



wwPDB X-ray Structure Validation Summary Report i

Oct 9, 2014 – 10:14 PM BST

PDB ID : 4U56
Title : Crystal structure of Blasticidin S bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.45 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>

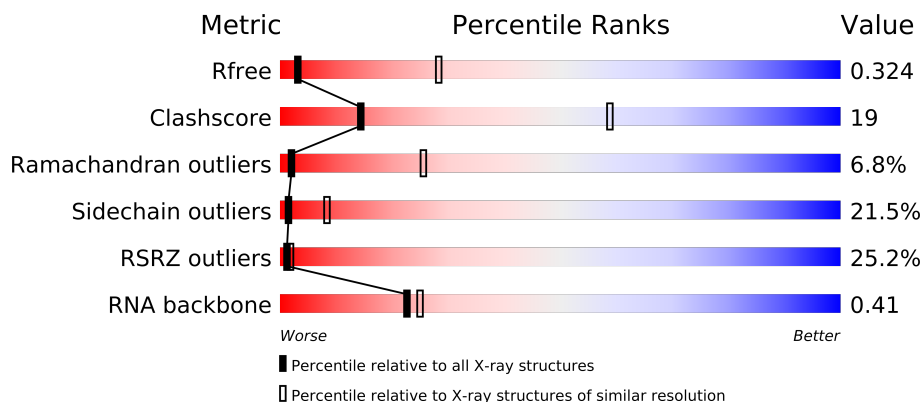
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.45 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	1149 (3.62-3.30)
Clashscore	79885	1012 (3.60-3.32)
Ramachandran outliers	78287	1401 (3.62-3.30)
Sidechain outliers	78261	1401 (3.62-3.30)
RSRZ outliers	66119	1149 (3.62-3.30)
RNA backbone	1838	1004 (4.10-2.76)

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

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

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

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

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

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

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

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3402	-	X
85	MG	1	3405	-	X
85	MG	1	3409	-	X
85	MG	1	3415	-	X
85	MG	1	3417	-	X
85	MG	1	3418	-	X
85	MG	1	3429	-	X
85	MG	1	3434	-	X
85	MG	1	3438	-	X
85	MG	1	3442	-	X
85	MG	1	3445	-	X
85	MG	1	3449	-	X
85	MG	1	3451	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3452	-	X
85	MG	1	3453	-	X
85	MG	1	3456	-	X
85	MG	1	3457	-	X
85	MG	1	3461	-	X
85	MG	1	3463	-	X
85	MG	1	3466	-	X
85	MG	1	3469	-	X
85	MG	1	3470	-	X
85	MG	1	3473	-	X
85	MG	1	3475	-	X
85	MG	1	3479	-	X
85	MG	1	3480	-	X
85	MG	1	3482	-	X
85	MG	1	3483	-	X
85	MG	1	3485	-	X
85	MG	1	3487	-	X
85	MG	1	3489	-	X
85	MG	1	3491	-	X
85	MG	1	3492	-	X
85	MG	1	3498	-	X
85	MG	1	3499	-	X
85	MG	1	3501	-	X
85	MG	1	3503	-	X
85	MG	1	3508	-	X
85	MG	1	3522	-	X
85	MG	1	3525	-	X
85	MG	1	3527	-	X
85	MG	1	3531	-	X
85	MG	1	3533	-	X
85	MG	1	3534	-	X
85	MG	1	3535	-	X
85	MG	1	3536	-	X
85	MG	1	3538	-	X
85	MG	1	3541	-	X
85	MG	1	3542	-	X
85	MG	1	3544	-	X
85	MG	1	3546	-	X
85	MG	1	3552	-	X
85	MG	1	3553	-	X
85	MG	1	3555	-	X
85	MG	1	3559	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3561	-	X
85	MG	1	3563	-	X
85	MG	1	3570	-	X
85	MG	1	3576	-	X
85	MG	1	3587	-	X
85	MG	1	3594	-	X
85	MG	1	3595	-	X
85	MG	1	3599	-	X
85	MG	1	3607	-	X
85	MG	1	3608	-	X
85	MG	1	3609	-	X
85	MG	1	3611	-	X
85	MG	1	3612	-	X
85	MG	1	3615	-	X
85	MG	1	3617	-	X
85	MG	1	3618	-	X
85	MG	1	3619	-	X
85	MG	1	3620	-	X
85	MG	1	3622	-	X
85	MG	1	3624	-	X
85	MG	1	3626	-	X
85	MG	1	3629	-	X
85	MG	1	3630	-	X
85	MG	1	3631	-	X
85	MG	1	3632	-	X
85	MG	1	3634	-	X
85	MG	1	3635	-	X
85	MG	1	3639	-	X
85	MG	1	3640	-	X
85	MG	1	3644	-	X
85	MG	1	3646	-	X
85	MG	1	3647	-	X
85	MG	1	3648	-	X
85	MG	1	3650	-	X
85	MG	1	3659	-	X
85	MG	1	3660	-	X
85	MG	1	3663	-	X
85	MG	1	3665	-	X
85	MG	1	3669	-	X
85	MG	1	3674	-	X
85	MG	1	3675	-	X
85	MG	1	3678	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3679	-	X
85	MG	1	3680	-	X
85	MG	1	3681	-	X
85	MG	1	3682	-	X
85	MG	1	3684	-	X
85	MG	1	3689	-	X
85	MG	1	3690	-	X
85	MG	1	3692	-	X
85	MG	1	3693	-	X
85	MG	1	3698	-	X
85	MG	1	3700	-	X
85	MG	1	3701	-	X
85	MG	1	3702	-	X
85	MG	1	3705	-	X
85	MG	1	3707	-	X
85	MG	1	3708	-	X
85	MG	1	3709	-	X
85	MG	1	3710	-	X
85	MG	1	3712	-	X
85	MG	1	3715	-	X
85	MG	1	3717	-	X
85	MG	1	3718	-	X
85	MG	1	3719	-	X
85	MG	1	3720	-	X
85	MG	1	3721	-	X
85	MG	1	3723	-	X
85	MG	1	3725	-	X
85	MG	1	3727	-	X
85	MG	1	3728	-	X
85	MG	1	3729	-	X
85	MG	1	3730	-	X
85	MG	1	3731	-	X
85	MG	1	3736	-	X
85	MG	1	3737	-	X
85	MG	1	3739	-	X
85	MG	1	3740	-	X
85	MG	1	3746	-	X
85	MG	1	3748	-	X
85	MG	1	3749	-	X
85	MG	1	3755	-	X
85	MG	1	3756	-	X
85	MG	1	3757	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3758	-	X
85	MG	1	3760	-	X
85	MG	1	3761	-	X
85	MG	1	3766	-	X
85	MG	1	3767	-	X
85	MG	1	3768	-	X
85	MG	1	3769	-	X
85	MG	1	3772	-	X
85	MG	1	3774	-	X
85	MG	1	3780	-	X
85	MG	1	3781	-	X
85	MG	1	3782	-	X
85	MG	1	3783	-	X
85	MG	1	3785	-	X
85	MG	1	3787	-	X
85	MG	1	3789	-	X
85	MG	1	3790	-	X
85	MG	1	3792	-	X
85	MG	1	3793	-	X
85	MG	1	3795	-	X
85	MG	1	3796	-	X
85	MG	1	3798	-	X
85	MG	1	3799	-	X
85	MG	1	3800	-	X
85	MG	1	3804	-	X
85	MG	1	3806	-	X
85	MG	1	3807	-	X
85	MG	1	3808	-	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	3817	-	X
85	MG	1	3818	-	X
85	MG	1	3819	-	X
85	MG	1	3821	-	X
85	MG	1	3827	-	X
85	MG	1	3828	-	X
85	MG	1	3829	-	X
85	MG	1	3834	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3835	-	X
85	MG	1	3837	-	X
85	MG	1	3839	-	X
85	MG	1	3842	-	X
85	MG	1	3844	-	X
85	MG	1	3848	-	X
85	MG	1	3849	-	X
85	MG	1	3850	-	X
85	MG	1	3852	-	X
85	MG	1	3855	-	X
85	MG	1	4215	-	X
85	MG	1	4217	-	X
85	MG	2	1902	-	X
85	MG	2	1903	-	X
85	MG	2	1904	-	X
85	MG	2	1905	-	X
85	MG	2	1914	-	X
85	MG	2	1915	-	X
85	MG	2	1916	-	X
85	MG	2	1917	-	X
85	MG	2	1918	-	X
85	MG	2	1921	-	X
85	MG	2	1923	-	X
85	MG	2	1925	-	X
85	MG	2	1926	-	X
85	MG	2	1929	-	X
85	MG	2	1932	-	X
85	MG	2	1933	-	X
85	MG	2	1935	-	X
85	MG	2	1936	-	X
85	MG	2	1938	-	X
85	MG	2	1944	-	X
85	MG	2	1945	-	X
85	MG	2	1949	-	X
85	MG	2	1950	-	X
85	MG	2	1952	-	X
85	MG	2	1954	-	X
85	MG	2	1955	-	X
85	MG	2	1958	-	X
85	MG	2	1959	-	X
85	MG	2	1961	-	X
85	MG	2	1963	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1965	-	X
85	MG	2	1966	-	X
85	MG	2	1967	-	X
85	MG	2	1968	-	X
85	MG	2	1969	-	X
85	MG	2	1970	-	X
85	MG	2	1971	-	X
85	MG	2	1973	-	X
85	MG	2	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	1987	-	X
85	MG	2	1988	-	X
85	MG	2	1994	-	X
85	MG	2	1995	-	X
85	MG	2	1996	-	X
85	MG	2	2001	-	X
85	MG	2	2002	-	X
85	MG	2	2003	-	X
85	MG	2	2004	-	X
85	MG	2	2006	-	X
85	MG	2	2008	-	X
85	MG	2	2009	-	X
85	MG	2	2010	-	X
85	MG	2	2012	-	X
85	MG	2	2013	-	X
85	MG	2	2014	-	X
85	MG	2	2016	-	X
85	MG	2	2017	-	X
85	MG	2	2018	-	X
85	MG	2	2021	-	X
85	MG	3	201	-	X
85	MG	3	202	-	X
85	MG	3	204	-	X
85	MG	3	205	-	X
85	MG	3	207	-	X
85	MG	3	208	-	X
85	MG	3	209	-	X
85	MG	3	212	-	X
85	MG	3	214	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	4	201	-	X
85	MG	4	203	-	X
85	MG	4	208	-	X
85	MG	4	210	-	X
85	MG	4	211	-	X
85	MG	4	212	-	X
85	MG	4	213	-	X
85	MG	4	214	-	X
85	MG	4	217	-	X
85	MG	4	218	-	X
85	MG	4	220	-	X
85	MG	5	3401	-	X
85	MG	5	3404	-	X
85	MG	5	3407	-	X
85	MG	5	3410	-	X
85	MG	5	3413	-	X
85	MG	5	3417	-	X
85	MG	5	3425	-	X
85	MG	5	3430	-	X
85	MG	5	3432	-	X
85	MG	5	3434	-	X
85	MG	5	3435	-	X
85	MG	5	3436	-	X
85	MG	5	3438	-	X
85	MG	5	3439	-	X
85	MG	5	3442	-	X
85	MG	5	3444	-	X
85	MG	5	3449	-	X
85	MG	5	3451	-	X
85	MG	5	3458	-	X
85	MG	5	3462	-	X
85	MG	5	3466	-	X
85	MG	5	3467	-	X
85	MG	5	3469	-	X
85	MG	5	3472	-	X
85	MG	5	3473	-	X
85	MG	5	3475	-	X
85	MG	5	3477	-	X
85	MG	5	3481	-	X
85	MG	5	3483	-	X
85	MG	5	3486	-	X
85	MG	5	3487	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3490	-	X
85	MG	5	3491	-	X
85	MG	5	3496	-	X
85	MG	5	3498	-	X
85	MG	5	3501	-	X
85	MG	5	3502	-	X
85	MG	5	3503	-	X
85	MG	5	3504	-	X
85	MG	5	3510	-	X
85	MG	5	3515	-	X
85	MG	5	3518	-	X
85	MG	5	3522	-	X
85	MG	5	3525	-	X
85	MG	5	3528	-	X
85	MG	5	3529	-	X
85	MG	5	3530	-	X
85	MG	5	3534	-	X
85	MG	5	3535	-	X
85	MG	5	3536	-	X
85	MG	5	3539	-	X
85	MG	5	3544	-	X
85	MG	5	3546	-	X
85	MG	5	3551	-	X
85	MG	5	3553	-	X
85	MG	5	3554	-	X
85	MG	5	3558	-	X
85	MG	5	3559	-	X
85	MG	5	3560	-	X
85	MG	5	3561	-	X
85	MG	5	3562	-	X
85	MG	5	3565	-	X
85	MG	5	3569	-	X
85	MG	5	3571	-	X
85	MG	5	3574	-	X
85	MG	5	3575	-	X
85	MG	5	3577	-	X
85	MG	5	3578	-	X
85	MG	5	3580	-	X
85	MG	5	3582	-	X
85	MG	5	3589	-	X
85	MG	5	3594	-	X
85	MG	5	3596	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3600	-	X
85	MG	5	3603	-	X
85	MG	5	3604	-	X
85	MG	5	3605	-	X
85	MG	5	3607	-	X
85	MG	5	3608	-	X
85	MG	5	3613	-	X
85	MG	5	3614	-	X
85	MG	5	3616	-	X
85	MG	5	3622	-	X
85	MG	5	3624	-	X
85	MG	5	3626	-	X
85	MG	5	3627	-	X
85	MG	5	3629	-	X
85	MG	5	3630	-	X
85	MG	5	3632	-	X
85	MG	5	3634	-	X
85	MG	5	3638	-	X
85	MG	5	3639	-	X
85	MG	5	3641	-	X
85	MG	5	3643	-	X
85	MG	5	3644	-	X
85	MG	5	3646	-	X
85	MG	5	3649	-	X
85	MG	5	3651	-	X
85	MG	5	3652	-	X
85	MG	5	3653	-	X
85	MG	5	3654	-	X
85	MG	5	3655	-	X
85	MG	5	3656	-	X
85	MG	5	3657	-	X
85	MG	5	3659	-	X
85	MG	5	3663	-	X
85	MG	5	3665	-	X
85	MG	5	3666	-	X
85	MG	5	3668	-	X
85	MG	5	3669	-	X
85	MG	5	3670	-	X
85	MG	5	3673	-	X
85	MG	5	3676	-	X
85	MG	5	3677	-	X
85	MG	5	3678	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3679	-	X
85	MG	5	3680	-	X
85	MG	5	3681	-	X
85	MG	5	3683	-	X
85	MG	5	3686	-	X
85	MG	5	3687	-	X
85	MG	5	3692	-	X
85	MG	5	3694	-	X
85	MG	5	3696	-	X
85	MG	5	3698	-	X
85	MG	5	3699	-	X
85	MG	5	3701	-	X
85	MG	5	3702	-	X
85	MG	5	3703	-	X
85	MG	5	3704	-	X
85	MG	5	3705	-	X
85	MG	5	3707	-	X
85	MG	5	3708	-	X
85	MG	5	3709	-	X
85	MG	5	3713	-	X
85	MG	5	3715	-	X
85	MG	5	3717	-	X
85	MG	5	3720	-	X
85	MG	5	3724	-	X
85	MG	5	3726	-	X
85	MG	5	3727	-	X
85	MG	5	3728	-	X
85	MG	5	3730	-	X
85	MG	5	3731	-	X
85	MG	5	3732	-	X
85	MG	5	3733	-	X
85	MG	5	3734	-	X
85	MG	5	3737	-	X
85	MG	5	3738	-	X
85	MG	5	3739	-	X
85	MG	5	3743	-	X
85	MG	5	3745	-	X
85	MG	5	3749	-	X
85	MG	5	3751	-	X
85	MG	5	3754	-	X
85	MG	5	3756	-	X
85	MG	5	3757	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3758	-	X
85	MG	5	3760	-	X
85	MG	5	3761	-	X
85	MG	5	3763	-	X
85	MG	5	3765	-	X
85	MG	5	3768	-	X
85	MG	5	3769	-	X
85	MG	5	3772	-	X
85	MG	5	3774	-	X
85	MG	5	3775	-	X
85	MG	5	3777	-	X
85	MG	5	3778	-	X
85	MG	5	3782	-	X
85	MG	5	3786	-	X
85	MG	5	3787	-	X
85	MG	5	3792	-	X
85	MG	5	3793	-	X
85	MG	5	3796	-	X
85	MG	5	3797	-	X
85	MG	5	3798	-	X
85	MG	5	3801	-	X
85	MG	5	3806	-	X
85	MG	5	3807	-	X
85	MG	5	3808	-	X
85	MG	5	3810	-	X
85	MG	5	3812	-	X
85	MG	5	3814	-	X
85	MG	5	3817	-	X
85	MG	5	3819	-	X
85	MG	5	3820	-	X
85	MG	5	3822	-	X
85	MG	5	3823	-	X
85	MG	5	3825	-	X
85	MG	5	3827	-	X
85	MG	5	3831	-	X
85	MG	5	3832	-	X
85	MG	5	3838	-	X
85	MG	5	3839	-	X
85	MG	5	3840	-	X
85	MG	5	3842	-	X
85	MG	5	3843	-	X
85	MG	5	3845	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3846	-	X
85	MG	5	3847	-	X
85	MG	5	3848	-	X
85	MG	5	3850	-	X
85	MG	5	3851	-	X
85	MG	5	3852	-	X
85	MG	5	3853	-	X
85	MG	5	3855	-	X
85	MG	5	3858	-	X
85	MG	5	3863	-	X
85	MG	5	3865	-	X
85	MG	5	3866	-	X
85	MG	5	3868	-	X
85	MG	5	3869	-	X
85	MG	5	3873	-	X
85	MG	5	3874	-	X
85	MG	5	3875	-	X
85	MG	5	3878	-	X
85	MG	5	3880	-	X
85	MG	5	3882	-	X
85	MG	5	3886	-	X
85	MG	5	3889	-	X
85	MG	5	3890	-	X
85	MG	5	3891	-	X
85	MG	5	4249	-	X
85	MG	6	1901	-	X
85	MG	6	1902	-	X
85	MG	6	1903	-	X
85	MG	6	1904	-	X
85	MG	6	1908	-	X
85	MG	6	1911	-	X
85	MG	6	1912	-	X
85	MG	6	1913	-	X
85	MG	6	1914	-	X
85	MG	6	1915	-	X
85	MG	6	1916	-	X
85	MG	6	1917	-	X
85	MG	6	1918	-	X
85	MG	6	1919	-	X
85	MG	6	1920	-	X
85	MG	6	1921	-	X
85	MG	6	1924	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1925	-	X
85	MG	6	1927	-	X
85	MG	6	1930	-	X
85	MG	6	1932	-	X
85	MG	6	1933	-	X
85	MG	6	1936	-	X
85	MG	6	1937	-	X
85	MG	6	1939	-	X
85	MG	6	1940	-	X
85	MG	6	1941	-	X
85	MG	6	1942	-	X
85	MG	6	1943	-	X
85	MG	6	1944	-	X
85	MG	6	1945	-	X
85	MG	6	1949	-	X
85	MG	6	1950	-	X
85	MG	6	1952	-	X
85	MG	6	1953	-	X
85	MG	6	1954	-	X
85	MG	6	1955	-	X
85	MG	6	1958	-	X
85	MG	6	1959	-	X
85	MG	6	1964	-	X
85	MG	6	1965	-	X
85	MG	6	1966	-	X
85	MG	6	1967	-	X
85	MG	6	1969	-	X
85	MG	6	1971	-	X
85	MG	6	1972	-	X
85	MG	6	1973	-	X
85	MG	6	1974	-	X
85	MG	6	1976	-	X
85	MG	6	1978	-	X
85	MG	6	1980	-	X
85	MG	6	1981	-	X
85	MG	6	1985	-	X
85	MG	6	1986	-	X
85	MG	6	1993	-	X
85	MG	6	1994	-	X
85	MG	6	1997	-	X
85	MG	6	1998	-	X
85	MG	6	2002	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	2005	-	X
85	MG	6	2007	-	X
85	MG	6	2008	-	X
85	MG	6	2009	-	X
85	MG	6	2010	-	X
85	MG	6	2013	-	X
85	MG	6	2014	-	X
85	MG	6	2018	-	X
85	MG	6	2021	-	X
85	MG	6	2024	-	X
85	MG	6	2027	-	X
85	MG	6	2028	-	X
85	MG	6	2030	-	X
85	MG	6	2032	-	X
85	MG	6	2035	-	X
85	MG	6	2038	-	X
85	MG	6	2039	-	X
85	MG	6	2040	-	X
85	MG	6	2042	-	X
85	MG	6	2044	-	X
85	MG	6	2045	-	X
85	MG	7	201	-	X
85	MG	7	202	-	X
85	MG	7	204	-	X
85	MG	7	206	-	X
85	MG	7	208	-	X
85	MG	7	209	-	X
85	MG	7	211	-	X
85	MG	7	213	-	X
85	MG	7	214	-	X
85	MG	7	216	-	X
85	MG	7	217	-	X
85	MG	8	204	-	X
85	MG	8	205	-	X
85	MG	8	207	-	X
85	MG	8	208	-	X
85	MG	8	209	-	X
85	MG	8	210	-	X
85	MG	8	211	-	X
85	MG	8	213	-	X
85	MG	8	214	-	X
85	MG	D0	201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	D3	201	-	X
85	MG	L3	401	-	X
85	MG	L4	401	-	X
85	MG	L4	403	-	X
85	MG	L7	302	-	X
85	MG	M0	302	-	X
85	MG	M1	201	-	X
85	MG	M3	201	-	X
85	MG	M7	202	-	X
85	MG	M7	205	-	X
85	MG	N3	201	-	X
85	MG	N3	202	-	X
85	MG	N8	202	-	X
85	MG	N8	203	-	X
85	MG	N8	204	-	X
85	MG	N8	205	-	X
85	MG	O2	201	-	X
85	MG	O2	202	-	X
85	MG	O5	201	-	X
85	MG	c4	201	-	X
85	MG	c9	201	-	X
85	MG	d3	202	-	X
85	MG	d3	203	-	X
85	MG	d6	102	-	X
85	MG	l2	301	-	X
85	MG	l2	303	-	X
85	MG	l3	402	-	X
85	MG	l3	403	-	X
85	MG	l4	401	-	X
85	MG	l5	302	-	X
85	MG	l7	301	-	X
85	MG	m0	301	-	X
85	MG	m4	201	-	X
85	MG	m5	303	-	X
85	MG	m5	305	-	X
85	MG	m7	205	-	X
85	MG	m7	206	-	X
85	MG	n8	201	-	X
85	MG	o3	201	-	X
85	MG	o3	202	-	X
85	MG	o7	101	-	X
85	MG	q0	3601	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	q0	3603	-	X
85	MG	s8	301	-	X
86	OHX	1	3859	-	X
86	OHX	1	3886	-	X
86	OHX	1	3891	-	X
86	OHX	1	3898	-	X
86	OHX	1	3913	-	X
86	OHX	1	4052	-	X
86	OHX	1	4058	-	X
86	OHX	1	4068	-	X
86	OHX	1	4074	-	X
86	OHX	1	4090	-	X
86	OHX	1	4121	-	X
86	OHX	1	4123	-	X
86	OHX	1	4135	-	X
86	OHX	1	4136	-	X
86	OHX	1	4137	-	X
86	OHX	1	4139	-	X
86	OHX	1	4167	-	X
86	OHX	1	4173	-	X
86	OHX	1	4183	-	X
86	OHX	1	4185	-	X
86	OHX	1	4186	-	X
86	OHX	1	4195	-	X
86	OHX	1	4203	-	X
86	OHX	1	4207	-	X
86	OHX	1	4209	-	X
86	OHX	2	2028	-	X
86	OHX	2	2052	-	X
86	OHX	2	2135	-	X
86	OHX	2	2143	-	X
86	OHX	2	2148	-	X
86	OHX	2	2157	-	X
86	OHX	2	2159	-	X
86	OHX	2	2160	-	X
86	OHX	2	2174	-	X
86	OHX	2	2176	-	X
86	OHX	4	231	-	X
86	OHX	4	236	-	X
86	OHX	5	3894	-	X
86	OHX	5	3901	-	X
86	OHX	5	3906	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4006	-	X
86	OHX	5	4091	-	X
86	OHX	5	4100	-	X
86	OHX	5	4106	-	X
86	OHX	5	4108	-	X
86	OHX	5	4146	-	X
86	OHX	5	4148	-	X
86	OHX	5	4149	-	X
86	OHX	5	4155	-	X
86	OHX	5	4160	-	X
86	OHX	5	4170	-	X
86	OHX	5	4179	-	X
86	OHX	5	4182	-	X
86	OHX	5	4190	-	X
86	OHX	5	4199	-	X
86	OHX	5	4201	-	X
86	OHX	5	4214	-	X
86	OHX	5	4217	-	X
86	OHX	5	4223	-	X
86	OHX	5	4225	-	X
86	OHX	5	4226	-	X
86	OHX	5	4230	-	X
86	OHX	5	4239	-	X
86	OHX	6	2054	-	X
86	OHX	6	2156	-	X
86	OHX	6	2160	-	X
86	OHX	6	2165	-	X
86	OHX	6	2180	-	X
86	OHX	6	2183	-	X
86	OHX	6	2204	-	X
86	OHX	7	227	-	X
86	OHX	8	225	-	X
86	OHX	8	228	-	X
86	OHX	m7	207	-	X
86	OHX	s9	201	-	X
87	ZN	d7	101	-	X
88	BLS	1	4211	-	X
88	BLS	5	4248	-	X

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411214 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	652	221	231				
35	sM	104	Total	C	N	O		0	0	0
			679	402	140	137				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	17	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	18	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	19	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 82 is a protein called unknown protein chain m2.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	2	Total	Mg	0	0
			2	2		
85	m6	2	Total	Mg	0	0
			2	2		
85	n8	3	Total	Mg	0	0
			3	3		
85	N5	1	Total	Mg	0	0
			1	1		
85	6	147	Total	Mg	0	0
			147	147		
85	sM	1	Total	Mg	0	0
			1	1		
85	m5	5	Total	Mg	0	0
			5	5		
85	l3	3	Total	Mg	0	0
			3	3		
85	C1	1	Total	Mg	0	0
			1	1		
85	M1	1	Total	Mg	0	0
			1	1		
85	d6	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	122	Total 122	Mg 122	0	0
85	n0	1	Total 1	Mg 1	0	0
85	L4	3	Total 3	Mg 3	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	2	Total 2	Mg 2	0	0
85	c9	1	Total 1	Mg 1	0	0
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	M9	1	Total 1	Mg 1	0	0
85	q0	2	Total 2	Mg 2	0	0
85	SM	1	Total 1	Mg 1	0	0
85	o4	3	Total 3	Mg 3	0	0
85	M0	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	n6	2	Total 2	Mg 2	0	0
85	5	495	Total 495	Mg 495	0	0
85	c8	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	n9	2	Total 2	Mg 2	0	0
85	1	462	Total 462	Mg 462	0	0

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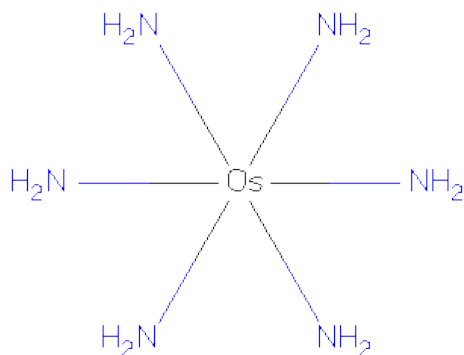
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	c4	1	Total 1	Mg 1	0	0
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	3	Total 3	Mg 3	0	0
85	O2	2	Total 2	Mg 2	0	0
85	o7	1	Total 1	Mg 1	0	0
85	o3	2	Total 2	Mg 2	0	0
85	d3	3	Total 3	Mg 3	0	0
85	M3	2	Total 2	Mg 2	0	0
85	N3	3	Total 3	Mg 3	0	0
85	4	23	Total 23	Mg 23	0	0
85	D4	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	2	Total 2	Mg 2	0	0
85	m1	1	Total 1	Mg 1	0	0
85	l5	3	Total 3	Mg 3	0	0
85	d0	1	Total 1	Mg 1	0	0
85	M7	5	Total 5	Mg 5	0	0
85	m4	1	Total 1	Mg 1	0	0
85	N8	5	Total 5	Mg 5	0	0
85	s1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	l9	1	Total 1	Mg 1	0	0
85	O1	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	17	Total 17	Mg 17	0	0
85	n3	1	Total 1	Mg 1	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	4	Total 4	Mg 4	0	0
85	O5	1	Total 1	Mg 1	0	0
85	N6	2	Total 2	Mg 2	0	0
85	8	14	Total 14	Mg 14	0	0
85	l4	1	Total 1	Mg 1	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0
85	m0	1	Total 1	Mg 1	0	0
85	3	15	Total 15	Mg 15	0	0
85	m7	6	Total 6	Mg 6	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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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
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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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
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
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			7	6	1		
86	C3	1	Total	N	Os	0	0
			7	6	1		
86	C5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	C8	1	Total	N	Os	0	0
			7	6	1		
86	D3	1	Total	N	Os	0	0
			7	6	1		
86	D9	1	Total	N	Os	0	0
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86	SR	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	M7	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
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86	6	1	Total 7	N 6	Os 1	0	0
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86	6	1	Total 7	N 6	Os 1	0	0
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86	s1	1	Total 7	N 6	Os 1	0	0
86	s4	1	Total 7	N 6	Os 1	0	0
86	s8	1	Total 7	N 6	Os 1	0	0
86	s9	1	Total 7	N 6	Os 1	0	0
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86	c5	1	Total 7	N 6	Os 1	0	0
86	c8	1	Total 7	N 6	Os 1	0	0
86	d4	1	Total 7	N 6	Os 1	0	0
86	d9	1	Total 7	N 6	Os 1	0	0
86	sR	1	Total 7	N 6	Os 1	0	0

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

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

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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		
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	l3	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	n1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

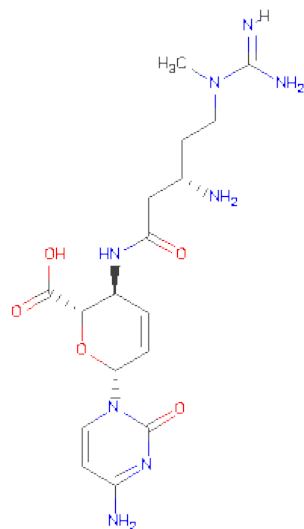
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0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

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

- Molecule 88 is BLASTICIDIN S (three-letter code: BLS) (formula: C₁₇H₂₆N₈O₅).

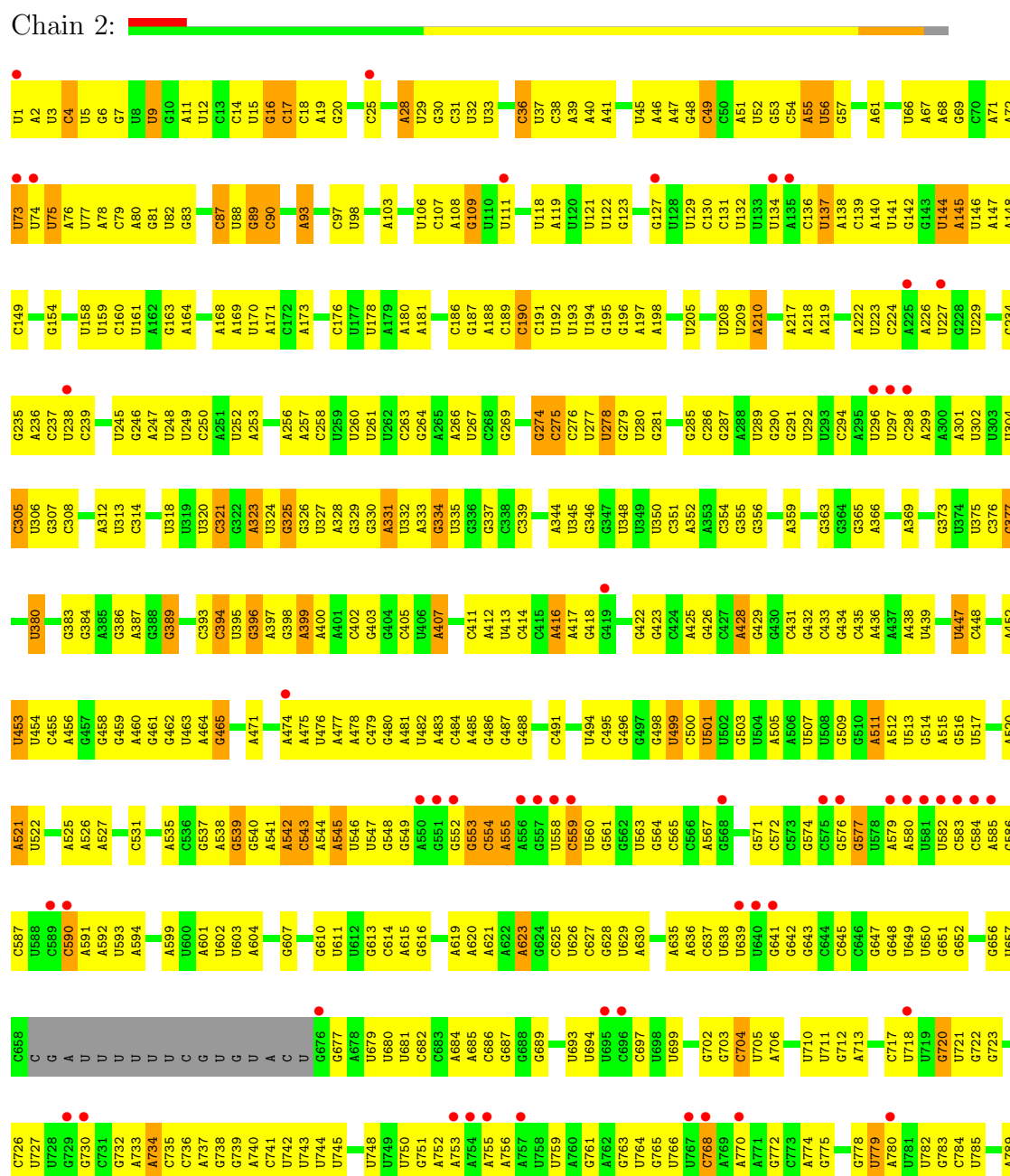


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total	C	N	O	0	0
			30	17	8	5		
88	5	1	Total	C	N	O	0	0
			30	17	8	5		

3 Residue-property plots

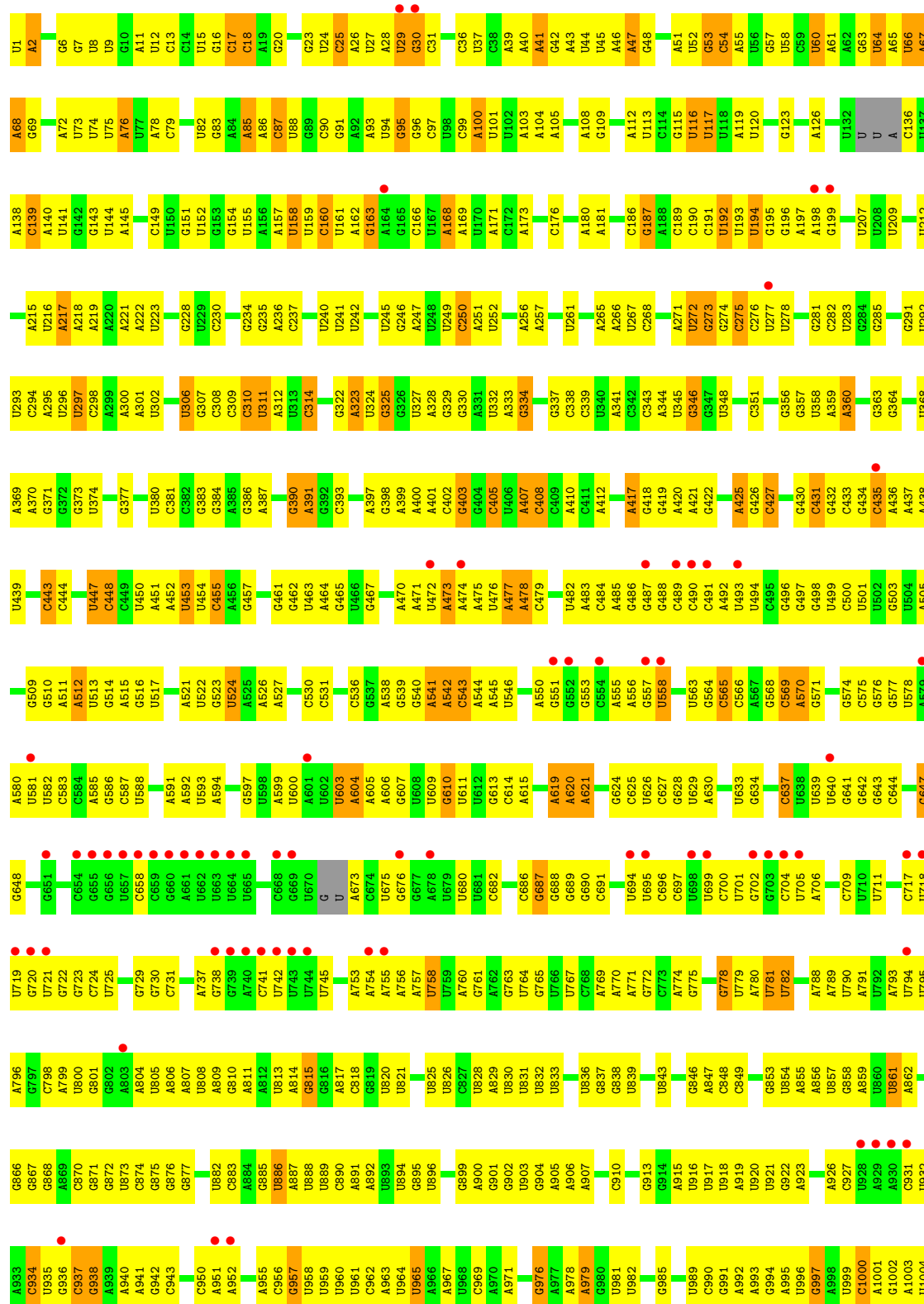
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

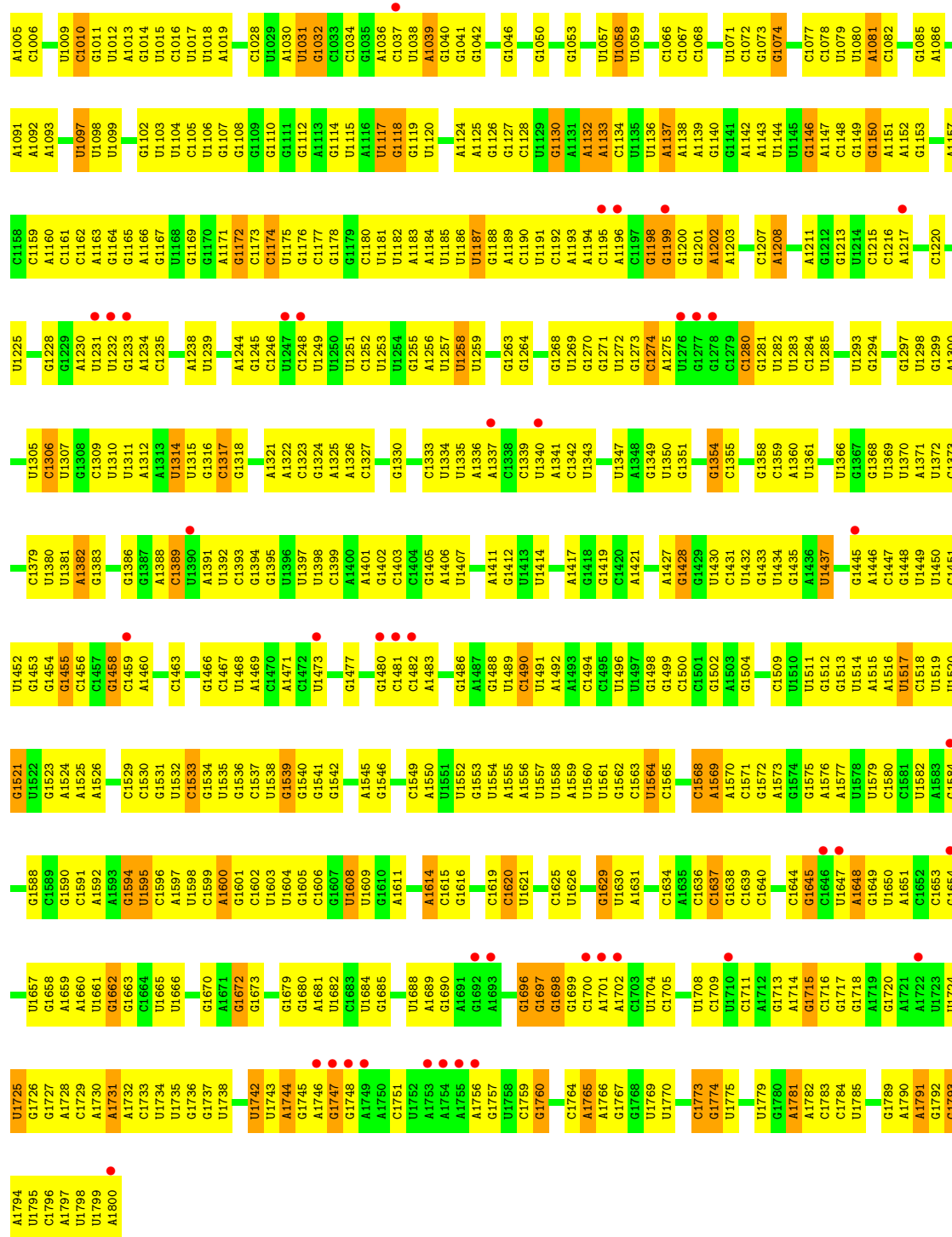
- Molecule 1: *Saccharomyces cerevisiae* chromosome XII cosmid 9634



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

Chain 6:

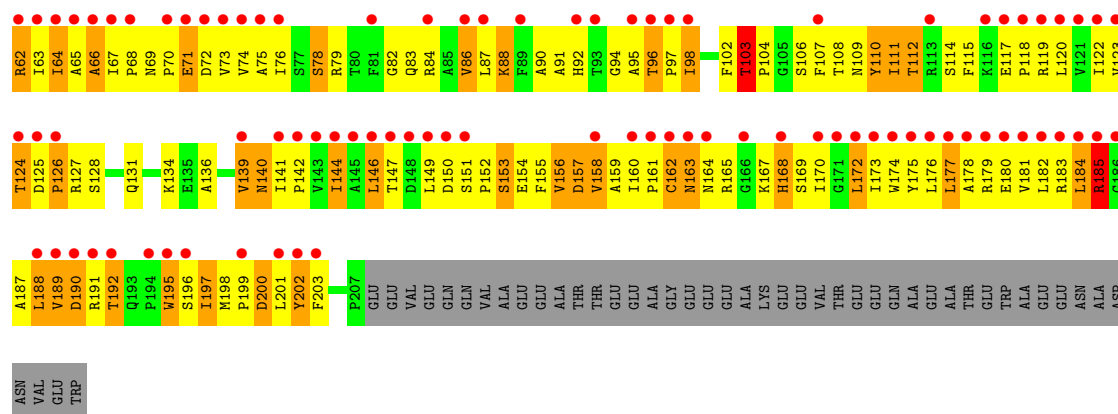




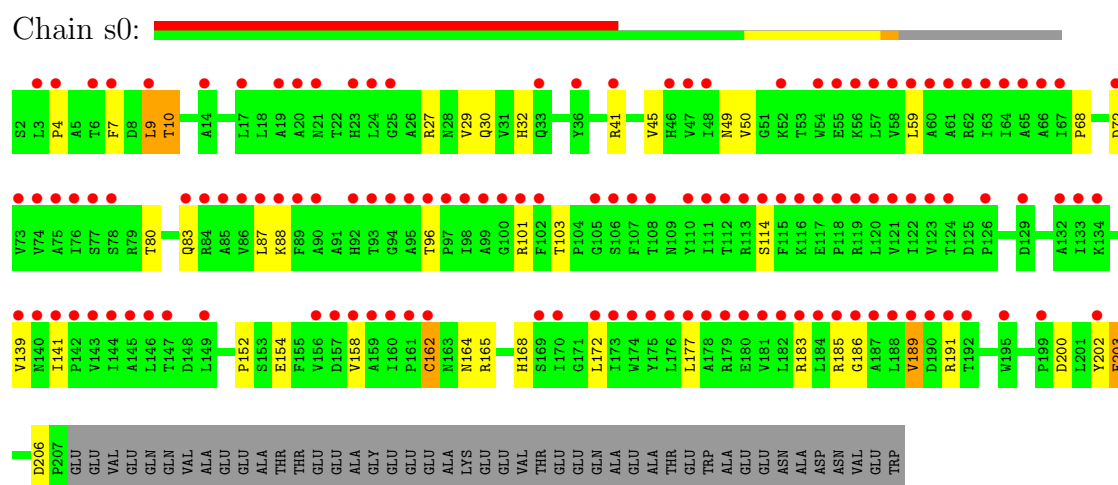
• Molecule 2: 40S ribosomal protein S0-A

Chain S0:

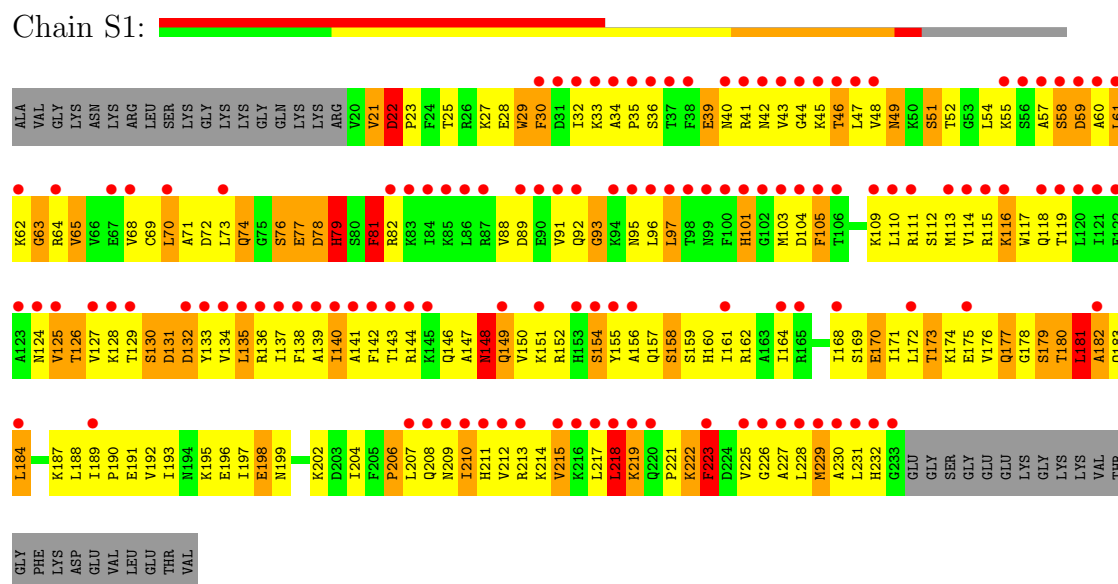




• Molecule 2: 40S ribosomal protein S0-A

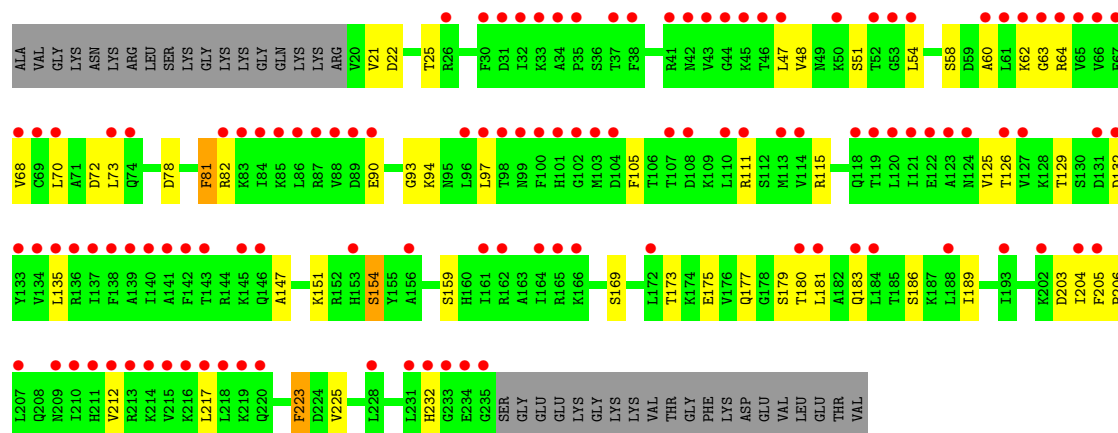


• Molecule 3: 40S ribosomal protein S1-A



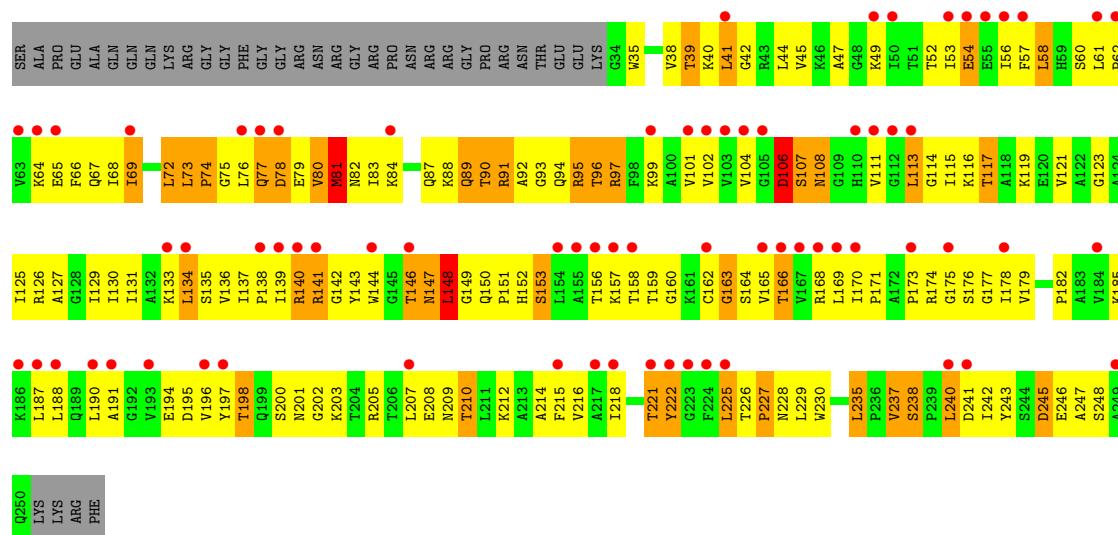
• Molecule 3: 40S ribosomal protein S1-A





