



wwPDB X-ray Structure Validation Summary Report i

Oct 9, 2014 – 10:16 PM BST

PDB ID : 4U52
Title : Crystal structure of Nagilactone C bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.00 Å(reported)

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

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

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

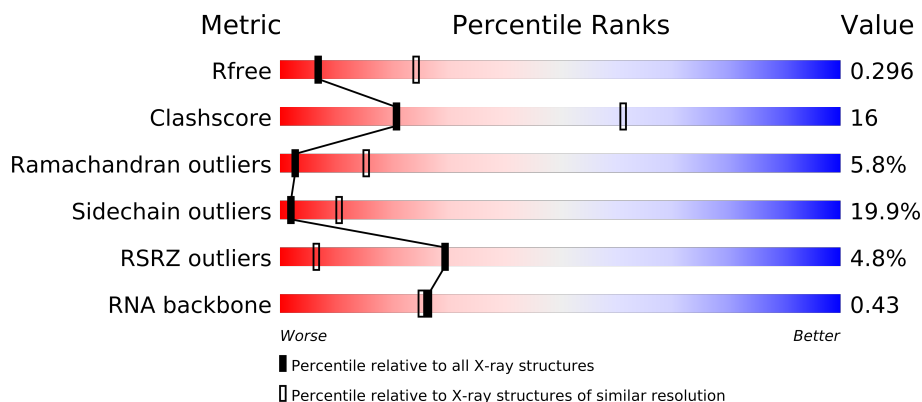
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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

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

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

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

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

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

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

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3402	-	X
85	MG	1	3405	-	X
85	MG	1	3408	-	X
85	MG	1	3409	-	X
85	MG	1	3412	-	X
85	MG	1	3413	-	X
85	MG	1	3418	-	X
85	MG	1	3419	-	X
85	MG	1	3429	-	X
85	MG	1	3430	-	X
85	MG	1	3432	-	X
85	MG	1	3442	-	X
85	MG	1	3443	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3450	-	X
85	MG	1	3452	-	X
85	MG	1	3455	-	X
85	MG	1	3460	-	X
85	MG	1	3462	-	X
85	MG	1	3463	-	X
85	MG	1	3468	-	X
85	MG	1	3469	-	X
85	MG	1	3472	-	X
85	MG	1	3474	-	X
85	MG	1	3480	-	X
85	MG	1	3484	-	X
85	MG	1	3499	-	X
85	MG	1	3500	-	X
85	MG	1	3502	-	X
85	MG	1	3504	-	X
85	MG	1	3506	-	X
85	MG	1	3509	-	X
85	MG	1	3510	-	X
85	MG	1	3511	-	X
85	MG	1	3513	-	X
85	MG	1	3515	-	X
85	MG	1	3518	-	X
85	MG	1	3521	-	X
85	MG	1	3522	-	X
85	MG	1	3523	-	X
85	MG	1	3524	-	X
85	MG	1	3525	-	X
85	MG	1	3526	-	X
85	MG	1	3529	-	X
85	MG	1	3535	-	X
85	MG	1	3536	-	X
85	MG	1	3537	-	X
85	MG	1	3538	-	X
85	MG	1	3540	-	X
85	MG	1	3542	-	X
85	MG	1	3543	-	X
85	MG	1	3545	-	X
85	MG	1	3546	-	X
85	MG	1	3548	-	X
85	MG	1	3552	-	X
85	MG	1	3556	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3559	-	X
85	MG	1	3562	-	X
85	MG	1	3566	-	X
85	MG	1	3570	-	X
85	MG	1	3572	-	X
85	MG	1	3573	-	X
85	MG	1	3574	-	X
85	MG	1	3578	-	X
85	MG	1	3579	-	X
85	MG	1	3585	-	X
85	MG	1	3586	-	X
85	MG	1	3587	-	X
85	MG	1	3589	-	X
85	MG	1	3590	-	X
85	MG	1	3591	-	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	3606	-	X
85	MG	1	3610	-	X
85	MG	1	3614	-	X
85	MG	1	3616	-	X
85	MG	1	3617	-	X
85	MG	1	3619	-	X
85	MG	1	3621	-	X
85	MG	1	3623	-	X
85	MG	1	3624	-	X
85	MG	1	3627	-	X
85	MG	1	3631	-	X
85	MG	1	3633	-	X
85	MG	1	3634	-	X
85	MG	1	3646	-	X
85	MG	1	3647	-	X
85	MG	1	3648	-	X
85	MG	1	3649	-	X
85	MG	1	3661	-	X
85	MG	1	3664	-	X
85	MG	1	3665	-	X
85	MG	1	3666	-	X
85	MG	1	3667	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3670	-	X
85	MG	1	3671	-	X
85	MG	1	3674	-	X
85	MG	1	3676	-	X
85	MG	1	3677	-	X
85	MG	1	3680	-	X
85	MG	1	3681	-	X
85	MG	1	3682	-	X
85	MG	1	3684	-	X
85	MG	1	3685	-	X
85	MG	1	3694	-	X
85	MG	1	3698	-	X
85	MG	1	3699	-	X
85	MG	1	3703	-	X
85	MG	1	3708	-	X
85	MG	1	3711	-	X
85	MG	1	3712	-	X
85	MG	1	3714	-	X
85	MG	1	3718	-	X
85	MG	1	3719	-	X
85	MG	1	3722	-	X
85	MG	1	3723	-	X
85	MG	1	3726	-	X
85	MG	1	3728	-	X
85	MG	1	3732	-	X
85	MG	1	3736	-	X
85	MG	1	3739	-	X
85	MG	1	3746	-	X
85	MG	1	3758	-	X
85	MG	1	3759	-	X
85	MG	1	3760	-	X
85	MG	1	3765	-	X
85	MG	1	3766	-	X
85	MG	1	3770	-	X
85	MG	1	3773	-	X
85	MG	1	3781	-	X
85	MG	1	3784	-	X
85	MG	1	3785	-	X
85	MG	1	3786	-	X
85	MG	1	3791	-	X
85	MG	1	3793	-	X
85	MG	1	3794	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3796	-	X
85	MG	1	3801	-	X
85	MG	1	3802	-	X
85	MG	1	3803	-	X
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	3815	-	X
85	MG	1	3816	-	X
85	MG	1	3818	-	X
85	MG	1	3819	-	X
85	MG	1	3820	-	X
85	MG	1	3821	-	X
85	MG	1	3822	-	X
85	MG	1	3828	-	X
85	MG	1	3830	-	X
85	MG	1	3833	-	X
85	MG	1	3834	-	X
85	MG	1	3836	-	X
85	MG	1	3838	-	X
85	MG	1	3839	-	X
85	MG	1	3843	-	X
85	MG	1	3845	-	X
85	MG	1	3850	-	X
85	MG	1	3855	-	X
85	MG	1	3856	-	X
85	MG	1	3858	-	X
85	MG	1	3860	-	X
85	MG	1	4212	-	X
85	MG	1	4215	-	X
85	MG	1	4216	-	X
85	MG	2	1902	-	X
85	MG	2	1903	-	X
85	MG	2	1904	-	X
85	MG	2	1905	-	X
85	MG	2	1908	-	X
85	MG	2	1913	-	X
85	MG	2	1914	-	X
85	MG	2	1915	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1918	-	X
85	MG	2	1919	-	X
85	MG	2	1926	-	X
85	MG	2	1929	-	X
85	MG	2	1932	-	X
85	MG	2	1934	-	X
85	MG	2	1935	-	X
85	MG	2	1936	-	X
85	MG	2	1938	-	X
85	MG	2	1941	-	X
85	MG	2	1943	-	X
85	MG	2	1945	-	X
85	MG	2	1947	-	X
85	MG	2	1951	-	X
85	MG	2	1952	-	X
85	MG	2	1954	-	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	1962	-	X
85	MG	2	1968	-	X
85	MG	2	1970	-	X
85	MG	2	1971	-	X
85	MG	2	1973	-	X
85	MG	2	1974	-	X
85	MG	2	1975	-	X
85	MG	2	1977	-	X
85	MG	2	1978	-	X
85	MG	2	1981	-	X
85	MG	2	1983	-	X
85	MG	2	1984	-	X
85	MG	2	1987	-	X
85	MG	2	1991	-	X
85	MG	2	1995	-	X
85	MG	2	1996	-	X
85	MG	2	1997	-	X
85	MG	2	2001	-	X
85	MG	2	2002	-	X
85	MG	2	2003	-	X
85	MG	2	2006	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	2007	-	X
85	MG	2	2009	-	X
85	MG	2	2013	-	X
85	MG	2	2014	-	X
85	MG	2	2017	-	X
85	MG	2	2018	-	X
85	MG	2	2019	-	X
85	MG	2	2022	-	X
85	MG	3	201	-	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	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	207	-	X
85	MG	4	212	-	X
85	MG	4	213	-	X
85	MG	4	215	-	X
85	MG	4	216	-	X
85	MG	4	220	-	X
85	MG	4	221	-	X
85	MG	4	222	-	X
85	MG	5	3403	-	X
85	MG	5	3404	-	X
85	MG	5	3409	-	X
85	MG	5	3410	-	X
85	MG	5	3414	-	X
85	MG	5	3416	-	X
85	MG	5	3418	-	X
85	MG	5	3420	-	X
85	MG	5	3429	-	X
85	MG	5	3431	-	X
85	MG	5	3433	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3434	-	X
85	MG	5	3438	-	X
85	MG	5	3440	-	X
85	MG	5	3441	-	X
85	MG	5	3445	-	X
85	MG	5	3448	-	X
85	MG	5	3449	-	X
85	MG	5	3451	-	X
85	MG	5	3453	-	X
85	MG	5	3463	-	X
85	MG	5	3466	-	X
85	MG	5	3468	-	X
85	MG	5	3472	-	X
85	MG	5	3473	-	X
85	MG	5	3475	-	X
85	MG	5	3482	-	X
85	MG	5	3483	-	X
85	MG	5	3485	-	X
85	MG	5	3486	-	X
85	MG	5	3489	-	X
85	MG	5	3496	-	X
85	MG	5	3498	-	X
85	MG	5	3500	-	X
85	MG	5	3503	-	X
85	MG	5	3504	-	X
85	MG	5	3505	-	X
85	MG	5	3506	-	X
85	MG	5	3512	-	X
85	MG	5	3517	-	X
85	MG	5	3518	-	X
85	MG	5	3519	-	X
85	MG	5	3524	-	X
85	MG	5	3529	-	X
85	MG	5	3530	-	X
85	MG	5	3532	-	X
85	MG	5	3535	-	X
85	MG	5	3536	-	X
85	MG	5	3539	-	X
85	MG	5	3540	-	X
85	MG	5	3544	-	X
85	MG	5	3545	-	X
85	MG	5	3546	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3547	-	X
85	MG	5	3552	-	X
85	MG	5	3554	-	X
85	MG	5	3556	-	X
85	MG	5	3560	-	X
85	MG	5	3561	-	X
85	MG	5	3562	-	X
85	MG	5	3563	-	X
85	MG	5	3566	-	X
85	MG	5	3567	-	X
85	MG	5	3569	-	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	3578	-	X
85	MG	5	3581	-	X
85	MG	5	3582	-	X
85	MG	5	3583	-	X
85	MG	5	3584	-	X
85	MG	5	3587	-	X
85	MG	5	3592	-	X
85	MG	5	3593	-	X
85	MG	5	3594	-	X
85	MG	5	3595	-	X
85	MG	5	3597	-	X
85	MG	5	3603	-	X
85	MG	5	3605	-	X
85	MG	5	3606	-	X
85	MG	5	3616	-	X
85	MG	5	3618	-	X
85	MG	5	3621	-	X
85	MG	5	3626	-	X
85	MG	5	3630	-	X
85	MG	5	3631	-	X
85	MG	5	3633	-	X
85	MG	5	3638	-	X
85	MG	5	3643	-	X
85	MG	5	3645	-	X
85	MG	5	3646	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3649	-	X
85	MG	5	3650	-	X
85	MG	5	3653	-	X
85	MG	5	3656	-	X
85	MG	5	3660	-	X
85	MG	5	3663	-	X
85	MG	5	3667	-	X
85	MG	5	3672	-	X
85	MG	5	3673	-	X
85	MG	5	3674	-	X
85	MG	5	3677	-	X
85	MG	5	3678	-	X
85	MG	5	3681	-	X
85	MG	5	3683	-	X
85	MG	5	3685	-	X
85	MG	5	3686	-	X
85	MG	5	3698	-	X
85	MG	5	3703	-	X
85	MG	5	3704	-	X
85	MG	5	3706	-	X
85	MG	5	3707	-	X
85	MG	5	3708	-	X
85	MG	5	3711	-	X
85	MG	5	3714	-	X
85	MG	5	3718	-	X
85	MG	5	3720	-	X
85	MG	5	3722	-	X
85	MG	5	3726	-	X
85	MG	5	3728	-	X
85	MG	5	3730	-	X
85	MG	5	3734	-	X
85	MG	5	3737	-	X
85	MG	5	3738	-	X
85	MG	5	3740	-	X
85	MG	5	3743	-	X
85	MG	5	3745	-	X
85	MG	5	3748	-	X
85	MG	5	3751	-	X
85	MG	5	3761	-	X
85	MG	5	3762	-	X
85	MG	5	3763	-	X
85	MG	5	3764	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3767	-	X
85	MG	5	3769	-	X
85	MG	5	3774	-	X
85	MG	5	3775	-	X
85	MG	5	3777	-	X
85	MG	5	3779	-	X
85	MG	5	3780	-	X
85	MG	5	3781	-	X
85	MG	5	3782	-	X
85	MG	5	3783	-	X
85	MG	5	3790	-	X
85	MG	5	3791	-	X
85	MG	5	3794	-	X
85	MG	5	3801	-	X
85	MG	5	3803	-	X
85	MG	5	3806	-	X
85	MG	5	3808	-	X
85	MG	5	3809	-	X
85	MG	5	3812	-	X
85	MG	5	3813	-	X
85	MG	5	3814	-	X
85	MG	5	3821	-	X
85	MG	5	3823	-	X
85	MG	5	3827	-	X
85	MG	5	3829	-	X
85	MG	5	3830	-	X
85	MG	5	3831	-	X
85	MG	5	3832	-	X
85	MG	5	3835	-	X
85	MG	5	3845	-	X
85	MG	5	3846	-	X
85	MG	5	3849	-	X
85	MG	5	3850	-	X
85	MG	5	3852	-	X
85	MG	5	3855	-	X
85	MG	5	3857	-	X
85	MG	5	3858	-	X
85	MG	5	3861	-	X
85	MG	5	3864	-	X
85	MG	5	3869	-	X
85	MG	5	3871	-	X
85	MG	5	3873	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3874	-	X
85	MG	5	3875	-	X
85	MG	5	3880	-	X
85	MG	5	3881	-	X
85	MG	5	3885	-	X
85	MG	5	3886	-	X
85	MG	5	3888	-	X
85	MG	5	3891	-	X
85	MG	5	3894	-	X
85	MG	5	3895	-	X
85	MG	5	3897	-	X
85	MG	5	4255	-	X
85	MG	5	4256	-	X
85	MG	6	1901	-	X
85	MG	6	1903	-	X
85	MG	6	1904	-	X
85	MG	6	1907	-	X
85	MG	6	1911	-	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	1922	-	X
85	MG	6	1923	-	X
85	MG	6	1924	-	X
85	MG	6	1928	-	X
85	MG	6	1929	-	X
85	MG	6	1931	-	X
85	MG	6	1934	-	X
85	MG	6	1940	-	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	1950	-	X
85	MG	6	1953	-	X
85	MG	6	1955	-	X
85	MG	6	1957	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1961	-	X
85	MG	6	1964	-	X
85	MG	6	1966	-	X
85	MG	6	1967	-	X
85	MG	6	1968	-	X
85	MG	6	1973	-	X
85	MG	6	1979	-	X
85	MG	6	1981	-	X
85	MG	6	1982	-	X
85	MG	6	1985	-	X
85	MG	6	1999	-	X
85	MG	6	2005	-	X
85	MG	6	2009	-	X
85	MG	6	2012	-	X
85	MG	6	2013	-	X
85	MG	6	2015	-	X
85	MG	6	2019	-	X
85	MG	6	2020	-	X
85	MG	6	2021	-	X
85	MG	6	2027	-	X
85	MG	6	2030	-	X
85	MG	6	2031	-	X
85	MG	6	2033	-	X
85	MG	6	2034	-	X
85	MG	6	2035	-	X
85	MG	6	2039	-	X
85	MG	6	2040	-	X
85	MG	6	2041	-	X
85	MG	6	2042	-	X
85	MG	6	2047	-	X
85	MG	7	201	-	X
85	MG	7	202	-	X
85	MG	7	203	-	X
85	MG	7	204	-	X
85	MG	7	205	-	X
85	MG	7	207	-	X
85	MG	7	208	-	X
85	MG	7	210	-	X
85	MG	7	215	-	X
85	MG	7	216	-	X
85	MG	7	217	-	X
85	MG	8	203	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	8	205	-	X
85	MG	8	207	-	X
85	MG	8	208	-	X
85	MG	8	209	-	X
85	MG	8	212	-	X
85	MG	L2	303	-	X
85	MG	L3	401	-	X
85	MG	L7	302	-	X
85	MG	L7	303	-	X
85	MG	M0	302	-	X
85	MG	M1	201	-	X
85	MG	M3	203	-	X
85	MG	M6	201	-	X
85	MG	M7	201	-	X
85	MG	M8	201	-	X
85	MG	N3	201	-	X
85	MG	N3	202	-	X
85	MG	N5	201	-	X
85	MG	N8	202	-	X
85	MG	N8	203	-	X
85	MG	N8	205	-	X
85	MG	c7	202	-	X
85	MG	d3	202	-	X
85	MG	d6	102	-	X
85	MG	l3	401	-	X
85	MG	l7	301	-	X
85	MG	m0	301	-	X
85	MG	m1	202	-	X
85	MG	m5	304	-	X
85	MG	m7	205	-	X
85	MG	n0	201	-	X
85	MG	n3	201	-	X
85	MG	o3	201	-	X
85	MG	q0	202	-	X
86	OHX	1	3864	-	X
86	OHX	1	3895	-	X
86	OHX	1	3919	-	X
86	OHX	1	4052	-	X
86	OHX	1	4057	-	X
86	OHX	1	4058	-	X
86	OHX	1	4068	-	X
86	OHX	1	4074	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4090	-	X
86	OHX	1	4107	-	X
86	OHX	1	4115	-	X
86	OHX	1	4121	-	X
86	OHX	1	4134	-	X
86	OHX	1	4135	-	X
86	OHX	1	4136	-	X
86	OHX	1	4137	-	X
86	OHX	1	4138	-	X
86	OHX	1	4155	-	X
86	OHX	1	4162	-	X
86	OHX	1	4164	-	X
86	OHX	1	4166	-	X
86	OHX	1	4167	-	X
86	OHX	1	4172	-	X
86	OHX	1	4173	-	X
86	OHX	1	4182	-	X
86	OHX	1	4184	-	X
86	OHX	1	4185	-	X
86	OHX	1	4187	-	X
86	OHX	1	4190	-	X
86	OHX	1	4194	-	X
86	OHX	1	4199	-	X
86	OHX	1	4201	-	X
86	OHX	1	4202	-	X
86	OHX	1	4204	-	X
86	OHX	1	4205	-	X
86	OHX	1	4207	-	X
86	OHX	1	4208	-	X
86	OHX	2	2092	-	X
86	OHX	2	2144	-	X
86	OHX	2	2149	-	X
86	OHX	2	2158	-	X
86	OHX	2	2160	-	X
86	OHX	2	2164	-	X
86	OHX	2	2172	-	X
86	OHX	2	2176	-	X
86	OHX	4	236	-	X
86	OHX	4	238	-	X
86	OHX	5	3906	-	X
86	OHX	5	3909	-	X
86	OHX	5	3953	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4052	-	X
86	OHX	5	4080	-	X
86	OHX	5	4087	-	X
86	OHX	5	4110	-	X
86	OHX	5	4141	-	X
86	OHX	5	4145	-	X
86	OHX	5	4148	-	X
86	OHX	5	4150	-	X
86	OHX	5	4152	-	X
86	OHX	5	4153	-	X
86	OHX	5	4157	-	X
86	OHX	5	4159	-	X
86	OHX	5	4161	-	X
86	OHX	5	4164	-	X
86	OHX	5	4175	-	X
86	OHX	5	4181	-	X
86	OHX	5	4186	-	X
86	OHX	5	4187	-	X
86	OHX	5	4195	-	X
86	OHX	5	4219	-	X
86	OHX	5	4221	-	X
86	OHX	5	4224	-	X
86	OHX	5	4229	-	X
86	OHX	5	4232	-	X
86	OHX	5	4235	-	X
86	OHX	5	4238	-	X
86	OHX	5	4239	-	X
86	OHX	5	4248	-	X
86	OHX	5	4249	-	X
86	OHX	6	2129	-	X
86	OHX	6	2159	-	X
86	OHX	6	2163	-	X
86	OHX	6	2171	-	X
86	OHX	6	2177	-	X
86	OHX	6	2184	-	X
86	OHX	6	2185	-	X
86	OHX	6	2187	-	X
86	OHX	6	2190	-	X
86	OHX	6	2194	-	X
86	OHX	6	2208	-	X
86	OHX	7	228	-	X
86	OHX	8	228	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	M7	204	-	X
86	OHX	l4	403	-	X
87	ZN	d7	101	-	X
88	3J2	1	4209	-	X
88	3J2	5	4254	-	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 TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence.

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
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- 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			
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			

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

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

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

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

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

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

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

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

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

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2441	1544	419	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			
35	sM	104	Total	C	N	O	0	0	0
			680	403	140	137			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
52	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	M7	183	Total	C	N	O	0	0	0
			1420	882	281	257			
53	m7	155	Total	C	N	O	0	0	0
			1227	764	238	225			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	110	GLU	-	expression tag	UNP P87262
O4	111	ALA	-	expression tag	UNP P87262
O4	112	ALA	-	expression tag	UNP P87262
O4	113	LYS	-	expression tag	UNP P87262
O4	114	SER	-	expression tag	UNP P87262
O4	115	GLU	-	expression tag	UNP P87262
O4	116	LYS	-	expression tag	UNP P87262
O4	117	LYS	-	expression tag	UNP P87262
O4	118	ALA	-	expression tag	UNP P87262

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Chain	Residue	Modelled	Actual	Comment	Reference
O4	119	LYS	-	expression tag	UNP P87262
O4	120	LYS	-	expression tag	UNP P87262
o4	110	GLU	-	expression tag	UNP P87262
o4	111	ALA	-	expression tag	UNP P87262
o4	112	ALA	-	expression tag	UNP P87262
o4	113	LYS	-	expression tag	UNP P87262
o4	114	SER	-	expression tag	UNP P87262
o4	115	GLU	-	expression tag	UNP P87262
o4	116	LYS	-	expression tag	UNP P87262
o4	117	LYS	-	expression tag	UNP P87262
o4	118	ALA	-	expression tag	UNP P87262
o4	119	LYS	-	expression tag	UNP P87262
o4	120	LYS	-	expression tag	UNP P87262

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e0	62	VAL	-	expression tag	UNP P0CX33
e0	63	GLN	-	expression tag	UNP P0CX33

- Molecule 81 is a protein called Unknown Protein m2.

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

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

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

- Molecule 83 is a protein called Unknown Protein p1.

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

- Molecule 84 is a protein called Unknown Protein p2.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	L7	3	Total 3 Mg 3	0	0
85	N9	1	Total 1 Mg 1	0	0
85	n8	5	Total 5 Mg 5	0	0
85	o1	1	Total 1 Mg 1	0	0
85	N5	1	Total 1 Mg 1	0	0
85	6	150	Total 150 Mg 150	0	0
85	sM	2	Total 2 Mg 2	0	0
85	O4	1	Total 1 Mg 1	0	0
85	m5	4	Total 4 Mg 4	0	0
85	l3	2	Total 2 Mg 2	0	0
85	M1	1	Total 1 Mg 1	0	0
85	n0	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	O3	1	Total 1 Mg 1	0	0
85	L4	2	Total 2 Mg 2	0	0
85	l7	1	Total 1 Mg 1	0	0
85	M5	3	Total 3 Mg 3	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	2	Total 2	Mg 2	0	0
85	5	502	Total 502	Mg 502	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	M4	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	3	Total 3	Mg 3	0	0
85	M8	1	Total 1	Mg 1	0	0
85	q3	1	Total 1	Mg 1	0	0
85	o3	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	3	Total 3	Mg 3	0	0
85	4	22	Total 22	Mg 22	0	0

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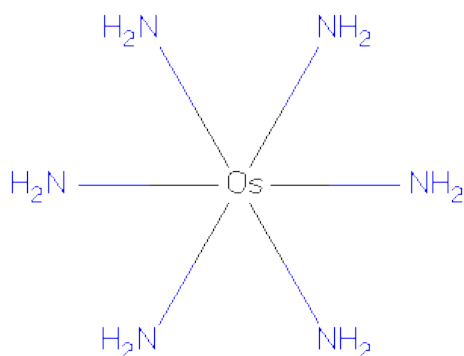
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	n6	1	Total 1	Mg 1	0	0
85	L2	3	Total 3	Mg 3	0	0
85	m1	2	Total 2	Mg 2	0	0
85	l5	1	Total 1	Mg 1	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	3	Total 3	Mg 3	0	0
85	N8	5	Total 5	Mg 5	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	O1	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	l8	1	Total 1	Mg 1	0	0
85	c7	2	Total 2	Mg 2	0	0
85	7	17	Total 17	Mg 17	0	0
85	n3	1	Total 1	Mg 1	0	0
85	L3	2	Total 2	Mg 2	0	0
85	m6	1	Total 1	Mg 1	0	0
85	N6	1	Total 1	Mg 1	0	0
85	8	15	Total 15	Mg 15	0	0
85	m0	1	Total 1	Mg 1	0	0
85	M6	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N0	1	Total	Mg	0	0
			1	1		
85	3	14	Total	Mg	0	0
			14	14		

- 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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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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	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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	L3	1	Total	N	Os	0	0
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86	L4	1	Total	N	Os	0	0
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86	M0	1	Total	N	Os	0	0
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86	M5	1	Total	N	Os	0	0
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86	M6	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	O3	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O9	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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	c5	1	Total	N	Os	0	0
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86	c8	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			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		
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		
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	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	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	19	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	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	m9	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n6	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	o7	1	Total	N	Os	0	0
			7	6	1		
86	q1	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

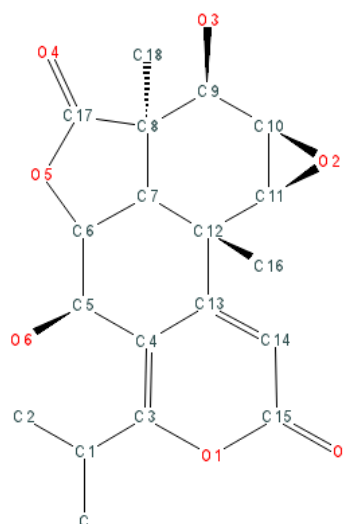
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0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

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

- Molecule 88 is Nagilactone C (three-letter code: 3J2) (formula: $C_{19}H_{22}O_7$).

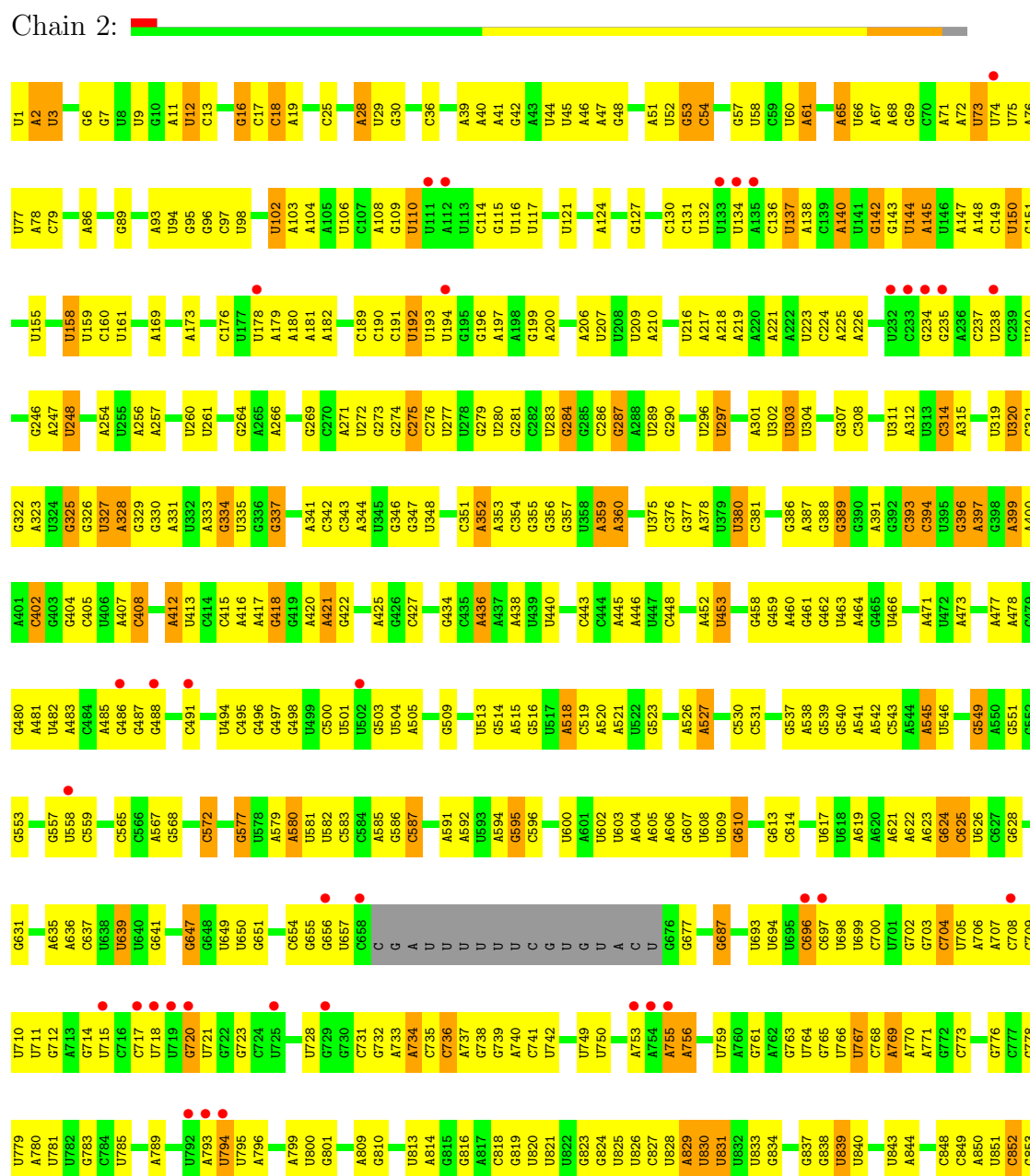


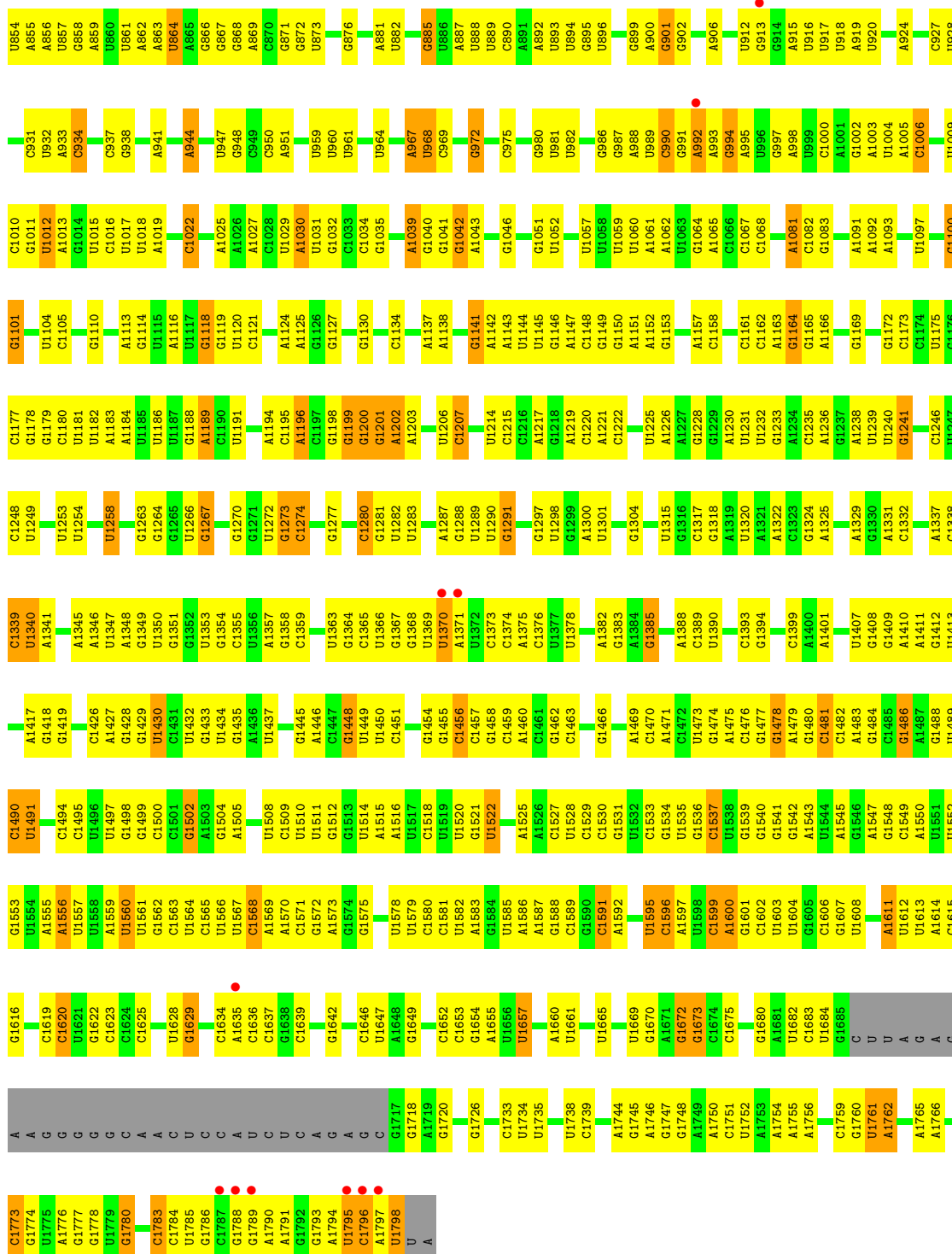
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			26	19	7		
88	5	1	Total	C	O	0	0
			26	19	7		

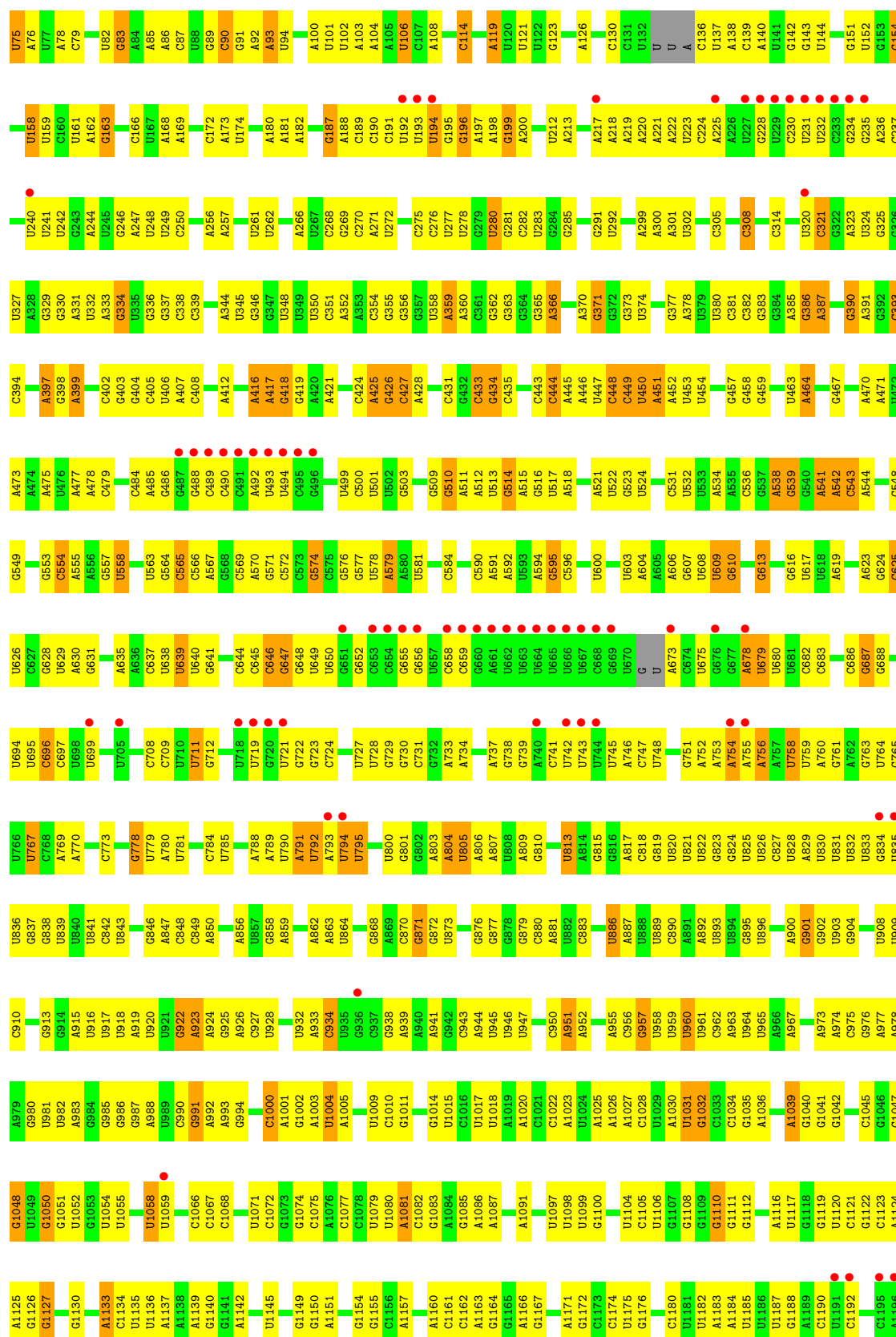
3 Residue-property plots

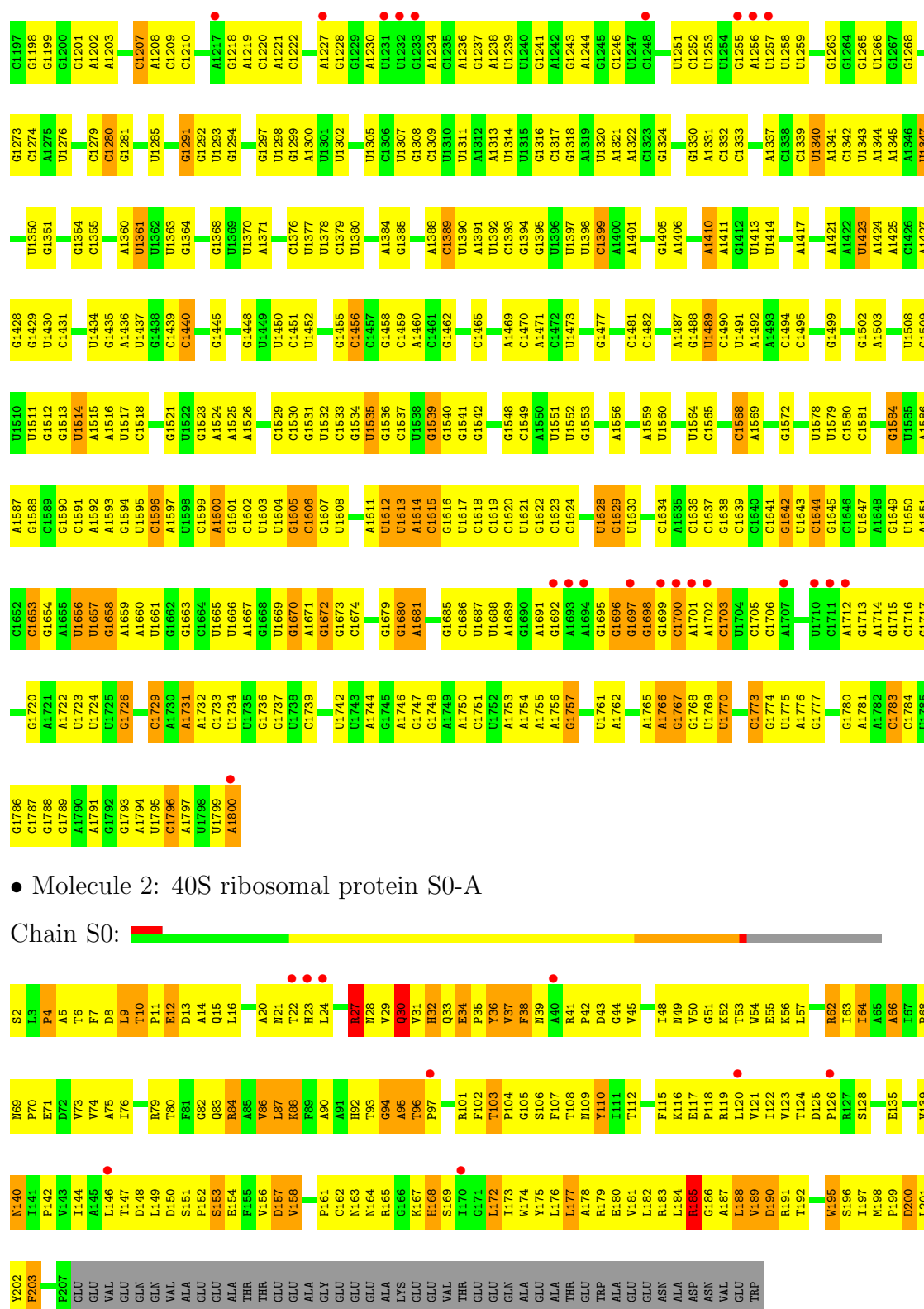
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

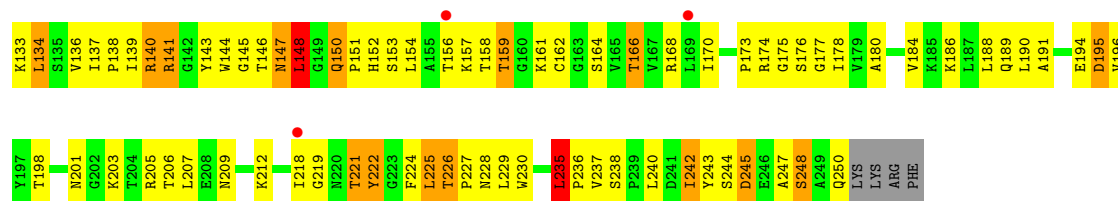
- Molecule 1: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence





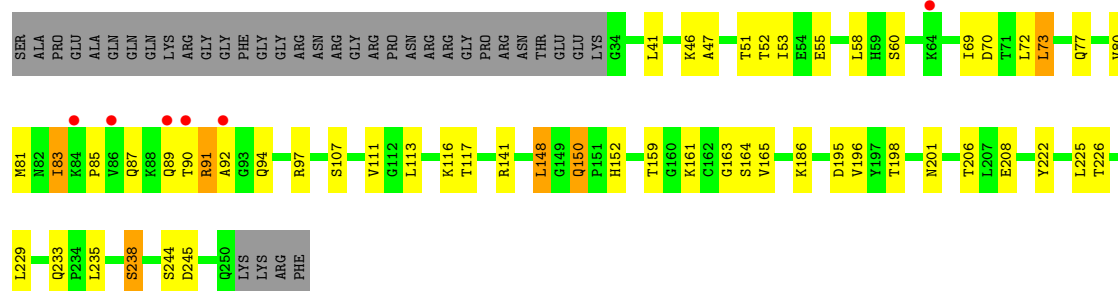






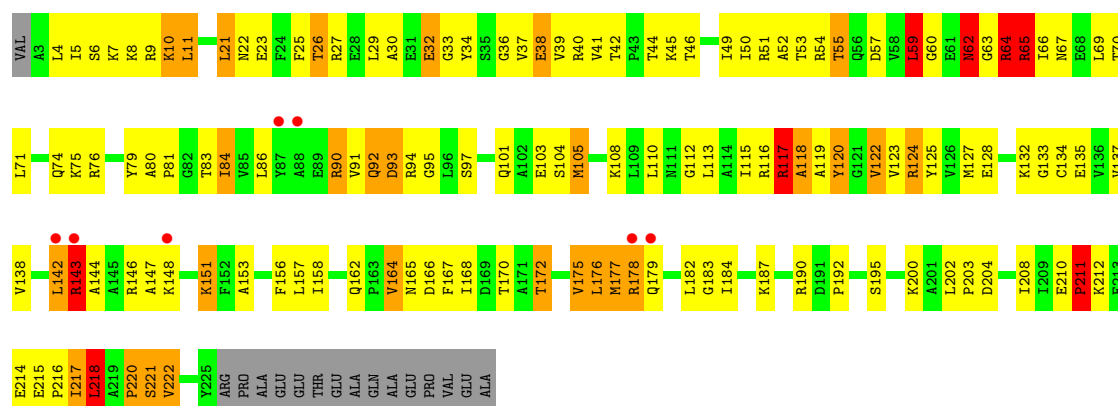
• Molecule 4: 40S ribosomal protein S2

Chain s2:



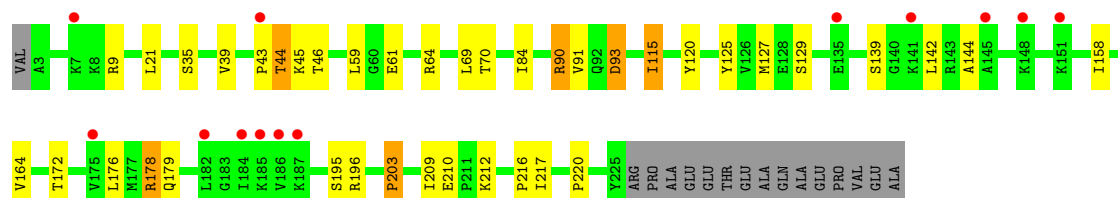
• Molecule 5: 40S ribosomal protein S3

Chain S3:



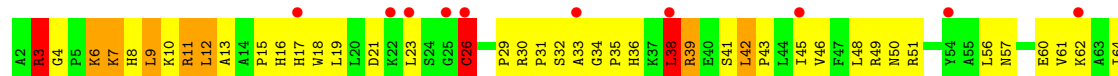
• Molecule 5: 40S ribosomal protein S3

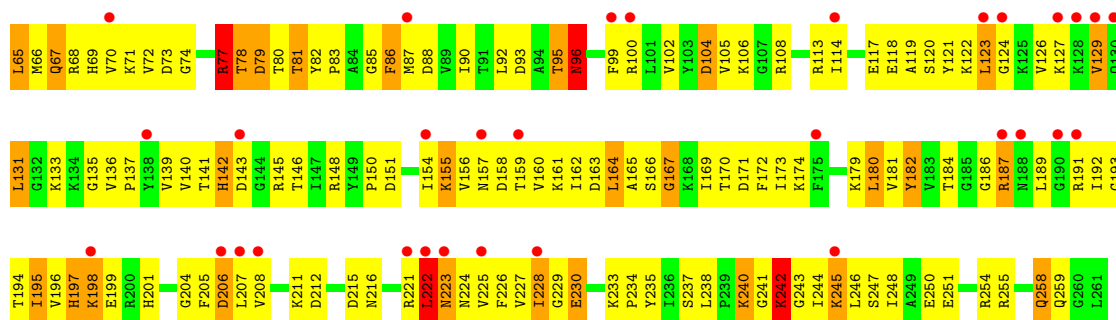
Chain s3:



• Molecule 6: 40S ribosomal protein S4-A

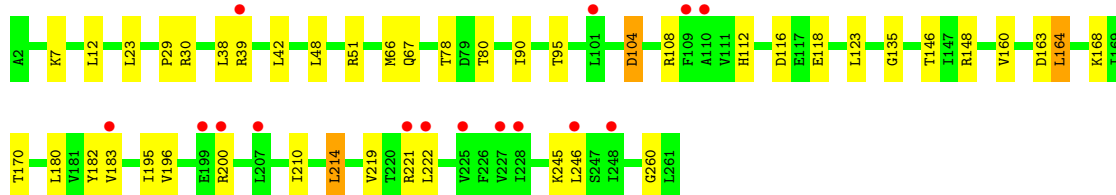
Chain S4:





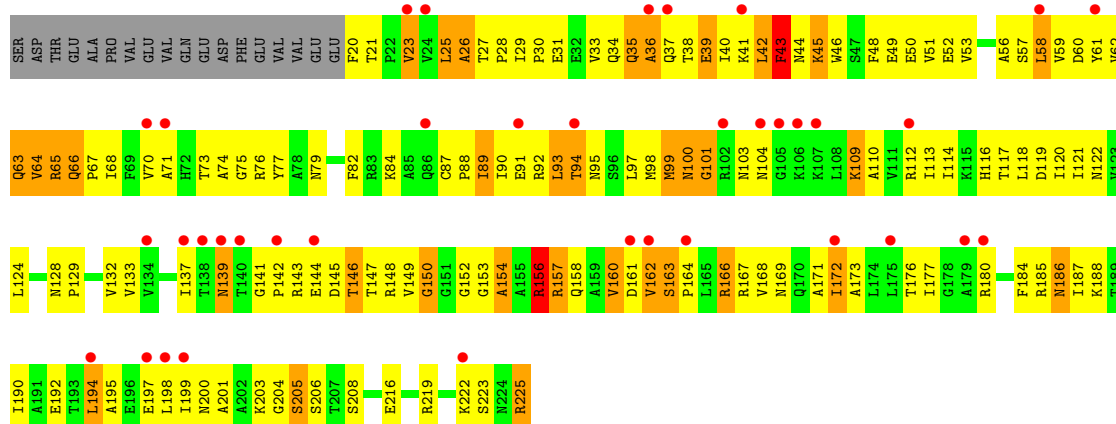
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



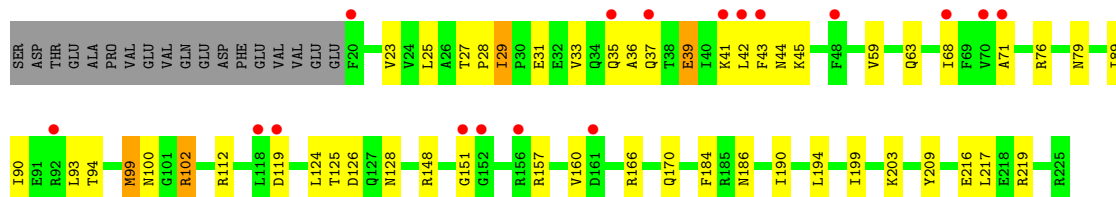
• Molecule 7: 40S ribosomal protein S5

Chain S5:



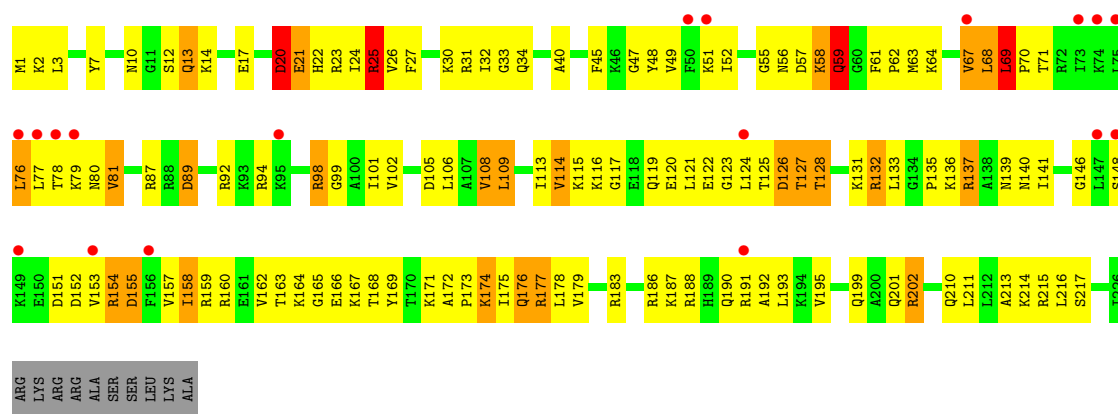
• Molecule 7: 40S ribosomal protein S5

Chain s5:



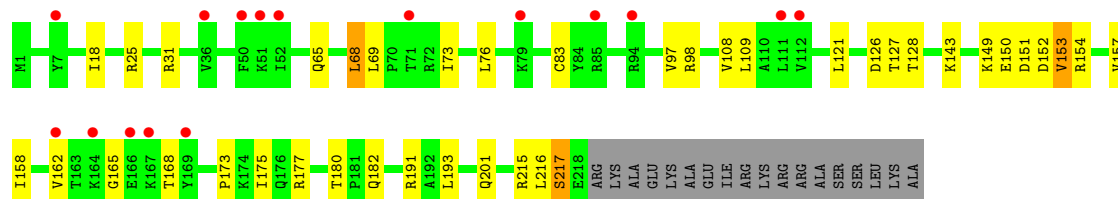
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



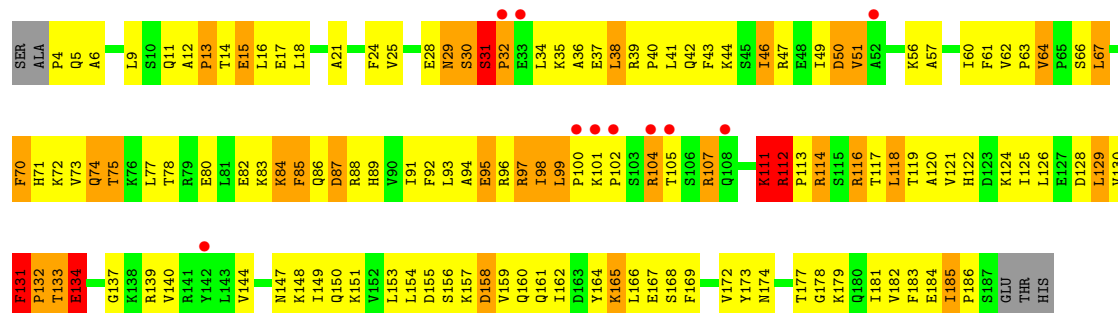
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



