,154,154	0
86	OHX	5	4194	7/7	0.33	5.67	133,133,133,133	0
85	MG	5	3702	1/1	0.31	5.62	37,37,37,37	0
85	MG	5	3419	1/1	0.47	5.59	34,34,34,34	0
85	MG	6	1978	1/1	0.32	5.55	50,50,50,50	0
86	OHX	5	4153	7/7	0.41	5.54	128,128,128,128	0
85	MG	1	3848	1/1	0.37	5.53	79,79,79,79	0
85	MG	5	3652	1/1	0.23	5.52	39,39,39,39	0
85	MG	5	3615	1/1	0.22	5.52	34,34,34,34	0
85	MG	6	2033	1/1	0.53	5.49	57,57,57,57	0
85	MG	1	3815	1/1	0.32	5.48	54,54,54,54	0
86	OHX	1	4193	7/7	0.21	5.48	143,143,143,143	0
85	MG	1	3711	1/1	0.34	5.47	38,38,38,38	0
85	MG	5	3566	1/1	0.28	5.46	28,28,28,28	0
86	OHX	1	4194	7/7	0.25	5.45	165,165,165,165	0
85	MG	5	3575	1/1	0.34	5.45	37,37,37,37	0
85	MG	5	3401	1/1	0.37	5.41	57,57,57,57	0
85	MG	1	3761	1/1	0.31	5.40	61,61,61,61	0
85	MG	1	3763	1/1	0.33	5.40	67,67,67,67	0
85	MG	5	3727	1/1	0.29	5.39	35,35,35,35	0
85	MG	5	3890	1/1	0.33	5.31	51,51,51,51	0
85	MG	6	1909	1/1	0.31	5.31	121,121,121,121	0
85	MG	2	1954	1/1	0.26	5.29	103,103,103,103	0
85	MG	6	1963	1/1	0.36	5.29	110,110,110,110	0
86	OHX	1	4183	7/7	0.31	5.28	137,137,137,137	0
85	MG	2	1968	1/1	0.71	5.28	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4234	7/7	0.29	5.27	144,144,144,144	0
85	MG	6	2035	1/1	0.62	5.26	90,90,90,90	0
85	MG	6	1983	1/1	0.36	5.24	55,55,55,55	0
86	OHX	5	4240	7/7	0.24	5.23	162,162,162,162	0
85	MG	5	3836	1/1	0.39	5.22	75,75,75,75	0
85	MG	1	3715	1/1	0.28	5.22	37,37,37,37	0
85	MG	2	1956	1/1	0.66	5.21	55,55,55,55	0
85	MG	1	3769	1/1	0.40	5.20	55,55,55,55	0
85	MG	6	2006	1/1	0.28	5.18	102,102,102,102	0
86	OHX	6	2178	7/7	0.30	5.18	152,152,152,152	0
85	MG	1	3571	1/1	0.46	5.17	36,36,36,36	0
85	MG	6	2022	1/1	0.52	5.16	70,70,70,70	0
86	OHX	1	4151	7/7	0.26	5.16	149,149,149,149	0
85	MG	1	3516	1/1	0.41	5.13	31,31,31,31	0
85	MG	1	3671	1/1	0.33	5.10	33,33,33,33	0
86	OHX	1	4161	7/7	0.37	5.09	150,150,150,150	0
85	MG	1	3733	1/1	0.26	5.09	36,36,36,36	0
85	MG	3	209	1/1	0.31	5.08	68,68,68,68	0
86	OHX	6	2187	7/7	0.32	5.07	172,172,172,172	0
85	MG	5	3514	1/1	0.32	5.01	64,64,64,64	0
86	OHX	1	4111	7/7	0.40	4.99	130,130,130,130	0
86	OHX	5	4188	7/7	0.26	4.98	136,136,136,136	0
85	MG	5	3775	1/1	0.26	4.98	83,83,83,83	0
86	OHX	1	4114	7/7	0.24	4.98	137,137,137,137	0
86	OHX	5	4218	7/7	0.28	4.97	156,156,156,156	0
85	MG	1	3660	1/1	0.28	4.95	43,43,43,43	0
85	MG	5	3832	1/1	0.30	4.94	28,28,28,28	0
86	OHX	7	227	7/7	0.25	4.93	142,142,142,142	0
85	MG	5	3628	1/1	0.34	4.91	66,66,66,66	0
85	MG	3	201	1/1	0.26	4.89	75,75,75,75	0
86	OHX	2	2122	7/7	0.19	4.85	151,151,151,151	0
85	MG	5	3706	1/1	0.28	4.84	73,73,73,73	0
86	OHX	2	2136	7/7	0.29	4.83	141,141,141,141	0
85	MG	N3	201	1/1	0.38	4.79	35,35,35,35	0
85	MG	1	3638	1/1	0.27	4.78	60,60,60,60	0
86	OHX	1	4107	7/7	0.21	4.78	130,130,130,130	0
86	OHX	1	4208	7/7	0.40	4.75	133,133,133,133	0
85	MG	5	3768	1/1	0.29	4.73	44,44,44,44	0
86	OHX	6	2160	7/7	0.33	4.71	136,136,136,136	0
85	MG	1	3540	1/1	0.29	4.69	60,60,60,60	0
85	MG	5	3745	1/1	0.37	4.69	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3438	1/1	0.39	4.68	48,48,48,48	0
86	OHX	5	4186	7/7	0.32	4.68	134,134,134,134	0
85	MG	6	1972	1/1	0.38	4.67	75,75,75,75	0
86	OHX	6	2147	7/7	0.27	4.66	119,119,119,119	0
85	MG	8	207	1/1	0.28	4.65	64,64,64,64	0
85	MG	L5	301	1/1	0.33	4.63	64,64,64,64	0
85	MG	1	3439	1/1	0.64	4.63	41,41,41,41	0
85	MG	1	3556	1/1	0.47	4.62	55,55,55,55	0
86	OHX	2	2177	7/7	0.40	4.61	154,154,154,154	0
86	OHX	M7	206	7/7	0.35	4.59	118,118,118,118	0
85	MG	5	3700	1/1	0.34	4.59	54,54,54,54	0
85	MG	2	1955	1/1	0.27	4.57	65,65,65,65	0
86	OHX	1	4060	7/7	0.26	4.57	148,148,148,148	0
86	OHX	1	4202	7/7	0.22	4.55	142,142,142,142	0
85	MG	5	3500	1/1	0.29	4.54	37,37,37,37	0
85	MG	1	3857	1/1	0.29	4.54	125,125,125,125	0
85	MG	5	3504	1/1	0.27	4.51	46,46,46,46	0
85	MG	5	3831	1/1	0.38	4.50	40,40,40,40	0
85	MG	1	3475	1/1	0.29	4.50	38,38,38,38	0
85	MG	1	3528	1/1	0.27	4.49	47,47,47,47	0
86	OHX	5	4252	7/7	0.29	4.48	153,153,153,153	0
85	MG	5	3454	1/1	0.40	4.45	34,34,34,34	0
85	MG	5	3559	1/1	0.32	4.42	49,49,49,49	0
86	OHX	5	4251	7/7	0.28	4.41	142,142,142,142	0
85	MG	5	3751	1/1	0.30	4.40	64,64,64,64	0
86	OHX	5	4206	7/7	0.32	4.40	149,149,149,149	0
86	OHX	1	4137	7/7	0.32	4.39	143,143,143,143	0
85	MG	5	3673	1/1	0.29	4.39	36,36,36,36	0
85	MG	o1	201	1/1	0.77	4.38	93,93,93,93	0
85	MG	2	1934	1/1	0.33	4.37	51,51,51,51	0
85	MG	1	3401	1/1	0.37	4.36	42,42,42,42	0
85	MG	2	1985	1/1	0.25	4.33	61,61,61,61	0
85	MG	5	3409	1/1	0.27	4.31	48,48,48,48	0
85	MG	1	3785	1/1	0.53	4.28	30,30,30,30	0
85	MG	N8	205	1/1	0.29	4.25	30,30,30,30	0
85	MG	1	3500	1/1	0.45	4.25	23,23,23,23	0
85	MG	5	3797	1/1	0.33	4.24	43,43,43,43	0
85	MG	5	3821	1/1	0.28	4.22	40,40,40,40	0
86	OHX	5	4099	7/7	0.16	4.22	155,155,155,155	0
85	MG	5	3595	1/1	0.31	4.21	41,41,41,41	0
85	MG	5	3793	1/1	0.35	4.21	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4238	7/7	0.61	4.20	157,157,157,157	0
86	OHX	6	2137	7/7	0.31	4.17	148,148,148,148	0
85	MG	1	3721	1/1	0.27	4.15	49,49,49,49	0
85	MG	5	3446	1/1	0.26	4.13	45,45,45,45	0
85	MG	5	3567	1/1	0.39	4.11	34,34,34,34	0
85	MG	M6	201	1/1	0.39	4.10	49,49,49,49	0
85	MG	2	1949	1/1	0.35	4.10	58,58,58,58	0
85	MG	6	2020	1/1	0.23	4.09	117,117,117,117	0
86	OHX	1	4158	7/7	0.20	4.09	158,158,158,158	0
85	MG	m7	205	1/1	0.49	4.09	45,45,45,45	0
85	MG	6	1916	1/1	0.38	4.08	60,60,60,60	0
85	MG	3	214	1/1	0.36	4.07	70,70,70,70	0
85	MG	5	3551	1/1	0.40	4.05	51,51,51,51	0
85	MG	5	3633	1/1	0.29	4.04	79,79,79,79	0
85	MG	5	3596	1/1	0.36	4.04	37,37,37,37	0
85	MG	5	3632	1/1	0.21	4.03	45,45,45,45	0
86	OHX	5	4233	7/7	0.24	4.03	167,167,167,167	0
85	MG	4	207	1/1	0.38	4.03	36,36,36,36	0
85	MG	5	3536	1/1	0.59	4.01	33,33,33,33	0
85	MG	1	3709	1/1	0.56	4.00	55,55,55,55	0
85	MG	6	1962	1/1	0.36	3.99	52,52,52,52	0
86	OHX	5	4198	7/7	0.28	3.98	155,155,155,155	0
85	MG	2	2009	1/1	0.33	3.98	77,77,77,77	0
86	OHX	1	4190	7/7	0.32	3.98	159,159,159,159	0
85	MG	5	3800	1/1	0.35	3.95	59,59,59,59	0
85	MG	5	3498	1/1	0.35	3.95	36,36,36,36	0
85	MG	1	3719	1/1	0.34	3.89	60,60,60,60	0
86	OHX	5	4142	7/7	0.28	3.89	137,137,137,137	0
85	MG	M7	204	1/1	0.31	3.86	41,41,41,41	0
85	MG	L8	301	1/1	0.38	3.84	50,50,50,50	0
85	MG	5	3747	1/1	0.28	3.82	34,34,34,34	0
86	OHX	5	3914	7/7	0.18	3.79	64,64,64,64	0
85	MG	5	3611	1/1	0.29	3.78	33,33,33,33	0
85	MG	5	3892	1/1	0.31	3.78	37,37,37,37	0
86	OHX	5	4212	7/7	0.26	3.77	154,154,154,154	0
85	MG	1	3782	1/1	0.40	3.77	56,56,56,56	0
85	MG	5	3785	1/1	0.53	3.77	81,81,81,81	0
85	MG	2	2007	1/1	0.68	3.76	51,51,51,51	0
85	MG	1	3699	1/1	0.30	3.70	39,39,39,39	0
86	OHX	1	4118	7/7	0.33	3.69	126,126,126,126	0
85	MG	7	202	1/1	0.24	3.68	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	1971	1/1	0.36	3.68	77,77,77,77	0
85	MG	1	3811	1/1	0.24	3.65	57,57,57,57	0
85	MG	5	3464	1/1	0.30	3.65	52,52,52,52	0
85	MG	2	1960	1/1	0.35	3.63	67,67,67,67	0
86	OHX	5	4123	7/7	0.26	3.62	131,131,131,131	0
86	OHX	6	2180	7/7	0.27	3.60	144,144,144,144	0
86	OHX	O9	101	7/7	0.32	3.60	134,134,134,134	0
86	OHX	1	4159	7/7	0.26	3.59	163,163,163,163	0
85	MG	6	1986	1/1	0.46	3.59	87,87,87,87	0
86	OHX	5	4224	7/7	0.27	3.57	168,168,168,168	0
85	MG	1	3579	1/1	0.32	3.56	44,44,44,44	0
85	MG	1	3759	1/1	0.39	3.55	48,48,48,48	0
85	MG	6	1949	1/1	0.54	3.55	52,52,52,52	0
85	MG	5	3772	1/1	0.29	3.54	44,44,44,44	0
85	MG	5	3459	1/1	0.27	3.53	64,64,64,64	0
85	MG	1	3853	1/1	0.33	3.52	90,90,90,90	0
85	MG	5	3549	1/1	0.26	3.51	50,50,50,50	0
85	MG	5	3718	1/1	0.34	3.50	52,52,52,52	0
86	OHX	2	2168	7/7	0.27	3.49	162,162,162,162	0
86	OHX	5	4116	7/7	0.26	3.48	120,120,120,120	0
86	OHX	5	4159	7/7	0.21	3.46	146,146,146,146	0
85	MG	n9	101	1/1	0.28	3.45	36,36,36,36	0
85	MG	1	3714	1/1	0.28	3.45	79,79,79,79	0
85	MG	1	3802	1/1	0.27	3.45	40,40,40,40	0
86	OHX	5	4250	7/7	0.27	3.45	154,154,154,154	0
86	OHX	5	4226	7/7	0.36	3.44	138,138,138,138	0
86	OHX	1	4117	7/7	0.29	3.43	136,136,136,136	0
86	OHX	5	4187	7/7	0.27	3.43	130,130,130,130	0
85	MG	5	3752	1/1	0.27	3.41	37,37,37,37	0
85	MG	1	4215	1/1	0.31	3.41	39,39,39,39	0
86	OHX	1	4141	7/7	0.16	3.38	142,142,142,142	0
85	MG	c7	201	1/1	0.42	3.37	87,87,87,87	0
86	OHX	M7	207	7/7	0.29	3.37	142,142,142,142	0
85	MG	1	3689	1/1	0.35	3.35	42,42,42,42	0
86	OHX	5	4163	7/7	0.24	3.34	129,129,129,129	0
85	MG	7	210	1/1	0.28	3.33	47,47,47,47	0
85	MG	l9	201	1/1	0.24	3.33	44,44,44,44	0
86	OHX	1	4042	7/7	0.28	3.32	115,115,115,115	0
85	MG	7	228	1/1	0.25	3.31	36,36,36,36	0
85	MG	6	1964	1/1	0.21	3.25	62,62,62,62	0
85	MG	L7	301	1/1	0.29	3.24	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3435	1/1	0.30	3.23	31,31,31,31	0
85	MG	1	3708	1/1	0.23	3.23	62,62,62,62	0
85	MG	1	3678	1/1	0.30	3.19	65,65,65,65	0
85	MG	1	3731	1/1	0.23	3.18	29,29,29,29	0
85	MG	8	212	1/1	0.23	3.17	105,105,105,105	0
85	MG	5	3760	1/1	0.22	3.15	60,60,60,60	0
85	MG	5	3529	1/1	0.21	3.15	34,34,34,34	0
85	MG	s6	301	1/1	0.28	3.14	77,77,77,77	0
86	OHX	5	4143	7/7	0.15	3.14	150,150,150,150	0
85	MG	5	3643	1/1	0.25	3.13	54,54,54,54	0
85	MG	8	208	1/1	0.28	3.13	54,54,54,54	0
85	MG	1	4217	1/1	0.28	3.12	48,48,48,48	0
85	MG	M7	205	1/1	0.33	3.09	41,41,41,41	0
86	OHX	6	2117	7/7	0.36	3.08	150,150,150,150	0
86	OHX	2	2156	7/7	0.28	3.07	128,128,128,128	0
85	MG	5	3630	1/1	0.30	3.07	69,69,69,69	0
86	OHX	5	4102	7/7	0.23	3.06	132,132,132,132	0
85	MG	2	1990	1/1	0.40	3.05	57,57,57,57	0
85	MG	1	3831	1/1	0.40	3.05	41,41,41,41	0
85	MG	n0	202	1/1	0.22	3.03	43,43,43,43	0
86	OHX	1	4172	7/7	0.22	3.02	172,172,172,172	0
85	MG	3	203	1/1	0.25	3.01	98,98,98,98	0
85	MG	5	3638	1/1	0.39	3.01	53,53,53,53	0
85	MG	6	2036	1/1	0.73	3.01	78,78,78,78	0
86	OHX	2	2159	7/7	0.41	3.00	145,145,145,145	0