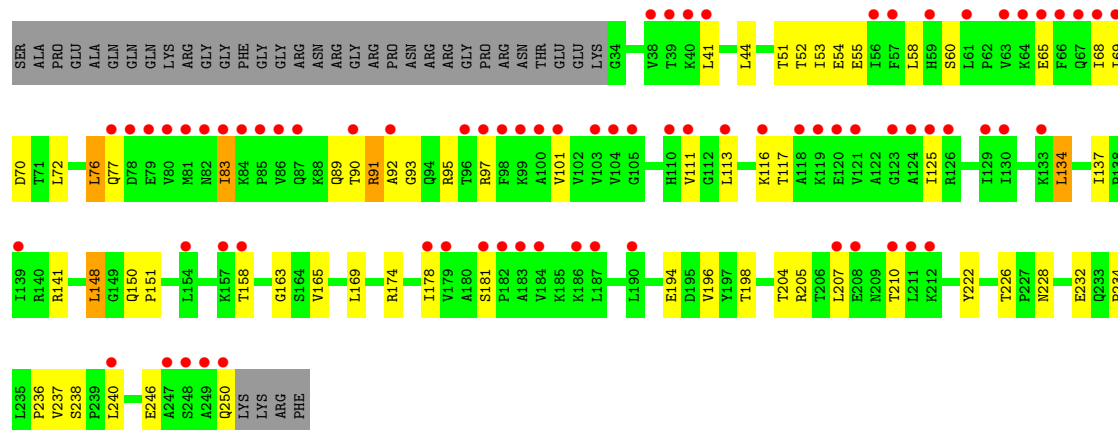
• Molecule 4: 40S ribosomal protein S2

Chain S2:



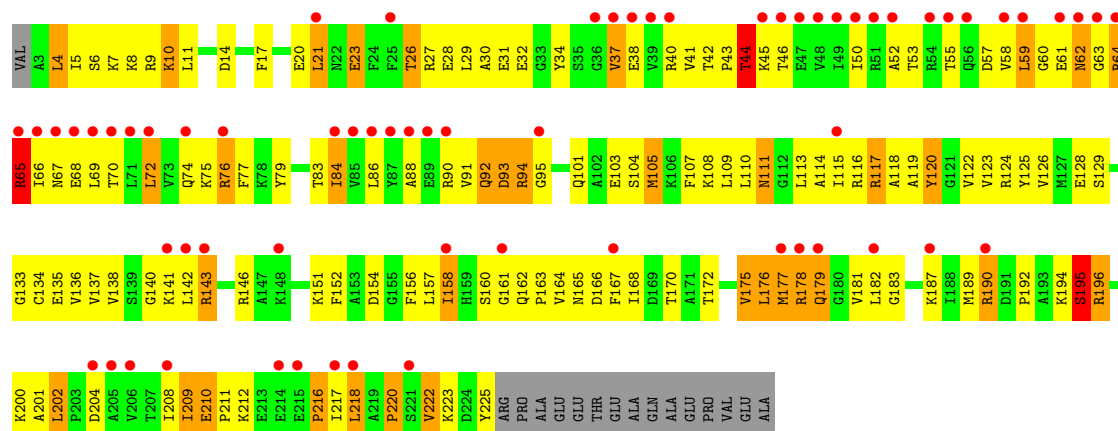
• Molecule 4: 40S ribosomal protein S2

Chain s2:



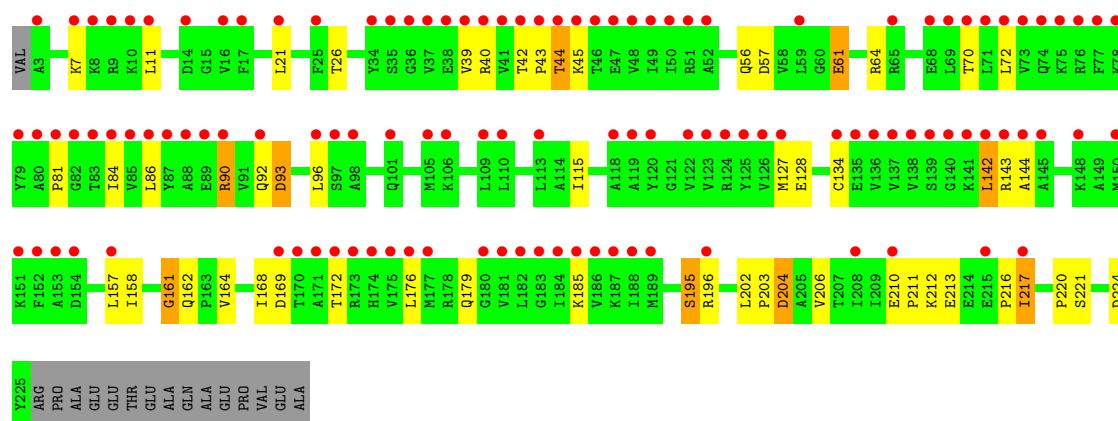
• Molecule 5: 40S ribosomal protein S3

Chain S3:



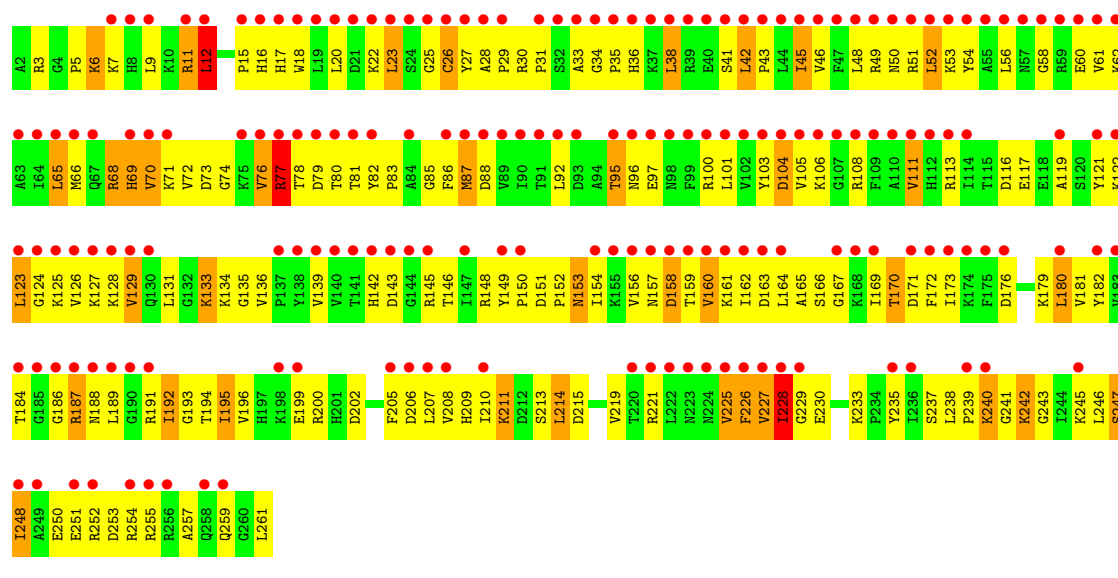
• Molecule 5: 40S ribosomal protein S3

Chain s3:



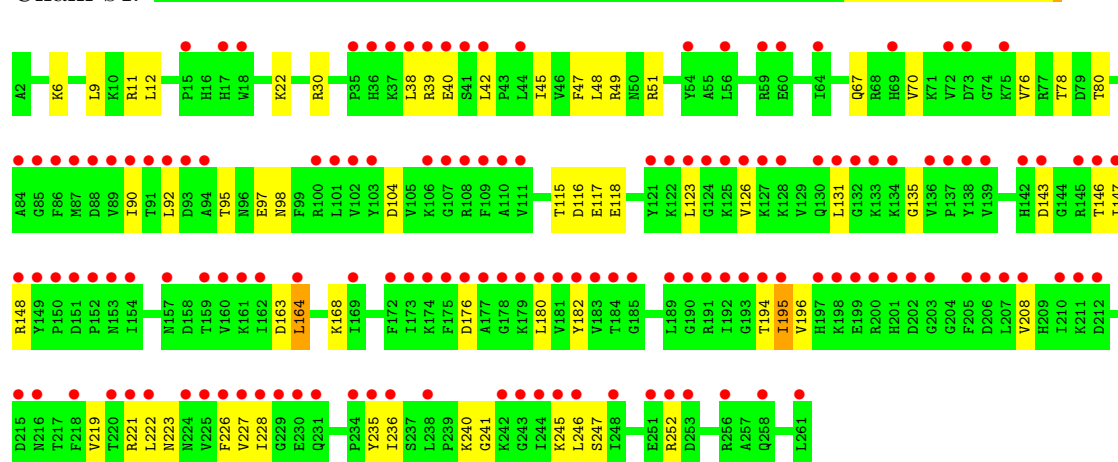
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



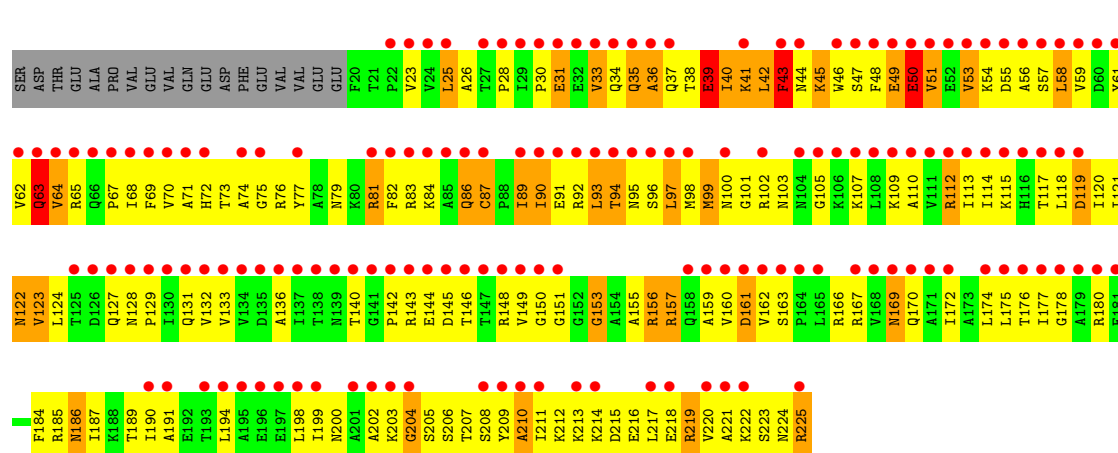
- Molecule 6: 40S ribosomal protein S4-A

Chain s4:



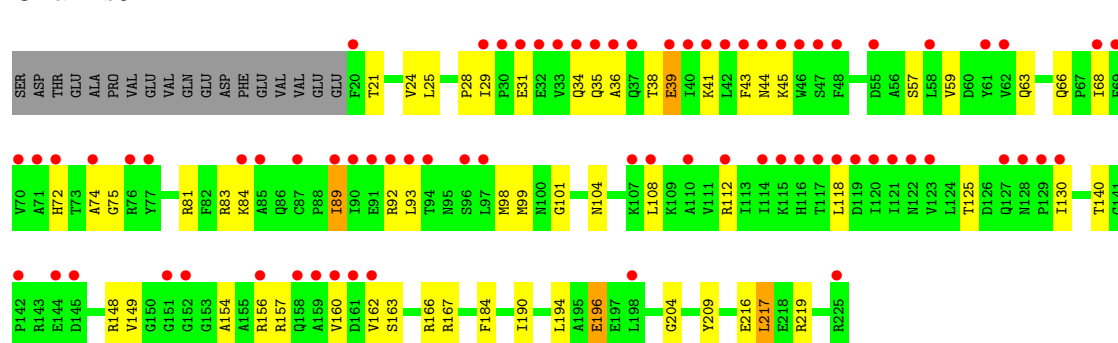
- Molecule 7: 40S ribosomal protein S5

Chain S5:



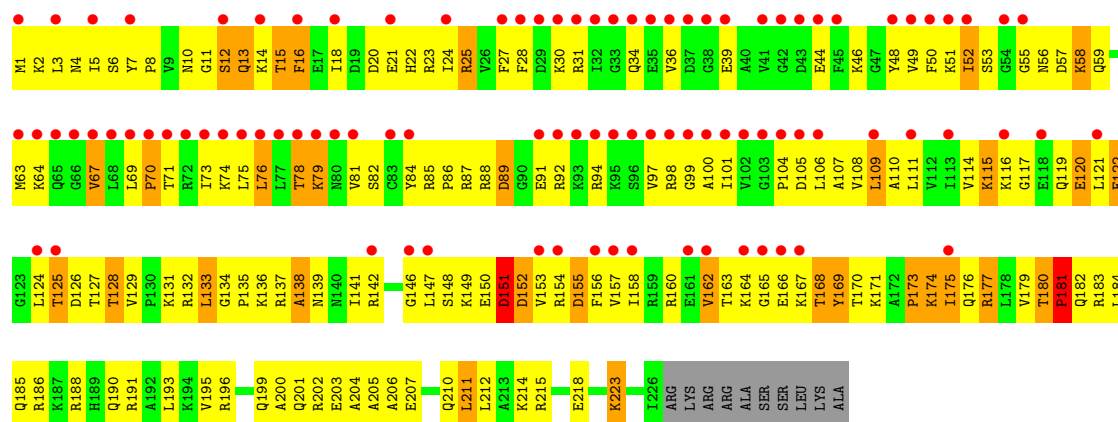
- Molecule 7: 40S ribosomal protein S5

Chain s5:



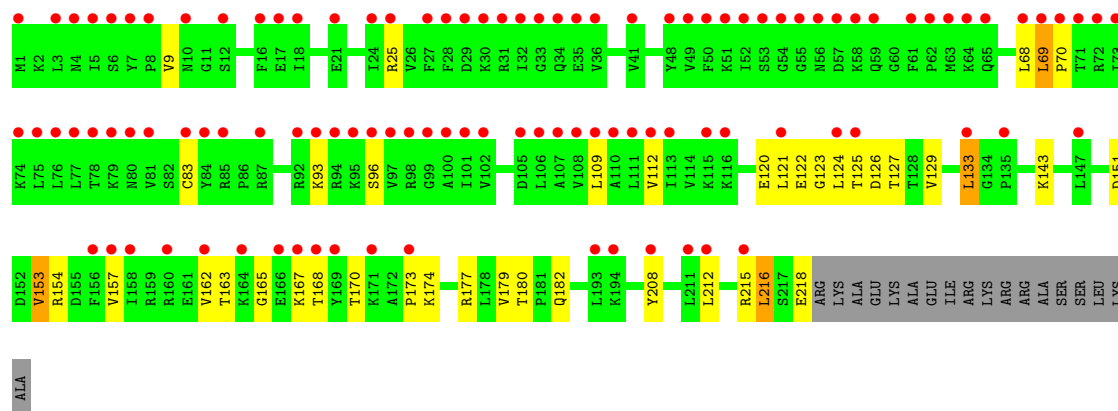
- Molecule 8: 40S ribosomal protein S6-A

Chain S6:



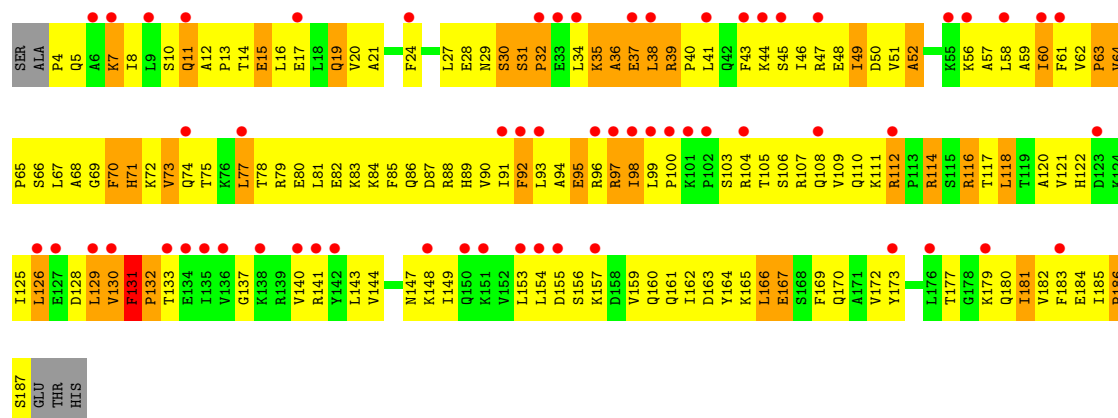
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



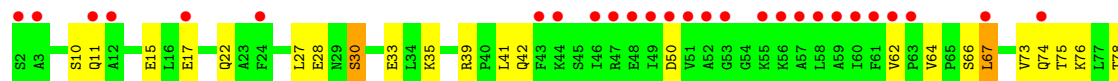
• Molecule 9: 40S ribosomal protein S7-A

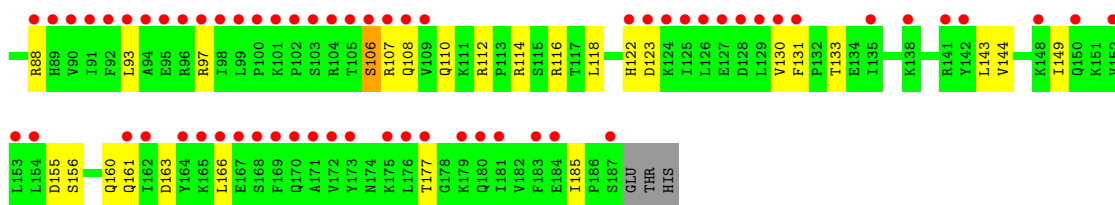
Chain S7:



• Molecule 9: 40S ribosomal protein S7-A

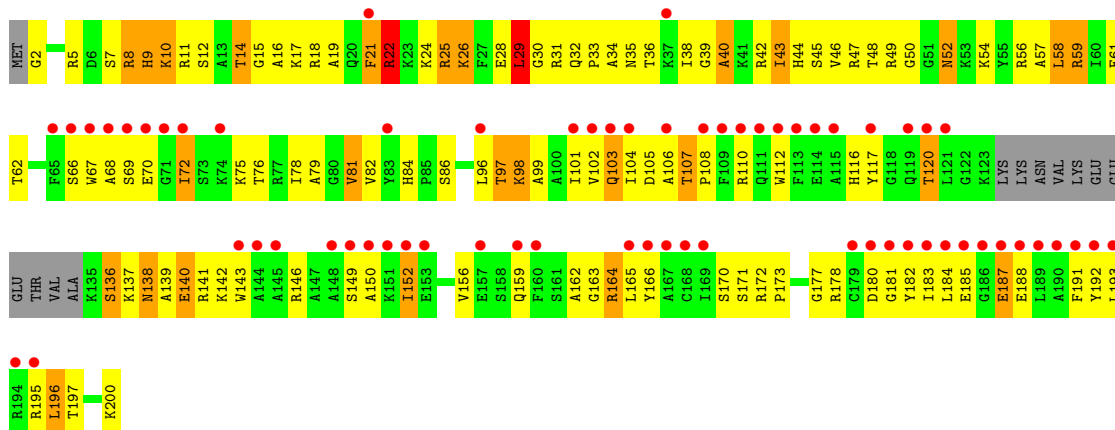
Chain s7:





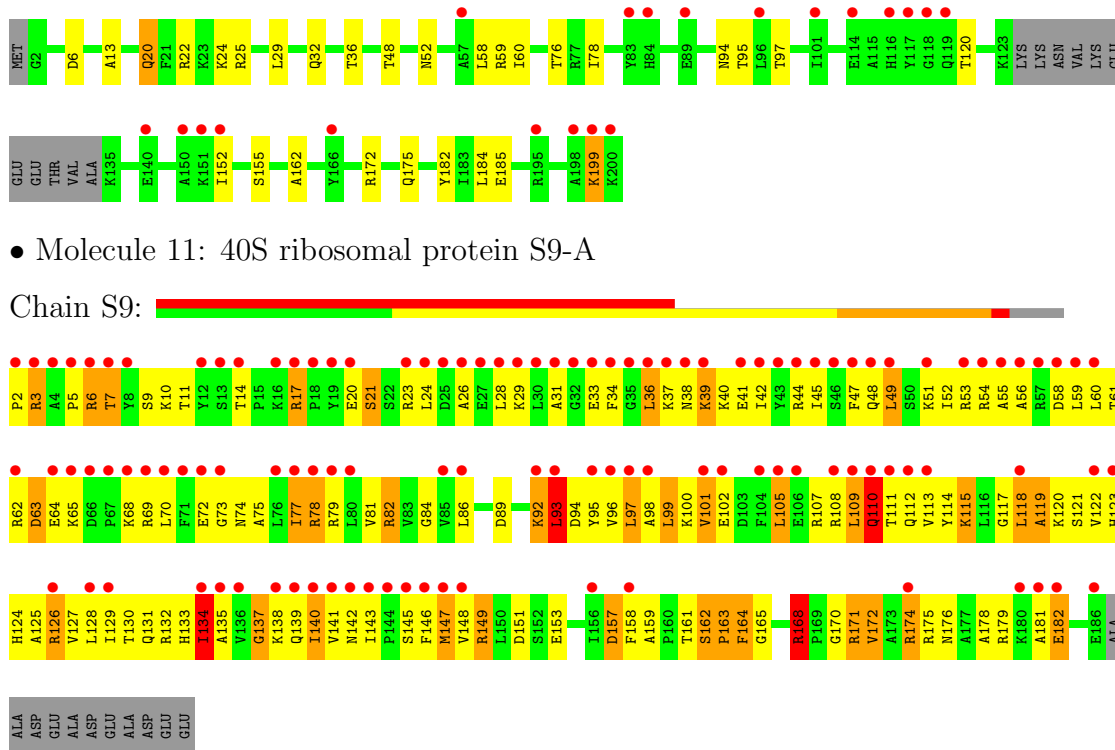
• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



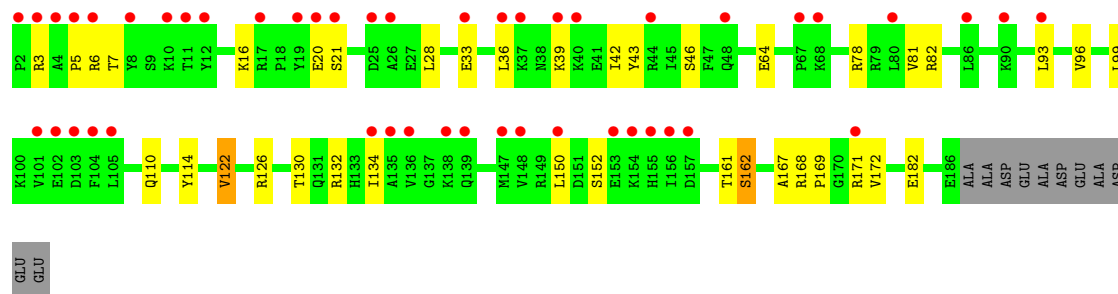
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



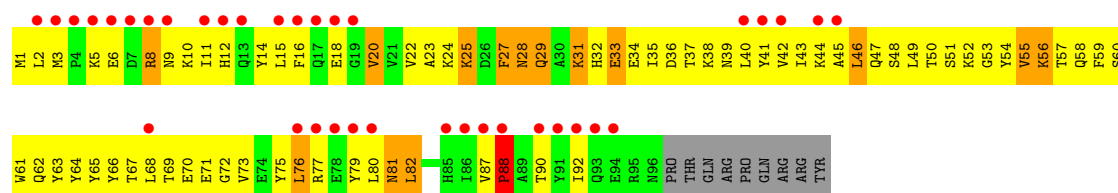
• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



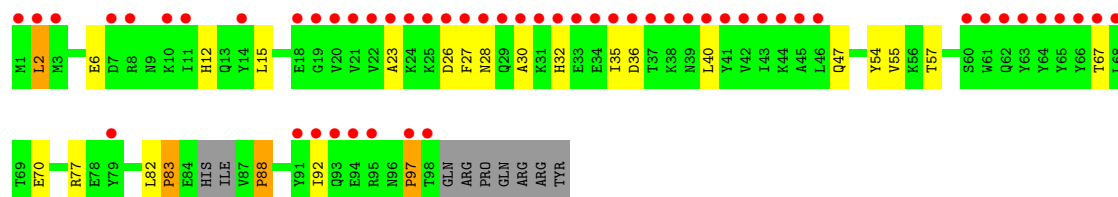
- Molecule 12: 40S ribosomal protein S10-A

Chain C0:



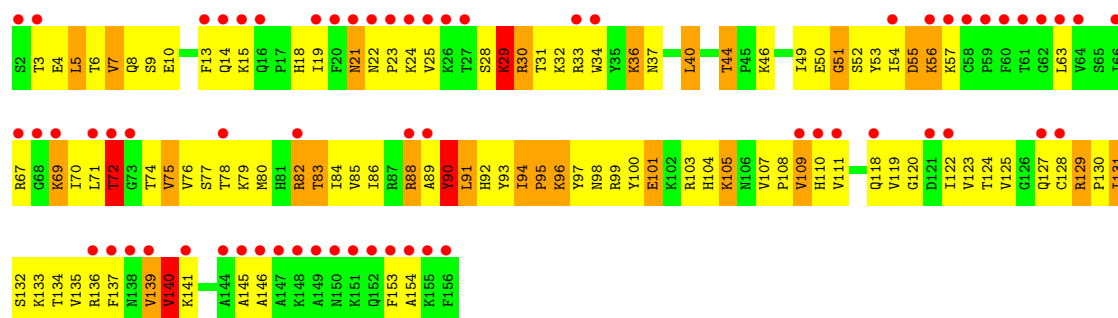
- Molecule 12: 40S ribosomal protein S10-A

Chain c0:



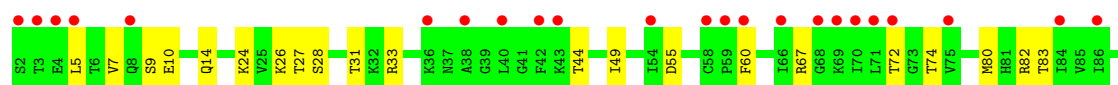
- Molecule 13: 40S ribosomal protein S11-A

Chain C1:



- Molecule 13: 40S ribosomal protein S11-A

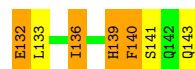
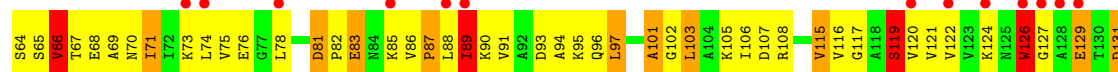
Chain c1:





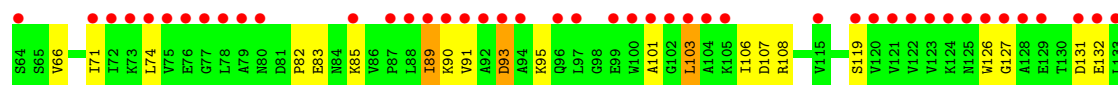
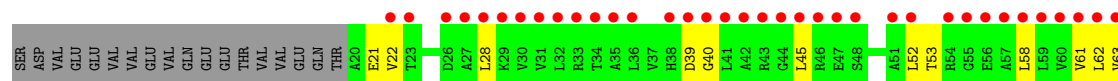
- Molecule 14: 40S ribosomal protein S12

Chain C2:



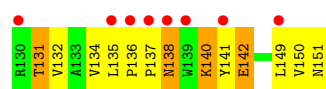
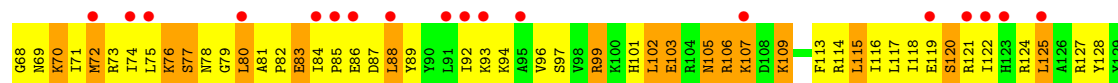
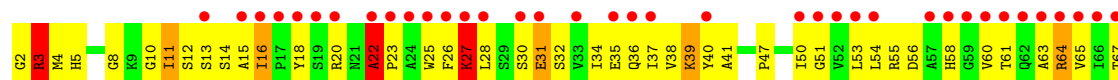
- Molecule 14: 40S ribosomal protein S12

Chain c2:



- Molecule 15: 40S ribosomal protein S13

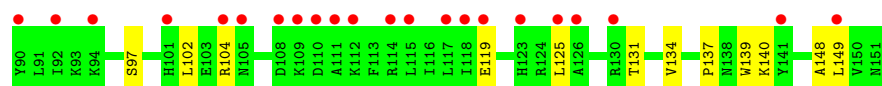
Chain C3:



- Molecule 15: 40S ribosomal protein S13

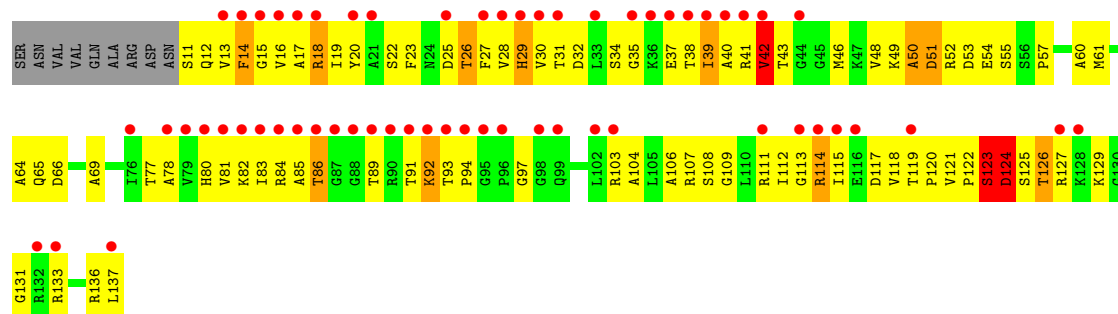
Chain c3:





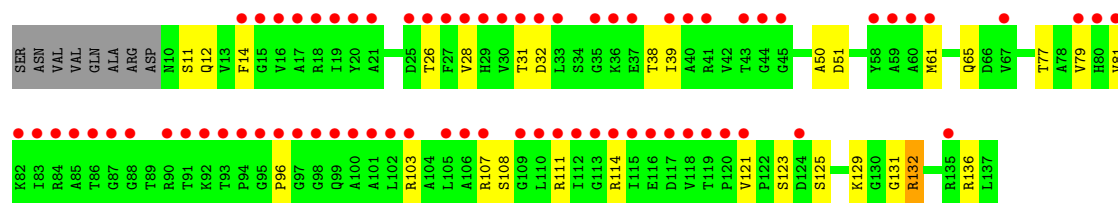
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



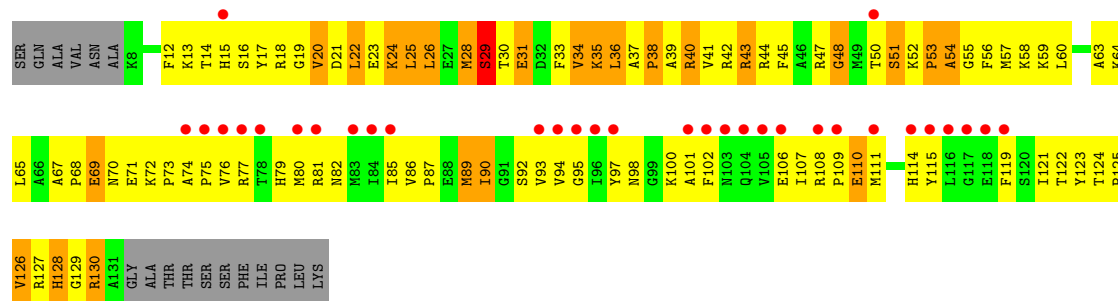
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



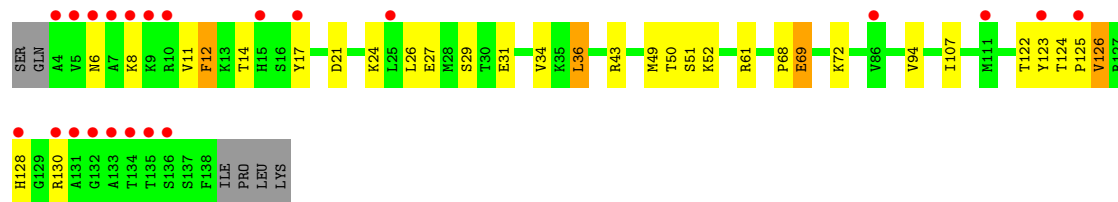
• Molecule 17: 40S ribosomal protein S15

Chain C5:



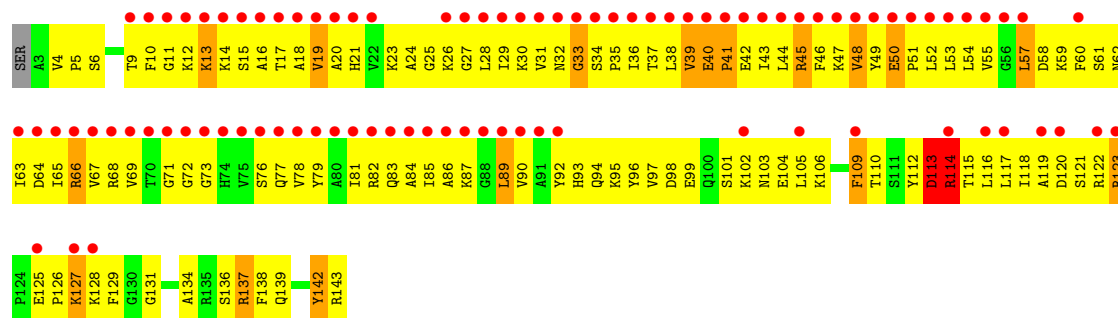
• Molecule 17: 40S ribosomal protein S15

Chain c5:



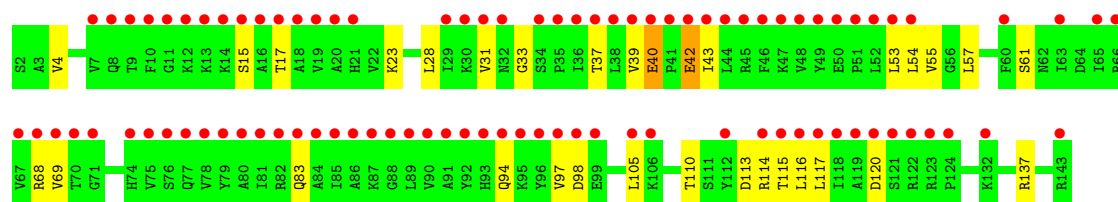
• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



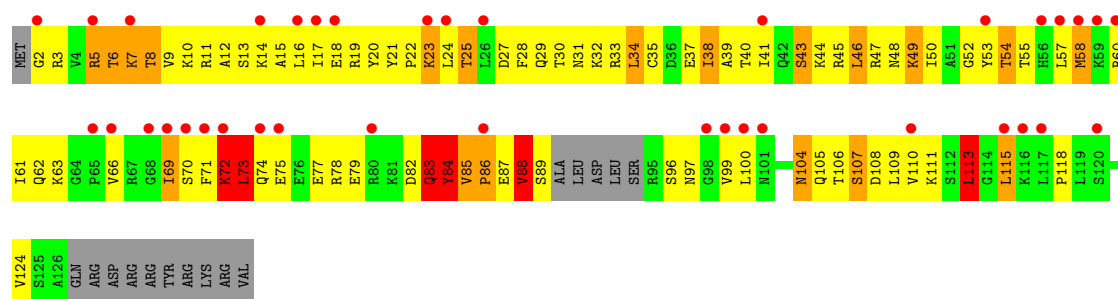
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:



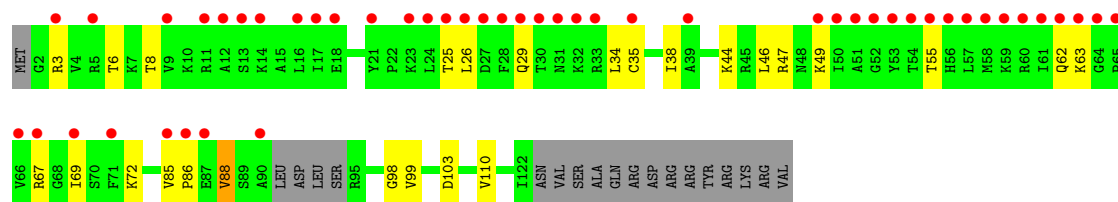
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:



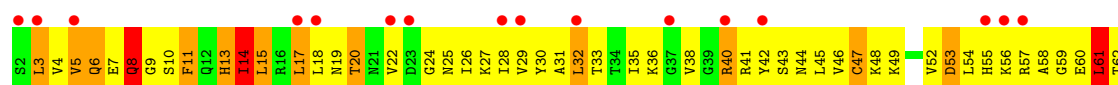
- Molecule 19: 40S ribosomal protein S17-A

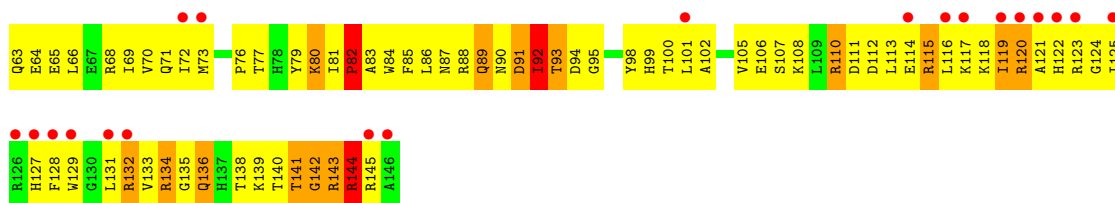
Chain c7:



- Molecule 20: 40S ribosomal protein S18-A

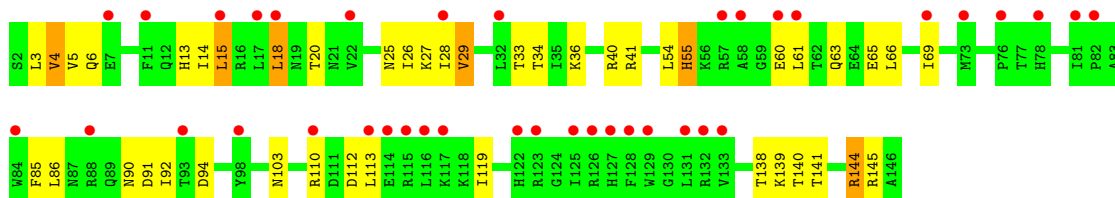
Chain C8:





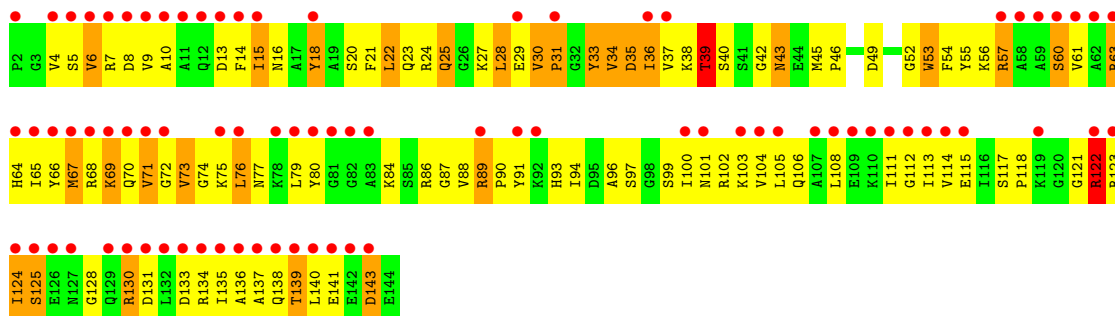
• Molecule 20: 40S ribosomal protein S18-A

Chain c8:



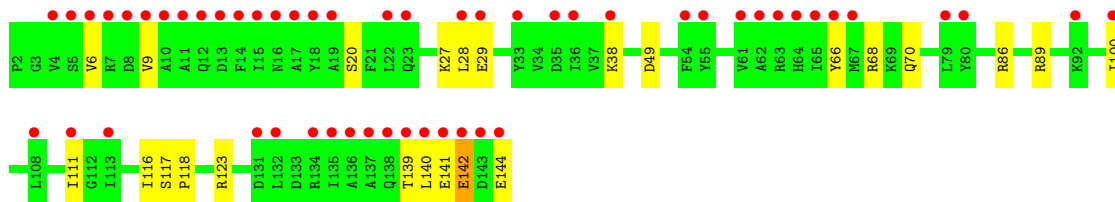
• Molecule 21: 40S ribosomal protein S19-A

Chain C9:



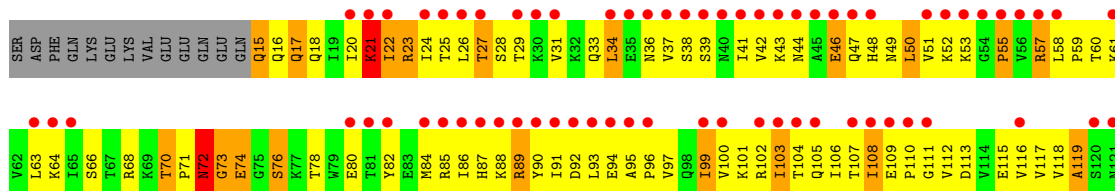
• Molecule 21: 40S ribosomal protein S19-A

Chain c9:



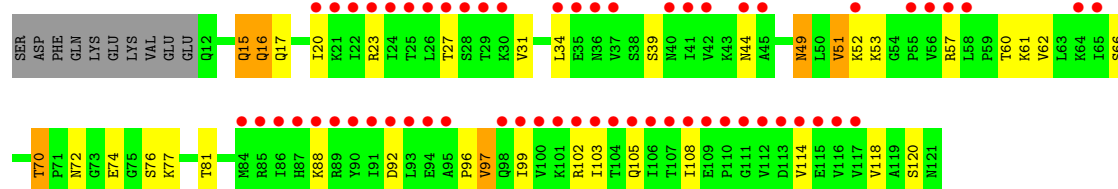
• Molecule 22: 40S ribosomal protein S20

Chain D0:



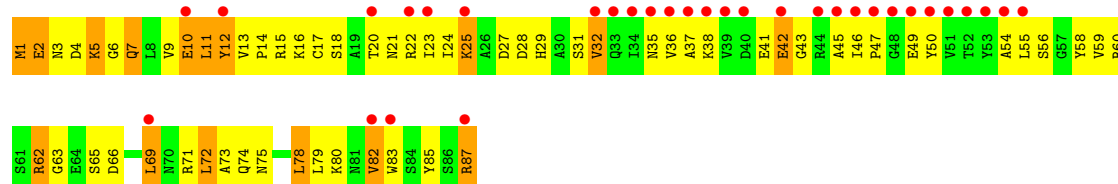
• Molecule 22: 40S ribosomal protein S20

Chain d0: 



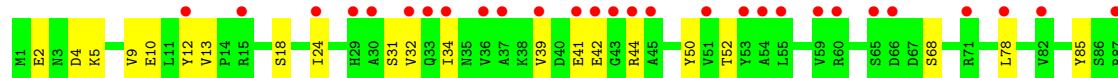
- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 



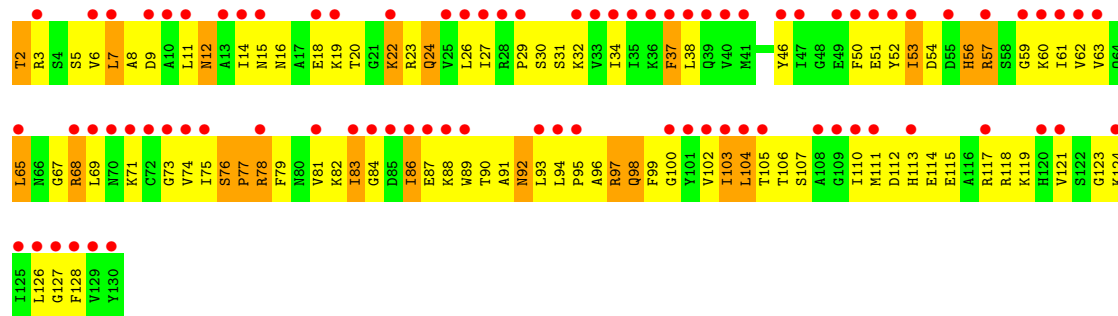
- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 



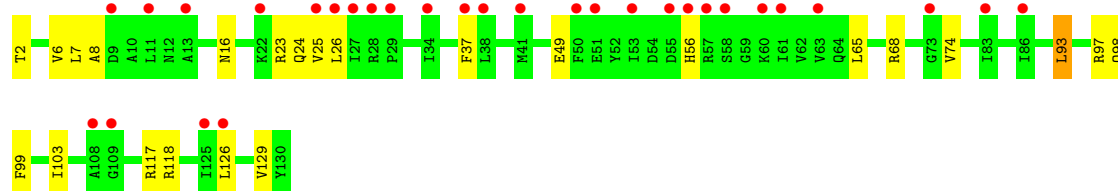
- Molecule 24: 40S ribosomal protein S22-A

Chain D2: 



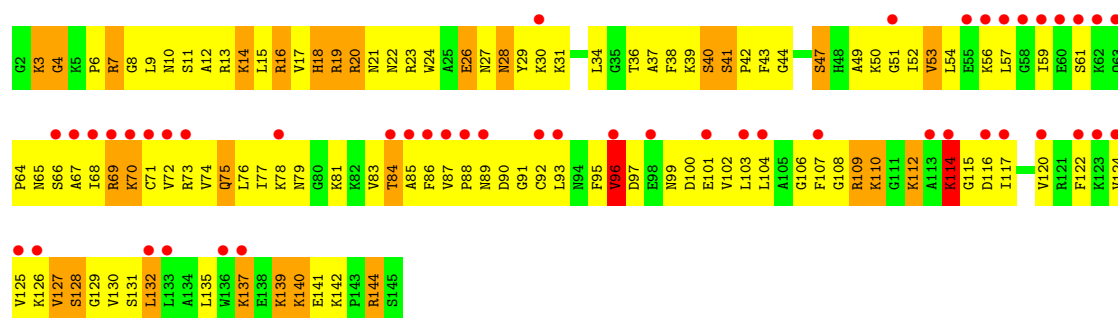
- Molecule 24: 40S ribosomal protein S22-A

Chain d2: 



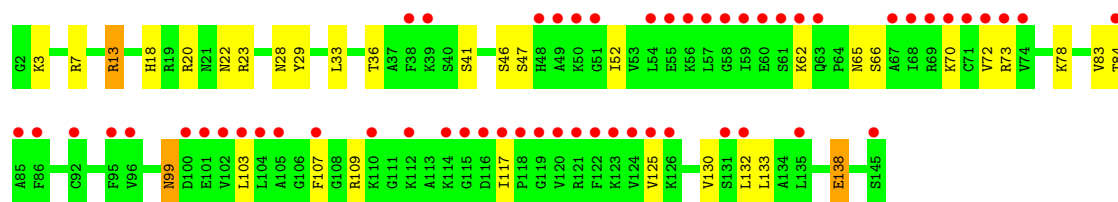
- Molecule 25: 40S ribosomal protein S23-A

Chain D3: 



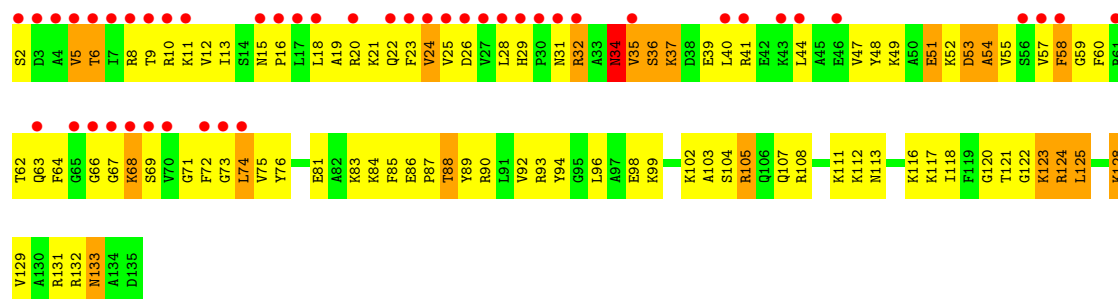
- Molecule 25: 40S ribosomal protein S23-A

Chain d3:



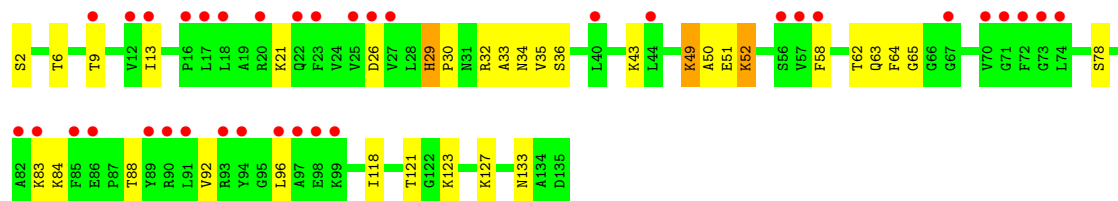
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:



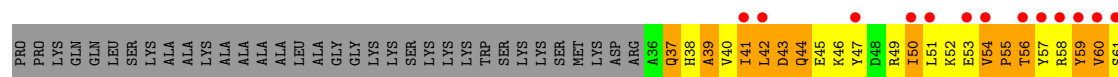
- Molecule 26: 40S ribosomal protein S24-A

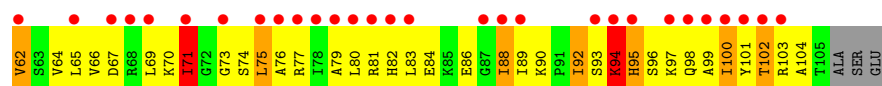
Chain d4:



- Molecule 27: 40S ribosomal protein S25-A

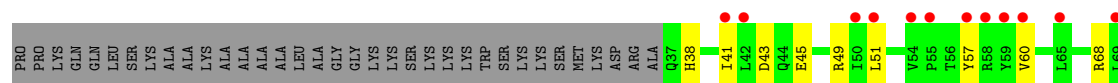
Chain D5:





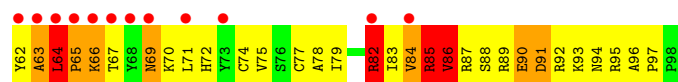
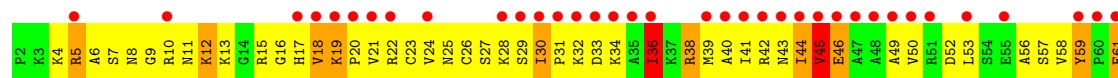
- Molecule 27: 40S ribosomal protein S25-A

Chain d5:



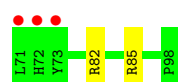
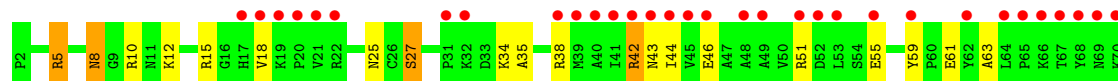
- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



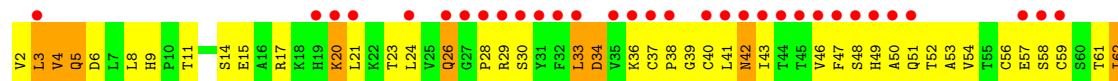
- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



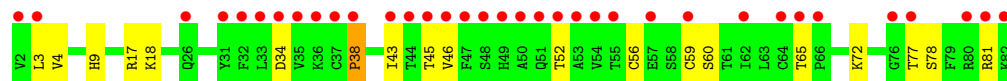
- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



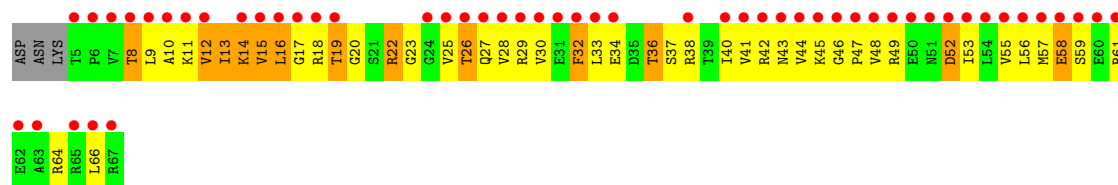
- Molecule 29: 40S ribosomal protein S27-A