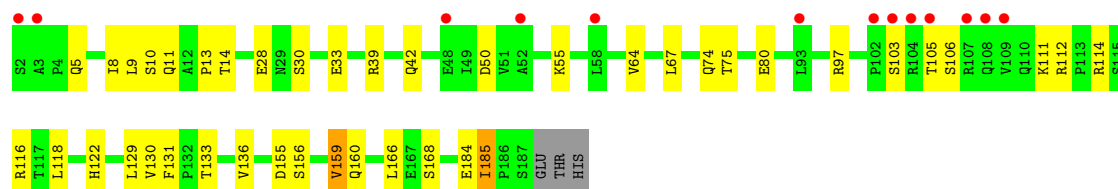
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



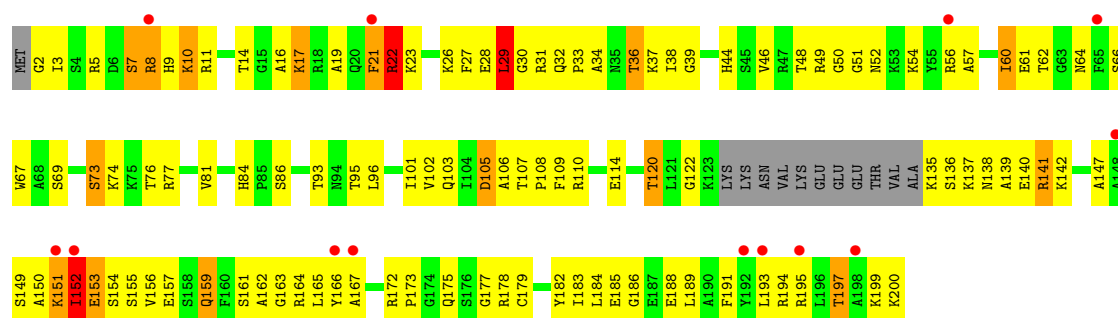
• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



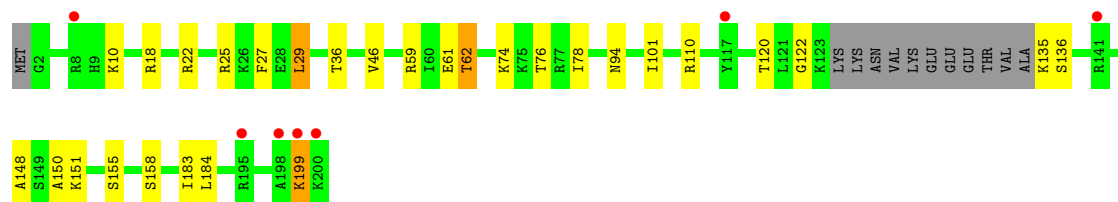
• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



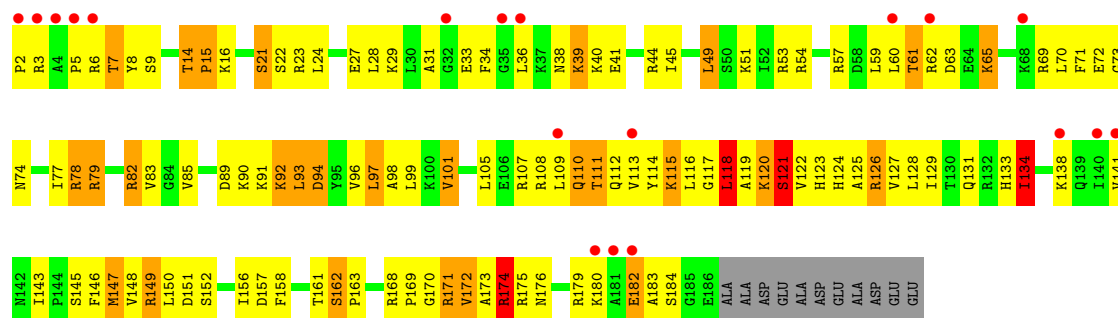
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



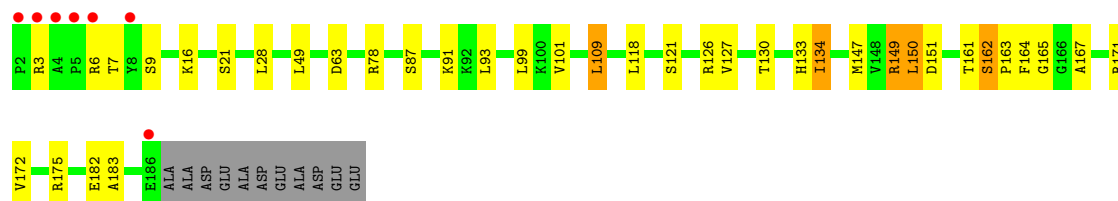
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



• Molecule 11: 40S ribosomal protein S9-A

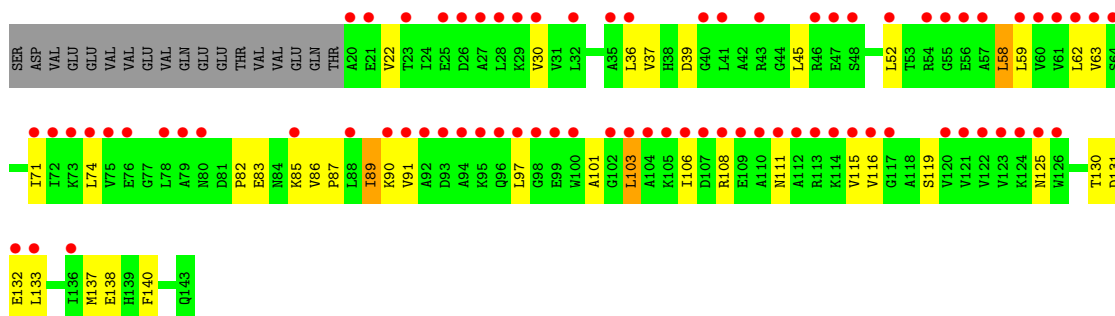
Chain s9:



• Molecule 12: 40S ribosomal protein S10-A

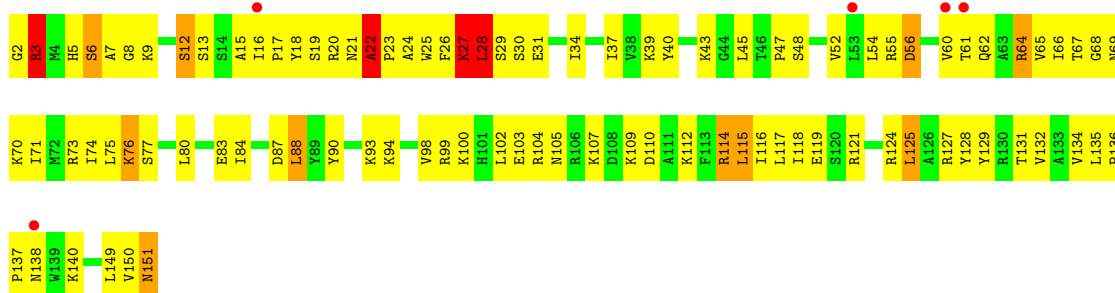
Chain C0:





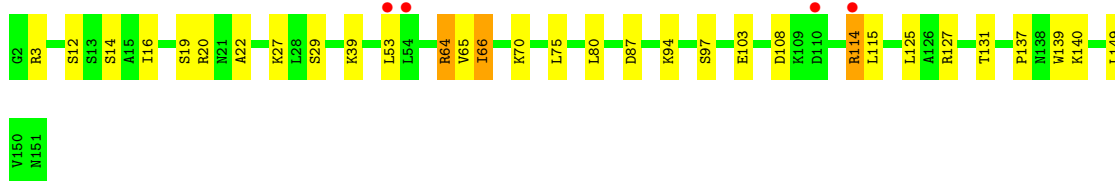
- Molecule 15: 40S ribosomal protein S13

Chain C3:



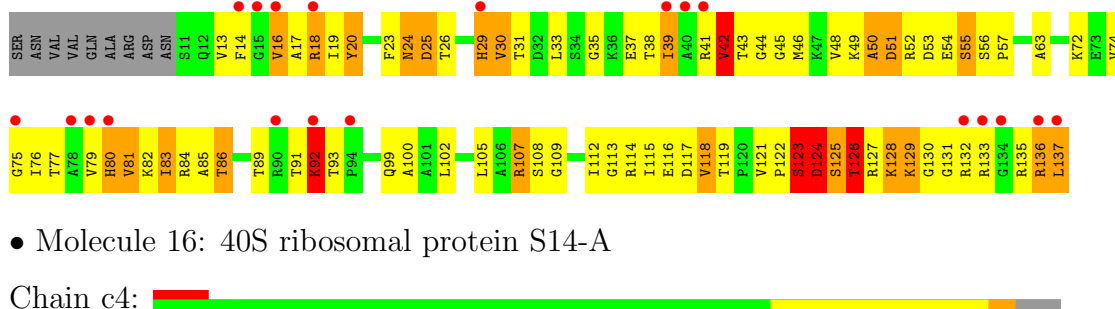
- Molecule 15: 40S ribosomal protein S13

Chain c3: 



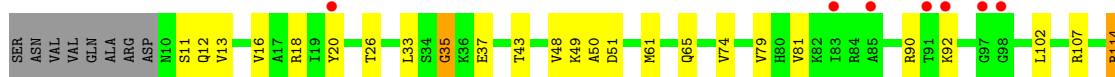
- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 



- Molecule 16: 40S ribosomal protein S14-A

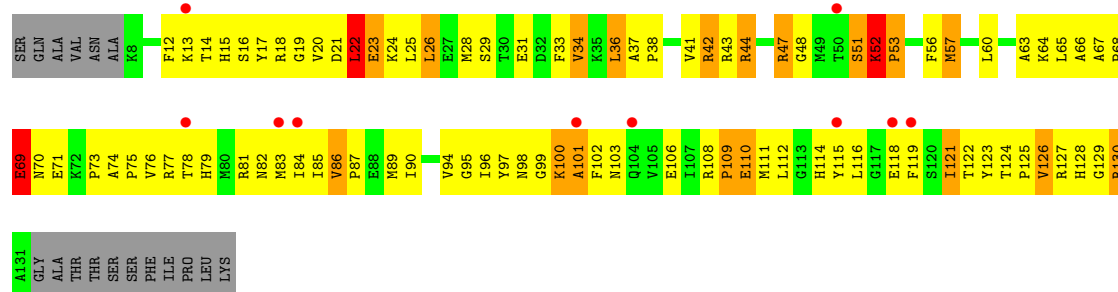
Chain c4:





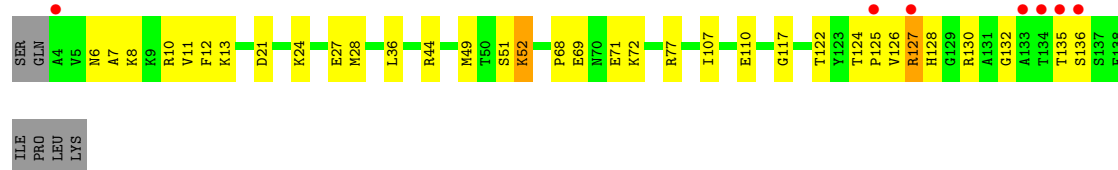
- Molecule 17: 40S ribosomal protein S15

Chain C5:



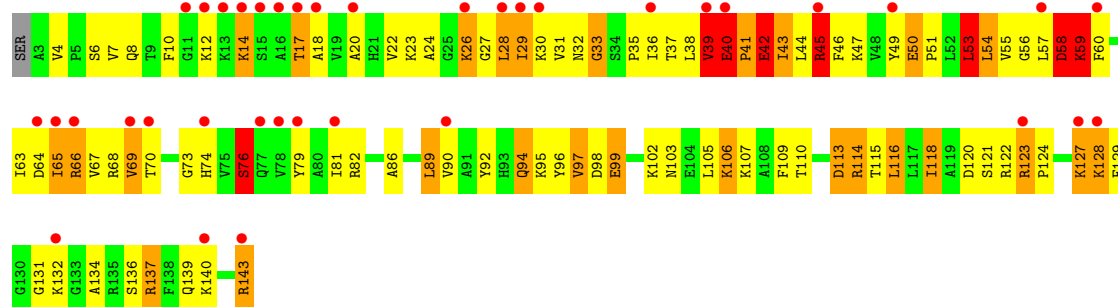
- Molecule 17: 40S ribosomal protein S15

Chain c5:



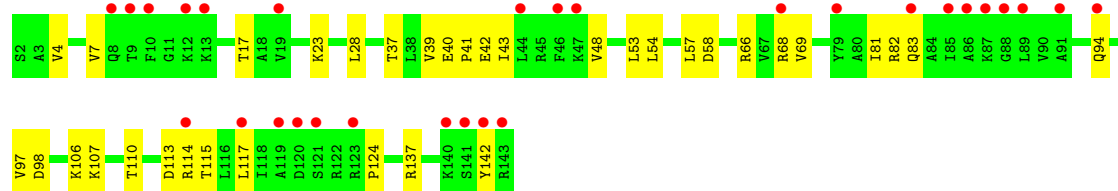
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:



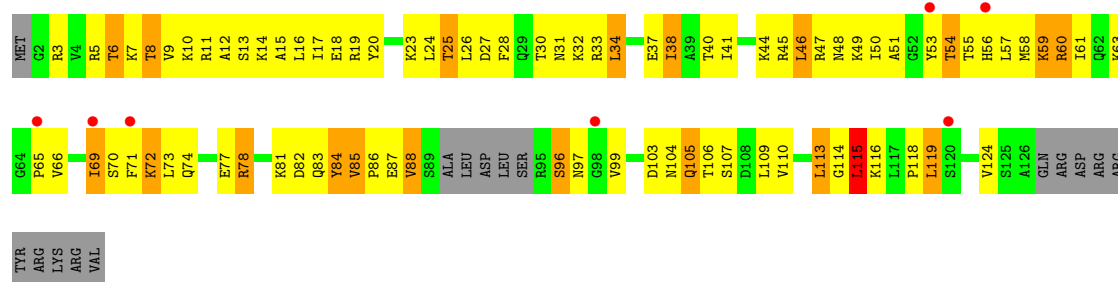
- Molecule 18: 40S ribosomal protein S16-A

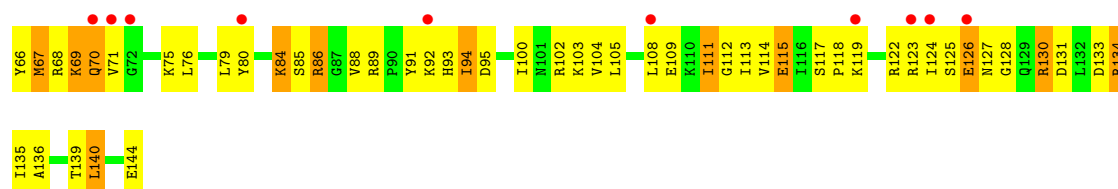
Chain c6:



- Molecule 19: 40S ribosomal protein S17-A

Chain C7:





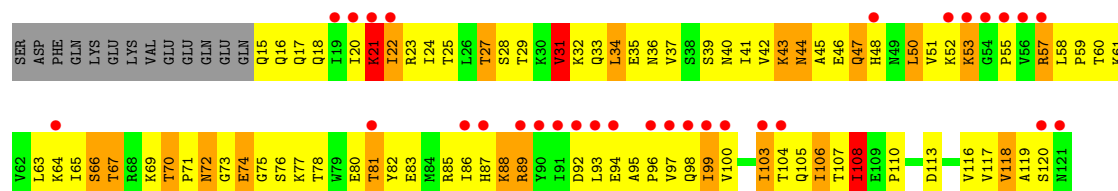
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



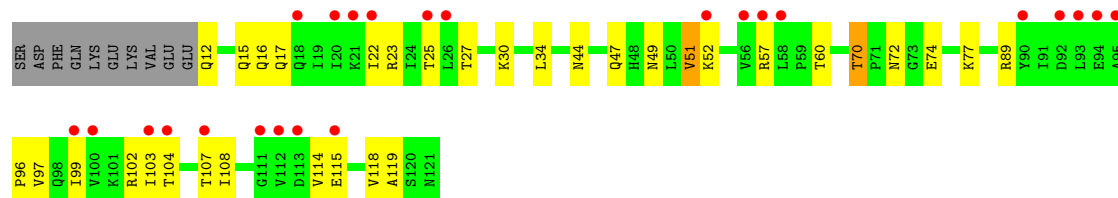
- Molecule 22: 40S ribosomal protein S20

Chain D0:



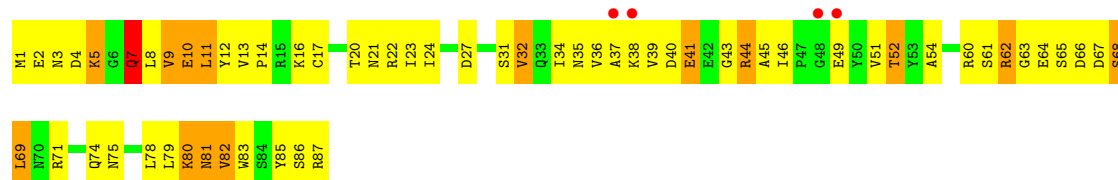
- Molecule 22: 40S ribosomal protein S20

Chain d0:



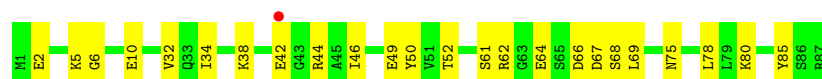
- Molecule 23: 40S ribosomal protein S21-A

Chain D1:



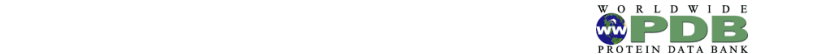
- Molecule 23: 40S ribosomal protein S21-A

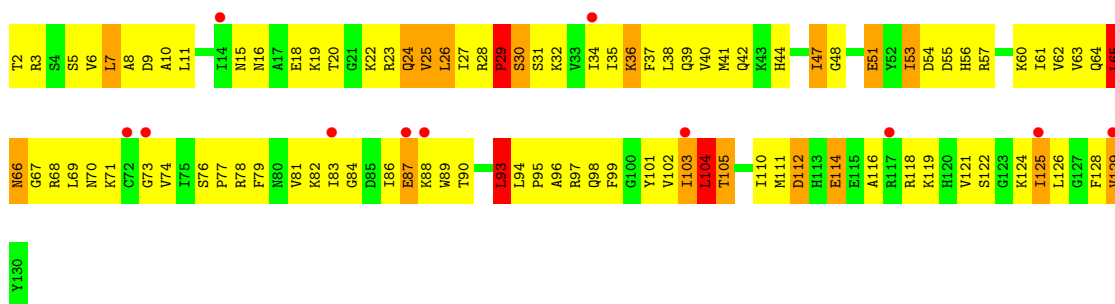
Chain d1:



- Molecule 24: 40S ribosomal protein S22-A

Chain D2:





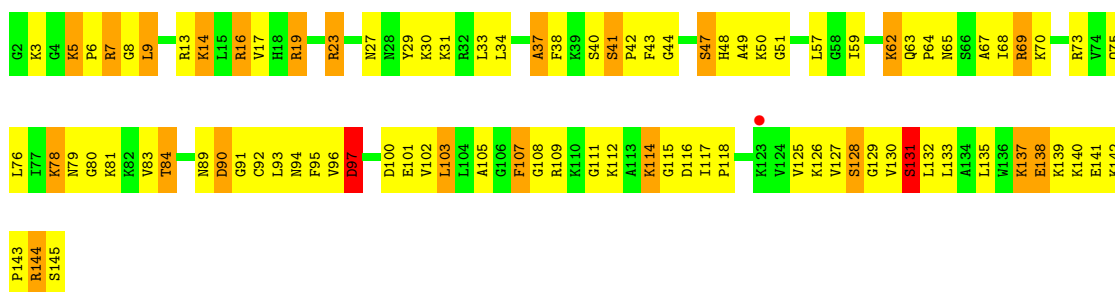
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:



- Molecule 25: 40S ribosomal protein S23-A

Chain D3:



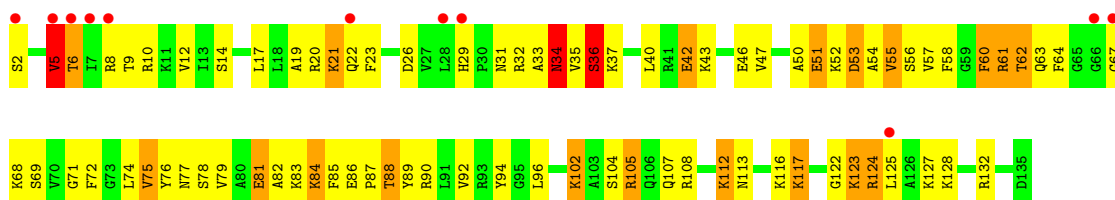
- Molecule 25: 40S ribosomal protein S23-A

Chain d3:



- Molecule 26: 40S ribosomal protein S24-A

Chain D4:



- Molecule 26: 40S ribosomal protein S24-A

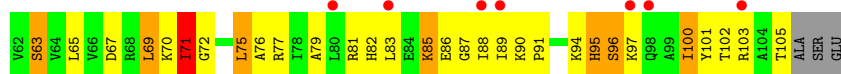
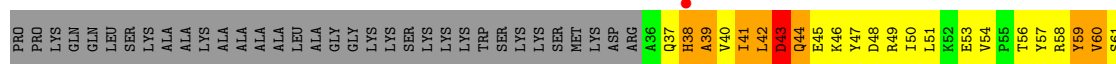
Chain d4:





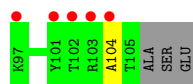
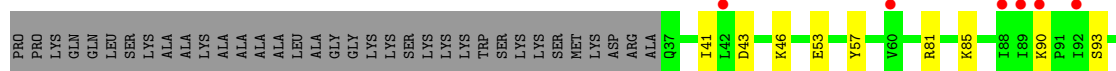
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:



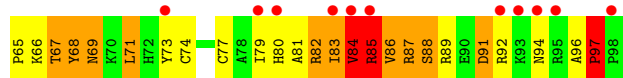
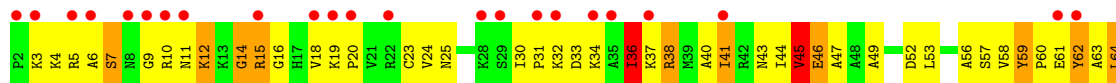
- Molecule 27: 40S ribosomal protein S25-A

Chain d5:



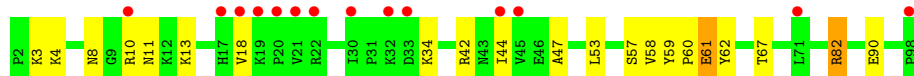
- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



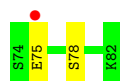
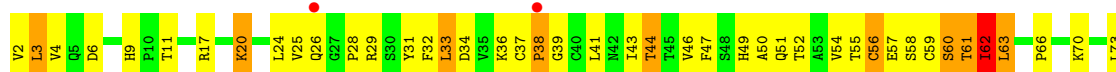
- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



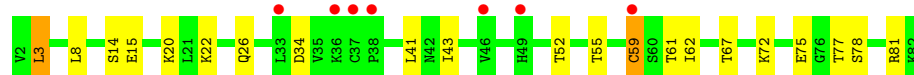
- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



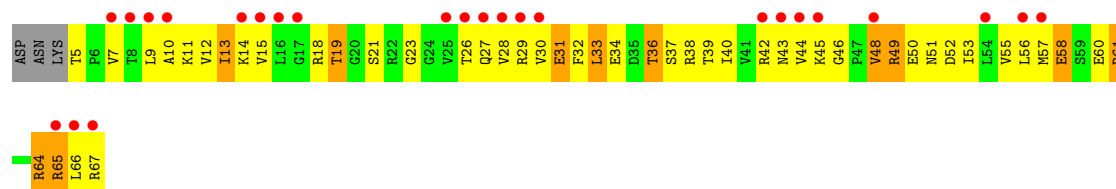
- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 



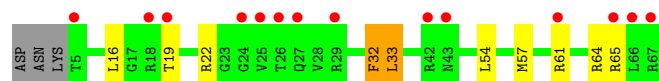
- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 



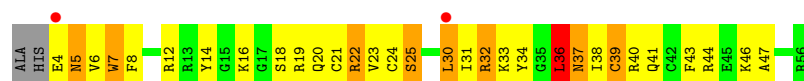
- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 



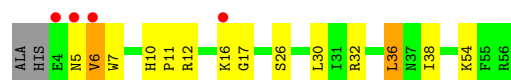
- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 



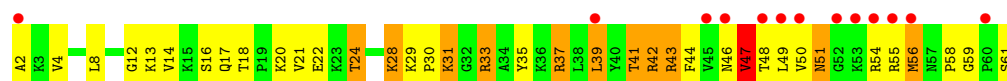
- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 



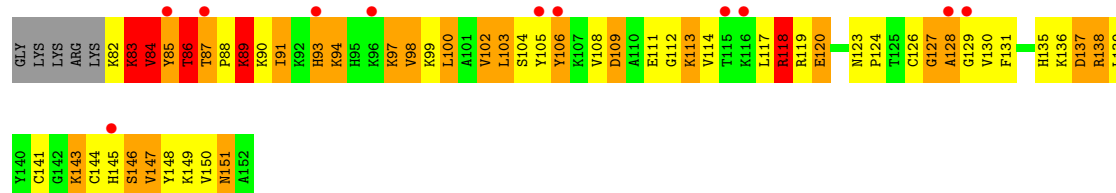
- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 



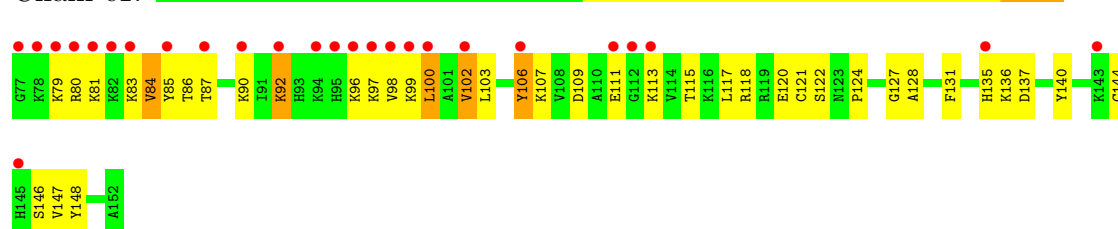
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 



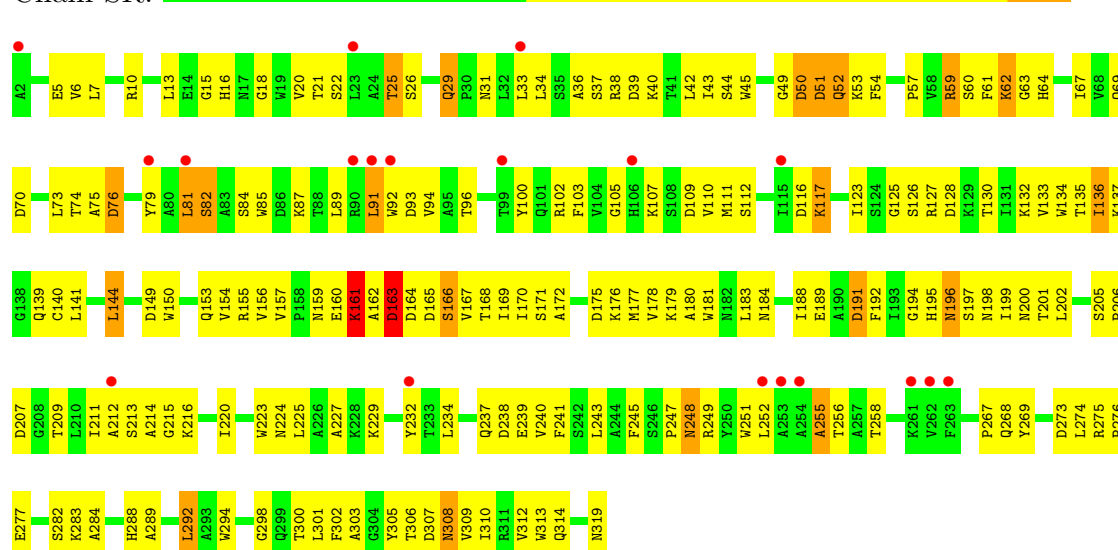
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:



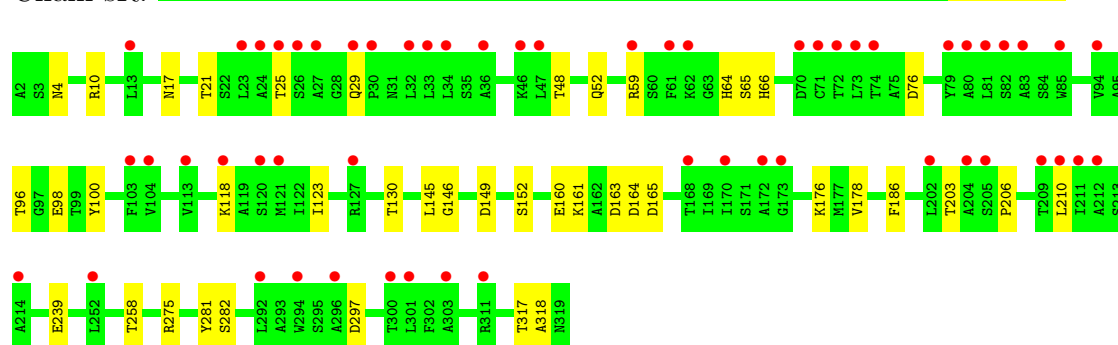
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



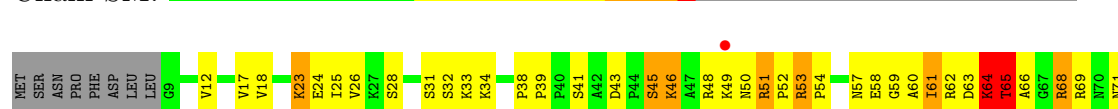
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

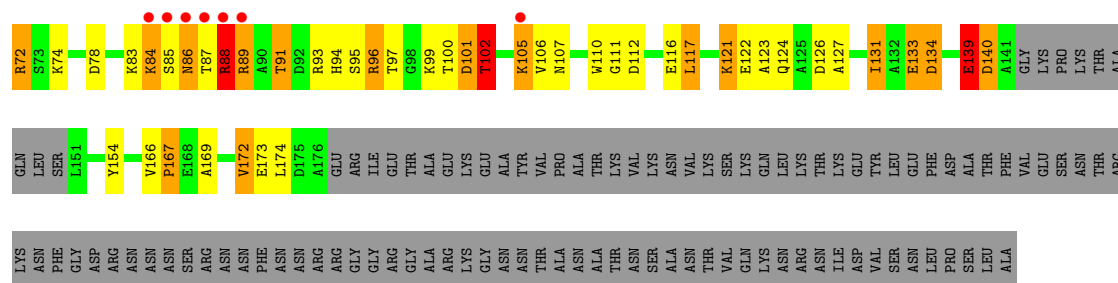
Chain sR:



- Molecule 35: Suppressor protein STM1

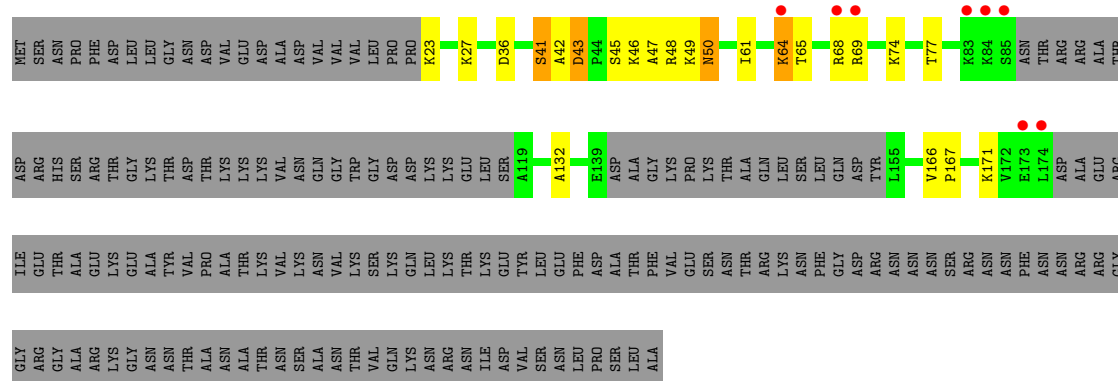
Chain SM:





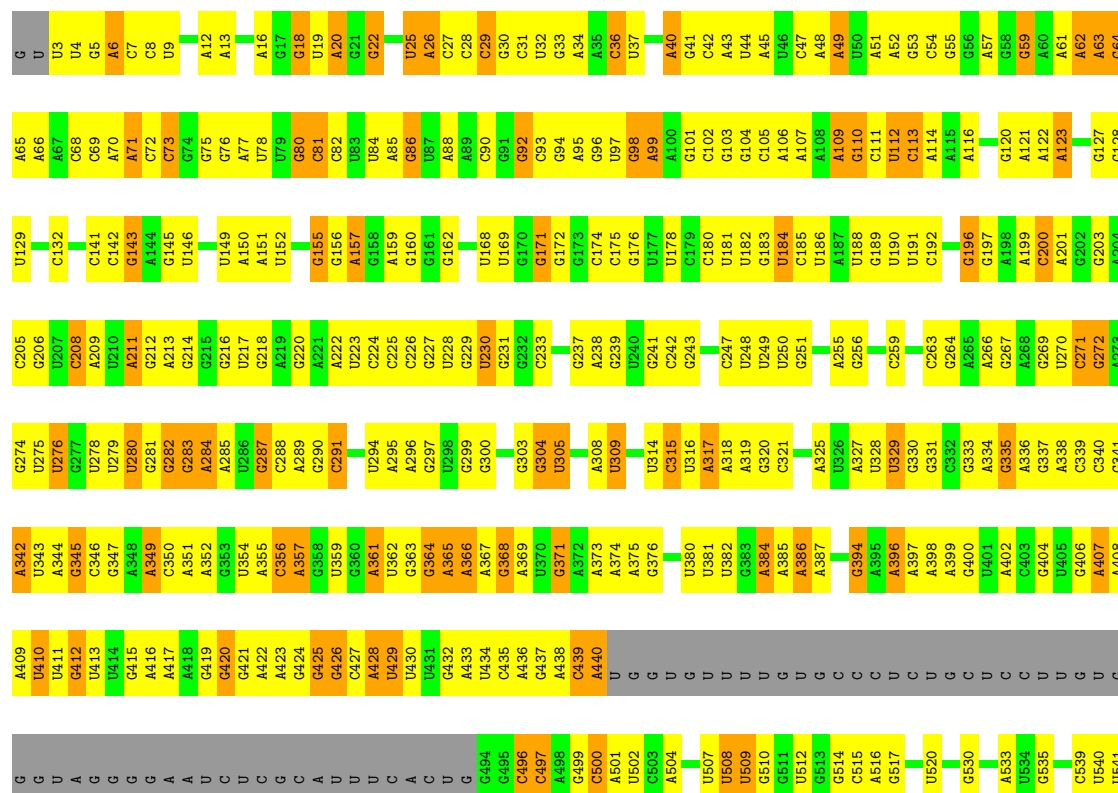
• Molecule 35: Suppressor protein STM1

Chain sM:



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

Chain 1:





U2541	C	A2413	U2282	A2352	A2142	U	G	A1895	U1819	U1740	G1653	G1577
U2544	A	G2414	G2283	G2353	A2143	C	C	A1896	U1820	A1741	A1654	C1578
C2545	G	C2415	C2284	C2354	A2144	G	U	G1897	U1821	U1742	G1655	C1579
G2546	U	U2416	C2285	G2355	A2145	C	A	G1898	G1822	G1743	A1656	A1580
A2547	G	G2417	U2286	U2356	C2146	U	G	G1899	A1823	G1744	C1657	C1581
C2548	A	U2418	C2287	G2357	A2147	U	G	A1900	G1829	G1747	G1658	C1582
U2549	A	C2419	A2291	C2358	U2148	G	C	A1901	G1830	G1748	A1583	A1584
G2550	A	C2420	U2292	A2220	A2149	C	C	G1902	G1831	G1749	C1660	U1585
U2551	U	U2421	C2293	A2223	A2150	U	G	G1903	U1832	A1752	G1661	U1586
C2552	A	C2422	U2294	A2224	G2151	C	A	C1904	G1833	G1759	G1662	A1587
U2553	C	U2423	A2295	U2225	A2152	C	U	G1905	G1834	C1760	G1668	A1588
A2554	C	A2424	A2296	U2226	U2153	A	U	G1906	U1835	A1760	C1669	A1589
U2555	A	U2425	U2297	C2227	G2154	U	A	C1907	G1836	C1761	U1671	G1592
U2556	C	U2426	U2298	A2228	G2155	U	C	A1908	U1837	C1762	C1670	G1593
U2557	U	A2427	U2299	A2229	G2156	A	U	A1910	G1838	U1763	U1672	U1594
U2558	A	U2428	C2300	A2230	U2157	C	U	G1911	U1839	U1764	U1673	U1595
C2559	C	C2431	G2301	A2232	G2160	A2093	C	A1912	U1840	U1765	G1674	C1596
U2560	U	A2432	A2302	A2233	G2161	C2094	G	G1913	U1841	G1766	G1675	C1597
A2561	C	U2433	C2303	G2234	U2162	G2095	U	G1914	A1842	G1769	A1676	G1598
U2562	U	U2434	C2304	A2242	C2163	U	C	A1915	U1843	G1770	U1680	U1599
U2563	U	G2435	G2305	A2243	G2164	A2099	C	U1916	G1844	C1771	U1681	U1600
U2564	U	U2436	C2306	A2244	G2165	A2100	C	G1917	G1845	U1777	U1682	A1603
U2565	C	U2437	G2307	A2245	A2166	C2101	U	C1918	C1846	G1778	G1687	G1604
U2566	A	A2443	A2308	C2246	A2167	U2102	C	G1919	A1847	C1779	U1688	A1605
U2567	C	C2444	U2310	G2247	A2168	U2103	G	U1920	C1848	G1780	U1689	U1606
U2568	U	U2445	G2311	G2248	U2169	A2104	U	A1921	U1849	C1781	U1690	C1607
U2569	A	U	U2314	G2249	U2170	A2105	C	G1922	G1851	U1782	C1608	C1609
U2570	C	G	U2315	A2252	A2171	A2106	U	U1923	U1852	U1783	G1700	G1610
U2571	A	A	A2317	C2252	U2175	C2108	A	G1924	U1853	G1784	G1611	G1612
U2572	C	C2445	U2318	G2253	U2176	G2111	C	U1925	C1854	G1785	C1614	C1615
C2573	U	U	U2319	U2254	U2177	U2112	U	G1926	U1855	G1786	G1701	U1620
C2574	C	G	A2320	A2255	G2178	U2113	C	G1927	U1856	A1787	U1702	A1621
C2575	U	G	C2321	C2256	A2179	A2113	G	G1928	C1857	G1788	U1703	U1622
C2576	C	U	C2322	C2257	G2179	G2116	C	U1929	A1858	G1789	A1715	G1623
C2577	A	U	C2323	U2258	C2180	A2117	U	A1930	G1790	G1790	U1716	U1630
C2578	C	A	C2324	A2259	C2181	A2118	C	G1931	G1791	U1797	U1717	C1631
C2579	U	G	G2325	U2260	A2182	C2119	U	A1932	C1792	A1800	G1718	G1634
C2580	C	U	A2326	C2261	A2183	C2120	C	G1933	G1793	U1720	G1719	U1635
C2581	A	A	C2331	C2262	G2187	A2121	G	A1934	G1794	U1721	U1721	U1636
C2582	C	C2400	C2332	U2263	U2188	G2122	U	G1935	U1795	C1802	U1722	A1637
C2583	U	A2401	C2333	C2264	U2189	A2123	C	U1936	G1796	C1803	A1723	A1638
C2584	G	G	U2334	C2265	U2190	G2124	U	U1937	A1797	C1804	U1724	C1639
C2585	C	U	C2337	U2266	U2191	A2125	C	U1938	G1872	C1805	C1725	C1640
C2586	A	U	C2338	C2267	C2192	G2126	G	G1939	U1877	A1806	C1726	U1641
C2587	C	G	C2339	U2268	U2193	A2127	U	C1940	G1878	G1801	U1732	A1642
C2588	U	C	U2340	A2270	G2194	U2128	C	U1941	A1879	C1802	G1733	G1646
C2589	C	A	C2343	C2271	C2195	U2129	U	U1942	U1880	C1803	U1738	G1650
C2590	C	U	U2344	G2272	G2196	G2130	G	C1943	A1881	A1723	U1739	
C2591	C	C	A2345	C2273	C2197	A2131	U	G1947	G1882	C1805		
C2592	U	U	C2346	U2274	A2198	G2134	C	G1948	A1883	A1806		
C2593	A	U	U2347	C2275	A2199	U2135	U	U1949	A1884	G1807		
C2594	C	C	A2348	G2276	G2205	G2135	A	U1950	U1885	A1729		
C2595	U	U	A2349	C2277	U2206	A2138	C	G1951	A1886	A1809		
C2596	C	C	U2350	U2278	A2207	A2139	C	U1952	A1887	U1732		
C2597	C	U	C2351	C2279	U2208	A2141	U	G1953	G1892	G1733		
C2598	C	C	U2352	A2280	A2209	U2140	C	U1954	A1893	C1738		
C2599	C	C	U2353	A2281	G2210	U2141	G	U1955	U1894	U1818		
C2600	C	C	U2354					A				
C2601	C	C	U2355									
C2602	C	C	U2356									
C2603	C	C	U2357									
C2604	C	C	U2358									
C2605	C	C	U2359									
C2606	C	C	U2360									
C2607	C	C	U2361									
C2608	C	C	U2362									
C2609	C	C	U2363									
C2610	C	C	U2364									
C2611	C	C	U2365									
C2612	C	C	U2366									
C2613	C	C	U2367									
C2614	C	C	U2368									
C2615	C	C	U2369									
C2616	C	C	U2370									
C2617	C	C	U2371									
C2618	C	C	U2372									
C2619	C	C	U2373									



G1212	G1213	G1216	G1217	A1221	G1222	G1230	G1231	G1232	G1233	G1234	U1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	U1258	A1259	G1260	G1261	G1264	A1270	A1271	C1277	A1278	C1279	G1284	G1285	G1289	A1290	A1291	C1292	G1293	A1294	G1296	C1296	G1297	U1298																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G1149	A1150	G1151	G1152	A1153	G1154	C1155	C1156	G1157	A1158	A1159	C1160	G1161	G1164	U1167	U1168	A1169	G1170	G1171	G1174	G1175	C1176	G1177	G1178	A1179	A1180	U1181	A1182	C1183	A1184	C1185	G1186	C1187	U1188	A1189	A1190	U1191	C1192	A1193	G1194	A1195	C1196	C1197	C1198	C1199	A1200	C1201	A1202	A1203	A1204	A1205	G1206	G1207	U1208	G1209	U1210	U1211																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G1087	U1088	G1089	C1092	A1093	U1094	C1095	U1096	G1097	A1098	A1099	U1100	G1101	A1102	A1103	G1104	C1107	U1108	U1109	U1110	U1111	A1112	G1113	U1114	G1115	A1116	G1117	G1118	C1119	A1120	U1121	U1122	U1123	U1124	U1125	G1126	U1127	U1128	A1129	A1130	G1131	G1132	A1133	A1134	A1135	U1136	C1137	C1201	A1202	A1203	A1204	A1205	G1206	G1207	U1208	G1209	U1210	U1211																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G1013	U1014	U1015	C1016	G1017	G1018	G1019	G1020	G1021	U1022	G1023	G1024	A1025	A1026	A1027	U1028	A1029	U1030	G1031	C1032	A1033	U1034	A1040	C1045	A1046	A1047	U1048	C1049	U1050	U1051	A1052	A1053	A1054	A1055	U1056	G1059	U1060	A1061	A1064	A1065	G1066	U1070	U1071	G1072	U1073	U1074	A1075	U1076	A1077	A1080	U1081	U1082	G1083																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
C949	G950	A951	A952	G953	U954	U955	U956	C957	C958	C959	U960	G961	A962	G963	U966	A967	G968	C969	A970	G971	A972	G974	G975	U976	C977	G978	U979	A980	U981	C982	A983	G984	U985	U986	U987	U988	A989	G991	A992	G993	G994	U995	A996	A997	U998	G999	C1000	U1001	A1002	A1003	U1004	U1008	A1011	G1012																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
A888	U889	C890	G891	U892	G893	G894	A895	A896	U897	G898	U899	G900	U903	A904	U905	A906	G907	G908	G909	G910	C911	G912	A913	A914	A915	U916	U917	G918	C919	U920	C923	G924	A925	A926	C927	C928	A929	U930	C931	U932	A933	G934	U935	A936	G937	C938	U939	G940	G941	U942	U943	G944	C945	U946	U947	C948																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C823	C824	U825	G826	A827	A828	U829	A830	G831	G832	G833	U834	G835	A836	A837	U838	C839	C840	A841	G845	A846	A847	A848	C849	U850	A851	U852	G853	G854	U855	G856	G857	G860	C861	U862	C863	G864	C868	G869	C870	U871	U872	C873	U874	G875	U876	C877	G878	U879	G880	C881	A882	A883	A884	U885	C886	G887																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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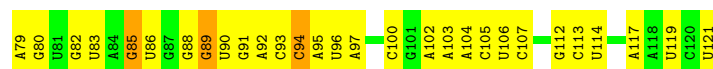
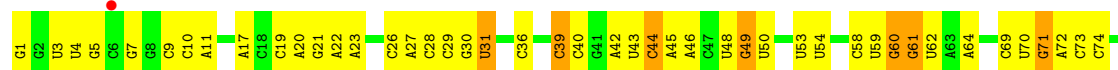


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A3210	C2346	U2541	C2615	U2752	U2818	C2881	G2947	G3077	A3078	G3143	G3210	A3210
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U3340	U2467	U2601	C2675	U2816	U2878	A2946	U3009	U3078	U3144	U3212	G3280	U3340
A3341	U2468	U2602	U2676	U2817	U2879	A2947	U3010	U3079	U3145	U3213	G3281	A3341
C3342	U2469	U2603	C2677	U2818	U2880	A2948	U3011	U3080	U3146	U3214	G3282	C3342
U3343	U2470	U2604	U2678	U2819	U2881	A2949	U3012	U3081	U3147	U3215	G3283	U3343
A3344	U2471	U2605	C2679	U2820	U2882	A2950	U3013	U3082	U3148	U3216	G3284	A3344
C3345	U2472	U2606	U2680	U2821	U2883	A2951	U3014	U3083	U3149	U3217	G3285	C3345
U3346	U2473	U2607	U2681	U2822	U2884	A2952	U3015	U3084	U3150	U3218	G3286	U3346
A3347	U2474	U2608	C2682	U2823	U2885	A2953	U3016	U3085	U3151	U3219	G3287	A3347
C3348	U2475	U2609	U2683	U2824	U2886	A2954	U3017	U3086	U3152	U3220	G3288	C3348
U3349	U2476	U2610	C2684	U2825	U2887	A2955	U3018	U3087	U3153	U3221	G3289	U3349
A3350	U2477	U2611	U2685	U2826	U2888	A2956	U3019	U3088	U3154	U3222	G3290	A3350
C3351	U2478	U2612	C2686	U2827	U2889	A2957	U3020	U3089	U3155	U3223	G3291	C3351
U3352	U2479	U2613	U2687	U2828	U2890	A2958	U3021	U3090	U3156	U3224	G3292	U3352
A3353	U2480	U2614	C2688	U2829	U2891	A2959	U3022	U3091	U3157	U3225	G3293	A3353
C3354	U2481	U2615	U2689	U2830	U2892	A2960	U3023	U3092	U3158	U3226	G3294	C3354
U3355	U2482	U2616	C2690	U2831	U2893	A2961	U3024	U3093	U3159	U3227	G3295	U3355
A3356	U2483	U2617	U2691	U2832	U2894	A2962	U3025	U3094	U3160	U3228	G3296	A3356
C3357	U2484	U2618	C2692	U2833	U2895	A2963	U3026	U3095	U3161	U3229	G3297	C3357
U3358	U2485	U2619	U2692	U2834	U2896	A2964	U3027	U3096	U3162	U3230	G3298	U3358
A3359	U2486	U2620	C2693	U2835	U2897	A2965	U3028	U3097	U3163	U3231	G3299	A3359
C3360	U2487	U2621	U2693	U2836	U2898	A2966	U3029	U3098	U3164	U3232	G3300	C3360
U3361	U2488	U2622	C2694	U2837	U2899	A2967	U3030	U3099	U3165	U3233	G3301	U3361
A3362	U2489	U2623	U2694	U2838	U2900	A2968	U3031	U3100	U3166	U3234	G3302	A3362
C3363	U2490	U2624	C2695	U2839	U2901	A2969	U3032	U3101	U3167	U3235	G3303	C3363
U3364	U2491	U2625	U2696	U2840	U2902	A2970	U3033	U3102	U3168	U3236	G3304	U3364
A3365	U2492	U2626	C2697	U2841	U2903	A2971	U3034	U3103	U3169	U3237	G3305	A3365
C3366	U2493	U2627	U2698	U2842	U2904	A2972	U3035	U3104	U3170	U3238	G3306	C3366
U3367	U2494	U2628	C2699	U2843	U2905	A2973	U3036	U3105	U3171	U3239	G3307	U3367
A3368	U2495	U2629	U2700	U2844	U2906	A2974	U3037	U3106	U3172	U3240	G3308	A3368
C3369	U2496	U2630	C2701	U2845	U2907	A2975	U3038	U3107	U3173	U3241	G3309	C3369
U3370	U2497	U2631	U2702	U2846	U2908	A2976	U3039	U3108	U3174	U3242	G3310	U3370
A3371	U2498	U2632	C2703	U2847	U2909	A2977	U3040	U3109	U3175	U3243	G3311	A3371
C3372	U2499	U2633	U2704	U2848	U2910	A2978	U3041	U3110	U3176	U3244	G3312	C3372
U3373	U2500	U2634	C2705	U2849	U2911	A2979	U3042	U3111				



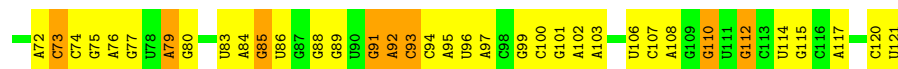
- Molecule 37: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 3:



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

Chain 7:



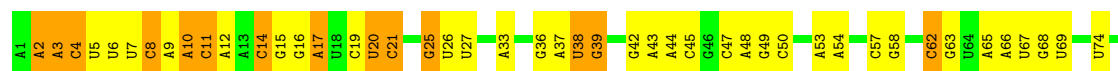
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 4:



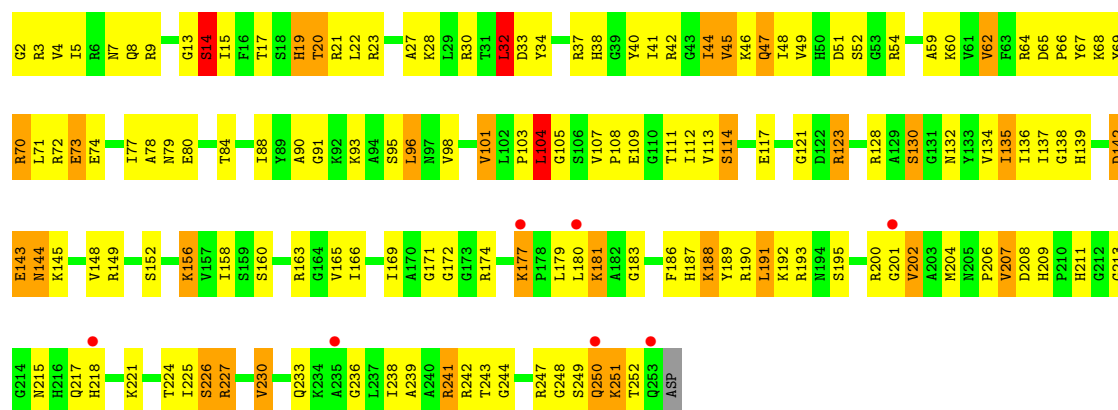
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 8:



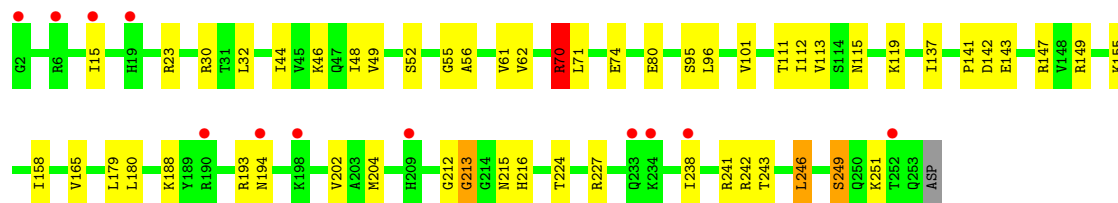
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