85	MG	5	3699	1/1	0.25	3.00	46,46,46,46	0
85	MG	5	3809	1/1	0.26	3.00	34,34,34,34	0
85	MG	5	3842	1/1	0.36	3.00	45,45,45,45	0
86	OHX	2	2131	7/7	0.24	3.00	140,140,140,140	0
86	OHX	6	2195	7/7	0.28	2.99	162,162,162,162	0
85	MG	5	3647	1/1	0.25	2.93	37,37,37,37	0
85	MG	5	3653	1/1	0.20	2.93	99,99,99,99	0
85	MG	5	3447	1/1	0.28	2.92	46,46,46,46	0
86	OHX	6	2121	7/7	0.26	2.91	124,124,124,124	0
85	MG	2	1993	1/1	0.46	2.90	75,75,75,75	0
86	OHX	5	4225	7/7	0.22	2.89	151,151,151,151	0
85	MG	5	3833	1/1	0.30	2.89	52,52,52,52	0
85	MG	1	3757	1/1	0.25	2.89	45,45,45,45	0
86	OHX	6	2125	7/7	0.28	2.85	141,141,141,141	0
85	MG	7	215	1/1	0.22	2.83	48,48,48,48	0
85	MG	1	3617	1/1	0.34	2.80	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4207	7/7	0.33	2.78	138,138,138,138	0
86	OHX	6	2189	7/7	0.30	2.78	151,151,151,151	0
85	MG	6	1905	1/1	0.52	2.78	59,59,59,59	0
86	OHX	1	4210	7/7	0.26	2.77	139,139,139,139	0
85	MG	1	3814	1/1	0.23	2.76	47,47,47,47	0
86	OHX	1	4201	7/7	0.28	2.76	139,139,139,139	0
85	MG	6	1938	1/1	0.34	2.76	48,48,48,48	0
86	OHX	1	4044	7/7	0.31	2.73	119,119,119,119	0
85	MG	5	3691	1/1	0.23	2.71	53,53,53,53	0
86	OHX	5	4053	7/7	0.20	2.70	116,116,116,116	0
85	MG	1	3684	1/1	0.28	2.69	84,84,84,84	0
86	OHX	6	2048	7/7	0.25	2.68	78,78,78,78	0
85	MG	5	3686	1/1	0.23	2.67	35,35,35,35	0
85	MG	7	214	1/1	0.36	2.66	52,52,52,52	0
85	MG	1	3790	1/1	0.27	2.65	42,42,42,42	0
85	MG	5	3581	1/1	0.24	2.65	37,37,37,37	0
85	MG	1	3794	1/1	0.23	2.64	49,49,49,49	0
85	MG	5	3635	1/1	0.21	2.64	35,35,35,35	0
85	MG	5	3731	1/1	0.32	2.64	31,31,31,31	0
85	MG	1	3569	1/1	0.33	2.63	24,24,24,24	0
86	OHX	5	4237	7/7	0.41	2.62	163,163,163,163	0
86	OHX	1	4125	7/7	0.24	2.61	150,150,150,150	0
86	OHX	5	4114	7/7	0.20	2.61	139,139,139,139	0
85	MG	1	3585	1/1	0.45	2.60	47,47,47,47	0
85	MG	5	3708	1/1	0.29	2.58	50,50,50,50	0
86	OHX	1	4113	7/7	0.23	2.58	129,129,129,129	0
85	MG	SM	301	1/1	0.36	2.56	58,58,58,58	0
85	MG	1	3485	1/1	0.22	2.56	44,44,44,44	0
86	OHX	6	2199	7/7	0.29	2.54	156,156,156,156	0
85	MG	5	3672	1/1	0.24	2.51	41,41,41,41	0
85	MG	2	1939	1/1	0.34	2.50	70,70,70,70	0
85	MG	6	1951	1/1	0.35	2.50	76,76,76,76	0
86	OHX	7	225	7/7	0.20	2.49	164,164,164,164	0
85	MG	6	1934	1/1	0.24	2.49	78,78,78,78	0
85	MG	1	3448	1/1	0.25	2.47	42,42,42,42	0
86	OHX	5	4158	7/7	0.24	2.46	136,136,136,136	0
86	OHX	6	2171	7/7	0.29	2.45	120,120,120,120	0
86	OHX	6	2177	7/7	0.25	2.44	130,130,130,130	0
85	MG	n3	201	1/1	0.31	2.44	26,26,26,26	0
85	MG	1	3416	1/1	0.31	2.43	36,36,36,36	0
85	MG	6	2026	1/1	0.32	2.42	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3776	1/1	0.22	2.40	54,54,54,54	0
85	MG	1	3648	1/1	0.31	2.39	49,49,49,49	0
85	MG	1	3681	1/1	0.22	2.37	44,44,44,44	0
86	OHX	1	4131	7/7	0.23	2.35	132,132,132,132	0
86	OHX	2	2140	7/7	0.30	2.33	166,166,166,166	0
86	OHX	6	2186	7/7	0.27	2.32	153,153,153,153	0
85	MG	1	3663	1/1	0.32	2.30	45,45,45,45	0
85	MG	1	3700	1/1	0.25	2.28	48,48,48,48	0
85	MG	1	3779	1/1	0.19	2.28	66,66,66,66	0
85	MG	5	3697	1/1	0.18	2.26	47,47,47,47	0
85	MG	5	3894	1/1	0.28	2.26	93,93,93,93	0
86	OHX	5	4246	7/7	0.32	2.26	165,165,165,165	0
85	MG	1	3744	1/1	0.32	2.25	53,53,53,53	0
85	MG	n8	201	1/1	0.29	2.23	30,30,30,30	0
85	MG	O7	102	1/1	0.37	2.20	70,70,70,70	0
85	MG	n8	203	1/1	0.34	2.19	44,44,44,44	0
85	MG	5	3527	1/1	0.20	2.18	47,47,47,47	0
86	OHX	5	4129	7/7	0.16	2.17	137,137,137,137	0
85	MG	1	3591	1/1	0.37	2.16	48,48,48,48	0
85	MG	5	3689	1/1	0.28	2.15	78,78,78,78	0
85	MG	5	3494	1/1	0.31	2.14	60,60,60,60	0
85	MG	1	3752	1/1	0.26	2.14	50,50,50,50	0
85	MG	2	1907	1/1	0.52	2.14	55,55,55,55	0
85	MG	1	3566	1/1	0.44	2.13	33,33,33,33	0
86	OHX	1	4167	7/7	0.26	2.11	126,126,126,126	0
86	OHX	1	4162	7/7	0.17	2.11	167,167,167,167	0
86	OHX	1	4076	7/7	0.31	2.08	132,132,132,132	0
86	OHX	14	402	7/7	0.25	2.07	171,171,171,171	0
86	OHX	2	2162	7/7	0.20	2.07	171,171,171,171	0
86	OHX	1	4165	7/7	0.26	2.07	121,121,121,121	0
86	OHX	2	2161	7/7	0.29	2.06	164,164,164,164	0
86	OHX	1	4200	7/7	0.33	2.05	151,151,151,151	0
86	OHX	2	2102	7/7	0.16	2.05	154,154,154,154	0
85	MG	6	2016	1/1	0.20	2.03	74,74,74,74	0
86	OHX	1	4080	7/7	0.18	2.03	146,146,146,146	0
85	MG	5	3845	1/1	0.26	2.03	41,41,41,41	0
86	OHX	1	4203	7/7	0.39	2.02	156,156,156,156	0
85	MG	5	3738	1/1	0.25	2.02	43,43,43,43	0
85	MG	2	1920	1/1	0.43	2.01	57,57,57,57	0
86	OHX	5	4108	7/7	0.34	2.00	115,115,115,115	0
86	OHX	6	2169	7/7	0.26	2.00	161,161,161,161	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3896	1/1	0.27	2.00	118,118,118,118	0
85	MG	2	1992	1/1	0.30	2.00	61,61,61,61	0
86	OHX	1	3861	7/7	0.21	1.99	46,46,46,46	0
85	MG	6	1991	1/1	0.30	1.99	70,70,70,70	0
85	MG	N8	202	1/1	0.34	1.99	27,27,27,27	0
86	OHX	1	4054	7/7	0.22	1.99	104,104,104,104	0
85	MG	L2	301	1/1	0.34	1.98	37,37,37,37	0
85	MG	1	3493	1/1	0.20	1.98	46,46,46,46	0
86	OHX	5	4167	7/7	0.22	1.97	195,195,195,195	0
86	OHX	5	4185	7/7	0.26	1.97	145,145,145,145	0
86	OHX	1	3946	7/7	0.19	1.96	125,125,125,125	0
86	OHX	5	3940	7/7	0.20	1.96	81,81,81,81	0
85	MG	l5	301	1/1	0.30	1.95	70,70,70,70	0
86	OHX	L4	402	7/7	0.27	1.94	154,154,154,154	0
85	MG	5	3669	1/1	0.24	1.94	49,49,49,49	0
85	MG	6	1992	1/1	0.29	1.93	85,85,85,85	0
85	MG	5	3469	1/1	0.25	1.93	36,36,36,36	0
86	OHX	2	2173	7/7	0.26	1.93	173,173,173,173	0
86	OHX	1	4093	7/7	0.18	1.91	134,134,134,134	0
86	OHX	5	3934	7/7	0.18	1.90	92,92,92,92	0
85	MG	5	3788	1/1	0.18	1.89	39,39,39,39	0
85	MG	6	1979	1/1	0.22	1.89	77,77,77,77	0
85	MG	2	1967	1/1	0.48	1.89	62,62,62,62	0
86	OHX	6	2157	7/7	0.38	1.88	146,146,146,146	0
86	OHX	8	230	7/7	0.25	1.87	130,130,130,130	0
85	MG	5	3781	1/1	0.41	1.86	59,59,59,59	0
86	OHX	5	3916	7/7	0.23	1.86	63,63,63,63	0
88	ZN	D7	101	1/1	0.44	1.86	166,166,166,166	0
85	MG	5	3900	1/1	0.28	1.86	50,50,50,50	0
86	OHX	1	4043	7/7	0.22	1.84	118,118,118,118	0
85	MG	1	3487	1/1	0.23	1.84	38,38,38,38	0
85	MG	3	210	1/1	0.32	1.84	68,68,68,68	0
85	MG	1	3662	1/1	0.26	1.83	56,56,56,56	0
85	MG	5	3848	1/1	0.38	1.83	53,53,53,53	0
85	MG	5	3582	1/1	0.28	1.82	33,33,33,33	0
85	MG	1	3604	1/1	0.21	1.80	45,45,45,45	0
86	OHX	1	4197	7/7	0.20	1.80	137,137,137,137	0
85	MG	5	3819	1/1	0.27	1.80	42,42,42,42	0
85	MG	5	3516	1/1	0.27	1.80	41,41,41,41	0
86	OHX	1	4128	7/7	0.25	1.80	176,176,176,176	0
85	MG	s8	301	1/1	0.34	1.77	62,62,62,62	0
86	OHX	1	3906	7/7	0.23	1.77	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3682	1/1	0.38	1.77	47,47,47,47	0
85	MG	5	3455	1/1	0.20	1.74	45,45,45,45	0
85	MG	1	3691	1/1	0.25	1.73	49,49,49,49	0
85	MG	5	4255	1/1	0.27	1.73	36,36,36,36	0
86	OHX	m7	206	7/7	0.36	1.73	132,132,132,132	0
85	MG	1	3631	1/1	0.40	1.73	76,76,76,76	0
85	MG	5	3687	1/1	0.53	1.73	50,50,50,50	0
86	OHX	6	2200	7/7	0.25	1.72	160,160,160,160	0
86	OHX	1	4099	7/7	0.18	1.72	164,164,164,164	0
85	MG	1	3753	1/1	0.35	1.70	37,37,37,37	0
86	OHX	6	2176	7/7	0.24	1.69	117,117,117,117	0
85	MG	5	3810	1/1	0.20	1.69	101,101,101,101	0
85	MG	2	1988	1/1	0.62	1.68	75,75,75,75	0
86	OHX	1	4109	7/7	0.28	1.67	118,118,118,118	0
86	OHX	5	3995	7/7	0.24	1.64	109,109,109,109	0
86	OHX	5	4243	7/7	0.22	1.64	196,196,196,196	0
86	OHX	1	3869	7/7	0.24	1.64	65,65,65,65	0
85	MG	1	3716	1/1	0.31	1.64	55,55,55,55	0
86	OHX	2	2025	7/7	0.23	1.63	91,91,91,91	0
86	OHX	1	4069	7/7	0.19	1.61	148,148,148,148	0
86	OHX	1	4136	7/7	0.22	1.61	130,130,130,130	0
85	MG	sM	301	1/1	0.59	1.59	50,50,50,50	0
85	MG	1	3697	1/1	0.22	1.59	44,44,44,44	0
86	OHX	1	4108	7/7	0.21	1.58	147,147,147,147	0
85	MG	5	3803	1/1	0.19	1.57	80,80,80,80	0
85	MG	1	3661	1/1	0.23	1.55	52,52,52,52	0
85	MG	1	3637	1/1	0.26	1.54	55,55,55,55	0
85	MG	1	3704	1/1	0.20	1.53	43,43,43,43	0
86	OHX	1	4173	7/7	0.24	1.52	145,145,145,145	0
85	MG	5	3753	1/1	0.22	1.51	54,54,54,54	0
86	OHX	6	2056	7/7	0.20	1.51	77,77,77,77	0
85	MG	5	3765	1/1	0.23	1.50	56,56,56,56	0
86	OHX	5	4136	7/7	0.28	1.48	128,128,128,128	0
86	OHX	M9	202	7/7	0.20	1.48	181,181,181,181	0
85	MG	1	3530	1/1	0.39	1.46	68,68,68,68	0
86	OHX	5	3903	7/7	0.18	1.45	50,50,50,50	0
85	MG	O5	201	1/1	0.24	1.45	56,56,56,56	0
86	OHX	5	4247	7/7	0.31	1.45	145,145,145,145	0
85	MG	1	4212	1/1	0.25	1.45	29,29,29,29	0
86	OHX	O2	202	7/7	0.29	1.44	153,153,153,153	0
86	OHX	5	4213	7/7	0.24	1.44	123,123,123,123	0
85	MG	5	3510	1/1	0.31	1.44	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3819	1/1	0.35	1.43	43,43,43,43	0
86	OHX	5	4034	7/7	0.20	1.43	117,117,117,117	0
86	OHX	5	4227	7/7	0.24	1.42	158,158,158,158	0
85	MG	1	3766	1/1	0.24	1.40	65,65,65,65	0
85	MG	5	3684	1/1	0.25	1.39	78,78,78,78	0
86	OHX	2	2115	7/7	0.24	1.39	154,154,154,154	0
85	MG	1	3628	1/1	0.22	1.39	67,67,67,67	0
85	MG	1	3748	1/1	0.19	1.38	63,63,63,63	0
86	OHX	5	4054	7/7	0.18	1.38	112,112,112,112	0
86	OHX	5	4208	7/7	0.51	1.37	150,150,150,150	0
86	OHX	5	3928	7/7	0.20	1.36	78,78,78,78	0
85	MG	5	3732	1/1	0.48	1.36	78,78,78,78	0
86	OHX	1	4139	7/7	0.20	1.35	136,136,136,136	0
86	OHX	1	4144	7/7	0.19	1.34	150,150,150,150	0
85	MG	1	3417	1/1	0.21	1.32	41,41,41,41	0
86	OHX	1	4157	7/7	0.18	1.31	138,138,138,138	0
86	OHX	6	2142	7/7	0.17	1.31	181,181,181,181	0
85	MG	L3	401	1/1	0.26	1.31	38,38,38,38	0
86	OHX	1	3892	7/7	0.21	1.31	83,83,83,83	0
85	MG	M3	202	1/1	0.39	1.27	102,102,102,102	0
85	MG	6	1996	1/1	0.18	1.27	47,47,47,47	0
88	ZN	d7	101	1/1	0.53	1.25	162,162,162,162	0
86	OHX	6	2203	7/7	0.56	1.24	158,158,158,158	0
85	MG	5	3690	1/1	0.23	1.24	42,42,42,42	0
85	MG	5	3487	1/1	0.24	1.23	52,52,52,52	0
85	MG	1	3601	1/1	0.31	1.22	34,34,34,34	0
86	OHX	6	2055	7/7	0.17	1.22	92,92,92,92	0
85	MG	5	3820	1/1	0.20	1.21	47,47,47,47	0
85	MG	5	3898	1/1	0.24	1.18	57,57,57,57	0
86	OHX	5	4103	7/7	0.18	1.18	133,133,133,133	0