Chain d7:



- Molecule 30: 40S ribosomal protein S28-A

Chain D8:



- Molecule 30: 40S ribosomal protein S28-A

Chain d8:



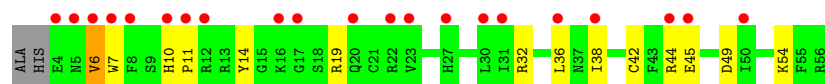
- Molecule 31: 40S ribosomal protein S29-A

Chain D9:



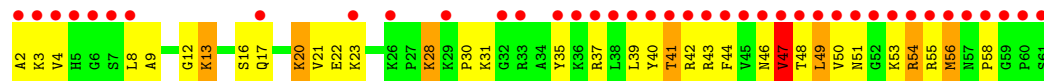
- Molecule 31: 40S ribosomal protein S29-A

Chain d9:



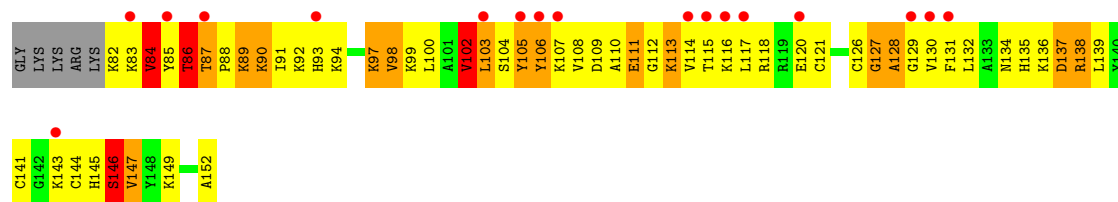
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:



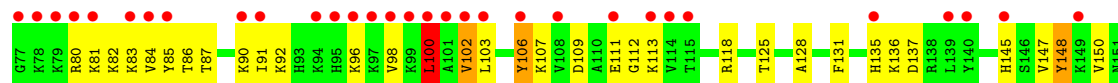
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



- Molecule 33: Ubiquitin-40S ribosomal protein S31

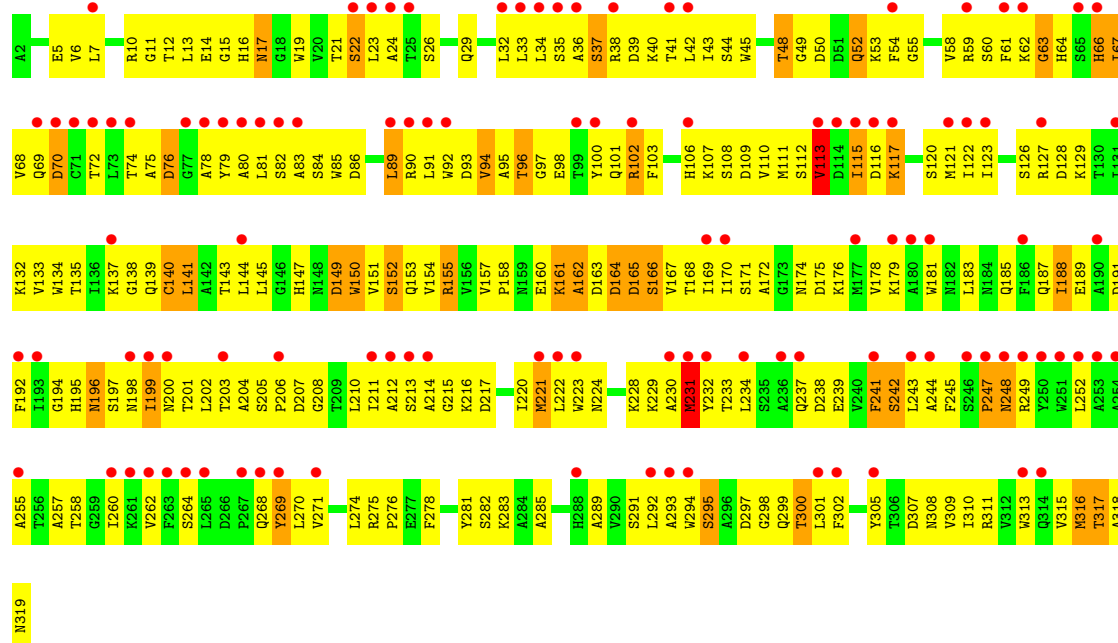
Chain e1:



A152

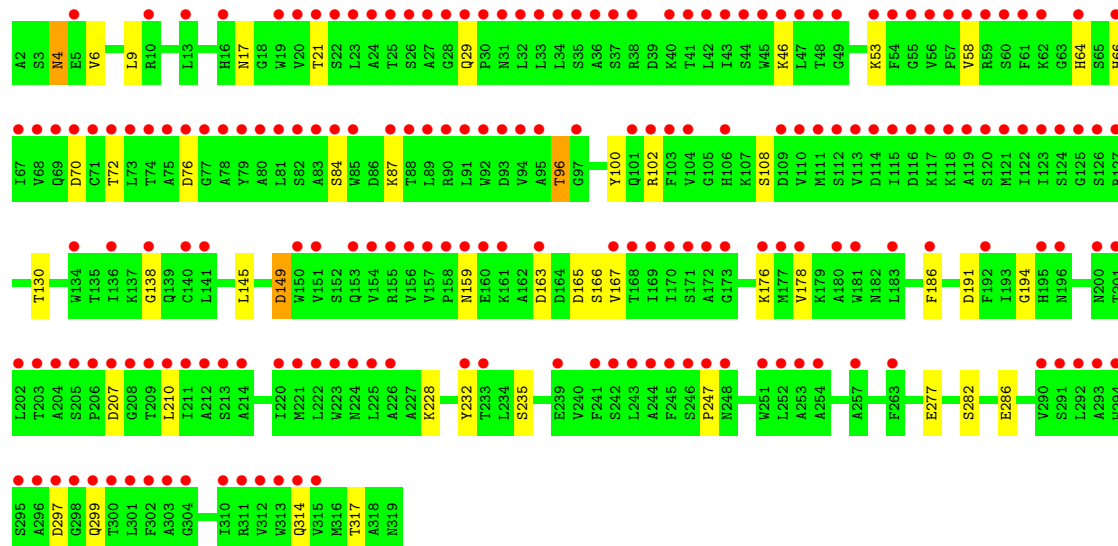
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



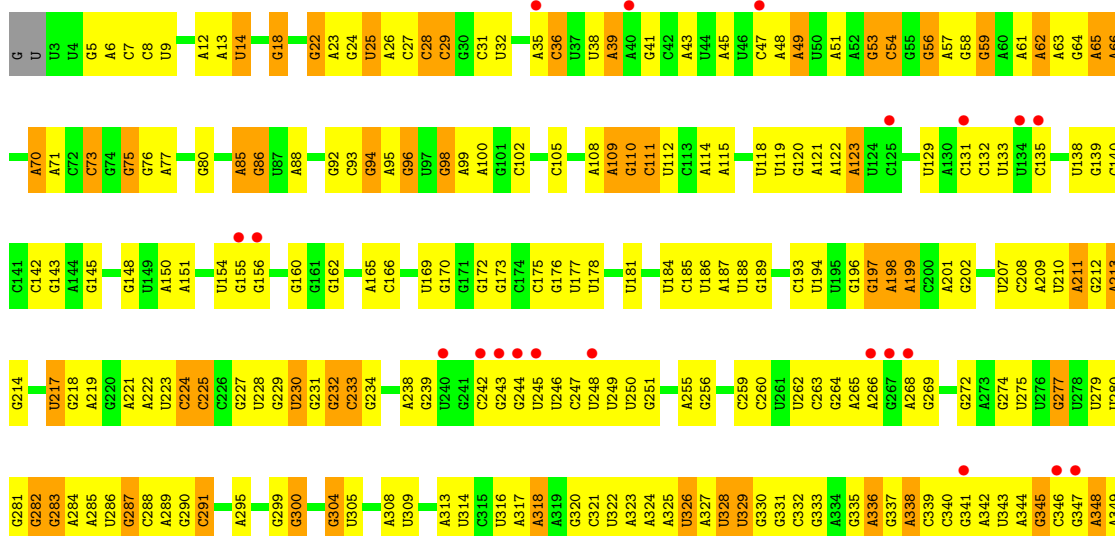
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



- Molecule 35: Suppressor protein STM1

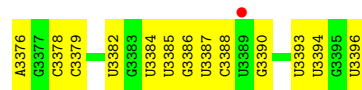
Chain SM:



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U1324	U1241	A1102	A1102	A1026	U960	A895	U829	U683	A621	A551	
U1325	G1242	A1170	G1103	A1027	C961	A896	G831	U684	G823	U555	
A1326	G1243	G1171	G1104	U1028	A962	A897	A830	U685	U622	U556	
C1327	A1244	G1172	A1105		C963	U898	G832	U686	G524	A557	
	U1245		G1106	C1032	U964	U899	G833	U687	G525	U558	
U1328	U1246	C1175	C1107	U1033	A965	U900	U834	U688	U626	A559	
U1329	U1247	C1176	U1108	G1265	U966	G901	U835	U689	U627	C560	
U1330	C1248	G1177	U1109	U1034	A967	G902	A836	U690	A428	C561	
A1331	U1249	G1178	U1110	G1035	C968	G902	A837	A691	U629	C562	
A1332	G1249	A1179	U1111		C969	U905	A837	A691	U629	C562	
C1333			U1112	U1039	C969	U905	G838	A692	A630	U563	U831
U1334	C1254	A1184	A1112	A1040	C969	A906	G838	A692	A630	U563	U831
	C1255	C1185	G1113	U1041	G971	A906	C839	A693	A631	U564	
G1340		G1185	G1113	U1041	G971	G907	C840	C594	G632	U565	G494
U1341	U1265	G1186	U1114		A972	G908	A841	C595	G633	U565	
C1342		C1187	G1115	C1045	A973	G909	A846	C596	G634	G567	C435
			G1116	U1046	G974	G910	A847	A697	G635	G568	A436
A1343		C1187	G1117	A1047	C975	C911	A847	U698	C636	C497	G437
U1344	U1288		C1118	U1048	U976	G912	A848	A699	C637	A498	
G1345	U1289	A1190	C1119	A1049	C977	A913	A849	U703	G638	U571	U506
	C1192	C1192	C1119	U1050	G978	A914	U850	U704	U640	A572	U507
U1346			U1122	U1051	U979	A915	C851	U705	U640	C573	U508
U1347			U1123	U1052	A980	G916	U852	A706	C641	U574	U509
U1348	C1196		U1124	U1053		A917	G853	A706	U642		U510
C1349	U1277	A1197	U1125	A1054	A983	A918	G854	U707	U643	A578	G511
A1350	U1278	C1198	G1126	U1055	U984	U919	G855	U708	G644	G579	U512
	C1279	C1199	G1126	U1056	U985	U920	U856	A709	G645	C580	U513
U1351	C1280	A1200	U1057	U1057	U986	A921	G857	U710	A646	U581	U514
C1352	G1281	C1201	A1057		U987	U922	U857	U711	A647	G582	U515
U1353	U1282	A1202	U1130	U1060	U988	C923	G860	G712	C648	G583	U516
G1354			G1131	A1061		G924	U860	U713	C649	G584	G517
A1355	A1286	A1204	U1134	A1062	G991	A925	C863	U714	C650	A519	U518
U1356	A1287	A1205	G1134	G1063	A992	A926	G864	G715	G651	C586	U520
C1360		G1206		U1064	G993	A927	U865	A716	G652	U587	C
G1361	C1292	G1207	C1137	A1065		C928	U866	C717	A653	A521	C
G1362	U1293	U1208	U1138	U1066	A996	C929	G867	U718	C654	A522	C
A1363	A1294	G1209	G1139	G1066	A997	A929	C868	U719	C655	G590	U
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			U1073		G1001	U935	U872	G723	G659	G595	C
A1368	A1302	A1217	U1073	U1073	A1002	A836	C873	A806	A660	C596	C
A1369	A1303		U1074	U1074	A1003	G937	U874	A807	A661	G597	U
G1370	A1304	U1220	C1146	A1075	C1003	C938	U875	G726	U662	A532	C
U1371	U1305	A1221	G1147	U1076	U1004	U939	A876	G727	A533	A598	C
C1372	G1306	G1221	G1148	C1076	G1005	G940	U877	G728	C563	U534	U
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G1374	A1308	A1223	A1150	U1078	U1008	G941	G878	U811	A665	U601	U
	U1309	C1224	U1151	A1079	A1009	U942	U879	U731	A666	A602	U
C1375	G1310		G1152	U1080	G1010	U943	G880	G732	C667	A603	G
C1376		C1227	A1153	U1081	U1011	C944	A883	G733	G668	G604	G
U1377	C1312	G1312	A1154	U1082	G1012	C945	U884	C734	U669	U540	U
G1378	G1313	G1230	C1155	G1083	U1013	U946	A884	A735	A607	A407	A
A1380	C1314	A1231	C1156	A1084	U1014	G947	U885	A817	G542	A408	
	U1315	G1232	C1157		U1015	C948	U886	A736	C609	A409	G
A1381	U1316	G1233	A1158	U1084	C1016		G887	C818	G674	A608	
G1382	C1317	G1234	A1159	U1095	U1016	G953	A888	U819	C875	A607	
C1383	U1318	U1235	C1160	U1096	G1017	U954	U889	A820	G676	A611	G
U1384	G1319	U1236	G1161	G1097	G1019	U955	C890	C822	A677	G612	U
C1385		C1237	U1162	U1098	G1020	U956	G891	C823	G678	G613	A
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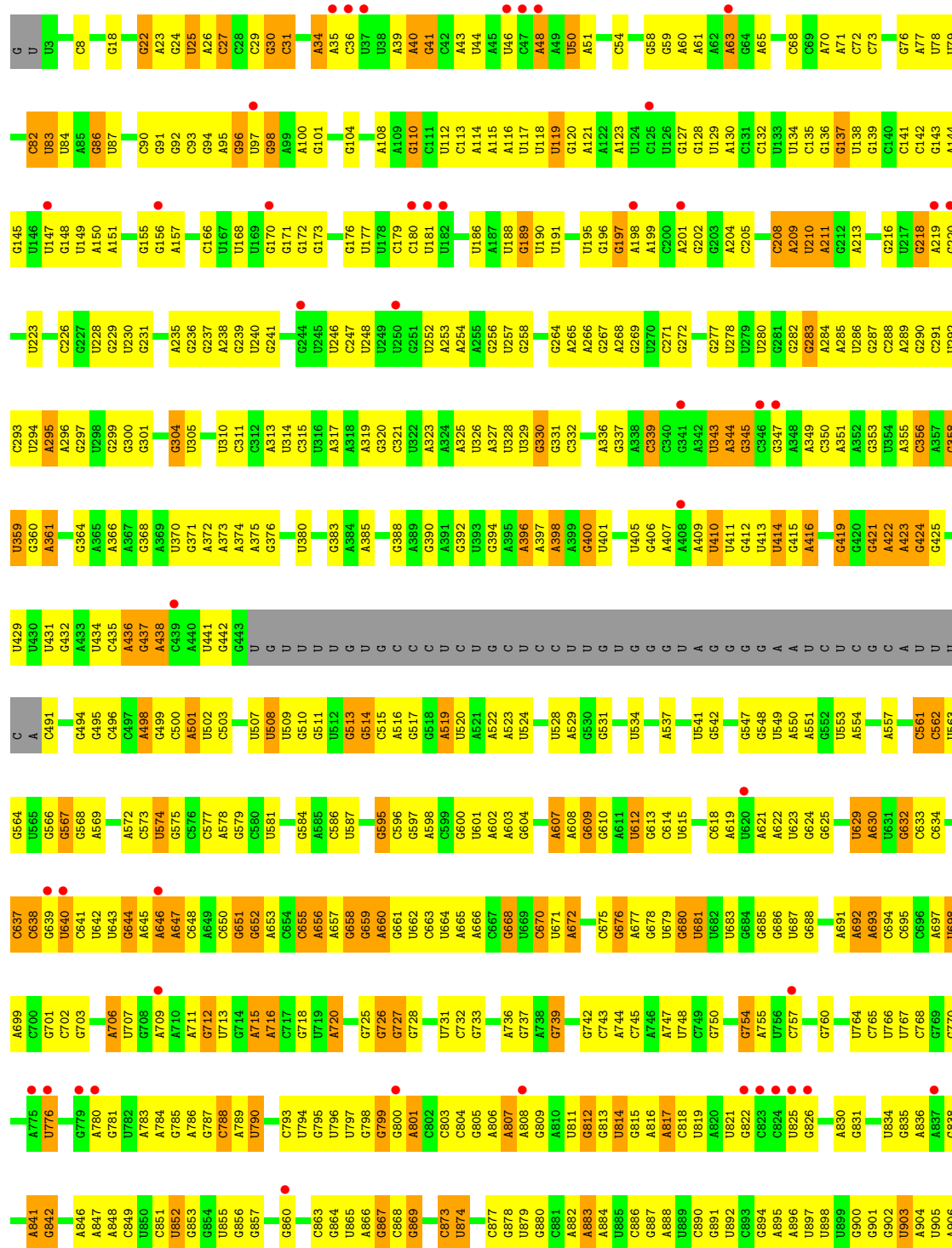


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G3309	C3082	G3245	U3154	C3081	G3015	U2944	C2877	A2811	A2746	U2613	A2404	
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G3327	A3094	A3243	U3167	C3028	C3028	C2959	C2891	G2823	U2758	A2626	G2418	
G3328	A3094	A3244	G3172	A3029	A3029	C2960	C2892	G2824	G2759	C2627	A2419	
U3329	G3098	A3245	A3173	G3030	G3030	U2961	C2893	U2827	G2760	C2628	C2420	
A3330	C3099	A3246	A3174	A3031	A3031	U2962	A2894	G2828	U2761	U2629	U2421	
G3333	G3101	G3247	U3175	A3032	A3032	U2963	A2895	U2829	U2762	U2630	A2422	
U3334	G3102	G3248	A3176	A3033	A3033	U2964	C2896	G2830	U2763	U2631	C2423	
A3335	U3104	G3249	A3177	A3034	A3034	U2965	C2897	A2831	U2764	U2632	U2424	
G3336	A3105	G3250	A3178	A3035	A3035	U2966	C2898	G2832	U2765	U2633	G2425	
A3337	U3106	G3251	A3179	A3036	A3036	U2967	C2899	A2833	U2766	U2634	U2426	
G3338	A3107	G3252	A3180	C3039	C3039	U2968	A2902	A2834	U2767	A2635	U2427	
U3339	A3108	G3253	C3181	A3040	A3040	C2970	A2903	G2835	U2768	C2556	A2430	
A3340	G3109	G3254	G3182	U3041	U3041	A2971	U2904	U2836	U2769	U2557	C2431	
G3341	U3110	G3255	A3186	U3042	U3042	U2972	U2905	A2837	U2770	U2558	A2432	
A3342	C3111	G3256	G3189	C3043	C3043	U2973	A2906	G2838	U2771	U2559	U2433	
G3343	U3112	G3257	C3190	A3044	A3044	U2974	U2907	A2839	U2772	U2560	U2434	
U3344	G3113	G3258	A3191	A3045	A3045	U2975	A2908	G2840	C2773	A2641	G2437	
A3345	A3114	G3259	C3192	C3046	C3046	U2976	U2909	U2841	C2774	U2642	A2438	
G3346	C3115	G3260	U3193	A3047	A3047	U2977	U2910	U2842	U2775	U2643	A2439	
U3347	U3116	G3261	C3194	A3048	A3048	U2978	U2911	U2843	U2776	U2644	G2442	
G3348	C3117	G3262	A3195	U3050	U3050	C2983	U2912	U2844	C2777	C2645	A2443	
C3349	U3118	G3263	U3196	U3051	U3051	C2984	U2913	A2845	G2778	U2646	C2444	
U3350	C3119	G3264	U3197	U3052	U3052	C2985	U2914	U2846	A2779	A2647	U	
A3351	U3120	G3265	C3198	G3053	G3053	U2986	U2915	A2847	U2780	U2501	A	
U3352	A3121	G3266	U3199	U3054	U3054	U2987	U2916	G2848	U2781	A2502	G	
G3353	G3122	G3267	C3200	U3057	U3057	U2988	U2917	U2849	U2782	G2503	A	
U3354	C3123	G3268	G3201	U3067	U3067	U2989	U2918	U2850	U2783	U2504	G	
G3355	A3124	G3269	C3202	C3068	C3068	U2990	U2919	U2851	U2784	U2505	U	
U3356	U3125	G3270	U3203	U3069	U3069	U2991	U2920	A2852	U2785	U2510	A	
A3357	C3126	G3271	C3204	C3070	C3070	U2992	U2921	U2853	C2786	A2511	G	
U3358	U3127	G3272	G3205	U3064	U3064	U2993	U2922	U2854	U2787	G2512	A	
A3359	C3128	G3273	U3206	U3065	U3065	U2994	U2923	U2855	U2788	U2513	G	
G3360	A3134	G3274	U3207	U3066	U3066	U2995	U2924	G2856	U2789	A2514	G	
U3361	U3138	G3275	C3208	C3067	C3067	U2996	U2925	U2857	C2790	U2515	U	
A3362	A3139	G3276	A3209	U3068	U3068	U2997	C2926	U2858	U2791	U2516	A	
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U3364	U3141	G3278	C3212	A3070	A3070	U2999	C2927	U2860	U2793	U2518	U	
G3365	A3142	G3279	U3213	U3071	U3071	U3000	U2928	U2861	U2794	C2519	A	
A3366	C3143	G3280	A3214	C3072	C3072	C3001	U2929	U2862	U2795	A2519	G	
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G3368	A3145	G3282	A3216	A3006	A3006	C3003	U2931	U2864	U2797	U2521	G	
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U3376	U3153	G3290	U3223	U3011	U3011	U3011	U2939	A2872	G2805	A2529	U	
A3377	A3154	G3291	A3224	U3012	U3012	U3012	U2940	U2873	A2806			
G3378	C3155	G3292	C3225	A3013	A3013	U3013	U2941		U2807			
U3379	U3156	G3293	U3226	U3014	U3014	U3014	U2942		C2741			
A3380	C3157	G3294	A3227	U3015	U3015	U3015	U2943		A2743			
G3381	U3158	G3295	C3227	U3016	U3016	U3016	U2944					
U3382	A3159	G3296	U3228	U3017	U3017	U3017	U2945					
A3383	C3160	G3297	A3229	U3018	U3018	U3018	U2946					
G3384	U3161	G3298	C3229	U3019	U3019	U3019	U2947					
U3385	A3162	G3299	U3230	U3020	U3020	U3020	U2948					
A3386	C3163	G3300	A3231	U3021	U3021	U3021	U2949					
G3387	U3164	G3301	C3232	U3022	U3022	U3022	U2950					
U3388	A3165	G3302	U3233	U3023	U3023	U3023	U2951					
A3389	C3166	G3303	A3234	U3024	U3024	U3024	U2952					
G3390	U3167	G3304	C3235	U3025	U3025	U3025	U2953					
U3391	A3168	G3305	U3236	U3026	U3026	U3026	U2954					
A3392	C3169	G3306	A3237	U3027	U3027	U3027	U2955					
G3393	U3170	G3307	C3237	U3028	U3028	U3028	U2956					
U3394	A3171	G3308	U3238	U3029	U3029	U3029	U2957					
A3395	C3172	G3309	A3238	U3030	U3030	U3030	U2958					
G3396	U3173	G3310	C3239	U3031	U3031	U3031	U2959					
U3397	A3174	G3311	U3240	U3032	U3032	U3032	U2960					
A3398	C3175	G3312	A3241	U3033	U3033	U3033	U2961					
G3399	U3176	G3313	C3242	A3034	A3034	U3034	U2962					
U3400	A3177	G3314	U3243	U3035	U3035	U3035	U2963					
A3401	C3178	G3315	A3244	U3036	U3036	U3036	U2964					
G3402	U3179	G3316	C3245	U3037	U3037	U3037	U2965					
U3403	A3180	G3317	A3246	U3038	U3038	U3038	U2966					
A3404	C3181	G3318	C3247	U3039	U3039	U3039	U2967					
G3405	U3182	G3319	U3248	U3040	U3040	U3040	U2968					
U3406	A3183	G3320	A3249	U3041	U3041	U3041	U2969					
A3407	C3184	G3321	C3250	U3042	U3042	U3042	U2970					
G3408	U3185	G3322	U3251	U3043	U3043	U3043	U2971					
U3409	A3186	G3323	A3252	U3044	U3044	U3044	U2972					
A3410	C3187	G3324	C3253	U3045	U3045	U3045	U2973					
G3411	U3188	G3325	U3254	U3046	U3046	U3046	U2974					
U3412	A3189	G3326	A3255	U3047	U3047	U3047	U2975					
A3413	C3189	G3327	U3256	U3048	U3048	U3048	U2976					
G3414	U3190	G3328	A3257	U3049	U3049	U3049	U2977					
U3415	A3191	G3329	C3258	U3050	U3050	U3050	U2978					
A3416	C3192	G3330	U3259	U3051	U3051	U3051	U2979					
G3417	U3193	G3331	A3260	U3052	U3052	U3052	U2980					
U3418	C3194	G3332	C3261	U3053	U3053	U3053	U2981					
A3419	U3195	G3333	U3262	U3054	U3054	U3054	U2982					
G3420	A3196	G3334	A3263	U3055	U3055	U3055	U2983					
U3421	C3197	G3335	C3264	U3056	U3056	U3056	U2984					
A3422	U3198	G3336	U3265	U3057	U3057	U3057	U2985					
G3423	A3199	G3337	A3266	U3058	U3058	U3058	U2986					
U3424	C3199	G3338	C3267	U3059	U3059	U3059	U2987					
A3425	U3200	G3339	U3268	U3060	U3060	U3060	U2988					
G3426	A3201	G3340	A3269	U3061	U3061	U3061	U2989					
U3427	C3202	G3341	C3270	U3062	U3062	U3062	U2990					
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G3429	C3204	G3343	A3272	U								



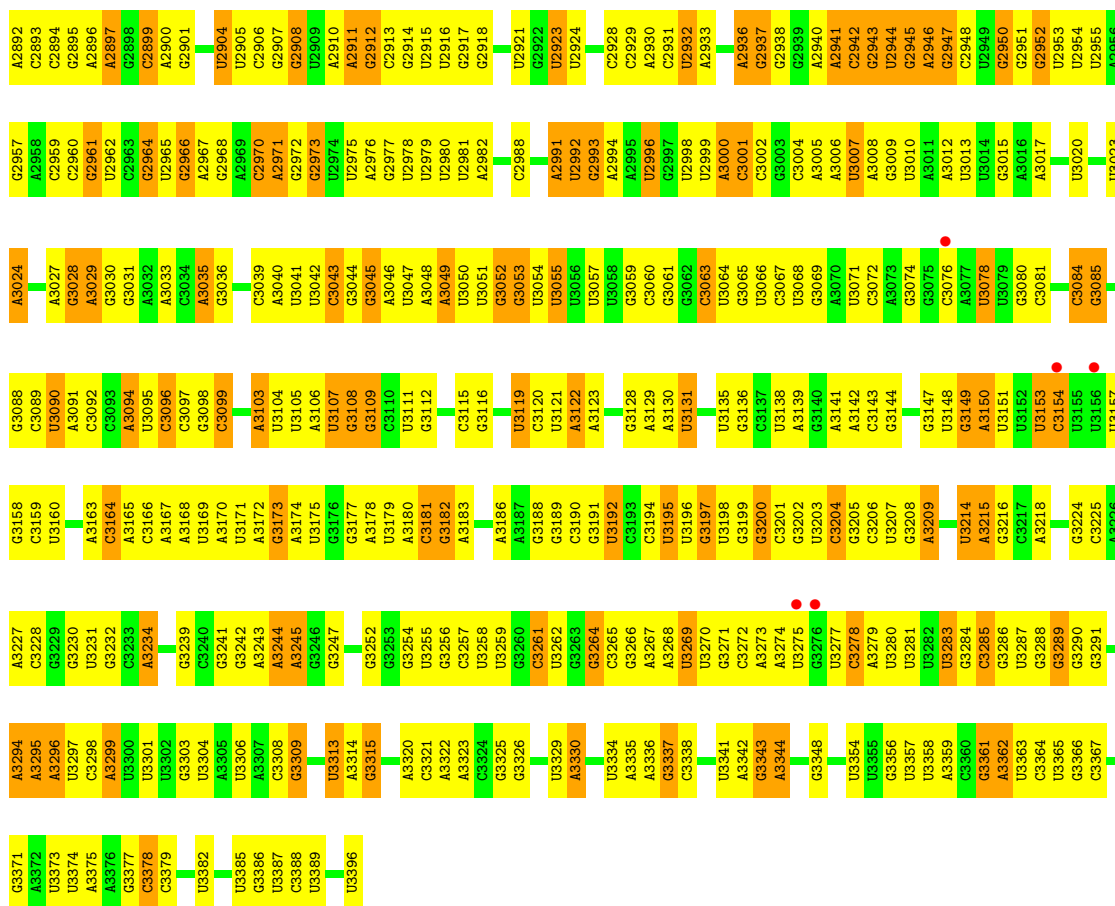
● Molecule 36: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 5:



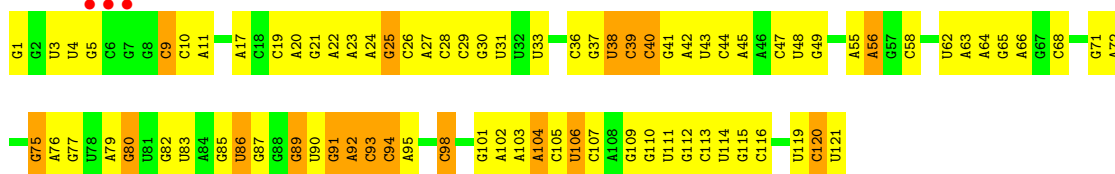
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C1844	G1775	G1700	G1562	U1495	A1434	A1370	A1308	C1231	A1103	A1103	G967
C1845	G1776	C1628	U1564	C1496	A1435	G1371	U1309	C1232	G1166	G1104	G968
C1846	U1777	U1629	G1565	C1497	A1436	C1372	G1310	U1167	U1166	A1105	G969
A1847	G1778	U1703	A1566	A1498	C1437	A1373	G1311	G1234	U1168	G1106	U1034
C1848	C1779	C1631	U1567	C1499	U1438	G1374	C1312	U1235	A1169	C1107	A972
C1849	G1780	U1705	U1568	G1500	U1439	G1375	G1313	G1236	U1170	U1108	A973
A1850	C1781	C1706	U1569	U1501	G1440	C1376	C1314	G1237	G1171	C1038	G974
G1851	A1707	A1707	U1570	C1502	G1441	G1377	U1315	C1238	U1172	U1039	C975
U1852	U1783				U1442	U1378	C1316	C1239	U1173	G1177	U976
C1853	G1784	A1638			G1443	G1379	A1317	A1240	G1174	A1112	A917
U1854	U1785	C1639			U1444	G1380	A1318	U1241	C1176	G1113	C918
C1855	G1786	G1640			U1445	G1381	G1319	G1242	C1175	U1114	G978
C1856	A1787	U1641			U1446	A1382	C1320	G1243	G1177	G1115	U919
U1857		A1643			G1447	G1383	G1321	A1244	U1178	A1110	A920
G1858	G1790	C1644			U1448	U1384	U1322	A1245	A1179	G1117	A921
A1859	U1791	U1716			U1449	C1385	G1323	G1246	A1180	A1046	C982
C1860	C1792	U1717			G1450	A1386	U1324		A1181	G1119	
U1861	G1793	A1648			C1451	G1387	U1325	G1249	A1182	C1120	U985
U1862	U1794	U1649			A1452	U1388	A1326	G1250	U1129	A1049	U986
C1863	U1795	C1650			U1453	G1389	C1327	C1255	C1185	U1051	U987
A1864		U1651			A1454	A1390	C1328	G1256	U1124	U1052	U988
A1865	U1798	U1652			U1455	C1391	U1329	C1257	U1126	A1053	C928
C1866	A1799	G1653			A1456	G1392	A1330	U1258	G1127	A1054	A929
U1867		A1654			U1457	A1393	U1035	C1259	U1128	A1055	G991
C1868	C1802	A1729			U1458	A1394	A1332	A1259	A1190	U1056	A992
C1869	U1796	A1656			C1459	G1395	C1333	A1260	U1129	U1056	G993
	A1804	A1731			A1460	U1334	U1335	G1261	A1130	G934	U995
C1872	C1805	U1659			A1461	A1401	U1336	G1262	G1131	U1061	U935
U1873	A1806	C1660			A1462	C1402	U1337	A1263	C1132	A1062	A936
A1874	G1807	G1661			U1463	A1403	A1337	G1264	A1133	G1063	G999
C1808	G1735	C1662			G1464	G1404	C1338	U1265	A1134	A1064	C1000
A1809	U1597	U1662			A1465	U1405	C1339	G1266	A1135	A1065	U939
A1810					U1466	A1406	G1340		A1136	G1066	A1002
	U1739	C1665			A1467	A1407	U1341	C1275	C1137	U1067	G940
U1877	U1740	C1666			A1468	G1408	C1342	U1276	U1138	A1003	G941
A1879	A1741	A1667			U1469	C1409		U1277	G1139	U1004	U942
U1880	U1814				A1534	G1409	G1345	A1276	C1201	G1068	U943
A1881	U1815	G1668			U1470	U1410	G1346	A1278	A1202	C1069	U944
C1882	A1816	C1669			U1471	U1411	U1347	C1284	A1203	U1070	C945
G1817	G1744	C1670			U1472	G1412	U1348	G1285	A1204	U1071	U1007
U1885	C1745	C1671			G1473	G1413	C1349		A1205	G1072	U946
A1886	U1746	U1672			U1474	G1414	C1349		G1206	U1073	G947
U1819	G1747	G1673			A1475	U1415	A1350	G1289	U1144	C1010	C948
U1820					G1476	C1416	U1351	A1290	G1145	A1011	C949
U1821	C1821	G1674			U1477	G1417	A1352	A1291	C1146	G1012	G950
U1888	A1750	G1675			A1478	A1418	U1353	C1292	G1147	G1013	G951
C1822	G1751	C1676			U1479	A1419	G1354	U1293	U1211	U1014	A952
U1890	A1752	A1679			G1480	A1419	A1355	U1294	G1149	C1015	G953
U1824		G1680			A1481	C1420	A1356	G1295	A1150	U1015	U954
	A1757				U1482	G1421	U1356		U1151	C1016	
C1830	G1758				U1483	G1422		C1296	G1152	C1017	U955
U1831		C1685			U1484	C1423	C1359	C1297	A1153	G1018	U956
C1832		C1686			U1485	G1424	A1360	U1298	U1214	C1019	U957
G1833	U1763	U1687			U1486	C1425	U1361	C1299	C1154	G1019	C957
U1834	U1764	U1688			G1487	U1426	G1362	U1299	U1155	G1020	C958
A1835	U1765	U1689			U1488	C1427	A1363		C1156	C1021	U959
U1836	G1766				U1489	C1428	G1364		U1157	G1024	C961
U1837		U1692			U1490	A1429	G1365		A1158	A1025	
U1838	U1768	C1693			A1491	U1430	A1366		C1159	A1026	
A1839	G1769	U1694			U1492	U1431	G1367		U1160	A1027	
U1840	G1770	U1695			C1493	G1432	U1368		U1161	U1028	
A1841		A1696			C1494	C1433	U1369		U1162	U1029	
U1842	C1773	A1697			U1495	G1434	U1370		U1163	U1030	U956





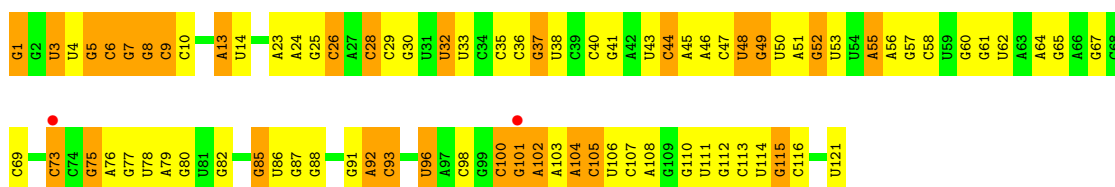
- Molecule 37: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 3:



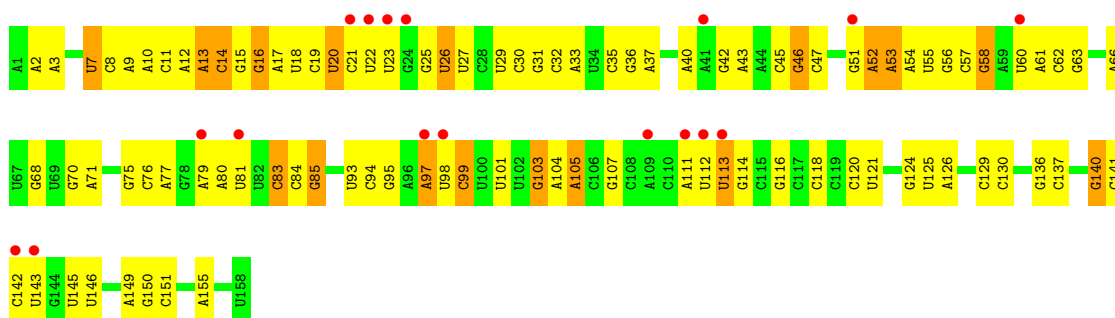
- Molecule 37: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 7:



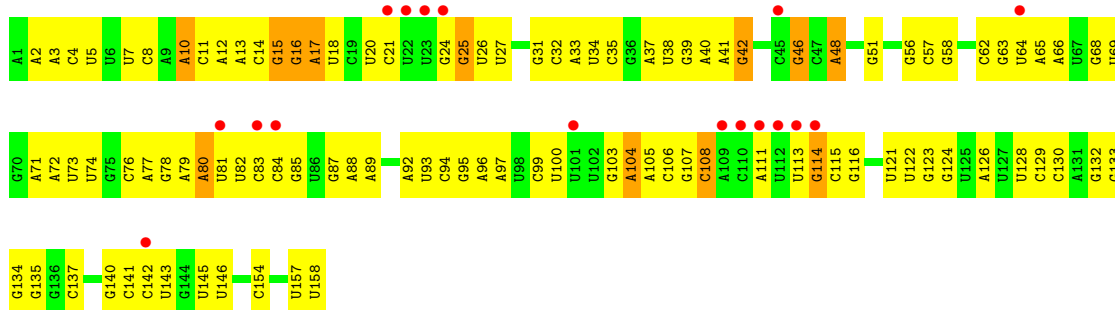
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 4:



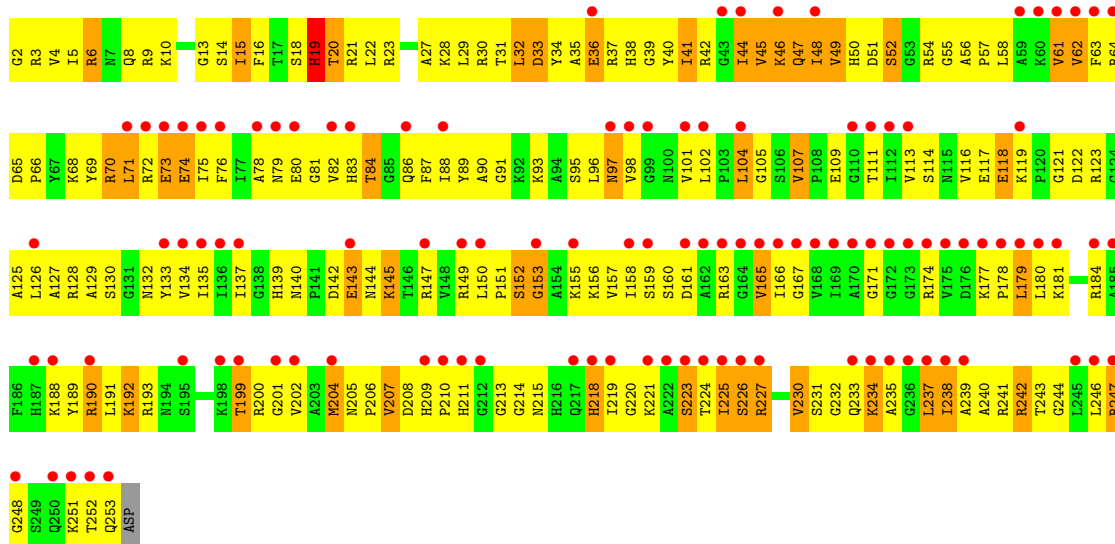
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 8:



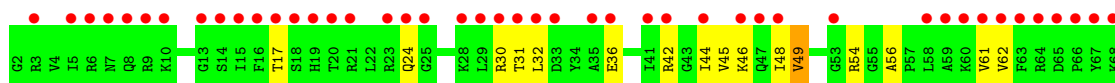
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:

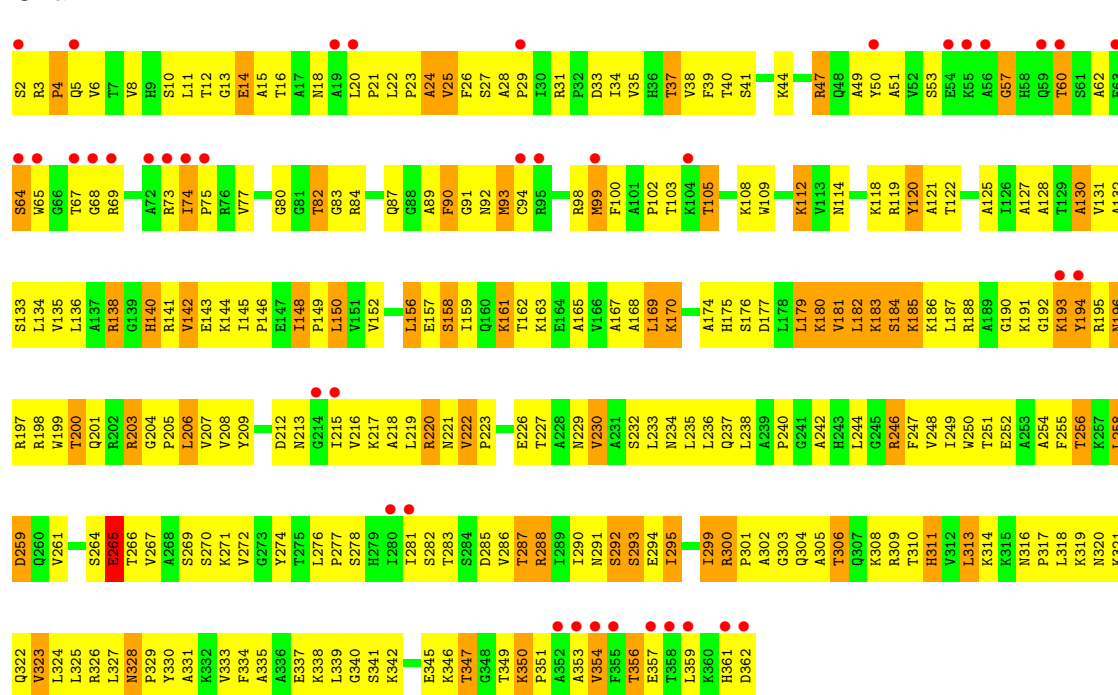


- Molecule 39: 60S ribosomal protein L2-A

Chain 12:



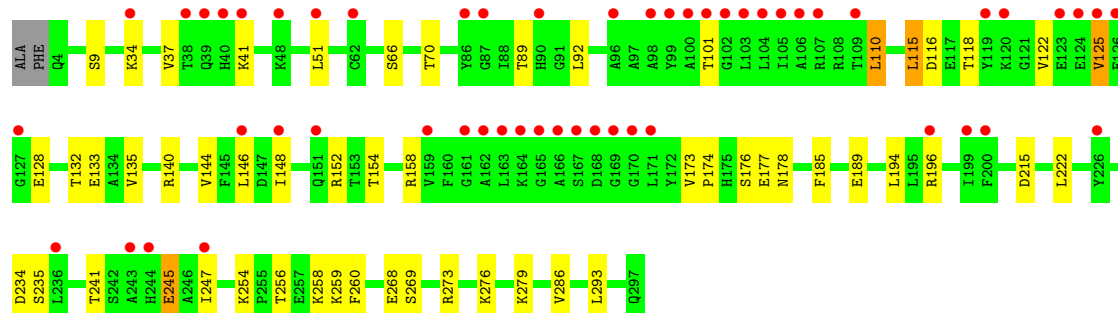
Chain L4:





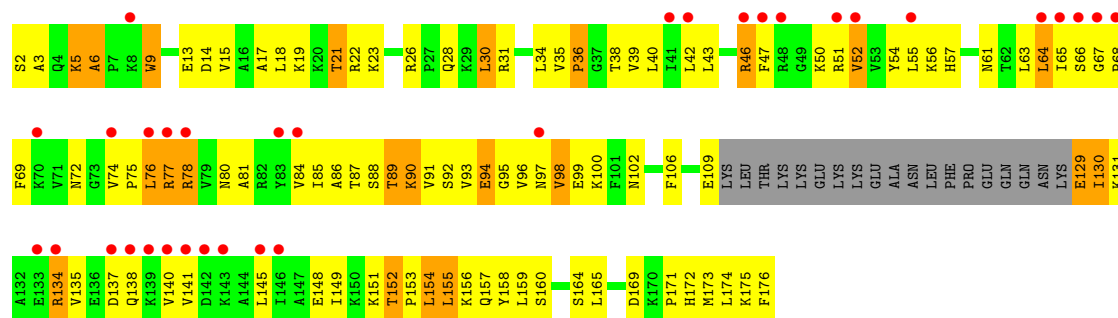
• Molecule 42: 60S ribosomal protein L5

Chain l5:



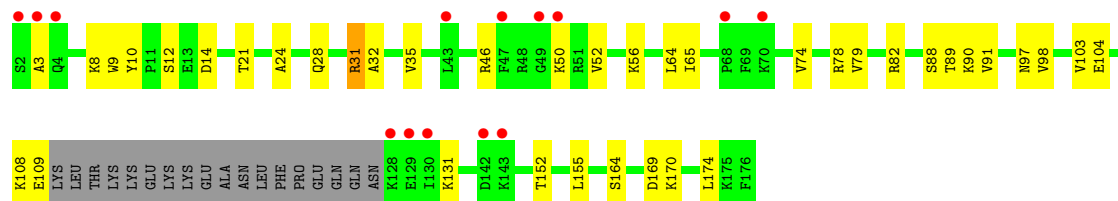
• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



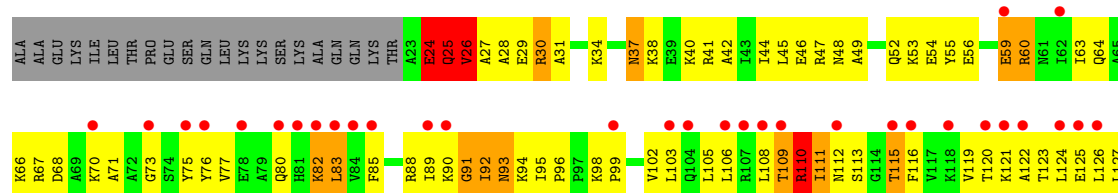
• Molecule 43: 60S ribosomal protein L6-A

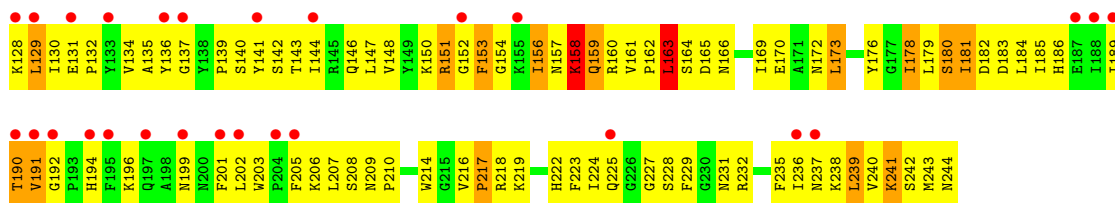
Chain l6:



• Molecule 44: 60S ribosomal protein L7-A

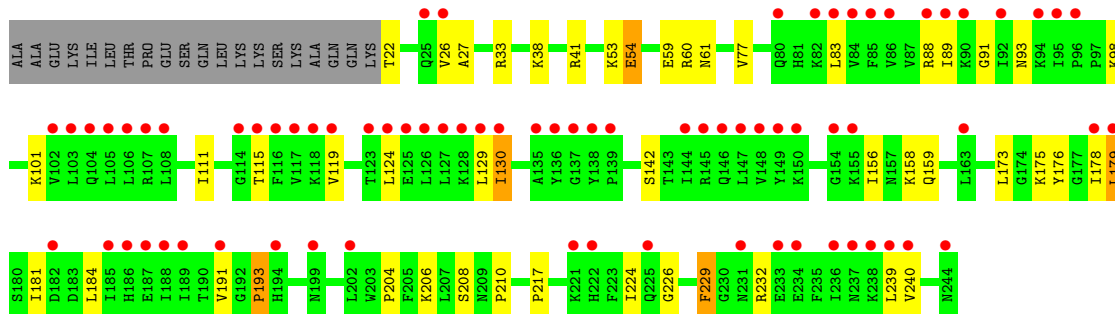
Chain L7:





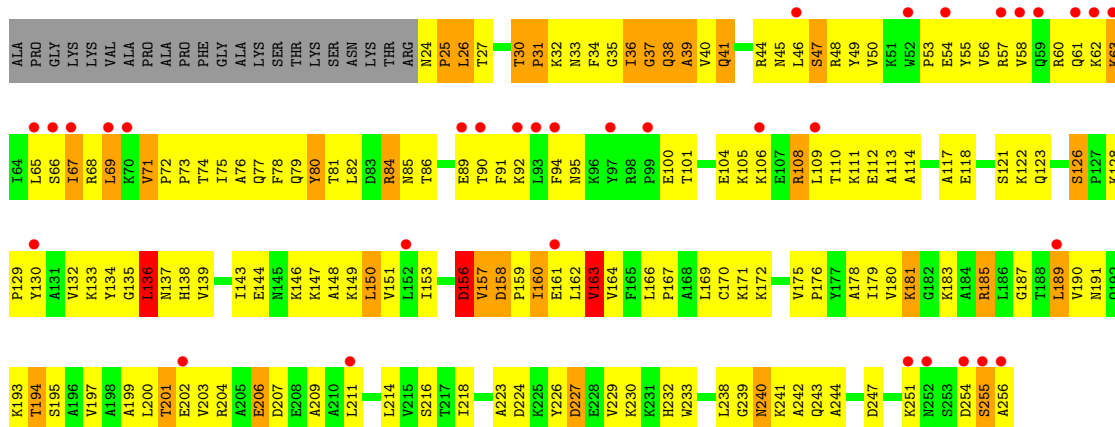
• Molecule 44: 60S ribosomal protein L7-A

Chain 17:



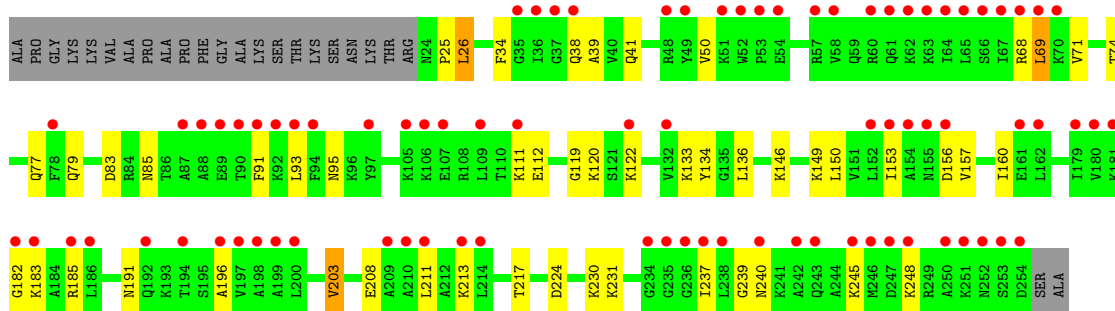
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



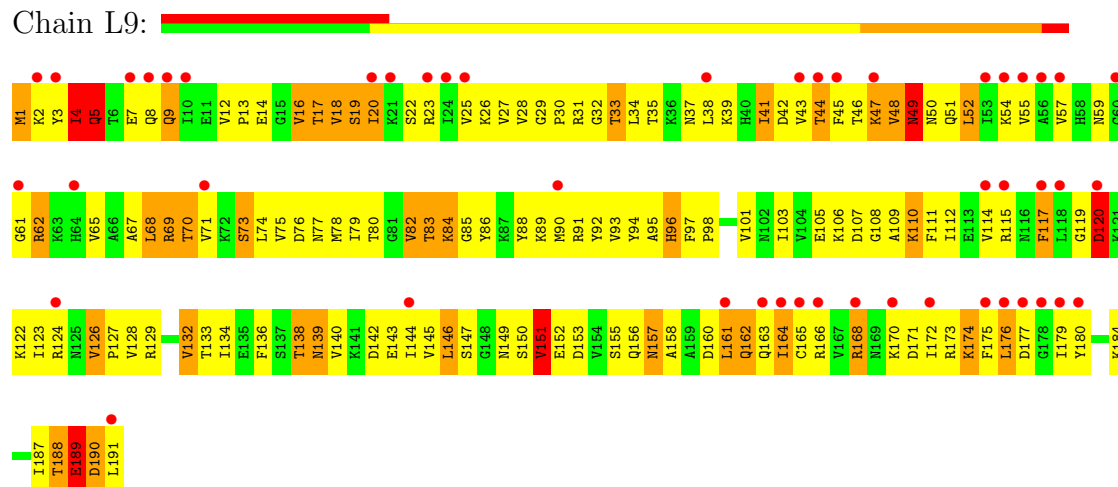
• Molecule 45: 60S ribosomal protein L8-A

Chain 18:



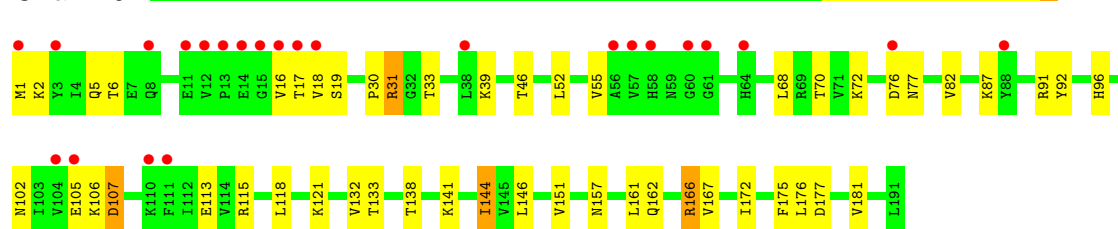
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



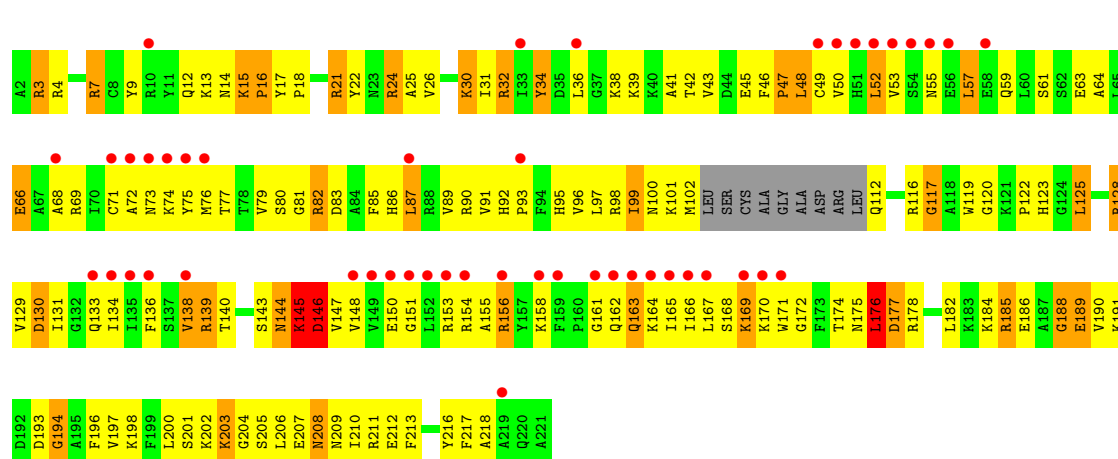
- Molecule 46: 60S ribosomal protein L9-A

Chain l9:



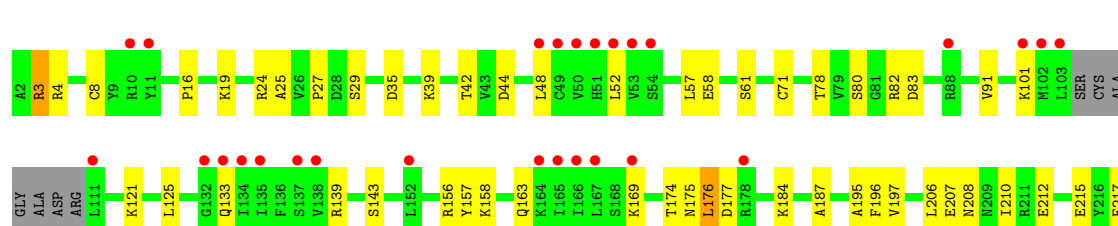
- Molecule 47: 60S ribosomal protein L10

Chain M0:



- Molecule 47: 60S ribosomal protein L10

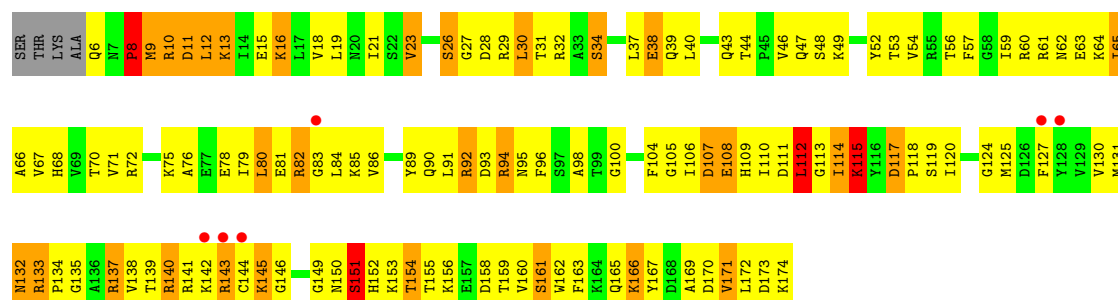
Chain m0:





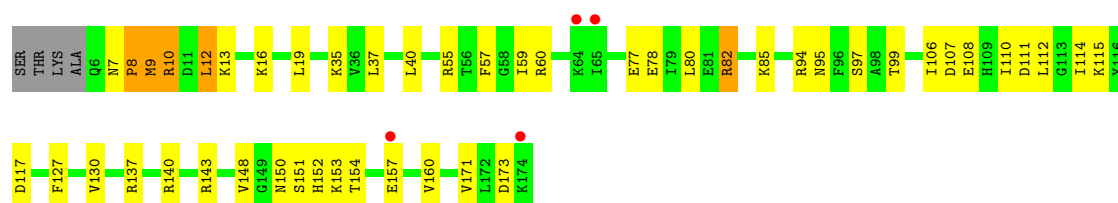
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



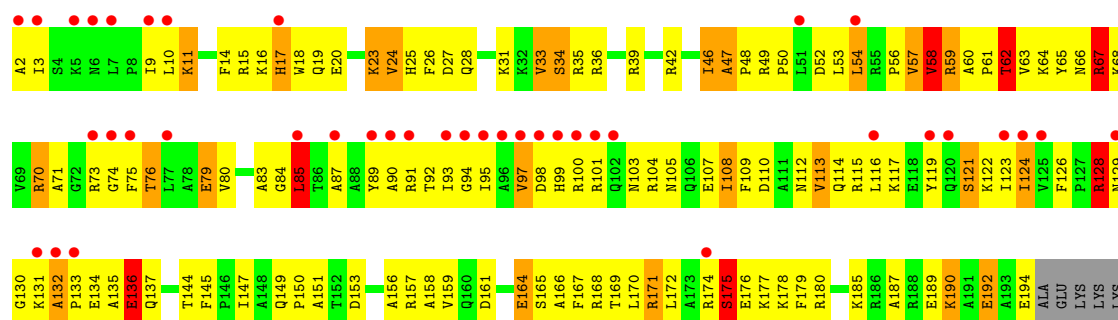
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



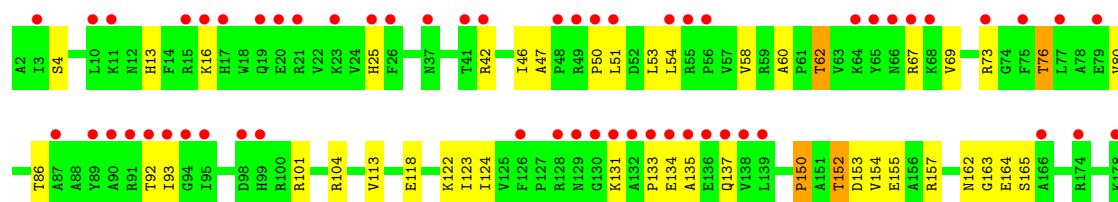
• Molecule 49: 60S ribosomal protein L13-A

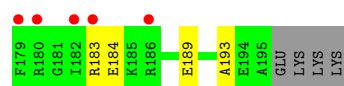
Chain M3:



• Molecule 49: 60S ribosomal protein L13-A

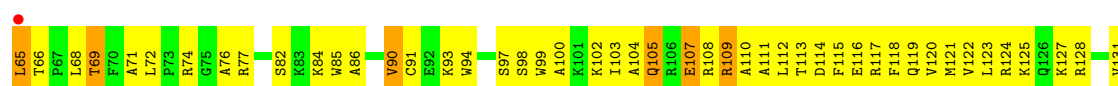
Chain m3:





• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



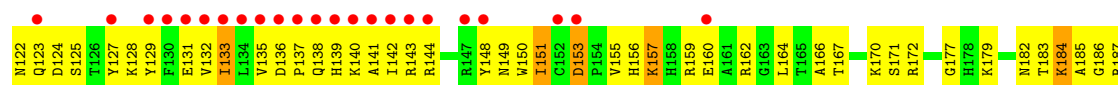
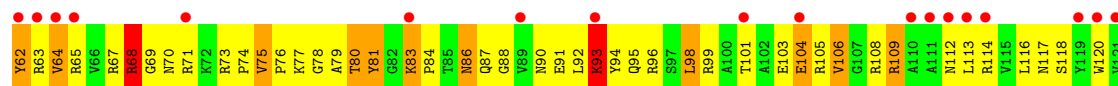
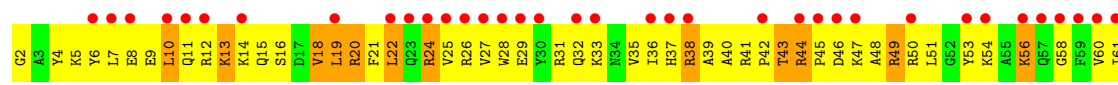
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



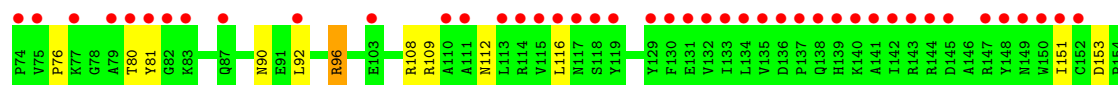
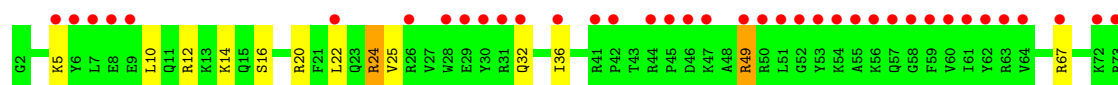
• Molecule 51: 60S ribosomal protein L15-A

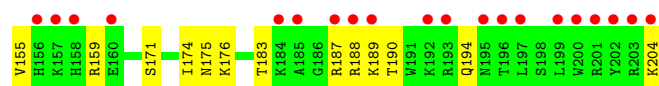
Chain M5:



• Molecule 51: 60S ribosomal protein L15-A

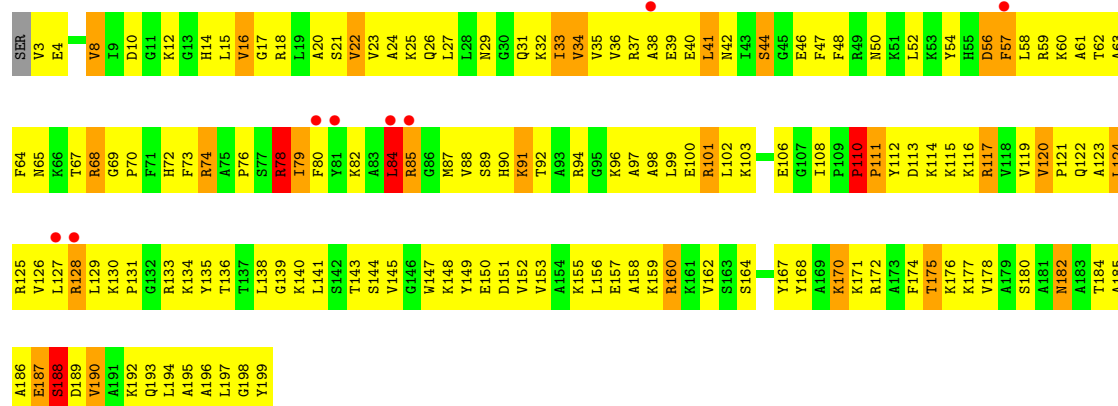
Chain m5:





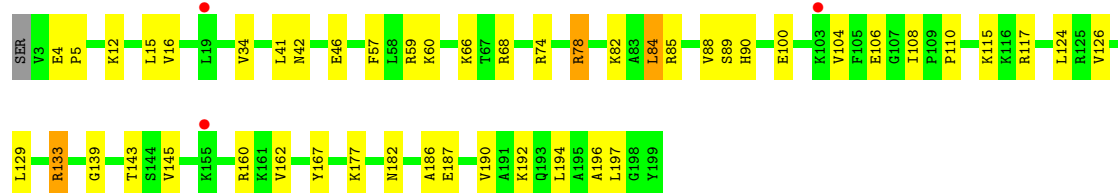
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:



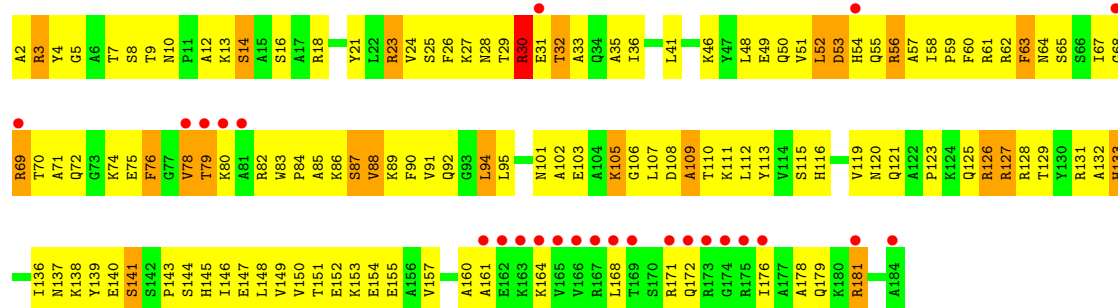
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:



- Molecule 53: 60S ribosomal protein L17-A

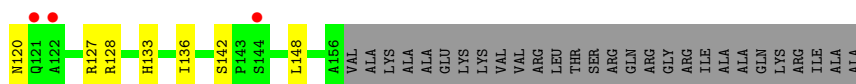
Chain M7:



- Molecule 53: 60S ribosomal protein L17-A

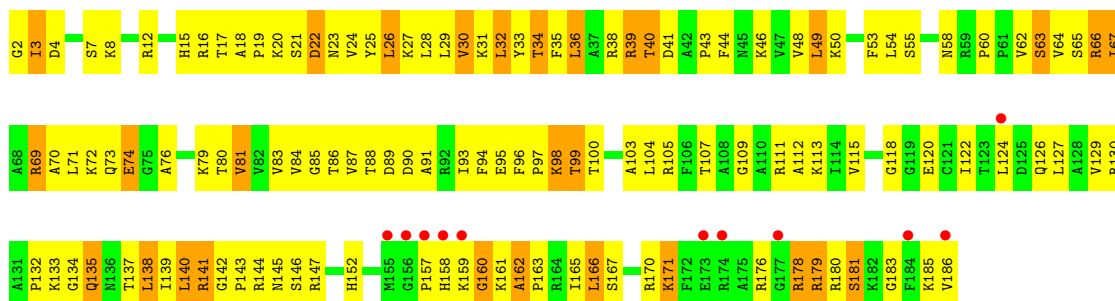
Chain m7:





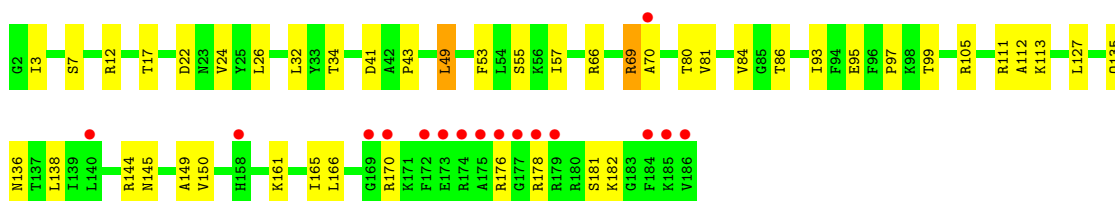
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



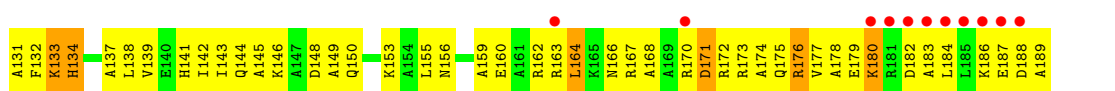
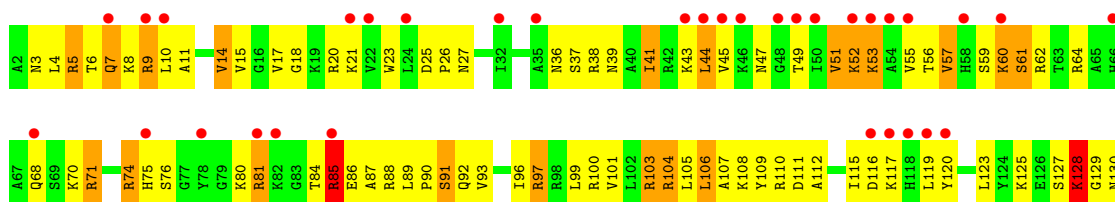
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



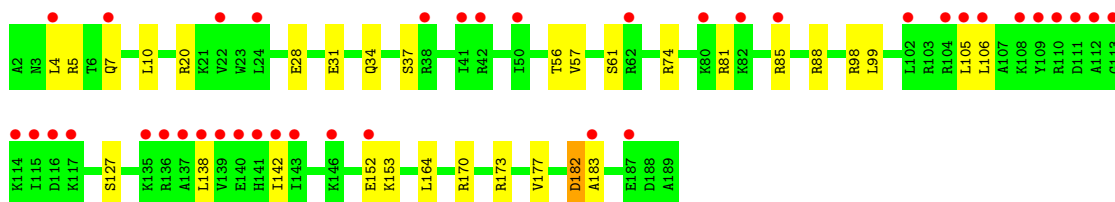
• Molecule 55: 60S ribosomal protein L19-A

Chain M9:

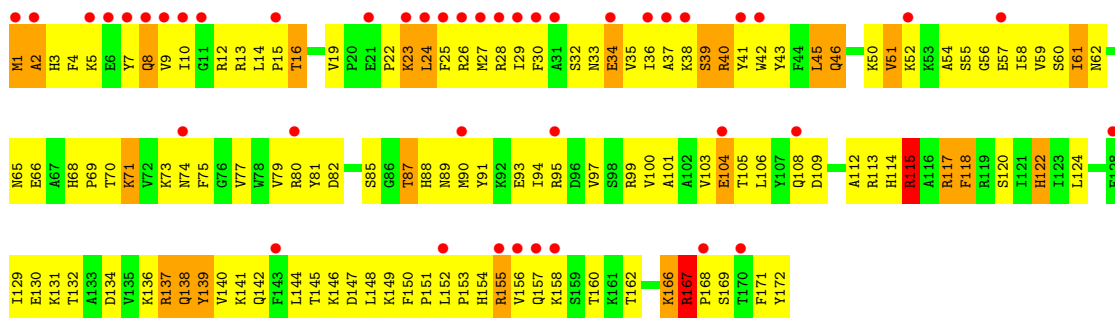


• Molecule 55: 60S ribosomal protein L19-A

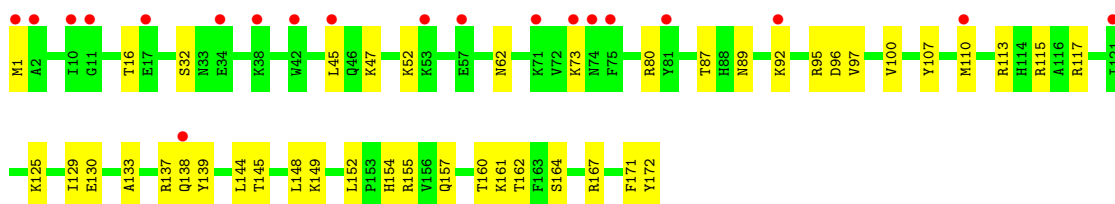
Chain m9:



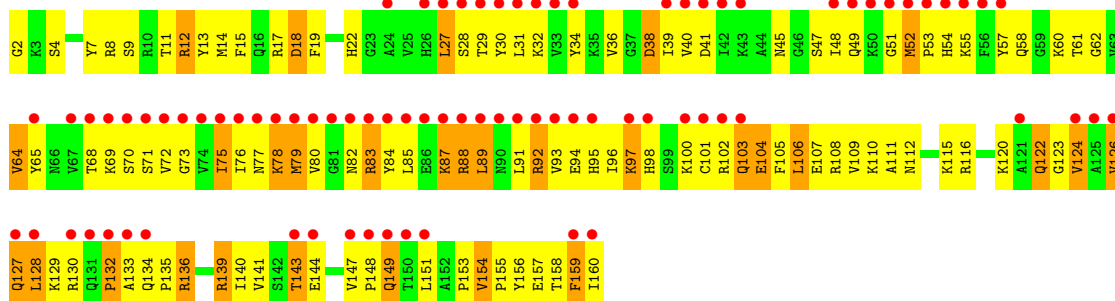
• Molecule 56: 60S ribosomal protein L20-A

Chain N0: 

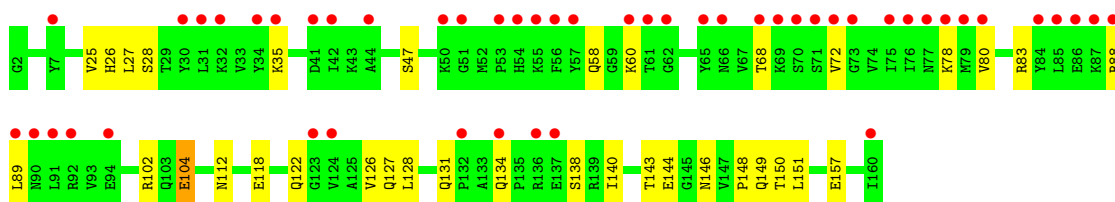
• Molecule 56: 60S ribosomal protein L20-A

Chain n0: 

• Molecule 57: 60S ribosomal protein L21-A

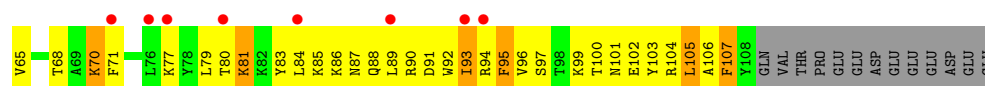
Chain N1: 

• Molecule 57: 60S ribosomal protein L21-A

Chain n1: 

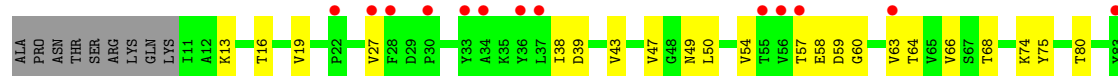
• Molecule 58: 60S ribosomal protein L22-A

Chain N2: 



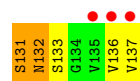
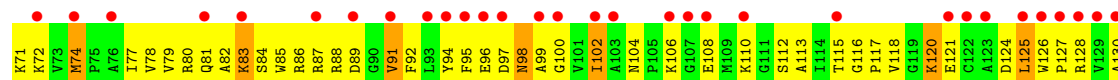
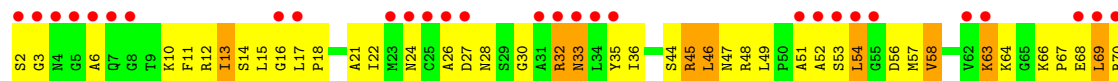
- Molecule 58: 60S ribosomal protein L22-A

Chain n2:



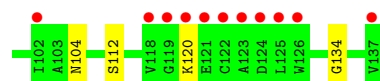
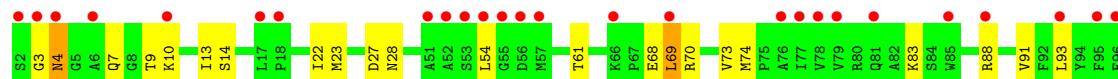
- Molecule 59: 60S ribosomal protein L23-A

Chain N3:



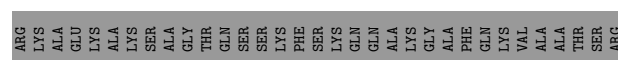
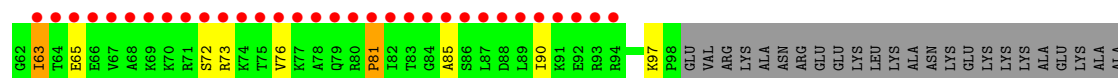
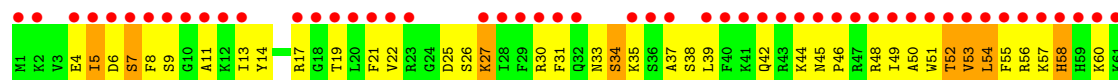
- Molecule 59: 60S ribosomal protein L23-A

Chain n3:



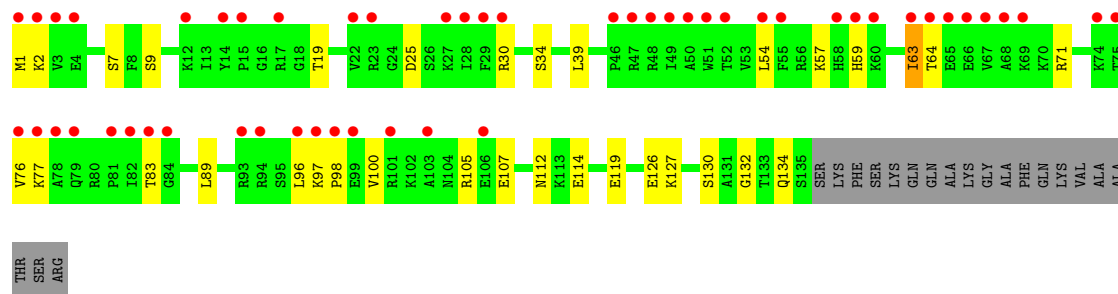
- Molecule 60: 60S ribosomal protein L24-A

Chain N4:



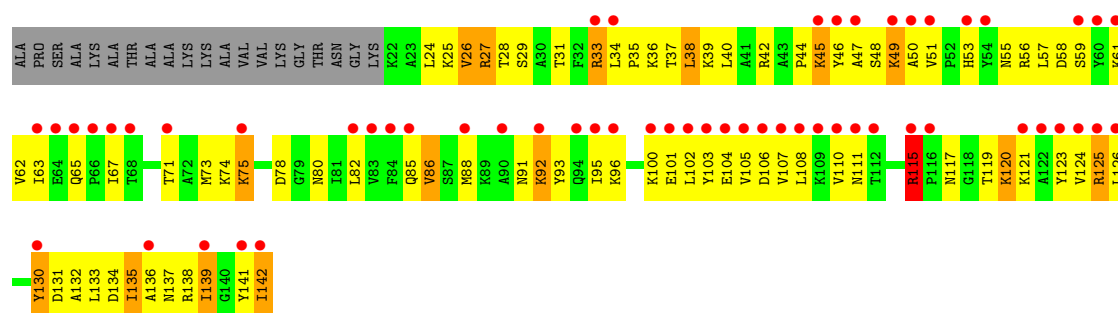
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:



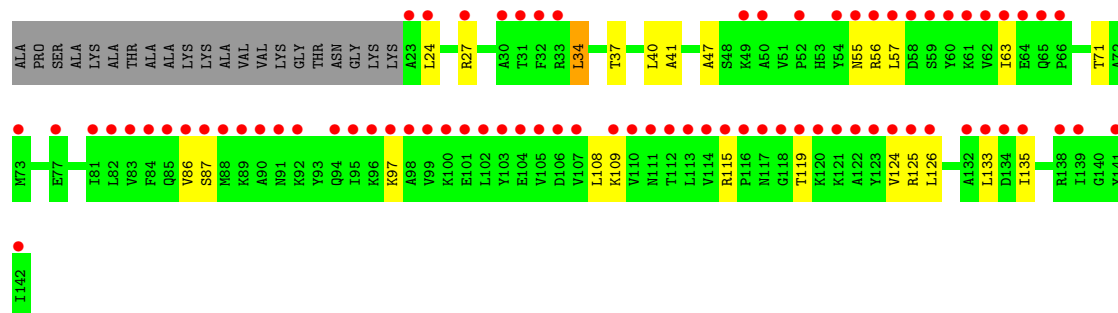
- Molecule 61: 60S ribosomal protein L25

Chain N5:



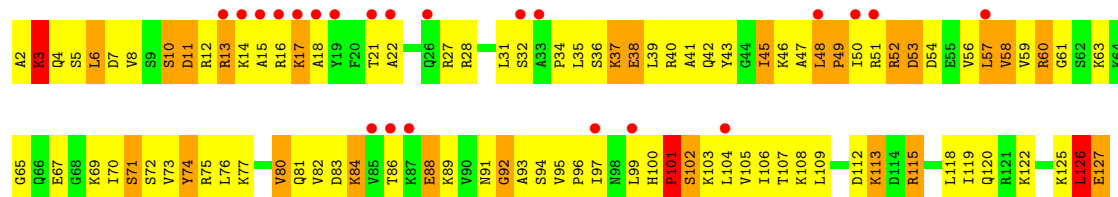
- Molecule 61: 60S ribosomal protein L25

Chain n5:



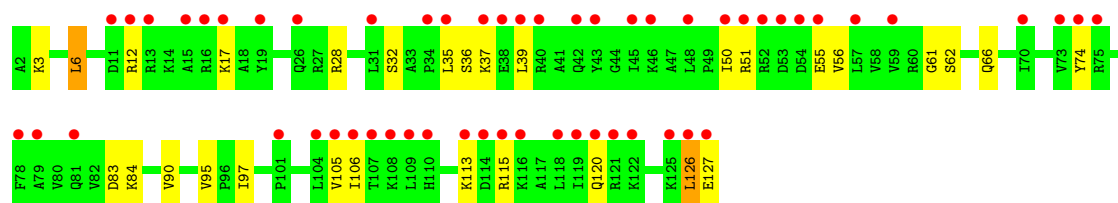
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



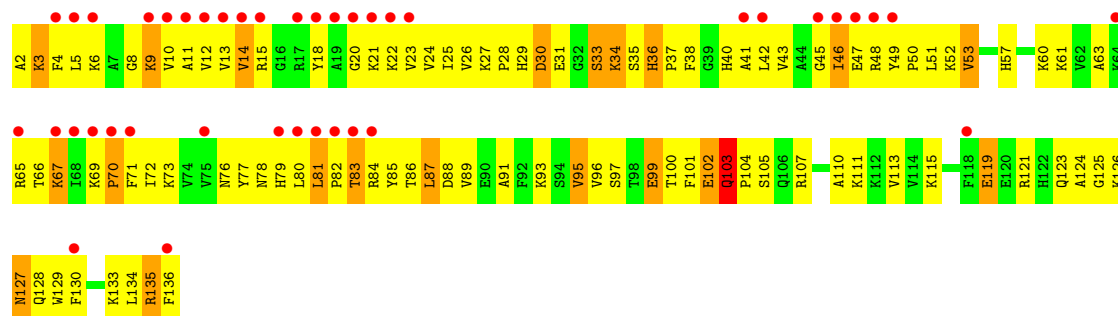
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



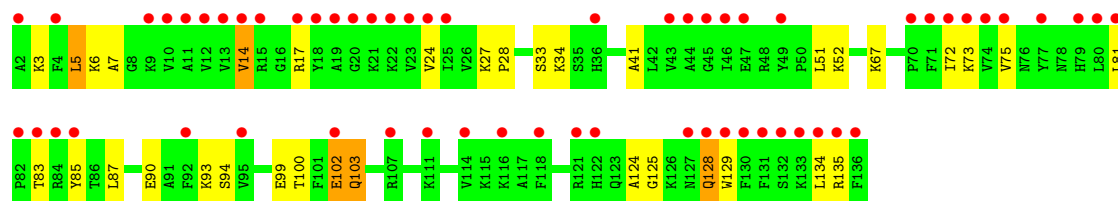
• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



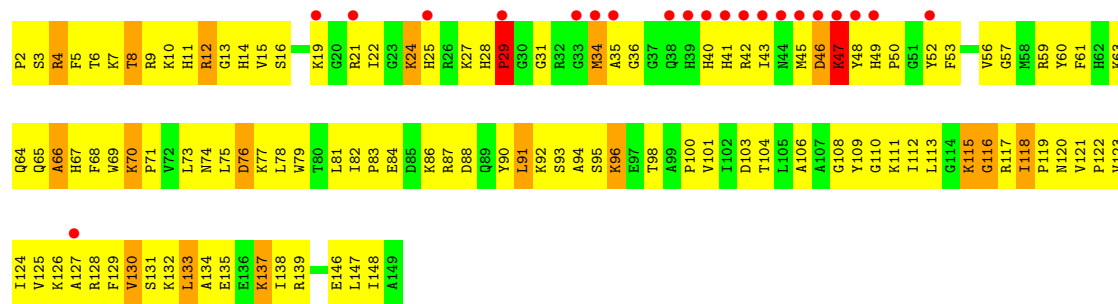
• Molecule 63: 60S ribosomal protein L27-A

Chain n7:



• Molecule 64: 60S ribosomal protein L28

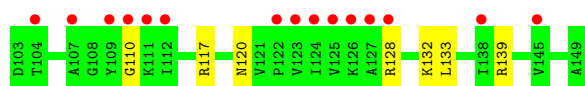
Chain N8:



• Molecule 64: 60S ribosomal protein L28

Chain n8:





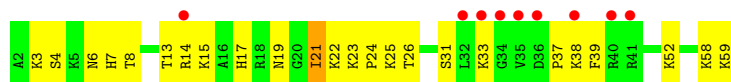
- Molecule 65: 60S ribosomal protein L29

Chain N9:



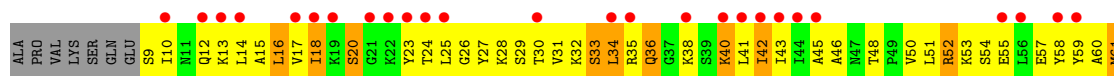
- Molecule 65: 60S ribosomal protein L29

Chain n9:



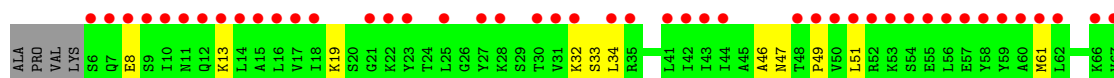
- Molecule 66: 60S ribosomal protein L30

Chain O0:



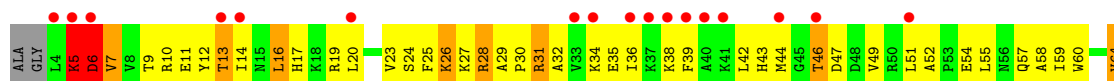
- Molecule 66: 60S ribosomal protein L30

Chain o0:



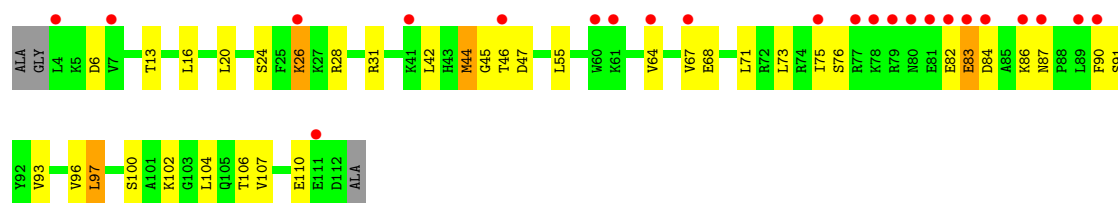
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:



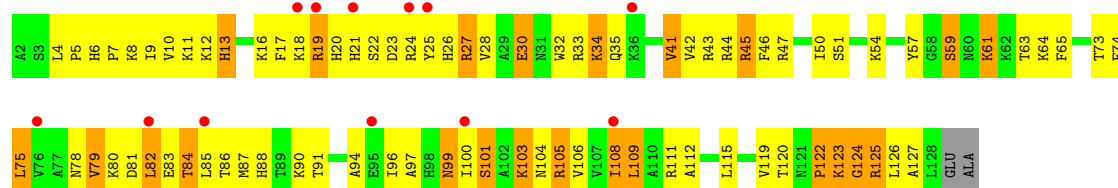
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



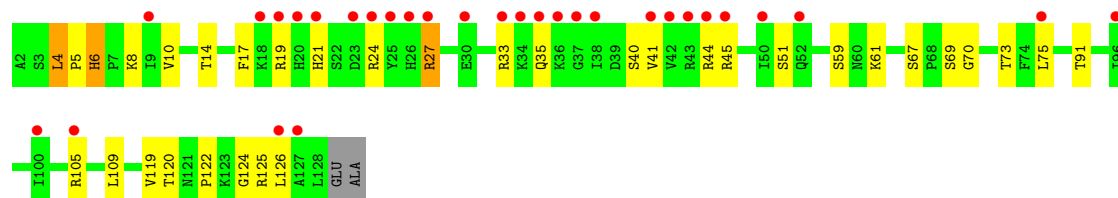
- Molecule 68: 60S ribosomal protein L32

Chain O2:



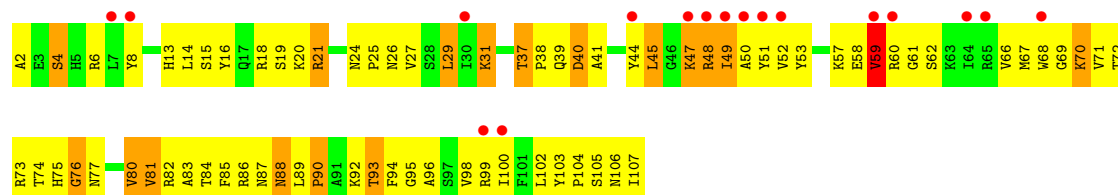
- Molecule 68: 60S ribosomal protein L32

Chain o2:



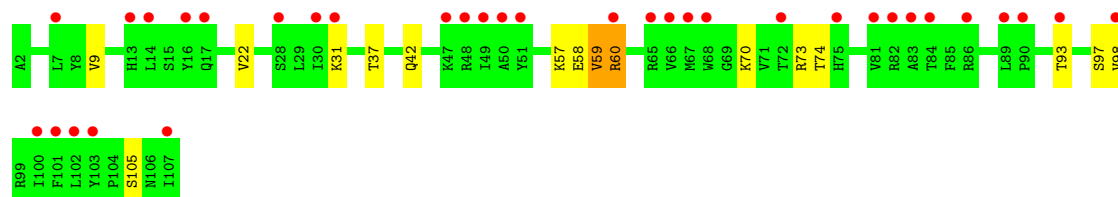
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



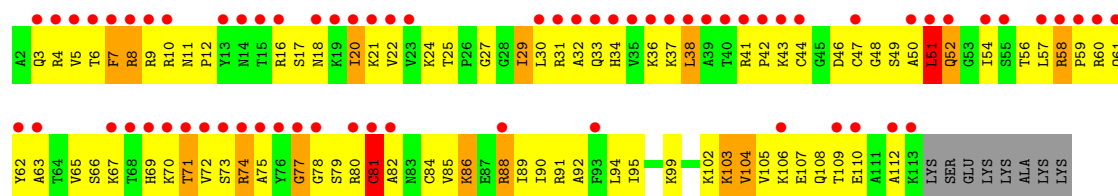
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



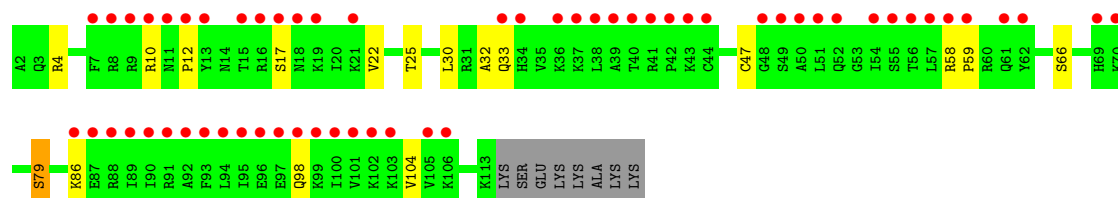
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



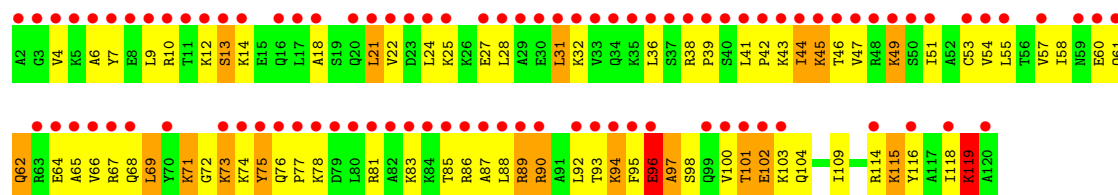
• Molecule 70: 60S ribosomal protein L34-A

Chain o4:



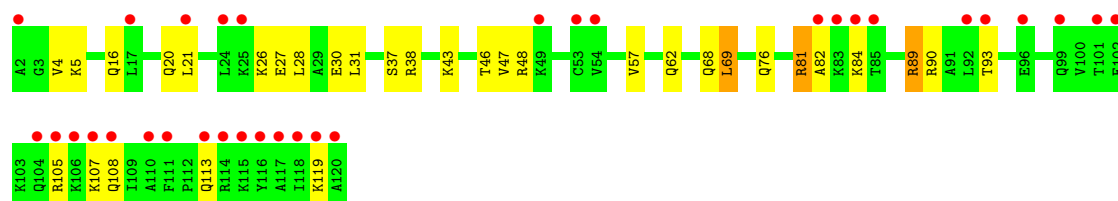
• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



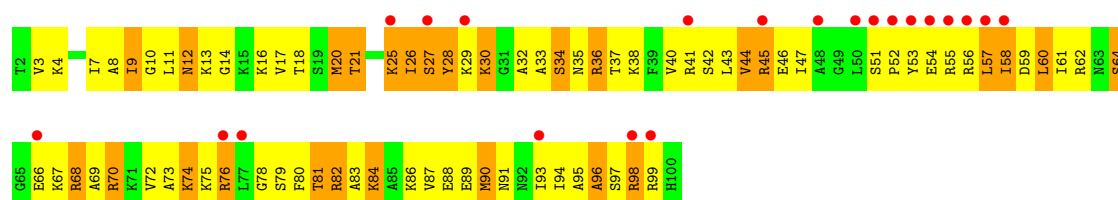
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



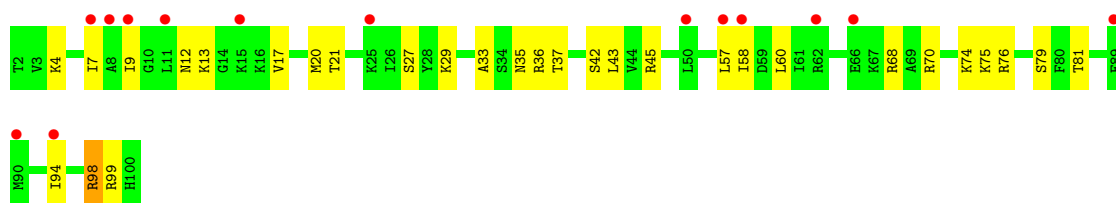
• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



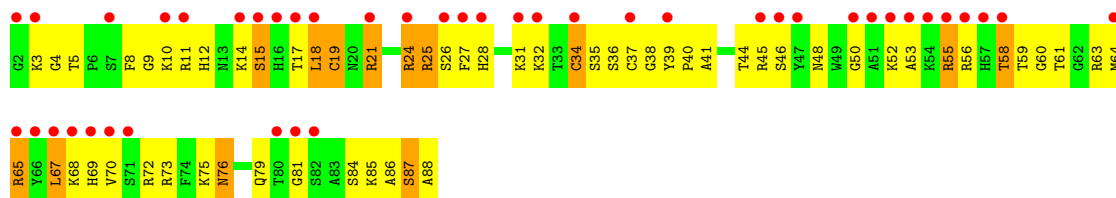
• Molecule 72: 60S ribosomal protein L36-A

Chain o6:



- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



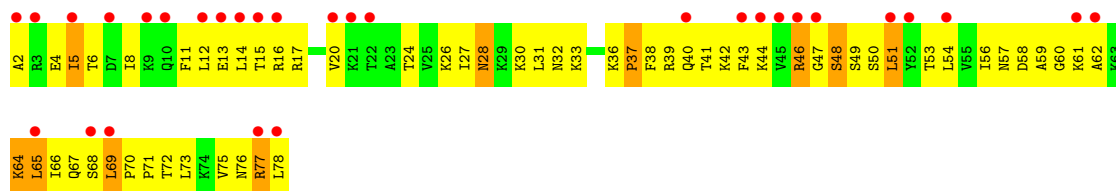
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



- Molecule 74: 60S ribosomal protein L38

Chain O8:



- Molecule 74: 60S ribosomal protein L38

Chain o8:



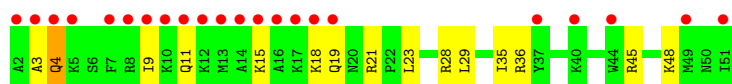
- Molecule 75: 60S ribosomal protein L39

Chain O9:



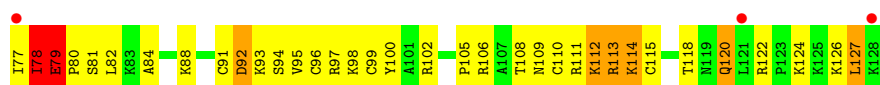
- Molecule 75: 60S ribosomal protein L39

Chain o9:



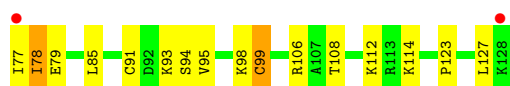
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



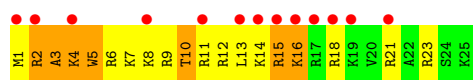
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



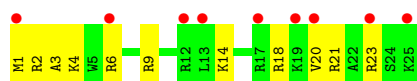
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



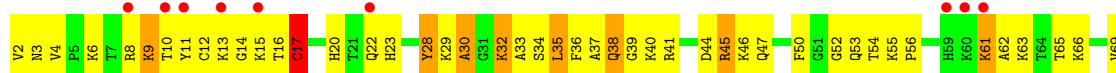
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:



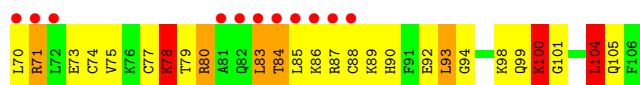
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



- Molecule 78: 60S ribosomal protein L42-A

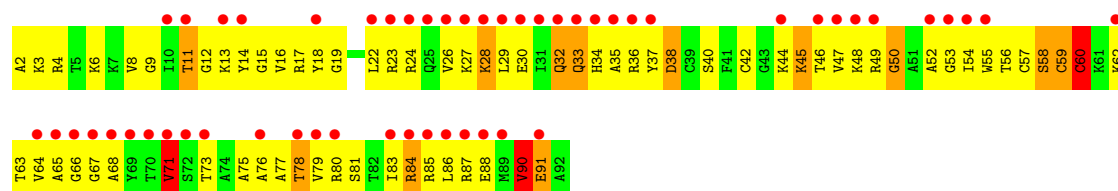
Chain q2:



- Molecule 79: 60S ribosomal protein L43-A

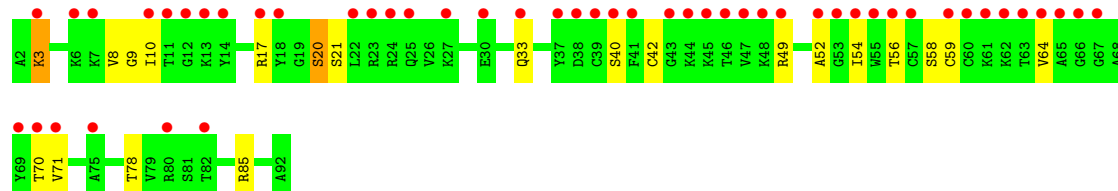
Chain Q3:





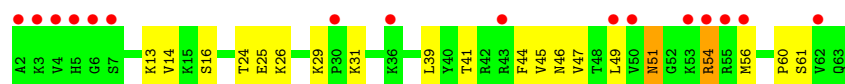
- Molecule 79: 60S ribosomal protein L43-A

Chain q3:



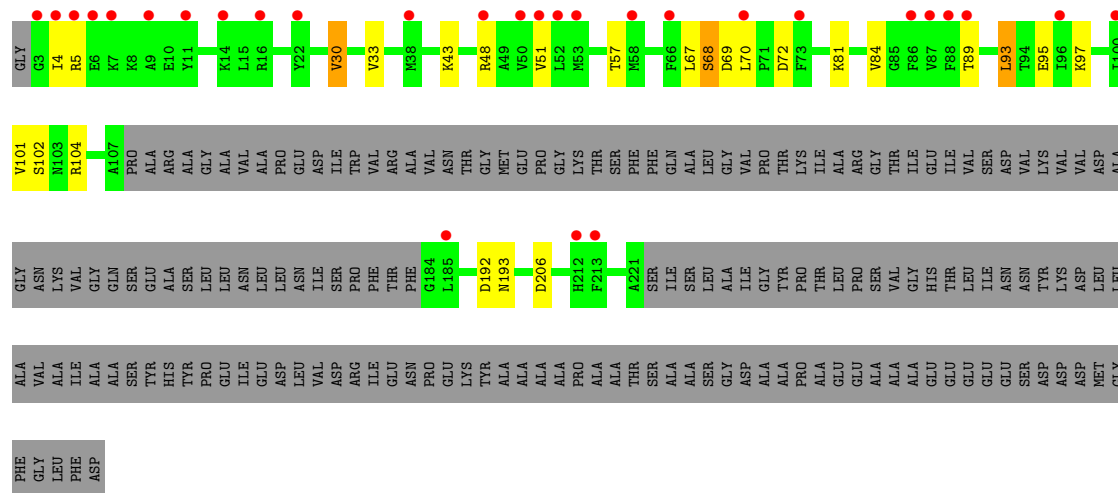
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:



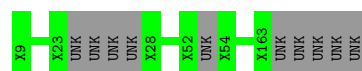
- Molecule 81: 60S acidic ribosomal protein P0

Chain p0:



- Molecule 82: unknown protein chain m2

Chain m2:



- Molecule 83: unknown protein chain p1

Chain p1:

There are no outlier residues recorded for this chain.