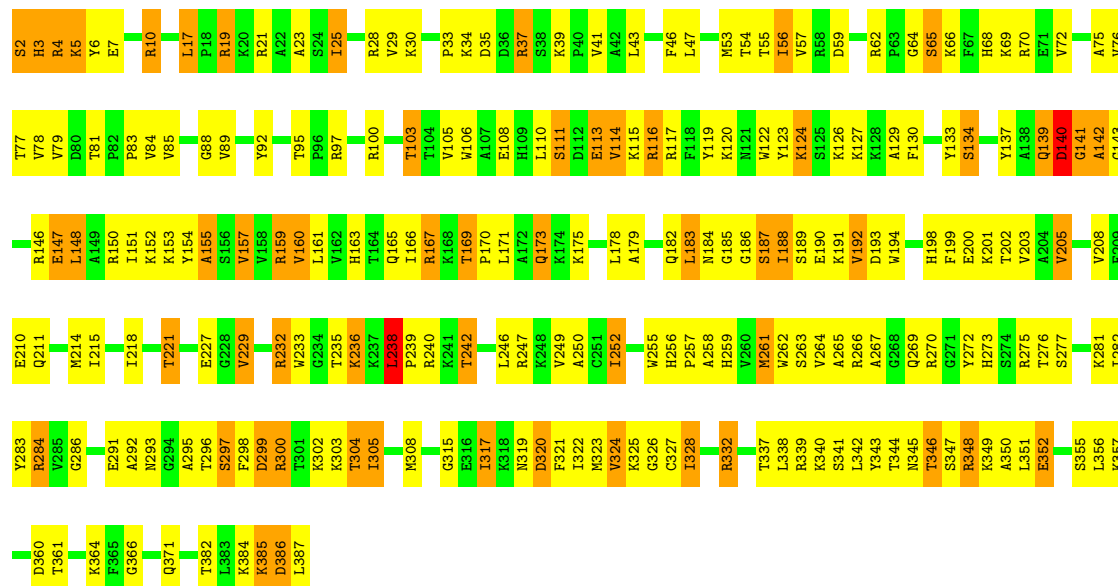
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:



• Molecule 40: 60S ribosomal protein L3

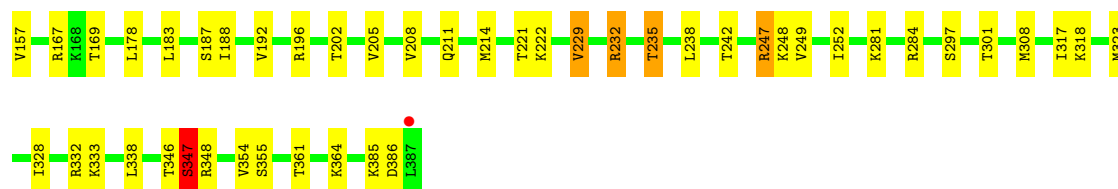
Chain l3:



• Molecule 40: 60S ribosomal protein L3

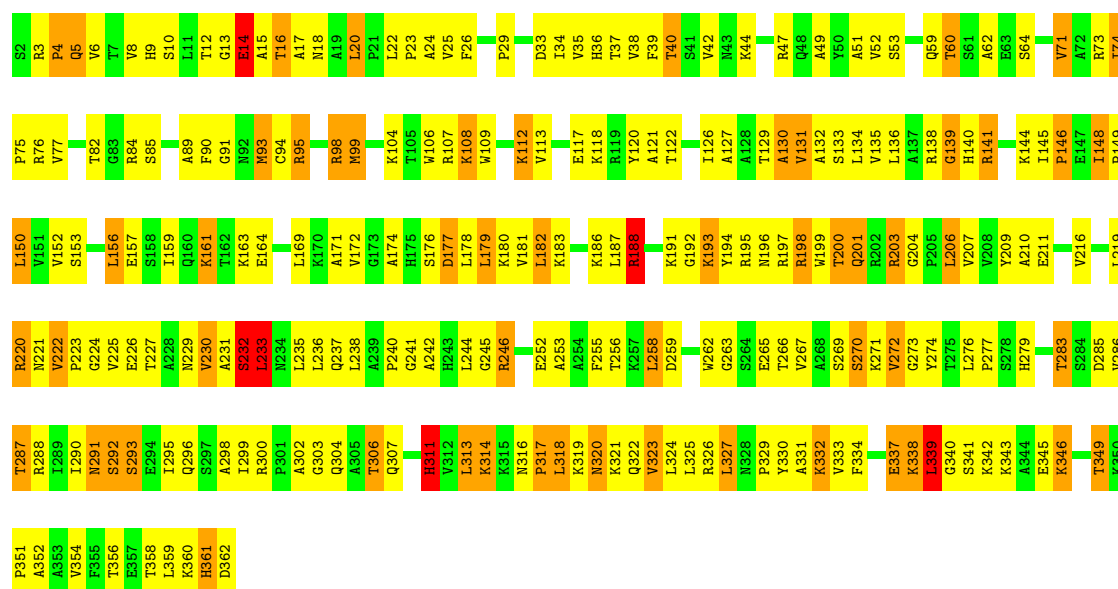
Chain l3:





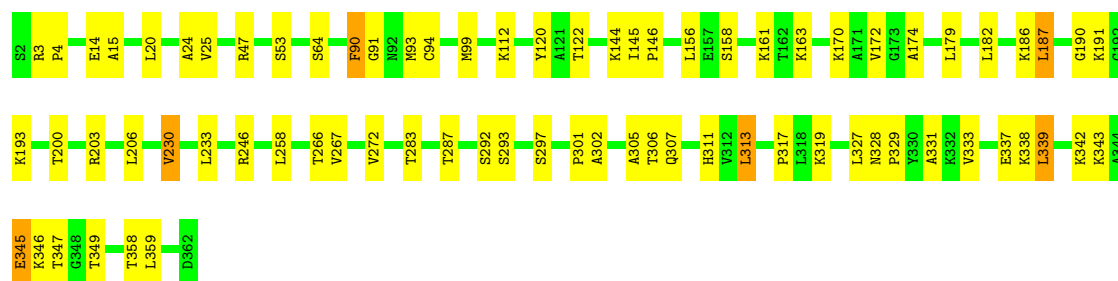
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



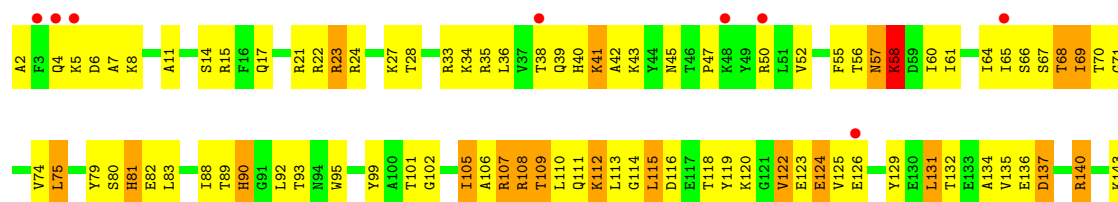
• Molecule 41: 60S ribosomal protein L4-A

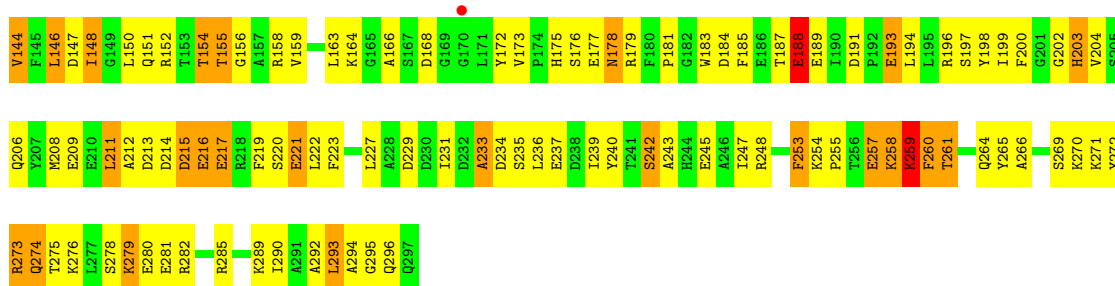
Chain l4:



• Molecule 42: 60S ribosomal protein L5

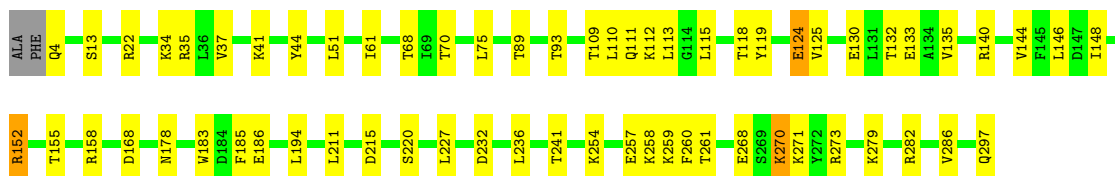
Chain L5:





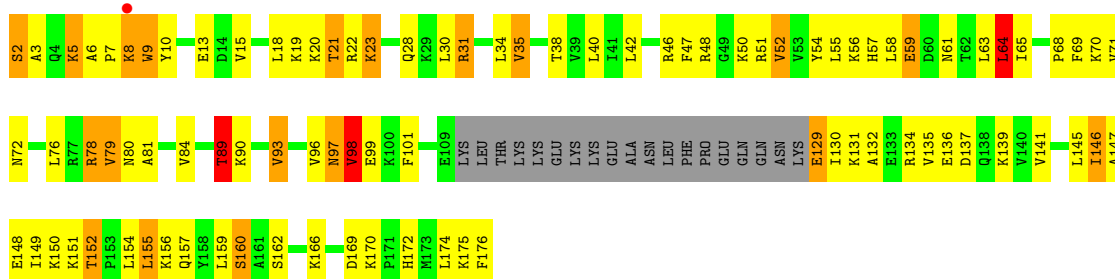
• Molecule 42: 60S ribosomal protein L5

Chain l5:



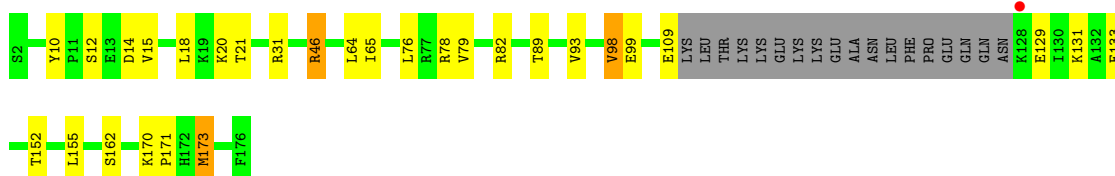
• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



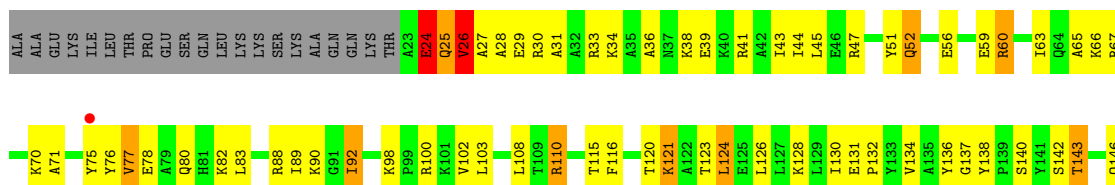
• Molecule 43: 60S ribosomal protein L6-A

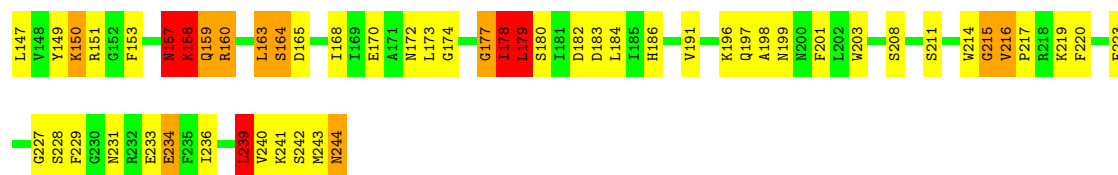
Chain l6:



• Molecule 44: 60S ribosomal protein L7-A

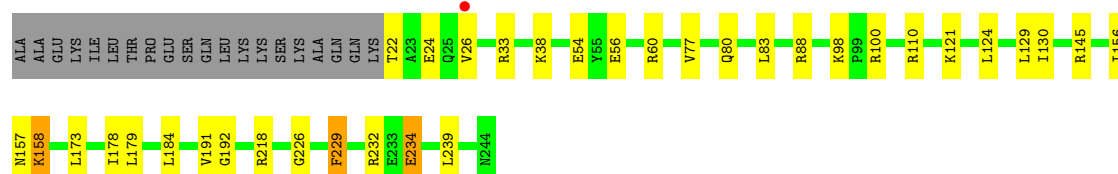
Chain L7:





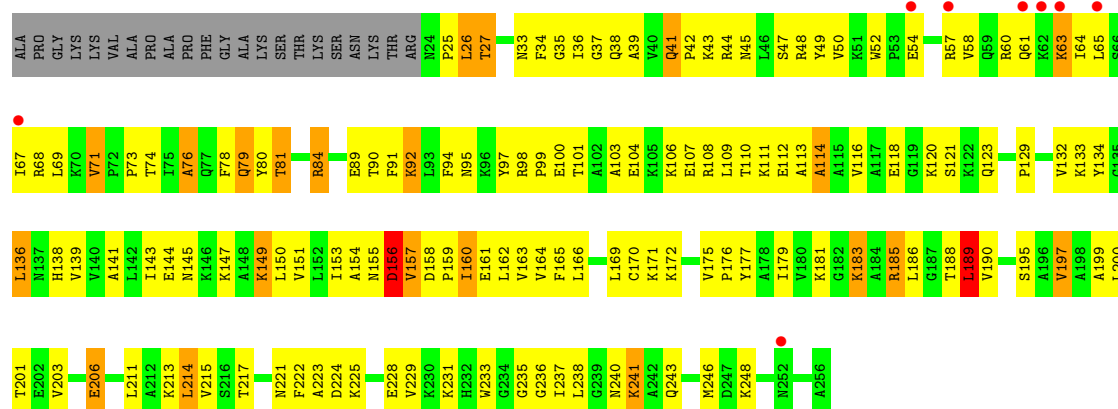
- Molecule 44: 60S ribosomal protein L7-A

Chain L7:



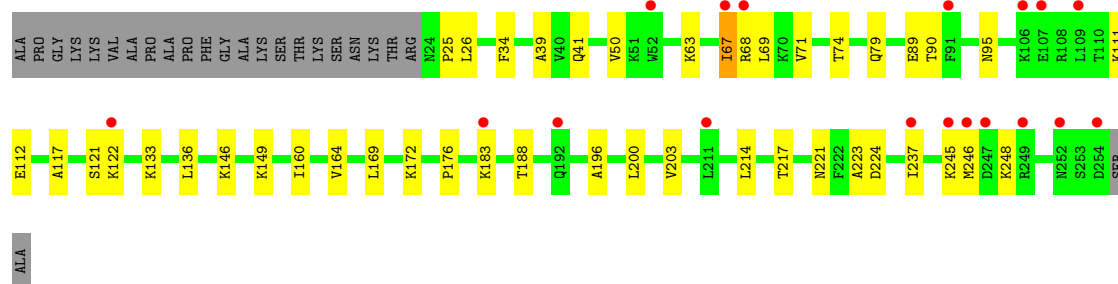
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:



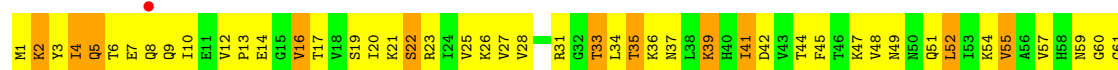
- Molecule 45: 60S ribosomal protein L8-A

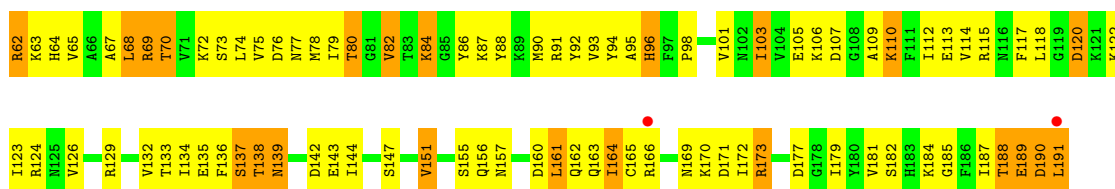
Chain l8:



- Molecule 46: 60S ribosomal protein L9-A

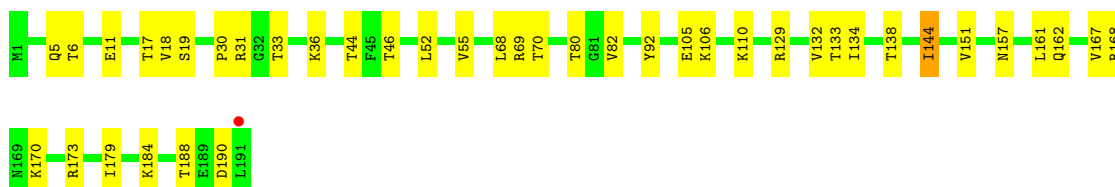
Chain L9:





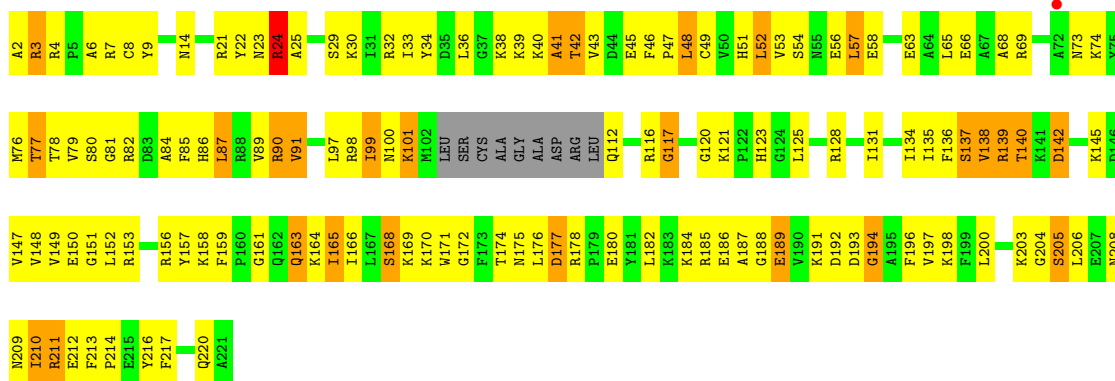
- Molecule 46: 60S ribosomal protein L9-A

Chain I9:



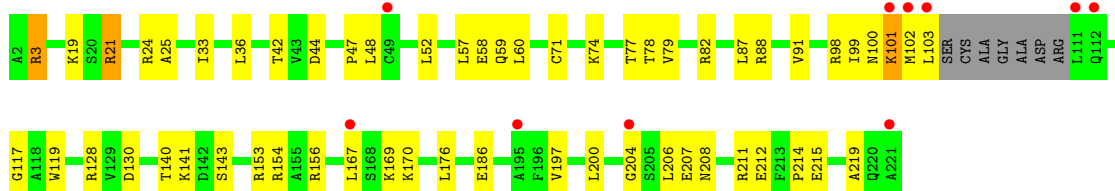
- Molecule 47: 60S ribosomal protein L10

Chain M0:



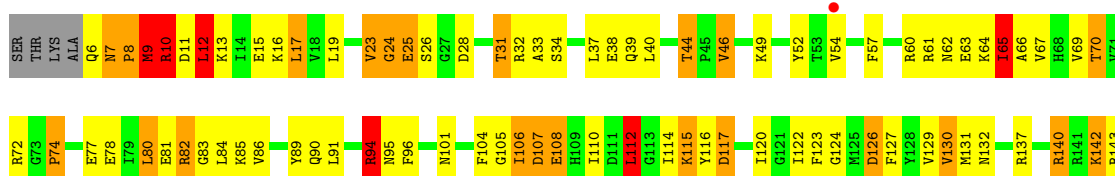
- Molecule 47: 60S ribosomal protein L10

Chain m0:



- Molecule 48: 60S ribosomal protein L11-B

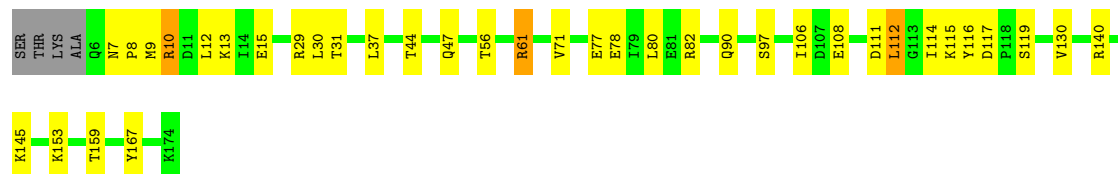
Chain M1:





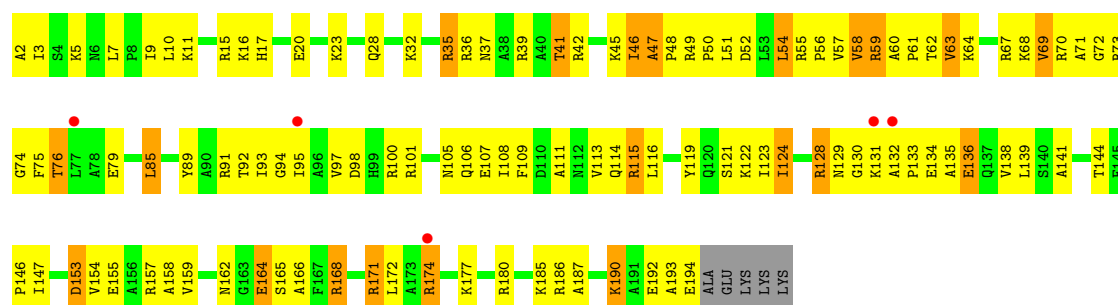
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



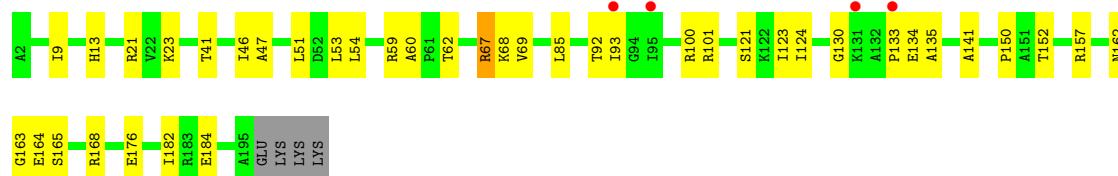
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



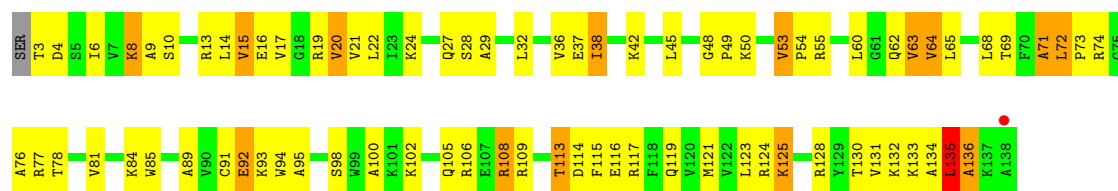
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



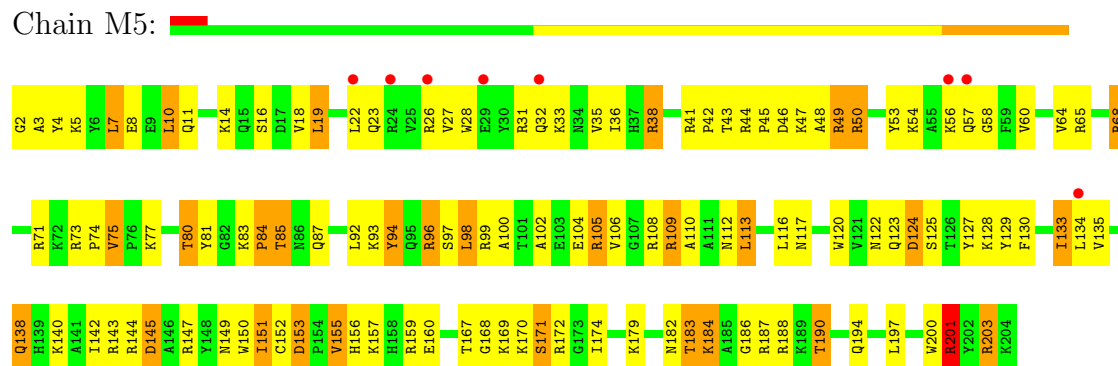
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



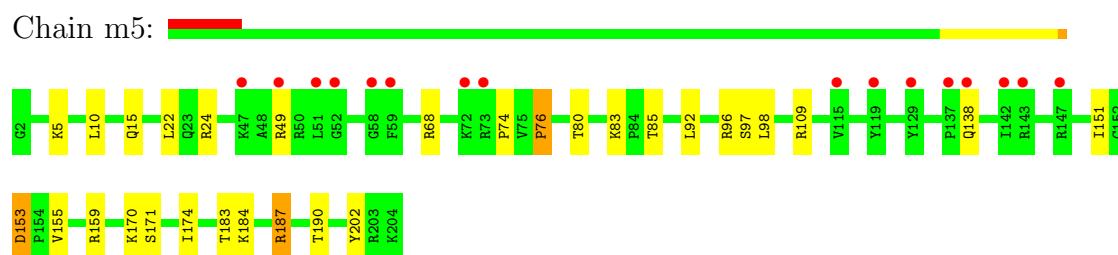
- Molecule 51: 60S ribosomal protein L15-A

Chain M5:



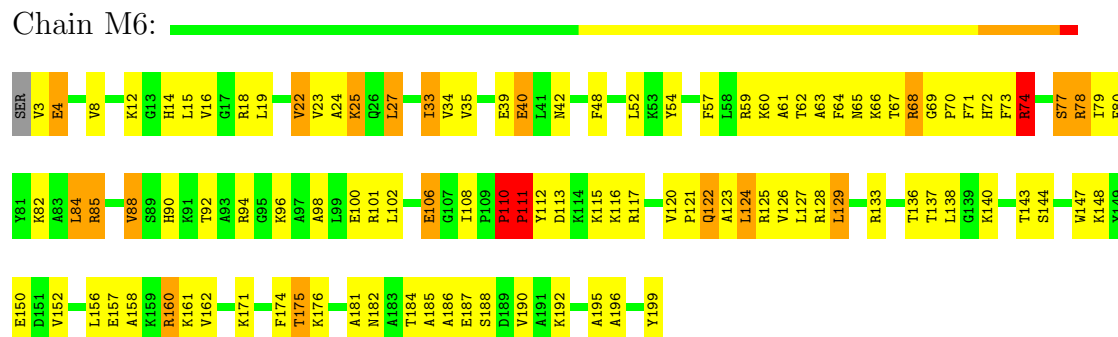
- Molecule 51: 60S ribosomal protein L15-A

Chain m5:



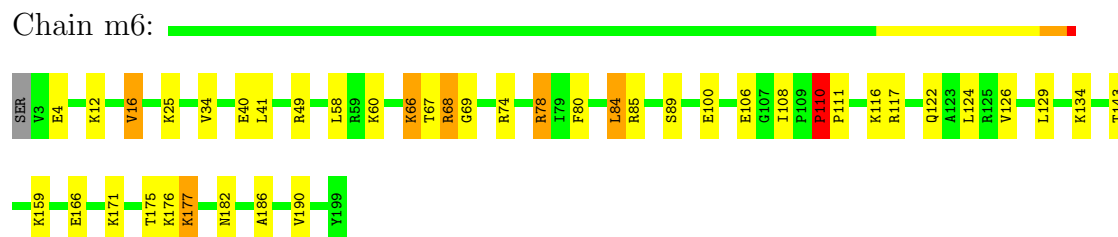
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:



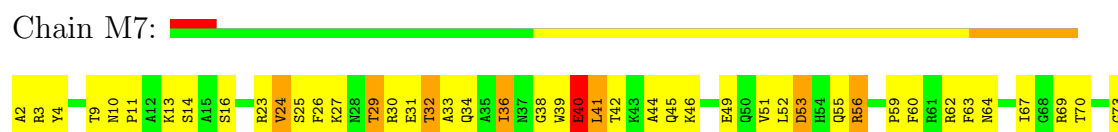
- Molecule 52: 60S ribosomal protein L16-A

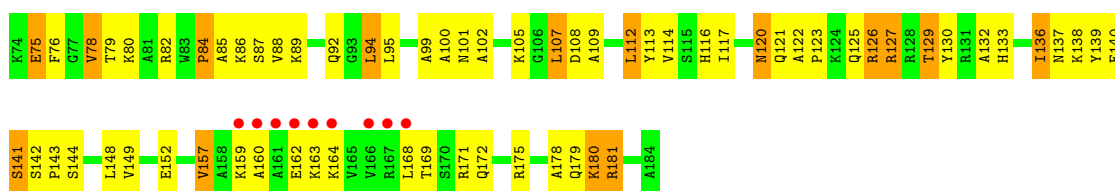
Chain m6:



- Molecule 53: 60S ribosomal protein L17-A

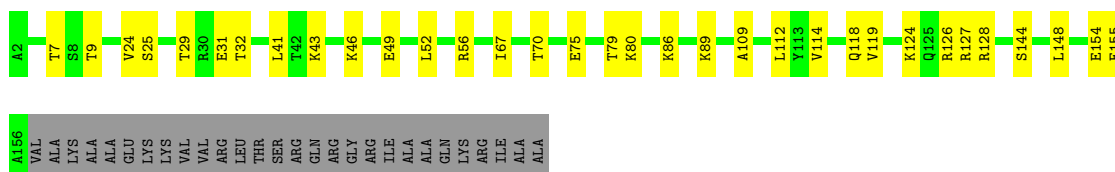
Chain M7:





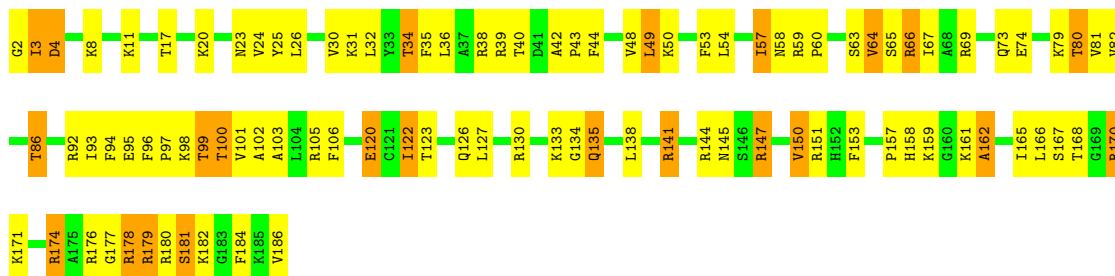
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:



- Molecule 54: 60S ribosomal protein L18-A

Chain M8:



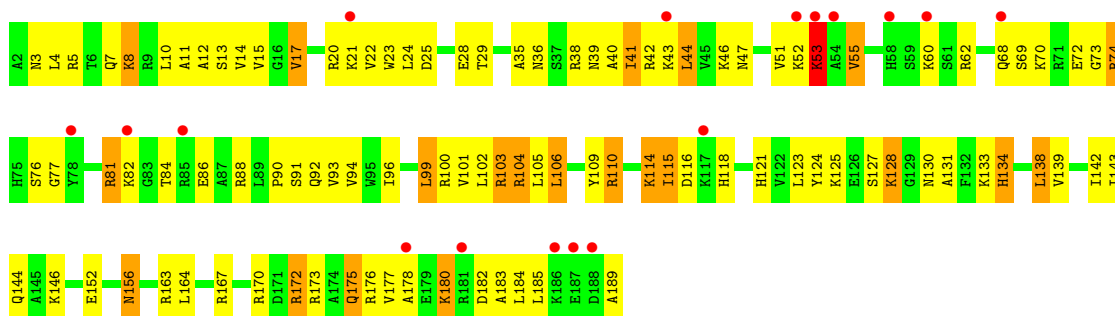
- Molecule 54: 60S ribosomal protein L18-A

Chain m8:



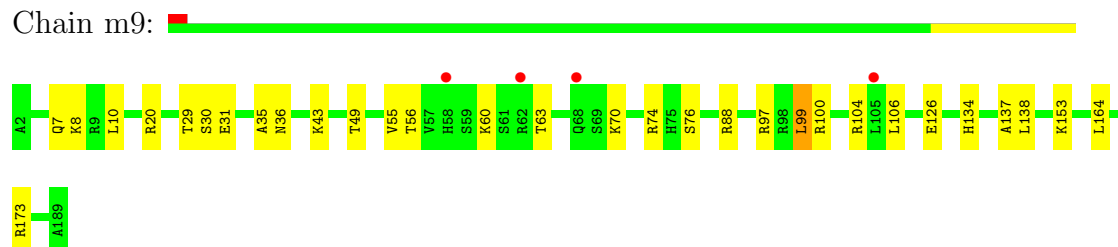
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:



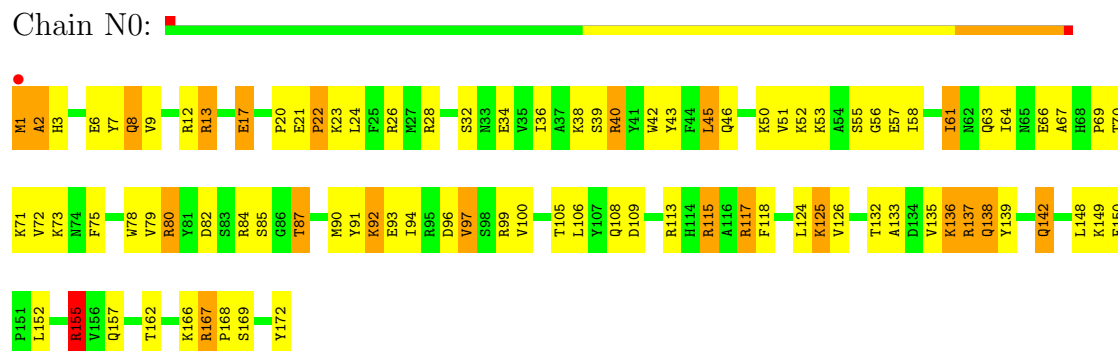
- Molecule 55: 60S ribosomal protein L19-A

Chain m9:



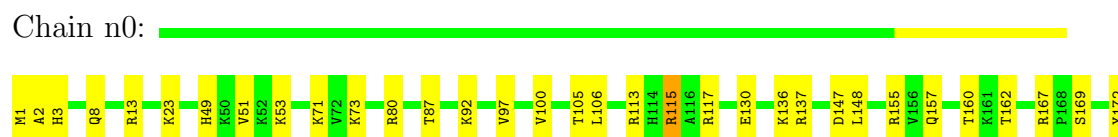
- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



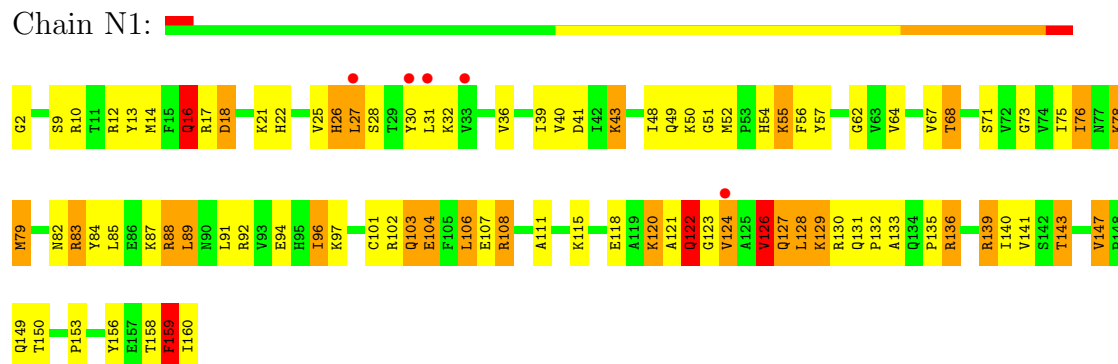
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:



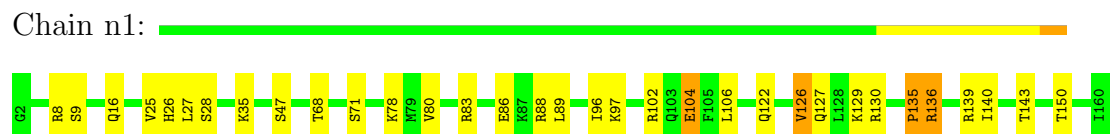
- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



- Molecule 57: 60S ribosomal protein L21-A

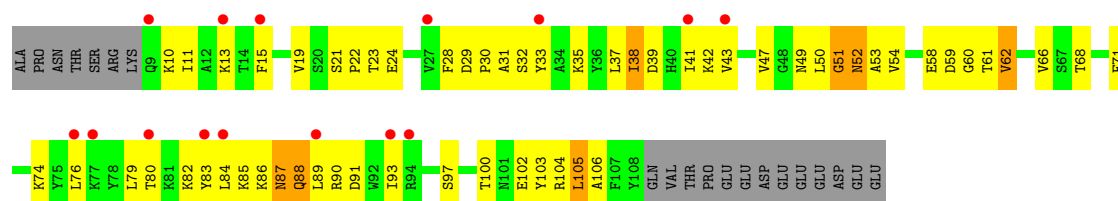
Chain n1:



- Molecule 58: 60S ribosomal protein L22-A

Chain N2:





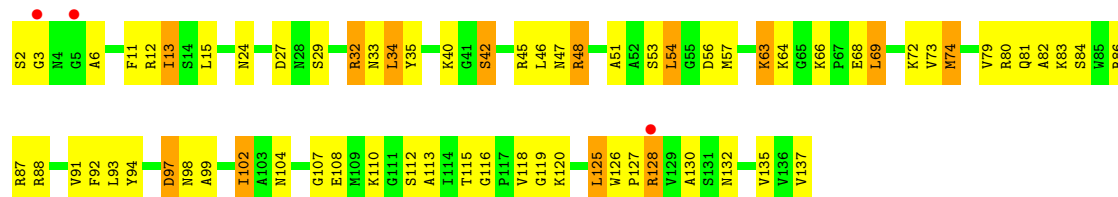
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



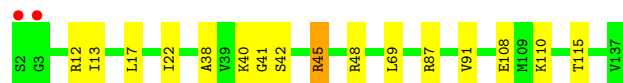
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



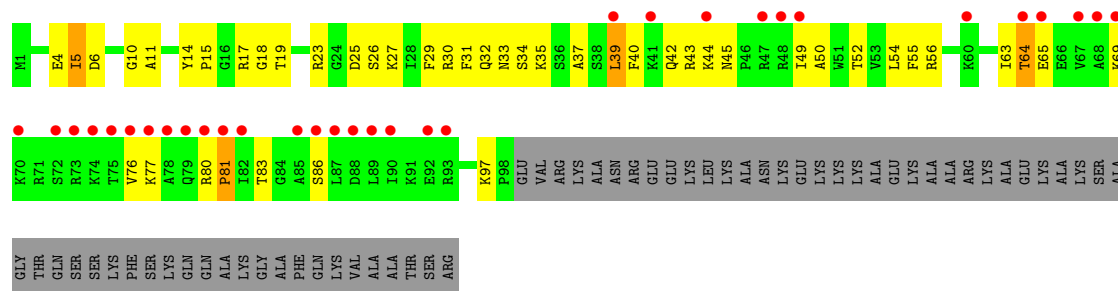
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



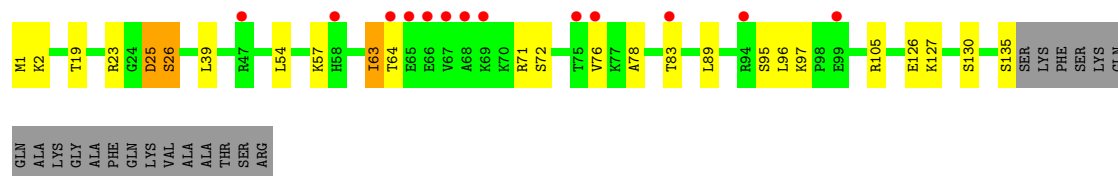
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



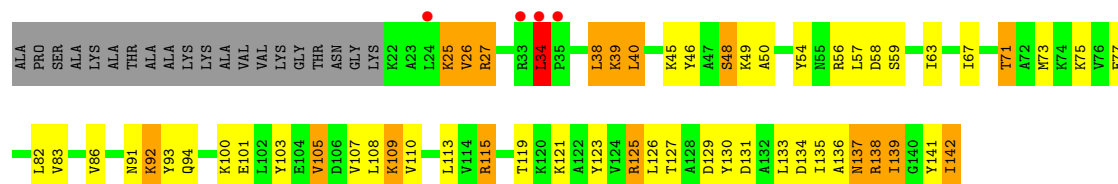
• Molecule 60: 60S ribosomal protein L24-A

Chain n4:



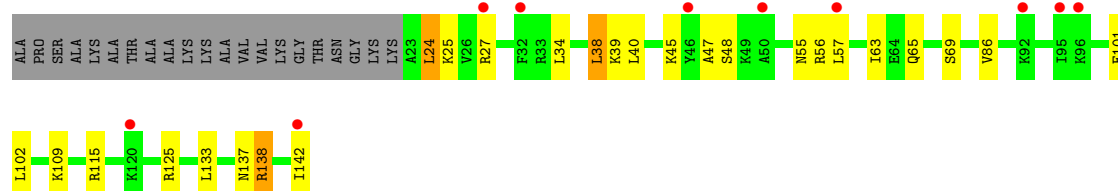
- Molecule 61: 60S ribosomal protein L25

Chain N5:



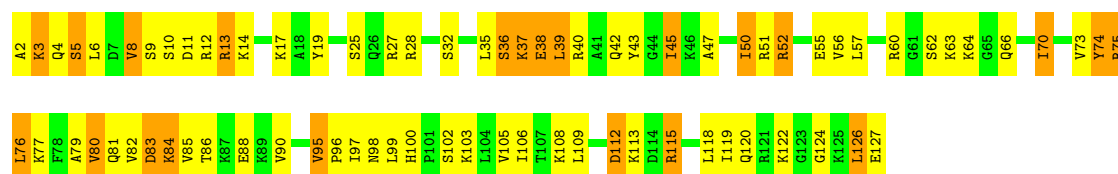
- Molecule 61: 60S ribosomal protein L25

Chain n5:



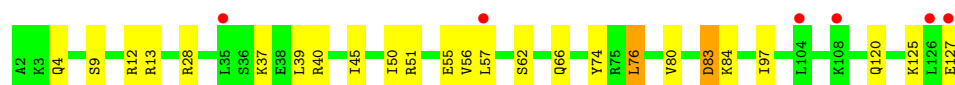
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



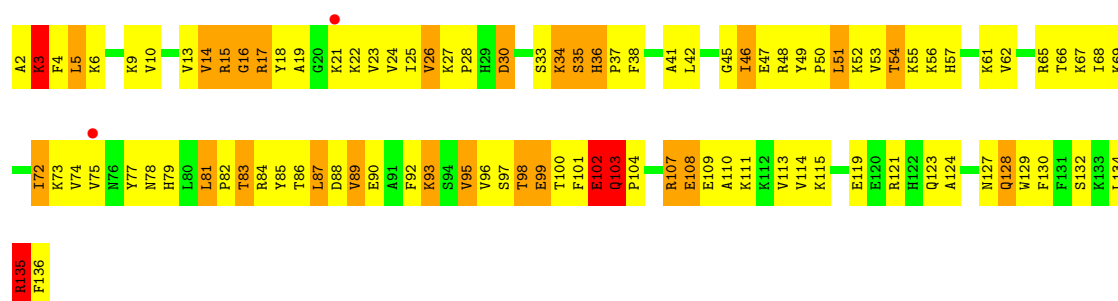
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



- Molecule 63: 60S ribosomal protein L27-A

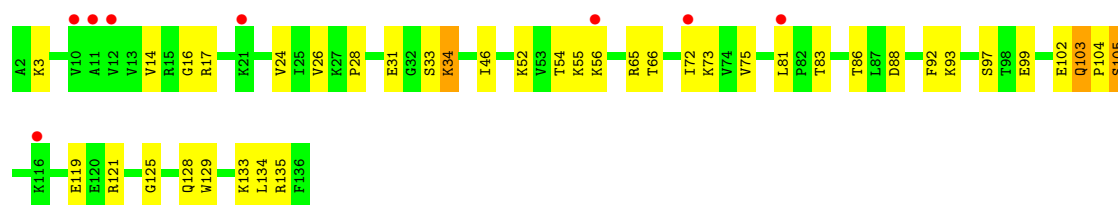
Chain N7:



- Molecule 63: 60S ribosomal protein L27-A

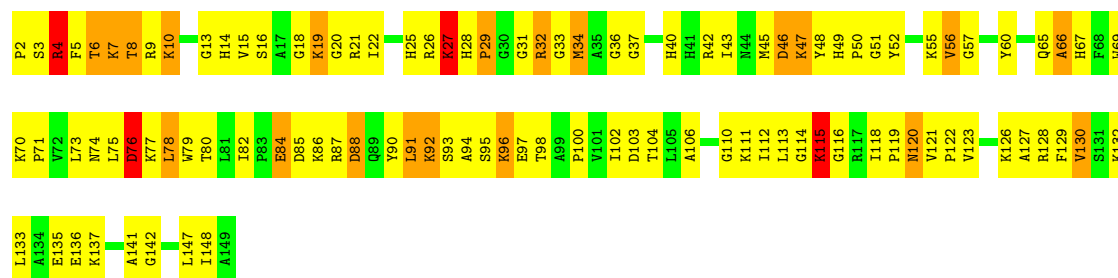
Chain n7:





- Molecule 64: 60S ribosomal protein L28

Chain N8:



- Molecule 64: 60S ribosomal protein L28

Chain n8:



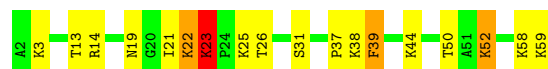
- Molecule 65: 60S ribosomal protein L29

Chain N9:



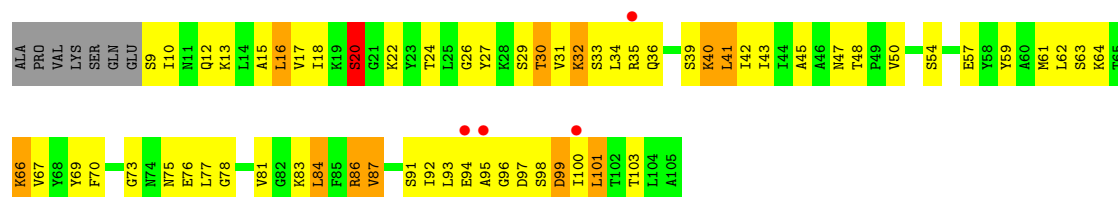
- Molecule 65: 60S ribosomal protein L29

Chain n9:



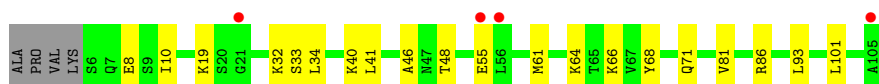
- Molecule 66: 60S ribosomal protein L30

Chain O0:



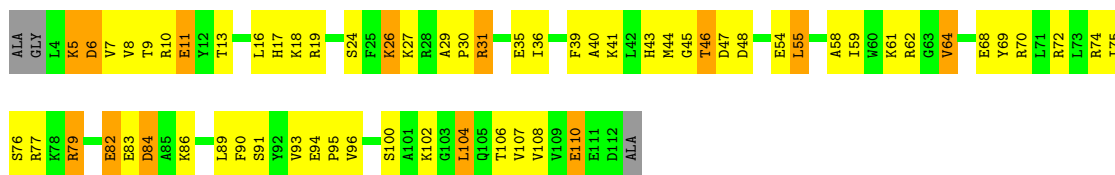
- Molecule 66: 60S ribosomal protein L30

Chain o0:



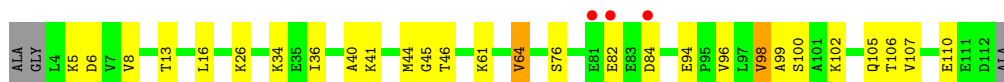
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:



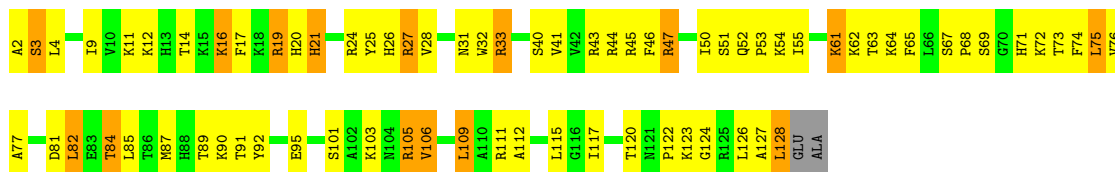
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



- Molecule 68: 60S ribosomal protein L32

Chain O2:



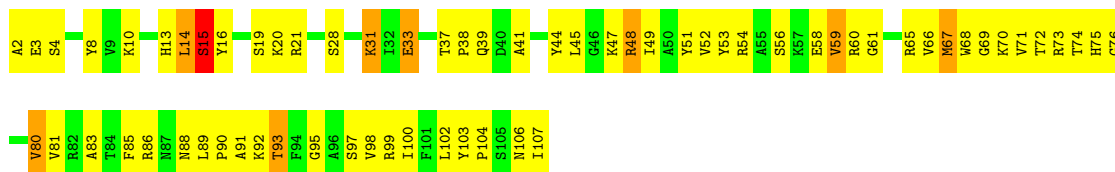
- Molecule 68: 60S ribosomal protein L32

Chain o2:



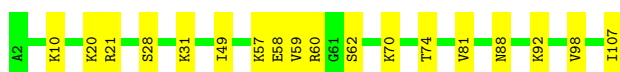
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



- Molecule 70: 60S ribosomal protein L34-A

G77	G78	G79	R80	R81	R82	R83	R84	R85	R86	R87	R88	R89	R90	R91	R92	R93	R94	R95	R96	R97	R98	R99	R100	R101	R102	R103	R104	R105	R106	R107	R108	R109	R110	R111	R112	R113	R114	R115	R116	R117	R118	R119	R120	R121	R122	R123	R124	R125	R126	R127	R128	R129	R130	R131	R132	R133	R134	R135	R136	R137	R138	R139	R140	R141	R142	R143	R144	R145	R146	R147	R148	R149	R150	R151	R152	R153	R154	R155	R156	R157	R158	R159	R160	R161	R162	R163	R164	R165	R166	R167	R168	R169	R170	R171	R172	R173	R174	R175	R176	R177	R178	R179	R180	R181	R182	R183	R184	R185	R186	R187	R188	R189	R190	R191	R192	R193	R194	R195	R196	R197	R198	R199	R200	R201	R202	R203	R204	R205	R206	R207	R208	R209	R210	R211	R212	R213	R214	R215	R216	R217	R218	R219	R220	R221	R222	R223	R224	R225	R226	R227	R228	R229	R230	R231	R232	R233	R234	R235	R236	R237	R238	R239	R240	R241	R242	R243	R244	R245	R246	R247	R248	R249	R250	R251	R252	R253	R254	R255	R256	R257	R258	R259	R260	R261	R262	R263	R264	R265	R266	R267	R268	R269	R270	R271	R272	R273	R274	R275	R276	R277	R278	R279	R280	R281	R282	R283	R284	R285	R286	R287	R288	R289	R290	R291	R292	R293	R294	R295	R296	R297	R298	R299	R300	R301	R302	R303	R304	R305	R306	R307	R308	R309	R310	R311	R312	R313	R314	R315	R316	R317	R318	R319	R320	R321	R322	R323	R324	R325	R326	R327	R328	R329	R330	R331	R332	R333	R334	R335	R336	R337	R338	R339	R340	R341	R342	R343	R344	R345	R346	R347	R348	R349	R350	R351	R352	R353	R354	R355	R356	R357	R358	R359	R360	R361	R362	R363	R364	R365	R366	R367	R368	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380	R381	R382	R383	R384	R385	R386	R387	R388	R389	R390	R391	R392	R393	R394	R395	R396	R397	R398	R399	R400	R401	R402	R403	R404	R405	R406	R407	R408	R409	R410	R411	R412	R413	R414	R415	R416	R417	R418	R419	R420	R421	R422	R423	R424	R425	R426	R427	R428	R429	R430	R431	R432	R433	R434	R435	R436	R437	R438	R439	R440	R441	R442	R443	R444	R445	R446	R447	R448	R449	R450	R451	R452	R453	R454	R455	R456	R457	R458	R459	R460	R461	R462	R463	R464	R465	R466	R467	R468	R469	R470	R471	R472	R473	R474	R475	R476	R477	R478	R479	R480	R481	R482	R483	R484	R485	R486	R487	R488	R489	R490	R491	R492	R493	R494	R495	R496	R497	R498	R499	R500	R501	R502	R503	R504	R505	R506	R507	R508	R509	R510	R511	R512	R513	R514	R515	R516	R517	R518	R519	R520	R521	R522	R523	R524	R525	R526	R527	R528	R529	R530	R531	R532	R533	R534	R535	R536	R537	R538	R539	R540	R541	R542	R543	R544	R545	R546	R547	R548	R549	R550	R551	R552	R553	R554	R555	R556	R557	R558	R559	R560	R561	R562	R563	R564	R565	R566	R567	R568	R569	R570	R571	R572	R573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584	R585	R586	R587	R588	R589	R590</
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- Chain o4: 

A2	V5	R16	K19	L20	K21	K24	L29	L30	Q33	R41	L51	R58	S66	G78	S79	N83	K86	Q98	K103	V104	V105	K106	K113	SER	GLU	LYS	LYS	ALA	LYS	LYS
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- Chain O5:

Category	Count
A2	10
G3	10
V4	10
K5	10
A6	10
K7	10
V8	10
E9	10
L9	10
T10	10
R11	10
K12	10
S13	10
K14	10
E15	10
Q16	10
L17	10
A18	10
S19	10
Q20	10
L21	10
V22	10
D23	10
L24	10
K25	10
K26	10
E27	10
L28	10
L31	10
K32	10
V33	10
Q34	10
K35	10
L36	10
S37	10
R38	10
S39	10
S40	10
L41	10
K42	10
K43	10
I44	10
K45	10
T46	10
V47	10
R48	10
K49	10
S50	10
L51	10
V54	10
L55	10
T56	10
V57	10
L58	10
N59	10
E60	10
Q61	10
Q62	10
R63	10