85	MG	1	3696	1/1	0.32	1.18	77,77,77,77	0
86	OHX	2	2075	7/7	0.24	1.17	150,150,150,150	0
85	MG	6	1985	1/1	0.19	1.16	82,82,82,82	0
86	OHX	5	4112	7/7	0.22	1.16	127,127,127,127	0
86	OHX	6	2127	7/7	0.27	1.15	110,110,110,110	0
86	OHX	5	4148	7/7	0.21	1.15	127,127,127,127	0
86	OHX	5	4174	7/7	0.24	1.14	109,109,109,109	0
86	OHX	s9	201	7/7	0.40	1.13	139,139,139,139	0
85	MG	m7	203	1/1	0.26	1.13	49,49,49,49	0
86	OHX	2	2116	7/7	0.23	1.12	148,148,148,148	0
86	OHX	1	3862	7/7	0.20	1.11	53,53,53,53	0
85	MG	1	3686	1/1	0.31	1.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2003	1/1	0.20	1.09	57,57,57,57	0
85	MG	5	3835	1/1	0.30	1.09	56,56,56,56	0
86	OHX	5	4111	7/7	0.28	1.09	141,141,141,141	0
86	OHX	1	4073	7/7	0.17	1.09	130,130,130,130	0
86	OHX	2	2151	7/7	0.32	1.08	154,154,154,154	0
86	OHX	5	3941	7/7	0.16	1.07	91,91,91,91	0
86	OHX	1	4133	7/7	0.23	1.07	126,126,126,126	0
85	MG	5	3606	1/1	0.27	1.07	26,26,26,26	0
86	OHX	2	2128	7/7	0.20	1.07	153,153,153,153	0
85	MG	5	3750	1/1	0.36	1.06	30,30,30,30	0
86	OHX	5	4178	7/7	0.27	1.06	145,145,145,145	0
85	MG	5	3886	1/1	0.22	1.06	48,48,48,48	0
86	OHX	8	215	7/7	0.21	1.06	62,62,62,62	0
85	MG	5	3534	1/1	0.18	1.06	55,55,55,55	0
85	MG	5	3725	1/1	0.16	1.05	54,54,54,54	0
85	MG	m1	201	1/1	0.19	1.05	62,62,62,62	0
86	OHX	6	2116	7/7	0.26	1.04	137,137,137,137	0
85	MG	5	3600	1/1	0.19	1.03	44,44,44,44	0
86	OHX	1	4206	7/7	0.21	1.03	133,133,133,133	0
86	OHX	5	3915	7/7	0.19	1.03	70,70,70,70	0
86	OHX	2	2134	7/7	0.29	1.03	146,146,146,146	0
86	OHX	5	4118	7/7	0.17	1.01	129,129,129,129	0
86	OHX	1	4153	7/7	0.26	1.01	135,135,135,135	0
86	OHX	6	2188	7/7	0.30	1.00	161,161,161,161	0
86	OHX	1	4182	7/7	0.17	1.00	151,151,151,151	0
85	MG	2	1964	1/1	0.30	0.99	98,98,98,98	0
85	MG	q3	502	1/1	0.34	0.99	73,73,73,73	0
86	OHX	1	4180	7/7	0.27	0.99	111,111,111,111	0
86	OHX	5	4214	7/7	0.23	0.99	142,142,142,142	0
87	3K8	2	2179	28/28	0.41	0.99	86,86,86,86	0
86	OHX	1	3884	7/7	0.18	0.99	78,78,78,78	0
86	OHX	5	4254	7/7	0.24	0.99	166,166,166,166	0
86	OHX	1	4081	7/7	0.23	0.95	139,139,139,139	0
86	OHX	1	4146	7/7	0.18	0.94	144,144,144,144	0
86	OHX	1	4074	7/7	0.17	0.93	133,133,133,133	0
86	OHX	1	4156	7/7	0.21	0.92	153,153,153,153	0
85	MG	1	3832	1/1	0.36	0.91	53,53,53,53	0
86	OHX	5	4193	7/7	0.24	0.91	130,130,130,130	0
86	OHX	5	4088	7/7	0.20	0.90	132,132,132,132	0
86	OHX	1	4147	7/7	0.22	0.89	142,142,142,142	0
85	MG	6	1984	1/1	0.37	0.88	60,60,60,60	0
86	OHX	D9	102	7/7	0.42	0.87	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4192	7/7	0.34	0.87	152,152,152,152	0
85	MG	5	3467	1/1	0.19	0.87	92,92,92,92	0
85	MG	5	3711	1/1	0.26	0.86	89,89,89,89	0
86	OHX	2	2099	7/7	0.26	0.85	163,163,163,163	0
85	MG	q0	202	1/1	0.28	0.85	42,42,42,42	0
86	OHX	5	3912	7/7	0.19	0.84	66,66,66,66	0
85	MG	5	3693	1/1	0.22	0.84	49,49,49,49	0
85	MG	1	3722	1/1	0.23	0.83	47,47,47,47	0
85	MG	6	1995	1/1	0.32	0.82	64,64,64,64	0
86	OHX	1	4149	7/7	0.20	0.82	118,118,118,118	0
85	MG	1	3581	1/1	0.43	0.82	38,38,38,38	0
85	MG	1	3726	1/1	0.25	0.82	33,33,33,33	0
86	OHX	1	4178	7/7	0.36	0.82	139,139,139,139	0
85	MG	1	3636	1/1	0.25	0.81	50,50,50,50	0
86	OHX	1	4078	7/7	0.29	0.81	132,132,132,132	0
86	OHX	5	4138	7/7	0.28	0.81	121,121,121,121	0
86	OHX	5	4235	7/7	0.28	0.81	170,170,170,170	0
86	OHX	5	4072	7/7	0.18	0.81	137,137,137,137	0
86	OHX	l5	305	7/7	0.28	0.79	156,156,156,156	0
86	OHX	5	4232	7/7	0.10	0.79	191,191,191,191	0
86	OHX	2	2129	7/7	0.22	0.78	204,204,204,204	0
86	OHX	5	4130	7/7	0.21	0.78	130,130,130,130	0
85	MG	5	3865	1/1	0.19	0.78	47,47,47,47	0
86	OHX	5	3902	7/7	0.19	0.77	47,47,47,47	0
86	OHX	2	2153	7/7	0.18	0.77	154,154,154,154	0
86	OHX	2	2024	7/7	0.17	0.76	83,83,83,83	0
86	OHX	1	4164	7/7	0.23	0.76	220,220,220,220	0
85	MG	6	1990	1/1	0.24	0.76	95,95,95,95	0
85	MG	6	2005	1/1	0.23	0.75	79,79,79,79	0
85	MG	5	3870	1/1	0.28	0.75	42,42,42,42	0
86	OHX	5	3906	7/7	0.20	0.74	58,58,58,58	0
85	MG	6	1941	1/1	0.24	0.74	52,52,52,52	0
86	OHX	1	4163	7/7	0.30	0.73	141,141,141,141	0
86	OHX	2	2112	7/7	0.20	0.73	137,137,137,137	0
86	OHX	1	3870	7/7	0.18	0.72	67,67,67,67	0
85	MG	1	3817	1/1	0.17	0.72	47,47,47,47	0
85	MG	5	3648	1/1	0.22	0.71	60,60,60,60	0
86	OHX	6	2173	7/7	0.46	0.71	163,163,163,163	0
86	OHX	2	2146	7/7	0.22	0.69	177,177,177,177	0
88	ZN	q2	501	1/1	0.30	0.69	97,97,97,97	0
85	MG	1	3488	1/1	0.33	0.69	57,57,57,57	0
85	MG	L5	302	1/1	0.42	0.68	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4132	7/7	0.22	0.68	144,144,144,144	0
85	MG	N8	201	1/1	0.25	0.68	33,33,33,33	0
86	OHX	1	4115	7/7	0.19	0.67	134,134,134,134	0
86	OHX	5	3990	7/7	0.15	0.67	122,122,122,122	0
85	MG	1	3415	1/1	0.24	0.67	49,49,49,49	0
85	MG	5	3871	1/1	0.26	0.66	35,35,35,35	0
85	MG	1	3584	1/1	0.26	0.66	54,54,54,54	0
88	ZN	q3	501	1/1	0.15	0.65	69,69,69,69	0
85	MG	M9	201	1/1	0.28	0.65	70,70,70,70	0
86	OHX	5	4078	7/7	0.22	0.64	134,134,134,134	0
85	MG	1	3800	1/1	0.20	0.64	58,58,58,58	0
86	OHX	5	4170	7/7	0.14	0.64	154,154,154,154	0
86	OHX	1	3871	7/7	0.21	0.63	62,62,62,62	0
86	OHX	1	4094	7/7	0.15	0.63	149,149,149,149	0
85	MG	1	3803	1/1	0.32	0.63	203,203,203,203	0
86	OHX	2	2028	7/7	0.23	0.61	100,100,100,100	0
86	OHX	2	2118	7/7	0.19	0.61	147,147,147,147	0
85	MG	1	3664	1/1	0.19	0.59	68,68,68,68	0
85	MG	1	3608	1/1	0.33	0.59	59,59,59,59	0
86	OHX	5	4109	7/7	0.23	0.59	121,121,121,121	0
85	MG	L3	402	1/1	0.31	0.58	66,66,66,66	0
86	OHX	1	4022	7/7	0.20	0.58	132,132,132,132	0
85	MG	5	3814	1/1	0.26	0.57	43,43,43,43	0
86	OHX	6	2128	7/7	0.21	0.57	129,129,129,129	0
85	MG	1	3621	1/1	0.18	0.56	36,36,36,36	0
86	OHX	1	3867	7/7	0.17	0.56	58,58,58,58	0
86	OHX	3	224	7/7	0.20	0.55	141,141,141,141	0
85	MG	5	3644	1/1	0.26	0.55	64,64,64,64	0
86	OHX	5	4166	7/7	0.19	0.55	149,149,149,149	0
86	OHX	d9	102	7/7	0.42	0.54	179,179,179,179	0
86	OHX	5	4140	7/7	0.32	0.54	138,138,138,138	0
85	MG	5	3841	1/1	0.20	0.54	36,36,36,36	0
86	OHX	6	2049	7/7	0.20	0.53	70,70,70,70	0
86	OHX	C1	201	7/7	0.24	0.52	141,141,141,141	0
85	MG	2	1977	1/1	0.18	0.52	85,85,85,85	0
85	MG	N8	204	1/1	0.33	0.52	47,47,47,47	0
85	MG	6	1904	1/1	0.33	0.52	75,75,75,75	0
85	MG	1	3742	1/1	0.15	0.52	40,40,40,40	0
85	MG	6	1939	1/1	0.33	0.52	69,69,69,69	0
85	MG	5	3860	1/1	0.25	0.51	45,45,45,45	0
86	OHX	1	4112	7/7	0.15	0.50	174,174,174,174	0
86	OHX	1	3924	7/7	0.18	0.49	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3519	1/1	0.21	0.48	37,37,37,37	0
86	OHX	5	4209	7/7	0.23	0.47	150,150,150,150	0
85	MG	1	3737	1/1	0.17	0.46	42,42,42,42	0
86	OHX	2	2145	7/7	0.22	0.46	132,132,132,132	0
85	MG	1	3454	1/1	0.32	0.46	48,48,48,48	0
85	MG	M7	201	1/1	0.47	0.45	67,67,67,67	0
86	OHX	1	4098	7/7	0.19	0.44	128,128,128,128	0
86	OHX	5	4192	7/7	0.14	0.44	141,141,141,141	0
86	OHX	2	2171	7/7	0.23	0.44	153,153,153,153	0
85	MG	1	3419	1/1	0.15	0.44	84,84,84,84	0
85	MG	2	1933	1/1	0.24	0.43	75,75,75,75	0
86	OHX	4	233	7/7	0.20	0.43	148,148,148,148	0
85	MG	5	3424	1/1	0.27	0.43	60,60,60,60	0
86	OHX	6	2191	7/7	0.22	0.42	175,175,175,175	0
86	OHX	1	4096	7/7	0.15	0.41	153,153,153,153	0
85	MG	5	3417	1/1	0.18	0.41	30,30,30,30	0
86	OHX	1	4079	7/7	0.26	0.40	123,123,123,123	0
86	OHX	1	3876	7/7	0.17	0.40	73,73,73,73	0
85	MG	m5	302	1/1	0.26	0.40	55,55,55,55	0
87	3K8	6	2205	28/28	0.24	0.39	67,67,67,67	0
86	OHX	2	2148	7/7	0.28	0.39	170,170,170,170	0
86	OHX	s4	301	7/7	0.22	0.38	154,154,154,154	0
86	OHX	5	4190	7/7	0.24	0.36	170,170,170,170	0
86	OHX	2	2170	7/7	0.18	0.36	150,150,150,150	0
86	OHX	1	4085	7/7	0.19	0.36	136,136,136,136	0
86	OHX	5	4253	7/7	0.23	0.36	152,152,152,152	0
85	MG	5	3824	1/1	0.23	0.36	56,56,56,56	0
86	OHX	s1	303	7/7	0.46	0.36	173,173,173,173	0
86	OHX	6	2201	7/7	0.24	0.35	151,151,151,151	0
86	OHX	1	4188	7/7	0.18	0.35	148,148,148,148	0
86	OHX	5	4149	7/7	0.21	0.35	124,124,124,124	0
86	OHX	1	4189	7/7	0.18	0.33	158,158,158,158	0
86	OHX	6	2170	7/7	0.19	0.33	167,167,167,167	0
86	OHX	2	2107	7/7	0.20	0.33	138,138,138,138	0
85	MG	o4	201	1/1	0.31	0.29	56,56,56,56	0
86	OHX	6	2051	7/7	0.24	0.29	79,79,79,79	0
86	OHX	1	4121	7/7	0.24	0.27	112,112,112,112	0
85	MG	2	1929	1/1	0.28	0.27	74,74,74,74	0
86	OHX	6	2052	7/7	0.22	0.27	72,72,72,72	0
85	MG	5	3695	1/1	0.21	0.27	46,46,46,46	0
86	OHX	2	2152	7/7	0.35	0.27	172,172,172,172	0
86	OHX	1	4134	7/7	0.20	0.27	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2104	7/7	0.23	0.25	127,127,127,127	0
85	MG	2	1951	1/1	0.32	0.25	98,98,98,98	0
86	OHX	1	3882	7/7	0.19	0.25	71,71,71,71	0
86	OHX	3	225	7/7	0.14	0.25	147,147,147,147	0
86	OHX	5	4127	7/7	0.20	0.24	149,149,149,149	0
85	MG	15	302	1/1	0.16	0.24	65,65,65,65	0
85	MG	M0	303	1/1	0.33	0.23	53,53,53,53	0
86	OHX	6	2153	7/7	0.16	0.22	150,150,150,150	0
86	OHX	2	2084	7/7	0.18	0.22	129,129,129,129	0
86	OHX	2	2037	7/7	0.14	0.21	129,129,129,129	0
85	MG	1	3603	1/1	0.20	0.20	40,40,40,40	0
85	MG	6	1981	1/1	0.24	0.20	80,80,80,80	0
85	MG	5	3816	1/1	0.16	0.20	87,87,87,87	0
86	OHX	1	4061	7/7	0.19	0.19	128,128,128,128	0
85	MG	7	209	1/1	0.16	0.19	50,50,50,50	0
86	OHX	6	2198	7/7	0.21	0.18	143,143,143,143	0
86	OHX	2	2040	7/7	0.16	0.16	109,109,109,109	0
86	OHX	1	3864	7/7	0.19	0.16	58,58,58,58	0
85	MG	5	3456	1/1	0.26	0.15	99,99,99,99	0
85	MG	1	4214	1/1	0.23	0.14	73,73,73,73	0
86	OHX	2	2164	7/7	0.12	0.14	177,177,177,177	0
85	MG	6	1914	1/1	0.42	0.14	78,78,78,78	0
86	OHX	1	3964	7/7	0.14	0.14	129,129,129,129	0
86	OHX	1	3958	7/7	0.12	0.14	129,129,129,129	0
86	OHX	1	3881	7/7	0.19	0.14	74,74,74,74	0
86	OHX	1	3875	7/7	0.15	0.14	68,68,68,68	0
85	MG	n6	201	1/1	0.36	0.13	55,55,55,55	0
85	MG	6	1915	1/1	0.24	0.12	42,42,42,42	0
86	OHX	5	4179	7/7	0.19	0.12	136,136,136,136	0