- Molecule 84: unknown protein chain p2

Chain p2: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.64Å 286.76Å 303.26Å 90.00° 98.72° 90.00°	Depositor
Resolution (Å)	299.76 – 3.45 299.75 – 3.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (299.76-3.45) 99.9 (299.75-3.45)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.196 , 0.260 0.270 , 0.324	Depositor DCC
R_{free} test set	12804 reflections (1.33%)	DCC
Wilson B-factor (Å ²)	93.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 963326 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	411214	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.74	4/41698 (0.0%)	1.34	362/64972 (0.6%)
1	6	0.83	14/42765 (0.0%)	1.39	467/66634 (0.7%)
2	S0	0.45	0/1617	0.68	0/2215
2	s0	0.47	0/1623	0.67	0/2222
3	S1	0.39	0/1735	0.66	1/2335 (0.0%)
3	s1	0.49	0/1748	0.68	0/2352
4	S2	0.49	0/1665	0.66	0/2263
4	s2	0.55	0/1665	0.77	0/2263
5	S3	0.50	0/1759	0.66	0/2368
5	s3	0.46	0/1759	0.64	1/2368 (0.0%)
6	S4	0.52	0/2109	0.73	0/2839
6	s4	0.53	0/2109	0.72	0/2839
7	S5	0.42	0/1629	0.64	0/2202
7	s5	0.45	0/1629	0.69	0/2202
8	S6	0.49	0/1823	0.65	0/2439
8	s6	0.59	1/1779 (0.1%)	0.72	1/2379 (0.0%)
9	S7	0.44	0/1506	0.68	0/2028
9	s7	0.45	0/1516	0.69	0/2043
10	S8	0.56	0/1514	0.74	1/2021 (0.0%)
10	s8	0.55	0/1514	0.71	0/2021
11	S9	0.48	0/1519	0.68	1/2035 (0.0%)
11	s9	0.54	0/1519	0.71	0/2035
12	C0	0.46	0/790	0.68	1/1069 (0.1%)
12	c0	0.41	0/777	0.69	3/1049 (0.3%)
13	C1	0.59	0/1240	0.76	1/1675 (0.1%)
13	c1	0.59	0/1194	0.76	0/1610
14	C2	0.41	0/900	0.65	0/1224
14	c2	0.32	0/900	0.60	0/1224
15	C3	0.52	0/1215	0.70	2/1638 (0.1%)
15	c3	0.55	0/1215	0.69	0/1638
16	C4	0.40	0/901	0.64	0/1217
16	c4	0.50	0/960	0.70	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.52	0/998	0.72	0/1341
17	c5	0.49	0/1060	0.69	1/1426 (0.1%)
18	C6	0.48	0/1125	0.68	2/1510 (0.1%)
18	c6	0.49	0/1131	0.71	0/1518
19	C7	0.48	0/935	0.68	1/1254 (0.1%)
19	c7	0.48	0/914	0.69	0/1224
20	C8	0.47	0/1211	0.70	0/1628
20	c8	0.50	0/1211	0.72	2/1628 (0.1%)
21	C9	0.44	0/1130	0.62	0/1517
21	c9	0.51	0/1130	0.67	0/1517
22	D0	0.45	0/865	0.71	1/1169 (0.1%)
22	d0	0.46	0/892	0.68	0/1205
23	D1	0.47	0/693	0.64	0/935
23	d1	0.51	0/693	0.68	0/935
24	D2	0.49	0/1038	0.71	0/1395
24	d2	0.59	0/1038	0.76	1/1395 (0.1%)
25	D3	0.61	0/1139	0.75	0/1518
25	d3	0.70	0/1139	0.83	1/1518 (0.1%)
26	D4	0.46	0/1087	0.65	0/1449
26	d4	0.55	0/1087	0.73	0/1449
27	D5	0.44	0/571	0.75	0/768
27	d5	0.45	0/566	0.68	0/761
28	D6	0.47	0/782	0.66	0/1047
28	d6	0.54	0/782	0.79	1/1047 (0.1%)
29	D7	0.42	0/620	0.65	0/838
29	d7	0.47	0/620	0.71	0/838
30	D8	0.42	0/499	0.64	0/670
30	d8	0.43	0/499	0.62	0/670
31	D9	0.53	0/452	0.67	0/600
31	d9	0.64	0/452	0.69	0/600
32	E0	0.48	0/483	0.65	0/643
33	E1	0.49	0/577	0.80	0/770
33	e1	0.42	0/619	0.75	1/822 (0.1%)
34	SR	0.40	0/2494	0.63	0/3393
34	sR	0.39	0/2495	0.58	0/3395
35	SM	0.53	0/1113	0.71	2/1502 (0.1%)
35	sM	0.49	0/682	0.69	1/921 (0.1%)
36	1	1.12	138/75394 (0.2%)	1.68	1938/117545 (1.6%)
36	5	1.11	157/75414 (0.2%)	1.68	1917/117575 (1.6%)
37	3	0.99	2/2883 (0.1%)	1.47	39/4491 (0.9%)
37	7	1.11	3/2883 (0.1%)	1.76	76/4491 (1.7%)
38	4	1.02	1/3746 (0.0%)	1.59	63/5832 (1.1%)
38	8	0.90	2/3746 (0.1%)	1.47	43/5832 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.68	0/1948	0.81	1/2617 (0.0%)
39	l2	0.60	0/1946	0.82	2/2614 (0.1%)
40	L3	0.74	0/3146	0.83	0/4228
40	l3	0.78	0/3146	0.86	2/4228 (0.0%)
41	L4	0.78	1/2800 (0.0%)	0.90	1/3790 (0.0%)
41	l4	0.73	1/2800 (0.0%)	0.88	3/3790 (0.1%)
42	L5	0.61	0/2425	0.73	0/3271
42	l5	0.72	0/2408	0.83	1/3248 (0.0%)
43	L6	0.78	0/1260	0.85	0/1694
43	l6	0.81	0/1269	0.87	0/1705
44	L7	0.83	0/1821	0.91	3/2451 (0.1%)
44	l7	0.87	0/1828	0.97	5/2461 (0.2%)
45	L8	0.54	0/1836	0.71	2/2481 (0.1%)
45	l8	0.48	0/1795	0.68	1/2429 (0.0%)
46	L9	0.69	0/1539	0.81	1/2073 (0.0%)
46	l9	0.76	0/1539	0.84	2/2073 (0.1%)
47	M0	0.76	0/1741	0.84	3/2335 (0.1%)
47	m0	0.76	1/1758 (0.1%)	0.82	0/2358
48	M1	0.56	0/1374	0.74	1/1842 (0.1%)
48	m1	0.70	0/1374	0.80	1/1842 (0.1%)
49	M3	0.72	0/1568	0.86	2/2106 (0.1%)
49	m3	0.64	0/1573	0.78	0/2113
50	M4	0.81	0/1068	0.88	1/1438 (0.1%)
50	m4	0.82	0/1074	0.84	1/1446 (0.1%)
51	M5	0.75	0/1757	0.86	2/2354 (0.1%)
51	m5	0.61	0/1757	0.79	2/2354 (0.1%)
52	M6	0.85	0/1585	0.92	4/2128 (0.2%)
52	m6	0.96	0/1585	0.98	4/2128 (0.2%)
53	M7	0.76	0/1443	0.83	0/1944
53	m7	0.83	0/1250	0.87	1/1683 (0.1%)
54	M8	0.75	0/1465	0.90	4/1965 (0.2%)
54	m8	0.72	0/1465	0.86	1/1965 (0.1%)
55	M9	0.60	0/1538	0.75	0/2050
55	m9	0.58	0/1538	0.69	0/2050
56	N0	0.78	0/1481	0.85	1/1990 (0.1%)
56	n0	0.88	0/1481	0.90	2/1990 (0.1%)
57	N1	0.74	0/1300	0.82	1/1743 (0.1%)
57	n1	0.81	1/1300 (0.1%)	0.88	0/1743
58	N2	0.48	0/812	0.63	0/1099
58	n2	0.49	0/794	0.68	0/1076
59	N3	0.69	0/1018	0.81	0/1369
59	n3	0.80	0/1018	0.82	0/1369
60	N4	0.62	0/712	0.74	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.65	0/1052	0.75	0/1398
61	N5	0.64	0/979	0.79	1/1321 (0.1%)
61	n5	0.60	0/974	0.77	1/1314 (0.1%)
62	N6	0.72	0/1004	0.86	1/1341 (0.1%)
62	n6	0.62	0/1004	0.81	0/1341
63	N7	0.54	0/1118	0.68	0/1497
63	n7	0.48	0/1118	0.66	0/1497
64	N8	0.73	0/1204	0.85	0/1612
64	n8	0.73	0/1204	0.84	1/1612 (0.1%)
65	N9	0.69	0/473	0.83	1/629 (0.2%)
65	n9	0.71	0/473	0.88	0/629
66	O0	0.49	0/751	0.68	0/1008
66	o0	0.53	0/775	0.69	0/1040
67	O1	0.65	0/890	0.80	0/1196
67	o1	0.71	0/897	0.86	2/1205 (0.2%)
68	O2	0.79	0/1041	0.87	0/1394
68	o2	0.87	0/1041	0.89	0/1394
69	O3	0.86	0/868	0.94	0/1168
69	o3	0.87	0/868	0.90	0/1168
70	O4	0.59	0/890	0.77	1/1189 (0.1%)
70	o4	0.52	0/890	0.74	0/1189
71	O5	0.67	0/978	0.78	0/1301
71	o5	0.58	0/974	0.77	2/1297 (0.2%)
72	O6	0.61	0/778	0.77	0/1034
72	o6	0.58	0/777	0.68	0/1033
73	O7	0.74	0/696	0.87	1/923 (0.1%)
73	o7	0.64	0/696	0.79	0/923
74	O8	0.53	0/618	0.66	0/826
74	o8	0.45	0/614	0.66	0/822
75	O9	0.64	0/443	0.82	0/588
75	o9	0.62	0/443	0.78	0/588
76	Q0	0.79	0/423	0.93	0/562
76	q0	0.90	1/423 (0.2%)	0.98	0/562
77	Q1	0.67	0/234	0.87	0/300
77	q1	0.58	0/234	0.89	0/300
78	Q2	0.83	1/860 (0.1%)	0.84	0/1136
78	q2	0.73	1/860 (0.1%)	0.83	2/1136 (0.2%)
79	Q3	0.71	0/701	0.83	0/934
79	q3	0.68	0/701	0.78	0/934
80	e0	0.51	0/499	0.75	0/665
81	p0	0.48	0/1091	0.64	0/1472
All	All	0.87	329/430072 (0.1%)	1.32	4999/631360 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	S1	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
10	S8	0	1
11	S9	0	1
16	C4	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	1
20	c8	0	1
22	d0	0	1
26	d4	0	1
27	D5	0	2
33	E1	0	1
39	L2	0	1
39	l2	0	1
40	L3	0	1
40	l3	0	1
42	L5	0	1
43	L6	0	1
44	l7	0	1
45	L8	0	1
47	M0	0	1
48	M1	0	1
48	m1	0	1
50	M4	0	1
52	M6	0	1
56	n0	0	2
64	n8	0	1
65	N9	0	1
67	O1	0	1
69	o3	0	1
80	e0	0	1
All	All	0	37

The worst 5 of 329 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	12.22	2.03	1.82
36	5	1152	G	N9-C4	-12.11	1.28	1.38
36	5	2145	A	N7-C5	-9.34	1.33	1.39
78	q2	17	CYS	CB-SG	9.04	1.97	1.82
36	5	3040	A	N9-C4	-8.70	1.32	1.37

The worst 5 of 4999 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-19.38	114.37	126.00
36	5	1152	G	N3-C4-C5	17.87	137.53	128.60
36	5	1152	G	C2-N3-C4	-16.63	103.58	111.90
36	1	645	A	N1-C6-N6	-16.45	108.73	118.60
36	1	343	U	O5'-P-OP2	-14.33	92.80	105.70

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
3	S1	177	GLN	Peptide
9	S7	131	PHE	Peptide
10	S8	8	ARG	Peptide
11	S9	137	GLY	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	18758	1135	1
1	6	38238	0	19241	1143	0
2	S0	1577	0	1567	185	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	191	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	155	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	199	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	198	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	192	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	154	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	137	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	160	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	74	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	116	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	76	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	133	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	100	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	115	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	137	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	107	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	147	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	140	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	105	0
22	d0	882	0	939	0	0
23	D1	684	0	672	88	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	111	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	103	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	68	0
27	d5	558	0	598	0	0
28	D6	769	0	814	123	0
28	d6	769	0	814	0	0
29	D7	610	0	631	59	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	40	0
33	E1	566	0	602	65	0
33	e1	608	0	656	0	0
34	SR	2441	0	2397	221	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	87	0
35	sM	679	0	603	0	0
36	1	67355	0	33845	1713	0
36	5	67376	0	33855	1695	1
37	3	2579	0	1304	81	0
37	7	2579	0	1303	73	0
38	4	3353	0	1695	85	0
38	8	3353	0	1695	98	0
39	L2	1914	0	1981	203	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	284	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	285	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	238	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	110	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	193	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	174	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	171	0
46	l9	1518	0	1587	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	M0	1705	0	1736	164	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	140	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	163	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	114	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	203	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	181	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	139	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	131	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1616	150	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	161	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	142	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	61	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	107	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	44	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	84	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	110	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	100	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	141	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	47	0
65	n9	462	0	491	0	0
66	O0	743	0	797	82	0
66	o0	767	0	816	0	0
67	O1	876	0	912	79	0
67	o1	883	0	918	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	O2	1020	0	1090	95	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	81	0
69	o3	850	0	880	0	0
70	O4	880	0	945	113	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	87	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	84	0
72	o6	770	0	846	0	0
73	O7	681	0	683	76	0
73	o7	681	0	683	0	0
74	O8	612	0	682	63	0
74	o8	608	0	671	0	0
75	O9	436	0	475	44	0
75	o9	436	0	475	0	0
76	Q0	417	0	457	47	0
76	q0	417	0	456	0	0
77	Q1	233	0	284	30	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	83	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	80	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	p0	1076	0	1040	0	0
82	m2	750	0	179	0	0
83	p1	235	0	50	0	0
84	p2	230	0	51	0	0
85	1	462	0	0	0	0
85	2	122	0	0	0	0
85	3	15	0	0	0	0
85	4	23	0	0	0	0
85	5	495	0	0	0	0
85	6	147	0	0	0	0
85	7	17	0	0	0	0
85	8	14	0	0	0	0
85	C1	1	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	D4	1	0	0	0	0
85	L2	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L3	4	0	0	0	0
85	L4	3	0	0	0	0
85	L7	2	0	0	0	0
85	L8	1	0	0	0	0
85	M0	3	0	0	0	0
85	M1	1	0	0	0	0
85	M3	2	0	0	0	0
85	M5	2	0	0	0	0
85	M6	1	0	0	0	0
85	M7	5	0	0	0	0
85	M9	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	2	0	0	0	0
85	N8	5	0	0	0	0
85	O1	1	0	0	0	0
85	O2	2	0	0	0	0
85	O5	1	0	0	0	0
85	O7	2	0	0	0	0
85	Q2	1	0	0	0	0
85	S4	1	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c4	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	1	0	0	0	0
85	c9	1	0	0	0	0
85	d0	1	0	0	0	0
85	d3	3	0	0	0	0
85	d6	1	0	0	0	0
85	l2	3	0	0	0	0
85	l3	3	0	0	0	0
85	l4	1	0	0	0	0
85	l5	3	0	0	0	0
85	l7	1	0	0	0	0
85	l9	1	0	0	0	0
85	m0	1	0	0	0	0
85	m1	1	0	0	0	0
85	m4	1	0	0	0	0
85	m5	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	m6	2	0	0	0	0
85	m7	6	0	0	0	0
85	n0	1	0	0	0	0
85	n3	1	0	0	0	0
85	n6	2	0	0	0	0
85	n8	3	0	0	0	0
85	n9	2	0	0	0	0
85	o3	2	0	0	0	0
85	o4	3	0	0	0	0
85	o7	1	0	0	0	0
85	q0	2	0	0	0	0
85	q1	1	0	0	0	0
85	s1	1	0	0	0	0
85	s8	1	0	0	0	0
85	sM	1	0	0	0	0
86	1	2478	0	0	204	0
86	2	1106	0	0	106	0
86	3	70	0	0	4	0
86	4	105	0	0	6	0
86	5	2492	0	0	217	0
86	6	1113	0	0	108	0
86	7	84	0	0	12	0
86	8	105	0	0	10	0
86	C3	7	0	0	1	0
86	C5	7	0	0	3	0
86	C8	7	0	0	0	0
86	D3	7	0	0	2	0
86	D9	7	0	0	0	0
86	L3	14	0	0	2	0
86	L4	7	0	0	2	0
86	M0	7	0	0	1	0
86	M5	7	0	0	1	0
86	M7	14	0	0	2	0
86	M9	7	0	0	1	0
86	N9	7	0	0	0	0
86	O1	7	0	0	7	0
86	O3	7	0	0	1	0
86	O7	14	0	0	7	0
86	Q2	7	0	0	2	0
86	S8	7	0	0	1	0
86	SR	7	0	0	0	0
86	c3	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	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	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	n1	7	0	0	0	0
86	n3	7	0	0	0	0
86	n9	7	0	0	0	0
86	o3	7	0	0	0	0
86	o7	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	0	0
86	sR	7	0	0	0	0
87	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	1	0
87	Q2	1	0	0	2	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	30	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	5	30	0	25	2	0
All	All	411214	0	297334	13265	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 19.

The worst 5 of 13265 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	2.03	1.47
78:Q2:17:CYS:CB	87:Q2:501:ZN:ZN	0.98	1.42
78:Q2:17:CYS:SG	87:Q2:501:ZN:ZN	1.30	1.18
36:5:2273:G:O6	86:5:4193:OHX:N5	1.90	1.05
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.53	1.04

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]	2.15	0.05

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%)	142 (70%)	37 (18%)	25 (12%)	1	9
2	s0	204/251 (81%)	150 (74%)	36 (18%)	18 (9%)	1	17
3	S1	212/254 (84%)	142 (67%)	42 (20%)	28 (13%)	0	7
3	s1	214/254 (84%)	165 (77%)	37 (17%)	12 (6%)	3	31
4	S2	215/253 (85%)	175 (81%)	23 (11%)	17 (8%)	1	20
4	s2	215/253 (85%)	169 (79%)	28 (13%)	18 (8%)	1	18
5	S3	221/239 (92%)	170 (77%)	37 (17%)	14 (6%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	s3	221/239 (92%)	174 (79%)	25 (11%)	22 (10%)	1	13
6	S4	258/260 (99%)	201 (78%)	43 (17%)	14 (5%)	3	33
6	s4	258/260 (99%)	206 (80%)	35 (14%)	17 (7%)	2	26
7	S5	204/224 (91%)	150 (74%)	33 (16%)	21 (10%)	1	12
7	s5	204/224 (91%)	140 (69%)	41 (20%)	23 (11%)	1	10
8	S6	224/236 (95%)	181 (81%)	33 (15%)	10 (4%)	4	39
8	s6	216/236 (92%)	172 (80%)	34 (16%)	10 (5%)	4	38
9	S7	182/189 (96%)	137 (75%)	27 (15%)	18 (10%)	1	13
9	s7	184/189 (97%)	133 (72%)	34 (18%)	17 (9%)	1	15
10	S8	184/200 (92%)	145 (79%)	29 (16%)	10 (5%)	3	33
10	s8	184/200 (92%)	149 (81%)	27 (15%)	8 (4%)	4	40
11	S9	183/196 (93%)	144 (79%)	27 (15%)	12 (7%)	2	26
11	s9	183/196 (93%)	133 (73%)	40 (22%)	10 (6%)	3	32
12	C0	94/105 (90%)	68 (72%)	19 (20%)	7 (7%)	2	23
12	c0	92/105 (88%)	68 (74%)	11 (12%)	13 (14%)	0	6
13	C1	153/155 (99%)	107 (70%)	27 (18%)	19 (12%)	1	9
13	c1	144/155 (93%)	114 (79%)	23 (16%)	7 (5%)	3	36
14	C2	122/142 (86%)	66 (54%)	39 (32%)	17 (14%)	0	6
14	c2	122/142 (86%)	72 (59%)	30 (25%)	20 (16%)	0	4
15	C3	148/150 (99%)	117 (79%)	24 (16%)	7 (5%)	4	37
15	c3	148/150 (99%)	107 (72%)	28 (19%)	13 (9%)	1	17
16	C4	125/136 (92%)	93 (74%)	23 (18%)	9 (7%)	2	24
16	c4	126/136 (93%)	99 (79%)	18 (14%)	9 (7%)	2	24
17	C5	122/141 (86%)	84 (69%)	24 (20%)	14 (12%)	1	10
17	c5	133/141 (94%)	92 (69%)	24 (18%)	17 (13%)	0	8
18	C6	139/142 (98%)	117 (84%)	16 (12%)	6 (4%)	4	40
18	c6	140/142 (99%)	106 (76%)	23 (16%)	11 (8%)	1	20
19	C7	116/136 (85%)	85 (73%)	18 (16%)	13 (11%)	1	10
19	c7	113/136 (83%)	84 (74%)	22 (20%)	7 (6%)	2	28
20	C8	143/145 (99%)	107 (75%)	23 (16%)	13 (9%)	1	16
20	c8	143/145 (99%)	105 (73%)	25 (18%)	13 (9%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	C9	141/143 (99%)	108 (77%)	27 (19%)	6 (4%)	4	40
21	c9	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	4	40
22	D0	105/120 (88%)	79 (75%)	20 (19%)	6 (6%)	3	31
22	d0	108/120 (90%)	83 (77%)	14 (13%)	11 (10%)	1	12
23	D1	85/87 (98%)	58 (68%)	19 (22%)	8 (9%)	1	15
23	d1	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	2	30
24	D2	127/129 (98%)	103 (81%)	17 (13%)	7 (6%)	3	32
24	d2	127/129 (98%)	101 (80%)	23 (18%)	3 (2%)	9	58
25	D3	142/144 (99%)	107 (75%)	22 (16%)	13 (9%)	1	15
25	d3	142/144 (99%)	115 (81%)	19 (13%)	8 (6%)	3	31
26	D4	132/134 (98%)	105 (80%)	17 (13%)	10 (8%)	2	21
26	d4	132/134 (98%)	100 (76%)	15 (11%)	17 (13%)	0	8
27	D5	68/107 (64%)	44 (65%)	14 (21%)	10 (15%)	0	5
27	d5	67/107 (63%)	47 (70%)	15 (22%)	5 (8%)	2	22
28	D6	95/97 (98%)	59 (62%)	23 (24%)	13 (14%)	0	7
28	d6	95/97 (98%)	70 (74%)	18 (19%)	7 (7%)	2	23
29	D7	79/81 (98%)	55 (70%)	18 (23%)	6 (8%)	2	21
29	d7	79/81 (98%)	53 (67%)	21 (27%)	5 (6%)	2	28
30	D8	61/66 (92%)	42 (69%)	14 (23%)	5 (8%)	1	19
30	d8	61/66 (92%)	43 (70%)	14 (23%)	4 (7%)	2	26
31	D9	51/55 (93%)	37 (72%)	10 (20%)	4 (8%)	1	20
31	d9	51/55 (93%)	39 (76%)	8 (16%)	4 (8%)	1	20
32	E0	58/60 (97%)	43 (74%)	10 (17%)	5 (9%)	1	17
33	E1	69/76 (91%)	32 (46%)	20 (29%)	17 (25%)	0	1
33	e1	74/76 (97%)	33 (45%)	21 (28%)	20 (27%)	0	0
34	SR	316/318 (99%)	231 (73%)	58 (18%)	27 (8%)	1	18
34	sR	316/318 (99%)	255 (81%)	49 (16%)	12 (4%)	5	45
35	SM	155/273 (57%)	99 (64%)	34 (22%)	22 (14%)	0	6
35	sM	98/273 (36%)	63 (64%)	23 (24%)	12 (12%)	1	9
39	L2	250/253 (99%)	214 (86%)	28 (11%)	8 (3%)	6	51
39	l2	250/253 (99%)	200 (80%)	32 (13%)	18 (7%)	2	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	L3	384/386 (100%)	324 (84%)	45 (12%)	15 (4%)	5	44
40	l3	384/386 (100%)	323 (84%)	42 (11%)	19 (5%)	3	36
41	L4	359/361 (99%)	279 (78%)	54 (15%)	26 (7%)	2	24
41	l4	359/361 (99%)	277 (77%)	56 (16%)	26 (7%)	2	24
42	L5	294/296 (99%)	237 (81%)	34 (12%)	23 (8%)	1	20
42	l5	292/296 (99%)	240 (82%)	39 (13%)	13 (4%)	4	39
43	L6	152/175 (87%)	121 (80%)	26 (17%)	5 (3%)	6	50
43	l6	153/175 (87%)	121 (79%)	25 (16%)	7 (5%)	4	38
44	L7	220/243 (90%)	183 (83%)	24 (11%)	13 (6%)	2	30
44	l7	221/243 (91%)	177 (80%)	30 (14%)	14 (6%)	2	28
45	L8	231/255 (91%)	179 (78%)	35 (15%)	17 (7%)	2	23
45	l8	229/255 (90%)	176 (77%)	36 (16%)	17 (7%)	2	23
46	L9	189/191 (99%)	150 (79%)	28 (15%)	11 (6%)	3	30
46	l9	189/191 (99%)	153 (81%)	27 (14%)	9 (5%)	4	36
47	M0	207/220 (94%)	167 (81%)	30 (14%)	10 (5%)	4	36
47	m0	209/220 (95%)	163 (78%)	27 (13%)	19 (9%)	1	16
48	M1	167/173 (96%)	126 (75%)	31 (19%)	10 (6%)	2	29
48	m1	167/173 (96%)	127 (76%)	25 (15%)	15 (9%)	1	16
49	M3	191/198 (96%)	140 (73%)	37 (19%)	14 (7%)	2	23
49	m3	192/198 (97%)	150 (78%)	24 (12%)	18 (9%)	1	15
50	M4	134/137 (98%)	106 (79%)	19 (14%)	9 (7%)	2	26
50	m4	135/137 (98%)	116 (86%)	16 (12%)	3 (2%)	10	60
51	M5	201/203 (99%)	170 (85%)	24 (12%)	7 (4%)	6	49
51	m5	201/203 (99%)	171 (85%)	25 (12%)	5 (2%)	9	57
52	M6	195/198 (98%)	167 (86%)	22 (11%)	6 (3%)	7	52
52	m6	195/198 (98%)	164 (84%)	23 (12%)	8 (4%)	4	42
53	M7	181/183 (99%)	142 (78%)	27 (15%)	12 (7%)	2	26
53	m7	153/183 (84%)	130 (85%)	20 (13%)	3 (2%)	11	62
54	M8	183/185 (99%)	148 (81%)	28 (15%)	7 (4%)	5	45
54	m8	183/185 (99%)	140 (76%)	30 (16%)	13 (7%)	2	24
55	M9	186/188 (99%)	160 (86%)	17 (9%)	9 (5%)	4	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	m9	186/188 (99%)	156 (84%)	26 (14%)	4 (2%)	10	60
56	N0	170/172 (99%)	149 (88%)	14 (8%)	7 (4%)	4	42
56	n0	170/172 (99%)	146 (86%)	19 (11%)	5 (3%)	7	54
57	N1	157/159 (99%)	136 (87%)	16 (10%)	5 (3%)	6	51
57	n1	157/159 (99%)	125 (80%)	26 (17%)	6 (4%)	5	45
58	N2	98/120 (82%)	74 (76%)	16 (16%)	8 (8%)	1	19
58	n2	96/120 (80%)	76 (79%)	17 (18%)	3 (3%)	7	52
59	N3	134/136 (98%)	114 (85%)	14 (10%)	6 (4%)	4	39
59	n3	134/136 (98%)	116 (87%)	9 (7%)	9 (7%)	2	26
60	N4	96/155 (62%)	68 (71%)	20 (21%)	8 (8%)	1	19
60	n4	133/155 (86%)	99 (74%)	21 (16%)	13 (10%)	1	14
61	N5	119/141 (84%)	98 (82%)	17 (14%)	4 (3%)	6	49
61	n5	118/141 (84%)	97 (82%)	16 (14%)	5 (4%)	4	41
62	N6	124/126 (98%)	99 (80%)	16 (13%)	9 (7%)	2	23
62	n6	124/126 (98%)	100 (81%)	16 (13%)	8 (6%)	2	27
63	N7	133/135 (98%)	104 (78%)	20 (15%)	9 (7%)	2	25
63	n7	133/135 (98%)	91 (68%)	30 (23%)	12 (9%)	1	16
64	N8	146/148 (99%)	114 (78%)	23 (16%)	9 (6%)	2	28
64	n8	146/148 (99%)	119 (82%)	19 (13%)	8 (6%)	3	32
65	N9	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	1	11
65	n9	56/58 (97%)	36 (64%)	11 (20%)	9 (16%)	0	4
66	O0	95/104 (91%)	76 (80%)	17 (18%)	2 (2%)	11	61
66	o0	98/104 (94%)	83 (85%)	11 (11%)	4 (4%)	4	42
67	O1	107/112 (96%)	87 (81%)	13 (12%)	7 (6%)	2	27
67	o1	107/112 (96%)	87 (81%)	12 (11%)	8 (8%)	2	22
68	O2	125/129 (97%)	99 (79%)	18 (14%)	8 (6%)	2	27
68	o2	125/129 (97%)	102 (82%)	14 (11%)	9 (7%)	2	24
69	O3	104/106 (98%)	86 (83%)	13 (12%)	5 (5%)	4	36
69	o3	104/106 (98%)	95 (91%)	7 (7%)	2 (2%)	12	63
70	O4	110/120 (92%)	92 (84%)	16 (14%)	2 (2%)	13	65
70	o4	110/120 (92%)	90 (82%)	15 (14%)	5 (4%)	4	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	O5	117/119 (98%)	99 (85%)	13 (11%)	5 (4%)	4	40
71	o5	117/119 (98%)	89 (76%)	22 (19%)	6 (5%)	3	35
72	O6	97/99 (98%)	70 (72%)	15 (16%)	12 (12%)	1	9
72	o6	97/99 (98%)	83 (86%)	10 (10%)	4 (4%)	4	42
73	O7	85/87 (98%)	66 (78%)	18 (21%)	1 (1%)	19	74
73	o7	85/87 (98%)	69 (81%)	12 (14%)	4 (5%)	4	37
74	O8	75/77 (97%)	61 (81%)	11 (15%)	3 (4%)	5	43
74	o8	75/77 (97%)	63 (84%)	10 (13%)	2 (3%)	8	55
75	O9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	11	61
75	o9	48/50 (96%)	38 (79%)	6 (12%)	4 (8%)	1	19
76	Q0	50/52 (96%)	42 (84%)	3 (6%)	5 (10%)	1	13
76	q0	50/52 (96%)	40 (80%)	8 (16%)	2 (4%)	5	43
77	Q1	23/25 (92%)	16 (70%)	5 (22%)	2 (9%)	1	17
77	q1	23/25 (92%)	19 (83%)	2 (9%)	2 (9%)	1	17
78	Q2	103/105 (98%)	77 (75%)	18 (18%)	8 (8%)	1	20
78	q2	103/105 (98%)	87 (84%)	11 (11%)	5 (5%)	3	36
79	Q3	89/91 (98%)	74 (83%)	8 (9%)	7 (8%)	1	20
79	q3	89/91 (98%)	70 (79%)	13 (15%)	6 (7%)	2	26
80	e0	60/62 (97%)	39 (65%)	15 (25%)	6 (10%)	1	13
81	p0	139/311 (45%)	108 (78%)	24 (17%)	7 (5%)	3	35
All	All	22333/24143 (92%)	17400 (78%)	3410 (15%)	1523 (7%)	2	25

5 of 1523 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	68	PRO
2	S0	139	VAL
2	S0	158	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	125 (76%)	39 (24%)	1	6
2	s0	165/209 (79%)	135 (82%)	30 (18%)	2	14
3	S1	191/223 (86%)	146 (76%)	45 (24%)	1	6
3	s1	192/223 (86%)	147 (77%)	45 (23%)	1	6
4	S2	176/204 (86%)	136 (77%)	40 (23%)	1	7
4	s2	176/204 (86%)	128 (73%)	48 (27%)	0	4
5	S3	182/194 (94%)	140 (77%)	42 (23%)	1	6
5	s3	182/194 (94%)	140 (77%)	42 (23%)	1	6
6	S4	221/221 (100%)	175 (79%)	46 (21%)	2	9
6	s4	221/221 (100%)	173 (78%)	48 (22%)	1	8
7	S5	173/190 (91%)	139 (80%)	34 (20%)	2	10
7	s5	173/190 (91%)	136 (79%)	37 (21%)	1	8
8	S6	188/201 (94%)	151 (80%)	37 (20%)	2	10
8	s6	187/201 (93%)	153 (82%)	34 (18%)	2	14
9	S7	165/169 (98%)	135 (82%)	30 (18%)	2	14
9	s7	165/169 (98%)	130 (79%)	35 (21%)	1	9
10	S8	150/161 (93%)	123 (82%)	27 (18%)	2	14
10	s8	150/161 (93%)	127 (85%)	23 (15%)	4	24
11	S9	158/165 (96%)	119 (75%)	39 (25%)	1	5
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	12
12	C0	77/98 (79%)	61 (79%)	16 (21%)	2	9
12	c0	73/98 (74%)	60 (82%)	13 (18%)	2	15
13	C1	129/136 (95%)	105 (81%)	24 (19%)	2	13
13	c1	129/136 (95%)	108 (84%)	21 (16%)	3	20
14	C2	88/118 (75%)	67 (76%)	21 (24%)	1	6
14	c2	88/118 (75%)	71 (81%)	17 (19%)	2	11
15	C3	127/127 (100%)	96 (76%)	31 (24%)	1	5
15	c3	127/127 (100%)	102 (80%)	25 (20%)	2	10
16	C4	81/104 (78%)	67 (83%)	14 (17%)	3	16
16	c4	97/104 (93%)	76 (78%)	21 (22%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	C5	101/117 (86%)	79 (78%)	22 (22%)	1	8
17	c5	103/117 (88%)	85 (82%)	18 (18%)	3	16
18	C6	117/118 (99%)	97 (83%)	20 (17%)	3	17
18	c6	118/118 (100%)	96 (81%)	22 (19%)	2	13
19	C7	94/124 (76%)	70 (74%)	24 (26%)	1	5
19	c7	92/124 (74%)	72 (78%)	20 (22%)	1	8
20	C8	128/128 (100%)	95 (74%)	33 (26%)	1	4
20	c8	128/128 (100%)	94 (73%)	34 (27%)	1	4
21	C9	115/115 (100%)	86 (75%)	29 (25%)	1	5
21	c9	115/115 (100%)	96 (84%)	19 (16%)	3	19
22	D0	100/113 (88%)	76 (76%)	24 (24%)	1	6
22	d0	103/113 (91%)	72 (70%)	31 (30%)	0	3
23	D1	74/74 (100%)	61 (82%)	13 (18%)	3	15
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	8
24	D2	110/110 (100%)	90 (82%)	20 (18%)	2	14
24	d2	110/110 (100%)	89 (81%)	21 (19%)	2	12
25	D3	119/119 (100%)	95 (80%)	24 (20%)	2	10
25	d3	119/119 (100%)	91 (76%)	28 (24%)	1	6
26	D4	112/112 (100%)	93 (83%)	19 (17%)	3	18
26	d4	112/112 (100%)	93 (83%)	19 (17%)	3	18
27	D5	61/88 (69%)	46 (75%)	15 (25%)	1	5
27	d5	61/88 (69%)	48 (79%)	13 (21%)	1	8
28	D6	83/83 (100%)	61 (74%)	22 (26%)	1	4
28	d6	83/83 (100%)	65 (78%)	18 (22%)	1	8
29	D7	70/70 (100%)	59 (84%)	11 (16%)	4	22
29	d7	70/70 (100%)	55 (79%)	15 (21%)	1	8
30	D8	56/59 (95%)	45 (80%)	11 (20%)	2	11
30	d8	56/59 (95%)	43 (77%)	13 (23%)	1	6
31	D9	47/48 (98%)	40 (85%)	7 (15%)	4	25
31	d9	47/48 (98%)	36 (77%)	11 (23%)	1	6
32	E0	51/51 (100%)	42 (82%)	9 (18%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	E1	62/66 (94%)	48 (77%)	14 (23%)	1	7
33	e1	66/66 (100%)	49 (74%)	17 (26%)	1	4
34	SR	260/261 (100%)	223 (86%)	37 (14%)	5	27
34	sR	260/261 (100%)	222 (85%)	38 (15%)	5	26
35	SM	97/228 (42%)	72 (74%)	25 (26%)	1	4
35	sM	54/228 (24%)	45 (83%)	9 (17%)	3	19
39	L2	193/195 (99%)	143 (74%)	50 (26%)	1	4
39	l2	192/195 (98%)	144 (75%)	48 (25%)	1	5
40	L3	320/322 (99%)	256 (80%)	64 (20%)	2	10
40	l3	320/322 (99%)	248 (78%)	72 (22%)	1	7
41	L4	288/288 (100%)	223 (77%)	65 (23%)	1	7
41	l4	288/288 (100%)	229 (80%)	59 (20%)	2	9
42	L5	244/244 (100%)	191 (78%)	53 (22%)	1	8
42	l5	243/244 (100%)	198 (82%)	45 (18%)	2	13
43	L6	134/152 (88%)	108 (81%)	26 (19%)	2	11
43	l6	135/152 (89%)	102 (76%)	33 (24%)	1	5
44	L7	186/204 (91%)	154 (83%)	32 (17%)	3	17
44	l7	187/204 (92%)	152 (81%)	35 (19%)	2	12
45	L8	187/207 (90%)	150 (80%)	37 (20%)	2	10
45	l8	177/207 (86%)	141 (80%)	36 (20%)	2	10
46	L9	171/171 (100%)	127 (74%)	44 (26%)	1	5
46	l9	171/171 (100%)	128 (75%)	43 (25%)	1	5
47	M0	177/186 (95%)	137 (77%)	40 (23%)	1	7
47	m0	179/186 (96%)	144 (80%)	35 (20%)	2	11
48	M1	147/150 (98%)	112 (76%)	35 (24%)	1	6
48	m1	147/150 (98%)	111 (76%)	36 (24%)	1	5
49	M3	154/158 (98%)	122 (79%)	32 (21%)	2	9
49	m3	154/158 (98%)	120 (78%)	34 (22%)	1	7
50	M4	107/108 (99%)	85 (79%)	22 (21%)	2	9
50	m4	108/108 (100%)	86 (80%)	22 (20%)	2	10
51	M5	175/175 (100%)	132 (75%)	43 (25%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	m5	175/175 (100%)	141 (81%)	34 (19%)	2	11
52	M6	160/161 (99%)	121 (76%)	39 (24%)	1	5
52	m6	160/161 (99%)	120 (75%)	40 (25%)	1	5
53	M7	140/145 (97%)	111 (79%)	29 (21%)	2	9
53	m7	125/145 (86%)	101 (81%)	24 (19%)	2	11
54	M8	150/150 (100%)	116 (77%)	34 (23%)	1	7
54	m8	150/150 (100%)	116 (77%)	34 (23%)	1	7
55	M9	153/153 (100%)	124 (81%)	29 (19%)	2	12
55	m9	153/153 (100%)	125 (82%)	28 (18%)	2	13
56	N0	156/156 (100%)	122 (78%)	34 (22%)	1	8
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1	8
57	N1	136/136 (100%)	102 (75%)	34 (25%)	1	5
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	8
58	N2	87/106 (82%)	73 (84%)	14 (16%)	3	21
58	n2	85/106 (80%)	58 (68%)	27 (32%)	0	3
59	N3	104/104 (100%)	84 (81%)	20 (19%)	2	11
59	n3	104/104 (100%)	85 (82%)	19 (18%)	2	13
60	N4	57/129 (44%)	47 (82%)	10 (18%)	3	16
60	n4	100/129 (78%)	79 (79%)	21 (21%)	1	9
61	N5	104/117 (89%)	78 (75%)	26 (25%)	1	5
61	n5	104/117 (89%)	85 (82%)	19 (18%)	2	13
62	N6	109/109 (100%)	88 (81%)	21 (19%)	2	11
62	n6	109/109 (100%)	85 (78%)	24 (22%)	1	7
63	N7	115/115 (100%)	94 (82%)	21 (18%)	2	13
63	n7	115/115 (100%)	87 (76%)	28 (24%)	1	5
64	N8	118/118 (100%)	98 (83%)	20 (17%)	3	18
64	n8	118/118 (100%)	91 (77%)	27 (23%)	1	7
65	N9	46/46 (100%)	35 (76%)	11 (24%)	1	6
65	n9	46/46 (100%)	30 (65%)	16 (35%)	0	2
66	O0	81/87 (93%)	66 (82%)	15 (18%)	2	13
66	o0	84/87 (97%)	69 (82%)	15 (18%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	O1	92/96 (96%)	69 (75%)	23 (25%)	1	5
67	o1	94/96 (98%)	63 (67%)	31 (33%)	0	2
68	O2	109/110 (99%)	87 (80%)	22 (20%)	2	10
68	o2	109/110 (99%)	81 (74%)	28 (26%)	1	5
69	O3	90/90 (100%)	71 (79%)	19 (21%)	1	9
69	o3	90/90 (100%)	75 (83%)	15 (17%)	3	19
70	O4	95/102 (93%)	75 (79%)	20 (21%)	1	9
70	o4	95/102 (93%)	82 (86%)	13 (14%)	5	29
71	O5	104/104 (100%)	83 (80%)	21 (20%)	2	10
71	o5	103/104 (99%)	76 (74%)	27 (26%)	1	4
72	O6	81/81 (100%)	56 (69%)	25 (31%)	0	3
72	o6	80/81 (99%)	53 (66%)	27 (34%)	0	2
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1	8
73	o7	70/70 (100%)	52 (74%)	18 (26%)	1	5
74	O8	68/68 (100%)	50 (74%)	18 (26%)	1	4
74	o8	67/68 (98%)	49 (73%)	18 (27%)	1	4
75	O9	45/45 (100%)	40 (89%)	5 (11%)	9	41
75	o9	45/45 (100%)	33 (73%)	12 (27%)	1	4
76	Q0	47/47 (100%)	41 (87%)	6 (13%)	6	32
76	q0	47/47 (100%)	32 (68%)	15 (32%)	0	3
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	3
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	1
78	Q2	90/90 (100%)	67 (74%)	23 (26%)	1	5
78	q2	90/90 (100%)	70 (78%)	20 (22%)	1	7
79	Q3	71/71 (100%)	55 (78%)	16 (22%)	1	7
79	q3	71/71 (100%)	54 (76%)	17 (24%)	1	6
80	e0	53/53 (100%)	38 (72%)	15 (28%)	0	4
81	p0	105/253 (42%)	84 (80%)	21 (20%)	2	10
All	All	18728/20241 (92%)	14710 (78%)	4018 (22%)	1	8

5 of 4018 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	O3	48	ARG
8	s6	133	LEU
64	n8	132	LYS
72	O6	20	MET
3	s1	154	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
58	N2	52	ASN
72	O6	91	ASN
62	n6	66	GLN
64	N8	74	ASN
2	s0	46	HIS

5.3.3 RNA ⓘ

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

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2557 ligands modelled in this entry, 1423 are monoatomic - leaving 1134 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	3857	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3858	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3859	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3860	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3861	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3862	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3863	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3887	-	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	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3930	-	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	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3973	-	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	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4016	-	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	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4059	-	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	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4102	-	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	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4145	-	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	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4188	-	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	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
88	BLS	1	4211	-	31,31,31	2.10	7 (22%)	40,43,43	2.43	13 (32%)
86	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2085	-	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	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2128	-	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	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2171	-	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	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	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	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
88	BLS	5	4248	-	31,31,31	1.44	3 (9%)	40,43,43	1.64	4 (10%)
86	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	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	-
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	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	215	-	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	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	D3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	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	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d4	201	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m6	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	103	-	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	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	-

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	3857	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3858	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3859	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3860	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3861	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3862	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3863	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3864	-	-	0/0/0/0	0/0/0/0

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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
88	BLS	1	4211	-	-	0/22/38/38	0/2/2/2
86	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2053	-	-	0/0/0/0	0/0/0/0

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2180	-	-	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	224	-	-	0/0/0/0	0/0/0/0
86	OHX	4	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	227	-	-	0/0/0/0	0/0/0/0
86	OHX	4	228	-	-	0/0/0/0	0/0/0/0
86	OHX	4	229	-	-	0/0/0/0	0/0/0/0
86	OHX	4	230	-	-	0/0/0/0	0/0/0/0
86	OHX	4	231	-	-	0/0/0/0	0/0/0/0
86	OHX	4	232	-	-	0/0/0/0	0/0/0/0
86	OHX	4	233	-	-	0/0/0/0	0/0/0/0
86	OHX	4	234	-	-	0/0/0/0	0/0/0/0
86	OHX	4	235	-	-	0/0/0/0	0/0/0/0
86	OHX	4	236	-	-	0/0/0/0	0/0/0/0
86	OHX	4	237	-	-	0/0/0/0	0/0/0/0
86	OHX	4	238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3892	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3893	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3894	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3895	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3896	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3897	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3907	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3949	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3991	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4033	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4075	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4117	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4159	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
88	BLS	5	4248	-	-	0/22/38/38	0/2/2/2
86	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2166	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	7	218	-	-	0/0/0/0	0/0/0/0
86	OHX	7	219	-	-	0/0/0/0	0/0/0/0
86	OHX	7	220	-	-	0/0/0/0	0/0/0/0
86	OHX	7	221	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	7	222	-	-	0/0/0/0	0/0/0/0
86	OHX	7	223	-	-	0/0/0/0	0/0/0/0
86	OHX	7	224	-	-	0/0/0/0	0/0/0/0
86	OHX	7	225	-	-	0/0/0/0	0/0/0/0
86	OHX	7	226	-	-	0/0/0/0	0/0/0/0
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	7	228	-	-	0/0/0/0	0/0/0/0
86	OHX	7	229	-	-	0/0/0/0	0/0/0/0
86	OHX	8	215	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	-	-	0/0/0/0	0/0/0/0
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0
86	OHX	8	219	-	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	-	-	0/0/0/0	0/0/0/0
86	OHX	8	222	-	-	0/0/0/0	0/0/0/0
86	OHX	8	223	-	-	0/0/0/0	0/0/0/0
86	OHX	8	224	-	-	0/0/0/0	0/0/0/0
86	OHX	8	225	-	-	0/0/0/0	0/0/0/0
86	OHX	8	226	-	-	0/0/0/0	0/0/0/0
86	OHX	8	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	229	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	D3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	406	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	404	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	304	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O1	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	201	-	-	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	Q2	503	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	202	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	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	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	306	-	-	0/0/0/0	0/0/0/0
86	OHX	m6	203	-	-	0/0/0/0	0/0/0/0
86	OHX	m7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	n1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	103	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	103	-	-	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	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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4211	BLS	C2-N1	6.52	1.45	1.38
88	5	4248	BLS	C11-N12	-5.01	1.36	1.47
88	1	4211	BLS	O2-C2	4.19	1.27	1.21
88	1	4211	BLS	C5-C4	3.85	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4211	BLS	C6-N1	3.76	1.41	1.35

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4211	BLS	C2-N3-C4	7.52	126.48	115.65
88	5	4248	BLS	O5'-C1'-C2'	-5.69	109.92	113.13
88	1	4211	BLS	C2-N1-C1'	5.54	121.68	118.21
88	1	4211	BLS	O5'-C5'-C4'	4.34	118.00	109.84
88	5	4248	BLS	C2-N1-C1'	-4.33	115.49	118.21