● E64
● A65
● V66
● R67
● Q68
● L69
● Y70
● K71
● G72
● W73
● T74
● Y75
● Q76
● P77
● K78
● D79
● L80
● R81
● A82
● T85
● R86
● A87
● L88
● R89
● R90
● A91
● L92
● T93
● K94
● F95
● S98
● Q99
● V100
● T101
● E102
● K103
● Q104
● K107
● Q108
● I109
● P112
● I113
● R114
● K115
● Y116
● A117
● I118
● K119
● A120

- Chain o5:

- Chain 06:

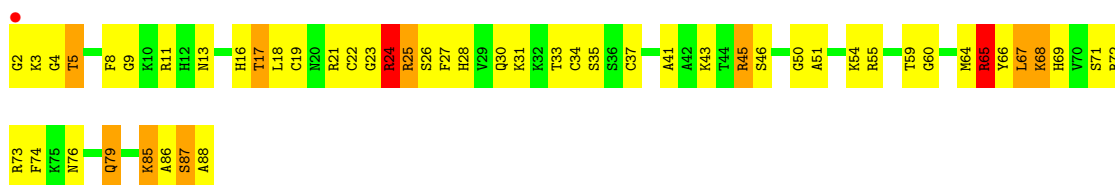
T2	V3	K4	T5	G6	I7	A8	G10	L11	N12	K13	K16	V17	T18	T21	P22	K25	I26	S27	Y28	K29	K30	A33	S34	L35	R36	T37	I47	Y53	E54	R55	R56	L57	I58	D59	L60	R61	R62	N63	S64	R68	A73	K74	K75	P76
----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SNP	reads
L77	100
G78	100
S79	100
F80	100
T81	100
K84	100
V87	100
E88	100
E89	100
M90	100
N91	100
I94	100
S97	100
R98	100
R99	100
H100	100

- Chain o6:

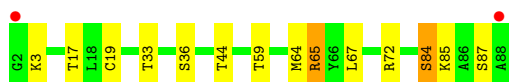
Year	Publications
1972	1
1973	1
1974	1
1975	1
1976	1
1977	1
1978	1
1979	1
1980	1
1981	1
1982	1
1983	1
1984	1
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2008	1
2009	1
2010	1
2011	1
2012	1
2013	1
2014	1
2015	1
2016	1
2017	1
2018	1
2019	1
2020	1
2021	1
2022	1

- Chain 07:



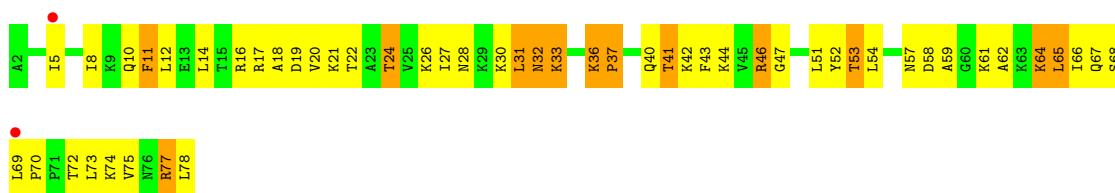
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



- Molecule 74: 60S ribosomal protein L38

Chain O8:



- Molecule 74: 60S ribosomal protein L38

Chain o8:



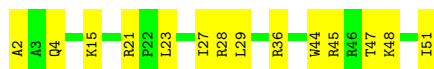
- Molecule 75: 60S ribosomal protein L39

Chain O9:



- Molecule 75: 60S ribosomal protein L39

Chain o9:



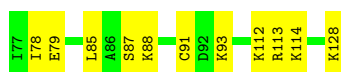
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



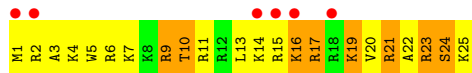
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



- Molecule 77: 60S ribosomal protein L41-A

Chain q1:



- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



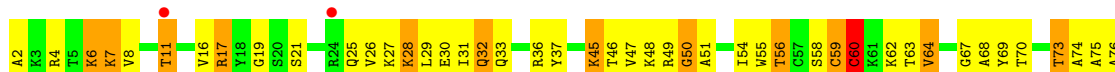
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:



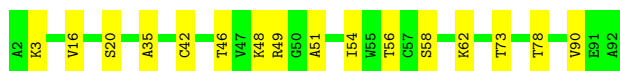
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



- Molecule 79: 60S ribosomal protein L43-A

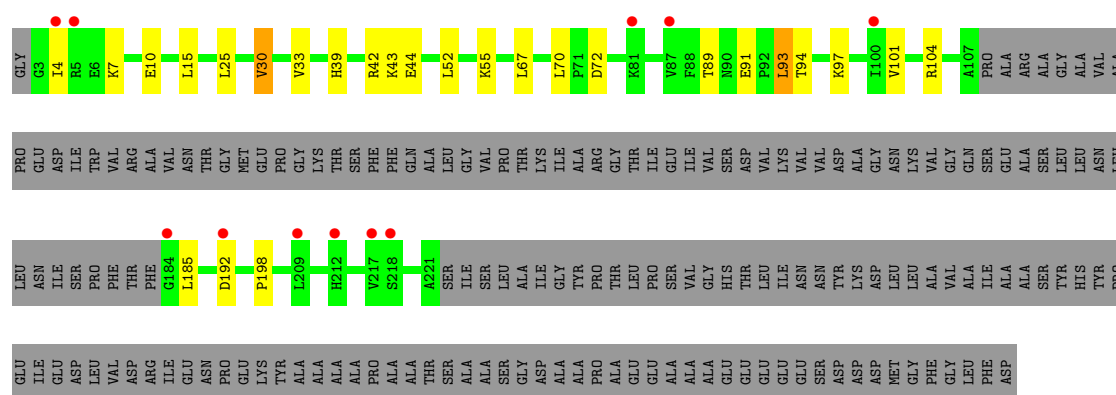
Chain q3:



- Molecule 80: 40S ribosomal protein S30-A

- [illegible]

- Chain p0: 



- 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	435.39Å 286.22Å 303.33Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	299.62 – 3.00 299.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (299.62-3.00) 99.9 (299.62-3.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.207 , 0.258 0.244 , 0.296	Depositor DCC
R_{free} test set	22130 reflections (1.52%)	DCC
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 1459481 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	411206	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: 3J2, ZN, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.87	13/41698 (0.0%)	1.42	462/64972 (0.7%)
1	6	0.97	33/42765 (0.1%)	1.48	645/66634 (1.0%)
2	S0	0.49	0/1617	0.69	0/2215
2	s0	0.52	0/1623	0.73	1/2222 (0.0%)
3	S1	0.42	0/1735	0.68	2/2335 (0.1%)
3	s1	0.54	0/1748	0.74	1/2352 (0.0%)
4	S2	0.54	0/1665	0.72	0/2263
4	s2	0.62	0/1665	0.81	2/2263 (0.1%)
5	S3	0.54	0/1759	0.72	1/2368 (0.0%)
5	s3	0.46	0/1759	0.65	0/2368
6	S4	0.56	0/2109	0.79	2/2839 (0.1%)
6	s4	0.56	0/2109	0.80	0/2839
7	S5	0.43	0/1629	0.63	0/2202
7	s5	0.47	0/1629	0.67	0/2202
8	S6	0.54	0/1823	0.72	0/2439
8	s6	0.64	1/1779 (0.1%)	0.74	0/2379
9	S7	0.48	0/1506	0.70	1/2028 (0.0%)
9	s7	0.52	0/1516	0.73	0/2043
10	S8	0.65	0/1514	0.82	1/2021 (0.0%)
10	s8	0.65	0/1514	0.79	1/2021 (0.0%)
11	S9	0.54	0/1519	0.74	1/2035 (0.0%)
11	s9	0.59	0/1519	0.80	4/2035 (0.2%)
12	C0	0.44	0/790	0.68	1/1069 (0.1%)
12	c0	0.39	0/777	0.66	3/1049 (0.3%)
13	C1	0.68	1/1239 (0.1%)	0.74	0/1673
13	c1	0.66	0/1194	0.82	1/1610 (0.1%)
14	C2	0.42	0/900	0.65	0/1224
14	c2	0.32	0/900	0.58	0/1224
15	C3	0.60	0/1215	0.73	2/1638 (0.1%)
15	c3	0.62	0/1215	0.82	2/1638 (0.1%)
16	C4	0.42	0/901	0.69	0/1217
16	c4	0.58	0/960	0.84	3/1290 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.54	0/998	0.78	1/1341 (0.1%)
17	c5	0.51	0/1060	0.69	0/1426
18	C6	0.50	0/1125	0.75	2/1510 (0.1%)
18	c6	0.52	0/1131	0.71	0/1518
19	C7	0.49	0/935	0.69	0/1254
19	c7	0.52	0/914	0.70	0/1224
20	C8	0.48	0/1211	0.72	1/1628 (0.1%)
20	c8	0.51	0/1211	0.73	2/1628 (0.1%)
21	C9	0.48	0/1130	0.69	0/1517
21	c9	0.52	0/1130	0.68	1/1517 (0.1%)
22	D0	0.51	0/865	0.70	0/1169
22	d0	0.53	0/892	0.69	0/1205
23	D1	0.55	0/693	0.70	0/935
23	d1	0.59	0/693	0.79	0/935
24	D2	0.58	0/1038	0.80	3/1395 (0.2%)
24	d2	0.66	0/1038	0.80	1/1395 (0.1%)
25	D3	0.73	0/1139	0.85	1/1518 (0.1%)
25	d3	0.74	0/1139	0.83	1/1518 (0.1%)
26	D4	0.53	0/1087	0.66	0/1449
26	d4	0.57	0/1087	0.78	0/1449
27	D5	0.43	0/571	0.75	0/768
27	d5	0.46	0/566	0.69	0/761
28	D6	0.48	0/782	0.72	0/1047
28	d6	0.60	0/782	0.75	0/1047
29	D7	0.50	0/620	0.70	0/838
29	d7	0.53	0/620	0.73	0/838
30	D8	0.43	0/499	0.62	0/670
30	d8	0.45	0/499	0.69	0/670
31	D9	0.63	0/452	0.85	1/600 (0.2%)
31	d9	0.57	0/452	0.75	1/600 (0.2%)
32	E0	0.54	0/483	0.68	0/643
33	E1	0.53	0/577	0.86	0/770
33	e1	0.42	0/619	0.72	0/822
34	SR	0.42	0/2494	0.63	1/3393 (0.0%)
34	sR	0.42	0/2495	0.59	0/3395
35	SM	0.58	0/1113	0.78	2/1502 (0.1%)
35	sM	0.55	0/683	0.78	2/923 (0.2%)
36	1	1.38	411/75394 (0.5%)	1.86	2927/117545 (2.5%)
36	5	1.40	457/75414 (0.6%)	1.87	2915/117575 (2.5%)
37	3	1.08	4/2883 (0.1%)	1.61	59/4491 (1.3%)
37	7	1.39	14/2883 (0.5%)	1.82	95/4491 (2.1%)
38	4	1.32	12/3746 (0.3%)	1.84	130/5832 (2.2%)
38	8	1.20	10/3746 (0.3%)	1.71	88/5832 (1.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.86	0/1948	0.93	2/2617 (0.1%)
39	l2	0.84	1/1946 (0.1%)	0.95	5/2614 (0.2%)
40	L3	0.87	1/3146 (0.0%)	0.93	2/4228 (0.0%)
40	l3	0.98	2/3146 (0.1%)	0.96	6/4228 (0.1%)
41	L4	0.93	0/2800	1.03	10/3790 (0.3%)
41	l4	0.90	1/2800 (0.0%)	0.95	5/3790 (0.1%)
42	L5	0.66	0/2425	0.75	0/3271
42	l5	0.87	2/2408 (0.1%)	0.89	2/3248 (0.1%)
43	L6	0.93	0/1260	0.91	1/1694 (0.1%)
43	l6	0.95	0/1269	0.97	4/1705 (0.2%)
44	L7	0.92	1/1821 (0.1%)	0.98	7/2451 (0.3%)
44	l7	1.01	4/1828 (0.2%)	0.98	3/2461 (0.1%)
45	L8	0.68	0/1836	0.76	1/2481 (0.0%)
45	l8	0.59	0/1795	0.71	0/2429
46	L9	0.77	0/1539	0.85	0/2073
46	l9	0.88	1/1539 (0.1%)	0.87	0/2073
47	M0	0.81	1/1741 (0.1%)	0.90	4/2335 (0.2%)
47	m0	0.88	1/1758 (0.1%)	0.98	6/2358 (0.3%)
48	M1	0.59	0/1374	0.80	1/1842 (0.1%)
48	m1	0.75	0/1374	0.85	2/1842 (0.1%)
49	M3	0.88	0/1568	0.93	1/2106 (0.0%)
49	m3	0.82	1/1573 (0.1%)	0.92	2/2113 (0.1%)
50	M4	0.88	0/1068	0.87	1/1438 (0.1%)
50	m4	0.96	0/1074	0.92	1/1446 (0.1%)
51	M5	0.90	0/1757	0.99	4/2354 (0.2%)
51	m5	0.78	1/1757 (0.1%)	0.91	2/2354 (0.1%)
52	M6	1.08	5/1585 (0.3%)	1.04	9/2128 (0.4%)
52	m6	1.18	4/1585 (0.3%)	1.08	6/2128 (0.3%)
53	M7	0.91	1/1443 (0.1%)	0.91	0/1944
53	m7	1.00	0/1250	0.97	0/1683
54	M8	0.90	0/1465	0.96	4/1965 (0.2%)
54	m8	0.90	0/1465	1.01	3/1965 (0.2%)
55	M9	0.69	0/1538	0.74	0/2050
55	m9	0.70	0/1538	0.77	0/2050
56	N0	0.89	0/1481	0.93	4/1990 (0.2%)
56	n0	1.01	0/1481	0.97	4/1990 (0.2%)
57	N1	0.87	0/1300	0.88	0/1743
57	n1	1.00	2/1300 (0.2%)	0.96	2/1743 (0.1%)
58	N2	0.49	0/812	0.66	0/1099
58	n2	0.54	0/794	0.72	0/1076
59	N3	0.87	0/1018	0.93	0/1369
59	n3	0.97	1/1018 (0.1%)	1.04	4/1369 (0.3%)
60	N4	0.70	0/712	0.77	1/958 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.75	0/1052	0.80	1/1398 (0.1%)
61	N5	0.80	0/979	0.91	1/1321 (0.1%)
61	n5	0.73	0/974	0.91	1/1314 (0.1%)
62	N6	0.83	0/1004	0.99	2/1341 (0.1%)
62	n6	0.87	1/1004 (0.1%)	0.98	2/1341 (0.1%)
63	N7	0.64	0/1118	0.78	1/1497 (0.1%)
63	n7	0.55	0/1118	0.71	0/1497
64	N8	0.93	0/1204	1.01	2/1612 (0.1%)
64	n8	0.90	1/1204 (0.1%)	0.95	2/1612 (0.1%)
65	N9	0.79	0/473	0.91	1/629 (0.2%)
65	n9	0.96	0/473	1.05	2/629 (0.3%)
66	O0	0.57	0/751	0.74	1/1008 (0.1%)
66	o0	0.55	0/775	0.69	0/1040
67	O1	0.75	0/890	0.80	1/1196 (0.1%)
67	o1	0.90	0/897	0.89	0/1205
68	O2	0.98	0/1041	1.04	4/1394 (0.3%)
68	o2	1.03	1/1041 (0.1%)	1.03	1/1394 (0.1%)
69	O3	1.14	3/868 (0.3%)	0.98	0/1168
69	o3	1.06	0/868	0.96	0/1168
70	O4	0.74	0/890	0.94	5/1189 (0.4%)
70	o4	0.69	0/890	0.82	1/1189 (0.1%)
71	O5	0.88	1/978 (0.1%)	0.91	2/1301 (0.2%)
71	o5	0.68	0/974	0.80	0/1297
72	O6	0.75	0/778	0.88	0/1034
72	o6	0.64	0/777	0.75	0/1033
73	O7	0.96	0/696	1.05	3/923 (0.3%)
73	o7	0.85	0/696	0.96	1/923 (0.1%)
74	O8	0.61	0/618	0.73	0/826
74	o8	0.53	0/614	0.76	1/822 (0.1%)
75	O9	0.91	0/443	0.93	0/588
75	o9	0.82	0/443	0.96	0/588
76	Q0	0.89	1/423 (0.2%)	0.95	1/562 (0.2%)
76	q0	1.00	0/423	1.01	0/562
77	Q1	0.75	0/234	0.96	1/300 (0.3%)
77	q1	0.92	0/234	1.15	3/300 (1.0%)
78	Q2	1.02	1/860 (0.1%)	0.94	1/1136 (0.1%)
78	q2	0.88	0/860	0.91	1/1136 (0.1%)
79	Q3	0.90	0/701	0.94	1/934 (0.1%)
79	q3	0.84	0/701	0.90	0/934
80	e0	0.60	0/499	0.78	0/665
82	p0	0.48	0/1092	0.61	0/1474
All	All	1.06	995/430073 (0.2%)	1.45	7522/631362 (1.2%)

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
3	S1	0	1
3	s1	0	1
5	s3	0	1
6	S4	0	1
7	S5	0	1
7	s5	0	2
9	S7	0	2
9	s7	0	1
16	C4	0	1
16	c4	0	1
18	c6	0	2
19	c7	0	1
22	d0	0	1
26	d4	0	1
27	D5	0	2
28	D6	0	2
33	E1	0	1
33	e1	0	1
39	L2	0	1
39	l2	0	3
41	L4	0	1
41	l4	0	1
42	L5	0	2
42	l5	0	1
43	L6	0	1
44	L7	0	1
44	l7	0	1
45	l8	0	1
48	M1	0	1
49	M3	0	1
51	M5	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
56	N0	0	1
56	n0	0	1
57	N1	0	1
59	n3	0	1
60	n4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	N7	0	1
64	N8	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	2
67	O1	0	2
67	o1	0	1
71	o5	0	1
72	O6	0	2
75	O9	0	1
75	o9	0	1
76	Q0	0	1
78	Q2	0	2
All	All	0	65

The worst 5 of 995 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	16.46	2.10	1.82
36	5	1152	G	N9-C4	-12.28	1.28	1.38
36	5	2872	A	N9-C4	-12.03	1.30	1.37
57	n1	104	GLU	CB-CG	10.19	1.71	1.52
36	1	3181	C	N3-C4	-9.73	1.27	1.33

The worst 5 of 7522 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	27.54	142.37	128.60
36	5	1152	G	N3-C4-N9	-26.81	109.91	126.00
36	1	2945	G	O5'-P-OP2	-22.04	84.25	110.70
36	5	1152	G	C2-N3-C4	-21.23	101.28	111.90
36	5	922	U	N3-C2-O2	-21.19	107.37	122.20

There are no chirality outliers.

5 of 65 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	S1	177	GLN	Peptide
6	S4	167	GLY	Peptide
7	S5	49	GLU	Peptide
9	S7	131	PHE	Peptide

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Mol	Chain	Res	Type	Group
9	S7	31	SER	Peptide

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	963	1
1	6	38238	0	19240	913	0
2	S0	1577	0	1567	167	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	170	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	158	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	127	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	195	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	185	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	150	0
8	s6	1755	0	1845	0	0
9	S7	1481	0	1572	148	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	119	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	132	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	74	0
12	c0	762	0	699	0	0
13	C1	1213	0	1257	76	0
13	c1	1168	0	1233	0	0
14	C2	892	0	891	71	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	100	0
15	c3	1192	0	1255	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	C4	891	0	883	100	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	103	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	118	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	83	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	113	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	110	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	94	0
22	d0	882	0	939	0	0
23	D1	684	0	672	82	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	112	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	98	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	93	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	54	0
27	d5	558	0	598	0	0
28	D6	769	0	814	104	0
28	d6	769	0	814	0	0
29	D7	610	0	631	44	0
29	d7	610	0	632	0	0
30	D8	497	0	535	55	0
30	d8	497	0	535	0	0
31	D9	442	0	428	42	0
31	d9	442	0	428	0	0
32	E0	475	0	525	36	0
33	E1	566	0	602	67	0
33	e1	608	0	656	0	0
34	SR	2441	0	2397	156	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	87	0
35	sM	680	0	607	0	0
36	1	67355	0	33835	1319	0
36	5	67376	0	33849	1295	1
37	3	2579	0	1304	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	7	2579	0	1304	53	0
38	4	3353	0	1695	60	0
38	8	3353	0	1695	84	0
39	L2	1914	0	1981	161	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	257	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	224	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	191	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	88	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	124	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	143	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	134	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	139	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	90	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	128	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	79	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	156	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	108	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	115	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	103	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	112	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	89	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	95	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	n2	778	0	791	0	0
59	N3	1003	0	1048	68	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	28	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	64	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	68	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	115	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	130	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	33	0
65	n9	462	0	491	0	0
66	O0	743	0	797	53	0
66	o0	767	0	816	0	0
67	O1	876	0	912	43	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	68	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	67	0
69	o3	850	0	880	0	0
70	O4	880	0	945	70	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	79	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	51	0
72	o6	770	0	846	0	0
73	O7	681	0	683	56	0
73	o7	681	0	683	0	0
74	O8	612	0	682	41	0
74	o8	608	0	671	0	0
75	O9	436	0	475	56	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	23	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	39	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	52	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	750	0	171	0	0
82	p0	1077	0	1041	0	0
83	p1	235	0	51	0	0
84	p2	230	0	51	0	0
85	1	469	0	0	0	0
85	2	125	0	0	0	0
85	3	14	0	0	0	0
85	4	22	0	0	0	0
85	5	502	0	0	0	0
85	6	150	0	0	0	0
85	7	17	0	0	0	0
85	8	15	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	L2	3	0	0	0	0
85	L3	2	0	0	0	0
85	L4	2	0	0	0	0
85	L5	1	0	0	0	0
85	L7	3	0	0	0	0
85	L8	1	0	0	0	0
85	M0	2	0	0	0	0
85	M1	1	0	0	0	0
85	M3	3	0	0	0	0
85	M4	1	0	0	0	0
85	M5	3	0	0	0	0
85	M6	1	0	0	0	0
85	M7	3	0	0	0	0
85	M8	1	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	3	0	0	0	0
85	N5	1	0	0	0	0
85	N6	1	0	0	0	0
85	N8	5	0	0	0	0
85	N9	1	0	0	0	0
85	O1	1	0	0	0	0
85	O3	1	0	0	0	0
85	O4	1	0	0	0	0
85	O7	2	0	0	0	0
85	S8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	SM	1	0	0	0	0
85	c7	2	0	0	0	0
85	c8	2	0	0	0	0
85	d3	2	0	0	0	0
85	d6	1	0	0	0	0
85	l2	3	0	0	0	0
85	l3	2	0	0	0	0
85	l4	1	0	0	0	0
85	l5	1	0	0	0	0
85	l7	1	0	0	0	0
85	l8	1	0	0	0	0
85	l9	1	0	0	0	0
85	m0	1	0	0	0	0
85	m1	2	0	0	0	0
85	m5	4	0	0	0	0
85	m6	1	0	0	0	0
85	m7	5	0	0	0	0
85	n0	1	0	0	0	0
85	n3	1	0	0	0	0
85	n6	1	0	0	0	0
85	n8	5	0	0	0	0
85	n9	1	0	0	0	0
85	o1	1	0	0	0	0
85	o3	1	0	0	0	0
85	o4	2	0	0	0	0
85	q0	1	0	0	0	0
85	q3	1	0	0	0	0
85	s1	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2422	0	0	309	0
86	2	1099	0	0	150	0
86	3	77	0	0	9	0
86	4	112	0	0	7	0
86	5	2478	0	0	247	0
86	6	1120	0	0	119	0
86	7	84	0	0	9	0
86	8	112	0	0	22	0
86	C1	7	0	0	6	0
86	C3	7	0	0	1	0
86	C5	7	0	0	5	0
86	C8	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	D9	7	0	0	1	0
86	L3	21	0	0	4	0
86	L4	7	0	0	2	0
86	M0	7	0	0	2	0
86	M5	7	0	0	1	0
86	M6	7	0	0	0	0
86	M7	14	0	0	2	0
86	M8	7	0	0	0	0
86	M9	7	0	0	1	0
86	N9	7	0	0	0	0
86	O2	7	0	0	0	0
86	O3	7	0	0	3	0
86	O7	14	0	0	4	0
86	O9	7	0	0	3	0
86	Q2	7	0	0	5	0
86	S8	7	0	0	1	0
86	S9	7	0	0	2	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	14	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	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	n3	7	0	0	0	0
86	n6	7	0	0	0	0
86	n9	7	0	0	0	0
86	o3	7	0	0	0	0
86	o7	7	0	0	0	0
86	q1	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	sR	7	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	1	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	0	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
88	1	26	0	0	0	0
88	5	26	0	0	0	0
All	All	411206	0	297263	10663	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 10663 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
52:M6:66:LYS:NZ	52:M6:66:LYS:CE	1.52	1.52
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.10	1.39
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.41	1.18
42:L5:152:ARG:HH11	42:L5:152:ARG:HG3	3.90	1.11
36:1:3182:G:OP1	52:M6:160:ARG:NH2	1.87	1.06

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]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	145 (71%)	36 (18%)	23 (11%)	1	3
2	s0	204/251 (81%)	151 (74%)	28 (14%)	25 (12%)	1	2
3	S1	212/254 (84%)	144 (68%)	40 (19%)	28 (13%)	0	2
3	s1	214/254 (84%)	169 (79%)	31 (14%)	14 (6%)	2	11
4	S2	215/253 (85%)	180 (84%)	23 (11%)	12 (6%)	3	16
4	s2	215/253 (85%)	183 (85%)	20 (9%)	12 (6%)	3	16
5	S3	221/239 (92%)	175 (79%)	32 (14%)	14 (6%)	2	12
5	s3	221/239 (92%)	182 (82%)	22 (10%)	17 (8%)	1	7
6	S4	258/260 (99%)	202 (78%)	36 (14%)	20 (8%)	1	7
6	s4	258/260 (99%)	211 (82%)	31 (12%)	16 (6%)	2	13
7	S5	204/224 (91%)	158 (78%)	25 (12%)	21 (10%)	1	4
7	s5	204/224 (91%)	152 (74%)	37 (18%)	15 (7%)	2	8
8	S6	224/236 (95%)	187 (84%)	28 (12%)	9 (4%)	5	25
8	s6	216/236 (92%)	180 (83%)	26 (12%)	10 (5%)	4	22
9	S7	182/189 (96%)	136 (75%)	28 (15%)	18 (10%)	1	4
9	s7	184/189 (97%)	133 (72%)	37 (20%)	14 (8%)	2	7
10	S8	184/200 (92%)	160 (87%)	16 (9%)	8 (4%)	4	23
10	s8	184/200 (92%)	157 (85%)	18 (10%)	9 (5%)	3	20
11	S9	183/196 (93%)	150 (82%)	25 (14%)	8 (4%)	4	22
11	s9	183/196 (93%)	143 (78%)	28 (15%)	12 (7%)	2	10
12	C0	94/105 (90%)	69 (73%)	16 (17%)	9 (10%)	1	4
12	c0	92/105 (88%)	67 (73%)	9 (10%)	16 (17%)	0	1
13	C1	153/155 (99%)	123 (80%)	19 (12%)	11 (7%)	2	8
13	c1	144/155 (93%)	121 (84%)	13 (9%)	10 (7%)	2	9
14	C2	122/142 (86%)	70 (57%)	28 (23%)	24 (20%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/142 (86%)	73 (60%)	32 (26%)	17 (14%)	0	2
15	C3	148/150 (99%)	120 (81%)	22 (15%)	6 (4%)	4	24
15	c3	148/150 (99%)	117 (79%)	20 (14%)	11 (7%)	2	8
16	C4	125/136 (92%)	81 (65%)	28 (22%)	16 (13%)	0	2
16	c4	126/136 (93%)	99 (79%)	14 (11%)	13 (10%)	1	4
17	C5	122/141 (86%)	91 (75%)	18 (15%)	13 (11%)	1	3
17	c5	133/141 (94%)	95 (71%)	20 (15%)	18 (14%)	0	2
18	C6	139/142 (98%)	111 (80%)	14 (10%)	14 (10%)	1	4
18	c6	140/142 (99%)	115 (82%)	17 (12%)	8 (6%)	3	16
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	1	4
19	c7	113/136 (83%)	86 (76%)	20 (18%)	7 (6%)	2	13
20	C8	143/145 (99%)	110 (77%)	20 (14%)	13 (9%)	1	5
20	c8	143/145 (99%)	112 (78%)	22 (15%)	9 (6%)	2	12
21	C9	141/143 (99%)	116 (82%)	17 (12%)	8 (6%)	3	16
21	c9	141/143 (99%)	120 (85%)	18 (13%)	3 (2%)	11	47
22	D0	105/120 (88%)	81 (77%)	16 (15%)	8 (8%)	2	7
22	d0	108/120 (90%)	80 (74%)	19 (18%)	9 (8%)	1	6
23	D1	85/87 (98%)	62 (73%)	15 (18%)	8 (9%)	1	5
23	d1	85/87 (98%)	68 (80%)	9 (11%)	8 (9%)	1	5
24	D2	127/129 (98%)	100 (79%)	23 (18%)	4 (3%)	7	34
24	d2	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	14	56
25	D3	142/144 (99%)	112 (79%)	17 (12%)	13 (9%)	1	5
25	d3	142/144 (99%)	121 (85%)	16 (11%)	5 (4%)	6	30
26	D4	132/134 (98%)	108 (82%)	17 (13%)	7 (5%)	3	18
26	d4	132/134 (98%)	104 (79%)	16 (12%)	12 (9%)	1	5
27	D5	68/107 (64%)	46 (68%)	13 (19%)	9 (13%)	0	2
27	d5	67/107 (63%)	52 (78%)	12 (18%)	3 (4%)	4	22
28	D6	95/97 (98%)	55 (58%)	24 (25%)	16 (17%)	0	1
28	d6	95/97 (98%)	73 (77%)	12 (13%)	10 (10%)	1	3
29	D7	79/81 (98%)	60 (76%)	14 (18%)	5 (6%)	2	12
29	d7	79/81 (98%)	63 (80%)	9 (11%)	7 (9%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D8	61/66 (92%)	47 (77%)	12 (20%)	2 (3%)	6	32
30	d8	61/66 (92%)	44 (72%)	13 (21%)	4 (7%)	2	10
31	D9	51/55 (93%)	43 (84%)	5 (10%)	3 (6%)	2	14
31	d9	51/55 (93%)	37 (72%)	9 (18%)	5 (10%)	1	4
32	E0	58/60 (97%)	44 (76%)	11 (19%)	3 (5%)	3	18
33	E1	69/76 (91%)	30 (44%)	19 (28%)	20 (29%)	0	0
33	e1	74/76 (97%)	37 (50%)	16 (22%)	21 (28%)	0	0
34	SR	316/318 (99%)	263 (83%)	45 (14%)	8 (2%)	9	40
34	sR	316/318 (99%)	256 (81%)	48 (15%)	12 (4%)	5	27
35	SM	155/273 (57%)	103 (66%)	29 (19%)	23 (15%)	0	1
35	sM	98/273 (36%)	57 (58%)	28 (29%)	13 (13%)	0	2
39	L2	250/253 (99%)	222 (89%)	19 (8%)	9 (4%)	5	29
39	l2	250/253 (99%)	211 (84%)	29 (12%)	10 (4%)	5	25
40	L3	384/386 (100%)	339 (88%)	29 (8%)	16 (4%)	4	24
40	l3	384/386 (100%)	342 (89%)	29 (8%)	13 (3%)	6	31
41	L4	359/361 (99%)	301 (84%)	39 (11%)	19 (5%)	3	18
41	l4	359/361 (99%)	303 (84%)	36 (10%)	20 (6%)	3	16
42	L5	294/296 (99%)	235 (80%)	37 (13%)	22 (8%)	2	8
42	l5	292/296 (99%)	247 (85%)	34 (12%)	11 (4%)	5	27
43	L6	152/175 (87%)	137 (90%)	12 (8%)	3 (2%)	11	48
43	l6	153/175 (87%)	129 (84%)	20 (13%)	4 (3%)	8	39
44	L7	220/243 (90%)	192 (87%)	20 (9%)	8 (4%)	5	29
44	l7	221/243 (91%)	201 (91%)	14 (6%)	6 (3%)	8	38
45	L8	231/255 (91%)	188 (81%)	36 (16%)	7 (3%)	7	34
45	l8	229/255 (90%)	180 (79%)	33 (14%)	16 (7%)	2	9
46	L9	189/191 (99%)	164 (87%)	21 (11%)	4 (2%)	11	47
46	l9	189/191 (99%)	169 (89%)	16 (8%)	4 (2%)	11	47
47	M0	207/220 (94%)	174 (84%)	25 (12%)	8 (4%)	5	26
47	m0	209/220 (95%)	167 (80%)	26 (12%)	16 (8%)	1	7
48	M1	167/173 (96%)	130 (78%)	21 (13%)	16 (10%)	1	4
48	m1	167/173 (96%)	139 (83%)	17 (10%)	11 (7%)	2	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	165 (86%)	17 (9%)	9 (5%)	4	21
49	m3	192/198 (97%)	152 (79%)	26 (14%)	14 (7%)	2	8
50	M4	134/137 (98%)	114 (85%)	10 (8%)	10 (8%)	2	8
50	m4	135/137 (98%)	122 (90%)	11 (8%)	2 (2%)	15	58
51	M5	201/203 (99%)	179 (89%)	17 (8%)	5 (2%)	9	40
51	m5	201/203 (99%)	180 (90%)	16 (8%)	5 (2%)	9	40
52	M6	195/198 (98%)	182 (93%)	10 (5%)	3 (2%)	15	58
52	m6	195/198 (98%)	172 (88%)	15 (8%)	8 (4%)	4	24
53	M7	181/183 (99%)	149 (82%)	21 (12%)	11 (6%)	2	14
53	m7	153/183 (84%)	133 (87%)	17 (11%)	3 (2%)	11	48
54	M8	183/185 (99%)	161 (88%)	16 (9%)	6 (3%)	6	32
54	m8	183/185 (99%)	148 (81%)	24 (13%)	11 (6%)	2	14
55	M9	186/188 (99%)	162 (87%)	21 (11%)	3 (2%)	14	56
55	m9	186/188 (99%)	156 (84%)	25 (13%)	5 (3%)	8	38
56	N0	170/172 (99%)	154 (91%)	14 (8%)	2 (1%)	19	64
56	n0	170/172 (99%)	153 (90%)	15 (9%)	2 (1%)	19	64
57	N1	157/159 (99%)	135 (86%)	13 (8%)	9 (6%)	3	16
57	n1	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	5	27
58	N2	98/120 (82%)	75 (76%)	18 (18%)	5 (5%)	3	18
58	n2	96/120 (80%)	77 (80%)	16 (17%)	3 (3%)	7	34
59	N3	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	15	58
59	n3	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
60	N4	96/155 (62%)	72 (75%)	16 (17%)	8 (8%)	1	6
60	n4	133/155 (86%)	101 (76%)	21 (16%)	11 (8%)	1	6
61	N5	119/141 (84%)	100 (84%)	17 (14%)	2 (2%)	14	54
61	n5	118/141 (84%)	103 (87%)	7 (6%)	8 (7%)	2	10
62	N6	124/126 (98%)	114 (92%)	8 (6%)	2 (2%)	14	56
62	n6	124/126 (98%)	109 (88%)	12 (10%)	3 (2%)	9	42
63	N7	133/135 (98%)	102 (77%)	21 (16%)	10 (8%)	2	8
63	n7	133/135 (98%)	101 (76%)	20 (15%)	12 (9%)	1	5
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	4	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	128 (88%)	14 (10%)	4 (3%)	8	38
65	N9	56/58 (97%)	43 (77%)	12 (21%)	1 (2%)	13	53
65	n9	56/58 (97%)	40 (71%)	9 (16%)	7 (12%)	1	2
66	O0	95/104 (91%)	88 (93%)	5 (5%)	2 (2%)	11	47
66	o0	98/104 (94%)	88 (90%)	8 (8%)	2 (2%)	11	48
67	O1	107/112 (96%)	95 (89%)	8 (8%)	4 (4%)	5	28
67	o1	107/112 (96%)	86 (80%)	14 (13%)	7 (6%)	2	11
68	O2	125/129 (97%)	113 (90%)	11 (9%)	1 (1%)	27	76
68	o2	125/129 (97%)	108 (86%)	12 (10%)	5 (4%)	5	25
69	O3	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	22	70
69	o3	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	12	51
70	O4	110/119 (92%)	100 (91%)	6 (6%)	4 (4%)	5	29
70	o4	110/119 (92%)	99 (90%)	7 (6%)	4 (4%)	5	29
71	O5	117/119 (98%)	108 (92%)	7 (6%)	2 (2%)	14	54
71	o5	117/119 (98%)	104 (89%)	7 (6%)	6 (5%)	3	18
72	O6	97/99 (98%)	79 (81%)	13 (13%)	5 (5%)	3	18
72	o6	97/99 (98%)	85 (88%)	10 (10%)	2 (2%)	11	47
73	O7	85/87 (98%)	71 (84%)	11 (13%)	3 (4%)	6	30
73	o7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	9	42
74	O8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	3	18
74	o8	75/77 (97%)	57 (76%)	15 (20%)	3 (4%)	5	25
75	O9	48/50 (96%)	42 (88%)	4 (8%)	2 (4%)	4	24
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	11	47
76	Q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	5	25
76	q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	11	48
77	Q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	4	23
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	84 (82%)	12 (12%)	7 (7%)	2	10
78	q2	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
79	Q3	89/91 (98%)	74 (83%)	11 (12%)	4 (4%)	4	22
79	q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	10	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	e0	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	1	4
82	p0	139/311 (45%)	113 (81%)	22 (16%)	4 (3%)	7	35
All	All	22333/24141 (92%)	18316 (82%)	2723 (12%)	1294 (6%)	3	15

5 of 1294 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	5	ALA
2	S0	30	GLN
2	S0	39	ASN
2	S0	66	ALA

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	132 (80%)	32 (20%)	2	11
2	s0	165/209 (79%)	120 (73%)	45 (27%)	0	3
3	S1	191/223 (86%)	152 (80%)	39 (20%)	2	9
3	s1	192/223 (86%)	152 (79%)	40 (21%)	2	8
4	S2	176/204 (86%)	142 (81%)	34 (19%)	2	12
4	s2	176/204 (86%)	129 (73%)	47 (27%)	1	4
5	S3	182/194 (94%)	136 (75%)	46 (25%)	1	4
5	s3	182/194 (94%)	154 (85%)	28 (15%)	4	19
6	S4	221/221 (100%)	179 (81%)	42 (19%)	2	12
6	s4	221/221 (100%)	190 (86%)	31 (14%)	5	23
7	S5	173/190 (91%)	140 (81%)	33 (19%)	2	12
7	s5	173/190 (91%)	135 (78%)	38 (22%)	1	7
8	S6	188/201 (94%)	150 (80%)	38 (20%)	2	10
8	s6	187/201 (93%)	155 (83%)	32 (17%)	3	15
9	S7	165/169 (98%)	132 (80%)	33 (20%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	s7	165/169 (98%)	136 (82%)	29 (18%)	3	14
10	S8	150/161 (93%)	132 (88%)	18 (12%)	7	30
10	s8	150/161 (93%)	128 (85%)	22 (15%)	4	21
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	5
11	s9	158/165 (96%)	130 (82%)	28 (18%)	3	14
12	C0	77/98 (79%)	63 (82%)	14 (18%)	2	13
12	c0	73/98 (74%)	62 (85%)	11 (15%)	4	20
13	C1	129/136 (95%)	106 (82%)	23 (18%)	2	14
13	c1	129/136 (95%)	101 (78%)	28 (22%)	1	8
14	C2	88/118 (75%)	64 (73%)	24 (27%)	0	3
14	c2	88/118 (75%)	64 (73%)	24 (27%)	0	3
15	C3	127/127 (100%)	106 (84%)	21 (16%)	3	16
15	c3	127/127 (100%)	106 (84%)	21 (16%)	3	16
16	C4	81/104 (78%)	55 (68%)	26 (32%)	0	2
16	c4	97/104 (93%)	74 (76%)	23 (24%)	1	5
17	C5	101/117 (86%)	81 (80%)	20 (20%)	2	11
17	c5	103/117 (88%)	85 (82%)	18 (18%)	3	14
18	C6	117/118 (99%)	86 (74%)	31 (26%)	1	4
18	c6	118/118 (100%)	93 (79%)	25 (21%)	1	8
19	C7	94/124 (76%)	75 (80%)	19 (20%)	2	10
19	c7	92/124 (74%)	76 (83%)	16 (17%)	3	14
20	C8	128/128 (100%)	97 (76%)	31 (24%)	1	5
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	5
21	C9	115/115 (100%)	89 (77%)	26 (23%)	1	6
21	c9	115/115 (100%)	96 (84%)	19 (16%)	3	16
22	D0	100/113 (88%)	71 (71%)	29 (29%)	0	3
22	d0	103/113 (91%)	77 (75%)	26 (25%)	1	4
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	8
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	8
24	D2	110/110 (100%)	85 (77%)	25 (23%)	1	6
24	d2	110/110 (100%)	95 (86%)	15 (14%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	D3	119/119 (100%)	97 (82%)	22 (18%)	2	13
25	d3	119/119 (100%)	94 (79%)	25 (21%)	1	8
26	D4	112/112 (100%)	89 (80%)	23 (20%)	2	9
26	d4	112/112 (100%)	90 (80%)	22 (20%)	2	11
27	D5	61/88 (69%)	44 (72%)	17 (28%)	0	3
27	d5	61/88 (69%)	54 (88%)	7 (12%)	8	32
28	D6	83/83 (100%)	65 (78%)	18 (22%)	1	8
28	d6	83/83 (100%)	70 (84%)	13 (16%)	4	18
29	D7	70/70 (100%)	60 (86%)	10 (14%)	5	22
29	d7	70/70 (100%)	54 (77%)	16 (23%)	1	6
30	D8	56/59 (95%)	42 (75%)	14 (25%)	1	4
30	d8	56/59 (95%)	48 (86%)	8 (14%)	5	22
31	D9	47/48 (98%)	38 (81%)	9 (19%)	2	12
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	8
32	E0	51/51 (100%)	36 (71%)	15 (29%)	0	2
33	E1	62/66 (94%)	42 (68%)	20 (32%)	0	2
33	e1	66/66 (100%)	43 (65%)	23 (35%)	0	1
34	SR	260/261 (100%)	227 (87%)	33 (13%)	6	27
34	sR	260/261 (100%)	230 (88%)	30 (12%)	8	32
35	SM	97/228 (42%)	68 (70%)	29 (30%)	0	2
35	sM	54/228 (24%)	42 (78%)	12 (22%)	1	7
39	L2	193/195 (99%)	158 (82%)	35 (18%)	2	13
39	l2	192/195 (98%)	152 (79%)	40 (21%)	2	8
40	L3	320/322 (99%)	252 (79%)	68 (21%)	1	8
40	l3	320/322 (99%)	249 (78%)	71 (22%)	1	7
41	L4	288/288 (100%)	229 (80%)	59 (20%)	2	9
41	l4	288/288 (100%)	234 (81%)	54 (19%)	2	12
42	L5	244/244 (100%)	193 (79%)	51 (21%)	1	8
42	l5	243/244 (100%)	193 (79%)	50 (21%)	2	9
43	L6	134/152 (88%)	108 (81%)	26 (19%)	2	11
43	l6	135/152 (89%)	110 (82%)	25 (18%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	L7	186/204 (91%)	159 (86%)	27 (14%)	5	22
44	l7	187/204 (92%)	160 (86%)	27 (14%)	5	22
45	L8	187/207 (90%)	158 (84%)	29 (16%)	4	19
45	l8	177/207 (86%)	149 (84%)	28 (16%)	4	18
46	L9	171/171 (100%)	133 (78%)	38 (22%)	1	7
46	l9	171/171 (100%)	134 (78%)	37 (22%)	1	8
47	M0	177/186 (95%)	140 (79%)	37 (21%)	1	8
47	m0	179/186 (96%)	141 (79%)	38 (21%)	1	8
48	M1	147/150 (98%)	114 (78%)	33 (22%)	1	7
48	m1	147/150 (98%)	120 (82%)	27 (18%)	2	13
49	M3	154/158 (98%)	128 (83%)	26 (17%)	3	15
49	m3	154/158 (98%)	130 (84%)	24 (16%)	4	18
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	14
50	m4	108/108 (100%)	90 (83%)	18 (17%)	3	16
51	M5	175/175 (100%)	145 (83%)	30 (17%)	3	15
51	m5	175/175 (100%)	150 (86%)	25 (14%)	5	22
52	M6	160/161 (99%)	134 (84%)	26 (16%)	3	17
52	m6	160/161 (99%)	127 (79%)	33 (21%)	2	9
53	M7	140/145 (97%)	111 (79%)	29 (21%)	2	8
53	m7	125/145 (86%)	95 (76%)	30 (24%)	1	5
54	M8	150/150 (100%)	122 (81%)	28 (19%)	2	12
54	m8	150/150 (100%)	118 (79%)	32 (21%)	1	8
55	M9	153/153 (100%)	124 (81%)	29 (19%)	2	12
55	m9	153/153 (100%)	126 (82%)	27 (18%)	3	14
56	N0	156/156 (100%)	126 (81%)	30 (19%)	2	12
56	n0	156/156 (100%)	129 (83%)	27 (17%)	3	14
57	N1	136/136 (100%)	101 (74%)	35 (26%)	1	4
57	n1	136/136 (100%)	108 (79%)	28 (21%)	2	9
58	N2	87/106 (82%)	77 (88%)	10 (12%)	8	32
58	n2	85/106 (80%)	75 (88%)	10 (12%)	8	30
59	N3	104/104 (100%)	83 (80%)	21 (20%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	n3	104/104 (100%)	92 (88%)	12 (12%)	8	32
60	N4	57/129 (44%)	52 (91%)	5 (9%)	14	48
60	n4	100/129 (78%)	85 (85%)	15 (15%)	4	20
61	N5	104/117 (89%)	80 (77%)	24 (23%)	1	6
61	n5	104/117 (89%)	84 (81%)	20 (19%)	2	12
62	N6	109/109 (100%)	79 (72%)	30 (28%)	0	3
62	n6	109/109 (100%)	88 (81%)	21 (19%)	2	12
63	N7	115/115 (100%)	85 (74%)	30 (26%)	1	4
63	n7	115/115 (100%)	84 (73%)	31 (27%)	1	3
64	N8	118/118 (100%)	95 (80%)	23 (20%)	2	11
64	n8	118/118 (100%)	94 (80%)	24 (20%)	2	9
65	N9	46/46 (100%)	35 (76%)	11 (24%)	1	5
65	n9	46/46 (100%)	34 (74%)	12 (26%)	1	4
66	O0	81/87 (93%)	67 (83%)	14 (17%)	3	14
66	o0	84/87 (97%)	66 (79%)	18 (21%)	1	8
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	6
67	o1	94/96 (98%)	72 (77%)	22 (23%)	1	5
68	O2	109/110 (99%)	86 (79%)	23 (21%)	1	8
68	o2	109/110 (99%)	87 (80%)	22 (20%)	2	10
69	O3	90/90 (100%)	78 (87%)	12 (13%)	6	25
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	14
70	O4	95/101 (94%)	77 (81%)	18 (19%)	2	12
70	o4	95/101 (94%)	82 (86%)	13 (14%)	5	24
71	O5	104/104 (100%)	72 (69%)	32 (31%)	0	2
71	o5	103/104 (99%)	84 (82%)	19 (18%)	2	13
72	O6	81/81 (100%)	58 (72%)	23 (28%)	0	3
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	2
73	O7	70/70 (100%)	58 (83%)	12 (17%)	3	15
73	o7	70/70 (100%)	57 (81%)	13 (19%)	2	13
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	7
74	o8	67/68 (98%)	49 (73%)	18 (27%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	O9	45/45 (100%)	36 (80%)	9 (20%)	2	10
75	o9	45/45 (100%)	33 (73%)	12 (27%)	1	4
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1	8
76	q0	47/47 (100%)	37 (79%)	10 (21%)	1	8
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	1	4
77	q1	23/23 (100%)	13 (56%)	10 (44%)	0	0
78	Q2	90/90 (100%)	73 (81%)	17 (19%)	2	12
78	q2	90/90 (100%)	74 (82%)	16 (18%)	2	14
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1	8
79	q3	71/71 (100%)	57 (80%)	14 (20%)	2	11
80	e0	53/53 (100%)	42 (79%)	11 (21%)	2	8
82	p0	105/253 (42%)	81 (77%)	24 (23%)	1	6
All	All	18728/20239 (92%)	14998 (80%)	3730 (20%)	2	10

5 of 3730 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
66	O0	87	VAL
6	s4	200	ARG
64	n8	27	LYS
69	O3	33	GLU
79	Q3	32	GLN

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

Mol	Chain	Res	Type
74	O8	32	ASN
9	s7	122	HIS
57	n1	131	GLN
2	s0	140	ASN
7	s5	186	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	0/1800	-	-

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

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2562 ligands modelled in this entry, 1429 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	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-
88	3J2	1	4209	-	30,30,30	3.06	5 (16%)	50,52,52	1.85	10 (20%)
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
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	86	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	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	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
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	86	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	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	-
88	3J2	5	4254	-	30,30,30	3.53	7 (23%)	50,52,52	1.63	10 (20%)
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	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	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M8	202	-	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	N9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	Q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	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	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	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	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	305	-	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	n3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	102	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q1	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	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	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4000	86	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4168	86	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
88	3J2	1	4209	-	-	0/4/65/65	0/4/5/5
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	86	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2147	86	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	3	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	223	-	-	0/0/0/0	0/0/0/0
86	OHX	4	224	-	-	0/0/0/0	0/0/0/0
86	OHX	4	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	227	-	-	0/0/0/0	0/0/0/0
86	OHX	4	228	-	-	0/0/0/0	0/0/0/0
86	OHX	4	229	-	-	0/0/0/0	0/0/0/0
86	OHX	4	230	-	-	0/0/0/0	0/0/0/0
86	OHX	4	231	-	-	0/0/0/0	0/0/0/0
86	OHX	4	232	-	-	0/0/0/0	0/0/0/0
86	OHX	4	233	-	-	0/0/0/0	0/0/0/0
86	OHX	4	234	-	-	0/0/0/0	0/0/0/0
86	OHX	4	235	-	-	0/0/0/0	0/0/0/0
86	OHX	4	236	-	-	0/0/0/0	0/0/0/0
86	OHX	4	237	-	-	0/0/0/0	0/0/0/0
86	OHX	4	238	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3941	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	86	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	86	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
88	3J2	5	4254	-	-	0/4/65/65	0/4/5/5
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2205	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2206	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2207	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2208	-	-	0/0/0/0	0/0/0/0
86	OHX	7	218	-	-	0/0/0/0	0/0/0/0
86	OHX	7	219	-	-	0/0/0/0	0/0/0/0
86	OHX	7	220	-	-	0/0/0/0	0/0/0/0
86	OHX	7	221	-	-	0/0/0/0	0/0/0/0
86	OHX	7	222	-	-	0/0/0/0	0/0/0/0
86	OHX	7	223	-	-	0/0/0/0	0/0/0/0
86	OHX	7	224	-	-	0/0/0/0	0/0/0/0
86	OHX	7	225	-	-	0/0/0/0	0/0/0/0
86	OHX	7	226	-	-	0/0/0/0	0/0/0/0
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	7	228	-	-	0/0/0/0	0/0/0/0
86	OHX	7	229	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	M6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	204	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	205	-	-	0/0/0/0	0/0/0/0
86	OHX	M8	202	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	O2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	105	-	-	0/0/0/0	0/0/0/0
86	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
86	OHX	S9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	203	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
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	302	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	305	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	n3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	n6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
86	OHX	q1	101	-	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	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	sR	401	-	-	0/0/0/0	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	4254	3J2	O1-C15	17.45	1.41	1.33
88	1	4209	3J2	O1-C15	14.72	1.40	1.33
88	5	4254	3J2	C4-C3	-4.23	1.34	1.39
88	1	4209	3J2	C3-C1	4.22	1.57	1.51
88	1	4209	3J2	C4-C13	3.94	1.47	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4209	3J2	O6-C5-C6	-5.40	97.42	109.55
88	5	4254	3J2	C18-C8-C9	-4.75	99.90	108.89
88	1	4209	3J2	O1-C3-C1	-4.74	107.25	112.57
88	1	4209	3J2	O2-C11-C12	4.48	123.51	117.83
88	5	4254	3J2	O6-C5-C6	-3.85	100.89	109.55