86	OHX	2	2172	7/7	0.20	0.10	159,159,159,159	0
86	OHX	5	3910	7/7	0.18	0.10	63,63,63,63	0
85	MG	1	3754	1/1	0.17	0.10	50,50,50,50	0
85	MG	N6	201	1/1	0.27	0.10	51,51,51,51	0
85	MG	1	3653	1/1	0.21	0.10	45,45,45,45	0
86	OHX	1	3886	7/7	0.18	0.10	80,80,80,80	0
86	OHX	1	4129	7/7	0.17	0.09	149,149,149,149	0
86	OHX	1	4035	7/7	0.18	0.08	121,121,121,121	0
86	OHX	2	2149	7/7	0.21	0.08	166,166,166,166	0
86	OHX	6	2115	7/7	0.23	0.07	134,134,134,134	0
86	OHX	6	2175	7/7	0.28	0.07	168,168,168,168	0
86	OHX	1	4198	7/7	0.20	0.07	171,171,171,171	0
85	MG	M7	202	1/1	0.30	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3659	1/1	0.17	0.07	45,45,45,45	0
86	OHX	1	4127	7/7	0.15	0.06	131,131,131,131	0
86	OHX	1	3905	7/7	0.20	0.06	79,79,79,79	0
86	OHX	5	4019	7/7	0.16	0.05	149,149,149,149	0
86	OHX	6	2144	7/7	0.19	0.05	157,157,157,157	0
86	OHX	6	2141	7/7	0.17	0.05	140,140,140,140	0
86	OHX	5	4191	7/7	0.33	0.05	131,131,131,131	0
86	OHX	1	4148	7/7	0.21	0.05	162,162,162,162	0
86	OHX	5	4215	7/7	0.20	0.05	154,154,154,154	0
85	MG	1	3629	1/1	0.22	0.05	35,35,35,35	0
85	MG	d6	102	1/1	0.30	0.04	65,65,65,65	0
85	MG	6	1982	1/1	0.29	0.03	50,50,50,50	0
88	ZN	Q2	501	1/1	0.24	0.03	95,95,95,95	0
85	MG	D3	201	1/1	0.32	0.03	61,61,61,61	0
86	OHX	1	4013	7/7	0.15	0.02	165,165,165,165	0
85	MG	1	3445	1/1	0.20	0.01	46,46,46,46	0
86	OHX	5	3942	7/7	0.14	0.01	90,90,90,90	0
86	OHX	5	4126	7/7	0.14	0.01	141,141,141,141	0
86	OHX	6	2129	7/7	0.26	0.01	160,160,160,160	0
86	OHX	2	2150	7/7	0.13	0.00	187,187,187,187	0
86	OHX	5	4171	7/7	0.19	-0.00	146,146,146,146	0
85	MG	5	3649	1/1	0.20	0.00	40,40,40,40	0
85	MG	2	1901	1/1	0.38	-0.01	76,76,76,76	0
85	MG	2	1987	1/1	0.18	-0.02	101,101,101,101	0
86	OHX	5	4202	7/7	0.24	-0.02	131,131,131,131	0
86	OHX	2	2144	7/7	0.27	-0.04	177,177,177,177	0
86	OHX	5	4169	7/7	0.17	-0.04	140,140,140,140	0
85	MG	1	3481	1/1	0.17	-0.05	32,32,32,32	0
85	MG	5	3601	1/1	0.17	-0.05	45,45,45,45	0
86	OHX	L3	404	7/7	0.24	-0.05	127,127,127,127	0
85	MG	6	1957	1/1	0.38	-0.06	61,61,61,61	0
86	OHX	1	4185	7/7	0.30	-0.07	148,148,148,148	0
86	OHX	1	4063	7/7	0.24	-0.07	112,112,112,112	0
86	OHX	6	2134	7/7	0.21	-0.07	163,163,163,163	0
86	OHX	2	2139	7/7	0.28	-0.07	169,169,169,169	0
85	MG	5	3477	1/1	0.20	-0.07	85,85,85,85	0
85	MG	1	3446	1/1	0.26	-0.07	39,39,39,39	0
86	OHX	8	223	7/7	0.20	-0.08	119,119,119,119	0
85	MG	1	3567	1/1	0.24	-0.08	34,34,34,34	0
85	MG	1	3643	1/1	0.23	-0.09	45,45,45,45	0
85	MG	2	2013	1/1	0.27	-0.09	56,56,56,56	0
86	OHX	1	4152	7/7	0.20	-0.10	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2024	1/1	0.23	-0.10	53,53,53,53	0
86	OHX	1	3935	7/7	0.15	-0.11	103,103,103,103	0
86	OHX	6	2182	7/7	0.28	-0.11	142,142,142,142	0
85	MG	5	3783	1/1	0.27	-0.12	74,74,74,74	0
86	OHX	6	2077	7/7	0.22	-0.12	118,118,118,118	0
86	OHX	6	2150	7/7	0.17	-0.12	153,153,153,153	0
86	OHX	6	2133	7/7	0.22	-0.13	135,135,135,135	0
85	MG	5	3755	1/1	0.20	-0.13	45,45,45,45	0
86	OHX	1	3920	7/7	0.18	-0.13	98,98,98,98	0
85	MG	2	1999	1/1	0.37	-0.14	76,76,76,76	0
85	MG	M0	301	1/1	0.17	-0.16	86,86,86,86	0
85	MG	1	3749	1/1	0.22	-0.16	45,45,45,45	0
86	OHX	2	2027	7/7	0.22	-0.19	78,78,78,78	0
86	OHX	2	2111	7/7	0.21	-0.20	164,164,164,164	0
86	OHX	5	4125	7/7	0.23	-0.20	145,145,145,145	0
85	MG	5	3407	1/1	0.15	-0.20	44,44,44,44	0
86	OHX	O3	201	7/7	0.22	-0.21	120,120,120,120	0
86	OHX	1	3865	7/7	0.18	-0.21	62,62,62,62	0
88	ZN	O7	101	1/1	0.18	-0.22	45,45,45,45	0
85	MG	1	3504	1/1	0.19	-0.22	39,39,39,39	0
86	OHX	5	4077	7/7	0.23	-0.23	130,130,130,130	0
85	MG	6	2038	1/1	0.26	-0.23	70,70,70,70	0
85	MG	6	1935	1/1	0.26	-0.23	57,57,57,57	0
86	OHX	5	3957	7/7	0.19	-0.23	100,100,100,100	0
86	OHX	s8	303	7/7	0.24	-0.25	167,167,167,167	0
85	MG	m7	202	1/1	0.23	-0.25	37,37,37,37	0
85	MG	M0	302	1/1	0.22	-0.25	41,41,41,41	0
86	OHX	7	226	7/7	0.17	-0.25	117,117,117,117	0
86	OHX	6	2165	7/7	0.17	-0.26	151,151,151,151	0
86	OHX	4	230	7/7	0.13	-0.27	133,133,133,133	0
86	OHX	6	2151	7/7	0.21	-0.27	127,127,127,127	0
86	OHX	1	4130	7/7	0.21	-0.27	169,169,169,169	0
86	OHX	5	4056	7/7	0.18	-0.28	116,116,116,116	0
86	OHX	2	2175	7/7	0.18	-0.28	182,182,182,182	0
86	OHX	6	2139	7/7	0.19	-0.28	130,130,130,130	0
86	OHX	1	3893	7/7	0.17	-0.31	81,81,81,81	0
86	OHX	1	3904	7/7	0.15	-0.31	90,90,90,90	0
86	OHX	5	4184	7/7	0.18	-0.32	154,154,154,154	0
85	MG	2	1912	1/1	0.18	-0.32	73,73,73,73	0
86	OHX	5	4245	7/7	0.26	-0.33	113,113,113,113	0
86	OHX	5	3968	7/7	0.14	-0.33	107,107,107,107	0
86	OHX	5	4070	7/7	0.21	-0.33	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	d4	202	7/7	0.18	-0.34	173,173,173,173	0
85	MG	5	3851	1/1	0.20	-0.34	57,57,57,57	0
86	OHX	1	3939	7/7	0.12	-0.34	107,107,107,107	0
85	MG	5	3792	1/1	0.23	-0.36	38,38,38,38	0
86	OHX	1	4027	7/7	0.19	-0.36	112,112,112,112	0
86	OHX	1	4077	7/7	0.17	-0.36	126,126,126,126	0
86	OHX	6	2110	7/7	0.19	-0.36	119,119,119,119	0
86	OHX	5	4061	7/7	0.17	-0.37	124,124,124,124	0
86	OHX	1	4100	7/7	0.25	-0.38	145,145,145,145	0
86	OHX	5	3909	7/7	0.26	-0.38	64,64,64,64	0
85	MG	5	3773	1/1	0.20	-0.38	52,52,52,52	0
85	MG	2	2181	1/1	0.32	-0.38	90,90,90,90	0
85	MG	5	3758	1/1	0.18	-0.38	54,54,54,54	0
86	OHX	1	4102	7/7	0.21	-0.39	133,133,133,133	0
86	OHX	5	3901	7/7	0.17	-0.39	52,52,52,52	0
86	OHX	5	4150	7/7	0.20	-0.39	141,141,141,141	0
86	OHX	m4	201	7/7	0.15	-0.40	221,221,221,221	0
86	OHX	6	2126	7/7	0.22	-0.40	149,149,149,149	0
85	MG	1	3420	1/1	0.39	-0.40	87,87,87,87	0
86	OHX	1	3866	7/7	0.23	-0.40	54,54,54,54	0
85	MG	5	3406	1/1	0.19	-0.40	44,44,44,44	0
86	OHX	2	2132	7/7	0.15	-0.41	163,163,163,163	0
86	OHX	L3	406	7/7	0.27	-0.41	163,163,163,163	0
86	OHX	1	4066	7/7	0.19	-0.42	135,135,135,135	0
85	MG	6	1976	1/1	0.23	-0.42	68,68,68,68	0
86	OHX	2	2160	7/7	0.31	-0.43	158,158,158,158	0
86	OHX	6	2107	7/7	0.20	-0.43	154,154,154,154	0
86	OHX	1	4170	7/7	0.23	-0.44	144,144,144,144	0
86	OHX	5	4090	7/7	0.17	-0.44	120,120,120,120	0
86	OHX	6	2185	7/7	0.15	-0.44	188,188,188,188	0
86	OHX	5	4228	7/7	0.19	-0.44	154,154,154,154	0
86	OHX	2	2120	7/7	0.22	-0.44	157,157,157,157	0
86	OHX	6	2064	7/7	0.15	-0.44	106,106,106,106	0
85	MG	5	3415	1/1	0.19	-0.45	53,53,53,53	0
86	OHX	2	2178	7/7	0.19	-0.45	172,172,172,172	0
85	MG	1	3651	1/1	0.19	-0.46	76,76,76,76	0
86	OHX	6	2071	7/7	0.13	-0.46	112,112,112,112	0
86	OHX	1	4155	7/7	0.15	-0.46	122,122,122,122	0
85	MG	2	2180	1/1	0.28	-0.47	72,72,72,72	0
86	OHX	5	3976	7/7	0.14	-0.47	113,113,113,113	0
86	OHX	n9	102	7/7	0.19	-0.48	70,70,70,70	0
86	OHX	6	2193	7/7	0.17	-0.49	188,188,188,188	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2167	7/7	0.16	-0.50	203,203,203,203	0
85	MG	5	3782	1/1	0.19	-0.51	55,55,55,55	0
86	OHX	1	3929	7/7	0.13	-0.51	107,107,107,107	0
86	OHX	2	2130	7/7	0.20	-0.51	127,127,127,127	0
85	MG	5	3402	1/1	0.21	-0.52	31,31,31,31	0
86	OHX	5	4097	7/7	0.18	-0.52	134,134,134,134	0
85	MG	M3	201	1/1	0.19	-0.53	43,43,43,43	0
86	OHX	5	4093	7/7	0.20	-0.53	112,112,112,112	0
86	OHX	2	2033	7/7	0.16	-0.53	109,109,109,109	0
86	OHX	1	3916	7/7	0.14	-0.54	113,113,113,113	0
86	OHX	2	2100	7/7	0.18	-0.54	150,150,150,150	0
86	OHX	5	3950	7/7	0.14	-0.54	97,97,97,97	0
86	OHX	7	217	7/7	0.16	-0.55	88,88,88,88	0
86	OHX	5	4217	7/7	0.12	-0.55	204,204,204,204	0
86	OHX	5	4098	7/7	0.16	-0.55	131,131,131,131	0
86	OHX	1	4160	7/7	0.20	-0.55	144,144,144,144	0
85	MG	5	3413	1/1	0.21	-0.55	45,45,45,45	0
86	OHX	5	4195	7/7	0.17	-0.55	125,125,125,125	0
86	OHX	2	2086	7/7	0.17	-0.56	123,123,123,123	0
86	OHX	1	4209	7/7	0.21	-0.56	163,163,163,163	0
85	MG	1	3425	1/1	0.20	-0.57	34,34,34,34	0
85	MG	1	3806	1/1	0.18	-0.57	39,39,39,39	0
86	OHX	m8	201	7/7	0.18	-0.58	143,143,143,143	0
86	OHX	5	4216	7/7	0.20	-0.59	127,127,127,127	0
86	OHX	1	4105	7/7	0.16	-0.59	124,124,124,124	0
86	OHX	6	2192	7/7	0.16	-0.60	162,162,162,162	0
85	MG	2	1941	1/1	0.22	-0.61	76,76,76,76	0
86	OHX	2	2035	7/7	0.16	-0.61	103,103,103,103	0
86	OHX	m9	201	7/7	0.18	-0.61	142,142,142,142	0
86	OHX	5	3907	7/7	0.18	-0.61	56,56,56,56	0
86	OHX	5	4132	7/7	0.15	-0.62	159,159,159,159	0
86	OHX	5	4120	7/7	0.22	-0.62	109,109,109,109	0
86	OHX	6	2168	7/7	0.21	-0.64	129,129,129,129	0
86	OHX	5	4001	7/7	0.13	-0.64	120,120,120,120	0
86	OHX	5	3921	7/7	0.16	-0.65	70,70,70,70	0
85	MG	M1	201	1/1	0.24	-0.65	76,76,76,76	0
86	OHX	2	2133	7/7	0.21	-0.66	163,163,163,163	0
86	OHX	5	4147	7/7	0.15	-0.66	123,123,123,123	0
86	OHX	m1	202	7/7	0.25	-0.66	163,163,163,163	0
85	MG	4	221	1/1	0.17	-0.66	54,54,54,54	0
86	OHX	2	2093	7/7	0.14	-0.67	157,157,157,157	0
86	OHX	6	2053	7/7	0.16	-0.67	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3988	7/7	0.17	-0.67	112,112,112,112	0
85	MG	c8	201	1/1	0.24	-0.69	80,80,80,80	0
86	OHX	5	4005	7/7	0.14	-0.69	117,117,117,117	0
86	OHX	1	4143	7/7	0.15	-0.69	165,165,165,165	0
86	OHX	sR	401	7/7	0.12	-0.69	169,169,169,169	0
86	OHX	1	3998	7/7	0.20	-0.70	105,105,105,105	0
86	OHX	5	4124	7/7	0.13	-0.70	148,148,148,148	0
86	OHX	6	2138	7/7	0.19	-0.70	128,128,128,128	0
86	OHX	1	4082	7/7	0.15	-0.71	146,146,146,146	0
85	MG	5	3767	1/1	0.16	-0.71	39,39,39,39	0
86	OHX	m0	303	7/7	0.21	-0.71	134,134,134,134	0
86	OHX	2	2043	7/7	0.20	-0.71	123,123,123,123	0
85	MG	6	1987	1/1	0.20	-0.71	51,51,51,51	0
86	OHX	5	4128	7/7	0.10	-0.71	153,153,153,153	0
85	MG	1	3758	1/1	0.20	-0.73	46,46,46,46	0
86	OHX	5	4239	7/7	0.19	-0.73	141,141,141,141	0
85	MG	1	3634	1/1	0.22	-0.73	80,80,80,80	0
86	OHX	6	2196	7/7	0.17	-0.74	172,172,172,172	0
86	OHX	1	4036	7/7	0.14	-0.74	125,125,125,125	0
86	OHX	6	2124	7/7	0.16	-0.74	116,116,116,116	0
86	OHX	1	3879	7/7	0.19	-0.76	70,70,70,70	0
86	OHX	2	2080	7/7	0.12	-0.76	172,172,172,172	0