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%)	0.29	122 (6%) 16 7	61, 94, 179, 258	0
1	6	1795/1800 (99%)	0.28	113 (6%) 19 8	51, 84, 200, 293	0
2	S0	206/251 (82%)	2.39	119 (57%) 0 1	102, 118, 131, 153	0
2	s0	206/251 (82%)	2.63	127 (61%) 0 1	85, 103, 119, 128	0
3	S1	214/254 (84%)	2.81	124 (57%) 0 1	103, 132, 156, 161	0
3	s1	216/254 (85%)	2.22	117 (54%) 0 1	77, 92, 120, 138	0
4	S2	217/253 (85%)	1.67	72 (33%) 1 1	78, 96, 115, 139	0
4	s2	217/253 (85%)	1.55	75 (34%) 1 1	63, 80, 107, 123	0
5	S3	223/239 (93%)	1.54	65 (29%) 1 1	79, 97, 128, 158	0
5	s3	223/239 (93%)	2.31	117 (52%) 0 1	83, 107, 137, 153	0
6	S4	260/260 (100%)	3.03	182 (70%) 0 1	69, 91, 105, 128	0
6	s4	260/260 (100%)	2.32	143 (55%) 0 1	59, 86, 103, 125	0
7	S5	206/224 (91%)	3.55	157 (76%) 0 0	96, 118, 140, 155	0
7	s5	206/224 (91%)	1.58	74 (35%) 1 1	75, 99, 130, 154	0
8	S6	226/236 (95%)	1.84	95 (42%) 1 1	69, 99, 127, 139	0
8	s6	218/236 (92%)	2.09	107 (49%) 1 1	58, 83, 114, 141	0
9	S7	184/189 (97%)	1.47	60 (32%) 1 1	92, 123, 146, 151	0
9	s7	186/189 (98%)	2.08	89 (47%) 1 1	80, 113, 142, 151	0
10	S8	188/200 (94%)	1.62	64 (34%) 1 1	60, 77, 123, 136	0
10	s8	188/200 (94%)	0.89	20 (10%) 7 4	54, 81, 135, 154	0
11	S9	185/196 (94%)	2.48	112 (60%) 0 1	89, 102, 138, 173	0
11	s9	185/196 (94%)	1.34	47 (25%) 1 2	69, 88, 131, 167	0
12	C0	96/105 (91%)	1.68	36 (37%) 1 1	83, 104, 134, 152	0
12	c0	96/105 (91%)	3.07	54 (56%) 0 1	95, 129, 149, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	2.28	64 (41%)	1	1	65, 80, 140, 148	0
13	c1	146/155 (94%)	1.61	46 (31%)	1	1	62, 79, 118, 142	0
14	C2	124/142 (87%)	1.28	33 (26%)	1	2	124, 142, 161, 171	0
14	c2	124/142 (87%)	3.62	81 (65%)	0	1	169, 188, 204, 211	0
15	C3	150/150 (100%)	1.91	63 (42%)	1	1	72, 94, 112, 115	0
15	c3	150/150 (100%)	1.32	40 (26%)	1	2	68, 85, 104, 122	0
16	C4	127/136 (93%)	2.04	59 (46%)	1	1	74, 135, 153, 161	0
16	c4	128/136 (94%)	2.44	73 (57%)	0	1	72, 92, 102, 107	0
17	C5	124/141 (87%)	0.97	32 (25%)	1	2	74, 92, 132, 145	0
17	c5	135/141 (95%)	0.91	22 (16%)	2	2	81, 102, 135, 190	0
18	C6	141/142 (99%)	3.24	90 (63%)	0	1	84, 113, 122, 128	0
18	c6	142/142 (100%)	3.07	91 (64%)	0	1	72, 93, 112, 135	0
19	C7	120/136 (88%)	1.53	37 (30%)	1	1	96, 117, 143, 147	0
19	c7	117/136 (86%)	1.77	49 (41%)	1	1	85, 102, 128, 141	0
20	C8	145/145 (100%)	1.24	36 (24%)	1	2	73, 102, 133, 142	0
20	c8	145/145 (100%)	1.30	38 (26%)	1	2	77, 89, 114, 130	0
21	C9	143/143 (100%)	2.57	81 (56%)	0	1	88, 104, 127, 141	0
21	c9	143/143 (100%)	1.62	53 (37%)	1	1	72, 85, 110, 134	0
22	D0	107/120 (89%)	2.54	67 (62%)	0	1	83, 115, 147, 151	0
22	d0	110/120 (91%)	2.60	59 (53%)	0	1	74, 109, 160, 202	0
23	D1	87/87 (100%)	1.81	32 (36%)	1	1	99, 107, 126, 139	0
23	d1	87/87 (100%)	1.62	28 (32%)	1	1	77, 88, 113, 129	0
24	D2	129/129 (100%)	2.67	83 (64%)	0	1	77, 89, 97, 104	0
24	d2	129/129 (100%)	1.32	30 (23%)	1	2	64, 75, 86, 99	0
25	D3	144/144 (100%)	1.57	48 (33%)	1	1	58, 70, 81, 106	0
25	d3	144/144 (100%)	1.65	56 (38%)	1	1	48, 58, 71, 90	0
26	D4	134/134 (100%)	1.74	46 (34%)	1	1	75, 103, 123, 132	0
26	d4	134/134 (100%)	1.11	36 (26%)	1	2	62, 85, 103, 139	0
27	D5	70/107 (65%)	2.81	42 (60%)	0	1	112, 130, 146, 148	0
27	d5	69/107 (64%)	2.69	38 (55%)	0	1	84, 114, 130, 133	0
28	D6	97/97 (100%)	2.28	48 (49%)	1	1	80, 100, 161, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
28	d6	97/97 (100%)	1.39	35 (36%)	1	1	65, 79, 105, 114	0
29	D7	81/81 (100%)	1.84	38 (46%)	1	1	90, 107, 150, 157	0
29	d7	81/81 (100%)	1.89	35 (43%)	1	1	81, 96, 135, 149	0
30	D8	63/66 (95%)	4.68	53 (84%)	0	0	110, 129, 144, 147	0
30	d8	63/66 (95%)	2.66	36 (57%)	0	1	92, 116, 134, 147	0
31	D9	53/55 (96%)	0.70	4 (7%)	14	7	80, 85, 105, 113	0
31	d9	53/55 (96%)	1.66	21 (39%)	1	1	74, 83, 126, 148	0
32	E0	60/60 (100%)	3.47	40 (66%)	0	1	76, 100, 140, 147	0
33	E1	71/76 (93%)	1.17	17 (23%)	1	2	99, 123, 139, 143	0
33	e1	76/76 (100%)	2.00	31 (40%)	1	1	127, 158, 172, 178	0
34	SR	318/318 (100%)	1.74	112 (35%)	1	1	69, 123, 149, 180	0
34	sR	318/318 (100%)	3.27	193 (60%)	0	1	103, 125, 145, 168	0
35	SM	159/273 (58%)	1.36	38 (23%)	1	2	64, 96, 143, 152	0
35	sM	104/273 (38%)	1.10	25 (24%)	1	2	67, 103, 179, 188	0
36	1	3149/3396 (92%)	0.43	189 (6%)	21	9	31, 56, 144, 283	0
36	5	3150/3396 (92%)	0.42	202 (6%)	19	8	32, 58, 136, 278	0
37	3	121/121 (100%)	0.43	3 (2%)	54	24	43, 68, 84, 89	0
37	7	121/121 (100%)	0.09	2 (1%)	67	32	40, 58, 74, 85	0
38	4	158/158 (100%)	0.70	17 (10%)	6	4	40, 60, 104, 160	0
38	8	158/158 (100%)	0.67	17 (10%)	6	4	45, 71, 119, 144	0
39	L2	252/253 (99%)	1.83	110 (43%)	1	1	42, 55, 74, 83	0
39	l2	252/253 (99%)	2.34	150 (59%)	0	1	45, 63, 86, 101	0
40	L3	386/386 (100%)	1.34	112 (29%)	1	1	36, 55, 73, 110	0
40	l3	386/386 (100%)	0.89	40 (10%)	7	5	33, 45, 61, 97	0
41	L4	361/361 (100%)	0.73	40 (11%)	6	4	35, 48, 64, 77	0
41	l4	361/361 (100%)	0.59	34 (9%)	9	5	41, 53, 76, 91	0
42	L5	296/296 (100%)	1.93	135 (45%)	1	1	52, 74, 96, 122	0
42	l5	294/296 (99%)	0.94	53 (18%)	2	2	44, 62, 93, 138	0
43	L6	156/175 (89%)	0.97	33 (21%)	1	2	41, 49, 76, 95	0
43	l6	157/175 (89%)	0.72	14 (8%)	10	6	41, 50, 74, 89	0
44	L7	222/243 (91%)	1.25	59 (26%)	1	2	34, 43, 82, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
44	l7	223/243 (91%)	1.46	75 (33%)	1	1	33, 41, 84, 138	0
45	L8	233/255 (91%)	0.77	34 (14%)	3	3	65, 81, 122, 138	0
45	l8	231/255 (90%)	1.63	83 (35%)	1	1	79, 95, 132, 141	0
46	L9	191/191 (100%)	1.17	48 (25%)	1	2	49, 59, 71, 92	0
46	l9	191/191 (100%)	0.96	24 (12%)	4	3	40, 49, 74, 111	0
47	M0	211/220 (95%)	1.18	47 (22%)	1	2	39, 50, 85, 123	0
47	m0	213/220 (96%)	0.87	28 (13%)	4	3	40, 60, 90, 105	0
48	M1	169/173 (97%)	0.34	6 (3%)	41	17	57, 77, 93, 106	0
48	m1	169/173 (97%)	0.36	4 (2%)	56	25	47, 65, 81, 95	0
49	M3	193/198 (97%)	0.95	40 (20%)	1	2	43, 59, 106, 135	0
49	m3	194/198 (97%)	1.45	62 (31%)	1	1	49, 70, 116, 144	0
50	M4	136/137 (99%)	0.66	13 (9%)	8	5	43, 50, 66, 81	0
50	m4	137/137 (100%)	0.29	4 (2%)	49	22	36, 45, 69, 82	0
51	M5	203/203 (100%)	1.79	78 (38%)	1	1	37, 54, 66, 73	0
51	m5	203/203 (100%)	2.16	101 (49%)	1	1	52, 66, 80, 88	0
52	M6	197/198 (99%)	0.50	8 (4%)	35	15	34, 41, 64, 68	0
52	m6	197/198 (99%)	0.47	3 (1%)	70	35	29, 35, 63, 71	0
53	M7	183/183 (100%)	0.93	25 (13%)	4	3	41, 49, 119, 148	0
53	m7	155/183 (84%)	0.93	23 (14%)	3	3	36, 46, 60, 95	0
54	M8	185/185 (100%)	0.69	11 (5%)	22	9	40, 49, 70, 86	0
54	m8	185/185 (100%)	0.66	16 (8%)	11	6	46, 54, 64, 69	0
55	M9	188/188 (100%)	1.26	44 (23%)	1	2	53, 73, 156, 164	0
55	m9	188/188 (100%)	1.05	39 (20%)	1	2	56, 71, 148, 159	0
56	N0	172/172 (100%)	1.48	43 (25%)	1	2	40, 49, 62, 68	0
56	n0	172/172 (100%)	0.98	20 (11%)	5	4	34, 42, 56, 71	0
57	N1	159/159 (100%)	2.20	81 (50%)	0	1	41, 52, 101, 110	0
57	n1	159/159 (100%)	1.34	50 (31%)	1	1	39, 48, 91, 102	0
58	N2	100/120 (83%)	0.79	16 (16%)	3	2	85, 104, 119, 154	0
58	n2	98/120 (81%)	1.14	19 (19%)	2	2	80, 94, 107, 115	0
59	N3	136/136 (100%)	2.03	63 (46%)	1	1	39, 52, 67, 81	0
59	n3	136/136 (100%)	1.53	37 (27%)	1	2	33, 45, 64, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	4.38	83 (84%)	0	0	50, 68, 177, 185	0
60	n4	135/155 (87%)	1.62	52 (38%)	1	1	44, 90, 137, 154	0
61	N5	121/141 (85%)	1.94	57 (47%)	1	1	50, 65, 87, 134	0
61	n5	120/141 (85%)	2.76	77 (64%)	0	1	57, 74, 101, 109	0
62	N6	126/126 (100%)	1.01	22 (17%)	2	2	47, 59, 72, 85	0
62	n6	126/126 (100%)	2.01	55 (43%)	1	1	50, 66, 87, 97	0
63	N7	135/135 (100%)	1.26	41 (30%)	1	1	74, 93, 114, 129	0
63	n7	135/135 (100%)	1.98	59 (43%)	1	1	91, 105, 124, 135	0
64	N8	148/148 (100%)	0.80	21 (14%)	3	3	40, 49, 77, 92	0
64	n8	148/148 (100%)	1.27	34 (22%)	1	2	42, 58, 81, 86	0
65	N9	58/58 (100%)	1.12	9 (15%)	3	2	51, 60, 102, 108	0
65	n9	58/58 (100%)	0.99	9 (15%)	3	2	47, 60, 90, 104	0
66	O0	97/104 (93%)	2.51	57 (58%)	0	1	74, 84, 116, 122	0
66	o0	100/104 (96%)	2.99	69 (69%)	0	1	79, 90, 123, 130	0
67	O1	109/112 (97%)	1.30	26 (23%)	1	2	50, 64, 105, 135	0
67	o1	109/112 (97%)	1.30	23 (21%)	1	2	45, 57, 103, 130	0
68	O2	127/129 (98%)	0.77	12 (9%)	9	5	33, 45, 62, 81	0
68	o2	127/129 (98%)	1.27	30 (23%)	1	2	35, 50, 65, 87	0
69	O3	106/106 (100%)	1.18	17 (16%)	3	2	35, 42, 64, 73	0
69	o3	106/106 (100%)	1.56	34 (32%)	1	1	31, 40, 68, 88	0
70	O4	112/120 (93%)	2.49	68 (60%)	0	1	53, 71, 108, 125	0
70	o4	112/120 (93%)	2.26	59 (52%)	0	1	59, 81, 123, 135	0
71	O5	119/119 (100%)	2.97	93 (78%)	0	0	47, 68, 77, 81	0
71	o5	119/119 (100%)	1.43	33 (27%)	1	1	60, 76, 92, 102	0
72	O6	99/99 (100%)	1.23	21 (21%)	1	2	58, 70, 99, 119	0
72	o6	99/99 (100%)	0.83	14 (14%)	3	3	66, 83, 112, 135	0
73	O7	87/87 (100%)	2.12	43 (49%)	1	1	41, 50, 82, 107	0
73	o7	87/87 (100%)	1.63	27 (31%)	1	1	52, 58, 92, 128	0
74	O8	77/77 (100%)	1.60	30 (38%)	1	1	76, 91, 115, 128	0
74	o8	77/77 (100%)	0.20	1 (1%)	74	39	86, 99, 111, 115	0
75	O9	50/50 (100%)	1.09	7 (14%)	3	3	49, 56, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	2.21	22 (44%) 1 1	57, 62, 74, 91	0
76	Q0	52/52 (100%)	0.65	3 (5%) 22 9	46, 53, 82, 94	0
76	q0	52/52 (100%)	0.20	2 (3%) 38 16	34, 42, 58, 69	0
77	Q1	25/25 (100%)	2.20	13 (52%) 0 1	59, 63, 68, 70	0
77	q1	25/25 (100%)	1.55	9 (36%) 1 1	53, 59, 73, 87	0
78	Q2	105/105 (100%)	1.01	20 (19%) 2 2	44, 62, 90, 129	0
78	q2	105/105 (100%)	0.88	15 (14%) 3 3	54, 64, 86, 114	0
79	Q3	91/91 (100%)	2.20	53 (58%) 0 1	49, 59, 82, 100	0
79	q3	91/91 (100%)	2.24	50 (54%) 0 1	48, 63, 79, 89	0
80	e0	62/62 (100%)	1.25	16 (25%) 1 2	63, 86, 124, 155	0
81	p0	143/311 (45%)	0.87	29 (20%) 1 2	89, 108, 197, 217	0
82	m2	0/160	-	-	-	-
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35346 (93%)	1.23	8340 (25%) 1 2	29, 75, 140, 293	0

The worst 5 of 8340 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	sR	24	ALA	14.9
14	c2	56	GLU	14.9
34	sR	25	THR	14.8
60	N4	76	VAL	13.9
36	1	3154	C	13.8