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%)	0.23	47 (2%)	52	10	40, 71, 144, 248	0
1	6	1795/1800 (99%)	0.31	90 (5%)	28	6	32, 64, 158, 254	0
2	S0	206/251 (82%)	0.61	9 (4%)	33	7	77, 91, 106, 127	0
2	s0	206/251 (82%)	0.40	6 (2%)	49	9	63, 82, 97, 107	0
3	S1	214/254 (84%)	0.95	39 (18%)	2	1	79, 111, 138, 142	0
3	s1	216/254 (85%)	0.47	5 (2%)	57	12	56, 69, 93, 103	0
4	S2	217/253 (85%)	0.33	4 (1%)	65	14	55, 70, 87, 99	0
4	s2	217/253 (85%)	0.27	6 (2%)	50	10	47, 63, 77, 92	0
5	S3	223/239 (93%)	0.28	7 (3%)	47	9	60, 75, 101, 122	0
5	s3	223/239 (93%)	0.41	13 (5%)	22	5	61, 88, 116, 129	0
6	S4	260/260 (100%)	1.12	41 (15%)	3	1	46, 71, 84, 121	0
6	s4	260/260 (100%)	0.62	15 (5%)	22	5	40, 65, 85, 121	0
7	S5	206/224 (91%)	1.05	37 (17%)	2	1	77, 99, 117, 137	0
7	s5	206/224 (91%)	0.64	17 (8%)	11	3	59, 84, 107, 126	0
8	S6	226/236 (95%)	0.67	18 (7%)	12	3	48, 80, 103, 143	0
8	s6	218/236 (92%)	0.68	16 (7%)	15	3	40, 70, 94, 117	0
9	S7	184/189 (97%)	0.53	10 (5%)	25	5	67, 96, 128, 138	0
9	s7	186/189 (98%)	0.51	13 (6%)	16	4	59, 91, 123, 135	0
10	S8	188/200 (94%)	0.79	13 (6%)	17	4	41, 54, 90, 108	0
10	s8	188/200 (94%)	0.54	7 (3%)	39	8	36, 57, 99, 112	0
11	S9	185/196 (94%)	0.89	19 (10%)	7	2	64, 80, 118, 154	0
11	s9	185/196 (94%)	0.32	7 (3%)	38	7	54, 70, 105, 140	0
12	C0	96/105 (91%)	0.15	2 (2%)	60	12	66, 86, 115, 126	0
12	c0	96/105 (91%)	1.07	22 (22%)	1	1	78, 108, 128, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	1.36	27 (17%)	2 1	44, 54, 128, 138	0
13	c1	146/155 (94%)	1.13	24 (16%)	2 1	40, 55, 86, 111	0
14	C2	124/142 (87%)	0.93	21 (16%)	2 1	108, 125, 144, 162	0
14	c2	124/142 (87%)	2.97	77 (62%)	0 0	151, 168, 191, 198	0
15	C3	150/150 (100%)	0.39	5 (3%)	44 8	51, 69, 83, 94	0
15	c3	150/150 (100%)	0.41	4 (2%)	52 10	48, 63, 81, 94	0
16	C4	127/136 (93%)	0.91	20 (15%)	3 1	54, 111, 128, 131	0
16	c4	128/136 (94%)	0.66	8 (6%)	19 5	39, 71, 79, 83	0
17	C5	124/141 (87%)	0.56	10 (8%)	12 3	59, 74, 114, 131	0
17	c5	135/141 (95%)	0.31	7 (5%)	26 6	63, 81, 106, 124	0
18	C6	141/142 (99%)	1.32	37 (26%)	1 1	66, 89, 95, 99	0
18	c6	142/142 (100%)	1.08	29 (20%)	1 1	53, 74, 92, 115	0
19	C7	120/136 (88%)	0.56	7 (5%)	22 5	75, 94, 121, 127	0
19	c7	117/136 (86%)	0.49	5 (4%)	34 7	66, 82, 112, 122	0
20	C8	145/145 (100%)	0.30	7 (4%)	29 6	59, 85, 112, 123	0
20	c8	145/145 (100%)	0.41	8 (5%)	24 5	57, 73, 105, 122	0
21	C9	143/143 (100%)	0.77	12 (8%)	11 3	69, 84, 102, 112	0
21	c9	143/143 (100%)	0.33	2 (1%)	72 18	55, 68, 91, 110	0
22	D0	107/120 (89%)	1.41	30 (28%)	1 0	57, 91, 131, 136	0
22	d0	110/120 (91%)	1.22	24 (21%)	1 1	54, 92, 136, 147	0
23	D1	87/87 (100%)	0.22	4 (4%)	31 7	73, 80, 99, 113	0
23	d1	87/87 (100%)	-0.04	1 (1%)	77 21	60, 68, 89, 97	0
24	D2	129/129 (100%)	0.82	11 (8%)	11 3	52, 64, 73, 84	0
24	d2	129/129 (100%)	0.26	1 (0%)	83 26	45, 55, 63, 75	0
25	D3	144/144 (100%)	0.26	1 (0%)	84 28	42, 48, 58, 75	0
25	d3	144/144 (100%)	0.44	1 (0%)	84 28	36, 40, 52, 68	0
26	D4	134/134 (100%)	0.57	11 (8%)	12 3	57, 83, 100, 110	0
26	d4	134/134 (100%)	0.31	2 (1%)	70 16	48, 72, 89, 114	0
27	D5	70/107 (65%)	0.82	8 (11%)	6 2	94, 111, 127, 132	0
27	d5	69/107 (64%)	1.03	11 (15%)	3 1	80, 101, 116, 120	0
28	D6	97/97 (100%)	1.63	34 (35%)	1 0	59, 75, 133, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.97	14 (14%) 3 1	44, 57, 85, 93	0
29	D7	81/81 (100%)	0.52	3 (3%) 39 8	67, 81, 121, 128	0
29	d7	81/81 (100%)	0.66	7 (8%) 11 3	57, 75, 124, 127	0
30	D8	63/66 (95%)	1.81	25 (39%) 1 0	93, 113, 129, 134	0
30	d8	63/66 (95%)	1.11	14 (22%) 1 1	79, 98, 116, 134	0
31	D9	53/55 (96%)	0.48	2 (3%) 38 7	59, 63, 82, 88	0
31	d9	53/55 (96%)	0.73	4 (7%) 14 3	58, 65, 104, 120	0
32	E0	60/60 (100%)	1.14	13 (21%) 1 1	48, 78, 135, 141	0
33	E1	71/76 (93%)	0.93	11 (15%) 3 1	86, 106, 121, 124	0
33	e1	76/76 (100%)	2.14	26 (34%) 1 0	128, 140, 151, 152	0
34	SR	318/318 (100%)	0.55	19 (5%) 21 5	58, 95, 118, 141	0
34	sR	318/318 (100%)	0.99	56 (17%) 2 1	82, 105, 122, 139	0
35	SM	159/273 (58%)	0.56	8 (5%) 28 6	51, 75, 129, 138	0
35	sM	104/273 (38%)	0.52	8 (7%) 13 3	44, 84, 157, 169	0
36	1	3149/3396 (92%)	0.25	76 (2%) 56 11	14, 36, 116, 249	0
36	5	3150/3396 (92%)	0.19	37 (1%) 75 20	14, 36, 105, 236	0
37	3	121/121 (100%)	-0.08	1 (0%) 83 26	29, 54, 69, 72	0
37	7	121/121 (100%)	-0.05	0 100 100	22, 38, 51, 58	0
38	4	158/158 (100%)	0.02	0 100 100	19, 36, 72, 114	0
38	8	158/158 (100%)	0.07	1 (0%) 86 32	25, 45, 79, 105	0
39	L2	252/253 (99%)	0.49	7 (2%) 50 10	20, 33, 48, 57	0
39	l2	252/253 (99%)	0.59	12 (4%) 29 6	23, 40, 56, 67	0
40	L3	386/386 (100%)	0.10	0 100 100	19, 38, 50, 83	0
40	l3	386/386 (100%)	0.04	1 (0%) 91 48	15, 28, 40, 73	0
41	L4	361/361 (100%)	0.02	0 100 100	17, 30, 48, 59	0
41	l4	361/361 (100%)	-0.01	0 100 100	19, 35, 52, 70	0
42	L5	296/296 (100%)	0.27	9 (3%) 48 9	37, 59, 77, 106	0
42	l5	294/296 (99%)	0.20	0 100 100	28, 42, 69, 113	0
43	L6	156/175 (89%)	0.18	1 (0%) 86 32	26, 33, 52, 72	0
43	l6	157/175 (89%)	0.00	1 (0%) 86 32	27, 34, 52, 65	0
44	L7	222/243 (91%)	0.13	1 (0%) 88 36	21, 28, 57, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	0.17	1 (0%) 90 41	18, 25, 64, 115	0
45	L8	233/255 (91%)	0.28	8 (3%) 43 8	41, 55, 91, 109	0
45	l8	231/255 (90%)	0.51	18 (7%) 13 3	53, 67, 101, 112	0
46	L9	191/191 (100%)	0.37	3 (1%) 68 16	34, 44, 55, 75	0
46	l9	191/191 (100%)	0.11	1 (0%) 88 36	25, 34, 55, 79	0
47	M0	211/220 (95%)	0.34	1 (0%) 88 36	26, 42, 77, 99	0
47	m0	213/220 (96%)	0.38	10 (4%) 30 6	27, 43, 67, 86	0
48	M1	169/173 (97%)	0.22	1 (0%) 86 32	46, 64, 75, 85	0
48	m1	169/173 (97%)	-0.02	0 100 100	31, 47, 59, 72	0
49	M3	193/198 (97%)	0.47	5 (2%) 53 10	19, 39, 81, 106	0
49	m3	194/198 (97%)	0.48	4 (2%) 60 12	26, 48, 86, 110	0
50	M4	136/137 (99%)	-0.04	1 (0%) 84 28	27, 35, 47, 55	0
50	m4	137/137 (100%)	-0.13	0 100 100	26, 29, 49, 59	0
51	M5	203/203 (100%)	0.63	8 (3%) 37 7	20, 32, 43, 47	0
51	m5	203/203 (100%)	0.88	16 (7%) 13 3	25, 42, 53, 58	0
52	M6	197/198 (99%)	-0.01	0 100 100	21, 27, 44, 46	0
52	m6	197/198 (99%)	0.03	0 100 100	16, 20, 44, 50	0
53	M7	183/183 (100%)	0.40	9 (4%) 28 6	22, 30, 93, 142	0
53	m7	155/183 (84%)	0.26	0 100 100	19, 26, 36, 69	0
54	M8	185/185 (100%)	0.13	0 100 100	22, 32, 48, 68	0
54	m8	185/185 (100%)	0.22	0 100 100	23, 34, 43, 49	0
55	M9	188/188 (100%)	0.73	17 (9%) 10 2	35, 50, 143, 153	0
55	m9	188/188 (100%)	0.48	4 (2%) 60 12	34, 47, 122, 132	0
56	N0	172/172 (100%)	0.13	1 (0%) 86 32	26, 34, 46, 56	0
56	n0	172/172 (100%)	-0.01	0 100 100	22, 28, 37, 44	0
57	N1	159/159 (100%)	0.50	5 (3%) 47 9	25, 35, 81, 91	0
57	n1	159/159 (100%)	0.18	0 100 100	22, 28, 67, 74	0
58	N2	100/120 (83%)	0.98	15 (15%) 3 1	65, 83, 97, 132	0
58	n2	98/120 (81%)	0.71	7 (7%) 16 4	59, 73, 82, 85	0
59	N3	136/136 (100%)	0.41	3 (2%) 59 12	24, 33, 44, 51	0
59	n3	136/136 (100%)	0.31	2 (1%) 70 16	17, 27, 40, 44	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	2.18	32 (32%) 1 0	34, 47, 138, 143	0
60	n4	135/155 (87%)	0.68	13 (9%) 8 2	27, 79, 124, 144	0
61	N5	121/141 (85%)	0.33	4 (3%) 44 8	32, 42, 61, 87	0
61	n5	120/141 (85%)	0.88	10 (8%) 11 3	36, 49, 71, 80	0
62	N6	126/126 (100%)	0.26	0 100 100	22, 38, 49, 53	0
62	n6	126/126 (100%)	0.75	6 (4%) 29 6	28, 43, 58, 65	0
63	N7	135/135 (100%)	0.32	2 (1%) 70 16	51, 65, 79, 90	0
63	n7	135/135 (100%)	0.58	8 (5%) 22 5	62, 75, 95, 105	0
64	N8	148/148 (100%)	0.40	0 100 100	15, 33, 56, 66	0
64	n8	148/148 (100%)	0.53	3 (2%) 62 12	17, 38, 52, 55	0
65	N9	58/58 (100%)	0.42	2 (3%) 43 8	23, 40, 89, 103	0
65	n9	58/58 (100%)	0.34	0 100 100	21, 38, 63, 69	0
66	O0	97/104 (93%)	0.25	4 (4%) 35 7	49, 59, 86, 97	0
66	o0	100/104 (96%)	0.47	4 (4%) 36 7	57, 67, 94, 98	0
67	O1	109/112 (97%)	0.20	0 100 100	32, 44, 83, 94	0
67	o1	109/112 (97%)	0.23	3 (2%) 50 10	27, 38, 73, 93	0
68	O2	127/129 (98%)	0.44	0 100 100	15, 29, 38, 56	0
68	o2	127/129 (98%)	0.54	4 (3%) 47 9	17, 32, 43, 67	0
69	O3	106/106 (100%)	0.22	0 100 100	21, 25, 47, 57	0
69	o3	106/106 (100%)	0.24	0 100 100	18, 25, 48, 54	0
70	O4	112/119 (94%)	0.79	11 (9%) 8 2	31, 47, 92, 111	0
70	o4	112/119 (94%)	0.70	5 (4%) 32 7	36, 54, 95, 108	0
71	O5	119/119 (100%)	0.81	7 (5%) 22 5	31, 45, 52, 57	0
71	o5	119/119 (100%)	0.54	4 (3%) 43 8	38, 52, 63, 71	0
72	O6	99/99 (100%)	0.62	4 (4%) 36 7	36, 46, 82, 98	0
72	o6	99/99 (100%)	0.33	2 (2%) 62 12	43, 57, 81, 95	0
73	O7	87/87 (100%)	0.30	1 (1%) 77 21	21, 25, 49, 71	0
73	o7	87/87 (100%)	0.27	2 (2%) 57 12	23, 31, 57, 93	0
74	O8	77/77 (100%)	0.44	2 (2%) 53 10	55, 67, 95, 106	0
74	o8	77/77 (100%)	0.61	3 (3%) 37 7	59, 72, 97, 101	0
75	O9	50/50 (100%)	0.04	1 (2%) 62 12	29, 32, 40, 41	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	0.18	0 100 100	34, 38, 45, 51	0
76	Q0	52/52 (100%)	0.20	0 100 100	30, 35, 47, 56	0
76	q0	52/52 (100%)	0.11	0 100 100	21, 25, 34, 41	0
77	Q1	25/25 (100%)	1.64	6 (24%) 1 1	40, 42, 45, 47	0
77	q1	25/25 (100%)	0.97	2 (8%) 12 3	32, 36, 44, 50	0
78	Q2	105/105 (100%)	0.36	2 (1%) 64 13	24, 39, 60, 83	0
78	q2	105/105 (100%)	0.56	4 (3%) 38 7	27, 38, 50, 78	0
79	Q3	91/91 (100%)	0.43	2 (2%) 59 12	27, 36, 50, 63	0
79	q3	91/91 (100%)	0.17	0 100 100	29, 41, 54, 63	0
80	e0	62/62 (100%)	0.26	3 (4%) 29 6	44, 69, 112, 130	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	0.64	11 (7%) 13 3	78, 94, 173, 179	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35344 (93%)	0.42	1576 (4%) 29 6	14, 53, 117, 254	0

The worst 5 of 1576 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	c2	112	ALA	12.1
60	N4	75	THR	12.0
1	6	662	U	11.9
60	N4	69	LYS	11.4
14	c2	63	VAL	11.4