86	OHX	5	4203	7/7	0.22	-0.76	123,123,123,123	0
86	OHX	5	4244	7/7	0.24	-0.77	246,246,246,246	0
86	OHX	3	223	7/7	0.13	-0.77	172,172,172,172	0
86	OHX	5	3953	7/7	0.15	-0.78	106,106,106,106	0
86	OHX	1	3952	7/7	0.09	-0.78	107,107,107,107	0
85	MG	5	3544	1/1	0.19	-0.78	71,71,71,71	0
86	OHX	5	4219	7/7	0.14	-0.78	110,110,110,110	0
86	OHX	1	4052	7/7	0.18	-0.79	118,118,118,118	0
85	MG	5	3813	1/1	0.19	-0.79	76,76,76,76	0
86	OHX	1	4086	7/7	0.18	-0.79	135,135,135,135	0
86	OHX	c3	201	7/7	0.15	-0.79	160,160,160,160	0
85	MG	5	3776	1/1	0.17	-0.80	73,73,73,73	0
86	OHX	2	2030	7/7	0.16	-0.80	100,100,100,100	0
86	OHX	1	4020	7/7	0.11	-0.80	150,150,150,150	0
86	OHX	5	4075	7/7	0.14	-0.80	121,121,121,121	0
85	MG	5	3495	1/1	0.14	-0.80	48,48,48,48	0
86	OHX	5	3905	7/7	0.18	-0.80	56,56,56,56	0
86	OHX	M8	201	7/7	0.17	-0.81	140,140,140,140	0
85	MG	5	3744	1/1	0.15	-0.81	61,61,61,61	0
86	OHX	6	2089	7/7	0.12	-0.81	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2031	7/7	0.13	-0.82	116,116,116,116	0
86	OHX	6	2179	7/7	0.14	-0.82	157,157,157,157	0
85	MG	1	3466	1/1	0.15	-0.83	55,55,55,55	0
86	OHX	1	3931	7/7	0.13	-0.83	106,106,106,106	0
85	MG	2	2004	1/1	0.17	-0.84	73,73,73,73	0
86	OHX	5	4230	7/7	0.14	-0.84	163,163,163,163	0
86	OHX	2	2110	7/7	0.19	-0.84	126,126,126,126	0
86	OHX	5	3975	7/7	0.12	-0.85	84,84,84,84	0
86	OHX	1	3919	7/7	0.14	-0.85	83,83,83,83	0
88	ZN	Q3	501	1/1	0.11	-0.85	63,63,63,63	0
86	OHX	1	3945	7/7	0.13	-0.86	122,122,122,122	0
86	OHX	2	2121	7/7	0.14	-0.86	144,144,144,144	0
86	OHX	1	4089	7/7	0.15	-0.86	156,156,156,156	0
85	MG	5	3404	1/1	0.18	-0.86	53,53,53,53	0
86	OHX	N9	101	7/7	0.17	-0.87	65,65,65,65	0
86	OHX	1	4097	7/7	0.23	-0.87	118,118,118,118	0
86	OHX	1	4032	7/7	0.19	-0.87	105,105,105,105	0
86	OHX	5	4106	7/7	0.10	-0.88	164,164,164,164	0
86	OHX	1	3979	7/7	0.06	-0.89	116,116,116,116	0
85	MG	5	3637	1/1	0.16	-0.89	58,58,58,58	0
86	OHX	6	2162	7/7	0.17	-0.89	129,129,129,129	0
86	OHX	1	4196	7/7	0.15	-0.90	138,138,138,138	0
86	OHX	5	4003	7/7	0.16	-0.90	108,108,108,108	0
86	OHX	5	4063	7/7	0.17	-0.90	114,114,114,114	0
86	OHX	S8	302	7/7	0.21	-0.91	165,165,165,165	0
86	OHX	1	3993	7/7	0.11	-0.91	165,165,165,165	0
86	OHX	2	2126	7/7	0.16	-0.91	144,144,144,144	0
86	OHX	5	4196	7/7	0.14	-0.91	182,182,182,182	0
86	OHX	5	3979	7/7	0.20	-0.92	100,100,100,100	0
85	MG	1	3823	1/1	0.17	-0.94	60,60,60,60	0
86	OHX	2	2123	7/7	0.12	-0.94	151,151,151,151	0
86	OHX	5	4236	7/7	0.16	-0.94	113,113,113,113	0
86	OHX	5	4241	7/7	0.12	-0.95	148,148,148,148	0
86	OHX	l5	303	7/7	0.12	-0.95	146,146,146,146	0
86	OHX	8	228	7/7	0.15	-0.95	143,143,143,143	0
88	ZN	D6	500	1/1	0.13	-0.96	83,83,83,83	0
85	MG	1	3580	1/1	0.19	-0.97	44,44,44,44	0
86	OHX	6	2148	7/7	0.17	-0.97	140,140,140,140	0
86	OHX	8	225	7/7	0.13	-0.97	130,130,130,130	0
86	OHX	c5	201	7/7	0.14	-0.98	169,169,169,169	0
85	MG	1	3635	1/1	0.13	-0.99	64,64,64,64	0
86	OHX	5	3911	7/7	0.19	-0.99	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3977	7/7	0.17	-1.00	104,104,104,104	0
86	OHX	6	2103	7/7	0.17	-1.00	128,128,128,128	0
86	OHX	5	4207	7/7	0.15	-1.01	142,142,142,142	0
86	OHX	2	2141	7/7	0.09	-1.01	174,174,174,174	0
86	OHX	5	4043	7/7	0.10	-1.01	163,163,163,163	0
86	OHX	5	4071	7/7	0.12	-1.02	141,141,141,141	0
85	MG	5	3728	1/1	0.13	-1.02	56,56,56,56	0
86	OHX	1	4046	7/7	0.12	-1.03	140,140,140,140	0
88	ZN	d9	101	1/1	0.10	-1.03	92,92,92,92	0
85	MG	5	3826	1/1	0.13	-1.04	99,99,99,99	0
85	MG	1	3467	1/1	0.16	-1.05	44,44,44,44	0
86	OHX	5	4220	7/7	0.16	-1.05	145,145,145,145	0
85	MG	sM	302	1/1	0.20	-1.05	51,51,51,51	0
86	OHX	5	4122	7/7	0.17	-1.05	123,123,123,123	0
86	OHX	5	4065	7/7	0.12	-1.06	132,132,132,132	0
85	MG	1	3602	1/1	0.18	-1.06	39,39,39,39	0
86	OHX	5	4013	7/7	0.16	-1.06	111,111,111,111	0
85	MG	q1	101	1/1	0.20	-1.07	50,50,50,50	0
86	OHX	1	3899	7/7	0.15	-1.07	81,81,81,81	0
86	OHX	1	3863	7/7	0.16	-1.07	52,52,52,52	0
85	MG	1	3826	1/1	0.18	-1.07	37,37,37,37	0
85	MG	1	3706	1/1	0.17	-1.08	55,55,55,55	0
86	OHX	2	2032	7/7	0.13	-1.08	105,105,105,105	0
85	MG	5	3642	1/1	0.17	-1.09	38,38,38,38	0
86	OHX	5	3998	7/7	0.19	-1.09	103,103,103,103	0
86	OHX	C8	201	7/7	0.14	-1.09	120,120,120,120	0
85	MG	1	3840	1/1	0.18	-1.10	37,37,37,37	0
88	ZN	Q0	500	1/1	0.14	-1.10	50,50,50,50	0
85	MG	5	3720	1/1	0.19	-1.10	49,49,49,49	0
85	MG	n8	204	1/1	0.18	-1.10	39,39,39,39	0
86	OHX	6	2130	7/7	0.19	-1.11	146,146,146,146	0
86	OHX	1	3933	7/7	0.19	-1.11	94,94,94,94	0
86	OHX	8	216	7/7	0.08	-1.11	121,121,121,121	0
86	OHX	5	3949	7/7	0.12	-1.11	91,91,91,91	0
86	OHX	1	3887	7/7	0.14	-1.11	71,71,71,71	0
86	OHX	5	3938	7/7	0.10	-1.11	72,72,72,72	0
86	OHX	1	3889	7/7	0.14	-1.12	75,75,75,75	0
86	OHX	2	2108	7/7	0.14	-1.12	157,157,157,157	0
86	OHX	5	4079	7/7	0.13	-1.12	163,163,163,163	0
88	ZN	q0	201	1/1	0.15	-1.14	36,36,36,36	0
86	OHX	5	4205	7/7	0.22	-1.14	136,136,136,136	0
86	OHX	1	4041	7/7	0.15	-1.15	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	N6	202	1/1	0.20	-1.15	47,47,47,47	0
86	OHX	5	4199	7/7	0.16	-1.15	131,131,131,131	0
86	OHX	2	2117	7/7	0.16	-1.16	160,160,160,160	0
85	MG	1	3797	1/1	0.20	-1.16	54,54,54,54	0
86	OHX	4	231	7/7	0.17	-1.16	124,124,124,124	0
86	OHX	5	4173	7/7	0.18	-1.16	175,175,175,175	0
86	OHX	2	2098	7/7	0.13	-1.17	122,122,122,122	0
85	MG	1	3616	1/1	0.12	-1.17	64,64,64,64	0
85	MG	2	2017	1/1	0.19	-1.18	79,79,79,79	0
86	OHX	13	404	7/7	0.17	-1.18	142,142,142,142	0
86	OHX	5	3981	7/7	0.17	-1.19	100,100,100,100	0
85	MG	6	2206	1/1	0.16	-1.19	60,60,60,60	0
86	OHX	5	4092	7/7	0.15	-1.20	101,101,101,101	0
86	OHX	2	2062	7/7	0.25	-1.20	133,133,133,133	0
86	OHX	2	2023	7/7	0.18	-1.20	76,76,76,76	0
86	OHX	M5	302	7/7	0.17	-1.20	120,120,120,120	0
85	MG	5	3486	1/1	0.15	-1.21	66,66,66,66	0
86	OHX	6	2197	7/7	0.17	-1.22	146,146,146,146	0
85	MG	5	3754	1/1	0.12	-1.22	51,51,51,51	0
85	MG	1	3428	1/1	0.11	-1.23	55,55,55,55	0
85	MG	5	3730	1/1	0.18	-1.23	94,94,94,94	0
86	OHX	1	4015	7/7	0.12	-1.24	134,134,134,134	0
86	OHX	5	3960	7/7	0.12	-1.24	94,94,94,94	0
85	MG	1	4213	1/1	0.21	-1.24	31,31,31,31	0
86	OHX	O7	105	7/7	0.09	-1.24	107,107,107,107	0
86	OHX	5	3986	7/7	0.22	-1.25	99,99,99,99	0
86	OHX	6	2050	7/7	0.15	-1.25	77,77,77,77	0
85	MG	1	3599	1/1	0.17	-1.25	41,41,41,41	0
86	OHX	1	4191	7/7	0.10	-1.25	174,174,174,174	0
86	OHX	1	4092	7/7	0.11	-1.25	148,148,148,148	0
86	OHX	2	2047	7/7	0.06	-1.26	133,133,133,133	0
86	OHX	6	2159	7/7	0.15	-1.26	124,124,124,124	0
86	OHX	5	4210	7/7	0.15	-1.27	161,161,161,161	0
86	OHX	2	2077	7/7	0.16	-1.27	125,125,125,125	0
86	OHX	1	3999	7/7	0.09	-1.28	126,126,126,126	0
86	OHX	1	4008	7/7	0.11	-1.28	130,130,130,130	0
86	OHX	2	2109	7/7	0.07	-1.28	136,136,136,136	0
86	OHX	2	2089	7/7	0.09	-1.29	119,119,119,119	0
86	OHX	5	3919	7/7	0.15	-1.30	65,65,65,65	0
86	OHX	1	4029	7/7	0.13	-1.30	107,107,107,107	0
85	MG	Q2	502	1/1	0.14	-1.31	65,65,65,65	0
86	OHX	1	3980	7/7	0.14	-1.31	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3725	1/1	0.21	-1.32	73,73,73,73	0
86	OHX	6	2047	7/7	0.17	-1.33	62,62,62,62	0
86	OHX	1	3953	7/7	0.14	-1.34	103,103,103,103	0
86	OHX	1	3968	7/7	0.12	-1.34	108,108,108,108	0
85	MG	5	3715	1/1	0.19	-1.34	75,75,75,75	0
86	OHX	O1	201	7/7	0.11	-1.34	121,121,121,121	0
86	OHX	1	4026	7/7	0.18	-1.35	135,135,135,135	0
86	OHX	6	2058	7/7	0.11	-1.35	94,94,94,94	0
86	OHX	19	202	7/7	0.18	-1.35	130,130,130,130	0
86	OHX	1	4009	7/7	0.09	-1.35	137,137,137,137	0
86	OHX	1	4083	7/7	0.14	-1.36	133,133,133,133	0
86	OHX	m0	302	7/7	0.12	-1.36	130,130,130,130	0
85	MG	1	3818	1/1	0.12	-1.36	58,58,58,58	0
86	OHX	1	3883	7/7	0.17	-1.37	72,72,72,72	0
86	OHX	1	4031	7/7	0.08	-1.38	153,153,153,153	0
86	OHX	2	2127	7/7	0.17	-1.38	141,141,141,141	0
86	OHX	1	3940	7/7	0.09	-1.38	95,95,95,95	0
86	OHX	1	3895	7/7	0.15	-1.39	91,91,91,91	0
86	OHX	5	4104	7/7	0.13	-1.39	150,150,150,150	0
86	OHX	1	4011	7/7	0.15	-1.39	124,124,124,124	0
86	OHX	1	3923	7/7	0.11	-1.40	88,88,88,88	0
86	OHX	4	227	7/7	0.14	-1.40	115,115,115,115	0
86	OHX	1	4057	7/7	0.07	-1.40	187,187,187,187	0
86	OHX	3	219	7/7	0.07	-1.41	120,120,120,120	0
85	MG	5	3822	1/1	0.12	-1.41	68,68,68,68	0
86	OHX	5	4031	7/7	0.16	-1.41	98,98,98,98	0
85	MG	1	3798	1/1	0.18	-1.41	62,62,62,62	0
86	OHX	1	3966	7/7	0.08	-1.42	110,110,110,110	0
85	MG	6	1952	1/1	0.13	-1.42	65,65,65,65	0
85	MG	s1	301	1/1	0.18	-1.42	80,80,80,80	0
85	MG	2	2182	1/1	0.10	-1.42	105,105,105,105	0
86	OHX	5	4119	7/7	0.18	-1.43	147,147,147,147	0
85	MG	1	3730	1/1	0.16	-1.43	63,63,63,63	0
88	ZN	d6	101	1/1	0.15	-1.45	64,64,64,64	0
86	OHX	5	4044	7/7	0.15	-1.45	134,134,134,134	0
86	OHX	L3	405	7/7	0.17	-1.47	116,116,116,116	0
86	OHX	2	2082	7/7	0.08	-1.47	156,156,156,156	0
86	OHX	5	3935	7/7	0.18	-1.47	74,74,74,74	0
86	OHX	SR	401	7/7	0.09	-1.47	174,174,174,174	0
86	OHX	6	2140	7/7	0.13	-1.47	142,142,142,142	0
86	OHX	5	4037	7/7	0.13	-1.47	130,130,130,130	0
86	OHX	4	229	7/7	0.07	-1.47	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3971	7/7	0.11	-1.48	106,106,106,106	0
85	MG	8	201	1/1	0.15	-1.48	45,45,45,45	0
86	OHX	8	231	7/7	0.16	-1.48	140,140,140,140	0
86	OHX	5	4033	7/7	0.08	-1.49	143,143,143,143	0
85	MG	5	3470	1/1	0.12	-1.49	111,111,111,111	0
86	OHX	6	2202	7/7	0.05	-1.49	204,204,204,204	0
86	OHX	5	4026	7/7	0.08	-1.50	120,120,120,120	0
86	OHX	6	2113	7/7	0.16	-1.50	114,114,114,114	0
85	MG	5	3671	1/1	0.19	-1.50	30,30,30,30	0
85	MG	2	1948	1/1	0.11	-1.51	90,90,90,90	0
86	OHX	5	4029	7/7	0.15	-1.52	107,107,107,107	0
86	OHX	2	2067	7/7	0.12	-1.52	144,144,144,144	0
86	OHX	2	2142	7/7	0.18	-1.52	153,153,153,153	0
86	OHX	5	4060	7/7	0.09	-1.52	144,144,144,144	0
86	OHX	6	2164	7/7	0.18	-1.53	203,203,203,203	0