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	4	217	1/1	0.86	1397.00	56,56,56,56	0
85	MG	2	1958	1/1	0.54	817.00	90,90,90,90	0
85	MG	7	217	1/1	0.47	517.00	74,74,74,74	0
85	MG	5	3882	1/1	0.38	419.00	33,33,33,33	0
85	MG	2	1970	1/1	0.35	383.00	69,69,69,69	0
85	MG	2	2001	1/1	0.39	246.17	91,91,91,91	0
85	MG	1	3785	1/1	0.32	241.00	66,66,66,66	0
85	MG	5	3763	1/1	1.23	169.80	104,104,104,104	0
85	MG	6	1939	1/1	0.42	161.00	90,90,90,90	0
85	MG	5	3473	1/1	0.31	145.00	60,60,60,60	0
85	MG	2	2017	1/1	0.44	125.00	83,83,83,83	0
85	MG	5	3875	1/1	0.53	121.33	97,97,97,97	0
85	MG	1	3700	1/1	0.32	101.67	41,41,41,41	0
85	MG	1	3850	1/1	0.50	93.86	53,53,53,53	0
85	MG	1	3844	1/1	0.75	91.33	95,95,95,95	0
85	MG	1	3499	1/1	0.54	88.56	73,73,73,73	0
85	MG	6	2040	1/1	0.45	85.29	59,59,59,59	0
85	MG	1	3646	1/1	0.98	76.69	50,50,50,50	0
85	MG	6	1976	1/1	0.21	75.00	67,67,67,67	0
85	MG	5	3430	1/1	0.38	73.00	73,73,73,73	0
85	MG	8	209	1/1	0.32	70.73	87,87,87,87	0
85	MG	2	1950	1/1	0.68	70.07	88,88,88,88	0
85	MG	1	3811	1/1	0.59	69.69	44,44,44,44	0
85	MG	1	3817	1/1	0.43	67.62	70,70,70,70	0
85	MG	5	3646	1/1	0.52	65.00	71,71,71,71	0
85	MG	5	3652	1/1	0.49	62.64	37,37,37,37	0
85	MG	5	3442	1/1	0.38	62.60	40,40,40,40	0
85	MG	5	3715	1/1	1.62	59.33	48,48,48,48	0
85	MG	6	1917	1/1	0.32	53.33	67,67,67,67	0
85	MG	1	3463	1/1	0.48	51.67	53,53,53,53	0
85	MG	1	3799	1/1	1.29	51.00	44,44,44,44	0
85	MG	1	3531	1/1	0.80	50.90	37,37,37,37	0
85	MG	1	3693	1/1	0.40	50.44	55,55,55,55	0
85	MG	5	3698	1/1	0.43	47.18	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	6	1942	1/1	0.41	47.12	42,42,42,42	0
85	MG	5	3678	1/1	0.26	45.65	41,41,41,41	0
85	MG	6	2028	1/1	0.59	44.75	80,80,80,80	0
85	MG	5	3444	1/1	0.73	43.92	36,36,36,36	0
85	MG	1	3818	1/1	0.91	42.60	51,51,51,51	0
85	MG	6	1980	1/1	0.44	42.17	57,57,57,57	0
85	MG	1	3680	1/1	0.47	39.41	50,50,50,50	0
85	MG	1	3766	1/1	0.33	38.35	60,60,60,60	0
85	MG	5	3732	1/1	0.50	35.75	80,80,80,80	0
85	MG	5	3840	1/1	0.61	35.58	58,58,58,58	0
85	MG	5	3629	1/1	0.58	35.18	90,90,90,90	0
85	MG	2	1923	1/1	0.50	35.09	61,61,61,61	0
85	MG	5	3851	1/1	0.83	34.05	50,50,50,50	0
85	MG	1	3757	1/1	0.88	32.66	52,52,52,52	0
85	MG	6	2014	1/1	0.50	32.22	149,149,149,149	0
85	MG	2	1988	1/1	0.39	31.93	64,64,64,64	0
85	MG	1	3789	1/1	0.46	31.88	60,60,60,60	0
85	MG	1	3449	1/1	0.43	31.80	50,50,50,50	0
85	MG	7	216	1/1	0.34	31.17	74,74,74,74	0
85	MG	5	3728	1/1	0.36	30.69	73,73,73,73	0
85	MG	5	3878	1/1	0.56	30.33	65,65,65,65	0
85	MG	1	3644	1/1	0.37	30.28	36,36,36,36	0
85	MG	7	211	1/1	0.31	30.00	43,43,43,43	0
85	MG	5	3758	1/1	0.95	29.70	50,50,50,50	0
85	MG	5	3726	1/1	0.40	29.00	60,60,60,60	0
85	MG	1	3793	1/1	0.27	29.00	89,89,89,89	0
85	MG	2	2013	1/1	0.36	27.71	57,57,57,57	0
85	MG	5	3772	1/1	0.61	27.60	82,82,82,82	0
85	MG	1	3587	1/1	0.57	27.53	46,46,46,46	0
85	MG	5	3796	1/1	0.44	26.89	77,77,77,77	0
85	MG	2	2002	1/1	0.28	26.53	102,102,102,102	0
85	MG	1	3576	1/1	0.62	26.53	28,28,28,28	0
85	MG	1	3723	1/1	0.53	26.46	40,40,40,40	0
85	MG	1	3675	1/1	0.39	26.44	42,42,42,42	0
85	MG	1	3608	1/1	0.54	26.39	45,45,45,45	0
85	MG	2	1975	1/1	0.57	26.36	77,77,77,77	0
85	MG	5	3544	1/1	0.65	26.26	51,51,51,51	0
85	MG	5	3775	1/1	1.18	26.14	66,66,66,66	0
85	MG	6	1943	1/1	0.51	25.99	75,75,75,75	0
85	MG	1	3756	1/1	0.42	25.77	61,61,61,61	0
85	MG	6	2008	1/1	0.44	25.50	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	6	2018	1/1	0.44	25.49	46,46,46,46	0
85	MG	5	3467	1/1	0.37	25.23	40,40,40,40	0
85	MG	1	3815	1/1	0.45	25.16	72,72,72,72	0
85	MG	5	3627	1/1	0.65	24.91	84,84,84,84	0
85	MG	1	3647	1/1	1.31	24.90	56,56,56,56	0
85	MG	5	3847	1/1	0.46	24.87	83,83,83,83	0
85	MG	1	3617	1/1	0.49	24.56	50,50,50,50	0
85	MG	1	3769	1/1	0.39	24.23	66,66,66,66	0
85	MG	5	3530	1/1	0.47	24.22	35,35,35,35	0
85	MG	5	3890	1/1	0.31	23.89	119,119,119,119	0
85	MG	5	3582	1/1	0.57	23.87	28,28,28,28	0
85	MG	1	3669	1/1	0.41	23.66	37,37,37,37	0
85	MG	1	3690	1/1	0.38	23.61	45,45,45,45	0
85	MG	5	3850	1/1	0.42	23.08	83,83,83,83	0
85	MG	5	3713	1/1	0.35	22.99	62,62,62,62	0
85	MG	2	1904	1/1	0.56	22.88	55,55,55,55	0
85	MG	1	3725	1/1	1.41	22.83	39,39,39,39	0
85	MG	1	3855	1/1	0.62	22.67	72,72,72,72	0
85	MG	2	1914	1/1	0.42	22.17	59,59,59,59	0
85	MG	5	3738	1/1	0.35	22.11	61,61,61,61	0
85	MG	5	3435	1/1	0.79	21.70	37,37,37,37	0
85	MG	5	3643	1/1	0.96	21.63	51,51,51,51	0
85	MG	5	3810	1/1	1.08	21.58	43,43,43,43	0
85	MG	1	3483	1/1	0.49	21.43	50,50,50,50	0
85	MG	5	3703	1/1	0.57	21.30	103,103,103,103	0
85	MG	6	1949	1/1	0.30	21.20	58,58,58,58	0
85	MG	5	3806	1/1	0.50	21.19	81,81,81,81	0
85	MG	1	3852	1/1	0.38	21.09	78,78,78,78	0
85	MG	D0	201	1/1	0.37	21.09	72,72,72,72	0
85	MG	4	213	1/1	0.40	21.00	57,57,57,57	0
85	MG	5	3848	1/1	0.43	20.81	63,63,63,63	0
85	MG	8	208	1/1	0.66	20.74	76,76,76,76	0
85	MG	1	3829	1/1	0.37	20.60	57,57,57,57	0
85	MG	6	1919	1/1	0.56	20.42	68,68,68,68	0
85	MG	5	3670	1/1	0.30	20.35	48,48,48,48	0
85	MG	1	3849	1/1	0.67	20.12	89,89,89,89	0
85	MG	2	1959	1/1	0.42	19.95	96,96,96,96	0
85	MG	5	3477	1/1	0.27	19.89	62,62,62,62	0
85	MG	m4	201	1/1	1.24	19.86	49,49,49,49	0
85	MG	5	3745	1/1	0.47	19.53	53,53,53,53	0
85	MG	5	3845	1/1	0.57	19.46	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3801	1/1	1.05	19.44	39,39,39,39	0
85	MG	2	1966	1/1	0.38	19.37	85,85,85,85	0
85	MG	5	3839	1/1	1.14	19.36	46,46,46,46	0
85	MG	4	201	1/1	0.40	19.29	61,61,61,61	0
85	MG	N8	204	1/1	0.27	18.89	35,35,35,35	0
85	MG	5	3868	1/1	0.54	18.89	31,31,31,31	0
85	MG	5	3842	1/1	0.59	18.66	74,74,74,74	0
85	MG	L4	401	1/1	0.36	18.65	98,98,98,98	0
85	MG	5	3638	1/1	0.21	18.33	59,59,59,59	0
85	MG	3	212	1/1	0.47	18.31	65,65,65,65	0
85	MG	5	3702	1/1	0.49	18.27	52,52,52,52	0
85	MG	5	3534	1/1	0.57	17.97	34,34,34,34	0
85	MG	2	2003	1/1	0.34	17.82	119,119,119,119	0
85	MG	5	3438	1/1	0.57	17.71	47,47,47,47	0
85	MG	5	3754	1/1	0.80	17.69	54,54,54,54	0
85	MG	1	3630	1/1	0.50	17.67	79,79,79,79	0
85	MG	1	3790	1/1	1.30	17.46	38,38,38,38	0
85	MG	6	1936	1/1	0.40	17.20	43,43,43,43	0
85	MG	5	3462	1/1	1.08	16.96	53,53,53,53	0
85	MG	2	1938	1/1	0.46	16.86	67,67,67,67	0
85	MG	1	3609	1/1	0.38	16.56	42,42,42,42	0
85	MG	5	3404	1/1	0.34	16.39	33,33,33,33	0
85	MG	6	1973	1/1	0.26	16.29	70,70,70,70	0
85	MG	1	3727	1/1	0.54	16.24	69,69,69,69	0
86	OHX	1	4183	7/7	0.55	16.18	201,201,201,201	0
85	MG	5	3858	1/1	0.51	15.87	78,78,78,78	0
85	MG	1	3648	1/1	0.49	15.81	95,95,95,95	0
85	MG	1	3848	1/1	0.28	15.68	51,51,51,51	0
85	MG	5	3679	1/1	1.23	15.65	44,44,44,44	0
85	MG	5	3683	1/1	0.84	15.56	58,58,58,58	0
85	MG	6	2027	1/1	0.31	15.54	66,66,66,66	0
85	MG	5	3757	1/1	1.26	15.30	49,49,49,49	0
85	MG	1	3563	1/1	0.46	15.27	24,24,24,24	0
85	MG	2	1968	1/1	0.64	15.08	137,137,137,137	0
85	MG	5	3865	1/1	0.53	14.92	44,44,44,44	0
85	MG	5	3649	1/1	0.51	14.91	69,69,69,69	0
85	MG	2	2014	1/1	0.44	14.89	54,54,54,54	0
85	MG	1	3795	1/1	0.56	14.68	67,67,67,67	0
85	MG	5	3874	1/1	0.43	14.62	56,56,56,56	0
85	MG	1	3780	1/1	1.03	14.39	49,49,49,49	0
85	MG	2	1973	1/1	0.59	14.32	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2045	1/1	0.61	14.21	98,98,98,98	0
85	MG	5	3565	1/1	0.45	14.21	32,32,32,32	0
85	MG	1	3418	1/1	0.27	14.15	91,91,91,91	0
85	MG	6	1901	1/1	0.42	14.14	55,55,55,55	0
85	MG	5	3680	1/1	0.53	14.06	67,67,67,67	0
85	MG	5	3739	1/1	0.32	13.84	68,68,68,68	0
85	MG	8	213	1/1	0.51	13.68	69,69,69,69	0
85	MG	1	3405	1/1	0.59	13.66	96,96,96,96	0
85	MG	3	214	1/1	0.44	13.58	49,49,49,49	0
85	MG	5	3768	1/1	0.77	13.53	34,34,34,34	0
85	MG	1	3736	1/1	0.47	13.37	55,55,55,55	0
85	MG	2	1965	1/1	0.49	13.34	51,51,51,51	0
85	MG	2	2004	1/1	0.49	13.33	89,89,89,89	0
85	MG	3	204	1/1	0.60	13.33	34,34,34,34	0
85	MG	5	3481	1/1	0.36	13.29	57,57,57,57	0
85	MG	1	3522	1/1	0.78	13.20	44,44,44,44	0
85	MG	6	1932	1/1	0.36	13.19	81,81,81,81	0
85	MG	5	3687	1/1	0.33	13.12	49,49,49,49	0
85	MG	1	3665	1/1	0.44	13.09	35,35,35,35	0
85	MG	5	3502	1/1	0.51	12.91	61,61,61,61	0
85	MG	5	3673	1/1	0.56	12.89	98,98,98,98	0
85	MG	1	3737	1/1	0.47	12.88	51,51,51,51	0
85	MG	5	3827	1/1	0.46	12.88	48,48,48,48	0
85	MG	5	3891	1/1	0.34	12.83	41,41,41,41	0
85	MG	5	3614	1/1	0.41	12.83	54,54,54,54	0
85	MG	5	3616	1/1	0.26	12.79	56,56,56,56	0
85	MG	5	3487	1/1	0.32	12.73	61,61,61,61	0
85	MG	1	3461	1/1	0.43	12.63	32,32,32,32	0
85	MG	5	3797	1/1	0.19	12.50	174,174,174,174	0
85	MG	2	1932	1/1	0.39	12.43	68,68,68,68	0
85	MG	5	3522	1/1	0.42	12.33	28,28,28,28	0
85	MG	1	3534	1/1	0.26	12.25	52,52,52,52	0
85	MG	6	1902	1/1	0.35	12.24	64,64,64,64	0
85	MG	1	3819	1/1	0.31	12.16	46,46,46,46	0
85	MG	7	209	1/1	0.30	12.14	65,65,65,65	0
85	MG	1	3492	1/1	0.38	12.13	84,84,84,84	0
85	MG	6	1971	1/1	0.43	12.00	75,75,75,75	0
85	MG	1	3758	1/1	0.71	11.98	61,61,61,61	0
85	MG	6	1959	1/1	0.37	11.92	47,47,47,47	0
85	MG	6	1993	1/1	0.36	11.91	62,62,62,62	0
85	MG	5	3449	1/1	0.37	11.87	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3546	1/1	0.42	11.74	45,45,45,45	0
85	MG	5	3596	1/1	0.51	11.74	28,28,28,28	0
85	MG	1	3559	1/1	0.32	11.72	28,28,28,28	0
86	OHX	1	4173	7/7	0.49	11.69	143,143,143,143	0
85	MG	1	3807	1/1	0.44	11.60	45,45,45,45	0
85	MG	6	1921	1/1	0.39	11.50	62,62,62,62	0
85	MG	5	3843	1/1	0.29	11.40	47,47,47,47	0
85	MG	2	1933	1/1	0.42	11.36	74,74,74,74	0
85	MG	1	3553	1/1	0.39	11.35	42,42,42,42	0
85	MG	5	3704	1/1	1.01	11.31	57,57,57,57	0
86	OHX	5	4223	7/7	0.29	11.27	152,152,152,152	0
85	MG	5	3503	1/1	0.38	11.25	30,30,30,30	0
85	MG	2	1994	1/1	0.46	11.15	125,125,125,125	0
85	MG	1	3813	1/1	0.34	11.12	59,59,59,59	0
85	MG	5	3832	1/1	0.26	11.00	55,55,55,55	0
85	MG	1	3538	1/1	0.38	10.95	55,55,55,55	0
85	MG	5	3410	1/1	0.28	10.95	52,52,52,52	0
85	MG	1	3442	1/1	0.30	10.92	54,54,54,54	0
85	MG	1	3821	1/1	0.27	10.92	31,31,31,31	0
86	OHX	1	4203	7/7	0.59	10.77	151,151,151,151	0
85	MG	5	3577	1/1	0.33	10.76	26,26,26,26	0
85	MG	1	4217	1/1	2.78	10.72	47,47,47,47	0
85	MG	5	3559	1/1	0.36	10.67	23,23,23,23	0
85	MG	6	1954	1/1	0.61	10.63	42,42,42,42	0
85	MG	5	3769	1/1	0.39	10.60	60,60,60,60	0
85	MG	2	1915	1/1	0.37	10.57	73,73,73,73	0
85	MG	1	3806	1/1	0.22	10.54	41,41,41,41	0
85	MG	5	3518	1/1	0.33	10.45	39,39,39,39	0
85	MG	1	3501	1/1	0.37	10.38	54,54,54,54	0
85	MG	1	3782	1/1	2.18	10.36	33,33,33,33	0
85	MG	1	3684	1/1	0.32	10.35	49,49,49,49	0
85	MG	2	2012	1/1	0.40	10.25	66,66,66,66	0
85	MG	5	3663	1/1	0.62	10.17	32,32,32,32	0
85	MG	1	3774	1/1	0.30	10.16	54,54,54,54	0
85	MG	1	3622	1/1	0.52	10.13	82,82,82,82	0
85	MG	1	3842	1/1	0.30	10.12	40,40,40,40	0
85	MG	5	3709	1/1	0.36	10.11	46,46,46,46	0
85	MG	2	1925	1/1	0.42	10.10	69,69,69,69	0
85	MG	7	208	1/1	0.47	10.10	44,44,44,44	0
85	MG	1	3612	1/1	0.78	10.08	47,47,47,47	0
85	MG	1	3798	1/1	0.81	10.03	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3787	1/1	0.97	10.01	48,48,48,48	0
85	MG	7	201	1/1	0.52	9.99	47,47,47,47	0
85	MG	1	3533	1/1	0.43	9.81	47,47,47,47	0
85	MG	7	202	1/1	0.37	9.77	52,52,52,52	0
86	OHX	5	4230	7/7	0.32	9.76	178,178,178,178	0
85	MG	2	2009	1/1	0.47	9.72	56,56,56,56	0
85	MG	1	3698	1/1	0.78	9.71	43,43,43,43	0
85	MG	1	3452	1/1	0.33	9.68	37,37,37,37	0
86	OHX	1	4139	7/7	0.34	9.60	153,153,153,153	0
85	MG	5	3705	1/1	0.43	9.52	100,100,100,100	0
86	OHX	2	2159	7/7	0.35	9.40	184,184,184,184	0
85	MG	2	1902	1/1	0.34	9.39	52,52,52,52	0
85	MG	5	3863	1/1	0.43	9.34	43,43,43,43	0
85	MG	6	2030	1/1	0.32	9.28	93,93,93,93	0
85	MG	5	3569	1/1	0.45	9.28	24,24,24,24	0
85	MG	1	3542	1/1	0.88	9.14	51,51,51,51	0
85	MG	2	1936	1/1	0.38	9.09	60,60,60,60	0
85	MG	8	204	1/1	0.41	9.05	60,60,60,60	0
85	MG	5	3603	1/1	0.29	9.04	35,35,35,35	0
85	MG	2	2021	1/1	0.52	9.04	89,89,89,89	0
85	MG	1	3740	1/1	0.31	8.92	50,50,50,50	0
85	MG	6	2013	1/1	0.28	8.92	82,82,82,82	0
85	MG	6	1944	1/1	0.48	8.91	33,33,33,33	0
85	MG	5	3560	1/1	0.39	8.75	24,24,24,24	0
85	MG	6	1966	1/1	0.34	8.71	82,82,82,82	0
85	MG	5	3852	1/1	0.34	8.69	100,100,100,100	0
85	MG	1	3730	1/1	0.45	8.69	45,45,45,45	0
85	MG	13	402	1/1	2.42	8.64	59,59,59,59	0
85	MG	5	4249	1/1	1.29	8.60	38,38,38,38	0
85	MG	6	1998	1/1	0.13	8.60	109,109,109,109	0
85	MG	6	1918	1/1	0.42	8.57	43,43,43,43	0
85	MG	1	3595	1/1	0.47	8.56	13,13,13,13	0
85	MG	5	3466	1/1	0.29	8.56	102,102,102,102	0
85	MG	8	207	1/1	1.58	8.51	62,62,62,62	0
88	BLS	5	4248	30/30	0.48	8.50	52,52,52,52	0
85	MG	1	3728	1/1	0.33	8.49	86,86,86,86	0
85	MG	5	3630	1/1	0.30	8.42	54,54,54,54	0
85	MG	1	3674	1/1	0.34	8.40	54,54,54,54	0
85	MG	2	1944	1/1	0.47	8.40	68,68,68,68	0
85	MG	5	3699	1/1	0.30	8.36	49,49,49,49	0
85	MG	5	3491	1/1	0.31	8.36	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3755	1/1	0.29	8.35	41,41,41,41	0
85	MG	1	3800	1/1	0.61	8.29	180,180,180,180	0
85	MG	1	3760	1/1	0.76	8.28	60,60,60,60	0
85	MG	7	204	1/1	0.33	8.27	50,50,50,50	0
85	MG	5	3777	1/1	0.31	8.27	37,37,37,37	0
85	MG	3	207	1/1	0.53	8.13	53,53,53,53	0
85	MG	5	3425	1/1	0.39	8.09	45,45,45,45	0
85	MG	5	3724	1/1	0.23	7.96	57,57,57,57	0
85	MG	5	3886	1/1	0.23	7.94	64,64,64,64	0
85	MG	2	1969	1/1	0.36	7.91	89,89,89,89	0
85	MG	4	218	1/1	0.57	7.89	67,67,67,67	0
85	MG	8	210	1/1	0.19	7.87	65,65,65,65	0
85	MG	1	3715	1/1	0.71	7.86	41,41,41,41	0
85	MG	5	3686	1/1	0.39	7.86	69,69,69,69	0
85	MG	1	4215	1/1	1.68	7.86	41,41,41,41	0
85	MG	8	211	1/1	1.41	7.82	49,49,49,49	0
85	MG	2	1983	1/1	0.31	7.81	74,74,74,74	0
85	MG	N8	205	1/1	1.27	7.80	39,39,39,39	0
85	MG	1	3555	1/1	0.29	7.80	46,46,46,46	0
85	MG	5	3644	1/1	0.24	7.80	31,31,31,31	0
85	MG	2	1996	1/1	0.47	7.76	98,98,98,98	0
85	MG	1	3536	1/1	0.36	7.73	44,44,44,44	0
85	MG	2	1981	1/1	0.46	7.69	60,60,60,60	0
85	MG	5	3574	1/1	0.38	7.64	30,30,30,30	0
86	OHX	1	4058	7/7	0.28	7.64	154,154,154,154	0
85	MG	6	1985	1/1	0.49	7.60	82,82,82,82	0
86	OHX	2	2143	7/7	0.40	7.59	148,148,148,148	0
85	MG	1	3615	1/1	0.31	7.56	72,72,72,72	0
85	MG	6	1908	1/1	0.35	7.55	56,56,56,56	0
85	MG	1	3709	1/1	2.41	7.55	54,54,54,54	0
85	MG	6	1940	1/1	0.28	7.54	60,60,60,60	0
85	MG	5	3575	1/1	0.32	7.51	30,30,30,30	0
85	MG	6	1941	1/1	1.14	7.49	46,46,46,46	0
85	MG	5	3751	1/1	0.56	7.47	107,107,107,107	0
86	OHX	1	4123	7/7	0.30	7.37	180,180,180,180	0
85	MG	m7	205	1/1	1.72	7.36	44,44,44,44	0
85	MG	1	3635	1/1	1.61	7.30	60,60,60,60	0
85	MG	1	3620	1/1	0.20	7.28	48,48,48,48	0
85	MG	5	3641	1/1	0.37	7.28	43,43,43,43	0
85	MG	5	3774	1/1	1.24	7.26	96,96,96,96	0
85	MG	6	1927	1/1	0.54	7.26	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3814	1/1	0.72	7.25	64,64,64,64	0
85	MG	5	3656	1/1	0.34	7.25	40,40,40,40	0
86	OHX	5	4006	7/7	0.22	7.18	161,161,161,161	0
85	MG	l3	403	1/1	0.98	7.16	39,39,39,39	0
85	MG	5	3571	1/1	0.30	7.12	37,37,37,37	0
85	MG	l5	302	1/1	0.38	7.09	71,71,71,71	0
85	MG	8	205	1/1	0.74	7.08	56,56,56,56	0
85	MG	5	3787	1/1	0.35	7.06	62,62,62,62	0
85	MG	6	1958	1/1	0.24	7.05	57,57,57,57	0
85	MG	5	3701	1/1	0.34	7.04	50,50,50,50	0
85	MG	6	1969	1/1	0.36	7.03	65,65,65,65	0
85	MG	5	3793	1/1	0.97	6.99	78,78,78,78	0
86	OHX	1	4186	7/7	0.42	6.98	167,167,167,167	0
85	MG	5	3694	1/1	0.86	6.98	41,41,41,41	0
85	MG	1	3816	1/1	1.57	6.95	46,46,46,46	0
85	MG	1	3810	1/1	0.58	6.94	133,133,133,133	0
85	MG	5	3707	1/1	0.26	6.91	72,72,72,72	0
85	MG	5	3749	1/1	0.32	6.90	67,67,67,67	0
85	MG	d3	202	1/1	1.08	6.87	63,63,63,63	0
85	MG	1	3429	1/1	0.38	6.87	52,52,52,52	0
85	MG	1	3639	1/1	0.41	6.85	49,49,49,49	0
85	MG	5	3669	1/1	0.30	6.85	68,68,68,68	0
85	MG	1	3473	1/1	0.32	6.84	79,79,79,79	0
85	MG	5	3639	1/1	0.30	6.82	41,41,41,41	0
85	MG	5	3554	1/1	0.34	6.75	36,36,36,36	0
85	MG	5	3624	1/1	0.47	6.74	69,69,69,69	0
85	MG	N8	202	1/1	0.41	6.68	41,41,41,41	0
85	MG	1	3689	1/1	0.33	6.64	45,45,45,45	0
85	MG	1	3718	1/1	0.53	6.62	74,74,74,74	0
85	MG	5	3717	1/1	0.42	6.58	52,52,52,52	0
85	MG	5	3838	1/1	0.27	6.57	31,31,31,31	0
85	MG	6	1911	1/1	0.29	6.50	87,87,87,87	0
85	MG	5	3472	1/1	0.73	6.49	40,40,40,40	0
85	MG	1	3710	1/1	0.33	6.43	78,78,78,78	0
85	MG	5	3889	1/1	0.31	6.41	56,56,56,56	0
85	MG	5	3659	1/1	0.48	6.40	75,75,75,75	0
85	MG	1	3678	1/1	0.35	6.40	43,43,43,43	0
85	MG	5	3580	1/1	0.37	6.30	33,33,33,33	0
85	MG	O5	201	1/1	1.88	6.25	56,56,56,56	0
85	MG	L7	302	1/1	1.85	6.23	47,47,47,47	0
85	MG	2	1978	1/1	0.38	6.21	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3401	1/1	0.69	6.20	54,54,54,54	0
85	MG	4	203	1/1	0.39	6.18	53,53,53,53	0
85	MG	1	3812	1/1	0.43	6.16	45,45,45,45	0
85	MG	3	208	1/1	0.26	6.15	50,50,50,50	0
85	MG	6	2042	1/1	0.30	6.14	71,71,71,71	0
85	MG	6	1953	1/1	0.30	6.10	63,63,63,63	0
85	MG	6	2024	1/1	0.57	6.09	74,74,74,74	0
85	MG	6	1924	1/1	0.39	6.09	46,46,46,46	0
85	MG	2	1929	1/1	0.37	6.07	65,65,65,65	0
85	MG	5	3483	1/1	0.32	6.07	51,51,51,51	0
85	MG	5	3731	1/1	0.32	5.98	39,39,39,39	0
85	MG	6	1920	1/1	0.30	5.97	44,44,44,44	0
85	MG	o7	101	1/1	1.05	5.97	47,47,47,47	0
85	MG	14	401	1/1	0.63	5.96	59,59,59,59	0
85	MG	1	3451	1/1	0.28	5.95	48,48,48,48	0
85	MG	1	3720	1/1	0.30	5.94	50,50,50,50	0
85	MG	6	1967	1/1	0.47	5.90	76,76,76,76	0
85	MG	1	3746	1/1	0.28	5.90	62,62,62,62	0
85	MG	6	2007	1/1	0.24	5.89	64,64,64,64	0
85	MG	5	3613	1/1	0.32	5.89	42,42,42,42	0
85	MG	6	1945	1/1	0.41	5.88	73,73,73,73	0
85	MG	6	1913	1/1	0.36	5.88	39,39,39,39	0
85	MG	L3	401	1/1	0.29	5.79	41,41,41,41	0
85	MG	2	1926	1/1	0.40	5.78	92,92,92,92	0
86	OHX	6	2160	7/7	0.32	5.77	158,158,158,158	0
85	MG	4	214	1/1	1.02	5.68	45,45,45,45	0
85	MG	5	3600	1/1	0.31	5.68	39,39,39,39	0
85	MG	2	1987	1/1	0.31	5.68	105,105,105,105	0
85	MG	6	1903	1/1	0.23	5.68	45,45,45,45	0
85	MG	5	3605	1/1	0.28	5.67	36,36,36,36	0
85	MG	6	2009	1/1	0.37	5.67	58,58,58,58	0
85	MG	1	3475	1/1	0.38	5.66	43,43,43,43	0
86	OHX	6	2183	7/7	0.74	5.65	177,177,177,177	0
85	MG	6	1986	1/1	0.83	5.59	51,51,51,51	0
86	OHX	5	4146	7/7	0.26	5.54	145,145,145,145	0
85	MG	5	3501	1/1	0.42	5.50	37,37,37,37	0
85	MG	3	209	1/1	0.37	5.49	56,56,56,56	0
86	OHX	5	3901	7/7	0.23	5.47	66,66,66,66	0
85	MG	2	1952	1/1	0.28	5.46	108,108,108,108	0
85	MG	1	3772	1/1	0.18	5.46	68,68,68,68	0
85	MG	m0	301	1/1	1.04	5.46	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3611	1/1	0.23	5.45	39,39,39,39	0
85	MG	1	3701	1/1	0.54	5.45	54,54,54,54	0
85	MG	5	3551	1/1	0.38	5.44	46,46,46,46	0
85	MG	5	3733	1/1	0.35	5.37	28,28,28,28	0
85	MG	5	3413	1/1	0.63	5.34	31,31,31,31	0
86	OHX	1	4090	7/7	0.24	5.33	158,158,158,158	0
85	MG	2	1921	1/1	0.40	5.29	61,61,61,61	0
86	OHX	1	3913	7/7	0.23	5.28	123,123,123,123	0
85	MG	2	2010	1/1	0.34	5.25	68,68,68,68	0
86	OHX	6	2054	7/7	0.24	5.25	101,101,101,101	0
86	OHX	1	4074	7/7	0.40	5.21	155,155,155,155	0
85	MG	O2	202	1/1	1.34	5.20	38,38,38,38	0
85	MG	1	3768	1/1	0.68	5.20	68,68,68,68	0
86	OHX	1	4207	7/7	0.31	5.19	154,154,154,154	0
85	MG	5	3782	1/1	1.00	5.15	65,65,65,65	0
86	OHX	5	4170	7/7	0.28	5.15	174,174,174,174	0
85	MG	1	3479	1/1	0.29	5.15	50,50,50,50	0
85	MG	1	3456	1/1	0.30	5.15	46,46,46,46	0
88	BLS	1	4211	30/30	0.33	5.14	52,52,52,52	0
86	OHX	5	4155	7/7	0.57	5.14	161,161,161,161	0
85	MG	5	3853	1/1	0.41	5.09	63,63,63,63	0
85	MG	1	3570	1/1	0.37	5.04	22,22,22,22	0
85	MG	5	3846	1/1	0.27	5.03	56,56,56,56	0
85	MG	2	1977	1/1	0.36	5.03	85,85,85,85	0
85	MG	5	3817	1/1	0.51	5.01	43,43,43,43	0
86	OHX	5	4217	7/7	0.29	5.00	179,179,179,179	0
85	MG	5	3486	1/1	0.37	4.99	40,40,40,40	0
85	MG	1	3748	1/1	0.32	4.97	47,47,47,47	0
85	MG	3	205	1/1	0.26	4.94	37,37,37,37	0
85	MG	5	3668	1/1	0.54	4.93	36,36,36,36	0
85	MG	6	1978	1/1	0.32	4.90	53,53,53,53	0
85	MG	5	3655	1/1	0.24	4.89	51,51,51,51	0
85	MG	1	3508	1/1	0.27	4.89	39,39,39,39	0
85	MG	1	3487	1/1	1.41	4.85	61,61,61,61	0
85	MG	1	3660	1/1	0.86	4.82	56,56,56,56	0
86	OHX	2	2052	7/7	0.24	4.81	148,148,148,148	0
86	OHX	1	4136	7/7	0.33	4.79	156,156,156,156	0
85	MG	5	3880	1/1	0.31	4.79	61,61,61,61	0
85	MG	7	213	1/1	0.29	4.79	59,59,59,59	0
85	MG	5	3653	1/1	0.27	4.76	60,60,60,60	0
85	MG	6	1965	1/1	0.24	4.69	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	5	3510	1/1	0.21	4.69	63,63,63,63	0
85	MG	5	3820	1/1	1.40	4.67	45,45,45,45	0
85	MG	1	3457	1/1	0.31	4.66	66,66,66,66	0
85	MG	3	201	1/1	0.46	4.65	66,66,66,66	0
85	MG	1	3828	1/1	0.34	4.62	41,41,41,41	0
85	MG	2	1935	1/1	0.36	4.62	55,55,55,55	0
85	MG	7	206	1/1	0.36	4.60	26,26,26,26	0
85	MG	1	3409	1/1	0.37	4.58	25,25,25,25	0
85	MG	5	3439	1/1	0.26	4.58	35,35,35,35	0
85	MG	6	1950	1/1	0.30	4.52	65,65,65,65	0
85	MG	5	3866	1/1	0.39	4.50	34,34,34,34	0
85	MG	1	3624	1/1	0.28	4.49	39,39,39,39	0
86	OHX	1	3886	7/7	0.24	4.48	82,82,82,82	0
85	MG	5	3786	1/1	1.30	4.48	45,45,45,45	0
85	MG	2	1903	1/1	0.44	4.47	47,47,47,47	0
85	MG	5	3608	1/1	0.33	4.45	45,45,45,45	0
85	MG	1	3402	1/1	0.44	4.43	54,54,54,54	0
85	MG	1	3781	1/1	0.48	4.37	37,37,37,37	0
85	MG	M1	201	1/1	0.41	4.34	64,64,64,64	0
86	OHX	1	4195	7/7	0.21	4.34	156,156,156,156	0
85	MG	4	220	1/1	0.35	4.34	44,44,44,44	0
85	MG	5	3831	1/1	0.37	4.32	36,36,36,36	0
85	MG	5	3677	1/1	0.38	4.28	89,89,89,89	0
85	MG	1	3561	1/1	0.35	4.27	37,37,37,37	0
85	MG	1	3729	1/1	0.61	4.25	61,61,61,61	0
85	MG	6	1994	1/1	0.23	4.18	56,56,56,56	0
85	MG	q0	3601	1/1	0.23	4.16	63,63,63,63	0
85	MG	1	3702	1/1	0.23	4.16	69,69,69,69	0
85	MG	5	3708	1/1	0.23	4.15	48,48,48,48	0
85	MG	5	3825	1/1	0.38	4.14	85,85,85,85	0
85	MG	6	1912	1/1	0.28	4.09	52,52,52,52	0
85	MG	2	1905	1/1	0.44	4.09	70,70,70,70	0
85	MG	1	3618	1/1	0.46	4.08	42,42,42,42	0
86	OHX	2	2176	7/7	0.20	4.08	169,169,169,169	0
85	MG	5	3651	1/1	0.24	4.07	44,44,44,44	0
85	MG	1	3827	1/1	0.43	4.07	45,45,45,45	0
86	OHX	5	4214	7/7	0.40	4.06	165,165,165,165	0
85	MG	2	1954	1/1	0.30	4.03	101,101,101,101	0
86	OHX	8	225	7/7	0.26	4.03	162,162,162,162	0
85	MG	c4	201	1/1	0.36	4.03	58,58,58,58	0
86	OHX	5	4160	7/7	0.30	4.00	208,208,208,208	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4106	7/7	0.26	4.00	155,155,155,155	0
85	MG	1	3783	1/1	0.24	4.00	81,81,81,81	0
86	OHX	1	4167	7/7	0.42	3.97	176,176,176,176	0
85	MG	5	3458	1/1	0.24	3.95	30,30,30,30	0
85	MG	5	3632	1/1	0.26	3.94	73,73,73,73	0
85	MG	1	3482	1/1	0.72	3.92	48,48,48,48	0
85	MG	5	3692	1/1	0.48	3.86	66,66,66,66	0
85	MG	6	1933	1/1	0.26	3.85	86,86,86,86	0
85	MG	5	3807	1/1	0.54	3.83	62,62,62,62	0
85	MG	5	3622	1/1	0.20	3.83	64,64,64,64	0
85	MG	2	1955	1/1	0.27	3.82	72,72,72,72	0
85	MG	q0	3603	1/1	0.54	3.81	47,47,47,47	0
85	MG	5	3869	1/1	0.30	3.80	46,46,46,46	0
85	MG	5	3734	1/1	0.24	3.80	64,64,64,64	0
85	MG	1	3466	1/1	0.34	3.78	45,45,45,45	0
85	MG	5	3778	1/1	0.23	3.78	43,43,43,43	0
85	MG	6	1981	1/1	0.29	3.76	90,90,90,90	0
85	MG	5	3496	1/1	0.28	3.72	40,40,40,40	0
85	MG	1	3708	1/1	0.34	3.72	66,66,66,66	0
85	MG	1	3717	1/1	0.30	3.71	41,41,41,41	0
86	OHX	4	236	7/7	0.24	3.70	166,166,166,166	0
86	OHX	5	3906	7/7	0.21	3.69	72,72,72,72	0
85	MG	6	1915	1/1	0.37	3.69	64,64,64,64	0
86	OHX	1	3898	7/7	0.24	3.67	103,103,103,103	0
86	OHX	1	3891	7/7	0.20	3.66	93,93,93,93	0
85	MG	1	3719	1/1	0.70	3.65	52,52,52,52	0
85	MG	5	3822	1/1	0.40	3.65	68,68,68,68	0
85	MG	5	3756	1/1	0.22	3.63	45,45,45,45	0
85	MG	6	2021	1/1	0.27	3.61	94,94,94,94	0
85	MG	L4	403	1/1	1.08	3.60	36,36,36,36	0
85	MG	2	1971	1/1	0.41	3.59	76,76,76,76	0
85	MG	5	3737	1/1	0.42	3.58	41,41,41,41	0
85	MG	6	1964	1/1	0.44	3.57	80,80,80,80	0
85	MG	6	1952	1/1	0.39	3.57	64,64,64,64	0
85	MG	1	3632	1/1	0.24	3.57	70,70,70,70	0
85	MG	6	2032	1/1	0.66	3.56	58,58,58,58	0
85	MG	1	3469	1/1	0.35	3.55	48,48,48,48	0
85	MG	1	3417	1/1	0.34	3.55	43,43,43,43	0
85	MG	5	3432	1/1	0.22	3.53	40,40,40,40	0
85	MG	5	3873	1/1	0.25	3.53	32,32,32,32	0
85	MG	O2	201	1/1	0.82	3.53	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4239	7/7	0.28	3.51	193,193,193,193	0
85	MG	1	3544	1/1	0.24	3.50	59,59,59,59	0
85	MG	2	1945	1/1	0.22	3.48	76,76,76,76	0
86	OHX	1	4137	7/7	0.26	3.46	154,154,154,154	0
85	MG	1	3839	1/1	0.28	3.45	54,54,54,54	0
85	MG	1	3659	1/1	0.24	3.41	48,48,48,48	0
85	MG	5	3730	1/1	0.24	3.41	48,48,48,48	0
85	MG	1	3607	1/1	0.59	3.39	45,45,45,45	0
85	MG	6	2002	1/1	0.28	3.37	84,84,84,84	0
85	MG	6	1916	1/1	0.30	3.35	65,65,65,65	0
85	MG	2	1961	1/1	0.25	3.34	65,65,65,65	0
85	MG	6	1955	1/1	0.38	3.33	51,51,51,51	0
85	MG	1	3527	1/1	0.36	3.33	23,23,23,23	0
85	MG	2	1995	1/1	0.33	3.32	57,57,57,57	0
85	MG	6	1904	1/1	0.36	3.30	73,73,73,73	0
85	MG	N3	201	1/1	0.26	3.29	35,35,35,35	0
85	MG	5	3855	1/1	0.73	3.28	48,48,48,48	0
85	MG	1	3692	1/1	0.31	3.28	52,52,52,52	0
85	MG	5	3498	1/1	0.29	3.26	29,29,29,29	0
85	MG	5	3562	1/1	0.27	3.25	31,31,31,31	0
85	MG	1	3552	1/1	0.36	3.25	23,23,23,23	0
85	MG	5	3720	1/1	0.24	3.24	42,42,42,42	0
85	MG	1	3837	1/1	0.33	3.22	49,49,49,49	0
85	MG	1	3594	1/1	0.33	3.21	38,38,38,38	0
85	MG	1	3438	1/1	0.27	3.20	22,22,22,22	0
85	MG	6	1914	1/1	0.28	3.19	57,57,57,57	0
85	MG	5	3515	1/1	0.32	3.19	24,24,24,24	0
85	MG	M3	201	1/1	0.78	3.19	45,45,45,45	0
85	MG	1	3445	1/1	0.29	3.19	34,34,34,34	0
85	MG	2	1963	1/1	0.24	3.16	175,175,175,175	0
85	MG	1	3541	1/1	0.30	3.15	41,41,41,41	0
86	OHX	1	4185	7/7	0.21	3.15	155,155,155,155	0
85	MG	1	3626	1/1	0.25	3.13	65,65,65,65	0
85	MG	6	1930	1/1	0.43	3.11	54,54,54,54	0
86	OHX	5	4179	7/7	0.34	3.11	141,141,141,141	0
85	MG	5	3553	1/1	0.42	3.10	43,43,43,43	0
85	MG	5	3451	1/1	0.30	3.09	43,43,43,43	0
85	MG	1	3834	1/1	0.35	3.09	54,54,54,54	0
85	MG	5	3539	1/1	0.31	3.05	28,28,28,28	0
86	OHX	5	4225	7/7	0.39	3.03	177,177,177,177	0
85	MG	5	3407	1/1	0.54	3.02	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	N8	203	1/1	0.45	3.02	46,46,46,46	0
85	MG	2	1918	1/1	0.42	3.02	57,57,57,57	0
86	OHX	2	2148	7/7	0.31	3.02	144,144,144,144	0
85	MG	5	3561	1/1	0.42	3.02	24,24,24,24	0
85	MG	1	3650	1/1	0.39	3.02	46,46,46,46	0
85	MG	5	3558	1/1	0.29	3.01	36,36,36,36	0
85	MG	5	3657	1/1	0.42	3.01	51,51,51,51	0
85	MG	d6	102	1/1	0.89	2.99	71,71,71,71	0
85	MG	2	1917	1/1	0.42	2.97	61,61,61,61	0
85	MG	1	3434	1/1	0.24	2.96	41,41,41,41	0
85	MG	1	3707	1/1	0.48	2.96	43,43,43,43	0
85	MG	1	3663	1/1	0.33	2.96	80,80,80,80	0
85	MG	5	3594	1/1	0.34	2.95	17,17,17,17	0
85	MG	3	202	1/1	0.35	2.93	42,42,42,42	0
85	MG	17	301	1/1	1.19	2.92	42,42,42,42	0
86	OHX	6	2165	7/7	0.23	2.91	165,165,165,165	0
85	MG	5	3808	1/1	0.21	2.89	69,69,69,69	0
85	MG	1	3835	1/1	0.43	2.89	45,45,45,45	0
85	MG	5	3589	1/1	0.34	2.89	48,48,48,48	0
85	MG	5	3654	1/1	0.26	2.89	35,35,35,35	0
85	MG	5	3665	1/1	0.49	2.88	51,51,51,51	0
85	MG	5	3535	1/1	0.36	2.86	42,42,42,42	0
85	MG	5	3823	1/1	0.31	2.85	86,86,86,86	0
85	MG	6	1997	1/1	0.25	2.82	73,73,73,73	0
85	MG	M7	202	1/1	0.32	2.81	33,33,33,33	0
85	MG	1	3721	1/1	0.61	2.80	48,48,48,48	0
86	OHX	1	4209	7/7	0.50	2.80	162,162,162,162	0
86	OHX	2	2174	7/7	0.24	2.80	169,169,169,169	0
85	MG	4	212	1/1	0.24	2.79	62,62,62,62	0
85	MG	1	3739	1/1	0.30	2.79	50,50,50,50	0
85	MG	N3	202	1/1	0.73	2.78	63,63,63,63	0
85	MG	2	1967	1/1	0.35	2.78	62,62,62,62	0
85	MG	5	3743	1/1	0.71	2.77	54,54,54,54	0
85	MG	1	3489	1/1	0.45	2.75	59,59,59,59	0
85	MG	5	3676	1/1	0.33	2.75	40,40,40,40	0
85	MG	1	3498	1/1	0.32	2.74	62,62,62,62	0
85	MG	5	3417	1/1	0.22	2.72	33,33,33,33	0
85	MG	2	2018	1/1	0.36	2.72	73,73,73,73	0
85	MG	5	3696	1/1	0.49	2.71	37,37,37,37	0
85	MG	5	3469	1/1	0.21	2.70	121,121,121,121	0
86	OHX	6	2156	7/7	0.37	2.68	203,203,203,203	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2180	7/7	0.38	2.68	164,164,164,164	0
86	OHX	5	4199	7/7	0.22	2.68	160,160,160,160	0
85	MG	5	3504	1/1	0.34	2.68	37,37,37,37	0
85	MG	2	2006	1/1	0.25	2.67	70,70,70,70	0
85	MG	5	3528	1/1	0.34	2.65	27,27,27,27	0
85	MG	1	3761	1/1	0.37	2.65	64,64,64,64	0
85	MG	1	3599	1/1	0.51	2.64	42,42,42,42	0
86	OHX	2	2157	7/7	0.26	2.62	138,138,138,138	0
85	MG	12	301	1/1	1.01	2.61	43,43,43,43	0
85	MG	5	3578	1/1	0.30	2.60	27,27,27,27	0
86	OHX	7	227	7/7	0.19	2.60	171,171,171,171	0
85	MG	5	3436	1/1	0.30	2.59	48,48,48,48	0
85	MG	1	3480	1/1	0.21	2.57	33,33,33,33	0
85	MG	6	2005	1/1	1.00	2.56	80,80,80,80	0
85	MG	1	3712	1/1	0.34	2.56	44,44,44,44	0
85	MG	1	3634	1/1	0.49	2.53	66,66,66,66	0
85	MG	5	3798	1/1	0.23	2.53	37,37,37,37	0
85	MG	D3	201	1/1	1.54	2.52	54,54,54,54	0
85	MG	5	3634	1/1	0.29	2.52	39,39,39,39	0
85	MG	1	3619	1/1	0.23	2.49	48,48,48,48	0
85	MG	1	3705	1/1	0.20	2.47	51,51,51,51	0
85	MG	1	3749	1/1	1.36	2.45	68,68,68,68	0
86	OHX	8	228	7/7	0.29	2.43	154,154,154,154	0
85	MG	1	3631	1/1	0.51	2.41	70,70,70,70	0
85	MG	1	3679	1/1	0.27	2.41	46,46,46,46	0
85	MG	6	1937	1/1	0.23	2.39	56,56,56,56	0
86	OHX	5	4091	7/7	0.26	2.39	172,172,172,172	0
86	OHX	5	4148	7/7	0.32	2.39	140,140,140,140	0
85	MG	1	3796	1/1	0.39	2.39	57,57,57,57	0
86	OHX	1	3859	7/7	0.20	2.37	55,55,55,55	0
85	MG	1	3535	1/1	0.35	2.35	34,34,34,34	0
85	MG	5	3536	1/1	0.29	2.34	38,38,38,38	0
85	MG	6	2039	1/1	0.61	2.33	112,112,112,112	0
85	MG	1	3767	1/1	0.69	2.31	64,64,64,64	0
85	MG	5	3529	1/1	0.34	2.31	41,41,41,41	0
86	OHX	1	4135	7/7	0.34	2.30	131,131,131,131	0
85	MG	5	3626	1/1	0.27	2.30	49,49,49,49	0
85	MG	5	3765	1/1	1.41	2.30	79,79,79,79	0
85	MG	6	1974	1/1	0.30	2.29	61,61,61,61	0
85	MG	2	1916	1/1	0.25	2.29	61,61,61,61	0
85	MG	5	3760	1/1	0.43	2.29	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	m5	303	1/1	0.60	2.28	53,53,53,53	0
85	MG	2	2008	1/1	0.47	2.28	55,55,55,55	0
86	OHX	2	2028	7/7	0.23	2.26	106,106,106,106	0
85	MG	2	1949	1/1	0.29	2.25	59,59,59,59	0
86	OHX	5	4182	7/7	0.36	2.25	144,144,144,144	0
85	MG	4	211	1/1	0.25	2.24	80,80,80,80	0
85	MG	1	3804	1/1	0.48	2.24	53,53,53,53	0
85	MG	5	3819	1/1	0.29	2.24	41,41,41,41	0
85	MG	5	3727	1/1	0.49	2.24	42,42,42,42	0
85	MG	2	2016	1/1	0.63	2.23	84,84,84,84	0
85	MG	s8	301	1/1	0.33	2.20	57,57,57,57	0
85	MG	1	3629	1/1	0.27	2.19	34,34,34,34	0
86	OHX	5	4226	7/7	0.38	2.18	154,154,154,154	0
85	MG	1	3792	1/1	0.27	2.17	47,47,47,47	0
85	MG	1	3503	1/1	0.40	2.17	46,46,46,46	0
85	MG	1	3808	1/1	0.25	2.17	67,67,67,67	0
85	MG	1	3525	1/1	0.30	2.17	31,31,31,31	0
85	MG	6	2010	1/1	0.23	2.15	61,61,61,61	0
85	MG	5	3812	1/1	0.44	2.14	63,63,63,63	0
85	MG	8	214	1/1	0.35	2.14	37,37,37,37	0
85	MG	1	3485	1/1	0.28	2.13	41,41,41,41	0
86	OHX	6	2204	7/7	0.29	2.13	173,173,173,173	0
86	OHX	2	2135	7/7	0.34	2.13	160,160,160,160	0
85	MG	5	3546	1/1	0.32	2.12	49,49,49,49	0
86	OHX	5	4100	7/7	0.40	2.12	129,129,129,129	0
85	MG	6	1972	1/1	0.56	2.10	72,72,72,72	0
86	OHX	5	4190	7/7	0.52	2.10	165,165,165,165	0
85	MG	5	3607	1/1	0.23	2.09	46,46,46,46	0
85	MG	1	3682	1/1	0.65	2.09	36,36,36,36	0
86	OHX	1	4052	7/7	0.23	2.09	136,136,136,136	0
86	OHX	5	4149	7/7	0.47	2.08	146,146,146,146	0
85	MG	5	3434	1/1	0.27	2.08	38,38,38,38	0
85	MG	5	3761	1/1	0.30	2.07	42,42,42,42	0
85	MG	1	3640	1/1	0.57	2.06	45,45,45,45	0
85	MG	5	3604	1/1	0.24	2.05	55,55,55,55	0
86	OHX	5	3894	7/7	0.21	2.05	53,53,53,53	0
85	MG	7	214	1/1	0.44	2.04	81,81,81,81	0
86	OHX	4	231	7/7	0.39	2.03	136,136,136,136	0
85	MG	5	3792	1/1	0.71	2.03	49,49,49,49	0
85	MG	6	1925	1/1	0.24	2.02	52,52,52,52	0
85	MG	5	3478	1/1	0.35	2.00	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4038	7/7	0.37	2.00	120,120,120,120	0
86	OHX	2	2179	7/7	0.21	2.00	168,168,168,168	0
86	OHX	6	2181	7/7	0.22	1.98	167,167,167,167	0
86	OHX	5	4077	7/7	0.34	1.97	143,143,143,143	0
85	MG	5	3618	1/1	0.22	1.97	62,62,62,62	0
85	MG	1	3454	1/1	0.38	1.96	63,63,63,63	0
86	OHX	2	2083	7/7	0.45	1.96	146,146,146,146	0
85	MG	5	3490	1/1	0.90	1.95	47,47,47,47	0
85	MG	6	1948	1/1	0.42	1.93	59,59,59,59	0
85	MG	6	1929	1/1	0.21	1.93	66,66,66,66	0
86	OHX	1	4121	7/7	0.51	1.92	143,143,143,143	0
86	OHX	5	4173	7/7	0.45	1.92	136,136,136,136	0
86	OHX	5	3932	7/7	0.26	1.91	98,98,98,98	0
86	OHX	6	2135	7/7	0.23	1.91	160,160,160,160	0
86	OHX	1	4011	7/7	0.24	1.90	160,160,160,160	0
86	OHX	1	3943	7/7	0.22	1.87	132,132,132,132	0
85	MG	1	3664	1/1	0.26	1.87	55,55,55,55	0
85	MG	1	3604	1/1	0.28	1.87	81,81,81,81	0
86	OHX	1	4193	7/7	0.36	1.87	157,157,157,157	0
85	MG	5	3771	1/1	0.26	1.87	54,54,54,54	0
86	OHX	5	4157	7/7	0.27	1.85	140,140,140,140	0
85	MG	1	3412	1/1	0.32	1.82	42,42,42,42	0
86	OHX	4	238	7/7	0.25	1.81	159,159,159,159	0
86	OHX	5	4181	7/7	0.22	1.78	153,153,153,153	0
85	MG	1	3515	1/1	0.38	1.77	38,38,38,38	0
85	MG	6	1946	1/1	0.33	1.77	61,61,61,61	0
86	OHX	5	3944	7/7	0.22	1.77	117,117,117,117	0
85	MG	1	3733	1/1	0.25	1.77	53,53,53,53	0
86	OHX	2	2133	7/7	0.20	1.77	180,180,180,180	0
85	MG	6	1960	1/1	0.32	1.75	76,76,76,76	0
85	MG	1	3413	1/1	0.26	1.75	66,66,66,66	0
85	MG	N5	201	1/1	0.32	1.75	69,69,69,69	0
86	OHX	1	3865	7/7	0.19	1.74	69,69,69,69	0
85	MG	m5	302	1/1	0.48	1.74	56,56,56,56	0
85	MG	1	3836	1/1	0.32	1.73	59,59,59,59	0
86	OHX	1	4206	7/7	0.29	1.72	161,161,161,161	0
85	MG	5	3781	1/1	0.36	1.72	61,61,61,61	0
86	OHX	6	2203	7/7	0.37	1.69	173,173,173,173	0
86	OHX	5	4176	7/7	0.32	1.69	169,169,169,169	0
86	OHX	5	4216	7/7	0.23	1.69	165,165,165,165	0
85	MG	1	3653	1/1	0.31	1.68	42,42,42,42	0
85	MG	1	3493	1/1	0.21	1.66	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4244	7/7	0.22	1.66	157,157,157,157	0
85	MG	1	3524	1/1	0.28	1.65	24,24,24,24	0
85	MG	1	3853	1/1	0.22	1.61	153,153,153,153	0
86	OHX	1	4200	7/7	0.34	1.60	162,162,162,162	0
85	MG	2	1992	1/1	0.29	1.60	66,66,66,66	0
86	OHX	5	3936	7/7	0.22	1.60	91,91,91,91	0
85	MG	1	3415	1/1	0.77	1.60	58,58,58,58	0
85	MG	5	3714	1/1	0.20	1.59	63,63,63,63	0
85	MG	5	3538	1/1	0.39	1.58	32,32,32,32	0
85	MG	5	3475	1/1	0.54	1.57	50,50,50,50	0
85	MG	5	3746	1/1	0.21	1.56	49,49,49,49	0
85	MG	5	3583	1/1	0.37	1.55	33,33,33,33	0
85	MG	5	3593	1/1	0.33	1.54	36,36,36,36	0
86	OHX	1	4182	7/7	0.27	1.54	180,180,180,180	0
86	OHX	1	4111	7/7	0.33	1.53	146,146,146,146	0
86	OHX	2	2042	7/7	0.23	1.53	132,132,132,132	0
85	MG	3	211	1/1	0.26	1.52	69,69,69,69	0
85	MG	5	3800	1/1	0.28	1.51	42,42,42,42	0
86	OHX	1	4131	7/7	0.24	1.50	141,141,141,141	0
85	MG	6	2006	1/1	0.28	1.49	69,69,69,69	0
86	OHX	2	2134	7/7	0.29	1.49	157,157,157,157	0
85	MG	M7	205	1/1	0.97	1.49	45,45,45,45	0
85	MG	2	1943	1/1	0.39	1.47	74,74,74,74	0
85	MG	5	3785	1/1	0.45	1.47	39,39,39,39	0
86	OHX	1	3866	7/7	0.22	1.47	68,68,68,68	0
85	MG	4	216	1/1	0.25	1.46	44,44,44,44	0
85	MG	S8	301	1/1	0.21	1.46	68,68,68,68	0
85	MG	5	3511	1/1	0.33	1.44	23,23,23,23	0
86	OHX	l5	306	7/7	0.22	1.44	170,170,170,170	0
85	MG	o3	202	1/1	0.58	1.43	38,38,38,38	0
85	MG	5	3492	1/1	0.30	1.43	34,34,34,34	0
86	OHX	2	2040	7/7	0.15	1.42	108,108,108,108	0
86	OHX	2	2142	7/7	0.20	1.42	163,163,163,163	0
86	OHX	5	4245	7/7	0.21	1.41	175,175,175,175	0
86	OHX	1	3896	7/7	0.18	1.40	88,88,88,88	0
86	OHX	1	4198	7/7	0.36	1.38	160,160,160,160	0
86	OHX	1	4022	7/7	0.25	1.37	131,131,131,131	0
85	MG	5	3464	1/1	0.37	1.36	38,38,38,38	0
85	MG	5	3681	1/1	0.57	1.36	94,94,94,94	0
85	MG	5	3834	1/1	0.26	1.35	40,40,40,40	0
85	MG	5	3409	1/1	0.23	1.34	36,36,36,36	0
85	MG	l3	401	1/1	0.32	1.34	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	6	2168	7/7	0.19	1.34	151,151,151,151	0
85	MG	1	3514	1/1	0.35	1.34	30,30,30,30	0
86	OHX	5	4188	7/7	0.25	1.34	143,143,143,143	0
86	OHX	6	2177	7/7	0.20	1.33	143,143,143,143	0
85	MG	7	210	1/1	0.45	1.33	51,51,51,51	0
85	MG	5	3719	1/1	0.31	1.32	66,66,66,66	0
85	MG	5	3516	1/1	0.28	1.32	26,26,26,26	0
85	MG	1	3691	1/1	0.27	1.31	36,36,36,36	0
86	OHX	1	4115	7/7	0.35	1.31	136,136,136,136	0
85	MG	1	3673	1/1	0.34	1.31	40,40,40,40	0
86	OHX	6	2187	7/7	0.19	1.30	177,177,177,177	0
86	OHX	1	4149	7/7	0.24	1.30	168,168,168,168	0
85	MG	2	1957	1/1	0.24	1.29	79,79,79,79	0
85	MG	5	3856	1/1	0.26	1.28	49,49,49,49	0
85	MG	1	3408	1/1	0.26	1.28	30,30,30,30	0
86	OHX	1	4179	7/7	0.29	1.27	157,157,157,157	0
85	MG	1	3470	1/1	0.68	1.27	44,44,44,44	0
85	MG	1	3462	1/1	0.30	1.27	61,61,61,61	0
85	MG	6	1963	1/1	0.18	1.27	58,58,58,58	0
86	OHX	5	4137	7/7	0.27	1.27	178,178,178,178	0
85	MG	5	3598	1/1	0.33	1.25	48,48,48,48	0
85	MG	1	3491	1/1	0.58	1.24	52,52,52,52	0
85	MG	n8	201	1/1	0.59	1.23	37,37,37,37	0
85	MG	5	3688	1/1	0.31	1.23	48,48,48,48	0
86	OHX	5	4201	7/7	0.51	1.22	181,181,181,181	0
85	MG	1	3597	1/1	0.44	1.22	31,31,31,31	0
86	OHX	5	3942	7/7	0.18	1.22	108,108,108,108	0
85	MG	O1	201	1/1	0.42	1.21	64,64,64,64	0
86	OHX	5	4242	7/7	0.25	1.20	175,175,175,175	0
85	MG	5	3791	1/1	0.24	1.19	42,42,42,42	0
85	MG	1	3428	1/1	0.27	1.18	37,37,37,37	0
85	MG	1	3649	1/1	0.28	1.18	66,66,66,66	0
85	MG	1	3530	1/1	0.32	1.18	42,42,42,42	0
85	MG	5	3592	1/1	0.25	1.18	44,44,44,44	0
85	MG	1	3444	1/1	0.41	1.17	50,50,50,50	0
86	OHX	5	4108	7/7	0.56	1.17	135,135,135,135	0
85	MG	7	207	1/1	0.24	1.16	45,45,45,45	0
86	OHX	1	4031	7/7	0.33	1.15	156,156,156,156	0
85	MG	5	3405	1/1	0.25	1.14	57,57,57,57	0
85	MG	1	3840	1/1	0.32	1.14	59,59,59,59	0
85	MG	5	3493	1/1	0.31	1.14	40,40,40,40	0
85	MG	6	1947	1/1	0.31	1.13	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	3457	1/1	0.31	1.12	35,35,35,35	0
85	MG	5	3783	1/1	0.24	1.12	35,35,35,35	0
85	MG	5	3666	1/1	0.57	1.11	39,39,39,39	0
86	OHX	5	3892	7/7	0.21	1.10	57,57,57,57	0
86	OHX	5	4110	7/7	0.20	1.09	145,145,145,145	0
85	MG	2	2015	1/1	0.45	1.09	57,57,57,57	0
85	MG	4	215	1/1	0.37	1.09	69,69,69,69	0
85	MG	1	3411	1/1	0.28	1.08	35,35,35,35	0
85	MG	6	1910	1/1	0.23	1.06	55,55,55,55	0
85	MG	4	210	1/1	0.71	1.06	54,54,54,54	0
85	MG	4	208	1/1	0.67	1.06	43,43,43,43	0
86	OHX	5	3959	7/7	0.21	1.05	112,112,112,112	0
85	MG	6	1989	1/1	0.40	1.04	88,88,88,88	0
85	MG	1	3636	1/1	0.32	1.03	55,55,55,55	0
85	MG	2	1922	1/1	0.32	1.03	65,65,65,65	0
85	MG	1	3558	1/1	0.32	1.03	28,28,28,28	0
86	OHX	1	4154	7/7	0.22	1.01	176,176,176,176	0
86	OHX	6	2126	7/7	0.18	1.01	136,136,136,136	0
86	OHX	2	2160	7/7	0.61	1.00	162,162,162,162	0
86	OHX	5	3898	7/7	0.23	1.00	69,69,69,69	0
85	MG	6	1906	1/1	0.40	1.00	45,45,45,45	0
85	MG	5	3418	1/1	0.32	0.99	31,31,31,31	0
85	MG	5	3606	1/1	0.27	0.99	35,35,35,35	0
86	OHX	5	3925	7/7	0.17	0.98	109,109,109,109	0
85	MG	1	3467	1/1	0.23	0.98	48,48,48,48	0
85	MG	1	3495	1/1	0.23	0.97	37,37,37,37	0
85	MG	1	3753	1/1	0.21	0.96	48,48,48,48	0
86	OHX	1	4133	7/7	0.28	0.94	154,154,154,154	0
86	OHX	5	4240	7/7	0.34	0.94	164,164,164,164	0
85	MG	6	1962	1/1	0.27	0.93	95,95,95,95	0
86	OHX	1	4168	7/7	0.26	0.93	162,162,162,162	0
85	MG	5	3525	1/1	0.85	0.91	64,64,64,64	0
86	OHX	1	4204	7/7	0.20	0.91	158,158,158,158	0
85	MG	6	1909	1/1	0.27	0.91	109,109,109,109	0
85	MG	5	3799	1/1	0.20	0.91	99,99,99,99	0
86	OHX	6	2136	7/7	0.22	0.91	168,168,168,168	0
85	MG	n0	201	1/1	0.30	0.90	40,40,40,40	0
86	OHX	5	4083	7/7	0.27	0.90	132,132,132,132	0
85	MG	15	303	1/1	0.32	0.89	63,63,63,63	0
85	MG	2	1913	1/1	0.40	0.89	78,78,78,78	0
85	MG	5	3773	1/1	0.24	0.89	81,81,81,81	0
85	MG	5	3521	1/1	0.32	0.88	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	6	2022	1/1	0.41	0.87	83,83,83,83	0
86	OHX	5	4132	7/7	0.30	0.87	161,161,161,161	0
86	OHX	5	3903	7/7	0.20	0.86	76,76,76,76	0
86	OHX	1	3995	7/7	0.34	0.86	135,135,135,135	0
86	OHX	5	4206	7/7	0.33	0.85	126,126,126,126	0
85	MG	5	3602	1/1	0.38	0.84	38,38,38,38	0
86	OHX	1	4159	7/7	0.24	0.84	169,169,169,169	0
85	MG	5	3441	1/1	0.26	0.84	38,38,38,38	0
85	MG	1	3516	1/1	0.28	0.84	35,35,35,35	0
85	MG	5	3860	1/1	0.39	0.84	48,48,48,48	0
86	OHX	7	228	7/7	0.25	0.83	142,142,142,142	0
86	OHX	M7	207	7/7	0.50	0.83	159,159,159,159	0
86	OHX	1	4073	7/7	0.21	0.83	147,147,147,147	0
85	MG	1	3711	1/1	0.42	0.83	40,40,40,40	0
85	MG	1	3430	1/1	0.25	0.83	42,42,42,42	0
85	MG	1	3432	1/1	0.32	0.82	39,39,39,39	0
85	MG	n3	201	1/1	0.27	0.82	24,24,24,24	0
86	OHX	1	4068	7/7	0.54	0.82	122,122,122,122	0
85	MG	5	3788	1/1	0.27	0.82	57,57,57,57	0
85	MG	n8	202	1/1	0.38	0.82	52,52,52,52	0
86	OHX	6	2052	7/7	0.20	0.81	95,95,95,95	0
85	MG	1	3672	1/1	0.28	0.81	68,68,68,68	0
85	MG	6	2206	1/1	0.23	0.80	80,80,80,80	0
85	MG	1	3403	1/1	0.27	0.80	41,41,41,41	0
85	MG	n9	101	1/1	0.29	0.79	40,40,40,40	0
85	MG	1	3562	1/1	0.31	0.78	39,39,39,39	0
85	MG	5	3517	1/1	0.25	0.77	30,30,30,30	0
86	OHX	6	2189	7/7	0.29	0.77	176,176,176,176	0
85	MG	2	1979	1/1	0.32	0.77	62,62,62,62	0
85	MG	1	3743	1/1	0.35	0.76	54,54,54,54	0
86	OHX	1	3858	7/7	0.21	0.76	62,62,62,62	0
86	OHX	6	2050	7/7	0.19	0.76	89,89,89,89	0
85	MG	1	3654	1/1	0.34	0.75	45,45,45,45	0
85	MG	2	1931	1/1	0.24	0.75	61,61,61,61	0
86	OHX	5	4243	7/7	0.38	0.75	171,171,171,171	0
85	MG	5	3729	1/1	0.22	0.75	47,47,47,47	0
85	MG	5	3722	1/1	0.29	0.75	35,35,35,35	0
85	MG	1	3788	1/1	0.36	0.74	35,35,35,35	0
85	MG	1	3716	1/1	0.34	0.74	52,52,52,52	0
85	MG	1	3643	1/1	0.26	0.74	76,76,76,76	0
85	MG	1	3464	1/1	0.28	0.73	49,49,49,49	0
86	OHX	5	4215	7/7	0.21	0.73	204,204,204,204	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	0.19	0.73	50,50,50,50	0
85	MG	1	3592	1/1	0.36	0.72	20,20,20,20	0
86	OHX	1	3857	7/7	0.23	0.71	52,52,52,52	0
86	OHX	2	2164	7/7	0.19	0.71	172,172,172,172	0
85	MG	2	1930	1/1	0.26	0.71	74,74,74,74	0
85	MG	6	2035	1/1	0.53	0.69	79,79,79,79	0
85	MG	1	3447	1/1	0.20	0.69	41,41,41,41	0
85	MG	5	3573	1/1	0.25	0.68	18,18,18,18	0
85	MG	5	3456	1/1	0.46	0.68	84,84,84,84	0
85	MG	5	3767	1/1	0.28	0.67	45,45,45,45	0
86	OHX	6	2147	7/7	0.22	0.66	141,141,141,141	0
85	MG	1	3603	1/1	0.26	0.66	45,45,45,45	0
85	MG	2	1951	1/1	0.27	0.66	96,96,96,96	0
86	OHX	1	4190	7/7	0.44	0.66	165,165,165,165	0
85	MG	1	3694	1/1	0.32	0.66	59,59,59,59	0
85	MG	5	3642	1/1	0.24	0.66	58,58,58,58	0
85	MG	m7	206	1/1	0.65	0.65	58,58,58,58	0
86	OHX	5	4153	7/7	0.28	0.65	155,155,155,155	0
85	MG	6	1977	1/1	0.21	0.63	53,53,53,53	0
85	MG	2	1984	1/1	0.18	0.63	76,76,76,76	0