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	2	2003	1/1	0.62	971.00	114,114,114,114	0
85	MG	7	217	1/1	0.40	403.00	39,39,39,39	0
85	MG	1	3718	1/1	0.30	275.00	38,38,38,38	0
85	MG	5	3730	1/1	0.29	232.64	40,40,40,40	0
85	MG	2	1997	1/1	0.27	215.00	83,83,83,83	0
85	MG	7	204	1/1	0.72	172.33	57,57,57,57	0
85	MG	6	1940	1/1	0.58	161.80	72,72,72,72	0
85	MG	5	3780	1/1	0.49	150.50	60,60,60,60	0
85	MG	6	2021	1/1	0.39	137.00	45,45,45,45	0
85	MG	5	3871	1/1	0.52	133.63	51,51,51,51	0
85	MG	1	3463	1/1	0.26	109.00	36,36,36,36	0
85	MG	1	3821	1/1	1.21	104.18	31,31,31,31	0
85	MG	1	3808	1/1	0.67	97.44	24,24,24,24	0
85	MG	L7	303	1/1	0.33	95.00	32,32,32,32	0
85	MG	1	3617	1/1	0.36	91.00	54,54,54,54	0
85	MG	5	3482	1/1	0.42	83.25	39,39,39,39	0
85	MG	3	209	1/1	0.42	81.86	51,51,51,51	0
85	MG	5	3703	1/1	0.42	81.42	59,59,59,59	0
85	MG	1	3736	1/1	0.38	77.92	44,44,44,44	0
85	MG	5	3630	1/1	0.57	76.46	67,67,67,67	0
85	MG	5	3858	1/1	0.40	74.93	74,74,74,74	0
85	MG	1	3548	1/1	0.33	72.20	30,30,30,30	0
85	MG	5	3410	1/1	0.41	67.57	33,33,33,33	0
85	MG	1	3674	1/1	0.35	61.50	59,59,59,59	0
85	MG	2	2014	1/1	0.58	56.22	64,64,64,64	0
85	MG	5	3857	1/1	0.34	55.29	66,66,66,66	0
85	MG	1	3703	1/1	0.25	55.06	47,47,47,47	0
85	MG	6	1945	1/1	0.45	51.73	29,29,29,29	0
85	MG	1	3578	1/1	0.51	50.19	25,25,25,25	0
85	MG	4	205	1/1	0.33	49.90	42,42,42,42	0
85	MG	6	2015	1/1	0.64	48.10	125,125,125,125	0
85	MG	5	3783	1/1	0.59	47.56	48,48,48,48	0
85	MG	6	1944	1/1	0.50	47.12	57,57,57,57	0
85	MG	5	3677	1/1	0.37	46.15	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1945	1/1	0.32	45.67	69,69,69,69	0
85	MG	1	3850	1/1	0.47	45.36	64,64,64,64	0
86	OHX	6	2187	7/7	0.42	42.45	121,121,121,121	0
85	MG	1	3770	1/1	0.23	41.67	40,40,40,40	0
85	MG	1	3856	1/1	1.33	41.16	50,50,50,50	0
85	MG	5	3779	1/1	0.54	41.12	61,61,61,61	0
85	MG	5	3448	1/1	0.34	40.10	49,49,49,49	0
85	MG	3	204	1/1	0.56	36.58	41,41,41,41	0
85	MG	6	2040	1/1	0.56	36.22	47,47,47,47	0
85	MG	5	3438	1/1	0.62	34.53	43,43,43,43	0
85	MG	5	3434	1/1	0.47	34.28	72,72,72,72	0
85	MG	5	3649	1/1	0.29	32.67	75,75,75,75	0
85	MG	6	1924	1/1	0.60	32.50	92,92,92,92	0
85	MG	2	1903	1/1	0.34	32.29	39,39,39,39	0
85	MG	5	3738	1/1	0.43	31.73	55,55,55,55	0
85	MG	1	3646	1/1	0.75	31.46	33,33,33,33	0
85	MG	3	214	1/1	0.52	30.74	50,50,50,50	0
85	MG	1	3839	1/1	0.39	30.50	36,36,36,36	0
85	MG	5	3808	1/1	0.76	30.46	24,24,24,24	0
85	MG	5	3616	1/1	0.38	30.40	33,33,33,33	0
85	MG	5	3881	1/1	0.53	30.36	77,77,77,77	0
85	MG	5	3885	1/1	0.53	30.09	53,53,53,53	0
85	MG	6	1953	1/1	0.42	30.00	54,54,54,54	0
85	MG	5	3674	1/1	0.30	29.50	29,29,29,29	0
85	MG	5	3873	1/1	0.37	29.48	36,36,36,36	0
85	MG	2	1957	1/1	0.42	29.00	60,60,60,60	0
85	MG	5	3540	1/1	0.37	28.69	26,26,26,26	0
85	MG	1	3813	1/1	0.54	27.67	101,101,101,101	0
85	MG	2	1904	1/1	0.52	27.38	55,55,55,55	0
85	MG	7	203	1/1	0.36	27.21	45,45,45,45	0
85	MG	8	205	1/1	0.41	27.14	40,40,40,40	0
85	MG	1	3855	1/1	0.37	26.75	44,44,44,44	0
85	MG	1	3726	1/1	0.61	26.44	24,24,24,24	0
85	MG	1	3540	1/1	0.36	26.29	52,52,52,52	0
85	MG	1	3443	1/1	0.41	26.17	42,42,42,42	0
85	MG	1	3818	1/1	0.34	26.15	48,48,48,48	0
85	MG	1	3500	1/1	0.31	25.60	63,63,63,63	0
85	MG	5	3475	1/1	0.41	25.50	73,73,73,73	0
85	MG	1	3681	1/1	0.30	25.22	30,30,30,30	0
85	MG	6	2031	1/1	0.54	24.22	74,74,74,74	0
85	MG	1	3759	1/1	0.45	24.21	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	4	213	1/1	0.31	23.67	46,46,46,46	0
85	MG	6	2047	1/1	0.54	23.29	79,79,79,79	0
85	MG	5	3874	1/1	0.50	23.27	31,31,31,31	0
85	MG	5	3583	1/1	0.41	22.87	21,21,21,21	0
85	MG	5	3561	1/1	0.41	22.48	21,21,21,21	0
85	MG	2	2019	1/1	0.45	22.44	60,60,60,60	0
85	MG	5	3656	1/1	0.39	22.33	39,39,39,39	0
85	MG	3	213	1/1	0.38	22.01	49,49,49,49	0
85	MG	5	3663	1/1	0.55	21.78	46,46,46,46	0
85	MG	6	2041	1/1	0.57	21.71	88,88,88,88	0
85	MG	3	203	1/1	0.38	21.64	76,76,76,76	0
85	MG	5	3849	1/1	0.40	21.58	48,48,48,48	0
85	MG	3	205	1/1	0.37	21.53	27,27,27,27	0
85	MG	1	3572	1/1	0.43	21.23	21,21,21,21	0
85	MG	1	3474	1/1	0.32	21.18	63,63,63,63	0
85	MG	5	3572	1/1	0.35	20.82	22,22,22,22	0
85	MG	5	3643	1/1	0.54	20.75	22,22,22,22	0
85	MG	1	3616	1/1	0.25	20.67	36,36,36,36	0
85	MG	5	3774	1/1	0.55	20.53	19,19,19,19	0
85	MG	5	3761	1/1	0.28	20.43	59,59,59,59	0
85	MG	3	207	1/1	0.44	20.14	56,56,56,56	0
85	MG	6	2030	1/1	0.33	20.04	61,61,61,61	0
85	MG	5	3466	1/1	0.58	19.90	86,86,86,86	0
85	MG	5	3751	1/1	0.41	19.61	34,34,34,34	0
86	OHX	1	4199	7/7	0.34	19.33	101,101,101,101	0
85	MG	1	3728	1/1	0.51	19.22	21,21,21,21	0
85	MG	1	3765	1/1	0.30	19.18	38,38,38,38	0
85	MG	6	1920	1/1	0.35	19.12	57,57,57,57	0
85	MG	5	3886	1/1	0.41	19.05	46,46,46,46	0
85	MG	5	3593	1/1	0.40	19.03	27,27,27,27	0
85	MG	5	3880	1/1	0.44	18.99	36,36,36,36	0
85	MG	5	3764	1/1	0.67	18.96	27,27,27,27	0
85	MG	1	3677	1/1	0.26	18.86	34,34,34,34	0
85	MG	3	206	1/1	0.42	18.80	26,26,26,26	0
85	MG	7	205	1/1	0.38	18.75	19,19,19,19	0
85	MG	5	3535	1/1	0.41	18.67	25,25,25,25	0
86	OHX	5	4219	7/7	0.32	18.66	114,114,114,114	0
85	MG	1	3860	1/1	0.50	18.57	51,51,51,51	0
85	MG	1	3666	1/1	0.31	18.43	35,35,35,35	0
85	MG	1	3619	1/1	0.24	18.33	31,31,31,31	0
85	MG	4	201	1/1	0.33	18.29	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	5	3864	1/1	0.29	18.20	58,58,58,58	0
85	MG	1	3614	1/1	0.40	18.20	26,26,26,26	0
85	MG	2	1943	1/1	0.68	17.91	53,53,53,53	0
85	MG	1	3732	1/1	0.29	17.83	69,69,69,69	0
85	MG	5	4255	1/1	1.32	17.63	17,17,17,17	0
85	MG	8	209	1/1	0.75	17.45	51,51,51,51	0
85	MG	2	2002	1/1	0.31	17.41	87,87,87,87	0
85	MG	c7	202	1/1	0.50	16.95	65,65,65,65	0
85	MG	5	3763	1/1	0.60	16.87	25,25,25,25	0
85	MG	6	1947	1/1	0.44	16.76	48,48,48,48	0
85	MG	6	1957	1/1	0.44	16.31	52,52,52,52	0
85	MG	5	3536	1/1	0.34	16.15	25,25,25,25	0
85	MG	5	3832	1/1	0.61	16.14	21,21,21,21	0
85	MG	5	3869	1/1	0.41	16.00	23,23,23,23	0
85	MG	2	1958	1/1	0.36	15.93	58,58,58,58	0
86	OHX	5	4229	7/7	0.47	15.85	100,100,100,100	0
85	MG	5	3473	1/1	0.27	15.62	48,48,48,48	0
85	MG	1	3830	1/1	0.42	15.53	43,43,43,43	0
85	MG	1	3685	1/1	0.31	15.46	37,37,37,37	0
85	MG	1	3784	1/1	0.65	15.44	27,27,27,27	0
85	MG	1	3546	1/1	0.28	15.38	51,51,51,51	0
85	MG	1	3801	1/1	0.80	15.36	25,25,25,25	0
85	MG	5	3574	1/1	0.32	15.31	18,18,18,18	0
85	MG	5	3734	1/1	0.19	15.29	64,64,64,64	0
85	MG	1	3699	1/1	0.47	15.25	31,31,31,31	0
85	MG	1	3719	1/1	0.28	15.23	39,39,39,39	0
85	MG	1	3810	1/1	0.29	15.23	42,42,42,42	0
85	MG	6	1918	1/1	0.33	14.63	61,61,61,61	0
85	MG	1	3524	1/1	0.39	14.47	27,27,27,27	0
85	MG	5	3809	1/1	0.27	14.34	44,44,44,44	0
85	MG	5	3595	1/1	0.39	14.30	14,14,14,14	0
85	MG	2	1934	1/1	0.46	14.28	37,37,37,37	0
85	MG	1	3442	1/1	0.34	14.27	75,75,75,75	0
85	MG	3	201	1/1	0.52	14.16	54,54,54,54	0
85	MG	2	2013	1/1	0.24	14.00	41,41,41,41	0
85	MG	5	3552	1/1	0.33	13.94	33,33,33,33	0
85	MG	1	3606	1/1	0.23	13.92	56,56,56,56	0
85	MG	5	3420	1/1	0.35	13.80	56,56,56,56	0
85	MG	5	3576	1/1	0.33	13.79	26,26,26,26	0
85	MG	2	1914	1/1	0.38	13.75	51,51,51,51	0
85	MG	5	3660	1/1	0.34	13.72	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3556	1/1	0.37	13.70	25,25,25,25	0
85	MG	5	3835	1/1	0.37	13.70	29,29,29,29	0
85	MG	5	3686	1/1	0.84	13.65	67,67,67,67	0
85	MG	6	1922	1/1	0.28	13.60	50,50,50,50	0
85	MG	5	3673	1/1	0.34	13.52	53,53,53,53	0
85	MG	1	3836	1/1	0.31	13.50	44,44,44,44	0
85	MG	6	1916	1/1	0.47	13.48	59,59,59,59	0
85	MG	5	3846	1/1	0.64	13.20	21,21,21,21	0
85	MG	5	3895	1/1	0.37	13.08	83,83,83,83	0
85	MG	6	1946	1/1	0.36	13.01	56,56,56,56	0
85	MG	5	3852	1/1	0.30	13.00	53,53,53,53	0
85	MG	1	3469	1/1	0.36	13.00	35,35,35,35	0
85	MG	6	1982	1/1	0.39	12.99	58,58,58,58	0
85	MG	6	1907	1/1	0.30	12.93	59,59,59,59	0
85	MG	1	3624	1/1	0.54	12.90	87,87,87,87	0
85	MG	6	2009	1/1	0.29	12.87	46,46,46,46	0
85	MG	1	3506	1/1	0.37	12.85	30,30,30,30	0
85	MG	5	3683	1/1	0.84	12.84	24,24,24,24	0
86	OHX	1	4166	7/7	0.41	12.70	139,139,139,139	0
85	MG	7	201	1/1	0.51	12.65	32,32,32,32	0
85	MG	5	3829	1/1	0.30	12.63	36,36,36,36	0
85	MG	5	3575	1/1	0.25	12.59	30,30,30,30	0
85	MG	1	3791	1/1	0.66	12.29	27,27,27,27	0
85	MG	6	2020	1/1	0.34	12.28	42,42,42,42	0
85	MG	5	3708	1/1	0.42	12.21	83,83,83,83	0
85	MG	5	3529	1/1	0.35	12.13	20,20,20,20	0
86	OHX	1	4172	7/7	0.39	12.12	89,89,89,89	0
86	OHX	7	228	7/7	0.32	12.06	94,94,94,94	0
85	MG	2	1913	1/1	0.42	11.94	70,70,70,70	0
85	MG	1	3597	1/1	0.47	11.93	12,12,12,12	0
85	MG	6	1973	1/1	0.46	11.92	58,58,58,58	0
85	MG	1	3671	1/1	0.34	11.83	50,50,50,50	0
86	OHX	1	4184	7/7	0.25	11.77	97,97,97,97	0
85	MG	8	208	1/1	0.78	11.76	44,44,44,44	0
85	MG	1	3511	1/1	0.31	11.69	33,33,33,33	0
86	OHX	5	4239	7/7	0.31	11.69	137,137,137,137	0
85	MG	4	220	1/1	0.29	11.62	26,26,26,26	0
85	MG	1	3712	1/1	0.33	11.59	70,70,70,70	0
85	MG	5	3718	1/1	0.42	11.50	53,53,53,53	0
85	MG	M0	302	1/1	1.02	11.44	43,43,43,43	0
85	MG	1	3766	1/1	0.23	11.33	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	3566	1/1	0.40	11.28	26,26,26,26	0
85	MG	5	3782	1/1	1.17	11.24	68,68,68,68	0
85	MG	4	203	1/1	0.35	11.19	38,38,38,38	0
85	MG	1	3502	1/1	0.40	11.17	34,34,34,34	0
85	MG	1	3714	1/1	0.54	11.15	28,28,28,28	0
85	MG	2	2018	1/1	0.27	11.12	62,62,62,62	0
85	MG	6	1904	1/1	0.40	11.06	57,57,57,57	0
85	MG	2	1952	1/1	0.29	11.05	85,85,85,85	0
85	MG	6	2019	1/1	0.42	11.00	39,39,39,39	0
85	MG	6	1928	1/1	0.37	10.99	61,61,61,61	0
85	MG	5	3539	1/1	0.36	10.96	19,19,19,19	0
85	MG	1	3408	1/1	0.31	10.95	24,24,24,24	0
85	MG	3	212	1/1	0.28	10.78	54,54,54,54	0
85	MG	2	1926	1/1	0.47	10.77	71,71,71,71	0
85	MG	2	1995	1/1	0.32	10.77	78,78,78,78	0
86	OHX	1	4137	7/7	0.31	10.76	102,102,102,102	0
85	MG	1	4215	1/1	0.51	10.73	18,18,18,18	0
85	MG	6	1934	1/1	0.36	10.71	65,65,65,65	0
85	MG	1	3589	1/1	0.29	10.70	27,27,27,27	0
85	MG	5	3891	1/1	0.31	10.70	50,50,50,50	0
85	MG	1	3509	1/1	0.28	10.69	33,33,33,33	0
85	MG	5	3489	1/1	0.32	10.64	28,28,28,28	0
85	MG	2	2022	1/1	0.43	10.56	70,70,70,70	0
85	MG	1	3537	1/1	0.40	10.51	26,26,26,26	0
85	MG	4	222	1/1	0.52	10.46	76,76,76,76	0
85	MG	1	3682	1/1	0.36	10.37	34,34,34,34	0
85	MG	1	3647	1/1	0.44	10.35	35,35,35,35	0
85	MG	1	3773	1/1	0.32	10.27	46,46,46,46	0
85	MG	1	3419	1/1	0.37	10.16	70,70,70,70	0
86	OHX	1	4207	7/7	0.37	10.10	103,103,103,103	0
85	MG	2	1973	1/1	0.36	10.09	65,65,65,65	0
85	MG	6	2027	1/1	0.38	10.06	60,60,60,60	0
85	MG	4	216	1/1	0.91	9.96	39,39,39,39	0
85	MG	17	301	1/1	0.34	9.87	30,30,30,30	0
85	MG	2	1984	1/1	0.35	9.85	62,62,62,62	0
85	MG	5	3433	1/1	0.33	9.82	38,38,38,38	0
85	MG	1	3793	1/1	0.27	9.68	39,39,39,39	0
85	MG	5	3587	1/1	0.51	9.67	42,42,42,42	0
85	MG	1	3468	1/1	0.29	9.64	48,48,48,48	0
85	MG	1	3845	1/1	0.34	9.64	38,38,38,38	0
85	MG	1	3665	1/1	0.32	9.57	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1977	1/1	0.36	9.56	73,73,73,73	0
85	MG	6	1950	1/1	0.30	9.53	38,38,38,38	0
85	MG	4	207	1/1	0.34	9.50	22,22,22,22	0
85	MG	6	1931	1/1	0.49	9.47	56,56,56,56	0
85	MG	1	3543	1/1	0.32	9.44	26,26,26,26	0
85	MG	2	1981	1/1	0.42	9.41	46,46,46,46	0
85	MG	5	3524	1/1	0.36	9.41	20,20,20,20	0
85	MG	2	2017	1/1	0.49	9.41	67,67,67,67	0
85	MG	7	210	1/1	0.33	9.40	31,31,31,31	0
85	MG	1	3523	1/1	0.35	9.37	17,17,17,17	0
85	MG	1	3529	1/1	0.39	9.31	27,27,27,27	0
85	MG	2	1987	1/1	0.46	9.28	88,88,88,88	0
85	MG	5	3403	1/1	0.36	9.27	38,38,38,38	0
85	MG	1	3402	1/1	0.44	9.24	35,35,35,35	0
88	3J2	5	4254	26/26	0.53	9.22	19,19,19,19	0
85	MG	N3	202	1/1	0.58	9.18	54,54,54,54	0
85	MG	5	3707	1/1	0.42	9.16	35,35,35,35	0
85	MG	2	1991	1/1	0.31	9.14	98,98,98,98	0
86	OHX	5	4175	7/7	0.27	9.13	108,108,108,108	0
85	MG	5	3720	1/1	0.40	9.13	30,30,30,30	0
85	MG	1	3649	1/1	0.54	9.04	95,95,95,95	0
86	OHX	5	4148	7/7	0.33	8.97	99,99,99,99	0
85	MG	5	3650	1/1	0.47	8.96	58,58,58,58	0
86	OHX	1	4201	7/7	0.46	8.91	90,90,90,90	0
85	MG	1	3684	1/1	0.29	8.91	70,70,70,70	0
85	MG	1	3570	1/1	0.41	8.74	34,34,34,34	0
85	MG	5	4256	1/1	0.39	8.73	23,23,23,23	0
85	MG	1	3413	1/1	0.34	8.72	47,47,47,47	0
85	MG	1	3535	1/1	0.36	8.71	34,34,34,34	0
85	MG	1	3796	1/1	0.31	8.67	33,33,33,33	0
85	MG	5	3618	1/1	0.23	8.64	33,33,33,33	0
85	MG	6	1901	1/1	0.36	8.57	41,41,41,41	0
85	MG	5	3814	1/1	0.30	8.56	50,50,50,50	0
85	MG	5	3728	1/1	0.22	8.52	81,81,81,81	0
85	MG	5	3449	1/1	0.33	8.49	56,56,56,56	0
85	MG	1	3739	1/1	0.44	8.47	49,49,49,49	0
85	MG	5	3504	1/1	0.30	8.36	43,43,43,43	0
85	MG	6	2034	1/1	0.23	8.20	53,53,53,53	0
86	OHX	2	2160	7/7	0.33	8.11	134,134,134,134	0
85	MG	6	1903	1/1	0.26	8.09	39,39,39,39	0
85	MG	2	1968	1/1	0.55	8.06	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3667	1/1	0.27	8.05	64,64,64,64	0
85	MG	5	3581	1/1	0.32	7.95	28,28,28,28	0
85	MG	5	3512	1/1	0.31	7.92	45,45,45,45	0
85	MG	1	3633	1/1	0.51	7.91	43,43,43,43	0
85	MG	5	3409	1/1	0.29	7.90	32,32,32,32	0
85	MG	1	3758	1/1	0.32	7.88	20,20,20,20	0
85	MG	5	3626	1/1	0.27	7.85	44,44,44,44	0
85	MG	6	1943	1/1	0.31	7.85	32,32,32,32	0
85	MG	5	3806	1/1	0.31	7.77	75,75,75,75	0
86	OHX	5	4187	7/7	0.41	7.74	86,86,86,86	0
85	MG	1	3822	1/1	0.25	7.74	31,31,31,31	0
85	MG	8	207	1/1	0.26	7.73	53,53,53,53	0
85	MG	5	3563	1/1	0.33	7.69	21,21,21,21	0
85	MG	1	3698	1/1	0.43	7.67	28,28,28,28	0
85	MG	5	3714	1/1	0.28	7.66	38,38,38,38	0
85	MG	5	3850	1/1	0.30	7.59	35,35,35,35	0
85	MG	1	3587	1/1	0.31	7.57	21,21,21,21	0
85	MG	6	1948	1/1	0.33	7.55	33,33,33,33	0
85	MG	5	3685	1/1	0.30	7.47	54,54,54,54	0
85	MG	1	3722	1/1	0.57	7.44	44,44,44,44	0
85	MG	5	3743	1/1	0.26	7.44	22,22,22,22	0
85	MG	1	3816	1/1	0.24	7.41	44,44,44,44	0
85	MG	1	3858	1/1	0.29	7.36	125,125,125,125	0
85	MG	7	216	1/1	0.32	7.34	55,55,55,55	0
85	MG	5	3897	1/1	0.27	7.29	34,34,34,34	0
85	MG	5	3672	1/1	0.52	7.16	19,19,19,19	0
85	MG	1	3838	1/1	0.31	7.15	49,49,49,49	0
85	MG	1	3661	1/1	0.49	7.11	37,37,37,37	0
85	MG	5	3597	1/1	0.42	7.08	23,23,23,23	0
86	OHX	5	4221	7/7	0.24	7.07	112,112,112,112	0
85	MG	1	3412	1/1	0.29	7.06	28,28,28,28	0
85	MG	2	1996	1/1	0.35	7.00	48,48,48,48	0
85	MG	5	3633	1/1	0.41	6.97	71,71,71,71	0
85	MG	2	2007	1/1	0.51	6.96	60,60,60,60	0
85	MG	7	202	1/1	0.30	6.95	15,15,15,15	0
85	MG	5	3468	1/1	0.26	6.93	24,24,24,24	0
85	MG	2	1932	1/1	0.32	6.87	48,48,48,48	0
86	OHX	6	2177	7/7	0.29	6.84	100,100,100,100	0
85	MG	5	3578	1/1	0.31	6.81	19,19,19,19	0
85	MG	5	3678	1/1	0.28	6.79	34,34,34,34	0
86	OHX	2	2164	7/7	0.30	6.79	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	6	2163	7/7	0.32	6.76	99,99,99,99	0
85	MG	5	3567	1/1	0.30	6.75	19,19,19,19	0
85	MG	5	3740	1/1	0.26	6.74	52,52,52,52	0
85	MG	5	3813	1/1	0.57	6.67	45,45,45,45	0
85	MG	5	3646	1/1	0.24	6.65	40,40,40,40	0
85	MG	1	3786	1/1	0.98	6.64	15,15,15,15	0
85	MG	1	3711	1/1	0.89	6.62	40,40,40,40	0
85	MG	2	1959	1/1	0.44	6.57	80,80,80,80	0
86	OHX	5	4181	7/7	0.22	6.55	112,112,112,112	0
85	MG	5	3812	1/1	0.21	6.54	69,69,69,69	0
85	MG	2	1902	1/1	0.31	6.51	30,30,30,30	0
85	MG	5	3888	1/1	0.44	6.51	27,27,27,27	0
85	MG	5	3875	1/1	0.28	6.50	31,31,31,31	0
85	MG	1	3429	1/1	0.36	6.49	35,35,35,35	0
85	MG	1	3834	1/1	0.32	6.47	24,24,24,24	0
85	MG	1	4212	1/1	0.96	6.45	22,22,22,22	0
85	MG	5	3830	1/1	0.24	6.45	63,63,63,63	0
86	OHX	1	4187	7/7	0.27	6.43	120,120,120,120	0
85	MG	1	3803	1/1	0.63	6.43	193,193,193,193	0
85	MG	5	3722	1/1	0.22	6.42	43,43,43,43	0
85	MG	1	3538	1/1	0.26	6.38	30,30,30,30	0
85	MG	2	1919	1/1	0.45	6.36	63,63,63,63	0
86	OHX	8	228	7/7	0.26	6.33	103,103,103,103	0
85	MG	6	1917	1/1	0.36	6.30	46,46,46,46	0
85	MG	1	3694	1/1	0.30	6.30	38,38,38,38	0
85	MG	1	3515	1/1	0.42	6.24	28,28,28,28	0
85	MG	6	2042	1/1	0.59	6.21	100,100,100,100	0
85	MG	5	3821	1/1	0.30	6.16	34,34,34,34	0
85	MG	5	3777	1/1	0.29	6.10	44,44,44,44	0
86	OHX	1	4190	7/7	0.24	6.10	108,108,108,108	0
85	MG	2	1956	1/1	0.41	6.09	48,48,48,48	0
86	OHX	5	4238	7/7	0.27	6.07	103,103,103,103	0
85	MG	1	3648	1/1	0.29	6.06	49,49,49,49	0
85	MG	5	3560	1/1	0.31	6.06	19,19,19,19	0
85	MG	2	1975	1/1	0.41	6.06	73,73,73,73	0
85	MG	5	3794	1/1	0.44	6.03	34,34,34,34	0
85	MG	6	1967	1/1	0.38	6.02	64,64,64,64	0
86	OHX	5	4232	7/7	0.36	5.90	96,96,96,96	0
85	MG	6	1919	1/1	0.36	5.90	34,34,34,34	0
86	OHX	2	2172	7/7	0.40	5.88	120,120,120,120	0
85	MG	1	3526	1/1	0.28	5.79	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3484	1/1	0.32	5.73	38,38,38,38	0
85	MG	5	3545	1/1	0.28	5.72	33,33,33,33	0
85	MG	1	3462	1/1	0.34	5.72	18,18,18,18	0
85	MG	5	3653	1/1	0.28	5.69	54,54,54,54	0
85	MG	5	3603	1/1	0.33	5.68	23,23,23,23	0
85	MG	1	3815	1/1	0.25	5.67	32,32,32,32	0
85	MG	1	3452	1/1	0.25	5.63	35,35,35,35	0
85	MG	5	3803	1/1	0.30	5.57	34,34,34,34	0
85	MG	5	3566	1/1	0.28	5.43	17,17,17,17	0
85	MG	4	212	1/1	0.25	5.43	43,43,43,43	0
85	MG	1	3562	1/1	0.27	5.39	19,19,19,19	0
85	MG	1	3802	1/1	0.30	5.39	21,21,21,21	0
86	OHX	1	4058	7/7	0.25	5.38	96,96,96,96	0
85	MG	5	3496	1/1	0.27	5.37	23,23,23,23	0
85	MG	5	3503	1/1	0.34	5.35	22,22,22,22	0
86	OHX	14	403	7/7	0.29	5.35	119,119,119,119	0
85	MG	1	3522	1/1	0.37	5.34	24,24,24,24	0
86	OHX	1	4052	7/7	0.24	5.32	90,90,90,90	0
85	MG	1	3723	1/1	0.31	5.31	33,33,33,33	0
86	OHX	5	4159	7/7	0.39	5.29	99,99,99,99	0
85	MG	5	3431	1/1	0.25	5.27	65,65,65,65	0
85	MG	1	3450	1/1	0.34	5.26	29,29,29,29	0
86	OHX	6	2185	7/7	0.28	5.26	115,115,115,115	0
85	MG	6	1966	1/1	0.33	5.25	75,75,75,75	0
85	MG	2	1938	1/1	0.33	5.24	55,55,55,55	0
85	MG	6	1999	1/1	0.28	5.21	51,51,51,51	0
85	MG	1	3794	1/1	0.42	5.18	18,18,18,18	0
86	OHX	1	4185	7/7	0.50	5.14	109,109,109,109	0
85	MG	2	2001	1/1	0.25	5.14	67,67,67,67	0
85	MG	6	1923	1/1	0.25	5.12	61,61,61,61	0
85	MG	5	3584	1/1	0.40	5.09	23,23,23,23	0
85	MG	1	3513	1/1	0.31	5.07	16,16,16,16	0
85	MG	1	3664	1/1	0.24	5.06	66,66,66,66	0
85	MG	5	3582	1/1	0.33	5.05	32,32,32,32	0
85	MG	2	1929	1/1	0.43	5.05	54,54,54,54	0
86	OHX	1	4134	7/7	0.21	5.04	101,101,101,101	0
85	MG	2	1918	1/1	0.40	5.02	40,40,40,40	0
85	MG	6	1985	1/1	0.26	5.01	72,72,72,72	0
85	MG	5	3790	1/1	0.40	5.01	35,35,35,35	0
85	MG	1	3586	1/1	0.28	4.99	18,18,18,18	0
85	MG	N8	205	1/1	0.54	4.98	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	2009	1/1	0.33	4.96	44,44,44,44	0
85	MG	5	3472	1/1	0.47	4.94	25,25,25,25	0
85	MG	1	3418	1/1	0.33	4.90	40,40,40,40	0
85	MG	5	3594	1/1	0.39	4.88	32,32,32,32	0
85	MG	L2	303	1/1	0.33	4.87	37,37,37,37	0
85	MG	1	3590	1/1	0.37	4.86	35,35,35,35	0
85	MG	5	3745	1/1	0.28	4.82	43,43,43,43	0
85	MG	5	3827	1/1	0.48	4.77	28,28,28,28	0
86	OHX	1	4173	7/7	0.26	4.76	122,122,122,122	0
85	MG	1	3409	1/1	0.32	4.75	22,22,22,22	0
85	MG	5	3404	1/1	0.29	4.74	37,37,37,37	0
85	MG	L3	401	1/1	0.28	4.72	22,22,22,22	0
85	MG	2	1974	1/1	0.23	4.71	55,55,55,55	0
85	MG	L7	302	1/1	0.63	4.68	30,30,30,30	0
85	MG	5	3855	1/1	0.20	4.63	44,44,44,44	0
85	MG	1	3585	1/1	0.34	4.62	29,29,29,29	0
85	MG	6	2012	1/1	0.31	4.61	48,48,48,48	0
85	MG	5	3505	1/1	0.30	4.54	21,21,21,21	0
85	MG	5	3769	1/1	0.41	4.54	90,90,90,90	0
85	MG	1	3809	1/1	0.20	4.53	41,41,41,41	0
86	OHX	1	4057	7/7	0.22	4.52	112,112,112,112	0
85	MG	2	1971	1/1	0.30	4.51	58,58,58,58	0
85	MG	6	1981	1/1	0.28	4.51	60,60,60,60	0
85	MG	6	1913	1/1	0.32	4.49	31,31,31,31	0
85	MG	1	3430	1/1	0.29	4.48	30,30,30,30	0
85	MG	2	1978	1/1	0.33	4.48	77,77,77,77	0
85	MG	1	3525	1/1	0.27	4.45	17,17,17,17	0
86	OHX	5	4224	7/7	0.48	4.44	95,95,95,95	0
85	MG	5	3681	1/1	0.36	4.44	71,71,71,71	0
85	MG	5	3573	1/1	0.28	4.43	31,31,31,31	0
85	MG	5	3737	1/1	0.24	4.41	36,36,36,36	0
85	MG	6	1911	1/1	0.32	4.41	69,69,69,69	0
86	OHX	5	4152	7/7	0.34	4.41	82,82,82,82	0
86	OHX	6	2184	7/7	0.34	4.38	109,109,109,109	0
86	OHX	5	4110	7/7	0.26	4.37	102,102,102,102	0
85	MG	1	3504	1/1	0.32	4.37	32,32,32,32	0
85	MG	1	3634	1/1	0.27	4.35	61,61,61,61	0
85	MG	1	3828	1/1	0.33	4.34	24,24,24,24	0
85	MG	N5	201	1/1	0.38	4.32	50,50,50,50	0
85	MG	1	3536	1/1	0.29	4.31	34,34,34,34	0
85	MG	5	3530	1/1	0.29	4.31	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	5	3429	1/1	0.27	4.31	18,18,18,18	0
85	MG	1	3521	1/1	0.32	4.28	65,65,65,65	0
85	MG	5	3519	1/1	0.28	4.26	26,26,26,26	0
86	OHX	5	4248	7/7	0.22	4.26	120,120,120,120	0
86	OHX	5	4153	7/7	0.30	4.24	86,86,86,86	0
85	MG	N3	201	1/1	0.35	4.24	23,23,23,23	0
85	MG	5	3592	1/1	0.28	4.20	21,21,21,21	0
85	MG	1	3785	1/1	0.22	4.19	26,26,26,26	0
86	OHX	1	4202	7/7	0.27	4.19	100,100,100,100	0
85	MG	m1	202	1/1	0.25	4.18	46,46,46,46	0
85	MG	1	3670	1/1	0.45	4.18	45,45,45,45	0
86	OHX	1	4074	7/7	0.25	4.17	91,91,91,91	0
85	MG	5	3532	1/1	0.24	4.15	23,23,23,23	0
85	MG	1	3545	1/1	0.25	4.12	39,39,39,39	0
85	MG	5	3704	1/1	0.24	4.11	39,39,39,39	0
85	MG	M6	201	1/1	0.30	4.10	36,36,36,36	0
85	MG	1	3574	1/1	0.29	4.10	12,12,12,12	0
85	MG	2	1941	1/1	0.27	4.07	65,65,65,65	0
85	MG	5	3861	1/1	0.27	4.07	29,29,29,29	0
85	MG	1	3405	1/1	0.60	4.06	89,89,89,89	0
85	MG	5	3845	1/1	0.28	4.05	22,22,22,22	0
85	MG	2	1935	1/1	0.33	4.05	39,39,39,39	0
85	MG	2	1947	1/1	0.43	4.01	45,45,45,45	0
85	MG	1	3627	1/1	0.48	3.96	46,46,46,46	0
85	MG	o3	201	1/1	0.41	3.94	21,21,21,21	0
85	MG	5	3823	1/1	0.26	3.91	49,49,49,49	0
85	MG	2	1960	1/1	0.38	3.90	52,52,52,52	0
85	MG	1	3610	1/1	0.21	3.88	33,33,33,33	0
85	MG	5	3562	1/1	0.40	3.88	27,27,27,27	0
85	MG	7	215	1/1	0.25	3.86	34,34,34,34	0
85	MG	5	3762	1/1	0.20	3.85	31,31,31,31	0
86	OHX	5	4157	7/7	0.24	3.78	113,113,113,113	0
85	MG	2	1936	1/1	0.31	3.76	47,47,47,47	0
85	MG	1	3593	1/1	0.30	3.72	16,16,16,16	0
85	MG	1	3781	1/1	0.24	3.71	50,50,50,50	0
85	MG	5	3606	1/1	0.29	3.70	20,20,20,20	0
85	MG	1	3746	1/1	0.33	3.70	36,36,36,36	0
85	MG	5	3416	1/1	0.40	3.67	22,22,22,22	0
85	MG	1	3432	1/1	0.26	3.67	23,23,23,23	0
85	MG	5	3645	1/1	0.25	3.67	26,26,26,26	0
85	MG	1	3579	1/1	0.30	3.66	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4135	7/7	0.35	3.65	84,84,84,84	0
85	MG	5	3546	1/1	0.30	3.60	40,40,40,40	0
85	MG	5	3711	1/1	0.34	3.59	28,28,28,28	0
85	MG	5	3791	1/1	0.38	3.54	45,45,45,45	0
85	MG	5	3506	1/1	0.29	3.52	25,25,25,25	0
85	MG	5	3441	1/1	0.33	3.48	21,21,21,21	0
85	MG	4	221	1/1	0.28	3.47	39,39,39,39	0
85	MG	1	3676	1/1	0.26	3.47	35,35,35,35	0
85	MG	8	212	1/1	0.59	3.43	27,27,27,27	0
86	OHX	1	4167	7/7	0.32	3.43	107,107,107,107	0
85	MG	5	3569	1/1	0.32	3.42	21,21,21,21	0
85	MG	5	3547	1/1	0.28	3.42	39,39,39,39	0
85	MG	5	3706	1/1	0.26	3.39	29,29,29,29	0
85	MG	6	2035	1/1	0.40	3.39	43,43,43,43	0
85	MG	1	3460	1/1	0.24	3.35	18,18,18,18	0
86	OHX	5	4052	7/7	0.39	3.35	92,92,92,92	0
85	MG	1	3455	1/1	0.29	3.32	46,46,46,46	0
85	MG	1	3552	1/1	0.35	3.32	29,29,29,29	0
85	MG	5	3781	1/1	0.59	3.32	32,32,32,32	0
85	MG	1	3480	1/1	0.30	3.31	31,31,31,31	0
86	OHX	1	4090	7/7	0.25	3.31	98,98,98,98	0
86	OHX	5	4249	7/7	0.40	3.30	128,128,128,128	0
86	OHX	6	2171	7/7	0.30	3.28	96,96,96,96	0
86	OHX	1	4205	7/7	0.38	3.27	88,88,88,88	0
85	MG	8	203	1/1	0.35	3.26	31,31,31,31	0
86	OHX	1	4204	7/7	0.33	3.26	97,97,97,97	0
86	OHX	1	4068	7/7	0.40	3.25	75,75,75,75	0
86	OHX	1	3895	7/7	0.23	3.21	60,60,60,60	0
85	MG	2	1962	1/1	0.28	3.20	67,67,67,67	0
86	OHX	1	4138	7/7	0.20	3.19	110,110,110,110	0
86	OHX	2	2144	7/7	0.28	3.19	96,96,96,96	0
86	OHX	5	3906	7/7	0.22	3.18	42,42,42,42	0
85	MG	1	3594	1/1	0.35	3.17	13,13,13,13	0
85	MG	2	1915	1/1	0.31	3.17	56,56,56,56	0
85	MG	1	3631	1/1	0.37	3.17	18,18,18,18	0
85	MG	5	3621	1/1	0.25	3.14	45,45,45,45	0
85	MG	5	3605	1/1	0.22	3.13	39,39,39,39	0
86	OHX	1	4121	7/7	0.32	3.13	88,88,88,88	0
86	OHX	6	2129	7/7	0.28	3.11	81,81,81,81	0
86	OHX	6	2194	7/7	0.24	3.09	116,116,116,116	0
85	MG	5	3554	1/1	0.32	3.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3542	1/1	0.29	3.08	24,24,24,24	0
85	MG	5	3418	1/1	0.29	3.06	14,14,14,14	0
85	MG	M1	201	1/1	0.34	3.06	64,64,64,64	0
88	3J2	1	4209	26/26	0.38	3.05	19,19,19,19	0
86	OHX	1	4107	7/7	0.26	3.00	109,109,109,109	0
85	MG	5	3517	1/1	0.31	3.00	18,18,18,18	0
86	OHX	1	4182	7/7	0.32	3.00	161,161,161,161	0
85	MG	5	3801	1/1	0.24	2.99	36,36,36,36	0
85	MG	1	3573	1/1	0.26	2.98	27,27,27,27	0
86	OHX	1	3919	7/7	0.20	2.98	92,92,92,92	0
86	OHX	6	2208	7/7	0.28	2.97	118,118,118,118	0
85	MG	1	3760	1/1	0.31	2.97	33,33,33,33	0
85	MG	1	3812	1/1	0.25	2.94	37,37,37,37	0
85	MG	5	3667	1/1	0.32	2.92	19,19,19,19	0
86	OHX	2	2158	7/7	0.32	2.92	91,91,91,91	0
85	MG	6	2039	1/1	0.26	2.92	59,59,59,59	0
85	MG	6	2005	1/1	0.30	2.91	80,80,80,80	0
86	OHX	5	4141	7/7	0.26	2.90	96,96,96,96	0
85	MG	2	1954	1/1	0.25	2.87	85,85,85,85	0
85	MG	5	3726	1/1	0.27	2.83	43,43,43,43	0
85	MG	1	4216	1/1	0.56	2.82	16,16,16,16	0
85	MG	5	3500	1/1	0.28	2.82	20,20,20,20	0
86	OHX	1	4115	7/7	0.41	2.81	80,80,80,80	0
85	MG	5	3414	1/1	0.29	2.81	22,22,22,22	0
85	MG	2	1970	1/1	0.28	2.81	61,61,61,61	0
85	MG	l3	401	1/1	0.46	2.80	19,19,19,19	0
86	OHX	5	4186	7/7	0.24	2.80	102,102,102,102	0
86	OHX	1	4208	7/7	0.30	2.79	116,116,116,116	0
85	MG	5	3453	1/1	0.26	2.75	33,33,33,33	0
85	MG	4	202	1/1	0.32	2.75	44,44,44,44	0
85	MG	5	3463	1/1	0.39	2.73	32,32,32,32	0
85	MG	4	215	1/1	0.22	2.72	43,43,43,43	0
85	MG	1	3833	1/1	0.55	2.71	29,29,29,29	0
86	OHX	4	238	7/7	0.33	2.70	106,106,106,106	0
85	MG	M3	203	1/1	0.39	2.69	22,22,22,22	0
85	MG	1	3708	1/1	0.27	2.67	22,22,22,22	0
85	MG	6	2033	1/1	0.27	2.65	65,65,65,65	0
85	MG	1	3623	1/1	0.20	2.65	42,42,42,42	0
85	MG	5	3544	1/1	0.35	2.64	41,41,41,41	0
85	MG	2	1905	1/1	0.32	2.64	52,52,52,52	0
85	MG	5	3638	1/1	0.29	2.64	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4080	7/7	0.24	2.63	82,82,82,82	0
85	MG	5	3451	1/1	0.25	2.63	25,25,25,25	0
85	MG	5	3556	1/1	0.30	2.63	16,16,16,16	0
85	MG	4	204	1/1	0.45	2.63	49,49,49,49	0
85	MG	5	3440	1/1	0.30	2.62	25,25,25,25	0
85	MG	6	1968	1/1	0.33	2.61	64,64,64,64	0
86	OHX	1	4164	7/7	0.25	2.61	91,91,91,91	0
85	MG	6	1964	1/1	0.25	2.59	48,48,48,48	0
85	MG	5	3631	1/1	0.47	2.58	34,34,34,34	0
86	OHX	5	4087	7/7	0.31	2.58	76,76,76,76	0
86	OHX	6	2159	7/7	0.32	2.58	134,134,134,134	0
86	OHX	5	4145	7/7	0.24	2.57	89,89,89,89	0
85	MG	2	2006	1/1	0.28	2.56	45,45,45,45	0
86	OHX	5	3953	7/7	0.20	2.55	95,95,95,95	0
85	MG	5	3775	1/1	0.20	2.53	46,46,46,46	0
85	MG	6	1979	1/1	0.31	2.53	38,38,38,38	0
85	MG	5	3498	1/1	0.24	2.52	21,21,21,21	0
85	MG	2	1908	1/1	0.28	2.51	55,55,55,55	0
85	MG	1	3843	1/1	0.27	2.51	41,41,41,41	0
85	MG	1	3680	1/1	0.28	2.50	31,31,31,31	0
86	OHX	5	4161	7/7	0.23	2.49	90,90,90,90	0
85	MG	7	207	1/1	0.20	2.46	48,48,48,48	0
86	OHX	1	4136	7/7	0.24	2.44	103,103,103,103	0
86	OHX	1	4155	7/7	0.20	2.44	126,126,126,126	0
86	OHX	2	2149	7/7	0.29	2.44	85,85,85,85	0
86	OHX	5	4235	7/7	0.40	2.43	126,126,126,126	0
86	OHX	1	4162	7/7	0.27	2.42	85,85,85,85	0
85	MG	5	3518	1/1	0.30	2.42	17,17,17,17	0
85	MG	5	3485	1/1	0.23	2.41	30,30,30,30	0
85	MG	5	3698	1/1	0.24	2.41	30,30,30,30	0
85	MG	d3	202	1/1	0.53	2.40	44,44,44,44	0
85	MG	1	3820	1/1	0.20	2.39	47,47,47,47	0
85	MG	1	3591	1/1	0.26	2.38	57,57,57,57	0
85	MG	6	1955	1/1	0.43	2.38	34,34,34,34	0
85	MG	1	3472	1/1	0.21	2.37	20,20,20,20	0
85	MG	M8	201	1/1	0.39	2.36	44,44,44,44	0
85	MG	7	208	1/1	0.23	2.36	54,54,54,54	0
85	MG	5	3767	1/1	0.26	2.36	28,28,28,28	0
85	MG	1	3595	1/1	0.34	2.34	17,17,17,17	0
85	MG	m0	301	1/1	0.40	2.33	21,21,21,21	0
85	MG	5	3831	1/1	0.25	2.32	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	5	3894	1/1	0.26	2.30	40,40,40,40	0
85	MG	6	1961	1/1	0.27	2.27	57,57,57,57	0
85	MG	5	3486	1/1	0.23	2.23	38,38,38,38	0
86	OHX	5	4164	7/7	0.23	2.23	169,169,169,169	0
85	MG	m5	304	1/1	0.86	2.22	70,70,70,70	0
85	MG	1	3499	1/1	0.27	2.22	56,56,56,56	0
86	OHX	2	2092	7/7	0.24	2.21	112,112,112,112	0
85	MG	1	3559	1/1	0.26	2.20	16,16,16,16	0
85	MG	6	1929	1/1	0.24	2.20	51,51,51,51	0
85	MG	q0	202	1/1	0.37	2.20	28,28,28,28	0
86	OHX	5	4150	7/7	0.31	2.20	85,85,85,85	0
86	OHX	5	4195	7/7	0.40	2.16	100,100,100,100	0
85	MG	1	3819	1/1	0.52	2.16	27,27,27,27	0
86	OHX	1	3864	7/7	0.21	2.15	39,39,39,39	0
85	MG	2	1983	1/1	0.27	2.14	66,66,66,66	0
85	MG	5	3445	1/1	0.20	2.14	32,32,32,32	0
86	OHX	M7	204	7/7	0.41	2.14	74,74,74,74	0
85	MG	n3	201	1/1	0.29	2.14	18,18,18,18	0
85	MG	1	3621	1/1	0.40	2.13	24,24,24,24	0
85	MG	1	3510	1/1	0.29	2.12	20,20,20,20	0
85	MG	1	3596	1/1	0.31	2.09	25,25,25,25	0
86	OHX	1	4194	7/7	0.23	2.09	99,99,99,99	0
85	MG	5	3571	1/1	0.25	2.09	29,29,29,29	0
86	OHX	4	236	7/7	0.20	2.09	112,112,112,112	0
85	MG	n0	201	1/1	0.29	2.08	32,32,32,32	0
85	MG	5	3748	1/1	0.27	2.08	37,37,37,37	0
85	MG	M7	201	1/1	0.47	2.07	55,55,55,55	0
86	OHX	5	3909	7/7	0.23	2.06	42,42,42,42	0
85	MG	1	3518	1/1	0.34	2.05	17,17,17,17	0
86	OHX	2	2176	7/7	0.21	2.05	111,111,111,111	0
85	MG	2	1951	1/1	0.31	2.04	79,79,79,79	0
85	MG	N8	203	1/1	0.26	2.03	23,23,23,23	0
85	MG	5	3483	1/1	0.31	2.02	18,18,18,18	0
85	MG	1	3811	1/1	0.20	2.02	37,37,37,37	0
86	OHX	6	2190	7/7	0.26	2.02	120,120,120,120	0
85	MG	6	2013	1/1	0.41	2.02	48,48,48,48	0
85	MG	1	3470	1/1	0.27	2.00	29,29,29,29	0
85	MG	6	2032	1/1	0.23	2.00	92,92,92,92	0
85	MG	5	3883	1/1	0.24	2.00	39,39,39,39	0
86	OHX	1	3892	7/7	0.19	1.99	54,54,54,54	0
86	OHX	5	3901	7/7	0.22	1.98	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	6	2003	1/1	0.26	1.98	46,46,46,46	0
85	MG	5	3402	1/1	0.24	1.96	17,17,17,17	0
86	OHX	1	4108	7/7	0.38	1.96	84,84,84,84	0
85	MG	5	3872	1/1	0.29	1.95	43,43,43,43	0
85	MG	5	3432	1/1	0.30	1.94	24,24,24,24	0
86	OHX	7	220	7/7	0.21	1.93	70,70,70,70	0
85	MG	5	3526	1/1	0.27	1.93	24,24,24,24	0
86	OHX	1	3949	7/7	0.19	1.93	98,98,98,98	0
86	OHX	6	2050	7/7	0.21	1.93	59,59,59,59	0
85	MG	L8	301	1/1	0.37	1.88	52,52,52,52	0
86	OHX	2	2179	7/7	0.24	1.86	115,115,115,115	0
85	MG	5	3531	1/1	0.29	1.86	37,37,37,37	0
85	MG	5	3446	1/1	0.21	1.85	23,23,23,23	0
85	MG	1	3775	1/1	0.29	1.84	36,36,36,36	0
86	OHX	5	4178	7/7	0.29	1.84	80,80,80,80	0
85	MG	5	3786	1/1	0.28	1.84	72,72,72,72	0
85	MG	m6	201	1/1	0.28	1.84	21,21,21,21	0
85	MG	5	3724	1/1	0.24	1.83	30,30,30,30	0
85	MG	6	1909	1/1	0.33	1.83	88,88,88,88	0
85	MG	1	3550	1/1	0.30	1.82	28,28,28,28	0
85	MG	1	3622	1/1	0.24	1.82	35,35,35,35	0
86	OHX	1	4192	7/7	0.33	1.80	108,108,108,108	0
87	ZN	d7	101	1/1	0.73	1.78	155,155,155,155	0
86	OHX	4	231	7/7	0.29	1.76	75,75,75,75	0
85	MG	1	3592	1/1	0.26	1.75	19,19,19,19	0
85	MG	6	1915	1/1	0.24	1.71	55,55,55,55	0
85	MG	5	3799	1/1	0.23	1.71	61,61,61,61	0
85	MG	5	3893	1/1	0.28	1.69	42,42,42,42	0
85	MG	1	3853	1/1	0.24	1.69	28,28,28,28	0
85	MG	d6	102	1/1	0.81	1.69	47,47,47,47	0
85	MG	5	3637	1/1	0.20	1.69	41,41,41,41	0
85	MG	6	2011	1/1	0.21	1.66	43,43,43,43	0
86	OHX	1	3869	7/7	0.20	1.66	43,43,43,43	0
86	OHX	5	4209	7/7	0.24	1.64	83,83,83,83	0
86	OHX	2	2136	7/7	0.32	1.63	103,103,103,103	0
85	MG	8	215	1/1	0.28	1.63	23,23,23,23	0
86	OHX	1	4165	7/7	0.20	1.63	125,125,125,125	0
85	MG	6	1986	1/1	0.29	1.61	64,64,64,64	0
86	OHX	5	4218	7/7	0.22	1.61	114,114,114,114	0
86	OHX	6	2052	7/7	0.21	1.60	60,60,60,60	0
86	OHX	6	2180	7/7	0.25	1.59	91,91,91,91	0
85	MG	6	1954	1/1	0.25	1.59	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	5	3499	1/1	0.29	1.59	28,28,28,28	0
86	OHX	1	4130	7/7	0.29	1.59	98,98,98,98	0
85	MG	1	3690	1/1	0.28	1.57	34,34,34,34	0
85	MG	O1	201	1/1	0.25	1.57	49,49,49,49	0
85	MG	5	3696	1/1	0.24	1.56	28,28,28,28	0
86	OHX	1	3871	7/7	0.21	1.56	46,46,46,46	0
85	MG	N8	202	1/1	0.56	1.55	40,40,40,40	0
85	MG	m7	205	1/1	0.51	1.55	27,27,27,27	0
85	MG	6	1989	1/1	0.21	1.55	42,42,42,42	0
85	MG	5	3625	1/1	0.22	1.54	52,52,52,52	0
85	MG	1	3497	1/1	0.23	1.54	30,30,30,30	0
85	MG	1	3829	1/1	0.33	1.53	15,15,15,15	0
85	MG	6	1908	1/1	0.24	1.53	38,38,38,38	0
86	OHX	2	2137	7/7	0.22	1.53	102,102,102,102	0
85	MG	2	1927	1/1	0.29	1.51	53,53,53,53	0
85	MG	5	3548	1/1	0.29	1.51	32,32,32,32	0
85	MG	1	3483	1/1	0.26	1.50	29,29,29,29	0
85	MG	2	1921	1/1	0.32	1.48	37,37,37,37	0
86	OHX	5	4237	7/7	0.24	1.48	115,115,115,115	0
85	MG	1	3824	1/1	0.20	1.47	17,17,17,17	0
86	OHX	6	2168	7/7	0.22	1.47	120,120,120,120	0
85	MG	2	1931	1/1	0.31	1.47	44,44,44,44	0
85	MG	5	3702	1/1	0.20	1.47	42,42,42,42	0
85	MG	5	3467	1/1	0.22	1.46	21,21,21,21	0
85	MG	2	1955	1/1	0.27	1.45	52,52,52,52	0
85	MG	5	3805	1/1	0.22	1.43	18,18,18,18	0
85	MG	5	3824	1/1	0.28	1.43	36,36,36,36	0
86	OHX	1	4178	7/7	0.29	1.43	108,108,108,108	0
86	OHX	6	2188	7/7	0.24	1.42	110,110,110,110	0
86	OHX	S9	201	7/7	0.42	1.41	110,110,110,110	0
85	MG	5	3457	1/1	0.21	1.41	25,25,25,25	0
85	MG	5	3596	1/1	0.26	1.41	24,24,24,24	0
85	MG	5	4257	1/1	0.32	1.41	19,19,19,19	0
86	OHX	5	4183	7/7	0.22	1.40	105,105,105,105	0
85	MG	1	3709	1/1	0.28	1.40	26,26,26,26	0
86	OHX	4	235	7/7	0.21	1.39	122,122,122,122	0
86	OHX	5	4231	7/7	0.24	1.38	138,138,138,138	0
85	MG	5	3549	1/1	0.26	1.38	43,43,43,43	0
85	MG	6	1960	1/1	0.28	1.37	38,38,38,38	0
85	MG	1	3440	1/1	0.29	1.36	29,29,29,29	0
85	MG	1	3779	1/1	0.19	1.36	41,41,41,41	0
86	OHX	2	2173	7/7	0.21	1.35	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	3863	7/7	0.22	1.35	32,32,32,32	0
85	MG	1	3636	1/1	0.31	1.33	41,41,41,41	0
85	MG	1	3445	1/1	0.32	1.31	32,32,32,32	0
86	OHX	5	4193	7/7	0.24	1.31	88,88,88,88	0
85	MG	5	3513	1/1	0.32	1.30	19,19,19,19	0
85	MG	5	3516	1/1	0.24	1.30	26,26,26,26	0
85	MG	3	202	1/1	0.22	1.29	36,36,36,36	0
85	MG	M4	201	1/1	0.26	1.28	44,44,44,44	0
85	MG	5	3847	1/1	0.33	1.25	42,42,42,42	0
85	MG	5	3610	1/1	0.23	1.25	37,37,37,37	0
85	MG	5	3428	1/1	0.26	1.24	38,38,38,38	0
86	OHX	1	4181	7/7	0.28	1.24	121,121,121,121	0
86	OHX	1	4131	7/7	0.26	1.24	86,86,86,86	0
86	OHX	6	2057	7/7	0.19	1.23	70,70,70,70	0
86	OHX	5	4216	7/7	0.24	1.22	113,113,113,113	0
85	MG	18	301	1/1	0.32	1.21	59,59,59,59	0
85	MG	1	3861	1/1	0.33	1.20	40,40,40,40	0
85	MG	1	3854	1/1	0.27	1.19	83,83,83,83	0
86	OHX	5	3900	7/7	0.24	1.19	36,36,36,36	0
86	OHX	O9	101	7/7	0.26	1.18	82,82,82,82	0
85	MG	1	3672	1/1	0.23	1.15	18,18,18,18	0
86	OHX	1	4154	7/7	0.22	1.15	99,99,99,99	0
85	MG	1	3555	1/1	0.31	1.15	19,19,19,19	0
85	MG	1	3635	1/1	0.27	1.15	34,34,34,34	0
85	MG	6	2210	1/1	0.29	1.14	58,58,58,58	0
85	MG	L4	402	1/1	0.38	1.14	18,18,18,18	0
85	MG	5	3841	1/1	0.22	1.14	23,23,23,23	0
85	MG	2	1916	1/1	0.24	1.14	43,43,43,43	0
86	OHX	5	4015	7/7	0.17	1.12	126,126,126,126	0
85	MG	1	3750	1/1	0.21	1.12	36,36,36,36	0
85	MG	4	211	1/1	0.31	1.11	33,33,33,33	0
85	MG	5	3553	1/1	0.28	1.10	23,23,23,23	0
85	MG	1	3401	1/1	0.34	1.10	33,33,33,33	0
85	MG	1	3465	1/1	0.24	1.09	42,42,42,42	0
85	MG	1	3640	1/1	0.25	1.09	26,26,26,26	0
85	MG	6	1951	1/1	0.31	1.05	59,59,59,59	0
86	OHX	1	4133	7/7	0.23	1.05	95,95,95,95	0
86	OHX	1	4197	7/7	0.29	1.04	109,109,109,109	0
85	MG	1	3534	1/1	0.34	1.03	17,17,17,17	0
85	MG	1	3612	1/1	0.28	1.03	25,25,25,25	0
86	OHX	2	2085	7/7	0.29	1.02	93,93,93,93	0
85	MG	5	3469	1/1	0.20	1.02	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	3601	1/1	0.37	1.01	24,24,24,24	0
86	OHX	14	402	7/7	0.26	1.01	117,117,117,117	0
86	OHX	6	2119	7/7	0.29	1.01	115,115,115,115	0
86	OHX	6	2191	7/7	0.20	1.01	136,136,136,136	0
85	MG	5	3509	1/1	0.30	1.00	23,23,23,23	0
85	MG	1	3479	1/1	0.24	1.00	67,67,67,67	0
86	OHX	6	2201	7/7	0.27	0.99	119,119,119,119	0
85	MG	5	3487	1/1	0.27	0.98	16,16,16,16	0
85	MG	13	402	1/1	0.33	0.98	17,17,17,17	0
85	MG	7	213	1/1	0.20	0.97	50,50,50,50	0
85	MG	6	2025	1/1	0.21	0.97	46,46,46,46	0
85	MG	1	4211	1/1	0.33	0.97	51,51,51,51	0
85	MG	5	3405	1/1	0.20	0.97	19,19,19,19	0
85	MG	5	3589	1/1	0.30	0.96	27,27,27,27	0
86	OHX	5	4204	7/7	0.23	0.96	115,115,115,115	0
85	MG	2	1999	1/1	0.26	0.93	85,85,85,85	0
85	MG	5	3543	1/1	0.21	0.93	21,21,21,21	0
86	OHX	1	3877	7/7	0.18	0.93	48,48,48,48	0
86	OHX	6	2205	7/7	0.33	0.92	123,123,123,123	0
85	MG	8	214	1/1	0.26	0.92	50,50,50,50	0
86	OHX	1	4073	7/7	0.28	0.92	89,89,89,89	0
86	OHX	1	4195	7/7	0.29	0.91	115,115,115,115	0
86	OHX	m7	206	7/7	0.34	0.90	94,94,94,94	0
86	OHX	5	3950	7/7	0.20	0.89	77,77,77,77	0
86	OHX	5	3915	7/7	0.21	0.89	47,47,47,47	0
86	OHX	6	2204	7/7	0.23	0.89	126,126,126,126	0
85	MG	5	3577	1/1	0.34	0.89	31,31,31,31	0
86	OHX	2	2138	7/7	0.21	0.89	139,139,139,139	0
86	OHX	5	4172	7/7	0.22	0.88	77,77,77,77	0
86	OHX	1	4078	7/7	0.32	0.86	92,92,92,92	0
86	OHX	5	3934	7/7	0.16	0.85	75,75,75,75	0
86	OHX	6	2181	7/7	0.45	0.85	103,103,103,103	0
85	MG	1	3651	1/1	0.25	0.83	30,30,30,30	0
85	MG	8	210	1/1	0.26	0.83	34,34,34,34	0
85	MG	4	217	1/1	0.17	0.82	51,51,51,51	0
85	MG	4	209	1/1	0.23	0.82	17,17,17,17	0
85	MG	5	3627	1/1	0.25	0.82	52,52,52,52	0
85	MG	2	2020	1/1	0.23	0.82	61,61,61,61	0
85	MG	1	3473	1/1	0.25	0.81	15,15,15,15	0
85	MG	5	3662	1/1	0.34	0.81	58,58,58,58	0
85	MG	2	1961	1/1	0.25	0.81	46,46,46,46	0
86	OHX	2	2029	7/7	0.19	0.80	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	6	1963	1/1	0.26	0.79	71,71,71,71	0
85	MG	5	3811	1/1	0.21	0.79	33,33,33,33	0
85	MG	2	1907	1/1	0.32	0.79	42,42,42,42	0
85	MG	2	1979	1/1	0.29	0.78	46,46,46,46	0
86	OHX	5	4155	7/7	0.23	0.78	104,104,104,104	0
85	MG	1	3652	1/1	0.29	0.77	19,19,19,19	0
85	MG	D0	201	1/1	0.31	0.77	61,61,61,61	0
86	OHX	1	4142	7/7	0.27	0.74	111,111,111,111	0
85	MG	s8	301	1/1	0.36	0.74	42,42,42,42	0
86	OHX	1	3948	7/7	0.17	0.74	103,103,103,103	0
85	MG	1	3438	1/1	0.30	0.74	20,20,20,20	0
85	MG	1	3800	1/1	0.23	0.74	53,53,53,53	0
85	MG	1	3608	1/1	0.18	0.74	32,32,32,32	0
85	MG	5	3819	1/1	0.24	0.73	46,46,46,46	0
86	OHX	5	4168	7/7	0.26	0.73	105,105,105,105	0
86	OHX	1	3939	7/7	0.20	0.72	75,75,75,75	0
85	MG	5	3825	1/1	0.21	0.72	26,26,26,26	0
85	MG	5	3439	1/1	0.23	0.71	21,21,21,21	0
85	MG	2	1988	1/1	0.44	0.71	63,63,63,63	0
86	OHX	5	4246	7/7	0.32	0.71	104,104,104,104	0
85	MG	6	1925	1/1	0.26	0.70	40,40,40,40	0
86	OHX	5	3989	7/7	0.17	0.70	93,93,93,93	0
86	OHX	1	4175	7/7	0.30	0.68	103,103,103,103	0
85	MG	5	3739	1/1	0.22	0.68	27,27,27,27	0
85	MG	6	1949	1/1	0.34	0.68	40,40,40,40	0
86	OHX	6	2202	7/7	0.27	0.66	114,114,114,114	0
85	MG	d3	201	1/1	0.31	0.66	36,36,36,36	0
86	OHX	1	4123	7/7	0.24	0.65	122,122,122,122	0
85	MG	6	1912	1/1	0.24	0.65	51,51,51,51	0
86	OHX	l5	304	7/7	0.23	0.65	115,115,115,115	0
85	MG	1	3482	1/1	0.29	0.64	39,39,39,39	0
85	MG	6	1902	1/1	0.23	0.64	46,46,46,46	0
85	MG	5	3537	1/1	0.28	0.64	25,25,25,25	0
86	OHX	5	4138	7/7	0.28	0.63	95,95,95,95	0
86	OHX	5	4211	7/7	0.28	0.62	85,85,85,85	0
86	OHX	5	4185	7/7	0.21	0.62	94,94,94,94	0
85	MG	1	3568	1/1	0.26	0.61	18,18,18,18	0
85	MG	1	3539	1/1	0.27	0.61	15,15,15,15	0
86	OHX	5	4225	7/7	0.36	0.61	110,110,110,110	0
85	MG	1	3561	1/1	0.28	0.60	25,25,25,25	0
85	MG	5	3407	1/1	0.20	0.60	29,29,29,29	0
86	OHX	5	4011	7/7	0.17	0.60	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2109	7/7	0.29	0.59	100,100,100,100	0
85	MG	2	1923	1/1	0.28	0.58	49,49,49,49	0
85	MG	5	3713	1/1	0.21	0.57	30,30,30,30	0
86	OHX	6	2150	7/7	0.23	0.57	87,87,87,87	0
85	MG	2	1928	1/1	0.24	0.56	66,66,66,66	0
86	OHX	5	3941	7/7	0.19	0.56	72,72,72,72	0
85	MG	1	3508	1/1	0.33	0.56	16,16,16,16	0
86	OHX	8	230	7/7	0.23	0.55	95,95,95,95	0
86	OHX	1	4198	7/7	0.26	0.55	101,101,101,101	0
86	OHX	1	4180	7/7	0.23	0.55	99,99,99,99	0
86	OHX	1	4158	7/7	0.25	0.55	124,124,124,124	0
85	MG	1	3609	1/1	0.20	0.55	31,31,31,31	0
85	MG	6	1965	1/1	0.24	0.55	60,60,60,60	0