86	OHX	6	2184	7/7	0.18	-1.54	150,150,150,150	0
86	OHX	6	2066	7/7	0.14	-1.54	121,121,121,121	0
86	OHX	1	3873	7/7	0.17	-1.54	65,65,65,65	0
86	OHX	1	3962	7/7	0.13	-1.54	125,125,125,125	0
86	OHX	2	2095	7/7	0.14	-1.54	157,157,157,157	0
85	MG	1	3787	1/1	0.15	-1.54	88,88,88,88	0
86	OHX	5	4248	7/7	0.18	-1.56	165,165,165,165	0
86	OHX	2	2061	7/7	0.11	-1.56	132,132,132,132	0
85	MG	6	1998	1/1	0.17	-1.57	55,55,55,55	0
86	OHX	1	3959	7/7	0.15	-1.58	102,102,102,102	0
85	MG	O4	201	1/1	0.12	-1.58	61,61,61,61	0
85	MG	5	3791	1/1	0.14	-1.58	51,51,51,51	0
86	OHX	5	4059	7/7	0.09	-1.59	132,132,132,132	0
86	OHX	6	2085	7/7	0.10	-1.60	137,137,137,137	0
85	MG	5	3679	1/1	0.14	-1.61	41,41,41,41	0
86	OHX	5	4152	7/7	0.14	-1.61	151,151,151,151	0
86	OHX	5	4007	7/7	0.13	-1.61	110,110,110,110	0
86	OHX	5	4048	7/7	0.15	-1.61	112,112,112,112	0
85	MG	2	1978	1/1	0.11	-1.62	96,96,96,96	0
86	OHX	2	2101	7/7	0.14	-1.62	146,146,146,146	0
86	OHX	6	2111	7/7	0.13	-1.62	133,133,133,133	0
86	OHX	5	4008	7/7	0.19	-1.63	123,123,123,123	0
86	OHX	15	304	7/7	0.12	-1.63	149,149,149,149	0
86	OHX	5	3948	7/7	0.12	-1.64	76,76,76,76	0
86	OHX	2	2049	7/7	0.07	-1.65	126,126,126,126	0
86	OHX	6	2132	7/7	0.18	-1.65	149,149,149,149	0
86	OHX	2	2138	7/7	0.10	-1.65	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2076	7/7	0.12	-1.65	135,135,135,135	0
86	OHX	1	4045	7/7	0.11	-1.65	127,127,127,127	0
86	OHX	5	3972	7/7	0.11	-1.65	106,106,106,106	0
86	OHX	1	3885	7/7	0.17	-1.66	73,73,73,73	0
86	OHX	6	2106	7/7	0.15	-1.66	124,124,124,124	0
86	OHX	5	4028	7/7	0.16	-1.67	115,115,115,115	0
86	OHX	5	3904	7/7	0.15	-1.68	56,56,56,56	0
86	OHX	q2	502	7/7	0.11	-1.68	85,85,85,85	0
86	OHX	1	4050	7/7	0.12	-1.69	148,148,148,148	0
85	MG	1	3746	1/1	0.16	-1.70	51,51,51,51	0
86	OHX	2	2085	7/7	0.12	-1.70	149,149,149,149	0
86	OHX	2	2154	7/7	0.15	-1.72	157,157,157,157	0
85	MG	1	3825	1/1	0.19	-1.72	58,58,58,58	0
86	OHX	5	3908	7/7	0.17	-1.72	66,66,66,66	0
86	OHX	6	2122	7/7	0.07	-1.73	152,152,152,152	0
86	OHX	5	4025	7/7	0.12	-1.74	115,115,115,115	0
85	MG	2	1986	1/1	0.19	-1.74	65,65,65,65	0
86	OHX	5	3958	7/7	0.11	-1.75	101,101,101,101	0
86	OHX	2	2039	7/7	0.12	-1.75	103,103,103,103	0
85	MG	6	2207	1/1	0.12	-1.75	76,76,76,76	0
86	OHX	2	2094	7/7	0.07	-1.75	146,146,146,146	0
86	OHX	1	3901	7/7	0.13	-1.77	94,94,94,94	0
86	OHX	l3	403	7/7	0.11	-1.77	127,127,127,127	0
86	OHX	5	3945	7/7	0.13	-1.77	88,88,88,88	0
86	OHX	5	4131	7/7	0.17	-1.78	135,135,135,135	0
86	OHX	5	3917	7/7	0.16	-1.78	72,72,72,72	0
86	OHX	1	3949	7/7	0.16	-1.78	107,107,107,107	0
88	ZN	D9	101	1/1	0.06	-1.78	84,84,84,84	0
85	MG	1	3436	1/1	0.16	-1.78	47,47,47,47	0
86	OHX	5	4000	7/7	0.10	-1.79	109,109,109,109	0
86	OHX	2	2066	7/7	0.11	-1.79	138,138,138,138	0
86	OHX	6	2101	7/7	0.07	-1.80	171,171,171,171	0
85	MG	5	3645	1/1	0.17	-1.80	42,42,42,42	0
86	OHX	5	3970	7/7	0.12	-1.81	93,93,93,93	0
86	OHX	6	2161	7/7	0.16	-1.81	134,134,134,134	0
88	ZN	o7	102	1/1	0.18	-1.82	44,44,44,44	0
86	OHX	1	3925	7/7	0.10	-1.82	107,107,107,107	0
85	MG	6	1923	1/1	0.13	-1.82	72,72,72,72	0
86	OHX	1	4047	7/7	0.15	-1.83	123,123,123,123	0
86	OHX	N1	201	7/7	0.15	-1.84	69,69,69,69	0
86	OHX	o3	202	7/7	0.12	-1.85	110,110,110,110	0
86	OHX	2	2048	7/7	0.07	-1.86	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	6	1997	1/1	0.17	-1.87	75,75,75,75	0
86	OHX	5	4067	7/7	0.14	-1.87	124,124,124,124	0
86	OHX	2	2091	7/7	0.17	-1.87	154,154,154,154	0
86	OHX	6	2069	7/7	0.18	-1.87	106,106,106,106	0
86	OHX	1	4038	7/7	0.07	-1.87	132,132,132,132	0
86	OHX	6	2105	7/7	0.15	-1.88	126,126,126,126	0
86	OHX	8	229	7/7	0.20	-1.88	137,137,137,137	0
86	OHX	1	4062	7/7	0.17	-1.89	133,133,133,133	0
86	OHX	5	4015	7/7	0.10	-1.89	154,154,154,154	0
86	OHX	1	4002	7/7	0.14	-1.89	122,122,122,122	0
86	OHX	1	3943	7/7	0.09	-1.89	118,118,118,118	0
86	OHX	5	4134	7/7	0.09	-1.90	119,119,119,119	0
86	OHX	2	2046	7/7	0.05	-1.90	121,121,121,121	0
86	OHX	1	3898	7/7	0.10	-1.90	81,81,81,81	0
86	OHX	1	3965	7/7	0.10	-1.91	107,107,107,107	0
86	OHX	5	3933	7/7	0.14	-1.92	78,78,78,78	0
85	MG	5	3428	1/1	0.21	-1.92	44,44,44,44	0
88	ZN	e1	501	1/1	0.12	-1.92	186,186,186,186	0
86	OHX	6	2135	7/7	0.16	-1.92	140,140,140,140	0
86	OHX	1	3984	7/7	0.13	-1.92	123,123,123,123	0
86	OHX	2	2041	7/7	0.12	-1.93	100,100,100,100	0
86	OHX	6	2155	7/7	0.10	-1.95	121,121,121,121	0
85	MG	1	3659	1/1	0.14	-1.95	35,35,35,35	0
85	MG	5	3801	1/1	0.15	-1.95	41,41,41,41	0
86	OHX	5	4229	7/7	0.15	-1.96	141,141,141,141	0
86	OHX	O7	106	7/7	0.11	-1.96	105,105,105,105	0
85	MG	6	1974	1/1	0.14	-1.97	53,53,53,53	0
88	ZN	E1	501	1/1	0.04	-1.97	124,124,124,124	0
85	MG	1	3434	1/1	0.14	-1.97	49,49,49,49	0
86	OHX	4	223	7/7	0.12	-1.98	83,83,83,83	0
86	OHX	C5	201	7/7	0.07	-1.99	168,168,168,168	0
85	MG	n0	201	1/1	0.16	-1.99	45,45,45,45	0
86	OHX	1	3897	7/7	0.15	-2.00	70,70,70,70	0
85	MG	5	3807	1/1	0.12	-2.02	50,50,50,50	0
85	MG	c9	201	1/1	0.17	-2.03	62,62,62,62	0
86	OHX	5	4117	7/7	0.13	-2.03	122,122,122,122	0
86	OHX	2	2165	7/7	0.14	-2.04	170,170,170,170	0
86	OHX	1	4003	7/7	0.12	-2.04	109,109,109,109	0
85	MG	6	1966	1/1	0.11	-2.04	88,88,88,88	0
86	OHX	1	3894	7/7	0.16	-2.06	77,77,77,77	0
85	MG	1	3478	1/1	0.10	-2.06	92,92,92,92	0
86	OHX	5	4121	7/7	0.14	-2.06	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4154	7/7	0.19	-2.06	157,157,157,157	0
86	OHX	1	3928	7/7	0.12	-2.06	110,110,110,110	0
85	MG	6	2046	1/1	0.11	-2.07	72,72,72,72	0
86	OHX	1	3909	7/7	0.09	-2.07	83,83,83,83	0
86	OHX	c8	202	7/7	0.10	-2.08	155,155,155,155	0
86	OHX	1	3872	7/7	0.20	-2.08	64,64,64,64	0
86	OHX	5	3989	7/7	0.09	-2.08	100,100,100,100	0
86	OHX	5	4146	7/7	0.14	-2.09	138,138,138,138	0
86	OHX	1	3982	7/7	0.17	-2.09	111,111,111,111	0
86	OHX	5	4105	7/7	0.15	-2.10	109,109,109,109	0
86	OHX	8	224	7/7	0.08	-2.11	143,143,143,143	0
86	OHX	1	3922	7/7	0.11	-2.11	111,111,111,111	0
86	OHX	M0	304	7/7	0.11	-2.12	121,121,121,121	0
86	OHX	1	4048	7/7	0.13	-2.12	120,120,120,120	0
86	OHX	s1	302	7/7	0.14	-2.12	88,88,88,88	0
86	OHX	1	4135	7/7	0.22	-2.12	114,114,114,114	0
86	OHX	2	2097	7/7	0.08	-2.13	155,155,155,155	0
85	MG	1	3609	1/1	0.13	-2.14	45,45,45,45	0
85	MG	5	3834	1/1	0.08	-2.14	77,77,77,77	0
86	OHX	6	2082	7/7	0.07	-2.15	111,111,111,111	0
86	OHX	1	3977	7/7	0.17	-2.17	116,116,116,116	0
86	OHX	1	3868	7/7	0.18	-2.18	57,57,57,57	0
86	OHX	5	4052	7/7	0.07	-2.18	133,133,133,133	0
86	OHX	6	2118	7/7	0.09	-2.18	116,116,116,116	0
86	OHX	5	3982	7/7	0.09	-2.19	114,114,114,114	0
86	OHX	1	3963	7/7	0.11	-2.19	107,107,107,107	0
86	OHX	6	2054	7/7	0.16	-2.20	84,84,84,84	0
86	OHX	8	221	7/7	0.13	-2.21	123,123,123,123	0
86	OHX	1	4004	7/7	0.10	-2.21	112,112,112,112	0
86	OHX	5	3951	7/7	0.11	-2.22	103,103,103,103	0
86	OHX	1	4088	7/7	0.10	-2.23	141,141,141,141	0
86	OHX	5	4084	7/7	0.14	-2.24	109,109,109,109	0
86	OHX	l3	402	7/7	0.09	-2.24	107,107,107,107	0
85	MG	5	3759	1/1	0.10	-2.24	53,53,53,53	0
86	OHX	1	4033	7/7	0.16	-2.24	132,132,132,132	0
86	OHX	1	4075	7/7	0.12	-2.24	142,142,142,142	0
86	OHX	5	3964	7/7	0.08	-2.25	96,96,96,96	0
86	OHX	6	2090	7/7	0.08	-2.25	116,116,116,116	0
86	OHX	1	3915	7/7	0.13	-2.25	88,88,88,88	0
86	OHX	2	2056	7/7	0.10	-2.25	133,133,133,133	0
86	OHX	5	4082	7/7	0.11	-2.25	122,122,122,122	0
86	OHX	5	4076	7/7	0.14	-2.26	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4009	7/7	0.07	-2.26	126,126,126,126	0
86	OHX	8	226	7/7	0.17	-2.27	147,147,147,147	0
86	OHX	5	4110	7/7	0.12	-2.27	126,126,126,126	0
86	OHX	5	3952	7/7	0.15	-2.28	87,87,87,87	0
86	OHX	1	3956	7/7	0.10	-2.28	113,113,113,113	0
86	OHX	1	4123	7/7	0.10	-2.29	151,151,151,151	0
86	OHX	2	2119	7/7	0.13	-2.29	144,144,144,144	0
86	OHX	1	4171	7/7	0.11	-2.30	111,111,111,111	0
85	MG	5	3840	1/1	0.16	-2.31	68,68,68,68	0
86	OHX	1	4103	7/7	0.14	-2.32	131,131,131,131	0
86	OHX	2	2166	7/7	0.11	-2.32	170,170,170,170	0
86	OHX	1	4211	7/7	0.19	-2.33	161,161,161,161	0
86	OHX	6	2074	7/7	0.09	-2.34	156,156,156,156	0
85	MG	5	3663	1/1	0.14	-2.36	36,36,36,36	0
85	MG	1	3426	1/1	0.11	-2.36	63,63,63,63	0
86	OHX	1	4067	7/7	0.14	-2.37	127,127,127,127	0
86	OHX	5	3965	7/7	0.16	-2.38	101,101,101,101	0
86	OHX	1	4091	7/7	0.13	-2.38	156,156,156,156	0
86	OHX	1	4012	7/7	0.13	-2.38	120,120,120,120	0
85	MG	1	3804	1/1	0.15	-2.38	58,58,58,58	0
86	OHX	5	3937	7/7	0.16	-2.40	83,83,83,83	0
86	OHX	1	3976	7/7	0.10	-2.41	112,112,112,112	0
86	OHX	m5	303	7/7	0.10	-2.41	131,131,131,131	0
86	OHX	5	3939	7/7	0.13	-2.41	77,77,77,77	0
86	OHX	1	4122	7/7	0.13	-2.41	143,143,143,143	0
86	OHX	1	3891	7/7	0.16	-2.41	84,84,84,84	0
86	OHX	6	2086	7/7	0.13	-2.42	112,112,112,112	0
86	OHX	2	2057	7/7	0.09	-2.42	146,146,146,146	0
86	OHX	5	4144	7/7	0.17	-2.42	135,135,135,135	0
85	MG	m6	201	1/1	0.11	-2.43	32,32,32,32	0
86	OHX	6	2194	7/7	0.14	-2.43	195,195,195,195	0
86	OHX	5	4115	7/7	0.15	-2.43	127,127,127,127	0
86	OHX	2	2106	7/7	0.08	-2.44	119,119,119,119	0
86	OHX	6	2114	7/7	0.14	-2.44	136,136,136,136	0
86	OHX	5	4157	7/7	0.15	-2.45	121,121,121,121	0
86	OHX	6	2084	7/7	0.07	-2.45	125,125,125,125	0
85	MG	5	3478	1/1	0.17	-2.46	38,38,38,38	0
86	OHX	2	2053	7/7	0.10	-2.47	135,135,135,135	0
86	OHX	1	4034	7/7	0.08	-2.47	143,143,143,143	0
86	OHX	5	4081	7/7	0.15	-2.47	138,138,138,138	0
86	OHX	5	4040	7/7	0.06	-2.48	135,135,135,135	0
86	OHX	1	4019	7/7	0.07	-2.48	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3918	7/7	0.12	-2.48	96,96,96,96	0
86	OHX	1	4056	7/7	0.17	-2.49	129,129,129,129	0
86	OHX	1	4104	7/7	0.06	-2.51	141,141,141,141	0
85	MG	4	209	1/1	0.13	-2.51	49,49,49,49	0
86	OHX	6	2083	7/7	0.09	-2.51	122,122,122,122	0
86	OHX	2	2157	7/7	0.12	-2.52	293,293,293,293	0
86	OHX	5	3956	7/7	0.13	-2.52	95,95,95,95	0
86	OHX	5	4200	7/7	0.16	-2.52	92,92,92,92	0
86	OHX	6	2154	7/7	0.10	-2.53	143,143,143,143	0
86	OHX	5	3984	7/7	0.10	-2.54	88,88,88,88	0
86	OHX	5	3922	7/7	0.13	-2.54	70,70,70,70	0
86	OHX	2	2088	7/7	0.11	-2.54	132,132,132,132	0
86	OHX	2	2051	7/7	0.09	-2.54	112,112,112,112	0
86	OHX	4	226	7/7	0.05	-2.55	128,128,128,128	0
86	OHX	4	234	7/7	0.16	-2.55	135,135,135,135	0
86	OHX	2	2069	7/7	0.08	-2.55	121,121,121,121	0
86	OHX	5	3923	7/7	0.15	-2.56	70,70,70,70	0
86	OHX	5	3996	7/7	0.10	-2.56	136,136,136,136	0
86	OHX	5	3962	7/7	0.10	-2.56	80,80,80,80	0
86	OHX	2	2054	7/7	0.12	-2.57	137,137,137,137	0
86	OHX	4	222	7/7	0.17	-2.58	58,58,58,58	0
86	OHX	1	3974	7/7	0.10	-2.58	96,96,96,96	0
85	MG	2	1997	1/1	0.12	-2.58	78,78,78,78	0
86	OHX	5	4133	7/7	0.07	-2.58	145,145,145,145	0
85	MG	1	3703	1/1	0.12	-2.59	65,65,65,65	0
86	OHX	7	223	7/7	0.07	-2.60	110,110,110,110	0
85	MG	5	3855	1/1	0.17	-2.61	46,46,46,46	0
86	OHX	6	2120	7/7	0.07	-2.61	131,131,131,131	0
86	OHX	1	4072	7/7	0.07	-2.62	128,128,128,128	0
86	OHX	5	4211	7/7	0.20	-2.63	134,134,134,134	0
86	OHX	5	3999	7/7	0.09	-2.64	120,120,120,120	0
86	OHX	1	4040	7/7	0.10	-2.64	104,104,104,104	0
86	OHX	8	222	7/7	0.08	-2.64	125,125,125,125	0
85	MG	5	3430	1/1	0.14	-2.64	33,33,33,33	0
86	OHX	1	3942	7/7	0.09	-2.66	93,93,93,93	0
86	OHX	5	4027	7/7	0.09	-2.66	117,117,117,117	0
85	MG	1	3851	1/1	0.14	-2.67	77,77,77,77	0
86	OHX	5	3943	7/7	0.12	-2.69	91,91,91,91	0
86	OHX	1	3983	7/7	0.16	-2.69	129,129,129,129	0
86	OHX	n1	201	7/7	0.15	-2.70	62,62,62,62	0
86	OHX	1	3911	7/7	0.09	-2.70	105,105,105,105	0
86	OHX	5	4062	7/7	0.06	-2.70	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	8	217	7/7	0.09	-2.70	108,108,108,108	0
86	OHX	1	3986	7/7	0.10	-2.70	102,102,102,102	0
86	OHX	5	3926	7/7	0.17	-2.72	72,72,72,72	0
86	OHX	5	4095	7/7	0.14	-2.72	125,125,125,125	0
86	OHX	1	4064	7/7	0.07	-2.73	152,152,152,152	0
85	MG	5	3703	1/1	0.11	-2.73	63,63,63,63	0
86	OHX	2	2063	7/7	0.10	-2.73	139,139,139,139	0
86	OHX	5	3946	7/7	0.12	-2.74	90,90,90,90	0
85	MG	2	1922	1/1	0.14	-2.74	65,65,65,65	0
86	OHX	2	2073	7/7	0.14	-2.75	148,148,148,148	0
85	MG	3	211	1/1	0.10	-2.75	80,80,80,80	0
86	OHX	2	2072	7/7	0.08	-2.76	126,126,126,126	0
86	OHX	6	2136	7/7	0.12	-2.76	148,148,148,148	0
86	OHX	1	3908	7/7	0.15	-2.76	86,86,86,86	0
86	OHX	1	3902	7/7	0.13	-2.78	94,94,94,94	0
86	OHX	6	2063	7/7	0.14	-2.78	91,91,91,91	0
85	MG	5	3423	1/1	0.11	-2.78	44,44,44,44	0
86	OHX	5	4172	7/7	0.08	-2.78	191,191,191,191	0
86	OHX	1	3932	7/7	0.14	-2.79	99,99,99,99	0
86	OHX	1	4142	7/7	0.13	-2.80	119,119,119,119	0
86	OHX	5	4049	7/7	0.12	-2.80	128,128,128,128	0
86	OHX	1	4017	7/7	0.16	-2.80	130,130,130,130	0
86	OHX	2	2124	7/7	0.12	-2.82	147,147,147,147	0
86	OHX	1	3874	7/7	0.13	-2.83	60,60,60,60	0
86	OHX	1	4120	7/7	0.15	-2.84	152,152,152,152	0
86	OHX	6	2057	7/7	0.13	-2.84	82,82,82,82	0
86	OHX	6	2059	7/7	0.11	-2.84	100,100,100,100	0
86	OHX	6	2102	7/7	0.08	-2.86	121,121,121,121	0
86	OHX	2	2029	7/7	0.12	-2.86	108,108,108,108	0
85	MG	1	3774	1/1	0.14	-2.87	70,70,70,70	0
86	OHX	5	4051	7/7	0.07	-2.87	113,113,113,113	0
86	OHX	1	3991	7/7	0.08	-2.88	134,134,134,134	0
86	OHX	5	3932	7/7	0.13	-2.88	70,70,70,70	0
85	MG	5	3603	1/1	0.10	-2.88	65,65,65,65	0
86	OHX	2	2026	7/7	0.11	-2.89	87,87,87,87	0
86	OHX	6	2096	7/7	0.09	-2.90	134,134,134,134	0
86	OHX	7	224	7/7	0.10	-2.92	135,135,135,135	0
86	OHX	1	3912	7/7	0.14	-2.92	99,99,99,99	0
86	OHX	3	222	7/7	0.09	-2.92	146,146,146,146	0
86	OHX	2	2059	7/7	0.09	-2.93	127,127,127,127	0
86	OHX	5	3913	7/7	0.16	-2.93	59,59,59,59	0
86	OHX	1	4205	7/7	0.16	-2.94	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3896	7/7	0.20	-2.94	87,87,87,87	0
86	OHX	5	4094	7/7	0.12	-2.95	114,114,114,114	0
86	OHX	5	4030	7/7	0.12	-2.95	92,92,92,92	0
86	OHX	2	2096	7/7	0.08	-2.98	174,174,174,174	0
86	OHX	6	2098	7/7	0.09	-2.98	129,129,129,129	0
86	OHX	1	3926	7/7	0.17	-2.99	94,94,94,94	0
86	OHX	n3	203	7/7	0.07	-3.00	97,97,97,97	0
85	MG	5	3602	1/1	0.10	-3.01	48,48,48,48	0
86	OHX	1	4037	7/7	0.17	-3.01	122,122,122,122	0
86	OHX	1	4055	7/7	0.16	-3.01	121,121,121,121	0
86	OHX	5	4073	7/7	0.14	-3.01	134,134,134,134	0
85	MG	5	3616	1/1	0.13	-3.01	55,55,55,55	0
86	OHX	2	2068	7/7	0.09	-3.05	163,163,163,163	0
86	OHX	1	3888	7/7	0.13	-3.05	70,70,70,70	0
86	OHX	1	3960	7/7	0.11	-3.05	77,77,77,77	0
86	OHX	1	3878	7/7	0.12	-3.07	74,74,74,74	0
86	OHX	5	3929	7/7	0.15	-3.10	80,80,80,80	0
86	OHX	5	4012	7/7	0.09	-3.10	105,105,105,105	0
86	OHX	6	2131	7/7	0.21	-3.10	131,131,131,131	0
86	OHX	2	2042	7/7	0.09	-3.11	103,103,103,103	0
86	OHX	1	3907	7/7	0.11	-3.11	99,99,99,99	0
86	OHX	1	3948	7/7	0.14	-3.12	113,113,113,113	0
86	OHX	2	2058	7/7	0.10	-3.12	120,120,120,120	0
86	OHX	7	218	7/7	0.11	-3.13	98,98,98,98	0
86	OHX	1	3941	7/7	0.09	-3.13	111,111,111,111	0
86	OHX	2	2036	7/7	0.10	-3.16	98,98,98,98	0
86	OHX	8	218	7/7	0.11	-3.16	113,113,113,113	0
86	OHX	6	2100	7/7	0.09	-3.16	181,181,181,181	0
86	OHX	5	4038	7/7	0.08	-3.17	137,137,137,137	0
86	OHX	5	3959	7/7	0.11	-3.17	87,87,87,87	0
85	MG	1	3807	1/1	0.09	-3.17	55,55,55,55	0
86	OHX	5	3936	7/7	0.10	-3.19	84,84,84,84	0
86	OHX	1	3995	7/7	0.12	-3.21	118,118,118,118	0
85	MG	1	3639	1/1	0.14	-3.22	69,69,69,69	0
86	OHX	5	4010	7/7	0.16	-3.25	76,76,76,76	0
86	OHX	1	3914	7/7	0.10	-3.25	101,101,101,101	0
86	OHX	1	3973	7/7	0.11	-3.26	113,113,113,113	0
86	OHX	6	2158	7/7	0.10	-3.29	151,151,151,151	0
86	OHX	1	3994	7/7	0.08	-3.29	152,152,152,152	0
86	OHX	1	4001	7/7	0.10	-3.31	128,128,128,128	0
86	OHX	2	2055	7/7	0.11	-3.31	122,122,122,122	0
86	OHX	5	4182	7/7	0.19	-3.31	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2169	7/7	0.13	-3.31	152,152,152,152	0
85	MG	7	213	1/1	0.15	-3.32	78,78,78,78	0
86	OHX	1	3944	7/7	0.15	-3.33	116,116,116,116	0
86	OHX	2	2090	7/7	0.13	-3.34	128,128,128,128	0
85	MG	5	3614	1/1	0.13	-3.35	37,37,37,37	0
86	OHX	6	2065	7/7	0.10	-3.36	115,115,115,115	0
85	MG	1	3723	1/1	0.10	-3.36	64,64,64,64	0
86	OHX	6	2092	7/7	0.09	-3.36	125,125,125,125	0
86	OHX	1	3910	7/7	0.14	-3.37	90,90,90,90	0
86	OHX	5	4042	7/7	0.09	-3.37	131,131,131,131	0
86	OHX	2	2155	7/7	0.14	-3.38	246,246,246,246	0
85	MG	5	3770	1/1	0.14	-3.39	66,66,66,66	0
86	OHX	5	4137	7/7	0.12	-3.42	145,145,145,145	0
86	OHX	6	2087	7/7	0.08	-3.43	118,118,118,118	0
86	OHX	5	4002	7/7	0.07	-3.43	118,118,118,118	0
86	OHX	5	4068	7/7	0.06	-3.44	119,119,119,119	0
86	OHX	4	228	7/7	0.12	-3.46	122,122,122,122	0
86	OHX	6	2088	7/7	0.09	-3.46	129,129,129,129	0
86	OHX	1	4053	7/7	0.08	-3.46	153,153,153,153	0
86	OHX	1	4084	7/7	0.07	-3.47	196,196,196,196	0
86	OHX	2	2074	7/7	0.16	-3.49	122,122,122,122	0
86	OHX	5	3993	7/7	0.09	-3.49	96,96,96,96	0
86	OHX	1	3997	7/7	0.11	-3.50	120,120,120,120	0
86	OHX	5	4139	7/7	0.14	-3.50	140,140,140,140	0
86	OHX	C3	201	7/7	0.08	-3.50	162,162,162,162	0
86	OHX	5	4024	7/7	0.09	-3.51	113,113,113,113	0
86	OHX	5	3985	7/7	0.13	-3.52	104,104,104,104	0
86	OHX	5	4039	7/7	0.10	-3.53	130,130,130,130	0
86	OHX	6	2097	7/7	0.07	-3.55	164,164,164,164	0
86	OHX	6	2076	7/7	0.08	-3.57	115,115,115,115	0
86	OHX	5	4023	7/7	0.09	-3.58	114,114,114,114	0
86	OHX	3	221	7/7	0.05	-3.58	132,132,132,132	0
86	OHX	8	219	7/7	0.10	-3.59	131,131,131,131	0
86	OHX	5	4087	7/7	0.10	-3.60	126,126,126,126	0
86	OHX	1	3985	7/7	0.06	-3.61	126,126,126,126	0
86	OHX	1	3989	7/7	0.12	-3.62	136,136,136,136	0
86	OHX	1	4014	7/7	0.15	-3.63	124,124,124,124	0
86	OHX	6	2152	7/7	0.12	-3.65	158,158,158,158	0
86	OHX	1	4028	7/7	0.11	-3.69	142,142,142,142	0
86	OHX	6	2060	7/7	0.10	-3.69	91,91,91,91	0
86	OHX	5	4050	7/7	0.09	-3.69	118,118,118,118	0
86	OHX	5	4004	7/7	0.13	-3.72	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2062	7/7	0.10	-3.72	96,96,96,96	0
86	OHX	2	2114	7/7	0.12	-3.74	131,131,131,131	0
86	OHX	5	3980	7/7	0.12	-3.74	87,87,87,87	0
86	OHX	1	3877	7/7	0.12	-3.78	69,69,69,69	0
86	OHX	5	3963	7/7	0.11	-3.78	96,96,96,96	0
86	OHX	1	3934	7/7	0.14	-3.78	94,94,94,94	0
86	OHX	5	4175	7/7	0.10	-3.81	91,91,91,91	0
86	OHX	6	2163	7/7	0.13	-3.82	136,136,136,136	0
86	OHX	5	3987	7/7	0.08	-3.83	89,89,89,89	0
86	OHX	2	2052	7/7	0.08	-3.84	117,117,117,117	0
86	OHX	5	3954	7/7	0.11	-3.85	108,108,108,108	0
86	OHX	6	2073	7/7	0.08	-3.87	146,146,146,146	0
86	OHX	5	3967	7/7	0.14	-3.88	98,98,98,98	0
86	OHX	5	3927	7/7	0.13	-3.89	62,62,62,62	0
86	OHX	1	4023	7/7	0.06	-3.90	126,126,126,126	0
86	OHX	5	4032	7/7	0.10	-3.91	128,128,128,128	0
86	OHX	2	2044	7/7	0.07	-3.92	104,104,104,104	0
86	OHX	5	4036	7/7	0.11	-3.95	114,114,114,114	0
86	OHX	5	4069	7/7	0.08	-3.95	132,132,132,132	0
85	MG	5	3766	1/1	0.19	-3.96	82,82,82,82	0
86	OHX	4	224	7/7	0.10	-3.96	107,107,107,107	0
86	OHX	2	2081	7/7	0.13	-3.96	143,143,143,143	0
85	MG	5	3858	1/1	0.11	-3.97	76,76,76,76	0
86	OHX	2	2034	7/7	0.10	-4.02	106,106,106,106	0
86	OHX	5	4016	7/7	0.09	-4.04	100,100,100,100	0
86	OHX	6	2104	7/7	0.09	-4.04	128,128,128,128	0
86	OHX	1	4005	7/7	0.13	-4.04	127,127,127,127	0
86	OHX	1	3955	7/7	0.08	-4.07	111,111,111,111	0
86	OHX	8	220	7/7	0.08	-4.07	123,123,123,123	0
86	OHX	1	4059	7/7	0.08	-4.07	155,155,155,155	0
86	OHX	3	215	7/7	0.11	-4.08	101,101,101,101	0
85	MG	2	1980	1/1	0.13	-4.08	68,68,68,68	0
86	OHX	6	2094	7/7	0.06	-4.09	140,140,140,140	0
86	OHX	3	220	7/7	0.05	-4.09	129,129,129,129	0
86	OHX	5	3961	7/7	0.15	-4.13	74,74,74,74	0
86	OHX	5	4083	7/7	0.10	-4.14	116,116,116,116	0
86	OHX	2	2045	7/7	0.11	-4.16	108,108,108,108	0
85	MG	5	3713	1/1	0.15	-4.17	90,90,90,90	0
86	OHX	1	3992	7/7	0.12	-4.20	101,101,101,101	0
86	OHX	1	3951	7/7	0.09	-4.21	102,102,102,102	0