86	OHX	6	2068	7/7	0.19	0.55	107,107,107,107	0
85	MG	2	1912	1/1	0.21	0.54	54,54,54,54	0
85	MG	5	3661	1/1	0.19	0.54	36,36,36,36	0
86	OHX	5	4196	7/7	0.21	0.54	129,129,129,129	0
85	MG	6	1906	1/1	0.28	0.53	40,40,40,40	0
85	MG	5	3426	1/1	0.21	0.53	31,31,31,31	0
86	OHX	5	4146	7/7	0.30	0.51	82,82,82,82	0
85	MG	1	3428	1/1	0.30	0.50	27,27,27,27	0
86	OHX	1	4189	7/7	0.23	0.50	114,114,114,114	0
86	OHX	1	4111	7/7	0.20	0.50	102,102,102,102	0
86	OHX	1	3889	7/7	0.20	0.50	63,63,63,63	0
85	MG	2	1964	1/1	0.21	0.49	80,80,80,80	0
85	MG	5	3570	1/1	0.26	0.49	17,17,17,17	0
85	MG	1	3710	1/1	0.29	0.49	51,51,51,51	0
85	MG	5	3629	1/1	0.21	0.49	29,29,29,29	0
86	OHX	2	2054	7/7	0.18	0.49	105,105,105,105	0
85	MG	2	1925	1/1	0.33	0.48	56,56,56,56	0
86	OHX	5	4206	7/7	0.36	0.48	112,112,112,112	0
86	OHX	1	4094	7/7	0.31	0.48	85,85,85,85	0
86	OHX	1	4169	7/7	0.17	0.47	146,146,146,146	0
85	MG	5	3585	1/1	0.27	0.47	15,15,15,15	0
85	MG	2	2008	1/1	0.29	0.47	39,39,39,39	0
86	OHX	5	3911	7/7	0.23	0.46	50,50,50,50	0
85	MG	1	3584	1/1	0.28	0.46	30,30,30,30	0
86	OHX	2	2103	7/7	0.19	0.46	117,117,117,117	0
85	MG	1	3831	1/1	0.22	0.45	20,20,20,20	0
86	OHX	6	2207	7/7	0.32	0.45	123,123,123,123	0
85	MG	6	1984	1/1	0.28	0.44	37,37,37,37	0
86	OHX	5	3940	7/7	0.20	0.44	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	n8	201	1/1	0.27	0.44	36,36,36,36	0
85	MG	2	1993	1/1	0.28	0.43	44,44,44,44	0
85	MG	5	3822	1/1	0.26	0.43	79,79,79,79	0
86	OHX	1	4096	7/7	0.16	0.43	129,129,129,129	0
86	OHX	6	2179	7/7	0.21	0.42	83,83,83,83	0
86	OHX	2	2141	7/7	0.18	0.42	132,132,132,132	0
85	MG	5	3580	1/1	0.22	0.42	22,22,22,22	0
86	OHX	5	4190	7/7	0.17	0.41	108,108,108,108	0
85	MG	1	3814	1/1	0.18	0.41	25,25,25,25	0
85	MG	2	1967	1/1	0.31	0.41	49,49,49,49	0
86	OHX	5	3916	7/7	0.20	0.40	45,45,45,45	0
85	MG	2	1946	1/1	0.32	0.40	48,48,48,48	0
85	MG	5	3642	1/1	0.24	0.39	41,41,41,41	0
86	OHX	1	4163	7/7	0.19	0.39	86,86,86,86	0
85	MG	N3	203	1/1	0.28	0.39	39,39,39,39	0
86	OHX	5	4250	7/7	0.21	0.36	101,101,101,101	0
86	OHX	5	4220	7/7	0.22	0.36	151,151,151,151	0
86	OHX	5	4036	7/7	0.16	0.35	106,106,106,106	0
85	MG	1	3655	1/1	0.21	0.35	29,29,29,29	0
86	OHX	1	3878	7/7	0.20	0.34	49,49,49,49	0
86	OHX	5	4136	7/7	0.28	0.34	103,103,103,103	0
85	MG	N0	201	1/1	0.25	0.33	36,36,36,36	0
85	MG	6	2036	1/1	0.27	0.33	55,55,55,55	0
86	OHX	1	3903	7/7	0.19	0.32	65,65,65,65	0
85	MG	5	3773	1/1	0.24	0.32	21,21,21,21	0
85	MG	1	3532	1/1	0.24	0.32	25,25,25,25	0
85	MG	1	3691	1/1	0.22	0.31	35,35,35,35	0
86	OHX	1	4065	7/7	0.29	0.31	87,87,87,87	0
86	OHX	1	3866	7/7	0.23	0.31	39,39,39,39	0
85	MG	1	3501	1/1	0.30	0.30	18,18,18,18	0
85	MG	2	1909	1/1	0.24	0.30	58,58,58,58	0
86	OHX	5	4112	7/7	0.24	0.30	74,74,74,74	0
85	MG	6	2044	1/1	0.33	0.30	63,63,63,63	0
85	MG	6	1905	1/1	0.30	0.30	47,47,47,47	0
86	OHX	2	2099	7/7	0.17	0.30	90,90,90,90	0
85	MG	2	1917	1/1	0.29	0.29	45,45,45,45	0
85	MG	m5	303	1/1	0.32	0.28	46,46,46,46	0
86	OHX	6	2055	7/7	0.21	0.28	64,64,64,64	0
86	OHX	1	3976	7/7	0.26	0.27	62,62,62,62	0
86	OHX	5	4132	7/7	0.18	0.27	86,86,86,86	0
86	OHX	2	2146	7/7	0.25	0.27	114,114,114,114	0
87	ZN	D7	101	1/1	0.30	0.27	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3583	1/1	0.30	0.26	40,40,40,40	0
85	MG	5	3742	1/1	0.24	0.26	26,26,26,26	0
85	MG	1	3533	1/1	0.22	0.26	19,19,19,19	0
85	MG	1	3620	1/1	0.23	0.25	27,27,27,27	0
85	MG	1	3716	1/1	0.17	0.25	57,57,57,57	0
86	OHX	5	3914	7/7	0.17	0.24	46,46,46,46	0
85	MG	5	3565	1/1	0.32	0.23	40,40,40,40	0
85	MG	1	3628	1/1	0.21	0.23	58,58,58,58	0
85	MG	m7	201	1/1	0.30	0.21	20,20,20,20	0
85	MG	2	1901	1/1	0.43	0.21	62,62,62,62	0
86	OHX	6	2160	7/7	0.19	0.21	113,113,113,113	0
85	MG	1	3689	1/1	0.33	0.21	24,24,24,24	0
86	OHX	5	4201	7/7	0.23	0.19	93,93,93,93	0
86	OHX	1	4176	7/7	0.20	0.19	106,106,106,106	0
86	OHX	5	3902	7/7	0.19	0.19	47,47,47,47	0
85	MG	6	1937	1/1	0.23	0.19	38,38,38,38	0
85	MG	1	3417	1/1	0.23	0.19	36,36,36,36	0
86	OHX	1	4203	7/7	0.21	0.19	99,99,99,99	0
85	MG	5	3701	1/1	0.20	0.18	26,26,26,26	0
85	MG	5	3756	1/1	0.20	0.18	37,37,37,37	0
85	MG	6	1976	1/1	0.21	0.18	52,52,52,52	0
86	OHX	6	2073	7/7	0.16	0.18	93,93,93,93	0
85	MG	5	3470	1/1	0.24	0.18	27,27,27,27	0
85	MG	5	3522	1/1	0.26	0.17	32,32,32,32	0
86	OHX	6	2139	7/7	0.19	0.17	108,108,108,108	0
85	MG	n8	204	1/1	0.26	0.16	30,30,30,30	0
85	MG	1	3851	1/1	0.23	0.16	13,13,13,13	0
86	OHX	M7	205	7/7	0.27	0.16	106,106,106,106	0
86	OHX	1	4143	7/7	0.20	0.15	127,127,127,127	0
86	OHX	1	4062	7/7	0.25	0.15	82,82,82,82	0
85	MG	1	3607	1/1	0.31	0.15	47,47,47,47	0
85	MG	1	3756	1/1	0.33	0.14	19,19,19,19	0
86	OHX	2	2135	7/7	0.28	0.14	109,109,109,109	0
85	MG	5	3721	1/1	0.24	0.13	29,29,29,29	0
85	MG	l5	301	1/1	0.22	0.13	50,50,50,50	0
85	MG	M3	201	1/1	0.34	0.13	35,35,35,35	0
85	MG	2	1933	1/1	0.23	0.12	58,58,58,58	0
85	MG	6	1983	1/1	0.35	0.11	37,37,37,37	0
85	MG	5	3413	1/1	0.23	0.11	32,32,32,32	0
86	OHX	5	4214	7/7	0.27	0.11	91,91,91,91	0
85	MG	2	2010	1/1	0.18	0.10	59,59,59,59	0
85	MG	1	3456	1/1	0.23	0.09	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2037	1/1	0.34	0.09	75,75,75,75	0
85	MG	6	1991	1/1	0.27	0.09	67,67,67,67	0
85	MG	5	3611	1/1	0.40	0.08	25,25,25,25	0
85	MG	5	3844	1/1	0.24	0.08	40,40,40,40	0
86	OHX	1	4087	7/7	0.21	0.08	85,85,85,85	0
86	OHX	7	218	7/7	0.21	0.07	70,70,70,70	0
86	OHX	5	4122	7/7	0.16	0.07	108,108,108,108	0
85	MG	7	209	1/1	0.24	0.07	43,43,43,43	0
86	OHX	1	3932	7/7	0.19	0.07	79,79,79,79	0
85	MG	5	3479	1/1	0.29	0.07	50,50,50,50	0
86	OHX	1	4128	7/7	0.23	0.06	89,89,89,89	0
85	MG	6	1996	1/1	0.21	0.06	35,35,35,35	0
86	OHX	2	2163	7/7	0.21	0.06	141,141,141,141	0
85	MG	S8	301	1/1	0.24	0.06	47,47,47,47	0
86	OHX	5	4212	7/7	0.20	0.06	106,106,106,106	0
86	OHX	6	2195	7/7	0.36	0.05	139,139,139,139	0
85	MG	1	3454	1/1	0.31	0.05	42,42,42,42	0
86	OHX	5	3905	7/7	0.20	0.04	43,43,43,43	0
86	OHX	5	4059	7/7	0.23	0.04	79,79,79,79	0
86	OHX	5	4173	7/7	0.22	0.04	64,64,64,64	0
85	MG	5	3838	1/1	0.30	0.03	23,23,23,23	0
85	MG	4	208	1/1	0.23	0.03	22,22,22,22	0
85	MG	1	3613	1/1	0.20	0.03	32,32,32,32	0
85	MG	5	3755	1/1	0.19	0.03	52,52,52,52	0
85	MG	1	3415	1/1	0.27	0.03	32,32,32,32	0
86	OHX	2	2100	7/7	0.26	0.01	124,124,124,124	0
85	MG	6	1935	1/1	0.26	0.01	54,54,54,54	0
85	MG	5	3551	1/1	0.25	0.00	34,34,34,34	0
86	OHX	1	4153	7/7	0.18	0.00	116,116,116,116	0
85	MG	5	3480	1/1	0.21	0.00	58,58,58,58	0
86	OHX	6	2098	7/7	0.17	0.00	105,105,105,105	0
85	MG	5	3796	1/1	0.25	0.00	44,44,44,44	0
86	OHX	6	2174	7/7	0.25	-0.00	85,85,85,85	0
86	OHX	4	237	7/7	0.21	0.00	102,102,102,102	0
85	MG	5	3422	1/1	0.24	-0.01	25,25,25,25	0
85	MG	1	3563	1/1	0.24	-0.01	33,33,33,33	0
86	OHX	6	2135	7/7	0.35	-0.01	104,104,104,104	0
85	MG	m1	201	1/1	0.27	-0.01	50,50,50,50	0
85	MG	5	3879	1/1	0.21	-0.02	26,26,26,26	0
85	MG	5	3802	1/1	0.19	-0.02	54,54,54,54	0
85	MG	1	3407	1/1	0.22	-0.02	30,30,30,30	0
85	MG	5	3599	1/1	0.19	-0.02	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	8	202	1/1	0.20	-0.03	22,22,22,22	0
85	MG	1	3771	1/1	0.26	-0.03	38,38,38,38	0
85	MG	1	3436	1/1	0.22	-0.03	21,21,21,21	0
86	OHX	2	2175	7/7	0.19	-0.05	144,144,144,144	0
85	MG	1	3743	1/1	0.19	-0.05	42,42,42,42	0
86	OHX	5	4114	7/7	0.20	-0.06	90,90,90,90	0
86	OHX	L4	403	7/7	0.19	-0.07	106,106,106,106	0
85	MG	5	3523	1/1	0.28	-0.07	27,27,27,27	0
85	MG	4	206	1/1	0.26	-0.07	21,21,21,21	0
86	OHX	6	2176	7/7	0.22	-0.07	122,122,122,122	0
85	MG	1	3817	1/1	0.20	-0.07	31,31,31,31	0
85	MG	2	1944	1/1	0.18	-0.08	53,53,53,53	0
86	OHX	6	2193	7/7	0.20	-0.08	110,110,110,110	0
86	OHX	5	4251	7/7	0.19	-0.08	129,129,129,129	0
86	OHX	1	3961	7/7	0.16	-0.08	101,101,101,101	0
85	MG	o1	201	1/1	0.23	-0.09	33,33,33,33	0
85	MG	1	3848	1/1	0.18	-0.09	29,29,29,29	0
85	MG	1	3696	1/1	0.21	-0.09	60,60,60,60	0
86	OHX	5	3951	7/7	0.17	-0.10	80,80,80,80	0
86	OHX	1	4070	7/7	0.18	-0.11	93,93,93,93	0
86	OHX	5	4207	7/7	0.26	-0.11	114,114,114,114	0
85	MG	6	1939	1/1	0.27	-0.11	52,52,52,52	0
86	OHX	5	4104	7/7	0.29	-0.11	83,83,83,83	0
86	OHX	1	4013	7/7	0.17	-0.12	133,133,133,133	0
86	OHX	1	4118	7/7	0.25	-0.13	73,73,73,73	0
85	MG	6	1956	1/1	0.28	-0.14	40,40,40,40	0
85	MG	5	3525	1/1	0.25	-0.14	33,33,33,33	0
86	OHX	s1	303	7/7	0.28	-0.15	141,141,141,141	0
86	OHX	1	4145	7/7	0.19	-0.15	126,126,126,126	0
85	MG	5	3732	1/1	0.22	-0.16	57,57,57,57	0
85	MG	O3	201	1/1	0.32	-0.16	56,56,56,56	0
86	OHX	1	3922	7/7	0.25	-0.16	80,80,80,80	0
86	OHX	5	4074	7/7	0.21	-0.17	99,99,99,99	0
85	MG	1	3488	1/1	0.34	-0.17	40,40,40,40	0
85	MG	M7	203	1/1	0.30	-0.18	27,27,27,27	0
85	MG	1	3420	1/1	0.38	-0.18	66,66,66,66	0
86	OHX	2	2153	7/7	0.21	-0.18	117,117,117,117	0
85	MG	6	1958	1/1	0.29	-0.18	43,43,43,43	0
85	MG	1	3629	1/1	0.21	-0.19	27,27,27,27	0
85	MG	6	2018	1/1	0.24	-0.19	42,42,42,42	0
86	OHX	1	4106	7/7	0.24	-0.19	79,79,79,79	0
85	MG	2	1980	1/1	0.25	-0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3826	1/1	0.19	-0.20	30,30,30,30	0
86	OHX	2	2034	7/7	0.20	-0.20	88,88,88,88	0
85	MG	1	3560	1/1	0.22	-0.21	32,32,32,32	0
86	OHX	6	2151	7/7	0.22	-0.21	109,109,109,109	0
86	OHX	2	2093	7/7	0.26	-0.21	91,91,91,91	0
86	OHX	2	2116	7/7	0.18	-0.21	115,115,115,115	0
85	MG	1	3494	1/1	0.18	-0.21	32,32,32,32	0
86	OHX	5	4107	7/7	0.22	-0.22	101,101,101,101	0
85	MG	5	3807	1/1	0.21	-0.23	24,24,24,24	0
85	MG	1	3478	1/1	0.22	-0.24	64,64,64,64	0
85	MG	5	3695	1/1	0.24	-0.24	56,56,56,56	0
85	MG	6	1933	1/1	0.26	-0.25	61,61,61,61	0
85	MG	6	1972	1/1	0.24	-0.25	60,60,60,60	0
86	OHX	1	3867	7/7	0.22	-0.25	44,44,44,44	0
86	OHX	1	4170	7/7	0.17	-0.25	108,108,108,108	0
86	OHX	5	4037	7/7	0.26	-0.26	64,64,64,64	0
85	MG	5	3622	1/1	0.23	-0.27	30,30,30,30	0
85	MG	s8	302	1/1	0.26	-0.27	37,37,37,37	0
86	OHX	5	4106	7/7	0.24	-0.27	95,95,95,95	0
85	MG	5	3877	1/1	0.24	-0.27	16,16,16,16	0
85	MG	2	1966	1/1	0.17	-0.28	69,69,69,69	0
86	OHX	5	3974	7/7	0.29	-0.28	76,76,76,76	0
85	MG	6	1952	1/1	0.24	-0.28	56,56,56,56	0
85	MG	5	3619	1/1	0.20	-0.29	44,44,44,44	0
85	MG	1	3844	1/1	0.19	-0.29	30,30,30,30	0
85	MG	1	3410	1/1	0.24	-0.29	35,35,35,35	0
85	MG	1	3404	1/1	0.24	-0.30	53,53,53,53	0
85	MG	sM	301	1/1	0.24	-0.30	31,31,31,31	0
86	OHX	2	2134	7/7	0.15	-0.31	132,132,132,132	0
86	OHX	1	4041	7/7	0.24	-0.31	82,82,82,82	0
85	MG	1	3441	1/1	0.23	-0.31	15,15,15,15	0
86	OHX	1	4139	7/7	0.21	-0.31	83,83,83,83	0
85	MG	5	3684	1/1	0.26	-0.32	36,36,36,36	0
86	OHX	1	3886	7/7	0.18	-0.32	62,62,62,62	0
85	MG	6	1995	1/1	0.23	-0.32	49,49,49,49	0
85	MG	m7	202	1/1	0.31	-0.32	24,24,24,24	0
85	MG	5	3541	1/1	0.21	-0.32	21,21,21,21	0
85	MG	6	1942	1/1	0.31	-0.33	28,28,28,28	0
85	MG	c8	201	1/1	0.23	-0.33	64,64,64,64	0
85	MG	2	2016	1/1	0.32	-0.33	57,57,57,57	0
85	MG	6	1936	1/1	0.21	-0.33	76,76,76,76	0
86	OHX	5	4247	7/7	0.20	-0.33	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3588	1/1	0.28	-0.34	31,31,31,31	0
86	OHX	6	2061	7/7	0.18	-0.34	79,79,79,79	0
85	MG	1	3558	1/1	0.20	-0.34	44,44,44,44	0
86	OHX	5	4245	7/7	0.20	-0.34	130,130,130,130	0
86	OHX	6	2197	7/7	0.21	-0.34	152,152,152,152	0
86	OHX	6	2178	7/7	0.19	-0.34	131,131,131,131	0
86	OHX	1	4059	7/7	0.18	-0.35	94,94,94,94	0
86	OHX	5	4039	7/7	0.18	-0.35	138,138,138,138	0
86	OHX	1	3902	7/7	0.17	-0.35	58,58,58,58	0
85	MG	2	2000	1/1	0.26	-0.35	59,59,59,59	0
86	OHX	6	2189	7/7	0.15	-0.35	146,146,146,146	0
85	MG	L5	301	1/1	0.32	-0.36	52,52,52,52	0
86	OHX	5	4226	7/7	0.21	-0.37	116,116,116,116	0
85	MG	1	3757	1/1	0.17	-0.37	35,35,35,35	0
85	MG	1	3446	1/1	0.24	-0.37	26,26,26,26	0
85	MG	1	3531	1/1	0.21	-0.37	17,17,17,17	0
85	MG	8	206	1/1	0.24	-0.37	42,42,42,42	0
86	OHX	5	4205	7/7	0.19	-0.37	110,110,110,110	0
85	MG	M9	201	1/1	0.23	-0.37	44,44,44,44	0
85	MG	1	3453	1/1	0.19	-0.37	25,25,25,25	0
85	MG	2	2023	1/1	0.23	-0.38	93,93,93,93	0
86	OHX	6	2186	7/7	0.20	-0.38	111,111,111,111	0
86	OHX	2	2177	7/7	0.29	-0.39	151,151,151,151	0
85	MG	2	1992	1/1	0.21	-0.39	82,82,82,82	0
86	OHX	1	3872	7/7	0.20	-0.39	43,43,43,43	0
86	OHX	5	4188	7/7	0.23	-0.39	137,137,137,137	0
85	MG	5	3417	1/1	0.19	-0.40	20,20,20,20	0
85	MG	M7	202	1/1	0.27	-0.40	23,23,23,23	0
86	OHX	5	4121	7/7	0.19	-0.40	108,108,108,108	0
86	OHX	5	3908	7/7	0.18	-0.40	47,47,47,47	0
86	OHX	6	2203	7/7	0.21	-0.41	123,123,123,123	0
85	MG	3	210	1/1	0.20	-0.41	49,49,49,49	0
86	OHX	d9	102	7/7	0.23	-0.41	135,135,135,135	0
85	MG	5	3602	1/1	0.20	-0.42	27,27,27,27	0
86	OHX	6	2192	7/7	0.30	-0.42	125,125,125,125	0
85	MG	L2	301	1/1	0.25	-0.43	20,20,20,20	0
86	OHX	1	4156	7/7	0.17	-0.43	122,122,122,122	0
86	OHX	1	4102	7/7	0.21	-0.43	88,88,88,88	0
85	MG	5	3568	1/1	0.24	-0.44	24,24,24,24	0
86	OHX	5	3912	7/7	0.20	-0.44	40,40,40,40	0
86	OHX	2	2169	7/7	0.17	-0.44	129,129,129,129	0
85	MG	6	1974	1/1	0.18	-0.44	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3907	7/7	0.20	-0.45	45,45,45,45	0
86	OHX	2	2145	7/7	0.18	-0.45	139,139,139,139	0
85	MG	5	3491	1/1	0.24	-0.45	51,51,51,51	0
85	MG	1	3581	1/1	0.24	-0.45	26,26,26,26	0
86	OHX	D9	102	7/7	0.23	-0.45	118,118,118,118	0
86	OHX	2	2151	7/7	0.20	-0.46	133,133,133,133	0
86	OHX	1	4188	7/7	0.16	-0.46	153,153,153,153	0
85	MG	5	3527	1/1	0.22	-0.47	46,46,46,46	0
86	OHX	5	4222	7/7	0.16	-0.47	132,132,132,132	0
85	MG	5	3478	1/1	0.17	-0.47	54,54,54,54	0
85	MG	5	3747	1/1	0.23	-0.48	30,30,30,30	0
86	OHX	2	2174	7/7	0.23	-0.48	132,132,132,132	0
86	OHX	1	4075	7/7	0.28	-0.48	91,91,91,91	0
86	OHX	5	3904	7/7	0.23	-0.49	39,39,39,39	0
85	MG	5	3771	1/1	0.21	-0.49	57,57,57,57	0
87	ZN	d9	101	1/1	0.17	-0.49	67,67,67,67	0
85	MG	2	2182	1/1	0.18	-0.49	70,70,70,70	0
86	OHX	5	3928	7/7	0.19	-0.50	54,54,54,54	0
85	MG	5	3839	1/1	0.15	-0.50	48,48,48,48	0
86	OHX	5	3975	7/7	0.17	-0.51	83,83,83,83	0
86	OHX	1	4160	7/7	0.21	-0.51	98,98,98,98	0
85	MG	M5	302	1/1	0.28	-0.51	39,39,39,39	0
85	MG	6	2024	1/1	0.26	-0.51	69,69,69,69	0
86	OHX	2	2180	7/7	0.34	-0.52	132,132,132,132	0
86	OHX	1	4179	7/7	0.16	-0.52	117,117,117,117	0
86	OHX	2	2166	7/7	0.15	-0.52	144,144,144,144	0
85	MG	6	1921	1/1	0.24	-0.53	41,41,41,41	0
85	MG	5	3510	1/1	0.24	-0.53	17,17,17,17	0
85	MG	5	3837	1/1	0.19	-0.53	46,46,46,46	0
86	OHX	5	4149	7/7	0.20	-0.53	122,122,122,122	0
86	OHX	1	3883	7/7	0.17	-0.54	53,53,53,53	0
86	OHX	1	4083	7/7	0.23	-0.54	95,95,95,95	0
86	OHX	1	3868	7/7	0.18	-0.54	40,40,40,40	0
85	MG	1	3557	1/1	0.19	-0.54	37,37,37,37	0
86	OHX	5	4042	7/7	0.18	-0.54	70,70,70,70	0
86	OHX	5	4119	7/7	0.16	-0.55	94,94,94,94	0
86	OHX	1	3925	7/7	0.16	-0.56	89,89,89,89	0
85	MG	5	3458	1/1	0.20	-0.56	61,61,61,61	0
85	MG	12	303	1/1	0.30	-0.57	28,28,28,28	0
86	OHX	5	4099	7/7	0.15	-0.57	101,101,101,101	0
86	OHX	O2	201	7/7	0.23	-0.57	70,70,70,70	0
86	OHX	m8	201	7/7	0.20	-0.57	104,104,104,104	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	0.23	-0.58	19,19,19,19	0
86	OHX	1	4084	7/7	0.27	-0.58	62,62,62,62	0
86	OHX	6	2049	7/7	0.19	-0.58	45,45,45,45	0
85	MG	1	3632	1/1	0.20	-0.58	49,49,49,49	0
86	OHX	1	3896	7/7	0.18	-0.59	57,57,57,57	0
85	MG	1	3639	1/1	0.17	-0.59	25,25,25,25	0
86	OHX	7	227	7/7	0.17	-0.59	127,127,127,127	0
86	OHX	M9	202	7/7	0.24	-0.59	142,142,142,142	0
85	MG	c7	201	1/1	0.19	-0.59	64,64,64,64	0
86	OHX	5	4098	7/7	0.20	-0.60	93,93,93,93	0
86	OHX	2	2161	7/7	0.16	-0.60	119,119,119,119	0
86	OHX	1	4053	7/7	0.19	-0.60	89,89,89,89	0
85	MG	N6	201	1/1	0.20	-0.61	33,33,33,33	0
85	MG	5	3694	1/1	0.16	-0.61	34,34,34,34	0
86	OHX	6	2053	7/7	0.19	-0.61	64,64,64,64	0
86	OHX	1	4177	7/7	0.19	-0.61	73,73,73,73	0
86	OHX	C8	201	7/7	0.17	-0.61	95,95,95,95	0
86	OHX	5	4244	7/7	0.13	-0.62	62,62,62,62	0
85	MG	5	3632	1/1	0.18	-0.62	23,23,23,23	0
85	MG	2	1920	1/1	0.23	-0.62	51,51,51,51	0
85	MG	5	3508	1/1	0.19	-0.62	30,30,30,30	0
86	OHX	m0	303	7/7	0.24	-0.62	92,92,92,92	0
85	MG	1	3527	1/1	0.28	-0.62	19,19,19,19	0
85	MG	5	3679	1/1	0.18	-0.62	33,33,33,33	0
85	MG	1	3514	1/1	0.26	-0.63	18,18,18,18	0
85	MG	1	3507	1/1	0.24	-0.63	20,20,20,20	0
86	OHX	1	4027	7/7	0.19	-0.64	101,101,101,101	0
86	OHX	1	4110	7/7	0.18	-0.64	90,90,90,90	0
85	MG	1	3605	1/1	0.22	-0.64	43,43,43,43	0
86	OHX	5	4191	7/7	0.16	-0.64	94,94,94,94	0
85	MG	1	3544	1/1	0.20	-0.64	28,28,28,28	0
86	OHX	5	3999	7/7	0.16	-0.64	84,84,84,84	0
86	OHX	2	2150	7/7	0.15	-0.65	134,134,134,134	0
86	OHX	6	2196	7/7	0.17	-0.65	131,131,131,131	0
86	OHX	6	2198	7/7	0.14	-0.65	152,152,152,152	0
85	MG	1	3686	1/1	0.28	-0.65	27,27,27,27	0
86	OHX	2	2121	7/7	0.18	-0.65	121,121,121,121	0
85	MG	1	3761	1/1	0.27	-0.66	36,36,36,36	0
85	MG	1	3748	1/1	0.17	-0.66	32,32,32,32	0
86	OHX	5	3967	7/7	0.16	-0.66	85,85,85,85	0
85	MG	6	2028	1/1	0.16	-0.67	76,76,76,76	0
85	MG	2	1972	1/1	0.24	-0.67	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4126	7/7	0.19	-0.68	124,124,124,124	0
86	OHX	2	2044	7/7	0.16	-0.68	94,94,94,94	0
86	OHX	6	2087	7/7	0.15	-0.68	116,116,116,116	0
86	OHX	6	2154	7/7	0.17	-0.68	91,91,91,91	0
86	OHX	5	4060	7/7	0.21	-0.68	102,102,102,102	0
86	OHX	5	4062	7/7	0.13	-0.68	127,127,127,127	0
85	MG	5	3863	1/1	0.19	-0.69	45,45,45,45	0
86	OHX	5	4151	7/7	0.20	-0.70	112,112,112,112	0
85	MG	5	3425	1/1	0.20	-0.70	27,27,27,27	0
86	OHX	1	3875	7/7	0.18	-0.70	43,43,43,43	0
85	MG	2	1990	1/1	0.24	-0.71	44,44,44,44	0
85	MG	5	3424	1/1	0.20	-0.71	47,47,47,47	0
86	OHX	5	4073	7/7	0.23	-0.71	86,86,86,86	0
85	MG	1	3505	1/1	0.22	-0.71	24,24,24,24	0
85	MG	5	3492	1/1	0.17	-0.71	30,30,30,30	0
86	OHX	1	4097	7/7	0.19	-0.71	102,102,102,102	0
85	MG	6	2023	1/1	0.19	-0.72	80,80,80,80	0
85	MG	N9	101	1/1	0.22	-0.72	19,19,19,19	0
85	MG	1	3416	1/1	0.18	-0.72	20,20,20,20	0
85	MG	5	3484	1/1	0.25	-0.73	32,32,32,32	0
86	OHX	8	216	7/7	0.18	-0.73	43,43,43,43	0
86	OHX	5	4202	7/7	0.16	-0.73	110,110,110,110	0
85	MG	5	3798	1/1	0.18	-0.74	32,32,32,32	0
85	MG	5	3495	1/1	0.20	-0.74	22,22,22,22	0
85	MG	1	3549	1/1	0.21	-0.74	26,26,26,26	0
85	MG	m7	204	1/1	0.24	-0.74	23,23,23,23	0
85	MG	5	3538	1/1	0.22	-0.74	15,15,15,15	0
86	OHX	1	4020	7/7	0.11	-0.74	115,115,115,115	0
85	MG	1	3720	1/1	0.22	-0.74	18,18,18,18	0
85	MG	1	3704	1/1	0.21	-0.75	55,55,55,55	0
86	OHX	5	3945	7/7	0.20	-0.75	63,63,63,63	0
85	MG	5	3856	1/1	0.22	-0.75	31,31,31,31	0
86	OHX	4	228	7/7	0.18	-0.75	87,87,87,87	0
86	OHX	2	2036	7/7	0.16	-0.75	80,80,80,80	0
85	MG	5	3715	1/1	0.18	-0.75	36,36,36,36	0
86	OHX	6	2182	7/7	0.18	-0.75	116,116,116,116	0
86	OHX	2	2128	7/7	0.17	-0.76	104,104,104,104	0
86	OHX	5	3966	7/7	0.17	-0.76	80,80,80,80	0
86	OHX	2	2117	7/7	0.20	-0.76	113,113,113,113	0
85	MG	n6	201	1/1	0.22	-0.77	47,47,47,47	0
86	OHX	2	2156	7/7	0.18	-0.77	118,118,118,118	0
85	MG	M3	202	1/1	0.32	-0.77	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	ZN	q3	501	1/1	0.14	-0.77	48,48,48,48	0
85	MG	2	1976	1/1	0.22	-0.77	44,44,44,44	0
86	OHX	1	4206	7/7	0.13	-0.78	126,126,126,126	0
85	MG	N8	201	1/1	0.24	-0.78	18,18,18,18	0
85	MG	5	3842	1/1	0.17	-0.79	40,40,40,40	0
85	MG	19	201	1/1	0.18	-0.79	27,27,27,27	0
86	OHX	2	2147	7/7	0.15	-0.79	97,97,97,97	0
85	MG	5	3710	1/1	0.20	-0.79	77,77,77,77	0
85	MG	1	3807	1/1	0.16	-0.79	36,36,36,36	0
85	MG	5	3579	1/1	0.23	-0.80	29,29,29,29	0
85	MG	5	3443	1/1	0.21	-0.80	16,16,16,16	0
85	MG	6	2001	1/1	0.19	-0.81	44,44,44,44	0
85	MG	6	1941	1/1	0.21	-0.81	42,42,42,42	0
86	OHX	5	4101	7/7	0.20	-0.81	74,74,74,74	0
85	MG	5	3768	1/1	0.17	-0.81	33,33,33,33	0
85	MG	1	3575	1/1	0.20	-0.82	17,17,17,17	0
85	MG	5	3601	1/1	0.16	-0.82	56,56,56,56	0
85	MG	5	3729	1/1	0.20	-0.82	19,19,19,19	0
86	OHX	2	2168	7/7	0.16	-0.83	93,93,93,93	0
85	MG	1	3517	1/1	0.21	-0.83	22,22,22,22	0
86	OHX	5	4089	7/7	0.24	-0.83	80,80,80,80	0
86	OHX	6	2085	7/7	0.16	-0.84	96,96,96,96	0
86	OHX	1	4183	7/7	0.20	-0.84	117,117,117,117	0
85	MG	5	3717	1/1	0.19	-0.84	38,38,38,38	0
85	MG	s1	301	1/1	0.23	-0.84	67,67,67,67	0
86	OHX	5	3919	7/7	0.19	-0.84	44,44,44,44	0
86	OHX	2	2086	7/7	0.13	-0.84	117,117,117,117	0
85	MG	D3	201	1/1	0.20	-0.84	41,41,41,41	0
86	OHX	m0	302	7/7	0.14	-0.84	102,102,102,102	0
85	MG	5	3648	1/1	0.18	-0.85	33,33,33,33	0
85	MG	5	3776	1/1	0.18	-0.85	44,44,44,44	0
86	OHX	1	3923	7/7	0.17	-0.86	66,66,66,66	0
85	MG	1	3458	1/1	0.16	-0.86	45,45,45,45	0
86	OHX	1	4127	7/7	0.15	-0.87	130,130,130,130	0
85	MG	1	3553	1/1	0.18	-0.87	33,33,33,33	0
86	OHX	2	2132	7/7	0.15	-0.87	95,95,95,95	0
85	MG	1	3679	1/1	0.19	-0.87	48,48,48,48	0
86	OHX	5	4140	7/7	0.19	-0.87	104,104,104,104	0
85	MG	7	212	1/1	0.18	-0.87	27,27,27,27	0
86	OHX	2	2048	7/7	0.12	-0.88	102,102,102,102	0
86	OHX	5	4144	7/7	0.22	-0.88	108,108,108,108	0
86	OHX	5	4233	7/7	0.17	-0.88	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	3949	7/7	0.15	-0.88	65,65,65,65	0
85	MG	5	3687	1/1	0.19	-0.88	30,30,30,30	0
86	OHX	2	2107	7/7	0.11	-0.88	86,86,86,86	0
86	OHX	1	4051	7/7	0.19	-0.89	72,72,72,72	0
86	OHX	6	2054	7/7	0.18	-0.89	53,53,53,53	0
85	MG	5	3733	1/1	0.16	-0.90	35,35,35,35	0
85	MG	5	3816	1/1	0.15	-0.90	30,30,30,30	0
86	OHX	1	3928	7/7	0.13	-0.90	86,86,86,86	0
86	OHX	1	4076	7/7	0.17	-0.90	88,88,88,88	0
86	OHX	13	404	7/7	0.17	-0.90	106,106,106,106	0
85	MG	6	2038	1/1	0.22	-0.91	71,71,71,71	0
86	OHX	5	3921	7/7	0.17	-0.91	52,52,52,52	0
85	MG	1	3774	1/1	0.17	-0.91	53,53,53,53	0
86	OHX	1	4140	7/7	0.14	-0.91	127,127,127,127	0
85	MG	5	3406	1/1	0.22	-0.92	33,33,33,33	0
85	MG	1	3444	1/1	0.22	-0.92	28,28,28,28	0
86	OHX	1	4171	7/7	0.15	-0.93	122,122,122,122	0
86	OHX	6	2199	7/7	0.14	-0.93	131,131,131,131	0
86	OHX	1	3921	7/7	0.12	-0.94	69,69,69,69	0
86	OHX	6	2140	7/7	0.17	-0.94	97,97,97,97	0
86	OHX	5	4171	7/7	0.19	-0.94	133,133,133,133	0
86	OHX	6	2127	7/7	0.09	-0.94	105,105,105,105	0
86	OHX	2	2075	7/7	0.20	-0.94	89,89,89,89	0
85	MG	5	3758	1/1	0.20	-0.95	55,55,55,55	0
85	MG	5	3620	1/1	0.24	-0.95	27,27,27,27	0
85	MG	5	3460	1/1	0.22	-0.95	19,19,19,19	0
86	OHX	2	2162	7/7	0.20	-0.95	132,132,132,132	0
86	OHX	6	2137	7/7	0.20	-0.96	105,105,105,105	0
86	OHX	6	2079	7/7	0.17	-0.97	91,91,91,91	0
85	MG	1	3727	1/1	0.19	-0.97	43,43,43,43	0
86	OHX	1	4161	7/7	0.11	-0.98	188,188,188,188	0
86	OHX	8	223	7/7	0.14	-0.98	87,87,87,87	0
86	OHX	5	4097	7/7	0.18	-0.98	110,110,110,110	0
86	OHX	5	4179	7/7	0.20	-0.98	110,110,110,110	0
86	OHX	6	2166	7/7	0.20	-0.98	102,102,102,102	0
86	OHX	1	4030	7/7	0.10	-0.98	118,118,118,118	0
85	MG	1	3567	1/1	0.19	-0.99	20,20,20,20	0
86	OHX	n9	102	7/7	0.17	-0.99	46,46,46,46	0
85	MG	1	3795	1/1	0.17	-0.99	40,40,40,40	0
85	MG	1	3554	1/1	0.20	-0.99	21,21,21,21	0
85	MG	6	1926	1/1	0.23	-0.99	42,42,42,42	0
86	OHX	C1	201	7/7	0.12	-0.99	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4189	7/7	0.15	-0.99	94,94,94,94	0
85	MG	5	3815	1/1	0.19	-0.99	29,29,29,29	0
86	OHX	s8	303	7/7	0.21	-1.00	136,136,136,136	0
85	MG	5	3749	1/1	0.12	-1.00	35,35,35,35	0
85	MG	1	3662	1/1	0.21	-1.00	35,35,35,35	0
85	MG	n9	101	1/1	0.19	-1.00	20,20,20,20	0
86	OHX	5	4072	7/7	0.15	-1.00	87,87,87,87	0
85	MG	1	3481	1/1	0.16	-1.00	24,24,24,24	0
85	MG	6	1970	1/1	0.17	-1.00	51,51,51,51	0
86	OHX	5	3997	7/7	0.14	-1.01	97,97,97,97	0
86	OHX	5	4117	7/7	0.17	-1.01	95,95,95,95	0
86	OHX	N9	102	7/7	0.17	-1.01	44,44,44,44	0
85	MG	5	3430	1/1	0.19	-1.02	19,19,19,19	0
85	MG	5	3697	1/1	0.19	-1.02	43,43,43,43	0
85	MG	1	3422	1/1	0.19	-1.02	21,21,21,21	0
86	OHX	8	231	7/7	0.19	-1.02	106,106,106,106	0
85	MG	5	3668	1/1	0.23	-1.02	29,29,29,29	0
86	OHX	1	3989	7/7	0.18	-1.02	80,80,80,80	0
85	MG	1	3862	1/1	0.21	-1.03	28,28,28,28	0
86	OHX	2	2124	7/7	0.15	-1.03	116,116,116,116	0
85	MG	5	3465	1/1	0.17	-1.03	50,50,50,50	0
86	OHX	1	4031	7/7	0.19	-1.03	95,95,95,95	0
85	MG	2	1910	1/1	0.19	-1.03	41,41,41,41	0
86	OHX	6	2165	7/7	0.14	-1.04	96,96,96,96	0
86	OHX	5	4147	7/7	0.18	-1.04	107,107,107,107	0
86	OHX	2	2069	7/7	0.12	-1.04	133,133,133,133	0
86	OHX	5	4066	7/7	0.17	-1.05	79,79,79,79	0
87	ZN	Q3	501	1/1	0.13	-1.05	43,43,43,43	0
85	MG	5	3411	1/1	0.22	-1.05	27,27,27,27	0
87	ZN	Q0	500	1/1	0.16	-1.05	31,31,31,31	0
86	OHX	1	3980	7/7	0.07	-1.05	86,86,86,86	0
86	OHX	1	4077	7/7	0.15	-1.06	110,110,110,110	0
85	MG	5	3609	1/1	0.23	-1.06	26,26,26,26	0
86	OHX	2	2031	7/7	0.17	-1.06	77,77,77,77	0
85	MG	5	3533	1/1	0.15	-1.06	39,39,39,39	0
86	OHX	5	3980	7/7	0.14	-1.06	70,70,70,70	0
85	MG	6	1997	1/1	0.16	-1.06	64,64,64,64	0
86	OHX	6	2144	7/7	0.12	-1.06	147,147,147,147	0
86	OHX	5	4090	7/7	0.19	-1.06	83,83,83,83	0
86	OHX	5	3917	7/7	0.16	-1.07	53,53,53,53	0
86	OHX	5	4169	7/7	0.17	-1.07	99,99,99,99	0
86	OHX	6	2114	7/7	0.20	-1.07	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3942	7/7	0.16	-1.07	70,70,70,70	0
86	OHX	1	3967	7/7	0.12	-1.08	98,98,98,98	0
85	MG	o4	201	1/1	0.18	-1.08	55,55,55,55	0
85	MG	5	3515	1/1	0.20	-1.08	20,20,20,20	0
86	OHX	2	2080	7/7	0.20	-1.08	93,93,93,93	0
85	MG	1	3406	1/1	0.23	-1.08	26,26,26,26	0
85	MG	1	3742	1/1	0.22	-1.08	35,35,35,35	0
86	OHX	1	3943	7/7	0.14	-1.08	82,82,82,82	0
85	MG	2	1939	1/1	0.09	-1.09	54,54,54,54	0
86	OHX	8	218	7/7	0.10	-1.10	89,89,89,89	0
86	OHX	2	2178	7/7	0.15	-1.10	152,152,152,152	0
85	MG	5	3664	1/1	0.20	-1.10	31,31,31,31	0
85	MG	1	3656	1/1	0.23	-1.11	19,19,19,19	0
86	OHX	S8	302	7/7	0.12	-1.11	133,133,133,133	0
85	MG	5	3727	1/1	0.22	-1.11	25,25,25,25	0
86	OHX	5	3903	7/7	0.18	-1.11	38,38,38,38	0
85	MG	5	3591	1/1	0.24	-1.12	18,18,18,18	0
85	MG	l2	302	1/1	0.20	-1.12	28,28,28,28	0
86	OHX	5	4069	7/7	0.23	-1.12	104,104,104,104	0
85	MG	1	3466	1/1	0.13	-1.12	37,37,37,37	0
86	OHX	6	2123	7/7	0.18	-1.12	84,84,84,84	0
86	OHX	6	2060	7/7	0.14	-1.12	72,72,72,72	0
86	OHX	2	2105	7/7	0.21	-1.13	89,89,89,89	0
85	MG	6	2014	1/1	0.21	-1.13	55,55,55,55	0
86	OHX	SR	401	7/7	0.12	-1.13	146,146,146,146	0
85	MG	5	3735	1/1	0.17	-1.13	27,27,27,27	0
86	OHX	2	2058	7/7	0.14	-1.13	114,114,114,114	0
86	OHX	2	2122	7/7	0.14	-1.14	116,116,116,116	0
87	ZN	q0	201	1/1	0.17	-1.14	21,21,21,21	0
85	MG	1	3615	1/1	0.14	-1.14	45,45,45,45	0
85	MG	1	3653	1/1	0.19	-1.14	36,36,36,36	0
87	ZN	e1	501	1/1	0.13	-1.15	143,143,143,143	0
85	MG	1	3683	1/1	0.19	-1.15	26,26,26,26	0
85	MG	O7	102	1/1	0.16	-1.15	27,27,27,27	0
86	OHX	1	4129	7/7	0.17	-1.15	108,108,108,108	0
85	MG	5	3488	1/1	0.18	-1.15	21,21,21,21	0
86	OHX	5	4194	7/7	0.17	-1.15	145,145,145,145	0
86	OHX	1	3917	7/7	0.14	-1.16	77,77,77,77	0
86	OHX	1	3981	7/7	0.17	-1.16	83,83,83,83	0
86	OHX	1	4003	7/7	0.12	-1.16	74,74,74,74	0
85	MG	1	3448	1/1	0.15	-1.16	27,27,27,27	0
86	OHX	2	2025	7/7	0.19	-1.16	65,65,65,65	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	0.17	-1.17	78,78,78,78	0
85	MG	2	1924	1/1	0.24	-1.17	67,67,67,67	0
86	OHX	1	4150	7/7	0.16	-1.18	98,98,98,98	0
86	OHX	5	4163	7/7	0.17	-1.18	117,117,117,117	0
86	OHX	5	3923	7/7	0.15	-1.18	47,47,47,47	0
85	MG	1	3675	1/1	0.19	-1.18	31,31,31,31	0
86	OHX	1	3998	7/7	0.22	-1.18	71,71,71,71	0
86	OHX	2	2043	7/7	0.11	-1.19	75,75,75,75	0
85	MG	4	218	1/1	0.15	-1.19	51,51,51,51	0
86	OHX	1	3884	7/7	0.17	-1.19	51,51,51,51	0
85	MG	2	1982	1/1	0.25	-1.19	59,59,59,59	0
85	MG	1	3496	1/1	0.21	-1.20	19,19,19,19	0
86	OHX	1	3969	7/7	0.18	-1.20	81,81,81,81	0
86	OHX	6	2131	7/7	0.16	-1.20	118,118,118,118	0
86	OHX	5	3956	7/7	0.14	-1.20	73,73,73,73	0
86	OHX	2	2033	7/7	0.14	-1.20	79,79,79,79	0
86	OHX	1	4060	7/7	0.21	-1.20	75,75,75,75	0
86	OHX	2	2087	7/7	0.15	-1.21	90,90,90,90	0
86	OHX	8	226	7/7	0.13	-1.21	96,96,96,96	0
85	MG	1	3678	1/1	0.21	-1.21	39,39,39,39	0
86	OHX	5	3913	7/7	0.19	-1.23	42,42,42,42	0
85	MG	2	1949	1/1	0.18	-1.23	43,43,43,43	0
86	OHX	6	2162	7/7	0.12	-1.23	89,89,89,89	0
86	OHX	1	3904	7/7	0.13	-1.23	54,54,54,54	0
86	OHX	5	3970	7/7	0.12	-1.23	78,78,78,78	0
85	MG	14	401	1/1	0.21	-1.24	22,22,22,22	0
86	OHX	s1	302	7/7	0.18	-1.24	71,71,71,71	0
86	OHX	2	2131	7/7	0.21	-1.24	92,92,92,92	0
85	MG	sM	302	1/1	0.13	-1.25	30,30,30,30	0
86	OHX	5	3976	7/7	0.15	-1.25	79,79,79,79	0
86	OHX	5	4197	7/7	0.16	-1.25	103,103,103,103	0
86	OHX	6	2124	7/7	0.09	-1.25	119,119,119,119	0
85	MG	q3	502	1/1	0.21	-1.25	66,66,66,66	0
86	OHX	1	3955	7/7	0.10	-1.25	75,75,75,75	0
86	OHX	5	4016	7/7	0.11	-1.25	101,101,101,101	0
85	MG	5	3691	1/1	0.20	-1.25	39,39,39,39	0
85	MG	1	3471	1/1	0.19	-1.25	28,28,28,28	0
85	MG	5	3419	1/1	0.17	-1.26	24,24,24,24	0
85	MG	1	4214	1/1	0.16	-1.26	42,42,42,42	0
86	OHX	M5	304	7/7	0.17	-1.26	85,85,85,85	0
86	OHX	5	4243	7/7	0.15	-1.26	213,213,213,213	0
85	MG	5	3586	1/1	0.18	-1.27	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	5	3557	1/1	0.24	-1.27	39,39,39,39	0
85	MG	1	3421	1/1	0.20	-1.28	24,24,24,24	0
86	OHX	7	219	7/7	0.16	-1.28	66,66,66,66	0
85	MG	6	1930	1/1	0.19	-1.28	50,50,50,50	0
86	OHX	5	4200	7/7	0.15	-1.29	89,89,89,89	0
85	MG	5	3731	1/1	0.17	-1.29	27,27,27,27	0
85	MG	5	3454	1/1	0.20	-1.29	35,35,35,35	0
85	MG	m5	302	1/1	0.17	-1.29	31,31,31,31	0
85	MG	5	3898	1/1	0.20	-1.29	23,23,23,23	0
86	OHX	5	4061	7/7	0.14	-1.29	99,99,99,99	0
86	OHX	1	3934	7/7	0.15	-1.29	78,78,78,78	0
85	MG	6	2006	1/1	0.19	-1.29	66,66,66,66	0
86	OHX	6	2152	7/7	0.19	-1.29	84,84,84,84	0
85	MG	5	3641	1/1	0.18	-1.29	25,25,25,25	0
86	OHX	1	3916	7/7	0.17	-1.30	77,77,77,77	0
85	MG	5	3608	1/1	0.17	-1.30	22,22,22,22	0
86	OHX	5	4176	7/7	0.16	-1.30	112,112,112,112	0
86	OHX	1	3865	7/7	0.16	-1.30	43,43,43,43	0
85	MG	5	3754	1/1	0.15	-1.30	35,35,35,35	0
86	OHX	c3	201	7/7	0.15	-1.30	128,128,128,128	0
85	MG	L7	301	1/1	0.17	-1.30	30,30,30,30	0
85	MG	1	3700	1/1	0.21	-1.31	35,35,35,35	0
85	MG	1	3641	1/1	0.14	-1.32	31,31,31,31	0
85	MG	n8	203	1/1	0.20	-1.32	16,16,16,16	0
86	OHX	1	3890	7/7	0.16	-1.32	49,49,49,49	0
86	OHX	2	2133	7/7	0.10	-1.32	123,123,123,123	0
86	OHX	5	4182	7/7	0.15	-1.32	119,119,119,119	0
86	OHX	5	4228	7/7	0.14	-1.32	133,133,133,133	0
85	MG	1	3431	1/1	0.21	-1.32	29,29,29,29	0
86	OHX	2	2068	7/7	0.13	-1.32	112,112,112,112	0
86	OHX	2	2140	7/7	0.20	-1.32	138,138,138,138	0
86	OHX	1	4119	7/7	0.14	-1.32	107,107,107,107	0
86	OHX	5	4203	7/7	0.15	-1.33	101,101,101,101	0
86	OHX	5	4006	7/7	0.12	-1.33	43,43,43,43	0
86	OHX	6	2136	7/7	0.17	-1.34	129,129,129,129	0
85	MG	5	3725	1/1	0.21	-1.34	26,26,26,26	0
86	OHX	2	2035	7/7	0.17	-1.35	79,79,79,79	0
85	MG	2	1994	1/1	0.16	-1.35	59,59,59,59	0
85	MG	5	3617	1/1	0.13	-1.35	32,32,32,32	0
86	OHX	6	2051	7/7	0.18	-1.35	51,51,51,51	0
86	OHX	1	3888	7/7	0.17	-1.35	47,47,47,47	0
86	OHX	2	2170	7/7	0.13	-1.35	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4029	7/7	0.12	-1.36	113,113,113,113	0
85	MG	n8	202	1/1	0.18	-1.36	24,24,24,24	0
86	OHX	1	4029	7/7	0.21	-1.37	80,80,80,80	0
85	MG	1	3414	1/1	0.19	-1.37	21,21,21,21	0
85	MG	1	3713	1/1	0.17	-1.38	22,22,22,22	0
86	OHX	2	2028	7/7	0.17	-1.38	56,56,56,56	0
85	MG	1	3530	1/1	0.16	-1.39	48,48,48,48	0
86	OHX	5	4137	7/7	0.15	-1.39	105,105,105,105	0
86	OHX	1	4026	7/7	0.16	-1.39	76,76,76,76	0
85	MG	o4	202	1/1	0.14	-1.40	61,61,61,61	0
85	MG	SM	3401	1/1	0.17	-1.41	41,41,41,41	0
85	MG	5	3612	1/1	0.17	-1.42	25,25,25,25	0
86	OHX	1	4079	7/7	0.11	-1.42	115,115,115,115	0
86	OHX	1	3931	7/7	0.14	-1.42	76,76,76,76	0
85	MG	5	3542	1/1	0.15	-1.42	57,57,57,57	0
86	OHX	2	2091	7/7	0.14	-1.42	93,93,93,93	0
85	MG	5	3870	1/1	0.22	-1.42	18,18,18,18	0
86	OHX	6	2091	7/7	0.10	-1.42	107,107,107,107	0
86	OHX	6	2103	7/7	0.10	-1.42	155,155,155,155	0
85	MG	l2	301	1/1	0.23	-1.43	32,32,32,32	0
86	OHX	1	4091	7/7	0.17	-1.43	118,118,118,118	0
86	OHX	1	4193	7/7	0.13	-1.43	104,104,104,104	0
86	OHX	1	3956	7/7	0.15	-1.43	68,68,68,68	0
85	MG	O4	201	1/1	0.12	-1.43	45,45,45,45	0
85	MG	L2	302	1/1	0.17	-1.44	23,23,23,23	0
86	OHX	6	2122	7/7	0.09	-1.45	95,95,95,95	0
86	OHX	1	4157	7/7	0.20	-1.45	115,115,115,115	0
85	MG	1	3764	1/1	0.12	-1.45	48,48,48,48	0
85	MG	2	1998	1/1	0.16	-1.45	63,63,63,63	0
86	OHX	6	2107	7/7	0.17	-1.45	92,92,92,92	0
86	OHX	1	4114	7/7	0.18	-1.45	96,96,96,96	0
85	MG	2	1965	1/1	0.19	-1.46	48,48,48,48	0
86	OHX	6	2155	7/7	0.17	-1.46	136,136,136,136	0
86	OHX	5	3933	7/7	0.18	-1.46	53,53,53,53	0
86	OHX	1	3975	7/7	0.18	-1.46	66,66,66,66	0
85	MG	5	3671	1/1	0.19	-1.46	42,42,42,42	0
86	OHX	6	2088	7/7	0.16	-1.46	82,82,82,82	0
85	MG	1	3600	1/1	0.15	-1.46	21,21,21,21	0
86	OHX	5	4088	7/7	0.10	-1.47	68,68,68,68	0
85	MG	m5	301	1/1	0.16	-1.47	38,38,38,38	0
85	MG	1	3551	1/1	0.22	-1.48	23,23,23,23	0
86	OHX	1	3965	7/7	0.13	-1.48	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	6	2173	7/7	0.18	-1.48	124,124,124,124	0
86	OHX	1	4122	7/7	0.16	-1.49	116,116,116,116	0
86	OHX	2	2030	7/7	0.16	-1.49	79,79,79,79	0
86	OHX	M8	202	7/7	0.14	-1.49	103,103,103,103	0
85	MG	2	1940	1/1	0.17	-1.49	50,50,50,50	0
85	MG	6	1969	1/1	0.19	-1.49	36,36,36,36	0
86	OHX	1	4072	7/7	0.11	-1.49	108,108,108,108	0
85	MG	1	3724	1/1	0.14	-1.49	32,32,32,32	0
85	MG	O7	103	1/1	0.20	-1.49	27,27,27,27	0
85	MG	5	3437	1/1	0.17	-1.49	35,35,35,35	0
85	MG	1	3734	1/1	0.18	-1.49	50,50,50,50	0
86	OHX	5	3959	7/7	0.15	-1.49	63,63,63,63	0
85	MG	1	3660	1/1	0.16	-1.50	46,46,46,46	0
86	OHX	5	4022	7/7	0.10	-1.50	97,97,97,97	0
85	MG	5	3474	1/1	0.15	-1.50	42,42,42,42	0
86	OHX	1	4056	7/7	0.10	-1.50	125,125,125,125	0
85	MG	5	3639	1/1	0.21	-1.51	28,28,28,28	0
86	OHX	6	2069	7/7	0.10	-1.51	73,73,73,73	0
86	OHX	1	4095	7/7	0.18	-1.52	90,90,90,90	0
85	MG	6	1994	1/1	0.14	-1.52	47,47,47,47	0
86	OHX	1	3927	7/7	0.17	-1.52	78,78,78,78	0
86	OHX	6	2075	7/7	0.12	-1.52	103,103,103,103	0
86	OHX	5	4234	7/7	0.13	-1.53	76,76,76,76	0
86	OHX	6	2115	7/7	0.18	-1.53	85,85,85,85	0
86	OHX	n6	202	7/7	0.11	-1.53	105,105,105,105	0
86	OHX	4	223	7/7	0.20	-1.53	41,41,41,41	0
86	OHX	1	3938	7/7	0.13	-1.53	93,93,93,93	0
85	MG	2	2005	1/1	0.16	-1.53	58,58,58,58	0
85	MG	1	3571	1/1	0.20	-1.53	23,23,23,23	0
85	MG	1	3799	1/1	0.18	-1.54	42,42,42,42	0
85	MG	M0	301	1/1	0.19	-1.54	32,32,32,32	0
86	OHX	5	4242	7/7	0.18	-1.54	164,164,164,164	0
85	MG	5	3640	1/1	0.12	-1.54	36,36,36,36	0
86	OHX	1	3911	7/7	0.13	-1.55	61,61,61,61	0
85	MG	1	3782	1/1	0.20	-1.55	35,35,35,35	0
86	OHX	5	4075	7/7	0.13	-1.56	141,141,141,141	0
86	OHX	2	2076	7/7	0.21	-1.56	115,115,115,115	0
85	MG	5	3415	1/1	0.16	-1.57	39,39,39,39	0
86	OHX	5	4199	7/7	0.18	-1.57	86,86,86,86	0
86	OHX	1	3909	7/7	0.18	-1.57	66,66,66,66	0
87	ZN	D9	101	1/1	0.13	-1.57	60,60,60,60	0
86	OHX	s4	301	7/7	0.18	-1.57	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3607	1/1	0.18	-1.58	19,19,19,19	0
86	OHX	5	4162	7/7	0.18	-1.58	87,87,87,87	0
86	OHX	5	3988	7/7	0.11	-1.58	71,71,71,71	0
86	OHX	1	3990	7/7	0.13	-1.58	112,112,112,112	0
86	OHX	m1	203	7/7	0.12	-1.58	119,119,119,119	0
85	MG	6	2026	1/1	0.24	-1.59	40,40,40,40	0
86	OHX	2	2171	7/7	0.14	-1.59	122,122,122,122	0
86	OHX	2	2032	7/7	0.17	-1.59	94,94,94,94	0
85	MG	5	3490	1/1	0.21	-1.60	39,39,39,39	0
85	MG	6	1992	1/1	0.23	-1.60	62,62,62,62	0
85	MG	1	3437	1/1	0.16	-1.60	36,36,36,36	0
86	OHX	2	2040	7/7	0.12	-1.60	74,74,74,74	0
86	OHX	1	4009	7/7	0.09	-1.60	112,112,112,112	0
86	OHX	1	3915	7/7	0.13	-1.61	64,64,64,64	0
86	OHX	5	4134	7/7	0.17	-1.61	92,92,92,92	0
86	OHX	5	3936	7/7	0.17	-1.62	60,60,60,60	0
87	ZN	d6	101	1/1	0.14	-1.62	49,49,49,49	0
85	MG	1	3459	1/1	0.21	-1.62	18,18,18,18	0
85	MG	1	3747	1/1	0.18	-1.62	35,35,35,35	0
86	OHX	1	4039	7/7	0.11	-1.62	85,85,85,85	0
85	MG	5	3514	1/1	0.16	-1.63	27,27,27,27	0
86	OHX	4	232	7/7	0.09	-1.63	121,121,121,121	0
86	OHX	2	2071	7/7	0.12	-1.63	102,102,102,102	0
87	ZN	E1	501	1/1	0.10	-1.64	104,104,104,104	0
86	OHX	7	224	7/7	0.07	-1.64	81,81,81,81	0
85	MG	3	211	1/1	0.17	-1.64	57,57,57,57	0
85	MG	6	1914	1/1	0.19	-1.64	61,61,61,61	0
85	MG	1	3427	1/1	0.10	-1.64	41,41,41,41	0
87	ZN	D6	500	1/1	0.10	-1.65	67,67,67,67	0
85	MG	5	3534	1/1	0.18	-1.65	29,29,29,29	0
85	MG	6	1959	1/1	0.17	-1.66	50,50,50,50	0
85	MG	5	3635	1/1	0.16	-1.66	36,36,36,36	0
85	MG	5	3818	1/1	0.17	-1.66	49,49,49,49	0
85	MG	5	3723	1/1	0.20	-1.66	34,34,34,34	0
85	MG	5	3752	1/1	0.16	-1.66	31,31,31,31	0
85	MG	1	3643	1/1	0.12	-1.67	51,51,51,51	0
87	ZN	Q2	501	1/1	0.06	-1.67	56,56,56,56	0
86	OHX	6	2086	7/7	0.07	-1.67	96,96,96,96	0
85	MG	2	1948	1/1	0.19	-1.68	72,72,72,72	0
85	MG	5	3785	1/1	0.16	-1.68	24,24,24,24	0
86	OHX	2	2078	7/7	0.13	-1.68	95,95,95,95	0
86	OHX	4	227	7/7	0.10	-1.68	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	3569	1/1	0.13	-1.68	15,15,15,15	0
86	OHX	1	3899	7/7	0.15	-1.69	63,63,63,63	0
86	OHX	6	2200	7/7	0.12	-1.69	148,148,148,148	0
86	OHX	5	4001	7/7	0.16	-1.70	51,51,51,51	0
85	MG	6	1938	1/1	0.15	-1.70	36,36,36,36	0
86	OHX	6	2071	7/7	0.13	-1.71	83,83,83,83	0
85	MG	5	3497	1/1	0.18	-1.71	38,38,38,38	0
86	OHX	1	4015	7/7	0.12	-1.71	105,105,105,105	0
87	ZN	O7	101	1/1	0.14	-1.71	22,22,22,22	0
85	MG	5	3853	1/1	0.22	-1.72	38,38,38,38	0
86	OHX	5	3983	7/7	0.10	-1.72	58,58,58,58	0
85	MG	2	1937	1/1	0.19	-1.72	47,47,47,47	0
86	OHX	6	2076	7/7	0.12	-1.72	123,123,123,123	0
86	OHX	5	4124	7/7	0.09	-1.72	124,124,124,124	0
86	OHX	6	2147	7/7	0.15	-1.73	107,107,107,107	0
86	OHX	1	3874	7/7	0.17	-1.73	47,47,47,47	0
85	MG	n8	205	1/1	0.16	-1.74	24,24,24,24	0
86	OHX	c8	203	7/7	0.07	-1.74	119,119,119,119	0
87	ZN	o7	501	1/1	0.15	-1.74	31,31,31,31	0
85	MG	1	3687	1/1	0.17	-1.74	38,38,38,38	0
85	MG	5	3464	1/1	0.21	-1.74	28,28,28,28	0
86	OHX	2	2152	7/7	0.13	-1.74	162,162,162,162	0
85	MG	1	3783	1/1	0.12	-1.75	40,40,40,40	0
85	MG	2	2181	1/1	0.12	-1.75	56,56,56,56	0
86	OHX	2	2038	7/7	0.14	-1.75	110,110,110,110	0
86	OHX	1	4116	7/7	0.14	-1.75	105,105,105,105	0
86	OHX	6	2056	7/7	0.17	-1.75	64,64,64,64	0
86	OHX	1	3873	7/7	0.17	-1.75	42,42,42,42	0
85	MG	5	3753	1/1	0.13	-1.76	38,38,38,38	0
86	OHX	1	4117	7/7	0.17	-1.76	115,115,115,115	0
85	MG	1	3697	1/1	0.18	-1.76	31,31,31,31	0
86	OHX	5	4128	7/7	0.09	-1.76	123,123,123,123	0
86	OHX	2	2047	7/7	0.10	-1.76	87,87,87,87	0
86	OHX	O7	104	7/7	0.11	-1.76	77,77,77,77	0
86	OHX	5	4131	7/7	0.09	-1.76	155,155,155,155	0
85	MG	1	3663	1/1	0.09	-1.76	26,26,26,26	0
85	MG	5	3604	1/1	0.17	-1.77	29,29,29,29	0
86	OHX	2	2097	7/7	0.12	-1.77	140,140,140,140	0
86	OHX	m9	201	7/7	0.16	-1.77	78,78,78,78	0
86	OHX	1	4048	7/7	0.14	-1.77	105,105,105,105	0
85	MG	1	3755	1/1	0.13	-1.77	36,36,36,36	0
86	OHX	2	2098	7/7	0.09	-1.77	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	3994	7/7	0.12	-1.77	141,141,141,141	0
86	OHX	5	4230	7/7	0.12	-1.78	158,158,158,158	0
85	MG	1	3837	1/1	0.18	-1.78	20,20,20,20	0
86	OHX	3	215	7/7	0.14	-1.78	77,77,77,77	0
85	MG	2	1930	1/1	0.17	-1.78	55,55,55,55	0
86	OHX	1	3881	7/7	0.16	-1.78	46,46,46,46	0
86	OHX	1	4099	7/7	0.10	-1.79	93,93,93,93	0
86	OHX	2	2157	7/7	0.13	-1.79	212,212,212,212	0
85	MG	1	3832	1/1	0.15	-1.79	29,29,29,29	0
85	MG	1	3642	1/1	0.13	-1.80	30,30,30,30	0
86	OHX	2	2042	7/7	0.13	-1.80	78,78,78,78	0
86	OHX	2	2024	7/7	0.18	-1.80	57,57,57,57	0
85	MG	5	3555	1/1	0.20	-1.81	38,38,38,38	0
86	OHX	2	2026	7/7	0.19	-1.81	71,71,71,71	0
85	MG	1	3495	1/1	0.18	-1.81	34,34,34,34	0
85	MG	1	3657	1/1	0.16	-1.81	19,19,19,19	0
86	OHX	5	4217	7/7	0.10	-1.82	74,74,74,74	0
86	OHX	1	3970	7/7	0.14	-1.84	73,73,73,73	0
86	OHX	1	4196	7/7	0.16	-1.84	108,108,108,108	0