86	OHX	5	4113	7/7	0.08	-4.22	100,100,100,100	0
86	OHX	5	4101	7/7	0.10	-4.22	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3921	7/7	0.15	-4.25	80,80,80,80	0
86	OHX	6	2067	7/7	0.05	-4.27	98,98,98,98	0
86	OHX	1	4030	7/7	0.12	-4.28	117,117,117,117	0
86	OHX	5	4018	7/7	0.10	-4.29	113,113,113,113	0
86	OHX	1	4051	7/7	0.09	-4.29	136,136,136,136	0
86	OHX	1	4025	7/7	0.11	-4.32	135,135,135,135	0
86	OHX	6	2072	7/7	0.09	-4.32	94,94,94,94	0
86	OHX	5	3978	7/7	0.11	-4.32	107,107,107,107	0
86	OHX	6	2109	7/7	0.09	-4.33	126,126,126,126	0
86	OHX	2	2167	7/7	0.14	-4.35	132,132,132,132	0
86	OHX	6	2080	7/7	0.08	-4.35	110,110,110,110	0
85	MG	6	1961	1/1	0.16	-4.35	85,85,85,85	0
86	OHX	6	2119	7/7	0.10	-4.36	148,148,148,148	0
86	OHX	5	4201	7/7	0.15	-4.37	123,123,123,123	0
86	OHX	5	3947	7/7	0.10	-4.41	79,79,79,79	0
86	OHX	5	3992	7/7	0.11	-4.41	107,107,107,107	0
86	OHX	1	4039	7/7	0.11	-4.41	128,128,128,128	0
86	OHX	5	4089	7/7	0.09	-4.42	130,130,130,130	0
86	OHX	5	3974	7/7	0.09	-4.45	86,86,86,86	0
86	OHX	2	2079	7/7	0.12	-4.46	126,126,126,126	0
86	OHX	6	2149	7/7	0.12	-4.47	118,118,118,118	0
86	OHX	5	4085	7/7	0.14	-4.47	114,114,114,114	0
86	OHX	5	4041	7/7	0.17	-4.49	94,94,94,94	0
85	MG	1	3738	1/1	0.10	-4.51	43,43,43,43	0
86	OHX	5	3924	7/7	0.14	-4.52	69,69,69,69	0
86	OHX	2	2038	7/7	0.10	-4.54	103,103,103,103	0
86	OHX	2	2064	7/7	0.08	-4.57	119,119,119,119	0
86	OHX	1	3990	7/7	0.07	-4.60	127,127,127,127	0
86	OHX	5	3994	7/7	0.12	-4.62	111,111,111,111	0
86	OHX	1	4177	7/7	0.17	-4.65	253,253,253,253	0
86	OHX	5	3931	7/7	0.15	-4.66	84,84,84,84	0
85	MG	5	3764	1/1	0.09	-4.67	46,46,46,46	0
86	OHX	7	219	7/7	0.07	-4.70	105,105,105,105	0
85	MG	1	3728	1/1	0.15	-4.70	62,62,62,62	0
86	OHX	1	3913	7/7	0.13	-4.74	102,102,102,102	0
86	OHX	6	2123	7/7	0.08	-4.78	146,146,146,146	0
86	OHX	1	3957	7/7	0.08	-4.80	101,101,101,101	0
86	OHX	1	4116	7/7	0.13	-4.83	132,132,132,132	0
86	OHX	5	4057	7/7	0.06	-4.84	110,110,110,110	0
86	OHX	5	4011	7/7	0.09	-4.85	100,100,100,100	0
86	OHX	5	3966	7/7	0.13	-4.89	84,84,84,84	0
86	OHX	1	3969	7/7	0.06	-4.97	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3930	7/7	0.09	-4.97	83,83,83,83	0
86	OHX	5	4020	7/7	0.09	-4.97	124,124,124,124	0
86	OHX	2	2103	7/7	0.07	-5.03	204,204,204,204	0
86	OHX	6	2146	7/7	0.09	-5.04	139,139,139,139	0
86	OHX	1	4090	7/7	0.11	-5.05	126,126,126,126	0
86	OHX	1	3937	7/7	0.07	-5.06	99,99,99,99	0
86	OHX	5	3997	7/7	0.12	-5.07	118,118,118,118	0
85	MG	6	2027	1/1	0.07	-5.08	95,95,95,95	0
86	OHX	5	4165	7/7	0.08	-5.08	122,122,122,122	0
86	OHX	1	4006	7/7	0.09	-5.09	133,133,133,133	0
86	OHX	1	4024	7/7	0.15	-5.09	125,125,125,125	0
86	OHX	5	3944	7/7	0.09	-5.09	101,101,101,101	0
86	OHX	1	3971	7/7	0.10	-5.13	84,84,84,84	0
86	OHX	1	3917	7/7	0.10	-5.14	97,97,97,97	0
86	OHX	5	4066	7/7	0.07	-5.14	156,156,156,156	0
85	MG	1	3619	1/1	0.08	-5.16	67,67,67,67	0
86	OHX	2	2070	7/7	0.06	-5.22	130,130,130,130	0
86	OHX	1	3972	7/7	0.07	-5.22	110,110,110,110	0
86	OHX	1	3981	7/7	0.09	-5.23	102,102,102,102	0
85	MG	1	3605	1/1	0.13	-5.27	54,54,54,54	0
86	OHX	1	3975	7/7	0.10	-5.27	93,93,93,93	0
86	OHX	1	3967	7/7	0.10	-5.28	120,120,120,120	0
85	MG	5	3844	1/1	0.12	-5.28	77,77,77,77	0
86	OHX	6	2145	7/7	0.08	-5.31	138,138,138,138	0
86	OHX	3	217	7/7	0.09	-5.31	108,108,108,108	0
86	OHX	6	2095	7/7	0.12	-5.31	139,139,139,139	0
86	OHX	2	2092	7/7	0.09	-5.35	116,116,116,116	0
86	OHX	1	3900	7/7	0.09	-5.36	76,76,76,76	0
86	OHX	5	4046	7/7	0.09	-5.38	105,105,105,105	0
86	OHX	5	3955	7/7	0.10	-5.40	79,79,79,79	0
86	OHX	1	4007	7/7	0.10	-5.45	135,135,135,135	0
86	OHX	5	4135	7/7	0.07	-5.46	184,184,184,184	0
86	OHX	6	2143	7/7	0.07	-5.50	139,139,139,139	0
85	MG	1	3449	1/1	0.12	-5.50	43,43,43,43	0
86	OHX	m6	202	7/7	0.10	-5.57	98,98,98,98	0
86	OHX	6	2112	7/7	0.07	-5.58	125,125,125,125	0
86	OHX	5	4045	7/7	0.15	-5.58	122,122,122,122	0
86	OHX	6	2070	7/7	0.10	-5.59	96,96,96,96	0
86	OHX	5	4096	7/7	0.09	-5.62	120,120,120,120	0
86	OHX	1	4010	7/7	0.07	-5.62	124,124,124,124	0
86	OHX	1	3961	7/7	0.09	-5.63	109,109,109,109	0
86	OHX	2	2087	7/7	0.08	-5.72	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4070	7/7	0.15	-5.72	148,148,148,148	0
86	OHX	1	3890	7/7	0.08	-5.75	79,79,79,79	0
86	OHX	1	4150	7/7	0.08	-5.76	135,135,135,135	0
86	OHX	5	4022	7/7	0.12	-5.83	105,105,105,105	0
86	OHX	5	4014	7/7	0.09	-5.83	118,118,118,118	0
86	OHX	1	4058	7/7	0.12	-5.86	134,134,134,134	0
86	OHX	1	3903	7/7	0.11	-5.87	87,87,87,87	0
86	OHX	1	4101	7/7	0.14	-5.87	144,144,144,144	0
86	OHX	6	2078	7/7	0.10	-5.88	101,101,101,101	0
86	OHX	5	3991	7/7	0.07	-5.89	89,89,89,89	0
86	OHX	5	3969	7/7	0.12	-5.91	102,102,102,102	0
85	MG	5	3790	1/1	0.07	-5.94	46,46,46,46	0
86	OHX	1	3936	7/7	0.09	-6.04	101,101,101,101	0
86	OHX	5	3930	7/7	0.09	-6.08	80,80,80,80	0
86	OHX	7	222	7/7	0.08	-6.09	109,109,109,109	0
86	OHX	1	4000	7/7	0.08	-6.10	111,111,111,111	0
86	OHX	6	2099	7/7	0.09	-6.14	172,172,172,172	0
86	OHX	2	2125	7/7	0.12	-6.16	136,136,136,136	0
86	OHX	1	4119	7/7	0.14	-6.16	139,139,139,139	0
86	OHX	5	4168	7/7	0.13	-6.16	139,139,139,139	0
86	OHX	6	2166	7/7	0.11	-6.25	154,154,154,154	0
86	OHX	2	2078	7/7	0.07	-6.27	130,130,130,130	0
86	OHX	5	3983	7/7	0.15	-6.32	91,91,91,91	0
86	OHX	1	4154	7/7	0.09	-6.33	108,108,108,108	0
86	OHX	5	4021	7/7	0.06	-6.43	107,107,107,107	0
86	OHX	6	2075	7/7	0.10	-6.47	91,91,91,91	0
86	OHX	2	2113	7/7	0.14	-6.50	162,162,162,162	0
85	MG	5	3682	1/1	0.10	-6.54	50,50,50,50	0
86	OHX	2	2060	7/7	0.07	-6.58	113,113,113,113	0
86	OHX	1	3978	7/7	0.08	-6.60	84,84,84,84	0
85	MG	5	3707	1/1	0.09	-6.63	47,47,47,47	0
86	OHX	5	4107	7/7	0.10	-6.65	141,141,141,141	0
86	OHX	1	3996	7/7	0.09	-6.65	90,90,90,90	0
86	OHX	1	3954	7/7	0.07	-6.76	79,79,79,79	0
86	OHX	3	216	7/7	0.07	-6.86	118,118,118,118	0
85	MG	1	3705	1/1	0.11	-6.90	55,55,55,55	0
86	OHX	4	225	7/7	0.06	-6.90	120,120,120,120	0
86	OHX	6	2093	7/7	0.07	-6.96	112,112,112,112	0
86	OHX	6	2091	7/7	0.10	-7.07	126,126,126,126	0
86	OHX	5	3918	7/7	0.13	-7.13	66,66,66,66	0
86	OHX	1	3938	7/7	0.09	-7.22	92,92,92,92	0
86	OHX	2	2083	7/7	0.08	-7.26	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4055	7/7	0.08	-7.31	106,106,106,106	0
86	OHX	1	3947	7/7	0.09	-7.32	101,101,101,101	0
85	MG	2	1998	1/1	0.09	-7.32	107,107,107,107	0
86	OHX	1	4016	7/7	0.07	-7.39	113,113,113,113	0
86	OHX	6	2108	7/7	0.08	-7.59	118,118,118,118	0
86	OHX	5	3988	7/7	0.09	-7.76	96,96,96,96	0
86	OHX	6	2061	7/7	0.11	-7.80	92,92,92,92	0
86	OHX	5	4064	7/7	0.13	-7.80	133,133,133,133	0
86	OHX	1	4049	7/7	0.10	-7.83	134,134,134,134	0
86	OHX	5	4176	7/7	0.11	-7.85	126,126,126,126	0
86	OHX	6	2068	7/7	0.10	-7.89	100,100,100,100	0
86	OHX	2	2071	7/7	0.08	-7.91	132,132,132,132	0
85	MG	5	3651	1/1	0.17	-7.91	47,47,47,47	0
86	OHX	1	3987	7/7	0.12	-8.12	117,117,117,117	0
86	OHX	1	4018	7/7	0.09	-8.21	116,116,116,116	0
86	OHX	1	4087	7/7	0.06	-8.24	93,93,93,93	0
86	OHX	1	3970	7/7	0.09	-8.28	122,122,122,122	0
86	OHX	1	4110	7/7	0.15	-8.36	144,144,144,144	0
86	OHX	1	3927	7/7	0.10	-8.45	91,91,91,91	0
86	OHX	6	2079	7/7	0.07	-8.47	112,112,112,112	0
86	OHX	5	4100	7/7	0.11	-8.54	125,125,125,125	0
86	OHX	5	4058	7/7	0.11	-8.60	117,117,117,117	0
86	OHX	5	3973	7/7	0.07	-8.68	97,97,97,97	0
86	OHX	2	2105	7/7	0.14	-8.71	141,141,141,141	0
86	OHX	3	218	7/7	0.08	-8.82	107,107,107,107	0
86	OHX	7	220	7/7	0.08	-8.86	98,98,98,98	0
86	OHX	1	3880	7/7	0.13	-8.88	65,65,65,65	0
85	MG	1	3672	1/1	0.09	-8.91	72,72,72,72	0
86	OHX	2	2050	7/7	0.07	-9.09	121,121,121,121	0
86	OHX	5	4006	7/7	0.07	-9.24	104,104,104,104	0
86	OHX	5	4017	7/7	0.10	-9.32	111,111,111,111	0
86	OHX	5	4080	7/7	0.10	-9.81	95,95,95,95	0
85	MG	6	2002	1/1	0.15	-10.38	98,98,98,98	0
86	OHX	6	2081	7/7	0.12	-10.71	106,106,106,106	0
86	OHX	5	4086	7/7	0.09	-11.15	140,140,140,140	0
86	OHX	1	3950	7/7	0.10	-11.70	99,99,99,99	0
85	MG	5	3864	1/1	0.14	-11.80	68,68,68,68	0
85	MG	5	3859	1/1	0.09	-13.44	64,64,64,64	0
86	OHX	1	4021	7/7	0.08	-13.83	114,114,114,114	0
85	MG	1	3764	1/1	0.11	-14.24	92,92,92,92	0
86	OHX	7	221	7/7	0.07	-15.23	103,103,103,103	0
86	OHX	5	4035	7/7	0.07	-15.29	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2172	7/7	0.10	-15.47	152,152,152,152	0
86	OHX	2	2065	7/7	0.06	-16.75	114,114,114,114	0
86	OHX	5	3920	7/7	0.12	-18.20	76,76,76,76	0
85	MG	1	3788	1/1	0.07	-19.00	62,62,62,62	0
85	MG	5	3888	1/1	0.12	-43.44	62,62,62,62	0
86	OHX	5	4074	7/7	0.08	-47.04	123,123,123,123	0
85	MG	1	3845	1/1	0.43	-	38,38,38,38	0
85	MG	1	3849	1/1	1.95	-	111,111,111,111	0
85	MG	1	3786	1/1	0.12	-	73,73,73,73	0
85	MG	5	3442	1/1	0.41	-	42,42,42,42	0
85	MG	6	2045	1/1	0.39	-	83,83,83,83	0
85	MG	8	214	1/1	0.46	-	34,34,34,34	0
85	MG	L3	403	1/1	0.44	-	52,52,52,52	0
85	MG	1	3859	1/1	0.55	-	63,63,63,63	0
85	MG	1	3658	1/1	0.74	-	43,43,43,43	0
85	MG	1	3751	1/1	0.52	-	86,86,86,86	0
85	MG	6	2000	1/1	0.21	-	109,109,109,109	0
85	MG	5	3784	1/1	1.20	-	90,90,90,90	0
85	MG	1	3789	1/1	0.30	-	69,69,69,69	0
85	MG	5	3868	1/1	0.29	-	68,68,68,68	0
85	MG	5	3804	1/1	0.22	-	39,39,39,39	0
85	MG	5	3421	1/1	0.55	-	104,104,104,104	0
85	MG	2	1953	1/1	0.25	-	84,84,84,84	0
85	MG	1	3767	1/1	0.27	-	44,44,44,44	0
85	MG	5	3880	1/1	0.67	-	40,40,40,40	0
85	MG	1	3796	1/1	0.16	-	87,87,87,87	0
85	MG	1	3732	1/1	0.20	-	51,51,51,51	0
85	MG	1	3612	1/1	0.41	-	56,56,56,56	0
85	MG	6	2015	1/1	0.59	-	51,51,51,51	0
85	MG	2	1904	1/1	0.33	-	68,68,68,68	0
85	MG	6	2041	1/1	0.77	-	68,68,68,68	0
85	MG	2	1969	1/1	0.58	-	98,98,98,98	0
85	MG	1	3489	1/1	1.66	-	62,62,62,62	0
85	MG	5	3895	1/1	0.45	-	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.