87	ZN	q2	501	1/1	0.06	-1.85	51,51,51,51	0
86	OHX	6	2077	7/7	0.11	-1.85	67,67,67,67	0
86	OHX	2	2037	7/7	0.10	-1.86	72,72,72,72	0
86	OHX	5	4027	7/7	0.14	-1.86	68,68,68,68	0
85	MG	5	3868	1/1	0.20	-1.87	19,19,19,19	0
86	OHX	2	2090	7/7	0.11	-1.88	86,86,86,86	0
85	MG	5	3452	1/1	0.17	-1.88	23,23,23,23	0
85	MG	1	3424	1/1	0.19	-1.88	33,33,33,33	0
85	MG	1	3503	1/1	0.19	-1.88	17,17,17,17	0
85	MG	6	1990	1/1	0.14	-1.88	69,69,69,69	0
86	OHX	5	4044	7/7	0.17	-1.89	72,72,72,72	0
86	OHX	6	2099	7/7	0.13	-1.89	125,125,125,125	0
85	MG	5	3462	1/1	0.18	-1.89	23,23,23,23	0
85	MG	1	3702	1/1	0.18	-1.89	50,50,50,50	0
86	OHX	5	4068	7/7	0.16	-1.89	95,95,95,95	0
86	OHX	6	2084	7/7	0.11	-1.90	81,81,81,81	0
85	MG	1	3528	1/1	0.19	-1.90	35,35,35,35	0
86	OHX	5	4077	7/7	0.20	-1.90	97,97,97,97	0
86	OHX	1	3963	7/7	0.14	-1.91	46,46,46,46	0
85	MG	1	3733	1/1	0.16	-1.92	28,28,28,28	0
85	MG	1	3788	1/1	0.16	-1.92	73,73,73,73	0
86	OHX	1	3944	7/7	0.13	-1.92	68,68,68,68	0
86	OHX	q1	101	7/7	0.17	-1.93	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4109	7/7	0.16	-1.93	67,67,67,67	0
86	OHX	1	4100	7/7	0.15	-1.93	94,94,94,94	0
86	OHX	1	4036	7/7	0.12	-1.94	102,102,102,102	0
85	MG	4	214	1/1	0.15	-1.94	27,27,27,27	0
86	OHX	2	2094	7/7	0.13	-1.94	121,121,121,121	0
86	OHX	1	4124	7/7	0.14	-1.94	95,95,95,95	0
85	MG	M5	301	1/1	0.11	-1.94	26,26,26,26	0
86	OHX	1	4066	7/7	0.18	-1.94	102,102,102,102	0
86	OHX	4	234	7/7	0.15	-1.95	88,88,88,88	0
86	OHX	3	219	7/7	0.08	-1.96	95,95,95,95	0
85	MG	5	3757	1/1	0.17	-1.96	53,53,53,53	0
85	MG	1	3823	1/1	0.14	-1.97	44,44,44,44	0
85	MG	2	2004	1/1	0.15	-1.98	66,66,66,66	0
86	OHX	1	4151	7/7	0.16	-1.98	77,77,77,77	0
85	MG	1	3576	1/1	0.13	-1.99	17,17,17,17	0
86	OHX	1	4152	7/7	0.13	-1.99	84,84,84,84	0
85	MG	2	1911	1/1	0.21	-1.99	45,45,45,45	0
86	OHX	O3	202	7/7	0.17	-1.99	81,81,81,81	0
85	MG	5	3657	1/1	0.18	-2.00	34,34,34,34	0
86	OHX	5	3935	7/7	0.16	-2.00	52,52,52,52	0
85	MG	1	3476	1/1	0.14	-2.01	38,38,38,38	0
85	MG	5	3741	1/1	0.21	-2.02	17,17,17,17	0
86	OHX	1	4120	7/7	0.09	-2.02	117,117,117,117	0
85	MG	5	3665	1/1	0.15	-2.03	40,40,40,40	0
85	MG	1	3599	1/1	0.16	-2.03	17,17,17,17	0
86	OHX	5	4160	7/7	0.17	-2.04	95,95,95,95	0
86	OHX	6	2175	7/7	0.15	-2.04	122,122,122,122	0
86	OHX	5	4113	7/7	0.13	-2.04	87,87,87,87	0
86	OHX	1	3907	7/7	0.15	-2.04	70,70,70,70	0
86	OHX	C3	201	7/7	0.11	-2.04	131,131,131,131	0
86	OHX	2	2159	7/7	0.12	-2.05	255,255,255,255	0
85	MG	c8	202	1/1	0.17	-2.05	59,59,59,59	0
85	MG	1	3498	1/1	0.14	-2.05	23,23,23,23	0
85	MG	6	2209	1/1	0.10	-2.05	48,48,48,48	0
85	MG	5	3456	1/1	0.17	-2.05	16,16,16,16	0
86	OHX	1	3882	7/7	0.15	-2.06	42,42,42,42	0
85	MG	1	3457	1/1	0.16	-2.06	30,30,30,30	0
85	MG	1	3580	1/1	0.11	-2.06	27,27,27,27	0
85	MG	5	3520	1/1	0.20	-2.06	29,29,29,29	0
86	OHX	2	2095	7/7	0.10	-2.06	133,133,133,133	0
86	OHX	7	226	7/7	0.20	-2.07	84,84,84,84	0
85	MG	1	3804	1/1	0.14	-2.08	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	1	3492	1/1	0.16	-2.08	37,37,37,37	0
85	MG	5	3712	1/1	0.16	-2.08	53,53,53,53	0
85	MG	1	3658	1/1	0.17	-2.08	22,22,22,22	0
85	MG	1	3541	1/1	0.17	-2.09	17,17,17,17	0
85	MG	2	1985	1/1	0.14	-2.09	49,49,49,49	0
86	OHX	1	4105	7/7	0.14	-2.09	104,104,104,104	0
86	OHX	1	3952	7/7	0.16	-2.09	72,72,72,72	0
85	MG	m7	203	1/1	0.10	-2.09	35,35,35,35	0
86	OHX	2	2041	7/7	0.16	-2.09	80,80,80,80	0
86	OHX	5	3955	7/7	0.11	-2.09	72,72,72,72	0
85	MG	5	3521	1/1	0.20	-2.10	23,23,23,23	0
86	OHX	5	3957	7/7	0.17	-2.10	70,70,70,70	0
86	OHX	6	2067	7/7	0.14	-2.10	87,87,87,87	0
85	MG	5	3655	1/1	0.17	-2.11	32,32,32,32	0
86	OHX	5	4240	7/7	0.12	-2.11	116,116,116,116	0
86	OHX	2	2049	7/7	0.09	-2.11	90,90,90,90	0
86	OHX	1	3947	7/7	0.13	-2.11	89,89,89,89	0
86	OHX	2	2142	7/7	0.07	-2.11	146,146,146,146	0
86	OHX	1	4028	7/7	0.11	-2.12	77,77,77,77	0
86	OHX	n3	202	7/7	0.10	-2.12	64,64,64,64	0
85	MG	1	3423	1/1	0.18	-2.12	28,28,28,28	0
86	OHX	5	4051	7/7	0.20	-2.13	74,74,74,74	0
85	MG	1	3777	1/1	0.16	-2.13	46,46,46,46	0
86	OHX	sR	401	7/7	0.08	-2.13	142,142,142,142	0
86	OHX	5	3981	7/7	0.12	-2.13	80,80,80,80	0
86	OHX	1	4024	7/7	0.18	-2.14	85,85,85,85	0
85	MG	5	3459	1/1	0.19	-2.14	21,21,21,21	0
86	OHX	5	3925	7/7	0.17	-2.14	55,55,55,55	0
86	OHX	6	2097	7/7	0.09	-2.14	109,109,109,109	0
85	MG	1	3411	1/1	0.20	-2.15	20,20,20,20	0
86	OHX	1	4109	7/7	0.10	-2.16	148,148,148,148	0
85	MG	6	1978	1/1	0.16	-2.16	37,37,37,37	0
86	OHX	6	2132	7/7	0.12	-2.16	117,117,117,117	0
85	MG	1	3673	1/1	0.19	-2.16	51,51,51,51	0
86	OHX	1	4034	7/7	0.08	-2.16	87,87,87,87	0
86	OHX	2	2165	7/7	0.09	-2.17	153,153,153,153	0
85	MG	1	3792	1/1	0.20	-2.17	16,16,16,16	0
85	MG	6	1932	1/1	0.16	-2.18	37,37,37,37	0
86	OHX	2	2104	7/7	0.10	-2.18	185,185,185,185	0
86	OHX	1	4148	7/7	0.17	-2.18	107,107,107,107	0
86	OHX	M0	303	7/7	0.12	-2.18	92,92,92,92	0
85	MG	5	3636	1/1	0.12	-2.19	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	4210	1/1	0.14	-2.19	20,20,20,20	0
85	MG	5	3833	1/1	0.10	-2.20	60,60,60,60	0
85	MG	6	1927	1/1	0.21	-2.20	45,45,45,45	0
86	OHX	6	2206	7/7	0.06	-2.20	184,184,184,184	0
86	OHX	6	2121	7/7	0.11	-2.20	116,116,116,116	0
85	MG	L3	402	1/1	0.15	-2.20	38,38,38,38	0
85	MG	1	3840	1/1	0.15	-2.20	40,40,40,40	0
85	MG	1	3625	1/1	0.17	-2.20	25,25,25,25	0
85	MG	1	3491	1/1	0.18	-2.21	19,19,19,19	0
85	MG	1	3487	1/1	0.17	-2.21	24,24,24,24	0
86	OHX	1	4200	7/7	0.17	-2.21	104,104,104,104	0
86	OHX	5	4100	7/7	0.16	-2.21	125,125,125,125	0
85	MG	1	3604	1/1	0.13	-2.22	44,44,44,44	0
85	MG	5	3867	1/1	0.22	-2.22	15,15,15,15	0
85	MG	5	3766	1/1	0.13	-2.25	29,29,29,29	0
85	MG	5	3828	1/1	0.16	-2.26	18,18,18,18	0
86	OHX	d4	201	7/7	0.18	-2.27	133,133,133,133	0
86	OHX	5	3962	7/7	0.08	-2.27	71,71,71,71	0
85	MG	1	3669	1/1	0.22	-2.27	39,39,39,39	0
85	MG	1	3859	1/1	0.13	-2.27	55,55,55,55	0
86	OHX	1	4149	7/7	0.14	-2.28	112,112,112,112	0
85	MG	6	2017	1/1	0.16	-2.28	58,58,58,58	0
86	OHX	l5	302	7/7	0.09	-2.29	114,114,114,114	0
85	MG	1	3433	1/1	0.15	-2.29	37,37,37,37	0
85	MG	5	3455	1/1	0.09	-2.30	89,89,89,89	0
86	OHX	5	4035	7/7	0.09	-2.30	96,96,96,96	0
86	OHX	1	3993	7/7	0.19	-2.30	72,72,72,72	0
86	OHX	L3	404	7/7	0.09	-2.31	83,83,83,83	0
86	OHX	m5	305	7/7	0.17	-2.31	97,97,97,97	0
85	MG	5	3669	1/1	0.17	-2.31	24,24,24,24	0
86	OHX	O7	105	7/7	0.11	-2.32	68,68,68,68	0
86	OHX	6	2161	7/7	0.11	-2.32	111,111,111,111	0
85	MG	L4	401	1/1	0.17	-2.32	40,40,40,40	0
86	OHX	6	2142	7/7	0.14	-2.33	108,108,108,108	0
86	OHX	1	4002	7/7	0.15	-2.33	88,88,88,88	0
86	OHX	1	4043	7/7	0.07	-2.34	109,109,109,109	0
86	OHX	3	217	7/7	0.13	-2.34	81,81,81,81	0
86	OHX	1	3995	7/7	0.08	-2.35	123,123,123,123	0
85	MG	1	3725	1/1	0.14	-2.35	49,49,49,49	0
86	OHX	2	2139	7/7	0.12	-2.35	110,110,110,110	0
86	OHX	8	229	7/7	0.09	-2.35	111,111,111,111	0
86	OHX	5	3932	7/7	0.13	-2.35	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4034	7/7	0.13	-2.35	100,100,100,100	0
86	OHX	2	2062	7/7	0.09	-2.36	106,106,106,106	0
86	OHX	6	2143	7/7	0.15	-2.36	109,109,109,109	0
85	MG	5	3444	1/1	0.17	-2.36	21,21,21,21	0
86	OHX	13	403	7/7	0.11	-2.36	73,73,73,73	0
85	MG	5	3588	1/1	0.21	-2.36	17,17,17,17	0
86	OHX	1	3905	7/7	0.15	-2.37	66,66,66,66	0
85	MG	1	3645	1/1	0.18	-2.37	24,24,24,24	0
86	OHX	2	2089	7/7	0.14	-2.37	99,99,99,99	0
86	OHX	5	4108	7/7	0.14	-2.38	85,85,85,85	0
86	OHX	2	2070	7/7	0.12	-2.38	89,89,89,89	0
86	OHX	6	2102	7/7	0.10	-2.38	147,147,147,147	0
86	OHX	5	4170	7/7	0.08	-2.38	163,163,163,163	0
86	OHX	1	3908	7/7	0.17	-2.39	54,54,54,54	0
86	OHX	2	2109	7/7	0.12	-2.40	123,123,123,123	0
86	OHX	5	4103	7/7	0.08	-2.40	107,107,107,107	0
86	OHX	2	2120	7/7	0.13	-2.40	110,110,110,110	0
86	OHX	1	4022	7/7	0.12	-2.40	96,96,96,96	0
86	OHX	5	3929	7/7	0.15	-2.41	56,56,56,56	0
86	OHX	5	3971	7/7	0.13	-2.41	76,76,76,76	0
86	OHX	1	3900	7/7	0.16	-2.42	48,48,48,48	0
85	MG	1	3827	1/1	0.20	-2.43	17,17,17,17	0
85	MG	1	3692	1/1	0.18	-2.43	25,25,25,25	0
85	MG	1	3767	1/1	0.15	-2.44	17,17,17,17	0
86	OHX	q2	502	7/7	0.12	-2.44	57,57,57,57	0
86	OHX	2	2027	7/7	0.15	-2.45	66,66,66,66	0
86	OHX	5	4086	7/7	0.14	-2.46	82,82,82,82	0
86	OHX	5	4085	7/7	0.11	-2.46	100,100,100,100	0
85	MG	1	3626	1/1	0.15	-2.46	26,26,26,26	0
86	OHX	o3	202	7/7	0.11	-2.47	79,79,79,79	0
85	MG	5	3477	1/1	0.18	-2.48	16,16,16,16	0
86	OHX	5	4033	7/7	0.16	-2.48	102,102,102,102	0
86	OHX	1	3876	7/7	0.16	-2.49	41,41,41,41	0
86	OHX	5	3969	7/7	0.16	-2.49	64,64,64,64	0
86	OHX	1	4061	7/7	0.14	-2.49	123,123,123,123	0
86	OHX	5	4048	7/7	0.07	-2.50	109,109,109,109	0
86	OHX	1	4093	7/7	0.12	-2.51	124,124,124,124	0
86	OHX	1	3906	7/7	0.16	-2.51	62,62,62,62	0
86	OHX	5	4184	7/7	0.16	-2.53	94,94,94,94	0
86	OHX	5	3993	7/7	0.17	-2.53	65,65,65,65	0
86	OHX	5	4055	7/7	0.10	-2.53	105,105,105,105	0
86	OHX	1	3914	7/7	0.12	-2.53	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4063	7/7	0.17	-2.53	87,87,87,87	0
86	OHX	8	225	7/7	0.07	-2.54	119,119,119,119	0
85	MG	5	3427	1/1	0.15	-2.54	28,28,28,28	0
85	MG	5	3659	1/1	0.14	-2.54	32,32,32,32	0
85	MG	5	3836	1/1	0.15	-2.54	28,28,28,28	0
85	MG	5	3789	1/1	0.16	-2.55	16,16,16,16	0
86	OHX	2	2129	7/7	0.14	-2.55	125,125,125,125	0
86	OHX	L3	405	7/7	0.11	-2.55	130,130,130,130	0
86	OHX	15	303	7/7	0.14	-2.55	117,117,117,117	0
85	MG	5	3759	1/1	0.13	-2.55	30,30,30,30	0
86	OHX	5	4129	7/7	0.10	-2.55	118,118,118,118	0
86	OHX	5	3946	7/7	0.16	-2.55	68,68,68,68	0
86	OHX	1	3913	7/7	0.14	-2.56	63,63,63,63	0
86	OHX	8	219	7/7	0.09	-2.56	81,81,81,81	0
86	OHX	6	2059	7/7	0.16	-2.56	59,59,59,59	0
86	OHX	5	4038	7/7	0.10	-2.56	96,96,96,96	0
85	MG	5	3834	1/1	0.17	-2.57	29,29,29,29	0
85	MG	5	3666	1/1	0.17	-2.57	21,21,21,21	0
86	OHX	5	4177	7/7	0.17	-2.57	100,100,100,100	0
85	MG	6	1977	1/1	0.17	-2.58	60,60,60,60	0
86	OHX	6	2066	7/7	0.16	-2.58	76,76,76,76	0
85	MG	7	211	1/1	0.15	-2.58	23,23,23,23	0
85	MG	5	3658	1/1	0.17	-2.58	19,19,19,19	0
86	OHX	5	4091	7/7	0.18	-2.59	84,84,84,84	0
85	MG	2	1986	1/1	0.16	-2.59	49,49,49,49	0
85	MG	1	3650	1/1	0.14	-2.59	57,57,57,57	0
86	OHX	2	2065	7/7	0.14	-2.60	85,85,85,85	0
86	OHX	2	2113	7/7	0.14	-2.60	107,107,107,107	0
86	OHX	2	2154	7/7	0.11	-2.61	141,141,141,141	0
86	OHX	1	4086	7/7	0.11	-2.62	120,120,120,120	0
85	MG	1	3630	1/1	0.11	-2.62	18,18,18,18	0
86	OHX	6	2090	7/7	0.11	-2.63	99,99,99,99	0
86	OHX	2	2143	7/7	0.12	-2.63	113,113,113,113	0
85	MG	1	3486	1/1	0.21	-2.63	19,19,19,19	0
85	MG	5	3840	1/1	0.14	-2.63	51,51,51,51	0
86	OHX	2	2127	7/7	0.12	-2.63	109,109,109,109	0
86	OHX	5	4118	7/7	0.13	-2.65	89,89,89,89	0
86	OHX	6	2120	7/7	0.09	-2.65	84,84,84,84	0
85	MG	1	3516	1/1	0.28	-2.66	27,27,27,27	0
85	MG	5	3851	1/1	0.15	-2.66	37,37,37,37	0
86	OHX	5	4116	7/7	0.16	-2.66	78,78,78,78	0
85	MG	5	3623	1/1	0.19	-2.67	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2070	7/7	0.15	-2.67	67,67,67,67	0
85	MG	1	3439	1/1	0.15	-2.67	28,28,28,28	0
85	MG	5	3481	1/1	0.20	-2.67	32,32,32,32	0
86	OHX	5	3985	7/7	0.15	-2.67	67,67,67,67	0
86	OHX	1	4019	7/7	0.12	-2.68	111,111,111,111	0
86	OHX	6	2164	7/7	0.18	-2.68	101,101,101,101	0
85	MG	5	3676	1/1	0.13	-2.69	25,25,25,25	0
86	OHX	1	3945	7/7	0.11	-2.69	85,85,85,85	0
85	MG	5	3820	1/1	0.14	-2.69	42,42,42,42	0
85	MG	5	3494	1/1	0.13	-2.70	17,17,17,17	0
86	OHX	2	2118	7/7	0.11	-2.70	134,134,134,134	0
86	OHX	6	2110	7/7	0.11	-2.70	87,87,87,87	0
85	MG	5	3501	1/1	0.16	-2.70	30,30,30,30	0
86	OHX	1	4040	7/7	0.17	-2.71	82,82,82,82	0
86	OHX	1	3951	7/7	0.15	-2.71	81,81,81,81	0
85	MG	1	3565	1/1	0.20	-2.71	27,27,27,27	0
85	MG	5	3670	1/1	0.12	-2.72	22,22,22,22	0
85	MG	1	3582	1/1	0.16	-2.72	28,28,28,28	0
86	OHX	2	2050	7/7	0.11	-2.73	95,95,95,95	0
86	OHX	6	2072	7/7	0.11	-2.73	68,68,68,68	0
86	OHX	5	3926	7/7	0.14	-2.73	47,47,47,47	0
86	OHX	2	2067	7/7	0.12	-2.73	109,109,109,109	0
85	MG	1	3740	1/1	0.14	-2.74	33,33,33,33	0
86	OHX	1	4038	7/7	0.12	-2.74	70,70,70,70	0
86	OHX	5	4056	7/7	0.07	-2.75	111,111,111,111	0
86	OHX	1	4104	7/7	0.13	-2.75	94,94,94,94	0
86	OHX	6	2096	7/7	0.10	-2.75	110,110,110,110	0
86	OHX	m6	202	7/7	0.10	-2.77	67,67,67,67	0
86	OHX	1	3901	7/7	0.13	-2.77	57,57,57,57	0
86	OHX	1	3897	7/7	0.15	-2.78	55,55,55,55	0
85	MG	5	3889	1/1	0.15	-2.78	15,15,15,15	0
85	MG	5	3716	1/1	0.14	-2.78	51,51,51,51	0
85	MG	2	1922	1/1	0.11	-2.79	55,55,55,55	0
86	OHX	5	4054	7/7	0.16	-2.79	83,83,83,83	0
86	OHX	1	4047	7/7	0.07	-2.79	111,111,111,111	0
86	OHX	1	4101	7/7	0.08	-2.79	123,123,123,123	0
86	OHX	5	4081	7/7	0.18	-2.80	88,88,88,88	0
86	OHX	1	3996	7/7	0.14	-2.81	81,81,81,81	0
86	OHX	1	4054	7/7	0.06	-2.81	148,148,148,148	0
85	MG	1	3741	1/1	0.10	-2.81	26,26,26,26	0
86	OHX	6	2108	7/7	0.12	-2.82	93,93,93,93	0
86	OHX	5	4023	7/7	0.12	-2.83	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4004	7/7	0.14	-2.83	93,93,93,93	0
86	OHX	6	2167	7/7	0.14	-2.83	181,181,181,181	0
86	OHX	6	2170	7/7	0.09	-2.83	156,156,156,156	0
85	MG	1	3749	1/1	0.15	-2.83	43,43,43,43	0
86	OHX	1	4049	7/7	0.16	-2.84	76,76,76,76	0
86	OHX	5	4227	7/7	0.12	-2.84	108,108,108,108	0
85	MG	4	210	1/1	0.13	-2.84	34,34,34,34	0
85	MG	5	3600	1/1	0.15	-2.84	31,31,31,31	0
86	OHX	5	4058	7/7	0.09	-2.84	119,119,119,119	0
86	OHX	1	4081	7/7	0.11	-2.85	179,179,179,179	0
86	OHX	6	2080	7/7	0.11	-2.85	74,74,74,74	0
86	OHX	5	4028	7/7	0.12	-2.86	90,90,90,90	0
86	OHX	5	3995	7/7	0.14	-2.86	87,87,87,87	0
85	MG	1	3467	1/1	0.12	-2.87	33,33,33,33	0
86	OHX	6	2074	7/7	0.13	-2.87	69,69,69,69	0
86	OHX	8	220	7/7	0.09	-2.87	81,81,81,81	0
85	MG	1	3477	1/1	0.18	-2.88	27,27,27,27	0
85	MG	5	3624	1/1	0.15	-2.88	20,20,20,20	0
86	OHX	6	2125	7/7	0.10	-2.88	121,121,121,121	0
85	MG	6	2004	1/1	0.19	-2.88	65,65,65,65	0
85	MG	5	3817	1/1	0.15	-2.90	27,27,27,27	0
85	MG	5	3507	1/1	0.15	-2.91	19,19,19,19	0
86	OHX	6	2146	7/7	0.11	-2.91	116,116,116,116	0
85	MG	6	2010	1/1	0.15	-2.91	39,39,39,39	0
86	OHX	19	202	7/7	0.11	-2.91	92,92,92,92	0
86	OHX	5	4076	7/7	0.16	-2.91	67,67,67,67	0
86	OHX	1	3972	7/7	0.12	-2.91	92,92,92,92	0
86	OHX	6	2111	7/7	0.08	-2.92	98,98,98,98	0
86	OHX	1	4008	7/7	0.10	-2.93	97,97,97,97	0
86	OHX	1	4191	7/7	0.12	-2.93	149,149,149,149	0
85	MG	5	3442	1/1	0.19	-2.93	24,24,24,24	0
86	OHX	2	2148	7/7	0.11	-2.93	158,158,158,158	0
86	OHX	2	2055	7/7	0.11	-2.95	106,106,106,106	0
85	MG	1	3772	1/1	0.23	-2.95	44,44,44,44	0
86	OHX	1	3992	7/7	0.11	-2.95	101,101,101,101	0
86	OHX	2	2110	7/7	0.07	-2.96	107,107,107,107	0
86	OHX	2	2063	7/7	0.12	-2.96	96,96,96,96	0
86	OHX	4	226	7/7	0.10	-2.97	86,86,86,86	0
86	OHX	3	224	7/7	0.15	-2.97	103,103,103,103	0
86	OHX	5	3944	7/7	0.11	-2.97	74,74,74,74	0
86	OHX	1	4033	7/7	0.09	-2.97	88,88,88,88	0
86	OHX	2	2077	7/7	0.09	-2.98	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2062	7/7	0.13	-2.99	68,68,68,68	0
86	OHX	4	225	7/7	0.07	-2.99	75,75,75,75	0
86	OHX	1	4125	7/7	0.12	-2.99	133,133,133,133	0
86	OHX	5	3927	7/7	0.15	-3.00	42,42,42,42	0
86	OHX	2	2072	7/7	0.07	-3.02	102,102,102,102	0
86	OHX	6	2156	7/7	0.12	-3.02	113,113,113,113	0
86	OHX	1	4085	7/7	0.10	-3.02	109,109,109,109	0
86	OHX	1	3933	7/7	0.11	-3.02	57,57,57,57	0
86	OHX	8	222	7/7	0.09	-3.02	92,92,92,92	0
85	MG	6	1971	1/1	0.17	-3.03	51,51,51,51	0
86	OHX	5	3924	7/7	0.15	-3.04	53,53,53,53	0
86	OHX	1	3912	7/7	0.14	-3.05	60,60,60,60	0
85	MG	8	213	1/1	0.13	-3.05	42,42,42,42	0
86	OHX	5	4156	7/7	0.10	-3.05	110,110,110,110	0
86	OHX	1	3898	7/7	0.17	-3.06	65,65,65,65	0
86	OHX	6	2126	7/7	0.14	-3.07	83,83,83,83	0
85	MG	M5	303	1/1	0.10	-3.08	39,39,39,39	0
85	MG	1	3849	1/1	0.13	-3.08	48,48,48,48	0
86	OHX	1	4113	7/7	0.10	-3.09	99,99,99,99	0
85	MG	5	3705	1/1	0.21	-3.09	39,39,39,39	0
86	OHX	1	3958	7/7	0.10	-3.11	81,81,81,81	0
85	MG	5	3408	1/1	0.14	-3.11	18,18,18,18	0
86	OHX	1	3918	7/7	0.11	-3.11	61,61,61,61	0
86	OHX	4	229	7/7	0.13	-3.12	79,79,79,79	0
85	MG	5	3461	1/1	0.14	-3.12	29,29,29,29	0
86	OHX	5	4079	7/7	0.12	-3.12	79,79,79,79	0
86	OHX	1	3999	7/7	0.10	-3.12	92,92,92,92	0
86	OHX	2	2057	7/7	0.09	-3.13	104,104,104,104	0
85	MG	N8	204	1/1	0.09	-3.14	30,30,30,30	0
85	MG	1	3644	1/1	0.17	-3.14	23,23,23,23	0
86	OHX	1	4011	7/7	0.13	-3.14	90,90,90,90	0
86	OHX	6	2105	7/7	0.12	-3.14	92,92,92,92	0
86	OHX	2	2115	7/7	0.10	-3.15	95,95,95,95	0
85	MG	5	3899	1/1	0.12	-3.16	24,24,24,24	0
86	OHX	1	4103	7/7	0.13	-3.16	105,105,105,105	0
85	MG	5	3590	1/1	0.17	-3.17	28,28,28,28	0
86	OHX	5	3954	7/7	0.12	-3.17	82,82,82,82	0
85	MG	1	4213	1/1	0.10	-3.17	31,31,31,31	0
85	MG	5	3647	1/1	0.18	-3.17	33,33,33,33	0
86	OHX	1	3891	7/7	0.15	-3.17	47,47,47,47	0
85	MG	5	3887	1/1	0.14	-3.18	39,39,39,39	0
86	OHX	6	2064	7/7	0.14	-3.18	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3745	1/1	0.10	-3.18	29,29,29,29	0
86	OHX	5	3961	7/7	0.13	-3.18	52,52,52,52	0
85	MG	5	3564	1/1	0.15	-3.19	16,16,16,16	0
85	MG	5	3692	1/1	0.16	-3.19	34,34,34,34	0
86	OHX	5	3960	7/7	0.14	-3.20	49,49,49,49	0
85	MG	1	3449	1/1	0.15	-3.20	30,30,30,30	0
86	OHX	1	4017	7/7	0.15	-3.21	89,89,89,89	0
85	MG	1	3805	1/1	0.15	-3.21	27,27,27,27	0
86	OHX	5	3918	7/7	0.15	-3.21	45,45,45,45	0
86	OHX	Q2	502	7/7	0.12	-3.24	56,56,56,56	0
86	OHX	M6	202	7/7	0.08	-3.25	80,80,80,80	0
85	MG	5	3709	1/1	0.14	-3.26	31,31,31,31	0
86	OHX	5	4120	7/7	0.08	-3.26	112,112,112,112	0
86	OHX	5	4165	7/7	0.14	-3.29	104,104,104,104	0
86	OHX	5	3952	7/7	0.15	-3.29	62,62,62,62	0
85	MG	5	3746	1/1	0.14	-3.29	51,51,51,51	0
86	OHX	1	4037	7/7	0.12	-3.29	97,97,97,97	0
85	MG	1	3762	1/1	0.18	-3.30	34,34,34,34	0
85	MG	5	3550	1/1	0.19	-3.30	20,20,20,20	0
86	OHX	6	2169	7/7	0.10	-3.30	118,118,118,118	0
86	OHX	6	2145	7/7	0.13	-3.30	105,105,105,105	0
86	OHX	5	4158	7/7	0.16	-3.30	79,79,79,79	0
86	OHX	2	2155	7/7	0.11	-3.30	117,117,117,117	0
86	OHX	6	2130	7/7	0.20	-3.31	94,94,94,94	0
85	MG	1	3852	1/1	0.11	-3.32	59,59,59,59	0
86	OHX	5	3943	7/7	0.10	-3.32	62,62,62,62	0
85	MG	1	3577	1/1	0.14	-3.32	17,17,17,17	0
86	OHX	5	4025	7/7	0.14	-3.33	75,75,75,75	0
86	OHX	5	4102	7/7	0.11	-3.33	130,130,130,130	0
86	OHX	5	3973	7/7	0.10	-3.33	56,56,56,56	0
86	OHX	2	2167	7/7	0.10	-3.33	137,137,137,137	0
85	MG	5	3682	1/1	0.12	-3.34	18,18,18,18	0
85	MG	2	1906	1/1	0.14	-3.34	39,39,39,39	0
86	OHX	6	2158	7/7	0.08	-3.34	91,91,91,91	0
85	MG	2	2012	1/1	0.19	-3.34	59,59,59,59	0
85	MG	1	3520	1/1	0.11	-3.35	22,22,22,22	0
85	MG	1	3806	1/1	0.12	-3.35	24,24,24,24	0
86	OHX	1	4001	7/7	0.10	-3.35	94,94,94,94	0
86	OHX	6	2104	7/7	0.11	-3.35	96,96,96,96	0
86	OHX	1	3984	7/7	0.07	-3.36	93,93,93,93	0
85	MG	2	1942	1/1	0.08	-3.36	54,54,54,54	0
86	OHX	5	4192	7/7	0.12	-3.37	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4024	7/7	0.15	-3.38	80,80,80,80	0
85	MG	1	3768	1/1	0.18	-3.38	48,48,48,48	0
85	MG	1	3659	1/1	0.12	-3.38	30,30,30,30	0
86	OHX	4	224	7/7	0.08	-3.39	72,72,72,72	0
86	OHX	5	4046	7/7	0.10	-3.40	88,88,88,88	0
85	MG	6	1980	1/1	0.14	-3.41	69,69,69,69	0
85	MG	1	3730	1/1	0.10	-3.41	31,31,31,31	0
85	MG	1	3668	1/1	0.11	-3.42	41,41,41,41	0
86	OHX	1	3941	7/7	0.17	-3.44	66,66,66,66	0
86	OHX	1	4045	7/7	0.13	-3.45	87,87,87,87	0
86	OHX	5	4174	7/7	0.17	-3.45	91,91,91,91	0
86	OHX	1	3968	7/7	0.09	-3.46	84,84,84,84	0
86	OHX	1	3910	7/7	0.14	-3.46	72,72,72,72	0
86	OHX	L3	403	7/7	0.12	-3.46	90,90,90,90	0
85	MG	1	3654	1/1	0.14	-3.48	22,22,22,22	0
86	OHX	2	2045	7/7	0.08	-3.48	78,78,78,78	0
86	OHX	1	3929	7/7	0.10	-3.48	56,56,56,56	0
86	OHX	5	4050	7/7	0.12	-3.48	74,74,74,74	0
85	MG	1	3485	1/1	0.15	-3.48	29,29,29,29	0
85	MG	1	3707	1/1	0.13	-3.49	40,40,40,40	0
86	OHX	5	4053	7/7	0.08	-3.49	75,75,75,75	0
86	OHX	5	4105	7/7	0.15	-3.49	85,85,85,85	0
86	OHX	4	233	7/7	0.06	-3.49	105,105,105,105	0
86	OHX	1	4080	7/7	0.07	-3.50	96,96,96,96	0
86	OHX	5	3939	7/7	0.13	-3.50	52,52,52,52	0
85	MG	5	3778	1/1	0.17	-3.51	35,35,35,35	0
86	OHX	5	4115	7/7	0.12	-3.52	109,109,109,109	0
86	OHX	5	3963	7/7	0.12	-3.52	71,71,71,71	0
86	OHX	5	4252	7/7	0.11	-3.53	123,123,123,123	0
85	MG	5	3744	1/1	0.17	-3.56	34,34,34,34	0
85	MG	5	3848	1/1	0.14	-3.56	37,37,37,37	0
86	OHX	1	4064	7/7	0.10	-3.56	93,93,93,93	0
86	OHX	5	4208	7/7	0.11	-3.56	131,131,131,131	0
86	OHX	5	4142	7/7	0.10	-3.57	97,97,97,97	0
86	OHX	5	4043	7/7	0.11	-3.58	97,97,97,97	0
86	OHX	5	4041	7/7	0.13	-3.58	85,85,85,85	0
86	OHX	1	3887	7/7	0.12	-3.59	50,50,50,50	0
85	MG	5	3787	1/1	0.09	-3.59	31,31,31,31	0
86	OHX	1	4132	7/7	0.16	-3.60	85,85,85,85	0
86	OHX	1	3942	7/7	0.14	-3.62	60,60,60,60	0
86	OHX	c5	201	7/7	0.08	-3.62	130,130,130,130	0
86	OHX	1	4071	7/7	0.13	-3.63	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	6	2029	1/1	0.10	-3.63	68,68,68,68	0
86	OHX	o7	502	7/7	0.08	-3.63	74,74,74,74	0
86	OHX	8	227	7/7	0.13	-3.64	115,115,115,115	0
86	OHX	5	4143	7/7	0.11	-3.64	90,90,90,90	0
85	MG	5	3862	1/1	0.14	-3.64	30,30,30,30	0
86	OHX	2	2059	7/7	0.10	-3.65	89,89,89,89	0
85	MG	1	3564	1/1	0.18	-3.65	26,26,26,26	0
85	MG	1	3841	1/1	0.14	-3.66	24,24,24,24	0
86	OHX	5	4130	7/7	0.12	-3.66	84,84,84,84	0
86	OHX	5	4000	7/7	0.09	-3.66	91,91,91,91	0
85	MG	5	3614	1/1	0.13	-3.67	31,31,31,31	0
85	MG	5	3736	1/1	0.13	-3.67	35,35,35,35	0
85	MG	1	3602	1/1	0.18	-3.67	26,26,26,26	0
86	OHX	5	3998	7/7	0.09	-3.68	82,82,82,82	0
86	OHX	2	2074	7/7	0.09	-3.68	116,116,116,116	0
86	OHX	2	2046	7/7	0.09	-3.69	78,78,78,78	0
86	OHX	1	3880	7/7	0.14	-3.73	53,53,53,53	0
86	OHX	6	2058	7/7	0.15	-3.74	54,54,54,54	0
86	OHX	2	2039	7/7	0.14	-3.75	78,78,78,78	0
85	MG	5	3436	1/1	0.17	-3.75	23,23,23,23	0
85	MG	1	3729	1/1	0.12	-3.75	17,17,17,17	0
86	OHX	5	3992	7/7	0.11	-3.77	78,78,78,78	0
86	OHX	6	2065	7/7	0.12	-3.79	68,68,68,68	0
86	OHX	6	2089	7/7	0.08	-3.79	88,88,88,88	0
86	OHX	6	2149	7/7	0.12	-3.80	112,112,112,112	0
86	OHX	5	4092	7/7	0.11	-3.82	89,89,89,89	0
85	MG	5	3700	1/1	0.12	-3.82	45,45,45,45	0
85	MG	5	3558	1/1	0.17	-3.82	23,23,23,23	0
86	OHX	6	2133	7/7	0.12	-3.82	94,94,94,94	0
86	OHX	5	4008	7/7	0.09	-3.84	81,81,81,81	0
86	OHX	6	2083	7/7	0.12	-3.85	72,72,72,72	0
86	OHX	1	4023	7/7	0.09	-3.85	96,96,96,96	0
85	MG	6	2007	1/1	0.13	-3.85	51,51,51,51	0
85	MG	5	3699	1/1	0.15	-3.85	25,25,25,25	0
86	OHX	1	3977	7/7	0.11	-3.85	79,79,79,79	0
85	MG	1	3769	1/1	0.12	-3.86	39,39,39,39	0
86	OHX	2	2073	7/7	0.13	-3.88	85,85,85,85	0
86	OHX	1	3974	7/7	0.12	-3.88	77,77,77,77	0
85	MG	1	3618	1/1	0.13	-3.89	54,54,54,54	0
86	OHX	6	2116	7/7	0.10	-3.91	100,100,100,100	0
86	OHX	1	4144	7/7	0.12	-3.91	112,112,112,112	0
86	OHX	5	4018	7/7	0.09	-3.92	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4236	7/7	0.11	-3.93	197,197,197,197	0
86	OHX	5	3982	7/7	0.13	-3.93	59,59,59,59	0
86	OHX	5	3931	7/7	0.10	-3.93	62,62,62,62	0
86	OHX	5	4223	7/7	0.12	-3.96	112,112,112,112	0
85	MG	1	3751	1/1	0.14	-3.96	45,45,45,45	0
86	OHX	4	230	7/7	0.09	-3.97	89,89,89,89	0
86	OHX	1	4032	7/7	0.08	-3.98	117,117,117,117	0
86	OHX	C5	201	7/7	0.08	-3.99	137,137,137,137	0
85	MG	1	3451	1/1	0.14	-3.99	21,21,21,21	0
86	OHX	1	3935	7/7	0.12	-4.00	71,71,71,71	0
85	MG	5	3613	1/1	0.15	-4.00	38,38,38,38	0
85	MG	6	1987	1/1	0.17	-4.01	40,40,40,40	0
86	OHX	6	2101	7/7	0.10	-4.01	141,141,141,141	0
86	OHX	5	3920	7/7	0.15	-4.02	52,52,52,52	0
85	MG	5	3693	1/1	0.13	-4.03	33,33,33,33	0
86	OHX	2	2066	7/7	0.12	-4.03	85,85,85,85	0
86	OHX	2	2081	7/7	0.11	-4.05	145,145,145,145	0
86	OHX	6	2106	7/7	0.11	-4.05	101,101,101,101	0
86	OHX	2	2079	7/7	0.13	-4.06	99,99,99,99	0
85	MG	5	3760	1/1	0.14	-4.06	36,36,36,36	0
85	MG	6	2008	1/1	0.12	-4.08	50,50,50,50	0
85	MG	5	3502	1/1	0.14	-4.08	33,33,33,33	0
86	OHX	5	4040	7/7	0.14	-4.08	100,100,100,100	0
85	MG	1	3753	1/1	0.16	-4.09	15,15,15,15	0
85	MG	5	3719	1/1	0.17	-4.10	41,41,41,41	0
86	OHX	8	217	7/7	0.12	-4.11	67,67,67,67	0
86	OHX	1	3893	7/7	0.10	-4.11	53,53,53,53	0
86	OHX	1	3973	7/7	0.09	-4.11	81,81,81,81	0
85	MG	1	3426	1/1	0.11	-4.11	29,29,29,29	0
86	OHX	7	223	7/7	0.12	-4.12	73,73,73,73	0
86	OHX	2	2082	7/7	0.09	-4.14	108,108,108,108	0
86	OHX	6	2117	7/7	0.11	-4.15	94,94,94,94	0
85	MG	6	2045	1/1	0.16	-4.16	43,43,43,43	0
85	MG	5	3644	1/1	0.12	-4.16	47,47,47,47	0
85	MG	1	3489	1/1	0.09	-4.17	23,23,23,23	0
86	OHX	5	4093	7/7	0.09	-4.19	107,107,107,107	0
86	OHX	5	3938	7/7	0.11	-4.19	48,48,48,48	0
86	OHX	5	4049	7/7	0.11	-4.20	79,79,79,79	0
86	OHX	1	4089	7/7	0.10	-4.23	117,117,117,117	0
85	MG	1	3547	1/1	0.14	-4.24	30,30,30,30	0
86	OHX	5	4045	7/7	0.09	-4.25	97,97,97,97	0
86	OHX	5	4198	7/7	0.13	-4.26	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3860	1/1	0.16	-4.27	49,49,49,49	0
85	MG	5	3634	1/1	0.14	-4.28	42,42,42,42	0
85	MG	5	3423	1/1	0.13	-4.29	31,31,31,31	0
86	OHX	6	2172	7/7	0.10	-4.30	132,132,132,132	0
86	OHX	1	4088	7/7	0.12	-4.33	119,119,119,119	0
86	OHX	1	4018	7/7	0.09	-4.35	86,86,86,86	0
86	OHX	5	3947	7/7	0.11	-4.35	54,54,54,54	0
86	OHX	7	229	7/7	0.11	-4.37	109,109,109,109	0
86	OHX	2	2108	7/7	0.14	-4.37	105,105,105,105	0
86	OHX	1	4035	7/7	0.15	-4.37	83,83,83,83	0
86	OHX	1	3894	7/7	0.10	-4.38	60,60,60,60	0
85	MG	5	3651	1/1	0.14	-4.38	21,21,21,21	0
86	OHX	1	4044	7/7	0.16	-4.38	91,91,91,91	0
85	MG	5	3750	1/1	0.18	-4.41	31,31,31,31	0
85	MG	1	3744	1/1	0.13	-4.41	18,18,18,18	0
86	OHX	2	2052	7/7	0.11	-4.41	79,79,79,79	0
86	OHX	5	4180	7/7	0.07	-4.42	131,131,131,131	0
86	OHX	5	3978	7/7	0.13	-4.43	75,75,75,75	0
86	OHX	2	2083	7/7	0.06	-4.43	120,120,120,120	0
86	OHX	5	4139	7/7	0.10	-4.44	112,112,112,112	0
86	OHX	5	3972	7/7	0.12	-4.45	64,64,64,64	0
86	OHX	2	2088	7/7	0.07	-4.46	100,100,100,100	0
86	OHX	1	4069	7/7	0.09	-4.47	93,93,93,93	0
86	OHX	6	2128	7/7	0.09	-4.50	115,115,115,115	0
86	OHX	6	2153	7/7	0.12	-4.51	120,120,120,120	0
86	OHX	8	224	7/7	0.08	-4.52	98,98,98,98	0
85	MG	5	3559	1/1	0.18	-4.52	26,26,26,26	0
86	OHX	5	4210	7/7	0.14	-4.53	110,110,110,110	0
85	MG	1	3780	1/1	0.11	-4.54	34,34,34,34	0
86	OHX	5	3937	7/7	0.11	-4.56	56,56,56,56	0
85	MG	5	3788	1/1	0.14	-4.56	35,35,35,35	0
85	MG	5	3770	1/1	0.14	-4.58	55,55,55,55	0
86	OHX	5	4010	7/7	0.10	-4.59	78,78,78,78	0
85	MG	5	3843	1/1	0.15	-4.60	35,35,35,35	0
86	OHX	6	2100	7/7	0.09	-4.60	103,103,103,103	0
85	MG	1	3461	1/1	0.19	-4.60	19,19,19,19	0
85	MG	5	3810	1/1	0.10	-4.61	20,20,20,20	0
86	OHX	1	4046	7/7	0.10	-4.62	104,104,104,104	0
85	MG	5	3628	1/1	0.12	-4.63	29,29,29,29	0
86	OHX	5	4012	7/7	0.10	-4.63	69,69,69,69	0
86	OHX	6	2063	7/7	0.12	-4.64	65,65,65,65	0
86	OHX	1	4050	7/7	0.06	-4.64	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	1	3983	7/7	0.10	-4.65	76,76,76,76	0
86	OHX	5	4013	7/7	0.15	-4.65	75,75,75,75	0
86	OHX	1	3946	7/7	0.12	-4.67	60,60,60,60	0
86	OHX	5	4111	7/7	0.11	-4.68	95,95,95,95	0
85	MG	5	3866	1/1	0.23	-4.72	17,17,17,17	0
86	OHX	2	2126	7/7	0.09	-4.73	96,96,96,96	0
86	OHX	1	4186	7/7	0.10	-4.74	120,120,120,120	0
86	OHX	2	2064	7/7	0.07	-4.75	110,110,110,110	0
86	OHX	3	222	7/7	0.07	-4.78	120,120,120,120	0
86	OHX	1	3982	7/7	0.12	-4.78	68,68,68,68	0
86	OHX	5	4154	7/7	0.14	-4.79	89,89,89,89	0
85	MG	1	3475	1/1	0.13	-4.79	22,22,22,22	0
86	OHX	6	2112	7/7	0.12	-4.80	85,85,85,85	0
86	OHX	1	4141	7/7	0.13	-4.81	115,115,115,115	0
85	MG	5	3447	1/1	0.13	-4.81	26,26,26,26	0
86	OHX	6	2138	7/7	0.07	-4.83	113,113,113,113	0
85	MG	1	3435	1/1	0.14	-4.83	29,29,29,29	0
86	OHX	1	3870	7/7	0.14	-4.84	44,44,44,44	0
86	OHX	1	4146	7/7	0.10	-4.86	85,85,85,85	0
86	OHX	1	3964	7/7	0.10	-4.86	74,74,74,74	0
86	OHX	8	221	7/7	0.10	-4.88	108,108,108,108	0
85	MG	1	3715	1/1	0.14	-4.90	32,32,32,32	0
86	OHX	5	4020	7/7	0.07	-4.90	84,84,84,84	0
86	OHX	1	3991	7/7	0.08	-4.92	94,94,94,94	0
86	OHX	5	4078	7/7	0.08	-4.92	91,91,91,91	0
86	OHX	5	3996	7/7	0.12	-4.93	72,72,72,72	0
86	OHX	1	3959	7/7	0.10	-4.94	86,86,86,86	0
86	OHX	5	4095	7/7	0.16	-4.95	119,119,119,119	0
86	OHX	5	4094	7/7	0.12	-4.96	98,98,98,98	0
86	OHX	1	4007	7/7	0.12	-4.96	100,100,100,100	0
86	OHX	5	3958	7/7	0.09	-5.00	59,59,59,59	0
85	MG	1	3493	1/1	0.13	-5.00	68,68,68,68	0
86	OHX	1	3879	7/7	0.14	-5.01	44,44,44,44	0
86	OHX	6	2134	7/7	0.09	-5.01	125,125,125,125	0
86	OHX	1	3920	7/7	0.12	-5.01	67,67,67,67	0
86	OHX	5	4065	7/7	0.10	-5.05	96,96,96,96	0
86	OHX	5	3910	7/7	0.13	-5.06	42,42,42,42	0
86	OHX	2	2125	7/7	0.07	-5.07	114,114,114,114	0
85	MG	5	3892	1/1	0.12	-5.09	99,99,99,99	0
86	OHX	5	4026	7/7	0.10	-5.11	62,62,62,62	0
86	OHX	2	2061	7/7	0.08	-5.12	80,80,80,80	0
86	OHX	5	3968	7/7	0.13	-5.13	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2081	7/7	0.10	-5.18	85,85,85,85	0
86	OHX	5	4003	7/7	0.10	-5.20	72,72,72,72	0
86	OHX	5	4167	7/7	0.10	-5.21	124,124,124,124	0
86	OHX	5	3984	7/7	0.12	-5.24	71,71,71,71	0
86	OHX	5	4253	7/7	0.11	-5.26	139,139,139,139	0
86	OHX	6	2113	7/7	0.10	-5.27	102,102,102,102	0
86	OHX	1	3986	7/7	0.07	-5.30	95,95,95,95	0
86	OHX	5	4002	7/7	0.12	-5.33	82,82,82,82	0
85	MG	5	3800	1/1	0.14	-5.35	29,29,29,29	0
85	MG	1	3825	1/1	0.10	-5.37	35,35,35,35	0
86	OHX	1	4082	7/7	0.13	-5.37	104,104,104,104	0
85	MG	1	3425	1/1	0.13	-5.38	46,46,46,46	0
86	OHX	2	2102	7/7	0.07	-5.39	112,112,112,112	0
86	OHX	1	4055	7/7	0.10	-5.40	100,100,100,100	0
86	OHX	1	4092	7/7	0.06	-5.40	118,118,118,118	0
86	OHX	1	4112	7/7	0.12	-5.42	97,97,97,97	0
86	OHX	1	4012	7/7	0.09	-5.42	85,85,85,85	0
86	OHX	5	4014	7/7	0.11	-5.43	79,79,79,79	0
86	OHX	1	3997	7/7	0.07	-5.54	60,60,60,60	0
86	OHX	5	4021	7/7	0.08	-5.54	80,80,80,80	0
86	OHX	1	3978	7/7	0.15	-5.55	81,81,81,81	0
86	OHX	1	4147	7/7	0.13	-5.56	107,107,107,107	0
86	OHX	1	3953	7/7	0.10	-5.59	60,60,60,60	0
85	MG	5	3511	1/1	0.13	-5.59	19,19,19,19	0
86	OHX	5	4017	7/7	0.09	-5.60	76,76,76,76	0
86	OHX	5	4031	7/7	0.14	-5.60	79,79,79,79	0
86	OHX	1	3957	7/7	0.07	-5.62	52,52,52,52	0
85	MG	1	3857	1/1	0.14	-5.62	38,38,38,38	0
86	OHX	1	3937	7/7	0.10	-5.63	63,63,63,63	0
86	OHX	5	3990	7/7	0.08	-5.64	60,60,60,60	0
86	OHX	5	3991	7/7	0.08	-5.66	72,72,72,72	0
85	MG	1	3598	1/1	0.10	-5.66	27,27,27,27	0
85	MG	1	3688	1/1	0.17	-5.67	24,24,24,24	0
85	MG	6	1975	1/1	0.17	-5.67	41,41,41,41	0
85	MG	1	3735	1/1	0.24	-5.67	23,23,23,23	0
86	OHX	1	3885	7/7	0.16	-5.70	50,50,50,50	0
86	OHX	1	3960	7/7	0.09	-5.71	74,74,74,74	0
86	OHX	2	2084	7/7	0.08	-5.78	110,110,110,110	0
86	OHX	7	225	7/7	0.11	-5.81	107,107,107,107	0
86	OHX	1	3924	7/7	0.11	-5.83	51,51,51,51	0
85	MG	5	3476	1/1	0.11	-5.84	28,28,28,28	0
86	OHX	1	4016	7/7	0.08	-5.85	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3954	7/7	0.09	-5.85	74,74,74,74	0
86	OHX	5	3977	7/7	0.11	-5.86	79,79,79,79	0
86	OHX	5	4005	7/7	0.10	-5.90	105,105,105,105	0
85	MG	5	3675	1/1	0.12	-5.92	34,34,34,34	0
86	OHX	5	4030	7/7	0.11	-5.95	75,75,75,75	0
86	OHX	2	2060	7/7	0.10	-5.96	96,96,96,96	0
86	OHX	5	4133	7/7	0.14	-5.96	101,101,101,101	0
86	OHX	5	3930	7/7	0.10	-6.00	68,68,68,68	0
85	MG	6	1962	1/1	0.09	-6.05	42,42,42,42	0
85	MG	5	3412	1/1	0.17	-6.05	21,21,21,21	0
85	MG	6	1998	1/1	0.18	-6.06	45,45,45,45	0
86	OHX	7	221	7/7	0.09	-6.07	66,66,66,66	0
86	OHX	5	4166	7/7	0.11	-6.08	99,99,99,99	0
86	OHX	6	2093	7/7	0.12	-6.08	93,93,93,93	0
85	MG	1	3603	1/1	0.12	-6.15	29,29,29,29	0
86	OHX	2	2119	7/7	0.08	-6.17	112,112,112,112	0
86	OHX	1	3936	7/7	0.14	-6.20	67,67,67,67	0
85	MG	1	3798	1/1	0.10	-6.22	40,40,40,40	0
86	OHX	1	3950	7/7	0.13	-6.23	75,75,75,75	0
86	OHX	1	3926	7/7	0.12	-6.27	61,61,61,61	0
86	OHX	5	4047	7/7	0.08	-6.27	75,75,75,75	0
86	OHX	1	4010	7/7	0.08	-6.27	87,87,87,87	0
85	MG	1	3695	1/1	0.13	-6.33	43,43,43,43	0
86	OHX	5	3994	7/7	0.07	-6.33	102,102,102,102	0
86	OHX	2	2130	7/7	0.08	-6.36	168,168,168,168	0
85	MG	5	3793	1/1	0.09	-6.36	32,32,32,32	0
86	OHX	6	2094	7/7	0.09	-6.40	96,96,96,96	0
86	OHX	5	4082	7/7	0.07	-6.42	112,112,112,112	0
85	MG	5	3680	1/1	0.12	-6.42	26,26,26,26	0
86	OHX	2	2101	7/7	0.09	-6.47	117,117,117,117	0
86	OHX	5	3987	7/7	0.11	-6.49	56,56,56,56	0
85	MG	5	3882	1/1	0.11	-6.50	16,16,16,16	0
85	MG	1	3705	1/1	0.10	-6.50	28,28,28,28	0
86	OHX	6	2082	7/7	0.10	-6.52	80,80,80,80	0
86	OHX	2	2096	7/7	0.09	-6.54	121,121,121,121	0
86	OHX	5	4083	7/7	0.10	-6.55	89,89,89,89	0
85	MG	1	3638	1/1	0.12	-6.71	48,48,48,48	0
86	OHX	1	3966	7/7	0.11	-6.74	67,67,67,67	0
86	OHX	2	2106	7/7	0.10	-6.77	106,106,106,106	0
85	MG	1	3637	1/1	0.11	-6.79	44,44,44,44	0
86	OHX	5	4126	7/7	0.14	-6.79	89,89,89,89	0
85	MG	5	3792	1/1	0.15	-6.81	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3987	7/7	0.09	-6.82	72,72,72,72	0
85	MG	1	3789	1/1	0.12	-6.87	44,44,44,44	0
86	OHX	5	4123	7/7	0.08	-6.88	121,121,121,121	0
86	OHX	2	2111	7/7	0.11	-6.94	91,91,91,91	0
85	MG	1	3512	1/1	0.17	-7.01	17,17,17,17	0
85	MG	1	3738	1/1	0.12	-7.02	34,34,34,34	0
86	OHX	6	2095	7/7	0.11	-7.03	84,84,84,84	0
86	OHX	5	3922	7/7	0.16	-7.08	46,46,46,46	0
85	MG	6	2016	1/1	0.10	-7.08	37,37,37,37	0
86	OHX	2	2112	7/7	0.05	-7.11	130,130,130,130	0
85	MG	1	3731	1/1	0.05	-7.13	47,47,47,47	0
86	OHX	5	4067	7/7	0.06	-7.14	114,114,114,114	0
85	MG	1	3778	1/1	0.10	-7.19	30,30,30,30	0
86	OHX	1	4067	7/7	0.12	-7.19	115,115,115,115	0
86	OHX	5	4064	7/7	0.06	-7.24	89,89,89,89	0
86	OHX	1	4014	7/7	0.15	-7.24	90,90,90,90	0
86	OHX	5	4032	7/7	0.11	-7.27	84,84,84,84	0
85	MG	1	3826	1/1	0.14	-7.29	15,15,15,15	0
85	MG	6	1910	1/1	0.16	-7.29	40,40,40,40	0
86	OHX	5	3986	7/7	0.10	-7.30	60,60,60,60	0
85	MG	5	3688	1/1	0.13	-7.30	31,31,31,31	0
86	OHX	1	4025	7/7	0.09	-7.38	105,105,105,105	0
86	OHX	1	4021	7/7	0.09	-7.41	77,77,77,77	0
86	OHX	3	218	7/7	0.09	-7.46	74,74,74,74	0
86	OHX	6	2148	7/7	0.08	-7.47	109,109,109,109	0
85	MG	8	204	1/1	0.11	-7.51	48,48,48,48	0
86	OHX	1	4063	7/7	0.08	-7.51	89,89,89,89	0
86	OHX	5	3964	7/7	0.12	-7.52	71,71,71,71	0
85	MG	5	3528	1/1	0.10	-7.52	16,16,16,16	0
86	OHX	3	223	7/7	0.10	-7.60	146,146,146,146	0
85	MG	1	3403	1/1	0.12	-7.61	24,24,24,24	0
85	MG	1	3519	1/1	0.16	-7.65	25,25,25,25	0
85	MG	5	3471	1/1	0.15	-7.67	33,33,33,33	0
86	OHX	3	221	7/7	0.08	-7.71	98,98,98,98	0
86	OHX	1	3940	7/7	0.11	-7.72	74,74,74,74	0
85	MG	6	1988	1/1	0.12	-7.82	57,57,57,57	0
86	OHX	1	4098	7/7	0.09	-7.83	115,115,115,115	0
86	OHX	1	3979	7/7	0.09	-7.95	56,56,56,56	0
85	MG	5	3450	1/1	0.14	-7.96	22,22,22,22	0
85	MG	1	3706	1/1	0.10	-7.97	40,40,40,40	0
86	OHX	5	3965	7/7	0.10	-8.06	56,56,56,56	0
85	MG	7	206	1/1	0.13	-8.06	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2118	7/7	0.11	-8.15	101,101,101,101	0
85	MG	5	3865	1/1	0.12	-8.20	33,33,33,33	0
86	OHX	5	3979	7/7	0.10	-8.24	60,60,60,60	0
85	MG	5	3435	1/1	0.13	-8.32	17,17,17,17	0
85	MG	5	3401	1/1	0.13	-8.42	42,42,42,42	0
85	MG	8	211	1/1	0.09	-8.49	49,49,49,49	0
86	OHX	5	4057	7/7	0.17	-8.49	92,92,92,92	0
86	OHX	1	4005	7/7	0.13	-8.52	96,96,96,96	0
86	OHX	2	2056	7/7	0.11	-8.64	91,91,91,91	0
85	MG	1	3447	1/1	0.14	-8.65	21,21,21,21	0
85	MG	5	3690	1/1	0.10	-8.78	35,35,35,35	0
85	MG	1	3752	1/1	0.11	-8.96	29,29,29,29	0
85	MG	1	3721	1/1	0.07	-8.97	44,44,44,44	0
85	MG	1	3737	1/1	0.16	-9.05	38,38,38,38	0
85	MG	2	1963	1/1	0.14	-9.14	127,127,127,127	0
86	OHX	1	4042	7/7	0.08	-9.17	94,94,94,94	0
85	MG	1	3763	1/1	0.17	-9.27	30,30,30,30	0
86	OHX	5	4071	7/7	0.07	-9.32	86,86,86,86	0
86	OHX	6	2092	7/7	0.07	-9.34	85,85,85,85	0
86	OHX	6	2141	7/7	0.06	-9.51	98,98,98,98	0
85	MG	5	3652	1/1	0.08	-9.54	15,15,15,15	0
86	OHX	2	2123	7/7	0.14	-9.69	113,113,113,113	0
85	MG	5	3795	1/1	0.18	-9.69	59,59,59,59	0
86	OHX	5	4125	7/7	0.05	-9.77	111,111,111,111	0
85	MG	5	3765	1/1	0.10	-9.93	46,46,46,46	0
86	OHX	1	3988	7/7	0.07	-9.94	82,82,82,82	0
86	OHX	3	225	7/7	0.10	-10.11	110,110,110,110	0
85	MG	5	3797	1/1	0.07	-10.15	25,25,25,25	0
85	MG	5	3654	1/1	0.10	-10.16	47,47,47,47	0
86	OHX	2	2053	7/7	0.10	-10.18	85,85,85,85	0
86	OHX	1	3930	7/7	0.10	-10.22	63,63,63,63	0
85	MG	1	3717	1/1	0.13	-10.26	22,22,22,22	0
86	OHX	6	2183	7/7	0.10	-10.27	130,130,130,130	0
86	OHX	1	3962	7/7	0.14	-10.33	73,73,73,73	0
86	OHX	3	216	7/7	0.04	-10.50	79,79,79,79	0
85	MG	5	3784	1/1	0.12	-10.59	20,20,20,20	0
86	OHX	5	4007	7/7	0.10	-10.63	67,67,67,67	0
86	OHX	1	4168	7/7	0.10	-10.70	79,79,79,79	0
86	OHX	5	4084	7/7	0.14	-11.10	91,91,91,91	0
86	OHX	5	4127	7/7	0.11	-11.10	92,92,92,92	0
86	OHX	7	222	7/7	0.09	-11.31	65,65,65,65	0
86	OHX	5	4135	7/7	0.10	-11.52	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	1993	1/1	0.09	-11.82	44,44,44,44	0
86	OHX	5	4241	7/7	0.19	-12.02	112,112,112,112	0
86	OHX	1	4004	7/7	0.08	-12.04	79,79,79,79	0
85	MG	8	201	1/1	0.14	-12.51	31,31,31,31	0
86	OHX	1	3971	7/7	0.05	-12.75	78,78,78,78	0
86	OHX	6	2157	7/7	0.09	-12.84	114,114,114,114	0
85	MG	5	3598	1/1	0.12	-12.86	28,28,28,28	0
86	OHX	2	2051	7/7	0.07	-13.25	91,91,91,91	0
86	OHX	5	3948	7/7	0.15	-13.34	54,54,54,54	0
86	OHX	3	220	7/7	0.09	-14.10	98,98,98,98	0
85	MG	5	3878	1/1	0.11	-14.18	23,23,23,23	0
85	MG	1	3693	1/1	0.11	-14.84	31,31,31,31	0
86	OHX	1	4159	7/7	0.09	-14.98	135,135,135,135	0
86	OHX	5	4215	7/7	0.11	-15.49	179,179,179,179	0
86	OHX	6	2078	7/7	0.08	-16.26	81,81,81,81	0
86	OHX	5	4213	7/7	0.13	-16.41	123,123,123,123	0
86	OHX	5	4096	7/7	0.07	-16.44	92,92,92,92	0
86	OHX	1	4006	7/7	0.07	-18.79	101,101,101,101	0
86	OHX	1	3985	7/7	0.10	-19.60	89,89,89,89	0
86	OHX	5	4070	7/7	0.07	-20.68	89,89,89,89	0
86	OHX	1	4000	7/7	0.05	-21.62	80,80,80,80	0
86	OHX	5	4019	7/7	0.07	-21.85	71,71,71,71	0
85	MG	5	3689	1/1	0.15	-22.33	37,37,37,37	0
86	OHX	2	2114	7/7	0.12	-22.98	136,136,136,136	0
86	OHX	1	4174	7/7	0.10	-23.04	213,213,213,213	0
85	MG	1	3434	1/1	0.16	-23.04	30,30,30,30	0
85	MG	5	3890	1/1	0.10	-27.25	79,79,79,79	0
85	MG	7	214	1/1	0.10	-27.29	80,80,80,80	0
85	MG	5	3854	1/1	0.12	-101.00	71,71,71,71	0
85	MG	1	3701	1/1	0.12	-137.00	48,48,48,48	0
85	MG	4	219	1/1	0.30	-	44,44,44,44	0
85	MG	1	3846	1/1	0.20	-	35,35,35,35	0
85	MG	5	3772	1/1	0.42	-	87,87,87,87	0
85	MG	2	2015	1/1	0.42	-	48,48,48,48	0
85	MG	6	2043	1/1	0.39	-	52,52,52,52	0
85	MG	1	3490	1/1	0.11	-	45,45,45,45	0
85	MG	2	1969	1/1	0.40	-	78,78,78,78	0
85	MG	5	3896	1/1	0.58	-	100,100,100,100	0
85	MG	5	3876	1/1	0.25	-	32,32,32,32	0
85	MG	2	2021	1/1	0.42	-	64,64,64,64	0
85	MG	1	3611	1/1	0.31	-	42,42,42,42	0
85	MG	1	3790	1/1	0.13	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2002	1/1	0.10	-	87,87,87,87	0
85	MG	5	3615	1/1	0.27	-	18,18,18,18	0
85	MG	6	2000	1/1	0.18	-	91,91,91,91	0
85	MG	5	3859	1/1	0.39	-	46,46,46,46	0
85	MG	5	3421	1/1	0.30	-	82,82,82,82	0
85	MG	3	208	1/1	0.11	-	68,68,68,68	0
85	MG	2	1953	1/1	0.61	-	94,94,94,94	0
85	MG	2	1950	1/1	0.53	-	54,54,54,54	0
85	MG	1	3787	1/1	0.35	-	54,54,54,54	0
85	MG	1	3847	1/1	0.13	-	49,49,49,49	0
85	MG	5	3884	1/1	0.38	-	49,49,49,49	0
85	MG	1	3835	1/1	0.32	-	37,37,37,37	0
85	MG	6	2046	1/1	0.25	-	53,53,53,53	0
85	MG	6	2022	1/1	0.26	-	104,104,104,104	0
85	MG	5	3493	1/1	0.21	-	30,30,30,30	0
85	MG	1	3797	1/1	0.14	-	76,76,76,76	0
85	MG	2	1989	1/1	0.28	-	77,77,77,77	0
85	MG	1	3842	1/1	0.33	-	36,36,36,36	0
85	MG	5	3804	1/1	0.24	-	139,139,139,139	0
85	MG	1	3754	1/1	0.14	-	80,80,80,80	0
85	MG	1	3464	1/1	0.25	-	29,29,29,29	0
85	MG	6	2048	1/1	0.49	-	68,68,68,68	0
85	MG	2	2011	1/1	0.17	-	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.