85	MG	5	3497	1/1	0.28	0.63	48,48,48,48	0
86	OHX	1	3860	7/7	0.27	0.62	64,64,64,64	0
86	OHX	5	4128	7/7	0.31	0.62	141,141,141,141	0
85	MG	5	3429	1/1	0.37	0.61	41,41,41,41	0
85	MG	6	2011	1/1	0.24	0.61	65,65,65,65	0
85	MG	1	3585	1/1	0.24	0.60	29,29,29,29	0
86	OHX	6	2178	7/7	0.32	0.60	171,171,171,171	0
85	MG	5	3485	1/1	0.29	0.60	28,28,28,28	0
85	MG	5	3484	1/1	0.27	0.60	53,53,53,53	0
85	MG	1	3668	1/1	0.34	0.59	73,73,73,73	0
85	MG	4	202	1/1	0.35	0.58	49,49,49,49	0
85	MG	5	3828	1/1	0.22	0.58	43,43,43,43	0
86	OHX	1	4176	7/7	0.45	0.57	165,165,165,165	0
85	MG	1	3513	1/1	0.25	0.57	41,41,41,41	0
86	OHX	2	2149	7/7	0.28	0.56	199,199,199,199	0
86	OHX	2	2116	7/7	0.23	0.55	160,160,160,160	0
86	OHX	5	4130	7/7	0.32	0.55	143,143,143,143	0
86	OHX	1	4087	7/7	0.28	0.55	142,142,142,142	0
85	MG	5	3833	1/1	0.18	0.54	76,76,76,76	0
85	MG	2	1976	1/1	0.25	0.54	62,62,62,62	0
86	OHX	5	4229	7/7	0.25	0.54	180,180,180,180	0
85	MG	d3	203	1/1	0.63	0.53	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	l9	201	1/1	0.35	0.53	50,50,50,50	0
86	OHX	s9	201	7/7	0.52	0.53	160,160,160,160	0
85	MG	5	3706	1/1	0.37	0.53	44,44,44,44	0
86	OHX	5	3895	7/7	0.20	0.52	58,58,58,58	0
85	MG	1	3453	1/1	0.70	0.52	53,53,53,53	0
86	OHX	6	2095	7/7	0.21	0.52	142,142,142,142	0
86	OHX	1	4170	7/7	0.21	0.52	200,200,200,200	0
85	MG	5	3446	1/1	0.24	0.52	43,43,43,43	0
86	OHX	1	3942	7/7	0.17	0.51	128,128,128,128	0
85	MG	6	2037	1/1	0.40	0.50	52,52,52,52	0
86	OHX	5	4098	7/7	0.22	0.50	173,173,173,173	0
85	MG	c7	201	1/1	0.46	0.49	61,61,61,61	0
85	MG	1	3416	1/1	0.26	0.49	44,44,44,44	0
86	OHX	6	2064	7/7	0.17	0.49	127,127,127,127	0
86	OHX	M7	206	7/7	0.42	0.49	135,135,135,135	0
85	MG	5	3489	1/1	0.31	0.49	59,59,59,59	0
85	MG	5	3837	1/1	0.33	0.48	56,56,56,56	0
85	MG	1	3588	1/1	0.34	0.47	47,47,47,47	0
85	MG	5	3813	1/1	0.20	0.47	63,63,63,63	0
85	MG	1	3543	1/1	0.23	0.47	57,57,57,57	0
85	MG	1	3520	1/1	0.32	0.46	25,25,25,25	0
85	MG	2	1942	1/1	0.24	0.46	80,80,80,80	0
85	MG	n6	201	1/1	0.47	0.45	54,54,54,54	0
85	MG	6	2044	1/1	0.55	0.45	84,84,84,84	0
86	OHX	1	3871	7/7	0.19	0.45	69,69,69,69	0
85	MG	1	3713	1/1	0.31	0.45	48,48,48,48	0
85	MG	1	3641	1/1	0.17	0.43	54,54,54,54	0
86	OHX	1	4124	7/7	0.16	0.43	143,143,143,143	0
86	OHX	1	4174	7/7	0.45	0.43	177,177,177,177	0
86	OHX	7	226	7/7	0.30	0.42	132,132,132,132	0
86	OHX	5	4142	7/7	0.35	0.42	138,138,138,138	0
86	OHX	2	2172	7/7	0.30	0.41	174,174,174,174	0
85	MG	1	3505	1/1	0.26	0.41	35,35,35,35	0
85	MG	5	3718	1/1	0.25	0.41	28,28,28,28	0
85	MG	5	3633	1/1	0.25	0.40	45,45,45,45	0
86	OHX	1	4108	7/7	0.28	0.39	140,140,140,140	0
86	OHX	2	2034	7/7	0.18	0.39	110,110,110,110	0
86	OHX	6	2076	7/7	0.15	0.39	133,133,133,133	0
85	MG	5	3471	1/1	0.29	0.39	46,46,46,46	0
85	MG	5	3588	1/1	0.32	0.38	39,39,39,39	0
85	MG	5	3710	1/1	0.40	0.38	48,48,48,48	0
85	MG	5	3461	1/1	0.48	0.38	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4134	7/7	0.24	0.38	155,155,155,155	0
85	MG	5	3881	1/1	0.19	0.38	56,56,56,56	0
85	MG	5	3742	1/1	0.27	0.38	51,51,51,51	0
85	MG	5	3648	1/1	0.25	0.37	46,46,46,46	0
86	OHX	1	3877	7/7	0.20	0.36	83,83,83,83	0
85	MG	1	3651	1/1	0.30	0.36	45,45,45,45	0
85	MG	c9	201	1/1	0.72	0.36	65,65,65,65	0
85	MG	1	3490	1/1	0.22	0.36	36,36,36,36	0
85	MG	5	3488	1/1	0.41	0.35	49,49,49,49	0
85	MG	M6	201	1/1	0.27	0.35	43,43,43,43	0
86	OHX	1	4156	7/7	0.20	0.34	176,176,176,176	0
85	MG	l2	303	1/1	0.68	0.33	46,46,46,46	0
85	MG	5	3716	1/1	0.15	0.33	55,55,55,55	0
85	MG	5	3816	1/1	0.17	0.32	78,78,78,78	0
85	MG	1	3731	1/1	0.52	0.32	60,60,60,60	0
86	OHX	6	2200	7/7	0.22	0.32	174,174,174,174	0
85	MG	5	3693	1/1	0.24	0.32	43,43,43,43	0
86	OHX	5	4010	7/7	0.18	0.32	166,166,166,166	0
86	OHX	5	3992	7/7	0.19	0.31	122,122,122,122	0
85	MG	6	2012	1/1	0.20	0.31	54,54,54,54	0
85	MG	2	1920	1/1	0.44	0.31	68,68,68,68	0
85	MG	m7	204	1/1	0.38	0.31	40,40,40,40	0
85	MG	5	3406	1/1	0.22	0.31	36,36,36,36	0
85	MG	1	3512	1/1	0.24	0.31	25,25,25,25	0
86	OHX	5	3907	7/7	0.20	0.30	71,71,71,71	0
86	OHX	5	4087	7/7	0.34	0.30	137,137,137,137	0
86	OHX	1	4095	7/7	0.19	0.30	147,147,147,147	0
86	OHX	5	3897	7/7	0.21	0.30	68,68,68,68	0
86	OHX	2	2033	7/7	0.20	0.29	121,121,121,121	0
85	MG	o3	201	1/1	0.63	0.29	47,47,47,47	0
86	OHX	1	3863	7/7	0.20	0.29	66,66,66,66	0
85	MG	6	2038	1/1	0.58	0.29	96,96,96,96	0
85	MG	5	3824	1/1	0.29	0.29	56,56,56,56	0
85	MG	M5	302	1/1	0.45	0.29	55,55,55,55	0
85	MG	5	3635	1/1	0.29	0.28	54,54,54,54	0
85	MG	D4	201	1/1	0.30	0.28	72,72,72,72	0
85	MG	5	3725	1/1	0.20	0.27	41,41,41,41	0
85	MG	2	1962	1/1	0.40	0.27	76,76,76,76	0
85	MG	L2	301	1/1	0.26	0.27	40,40,40,40	0
85	MG	5	3747	1/1	0.39	0.27	60,60,60,60	0
85	MG	4	222	1/1	0.29	0.27	80,80,80,80	0
86	OHX	1	3961	7/7	0.19	0.26	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3448	1/1	0.22	0.26	52,52,52,52	0
85	MG	6	1979	1/1	0.21	0.26	81,81,81,81	0
86	OHX	6	2132	7/7	0.39	0.25	157,157,157,157	0
85	MG	5	3615	1/1	0.43	0.25	48,48,48,48	0
86	OHX	1	4102	7/7	0.48	0.24	142,142,142,142	0
85	MG	5	3549	1/1	0.25	0.24	29,29,29,29	0
85	MG	5	3660	1/1	0.41	0.24	44,44,44,44	0
85	MG	c8	201	1/1	0.48	0.24	68,68,68,68	0
85	MG	5	3453	1/1	0.26	0.23	45,45,45,45	0
86	OHX	14	403	7/7	0.19	0.23	175,175,175,175	0
86	OHX	1	4138	7/7	0.36	0.23	167,167,167,167	0
85	MG	1	3777	1/1	0.23	0.23	63,63,63,63	0
85	MG	6	1905	1/1	0.30	0.22	56,56,56,56	0
85	MG	1	3550	1/1	0.31	0.22	38,38,38,38	0
85	MG	3	213	1/1	0.32	0.22	59,59,59,59	0
85	MG	5	3723	1/1	0.42	0.21	84,84,84,84	0
86	OHX	2	2030	7/7	0.18	0.21	118,118,118,118	0
85	MG	1	3580	1/1	0.26	0.20	43,43,43,43	0
85	MG	5	3470	1/1	0.28	0.20	44,44,44,44	0
86	OHX	2	2146	7/7	0.24	0.20	153,153,153,153	0
86	OHX	1	3867	7/7	0.19	0.20	67,67,67,67	0
86	OHX	5	4070	7/7	0.22	0.20	156,156,156,156	0
86	OHX	6	2084	7/7	0.16	0.19	156,156,156,156	0
86	OHX	5	4221	7/7	0.21	0.19	167,167,167,167	0
86	OHX	1	4053	7/7	0.28	0.19	145,145,145,145	0
86	OHX	6	2148	7/7	0.29	0.19	157,157,157,157	0
86	OHX	1	4175	7/7	0.18	0.19	246,246,246,246	0
86	OHX	5	4183	7/7	0.18	0.19	195,195,195,195	0
85	MG	M7	203	1/1	0.28	0.19	38,38,38,38	0
85	MG	1	3549	1/1	0.29	0.19	37,37,37,37	0
86	OHX	5	4144	7/7	0.32	0.19	167,167,167,167	0
86	OHX	5	3991	7/7	0.19	0.18	115,115,115,115	0
85	MG	8	201	1/1	0.40	0.18	41,41,41,41	0
86	OHX	6	2047	7/7	0.21	0.18	85,85,85,85	0
85	MG	m7	203	1/1	0.36	0.18	48,48,48,48	0
86	OHX	1	4106	7/7	0.34	0.18	132,132,132,132	0
87	ZN	d7	101	1/1	0.58	0.18	160,160,160,160	0
86	OHX	M9	202	7/7	0.33	0.18	185,185,185,185	0
86	OHX	1	3936	7/7	0.17	0.18	111,111,111,111	0
86	OHX	1	4041	7/7	0.24	0.17	126,126,126,126	0
86	OHX	1	4199	7/7	0.29	0.17	164,164,164,164	0
86	OHX	5	3996	7/7	0.19	0.17	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4198	7/7	0.30	0.17	157,157,157,157	0
87	ZN	D7	101	1/1	0.48	0.17	176,176,176,176	0
85	MG	1	3582	1/1	0.40	0.17	49,49,49,49	0
86	OHX	1	4189	7/7	0.18	0.17	184,184,184,184	0
85	MG	5	3667	1/1	0.24	0.15	66,66,66,66	0
85	MG	2	1907	1/1	0.25	0.15	48,48,48,48	0
85	MG	2	1928	1/1	0.31	0.14	97,97,97,97	0
85	MG	5	3620	1/1	0.27	0.14	48,48,48,48	0
86	OHX	6	2191	7/7	0.29	0.14	192,192,192,192	0
86	OHX	5	3963	7/7	0.14	0.13	117,117,117,117	0
86	OHX	7	225	7/7	0.19	0.13	154,154,154,154	0
85	MG	1	3773	1/1	0.17	0.13	46,46,46,46	0
85	MG	5	3628	1/1	0.21	0.12	30,30,30,30	0
86	OHX	6	2070	7/7	0.14	0.12	125,125,125,125	0
85	MG	6	1922	1/1	0.19	0.12	78,78,78,78	0
85	MG	1	3568	1/1	0.36	0.11	43,43,43,43	0
85	MG	5	3835	1/1	0.40	0.11	60,60,60,60	0
85	MG	5	3805	1/1	0.23	0.11	44,44,44,44	0
86	OHX	1	4118	7/7	0.27	0.11	124,124,124,124	0
85	MG	6	1982	1/1	0.34	0.10	56,56,56,56	0
85	MG	5	3424	1/1	0.29	0.10	38,38,38,38	0
85	MG	7	203	1/1	0.23	0.10	23,23,23,23	0
85	MG	8	203	1/1	0.37	0.09	68,68,68,68	0
85	MG	6	1992	1/1	0.18	0.09	58,58,58,58	0
85	MG	2	1956	1/1	0.33	0.09	59,59,59,59	0
85	MG	5	3415	1/1	0.32	0.09	56,56,56,56	0
85	MG	5	3748	1/1	0.20	0.08	47,47,47,47	0
85	MG	1	3484	1/1	0.23	0.08	41,41,41,41	0
86	OHX	2	2027	7/7	0.20	0.08	89,89,89,89	0
86	OHX	1	4161	7/7	0.27	0.07	153,153,153,153	0
86	OHX	1	4144	7/7	0.33	0.07	159,159,159,159	0
86	OHX	6	2171	7/7	0.22	0.06	133,133,133,133	0
85	MG	1	3759	1/1	0.28	0.06	47,47,47,47	0
86	OHX	1	4166	7/7	0.15	0.06	179,179,179,179	0
86	OHX	6	2051	7/7	0.20	0.05	85,85,85,85	0
85	MG	5	3416	1/1	0.28	0.05	37,37,37,37	0
85	MG	1	3606	1/1	0.19	0.05	48,48,48,48	0
85	MG	2	1964	1/1	0.24	0.05	96,96,96,96	0
85	MG	2	1982	1/1	0.26	0.05	76,76,76,76	0
85	MG	6	2034	1/1	0.30	0.04	94,94,94,94	0
85	MG	2	1999	1/1	0.33	0.04	79,79,79,79	0
85	MG	5	3685	1/1	0.25	0.03	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2157	7/7	0.21	0.03	163,163,163,163	0
86	OHX	1	4059	7/7	0.25	0.03	149,149,149,149	0
85	MG	1	3623	1/1	0.24	0.03	36,36,36,36	0
85	MG	1	3677	1/1	0.26	0.02	70,70,70,70	0
86	OHX	m7	207	7/7	0.53	0.02	160,160,160,160	0
85	MG	4	206	1/1	0.22	0.02	19,19,19,19	0
85	MG	5	3826	1/1	0.34	0.02	48,48,48,48	0
86	OHX	5	4233	7/7	0.21	0.02	169,169,169,169	0
85	MG	5	3883	1/1	0.28	0.01	36,36,36,36	0
85	MG	1	3735	1/1	0.18	0.01	48,48,48,48	0
85	MG	5	3526	1/1	0.20	0.01	41,41,41,41	0
85	MG	1	3448	1/1	0.21	0.01	34,34,34,34	0
86	OHX	1	3926	7/7	0.17	0.01	108,108,108,108	0
86	OHX	6	2127	7/7	0.38	0.01	149,149,149,149	0
85	MG	5	3755	1/1	0.22	0.00	74,74,74,74	0
85	MG	1	3814	1/1	0.20	-0.02	51,51,51,51	0
85	MG	M0	302	1/1	0.57	-0.03	38,38,38,38	0
86	OHX	5	4118	7/7	0.17	-0.04	165,165,165,165	0
85	MG	5	3712	1/1	0.34	-0.04	54,54,54,54	0
85	MG	1	3476	1/1	0.20	-0.05	44,44,44,44	0
86	OHX	5	4035	7/7	0.19	-0.05	170,170,170,170	0
86	OHX	1	4093	7/7	0.15	-0.05	175,175,175,175	0
85	MG	L3	402	1/1	0.45	-0.05	71,71,71,71	0
85	MG	1	3770	1/1	0.29	-0.05	61,61,61,61	0
85	MG	l5	301	1/1	0.22	-0.05	39,39,39,39	0
86	OHX	2	2152	7/7	0.20	-0.06	166,166,166,166	0
86	OHX	6	2065	7/7	0.18	-0.06	146,146,146,146	0
85	MG	5	3402	1/1	0.22	-0.08	54,54,54,54	0
85	MG	2	1990	1/1	0.25	-0.09	110,110,110,110	0
85	MG	5	3545	1/1	0.23	-0.09	50,50,50,50	0
85	MG	1	3591	1/1	0.26	-0.09	21,21,21,21	0
85	MG	5	3770	1/1	0.48	-0.09	68,68,68,68	0
86	OHX	5	4094	7/7	0.18	-0.09	149,149,149,149	0
85	MG	5	3508	1/1	0.42	-0.09	28,28,28,28	0
85	MG	5	3499	1/1	0.24	-0.09	42,42,42,42	0
85	MG	1	3801	1/1	0.34	-0.09	62,62,62,62	0
86	OHX	2	2137	7/7	0.33	-0.09	182,182,182,182	0
85	MG	1	3627	1/1	0.24	-0.10	31,31,31,31	0
85	MG	4	207	1/1	0.26	-0.10	35,35,35,35	0
86	OHX	1	4177	7/7	0.24	-0.10	165,165,165,165	0
85	MG	6	1935	1/1	0.27	-0.10	86,86,86,86	0
86	OHX	1	3890	7/7	0.18	-0.11	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3576	1/1	0.32	-0.11	45,45,45,45	0
86	OHX	1	4210	7/7	0.25	-0.12	171,171,171,171	0
85	MG	5	3581	1/1	0.26	-0.12	46,46,46,46	0
85	MG	1	3526	1/1	0.22	-0.12	48,48,48,48	0
85	MG	1	3655	1/1	0.24	-0.13	47,47,47,47	0
85	MG	s1	301	1/1	0.39	-0.13	93,93,93,93	0
85	MG	1	3425	1/1	0.27	-0.14	69,69,69,69	0
86	OHX	2	2099	7/7	0.30	-0.14	170,170,170,170	0
85	MG	6	1984	1/1	0.19	-0.15	90,90,90,90	0
85	MG	1	3714	1/1	0.26	-0.16	82,82,82,82	0
86	OHX	5	4219	7/7	0.38	-0.16	176,176,176,176	0
86	OHX	5	4145	7/7	0.23	-0.16	166,166,166,166	0
85	MG	1	3838	1/1	0.20	-0.17	49,49,49,49	0
85	MG	5	3408	1/1	0.22	-0.17	46,46,46,46	0
85	MG	6	1931	1/1	0.20	-0.17	53,53,53,53	0
86	OHX	2	2104	7/7	0.34	-0.18	143,143,143,143	0
86	OHX	5	4202	7/7	0.34	-0.18	172,172,172,172	0
85	MG	O7	102	1/1	0.40	-0.18	66,66,66,66	0
86	OHX	1	4075	7/7	0.30	-0.18	150,150,150,150	0
85	MG	2	1960	1/1	0.23	-0.18	69,69,69,69	0
85	MG	5	3548	1/1	0.26	-0.18	60,60,60,60	0
86	OHX	2	2144	7/7	0.24	-0.18	182,182,182,182	0
85	MG	2	1908	1/1	0.36	-0.18	78,78,78,78	0
86	OHX	5	4103	7/7	0.28	-0.18	154,154,154,154	0
85	MG	5	4251	1/1	0.28	-0.19	47,47,47,47	0
85	MG	5	3454	1/1	0.31	-0.19	30,30,30,30	0
85	MG	5	3612	1/1	0.26	-0.19	54,54,54,54	0
86	OHX	2	2173	7/7	0.19	-0.19	168,168,168,168	0
85	MG	6	2019	1/1	0.23	-0.20	59,59,59,59	0
85	MG	2	2022	1/1	0.40	-0.20	134,134,134,134	0
85	MG	5	3861	1/1	0.29	-0.20	37,37,37,37	0
85	MG	3	206	1/1	0.23	-0.20	25,25,25,25	0
85	MG	2	1927	1/1	0.30	-0.21	49,49,49,49	0
85	MG	6	1907	1/1	0.19	-0.21	79,79,79,79	0
86	OHX	d9	102	7/7	0.24	-0.22	179,179,179,179	0
85	MG	1	3521	1/1	0.28	-0.22	28,28,28,28	0
85	MG	8	212	1/1	0.37	-0.22	67,67,67,67	0
85	MG	5	3674	1/1	0.26	-0.23	43,43,43,43	0
85	MG	1	3666	1/1	0.15	-0.23	89,89,89,89	0
86	OHX	1	4134	7/7	0.22	-0.23	166,166,166,166	0
86	OHX	6	2173	7/7	0.20	-0.24	164,164,164,164	0
85	MG	N8	201	1/1	0.32	-0.24	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	1	4049	7/7	0.23	-0.24	120,120,120,120	0
85	MG	1	3775	1/1	0.21	-0.25	49,49,49,49	0
85	MG	1	3851	1/1	0.21	-0.25	68,68,68,68	0
86	OHX	6	2192	7/7	0.17	-0.25	173,173,173,173	0
85	MG	1	3610	1/1	0.25	-0.25	37,37,37,37	0
86	OHX	1	4165	7/7	0.19	-0.25	141,141,141,141	0
85	MG	1	3600	1/1	0.20	-0.26	40,40,40,40	0
86	OHX	5	4127	7/7	0.14	-0.26	211,211,211,211	0
86	OHX	2	2102	7/7	0.17	-0.26	166,166,166,166	0
86	OHX	1	4030	7/7	0.24	-0.27	111,111,111,111	0
85	MG	5	3509	1/1	0.30	-0.27	44,44,44,44	0
86	OHX	2	2180	7/7	0.46	-0.27	186,186,186,186	0
85	MG	5	3790	1/1	0.22	-0.27	60,60,60,60	0
86	OHX	5	4080	7/7	0.26	-0.27	147,147,147,147	0
86	OHX	1	3872	7/7	0.18	-0.27	75,75,75,75	0
86	OHX	1	3892	7/7	0.15	-0.28	95,95,95,95	0
85	MG	1	3554	1/1	0.24	-0.28	50,50,50,50	0
86	OHX	5	4222	7/7	0.18	-0.28	184,184,184,184	0
86	OHX	8	227	7/7	0.22	-0.29	150,150,150,150	0
86	OHX	D9	102	7/7	0.20	-0.29	164,164,164,164	0
85	MG	1	4212	1/1	0.29	-0.29	34,34,34,34	0
85	MG	6	1938	1/1	0.24	-0.29	65,65,65,65	0
86	OHX	6	2201	7/7	0.16	-0.30	173,173,173,173	0
85	MG	M7	201	1/1	0.33	-0.30	69,69,69,69	0
85	MG	1	3805	1/1	0.26	-0.30	50,50,50,50	0
86	OHX	6	2128	7/7	0.22	-0.30	164,164,164,164	0
86	OHX	1	4180	7/7	0.15	-0.31	167,167,167,167	0
86	OHX	5	4058	7/7	0.14	-0.31	170,170,170,170	0
85	MG	6	1934	1/1	0.25	-0.31	61,61,61,61	0
86	OHX	5	4178	7/7	0.17	-0.32	168,168,168,168	0
85	MG	1	3832	1/1	0.25	-0.32	64,64,64,64	0
86	OHX	1	4114	7/7	0.20	-0.32	157,157,157,157	0
85	MG	1	3681	1/1	0.54	-0.32	53,53,53,53	0
86	OHX	1	3910	7/7	0.20	-0.32	107,107,107,107	0
85	MG	5	3695	1/1	0.21	-0.33	72,72,72,72	0
85	MG	m5	301	1/1	0.43	-0.33	42,42,42,42	0
85	MG	6	2036	1/1	0.32	-0.33	74,74,74,74	0
85	MG	6	2020	1/1	0.19	-0.33	128,128,128,128	0
85	MG	1	3633	1/1	0.33	-0.33	71,71,71,71	0
85	MG	M0	303	1/1	0.28	-0.33	41,41,41,41	0
86	OHX	2	2073	7/7	0.18	-0.33	135,135,135,135	0
85	MG	M7	204	1/1	0.27	-0.33	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2096	7/7	0.15	-0.34	163,163,163,163	0
86	OHX	5	3990	7/7	0.14	-0.34	136,136,136,136	0
86	OHX	5	4141	7/7	0.26	-0.35	141,141,141,141	0
86	OHX	1	4128	7/7	0.19	-0.35	142,142,142,142	0
86	OHX	1	4065	7/7	0.22	-0.35	140,140,140,140	0
86	OHX	5	4220	7/7	0.20	-0.36	177,177,177,177	0
85	MG	1	3579	1/1	0.28	-0.36	33,33,33,33	0
85	MG	1	3614	1/1	0.26	-0.36	54,54,54,54	0
85	MG	5	3803	1/1	0.30	-0.36	76,76,76,76	0
86	OHX	1	4097	7/7	0.33	-0.37	165,165,165,165	0
86	OHX	6	2175	7/7	0.18	-0.37	181,181,181,181	0
86	OHX	6	2170	7/7	0.19	-0.37	176,176,176,176	0
86	OHX	1	4188	7/7	0.14	-0.37	176,176,176,176	0
86	OHX	5	3933	7/7	0.17	-0.37	103,103,103,103	0
86	OHX	5	3910	7/7	0.19	-0.37	70,70,70,70	0
86	OHX	5	4136	7/7	0.18	-0.37	160,160,160,160	0
85	MG	5	3741	1/1	0.25	-0.38	47,47,47,47	0
86	OHX	2	2163	7/7	0.25	-0.38	183,183,183,183	0
86	OHX	6	2167	7/7	0.15	-0.38	194,194,194,194	0
85	MG	5	3531	1/1	0.18	-0.38	59,59,59,59	0
86	OHX	5	4040	7/7	0.26	-0.38	126,126,126,126	0
86	OHX	2	2177	7/7	0.28	-0.38	202,202,202,202	0
86	OHX	1	3880	7/7	0.19	-0.38	91,91,91,91	0
85	MG	S4	301	1/1	0.37	-0.38	71,71,71,71	0
86	OHX	5	4238	7/7	0.24	-0.38	125,125,125,125	0
85	MG	5	3609	1/1	0.49	-0.38	43,43,43,43	0
86	OHX	6	2141	7/7	0.14	-0.38	181,181,181,181	0
85	MG	1	3509	1/1	0.23	-0.39	34,34,34,34	0
85	MG	4	204	1/1	0.20	-0.39	79,79,79,79	0
85	MG	2	1912	1/1	0.17	-0.39	71,71,71,71	0
85	MG	o4	201	1/1	0.45	-0.39	45,45,45,45	0
86	OHX	5	4102	7/7	0.23	-0.39	143,143,143,143	0
85	MG	1	3744	1/1	0.24	-0.40	41,41,41,41	0
86	OHX	1	4151	7/7	0.25	-0.40	154,154,154,154	0
86	OHX	6	2116	7/7	0.29	-0.40	159,159,159,159	0
86	OHX	1	4141	7/7	0.32	-0.41	174,174,174,174	0
85	MG	5	3567	1/1	0.25	-0.42	37,37,37,37	0
86	OHX	5	4235	7/7	0.30	-0.42	204,204,204,204	0
85	MG	2	1939	1/1	0.21	-0.42	73,73,73,73	0
85	MG	5	3523	1/1	0.31	-0.42	57,57,57,57	0
86	OHX	5	4204	7/7	0.30	-0.42	150,150,150,150	0
85	MG	1	3500	1/1	0.25	-0.42	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	s4	301	7/7	0.36	-0.43	168,168,168,168	0
86	OHX	5	4164	7/7	0.17	-0.43	160,160,160,160	0
86	OHX	14	402	7/7	0.17	-0.43	182,182,182,182	0
85	MG	1	3401	1/1	0.30	-0.44	42,42,42,42	0
86	OHX	5	4090	7/7	0.20	-0.44	144,144,144,144	0
85	MG	1	3791	1/1	0.18	-0.44	53,53,53,53	0
86	OHX	5	4171	7/7	0.24	-0.44	160,160,160,160	0
85	MG	6	2033	1/1	0.30	-0.45	70,70,70,70	0
85	MG	m5	305	1/1	0.52	-0.45	87,87,87,87	0
85	MG	1	3422	1/1	0.24	-0.45	39,39,39,39	0
85	MG	6	1996	1/1	0.15	-0.45	67,67,67,67	0
86	OHX	5	4200	7/7	0.26	-0.46	162,162,162,162	0
85	MG	6	1990	1/1	0.21	-0.46	75,75,75,75	0
86	OHX	5	4167	7/7	0.20	-0.46	126,126,126,126	0
85	MG	m1	201	1/1	0.18	-0.46	63,63,63,63	0
86	OHX	4	237	7/7	0.34	-0.47	168,168,168,168	0
85	MG	m7	202	1/1	0.39	-0.47	35,35,35,35	0
86	OHX	2	2136	7/7	0.15	-0.47	164,164,164,164	0
86	OHX	1	4155	7/7	0.17	-0.47	148,148,148,148	0
86	OHX	5	3986	7/7	0.27	-0.47	108,108,108,108	0
85	MG	1	3414	1/1	0.22	-0.47	39,39,39,39	0
86	OHX	1	3916	7/7	0.20	-0.47	79,79,79,79	0
86	OHX	1	4066	7/7	0.19	-0.47	154,154,154,154	0
86	OHX	1	3861	7/7	0.20	-0.48	64,64,64,64	0
86	OHX	4	235	7/7	0.19	-0.48	168,168,168,168	0
85	MG	6	1995	1/1	0.17	-0.48	77,77,77,77	0
86	OHX	5	4192	7/7	0.16	-0.48	146,146,146,146	0
86	OHX	C8	201	7/7	0.17	-0.48	123,123,123,123	0
85	MG	5	3815	1/1	0.18	-0.48	114,114,114,114	0
86	OHX	6	2053	7/7	0.17	-0.48	97,97,97,97	0
85	MG	2	1947	1/1	0.31	-0.49	54,54,54,54	0
85	MG	1	3688	1/1	0.27	-0.49	43,43,43,43	0
85	MG	5	3570	1/1	0.20	-0.49	48,48,48,48	0
86	OHX	5	3958	7/7	0.21	-0.49	115,115,115,115	0
86	OHX	1	4026	7/7	0.22	-0.49	150,150,150,150	0
85	MG	5	3682	1/1	0.19	-0.50	49,49,49,49	0
85	MG	5	3474	1/1	0.18	-0.50	92,92,92,92	0
85	MG	1	3459	1/1	0.24	-0.50	31,31,31,31	0
85	MG	5	3690	1/1	0.37	-0.50	58,58,58,58	0
86	OHX	1	4184	7/7	0.18	-0.50	164,164,164,164	0
86	OHX	1	4083	7/7	0.30	-0.50	150,150,150,150	0
85	MG	2	1941	1/1	0.39	-0.50	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4211	7/7	0.17	-0.51	165,165,165,165	0
85	MG	6	1970	1/1	0.33	-0.51	72,72,72,72	0
86	OHX	5	4069	7/7	0.25	-0.51	143,143,143,143	0
85	MG	5	3684	1/1	0.21	-0.51	51,51,51,51	0
86	OHX	2	2046	7/7	0.14	-0.51	137,137,137,137	0
85	MG	6	1983	1/1	0.22	-0.51	59,59,59,59	0
86	OHX	1	3977	7/7	0.22	-0.51	111,111,111,111	0
85	MG	2	1980	1/1	0.23	-0.52	69,69,69,69	0
85	MG	C1	201	1/1	0.21	-0.52	69,69,69,69	0
86	OHX	2	2029	7/7	0.16	-0.53	109,109,109,109	0
86	OHX	6	2109	7/7	0.25	-0.53	131,131,131,131	0
85	MG	6	1961	1/1	0.18	-0.53	50,50,50,50	0
85	MG	6	1968	1/1	0.20	-0.53	64,64,64,64	0
86	OHX	5	4196	7/7	0.19	-0.53	144,144,144,144	0
86	OHX	2	2085	7/7	0.23	-0.53	137,137,137,137	0
85	MG	5	3625	1/1	0.34	-0.54	43,43,43,43	0
86	OHX	1	4009	7/7	0.27	-0.54	143,143,143,143	0
86	OHX	6	2146	7/7	0.12	-0.54	160,160,160,160	0
85	MG	N6	201	1/1	0.22	-0.54	46,46,46,46	0
85	MG	2	2019	1/1	0.19	-0.55	70,70,70,70	0
85	MG	5	3862	1/1	0.24	-0.56	51,51,51,51	0
86	OHX	1	4191	7/7	0.17	-0.56	165,165,165,165	0
86	OHX	5	4194	7/7	0.20	-0.56	147,147,147,147	0
85	MG	1	3846	1/1	0.22	-0.57	33,33,33,33	0
85	MG	5	3572	1/1	0.23	-0.57	41,41,41,41	0
86	OHX	5	4055	7/7	0.17	-0.57	128,128,128,128	0
85	MG	5	3422	1/1	0.18	-0.57	45,45,45,45	0
86	OHX	2	2066	7/7	0.14	-0.58	155,155,155,155	0
85	MG	SM	301	1/1	0.22	-0.58	55,55,55,55	0
85	MG	5	3519	1/1	0.26	-0.58	40,40,40,40	0
86	OHX	5	4237	7/7	0.20	-0.58	162,162,162,162	0
85	MG	1	3419	1/1	0.28	-0.59	86,86,86,86	0
85	MG	5	3468	1/1	0.20	-0.59	35,35,35,35	0
85	MG	1	3560	1/1	0.20	-0.59	50,50,50,50	0
85	MG	5	3871	1/1	0.21	-0.59	28,28,28,28	0
85	MG	5	3585	1/1	0.19	-0.60	25,25,25,25	0
86	OHX	1	3919	7/7	0.16	-0.60	121,121,121,121	0
85	MG	n6	202	1/1	0.37	-0.60	47,47,47,47	0
86	OHX	5	4195	7/7	0.19	-0.60	148,148,148,148	0
86	OHX	5	4161	7/7	0.21	-0.60	154,154,154,154	0
85	MG	1	3726	1/1	0.24	-0.60	34,34,34,34	0
86	OHX	5	4228	7/7	0.22	-0.60	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	c1	201	1/1	0.23	-0.61	55,55,55,55	0
86	OHX	5	4191	7/7	0.15	-0.61	190,190,190,190	0
85	MG	M5	301	1/1	0.25	-0.61	39,39,39,39	0
86	OHX	6	2198	7/7	0.20	-0.61	171,171,171,171	0
85	MG	5	3505	1/1	0.29	-0.61	31,31,31,31	0
85	MG	n8	203	1/1	0.22	-0.62	43,43,43,43	0
85	MG	1	3605	1/1	0.21	-0.62	69,69,69,69	0
86	OHX	5	3967	7/7	0.15	-0.62	125,125,125,125	0
86	OHX	1	4196	7/7	0.31	-0.62	175,175,175,175	0
86	OHX	1	4062	7/7	0.17	-0.62	136,136,136,136	0
86	OHX	1	3915	7/7	0.15	-0.63	111,111,111,111	0
85	MG	1	3764	1/1	0.18	-0.63	75,75,75,75	0
86	OHX	2	2084	7/7	0.14	-0.63	161,161,161,161	0
86	OHX	m0	302	7/7	0.13	-0.64	133,133,133,133	0
85	MG	2	1993	1/1	0.17	-0.64	77,77,77,77	0
85	MG	5	3658	1/1	0.33	-0.64	61,61,61,61	0
86	OHX	6	2153	7/7	0.16	-0.64	169,169,169,169	0
86	OHX	1	3976	7/7	0.24	-0.65	125,125,125,125	0
85	MG	3	210	1/1	0.18	-0.65	52,52,52,52	0
85	MG	5	3804	1/1	0.21	-0.65	47,47,47,47	0
86	OHX	2	2140	7/7	0.14	-0.65	173,173,173,173	0
86	OHX	2	2123	7/7	0.14	-0.65	166,166,166,166	0
86	OHX	2	2106	7/7	0.10	-0.65	129,129,129,129	0
85	MG	5	3431	1/1	0.18	-0.65	40,40,40,40	0
86	OHX	1	3978	7/7	0.22	-0.66	124,124,124,124	0
85	MG	1	3532	1/1	0.29	-0.66	33,33,33,33	0
85	MG	1	3581	1/1	0.21	-0.66	48,48,48,48	0
85	MG	1	3658	1/1	0.35	-0.66	35,35,35,35	0
85	MG	1	3616	1/1	0.21	-0.67	69,69,69,69	0
86	OHX	5	4147	7/7	0.28	-0.67	165,165,165,165	0
86	OHX	6	2172	7/7	0.15	-0.67	165,165,165,165	0
86	OHX	2	2161	7/7	0.23	-0.67	175,175,175,175	0
85	MG	2	1937	1/1	0.17	-0.68	66,66,66,66	0
85	MG	4	209	1/1	0.24	-0.68	52,52,52,52	0
86	OHX	1	4146	7/7	0.18	-0.68	180,180,180,180	0
86	OHX	5	4062	7/7	0.22	-0.68	131,131,131,131	0
86	OHX	8	229	7/7	0.16	-0.68	161,161,161,161	0
86	OHX	5	3902	7/7	0.19	-0.68	60,60,60,60	0
86	OHX	1	4040	7/7	0.17	-0.70	135,135,135,135	0
86	OHX	5	4018	7/7	0.12	-0.70	144,144,144,144	0
86	OHX	2	2130	7/7	0.18	-0.71	136,136,136,136	0
85	MG	1	3685	1/1	0.33	-0.71	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3752	1/1	0.21	-0.71	71,71,71,71	0
86	OHX	1	3985	7/7	0.25	-0.71	139,139,139,139	0
85	MG	1	3642	1/1	0.21	-0.72	42,42,42,42	0
86	OHX	5	3924	7/7	0.18	-0.72	85,85,85,85	0
85	MG	1	3465	1/1	0.20	-0.72	47,47,47,47	0
86	OHX	5	3973	7/7	0.15	-0.72	129,129,129,129	0
86	OHX	6	2046	7/7	0.18	-0.72	66,66,66,66	0
86	OHX	2	2054	7/7	0.16	-0.73	132,132,132,132	0
85	MG	1	3662	1/1	0.27	-0.73	40,40,40,40	0
85	MG	6	1999	1/1	0.18	-0.73	65,65,65,65	0
85	MG	6	2041	1/1	0.22	-0.73	72,72,72,72	0
86	OHX	5	3896	7/7	0.20	-0.73	59,59,59,59	0
85	MG	n9	102	1/1	0.20	-0.74	24,24,24,24	0
86	OHX	1	3925	7/7	0.16	-0.74	118,118,118,118	0
86	OHX	5	4085	7/7	0.24	-0.74	127,127,127,127	0
85	MG	6	2025	1/1	0.17	-0.75	91,91,91,91	0
85	MG	2	1909	1/1	0.22	-0.75	73,73,73,73	0
86	OHX	4	225	7/7	0.15	-0.76	86,86,86,86	0
86	OHX	L4	404	7/7	0.24	-0.76	160,160,160,160	0
86	OHX	5	3914	7/7	0.15	-0.76	84,84,84,84	0
86	OHX	1	4001	7/7	0.19	-0.77	123,123,123,123	0
86	OHX	5	4209	7/7	0.25	-0.77	141,141,141,141	0
85	MG	2	2007	1/1	0.33	-0.77	79,79,79,79	0
85	MG	2	1901	1/1	0.33	-0.77	77,77,77,77	0
85	MG	1	3406	1/1	0.25	-0.78	45,45,45,45	0
85	MG	5	3555	1/1	0.25	-0.78	25,25,25,25	0
86	OHX	6	2063	7/7	0.16	-0.78	114,114,114,114	0
85	MG	5	3426	1/1	0.26	-0.78	46,46,46,46	0
86	OHX	5	3981	7/7	0.23	-0.78	130,130,130,130	0
86	OHX	1	4078	7/7	0.20	-0.78	153,153,153,153	0
85	MG	5	3636	1/1	0.26	-0.78	70,70,70,70	0
86	OHX	1	3878	7/7	0.16	-0.78	86,86,86,86	0
85	MG	1	3841	1/1	0.20	-0.79	51,51,51,51	0
85	MG	6	1956	1/1	0.30	-0.79	60,60,60,60	0
86	OHX	1	4120	7/7	0.15	-0.79	168,168,168,168	0
85	MG	1	3820	1/1	0.18	-0.79	57,57,57,57	0
86	OHX	8	223	7/7	0.21	-0.79	153,153,153,153	0
86	OHX	1	4178	7/7	0.19	-0.80	124,124,124,124	0
86	OHX	5	3961	7/7	0.21	-0.80	110,110,110,110	0
86	OHX	5	3995	7/7	0.22	-0.80	89,89,89,89	0
86	OHX	5	3972	7/7	0.12	-0.81	109,109,109,109	0
86	OHX	O3	201	7/7	0.18	-0.81	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2097	7/7	0.09	-0.81	172,172,172,172	0
86	OHX	1	3894	7/7	0.15	-0.81	80,80,80,80	0
86	OHX	1	3922	7/7	0.14	-0.81	121,121,121,121	0
85	MG	5	3697	1/1	0.17	-0.82	59,59,59,59	0
86	OHX	5	4072	7/7	0.30	-0.82	120,120,120,120	0
86	OHX	1	3955	7/7	0.14	-0.82	142,142,142,142	0
86	OHX	5	4101	7/7	0.20	-0.82	141,141,141,141	0
86	OHX	5	4030	7/7	0.15	-0.83	157,157,157,157	0
86	OHX	1	4060	7/7	0.21	-0.83	126,126,126,126	0
86	OHX	2	2150	7/7	0.15	-0.83	175,175,175,175	0
86	OHX	2	2056	7/7	0.14	-0.83	157,157,157,157	0
86	OHX	6	2085	7/7	0.17	-0.84	124,124,124,124	0
85	MG	1	3628	1/1	0.16	-0.84	37,37,37,37	0
85	MG	5	3888	1/1	0.22	-0.84	61,61,61,61	0
86	OHX	1	3884	7/7	0.17	-0.84	73,73,73,73	0
86	OHX	1	3972	7/7	0.19	-0.84	130,130,130,130	0
86	OHX	6	2188	7/7	0.20	-0.84	170,170,170,170	0
86	OHX	2	2139	7/7	0.25	-0.84	192,192,192,192	0
86	OHX	1	3975	7/7	0.09	-0.85	129,129,129,129	0
85	MG	L7	301	1/1	0.19	-0.85	39,39,39,39	0
85	MG	1	3747	1/1	0.29	-0.85	34,34,34,34	0
86	OHX	2	2127	7/7	0.14	-0.85	174,174,174,174	0
85	MG	1	3776	1/1	0.19	-0.85	39,39,39,39	0
85	MG	1	3826	1/1	0.22	-0.85	32,32,32,32	0
85	MG	5	3631	1/1	0.46	-0.86	54,54,54,54	0
86	OHX	1	3911	7/7	0.15	-0.86	105,105,105,105	0
86	OHX	2	2132	7/7	0.12	-0.86	176,176,176,176	0
85	MG	5	3764	1/1	0.22	-0.86	79,79,79,79	0
87	ZN	d9	101	1/1	0.13	-0.86	87,87,87,87	0
85	MG	5	3750	1/1	0.16	-0.86	51,51,51,51	0
85	MG	1	3779	1/1	0.15	-0.86	50,50,50,50	0
85	MG	2	1911	1/1	0.24	-0.86	54,54,54,54	0
85	MG	1	3613	1/1	0.12	-0.87	66,66,66,66	0
86	OHX	1	4202	7/7	0.16	-0.87	163,163,163,163	0
86	OHX	m1	202	7/7	0.24	-0.87	180,180,180,180	0
86	OHX	1	3875	7/7	0.17	-0.87	81,81,81,81	0
86	OHX	5	4004	7/7	0.26	-0.87	129,129,129,129	0
85	MG	1	3823	1/1	0.21	-0.87	43,43,43,43	0
85	MG	2	1972	1/1	0.17	-0.87	95,95,95,95	0
85	MG	N6	202	1/1	0.29	-0.87	38,38,38,38	0
86	OHX	2	2115	7/7	0.14	-0.88	178,178,178,178	0
86	OHX	6	2163	7/7	0.18	-0.88	161,161,161,161	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2124	7/7	0.09	-0.88	161,161,161,161	0
85	MG	Q2	502	1/1	0.28	-0.89	77,77,77,77	0
86	OHX	m0	303	7/7	0.16	-0.89	145,145,145,145	0
87	ZN	e1	501	1/1	0.13	-0.89	158,158,158,158	0
86	OHX	6	2081	7/7	0.11	-0.89	109,109,109,109	0
85	MG	5	3552	1/1	0.22	-0.89	39,39,39,39	0
86	OHX	6	2061	7/7	0.15	-0.89	103,103,103,103	0
85	MG	1	3567	1/1	0.20	-0.89	24,24,24,24	0
86	OHX	6	2100	7/7	0.14	-0.89	192,192,192,192	0
86	OHX	1	4162	7/7	0.11	-0.90	211,211,211,211	0
85	MG	1	3510	1/1	0.29	-0.90	37,37,37,37	0
85	MG	5	3506	1/1	0.18	-0.90	41,41,41,41	0
85	MG	2	1986	1/1	0.16	-0.90	74,74,74,74	0
86	OHX	1	4018	7/7	0.10	-0.90	169,169,169,169	0
86	OHX	4	229	7/7	0.21	-0.90	126,126,126,126	0
86	OHX	5	3900	7/7	0.16	-0.90	73,73,73,73	0
85	MG	1	3703	1/1	0.17	-0.91	49,49,49,49	0
86	OHX	1	4098	7/7	0.19	-0.91	166,166,166,166	0
86	OHX	1	4113	7/7	0.14	-0.91	148,148,148,148	0
85	MG	2	1985	1/1	0.18	-0.91	67,67,67,67	0
86	OHX	6	2159	7/7	0.16	-0.91	137,137,137,137	0
86	OHX	5	4025	7/7	0.14	-0.91	166,166,166,166	0
86	OHX	2	2035	7/7	0.16	-0.91	112,112,112,112	0
86	OHX	1	4029	7/7	0.10	-0.92	163,163,163,163	0
86	OHX	2	2131	7/7	0.17	-0.92	153,153,153,153	0
85	MG	1	3676	1/1	0.26	-0.92	64,64,64,64	0
86	OHX	1	3932	7/7	0.18	-0.92	105,105,105,105	0
86	OHX	1	3928	7/7	0.14	-0.92	115,115,115,115	0
85	MG	d3	201	1/1	0.41	-0.92	49,49,49,49	0
85	MG	1	3440	1/1	0.21	-0.92	47,47,47,47	0
85	MG	6	2001	1/1	0.15	-0.92	58,58,58,58	0
86	OHX	5	4172	7/7	0.25	-0.92	152,152,152,152	0
86	OHX	5	3980	7/7	0.12	-0.92	119,119,119,119	0
86	OHX	2	2145	7/7	0.17	-0.92	166,166,166,166	0
85	MG	5	3586	1/1	0.18	-0.92	71,71,71,71	0
86	OHX	8	218	7/7	0.10	-0.92	153,153,153,153	0
86	OHX	1	3909	7/7	0.15	-0.93	109,109,109,109	0
86	OHX	2	2031	7/7	0.13	-0.93	127,127,127,127	0
86	OHX	5	3929	7/7	0.13	-0.93	83,83,83,83	0
85	MG	1	3481	1/1	0.22	-0.94	62,62,62,62	0
86	OHX	5	4096	7/7	0.14	-0.94	162,162,162,162	0
86	OHX	1	3996	7/7	0.20	-0.94	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3966	7/7	0.15	-0.94	92,92,92,92	0
86	OHX	5	3921	7/7	0.18	-0.95	89,89,89,89	0
86	OHX	1	4084	7/7	0.21	-0.95	107,107,107,107	0
85	MG	m6	201	1/1	0.20	-0.95	32,32,32,32	0
86	OHX	1	3917	7/7	0.15	-0.95	102,102,102,102	0
86	OHX	5	4143	7/7	0.21	-0.95	158,158,158,158	0
86	OHX	2	2023	7/7	0.17	-0.95	84,84,84,84	0
86	OHX	1	3988	7/7	0.17	-0.95	122,122,122,122	0
85	MG	2	1946	1/1	0.19	-0.96	92,92,92,92	0
86	OHX	6	2106	7/7	0.14	-0.96	151,151,151,151	0
85	MG	5	3547	1/1	0.23	-0.96	51,51,51,51	0
85	MG	5	3599	1/1	0.15	-0.97	53,53,53,53	0
85	MG	5	3428	1/1	0.22	-0.97	29,29,29,29	0
85	MG	5	3735	1/1	0.19	-0.97	49,49,49,49	0
86	OHX	1	4105	7/7	0.18	-0.98	156,156,156,156	0
86	OHX	2	2098	7/7	0.13	-0.99	141,141,141,141	0
86	OHX	2	2095	7/7	0.13	-0.99	159,159,159,159	0
86	OHX	6	2154	7/7	0.15	-0.99	162,162,162,162	0
86	OHX	1	4056	7/7	0.12	-0.99	169,169,169,169	0
86	OHX	8	222	7/7	0.13	-0.99	166,166,166,166	0
85	MG	1	3488	1/1	0.27	-1.00	36,36,36,36	0
86	OHX	8	217	7/7	0.20	-1.00	126,126,126,126	0
85	MG	2	2005	1/1	0.22	-1.00	67,67,67,67	0
86	OHX	5	4184	7/7	0.17	-1.00	149,149,149,149	0
86	OHX	1	3869	7/7	0.16	-1.00	80,80,80,80	0
86	OHX	5	3926	7/7	0.18	-1.00	85,85,85,85	0
85	MG	1	3424	1/1	0.24	-1.00	34,34,34,34	0
85	MG	1	3696	1/1	0.19	-1.00	49,49,49,49	0
85	MG	1	3797	1/1	0.18	-1.00	67,67,67,67	0
85	MG	5	3691	1/1	0.17	-1.00	44,44,44,44	0
85	MG	L2	302	1/1	0.23	-1.01	36,36,36,36	0
86	OHX	5	3949	7/7	0.16	-1.01	101,101,101,101	0
86	OHX	6	2202	7/7	0.16	-1.01	228,228,228,228	0
85	MG	5	3762	1/1	0.14	-1.02	58,58,58,58	0
85	MG	L3	403	1/1	0.17	-1.02	48,48,48,48	0
86	OHX	5	3994	7/7	0.19	-1.02	127,127,127,127	0
85	MG	N0	201	1/1	0.26	-1.02	45,45,45,45	0
86	OHX	1	4016	7/7	0.17	-1.02	135,135,135,135	0
86	OHX	5	3940	7/7	0.14	-1.03	97,97,97,97	0
85	MG	5	3818	1/1	0.15	-1.03	41,41,41,41	0
85	MG	2	2000	1/1	0.12	-1.03	91,91,91,91	0
86	OHX	2	2153	7/7	0.13	-1.03	186,186,186,186	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3436	1/1	0.18	-1.03	35,35,35,35	0
85	MG	5	3540	1/1	0.22	-1.03	34,34,34,34	0
86	OHX	2	2126	7/7	0.12	-1.03	158,158,158,158	0
86	OHX	1	4158	7/7	0.17	-1.03	155,155,155,155	0
85	MG	M0	301	1/1	0.15	-1.04	88,88,88,88	0
86	OHX	6	2162	7/7	0.09	-1.04	147,147,147,147	0
85	MG	1	3656	1/1	0.23	-1.04	38,38,38,38	0
86	OHX	2	2096	7/7	0.11	-1.04	186,186,186,186	0
86	OHX	1	3949	7/7	0.10	-1.05	115,115,115,115	0
85	MG	m5	304	1/1	0.20	-1.05	50,50,50,50	0
86	OHX	6	2094	7/7	0.13	-1.05	157,157,157,157	0
86	OHX	1	3873	7/7	0.16	-1.05	77,77,77,77	0
86	OHX	2	2156	7/7	0.15	-1.06	262,262,262,262	0
85	MG	8	202	1/1	0.27	-1.06	46,46,46,46	0
85	MG	m6	202	1/1	0.14	-1.06	39,39,39,39	0
85	MG	1	3765	1/1	0.16	-1.06	46,46,46,46	0
85	MG	5	3541	1/1	0.18	-1.06	78,78,78,78	0
85	MG	5	3780	1/1	0.15	-1.07	43,43,43,43	0
86	OHX	8	215	7/7	0.17	-1.07	68,68,68,68	0
85	MG	1	3421	1/1	0.17	-1.07	37,37,37,37	0
86	OHX	8	219	7/7	0.13	-1.07	149,149,149,149	0
85	MG	5	3661	1/1	0.11	-1.07	56,56,56,56	0
85	MG	5	3421	1/1	0.20	-1.07	45,45,45,45	0
86	OHX	5	4115	7/7	0.14	-1.08	139,139,139,139	0
86	OHX	1	3920	7/7	0.11	-1.08	101,101,101,101	0
85	MG	1	3545	1/1	0.19	-1.08	43,43,43,43	0
86	OHX	6	2195	7/7	0.13	-1.08	183,183,183,183	0
86	OHX	5	4076	7/7	0.18	-1.08	136,136,136,136	0
86	OHX	s1	303	7/7	0.43	-1.08	180,180,180,180	0
85	MG	5	3637	1/1	0.17	-1.08	30,30,30,30	0
86	OHX	1	4025	7/7	0.18	-1.08	126,126,126,126	0
86	OHX	1	4201	7/7	0.19	-1.08	158,158,158,158	0
85	MG	5	3836	1/1	0.24	-1.09	53,53,53,53	0
85	MG	2	1919	1/1	0.32	-1.09	65,65,65,65	0
86	OHX	2	2091	7/7	0.14	-1.09	134,134,134,134	0
85	MG	1	3504	1/1	0.21	-1.09	32,32,32,32	0
86	OHX	5	4031	7/7	0.12	-1.09	145,145,145,145	0
86	OHX	1	4076	7/7	0.15	-1.10	139,139,139,139	0
85	MG	5	3849	1/1	0.22	-1.10	45,45,45,45	0
85	MG	1	3528	1/1	0.16	-1.10	79,79,79,79	0
86	OHX	8	220	7/7	0.14	-1.10	140,140,140,140	0
85	MG	2	1997	1/1	0.21	-1.10	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4119	7/7	0.09	-1.11	164,164,164,164	0
86	OHX	6	2055	7/7	0.16	-1.11	90,90,90,90	0
86	OHX	6	2174	7/7	0.14	-1.11	161,161,161,161	0
85	MG	2	1974	1/1	0.11	-1.11	71,71,71,71	0
85	MG	6	1926	1/1	0.15	-1.11	51,51,51,51	0
86	OHX	1	4089	7/7	0.13	-1.11	161,161,161,161	0
85	MG	5	3452	1/1	0.18	-1.11	28,28,28,28	0
86	OHX	5	4168	7/7	0.17	-1.11	110,110,110,110	0
85	MG	1	3427	1/1	0.14	-1.11	56,56,56,56	0
85	MG	1	3856	1/1	0.20	-1.12	65,65,65,65	0
86	OHX	5	3941	7/7	0.15	-1.12	100,100,100,100	0
86	OHX	s1	302	7/7	0.15	-1.12	100,100,100,100	0
86	OHX	1	4077	7/7	0.14	-1.12	164,164,164,164	0
85	MG	1	3590	1/1	0.23	-1.12	35,35,35,35	0
85	MG	1	3517	1/1	0.25	-1.12	22,22,22,22	0
86	OHX	6	2182	7/7	0.10	-1.12	158,158,158,158	0
86	OHX	5	4047	7/7	0.17	-1.13	127,127,127,127	0
85	MG	5	3564	1/1	0.26	-1.13	50,50,50,50	0
86	OHX	5	4113	7/7	0.11	-1.14	154,154,154,154	0
86	OHX	5	4050	7/7	0.17	-1.14	140,140,140,140	0
86	OHX	2	2121	7/7	0.23	-1.14	170,170,170,170	0
86	OHX	5	4097	7/7	0.20	-1.14	125,125,125,125	0
86	OHX	5	3916	7/7	0.18	-1.14	89,89,89,89	0
85	MG	1	3564	1/1	0.18	-1.15	33,33,33,33	0
85	MG	5	3784	1/1	0.20	-1.15	78,78,78,78	0
85	MG	5	3809	1/1	0.16	-1.15	47,47,47,47	0
86	OHX	6	2117	7/7	0.16	-1.15	139,139,139,139	0
85	MG	5	3476	1/1	0.23	-1.15	30,30,30,30	0
86	OHX	2	2138	7/7	0.19	-1.15	159,159,159,159	0
86	OHX	6	2083	7/7	0.10	-1.16	135,135,135,135	0
85	MG	5	3877	1/1	0.20	-1.16	64,64,64,64	0
85	MG	1	3420	1/1	0.19	-1.16	40,40,40,40	0
86	OHX	6	2048	7/7	0.17	-1.16	83,83,83,83	0
85	MG	4	205	1/1	0.23	-1.16	46,46,46,46	0
86	OHX	1	3883	7/7	0.18	-1.16	95,95,95,95	0
87	ZN	d6	101	1/1	0.12	-1.17	68,68,68,68	0
86	OHX	1	3960	7/7	0.10	-1.17	112,112,112,112	0
85	MG	5	3821	1/1	0.17	-1.17	32,32,32,32	0
85	MG	5	3533	1/1	0.19	-1.17	30,30,30,30	0
86	OHX	5	4023	7/7	0.16	-1.17	105,105,105,105	0
85	MG	5	3795	1/1	0.18	-1.18	42,42,42,42	0
86	OHX	2	2068	7/7	0.13	-1.18	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2120	7/7	0.14	-1.18	169,169,169,169	0
85	MG	5	3579	1/1	0.20	-1.18	33,33,33,33	0
86	OHX	6	2119	7/7	0.14	-1.18	151,151,151,151	0
85	MG	1	3670	1/1	0.14	-1.18	36,36,36,36	0
85	MG	1	3621	1/1	0.17	-1.19	56,56,56,56	0
86	OHX	6	2194	7/7	0.13	-1.19	196,196,196,196	0
86	OHX	1	4024	7/7	0.15	-1.19	156,156,156,156	0
86	OHX	5	4001	7/7	0.12	-1.19	96,96,96,96	0
86	OHX	1	4181	7/7	0.16	-1.19	160,160,160,160	0
86	OHX	1	4067	7/7	0.12	-1.20	168,168,168,168	0
85	MG	1	3732	1/1	0.18	-1.20	35,35,35,35	0
87	ZN	D9	101	1/1	0.08	-1.20	83,83,83,83	0
86	OHX	1	4071	7/7	0.14	-1.20	154,154,154,154	0
85	MG	8	206	1/1	0.17	-1.20	74,74,74,74	0
86	OHX	n1	201	7/7	0.18	-1.20	69,69,69,69	0
85	MG	d0	201	1/1	0.21	-1.20	75,75,75,75	0
85	MG	1	3523	1/1	0.18	-1.20	34,34,34,34	0
86	OHX	2	2067	7/7	0.11	-1.21	194,194,194,194	0
85	MG	6	2029	1/1	0.17	-1.21	105,105,105,105	0
86	OHX	o7	103	7/7	0.14	-1.21	126,126,126,126	0
86	OHX	1	4122	7/7	0.16	-1.22	167,167,167,167	0
86	OHX	6	2102	7/7	0.18	-1.22	133,133,133,133	0
86	OHX	6	2097	7/7	0.12	-1.22	131,131,131,131	0
85	MG	5	3514	1/1	0.21	-1.22	43,43,43,43	0
87	ZN	E1	501	1/1	0.06	-1.23	118,118,118,118	0
86	OHX	6	2072	7/7	0.10	-1.23	142,142,142,142	0
86	OHX	1	3862	7/7	0.17	-1.23	61,61,61,61	0
85	MG	2	1910	1/1	0.17	-1.23	61,61,61,61	0
86	OHX	1	3889	7/7	0.19	-1.23	87,87,87,87	0
85	MG	5	3811	1/1	0.29	-1.24	70,70,70,70	0
86	OHX	1	4099	7/7	0.12	-1.24	138,138,138,138	0
85	MG	5	3664	1/1	0.17	-1.24	44,44,44,44	0
85	MG	q1	101	1/1	0.21	-1.24	50,50,50,50	0
86	OHX	5	3977	7/7	0.21	-1.24	108,108,108,108	0
85	MG	1	3657	1/1	0.18	-1.25	68,68,68,68	0
85	MG	5	3830	1/1	0.19	-1.25	44,44,44,44	0
86	OHX	5	4210	7/7	0.11	-1.25	221,221,221,221	0
85	MG	5	3494	1/1	0.23	-1.25	42,42,42,42	0
85	MG	5	3568	1/1	0.23	-1.25	34,34,34,34	0
86	OHX	7	223	7/7	0.14	-1.26	118,118,118,118	0
86	OHX	S8	302	7/7	0.24	-1.26	182,182,182,182	0
85	MG	5	3700	1/1	0.18	-1.26	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3611	1/1	0.09	-1.27	59,59,59,59	0
86	OHX	M5	303	7/7	0.36	-1.27	130,130,130,130	0
86	OHX	s8	302	7/7	0.24	-1.27	193,193,193,193	0
85	MG	5	3440	1/1	0.20	-1.27	40,40,40,40	0
86	OHX	5	3955	7/7	0.14	-1.27	109,109,109,109	0
86	OHX	5	4057	7/7	0.15	-1.28	148,148,148,148	0
86	OHX	3	216	7/7	0.13	-1.28	108,108,108,108	0
86	OHX	5	4154	7/7	0.15	-1.28	137,137,137,137	0
86	OHX	5	3948	7/7	0.14	-1.28	107,107,107,107	0
85	MG	o4	202	1/1	0.18	-1.28	79,79,79,79	0
86	OHX	5	3985	7/7	0.14	-1.29	124,124,124,124	0
86	OHX	5	3998	7/7	0.14	-1.29	116,116,116,116	0
86	OHX	5	3931	7/7	0.16	-1.30	95,95,95,95	0
85	MG	1	4214	1/1	0.15	-1.30	72,72,72,72	0
86	OHX	6	2133	7/7	0.15	-1.30	169,169,169,169	0
85	MG	1	4213	1/1	0.29	-1.31	35,35,35,35	0
86	OHX	5	4232	7/7	0.16	-1.31	175,175,175,175	0
85	MG	o4	203	1/1	0.20	-1.31	59,59,59,59	0
86	OHX	1	3901	7/7	0.14	-1.31	110,110,110,110	0
86	OHX	5	4107	7/7	0.14	-1.31	154,154,154,154	0
86	OHX	8	216	7/7	0.09	-1.32	131,131,131,131	0
86	OHX	L3	405	7/7	0.20	-1.32	141,141,141,141	0
86	OHX	l3	405	7/7	0.23	-1.32	170,170,170,170	0
85	MG	1	3574	1/1	0.22	-1.33	35,35,35,35	0
86	OHX	5	3951	7/7	0.14	-1.33	105,105,105,105	0
85	MG	1	3784	1/1	0.13	-1.33	94,94,94,94	0
85	MG	M9	201	1/1	0.14	-1.34	68,68,68,68	0
86	OHX	1	3962	7/7	0.10	-1.34	120,120,120,120	0
85	MG	1	3637	1/1	0.21	-1.34	63,63,63,63	0
86	OHX	1	4033	7/7	0.10	-1.35	144,144,144,144	0
86	OHX	7	218	7/7	0.17	-1.35	96,96,96,96	0
86	OHX	d4	201	7/7	0.12	-1.35	174,174,174,174	0
86	OHX	5	3908	7/7	0.14	-1.35	83,83,83,83	0
85	MG	6	2205	1/1	0.17	-1.36	65,65,65,65	0
86	OHX	1	4157	7/7	0.14	-1.36	179,179,179,179	0
86	OHX	1	4117	7/7	0.21	-1.36	170,170,170,170	0
86	OHX	6	2137	7/7	0.10	-1.36	148,148,148,148	0
86	OHX	5	3899	7/7	0.18	-1.37	70,70,70,70	0
86	OHX	1	3964	7/7	0.11	-1.37	131,131,131,131	0
86	OHX	1	4081	7/7	0.13	-1.37	192,192,192,192	0
86	OHX	5	4011	7/7	0.09	-1.37	145,145,145,145	0
86	OHX	5	3968	7/7	0.14	-1.37	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	C3	201	7/7	0.18	-1.37	174,174,174,174	0
86	OHX	5	4151	7/7	0.22	-1.37	168,168,168,168	0
86	OHX	5	4033	7/7	0.25	-1.38	112,112,112,112	0
85	MG	5	3563	1/1	0.26	-1.38	32,32,32,32	0
86	OHX	5	4028	7/7	0.13	-1.38	125,125,125,125	0
85	MG	1	3472	1/1	0.20	-1.38	28,28,28,28	0
86	OHX	2	2114	7/7	0.07	-1.38	146,146,146,146	0
86	OHX	5	4054	7/7	0.11	-1.39	169,169,169,169	0
86	OHX	1	3971	7/7	0.21	-1.39	109,109,109,109	0
86	OHX	2	2047	7/7	0.10	-1.39	127,127,127,127	0
86	OHX	6	2123	7/7	0.13	-1.39	135,135,135,135	0
86	OHX	1	3905	7/7	0.14	-1.39	101,101,101,101	0
85	MG	5	3520	1/1	0.21	-1.39	41,41,41,41	0
85	MG	5	3621	1/1	0.13	-1.39	38,38,38,38	0
86	OHX	6	2185	7/7	0.12	-1.40	203,203,203,203	0
85	MG	1	3539	1/1	0.20	-1.40	29,29,29,29	0
86	OHX	1	3957	7/7	0.20	-1.40	90,90,90,90	0
86	OHX	2	2092	7/7	0.14	-1.40	172,172,172,172	0
87	ZN	Q0	500	1/1	0.13	-1.41	52,52,52,52	0
86	OHX	5	3893	7/7	0.19	-1.41	51,51,51,51	0
86	OHX	O7	104	7/7	0.09	-1.41	112,112,112,112	0
86	OHX	1	4140	7/7	0.14	-1.41	145,145,145,145	0
86	OHX	5	4117	7/7	0.13	-1.41	166,166,166,166	0
86	OHX	5	3954	7/7	0.10	-1.42	119,119,119,119	0
86	OHX	m4	202	7/7	0.21	-1.42	223,223,223,223	0
85	MG	1	3565	1/1	0.18	-1.42	35,35,35,35	0
86	OHX	5	4124	7/7	0.10	-1.42	165,165,165,165	0
86	OHX	5	3988	7/7	0.14	-1.42	134,134,134,134	0
85	MG	O7	103	1/1	0.31	-1.42	35,35,35,35	0
86	OHX	2	2069	7/7	0.13	-1.42	139,139,139,139	0
85	MG	4	221	1/1	0.20	-1.43	58,58,58,58	0
86	OHX	1	4000	7/7	0.16	-1.43	137,137,137,137	0
86	OHX	5	4088	7/7	0.15	-1.43	141,141,141,141	0
86	OHX	8	226	7/7	0.11	-1.43	167,167,167,167	0
86	OHX	2	2032	7/7	0.14	-1.43	121,121,121,121	0
86	OHX	5	4081	7/7	0.16	-1.43	151,151,151,151	0
86	OHX	5	3911	7/7	0.15	-1.44	79,79,79,79	0
85	MG	5	3721	1/1	0.22	-1.44	98,98,98,98	0
86	OHX	2	2147	7/7	0.19	-1.44	205,205,205,205	0
86	OHX	6	2066	7/7	0.09	-1.44	112,112,112,112	0
86	OHX	1	3963	7/7	0.10	-1.44	125,125,125,125	0
86	OHX	4	224	7/7	0.17	-1.44	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4007	7/7	0.13	-1.44	157,157,157,157	0
86	OHX	5	3927	7/7	0.18	-1.44	93,93,93,93	0
85	MG	5	3617	1/1	0.23	-1.44	39,39,39,39	0
86	OHX	6	2082	7/7	0.13	-1.45	128,128,128,128	0
86	OHX	2	2037	7/7	0.13	-1.45	163,163,163,163	0
86	OHX	5	4189	7/7	0.07	-1.45	195,195,195,195	0
86	OHX	5	3969	7/7	0.16	-1.45	119,119,119,119	0
85	MG	1	3695	1/1	0.22	-1.45	81,81,81,81	0
86	OHX	1	4094	7/7	0.16	-1.45	134,134,134,134	0
86	OHX	1	4072	7/7	0.09	-1.46	153,153,153,153	0
86	OHX	1	4205	7/7	0.18	-1.46	146,146,146,146	0
86	OHX	6	2125	7/7	0.10	-1.46	166,166,166,166	0
85	MG	5	3619	1/1	0.11	-1.46	48,48,48,48	0
85	MG	5	3841	1/1	0.18	-1.46	42,42,42,42	0
85	MG	5	3455	1/1	0.17	-1.46	43,43,43,43	0
85	MG	5	3857	1/1	0.14	-1.46	58,58,58,58	0
86	OHX	6	2193	7/7	0.14	-1.46	209,209,209,209	0
85	MG	1	3638	1/1	0.15	-1.46	62,62,62,62	0
86	OHX	1	3945	7/7	0.15	-1.47	125,125,125,125	0
85	MG	1	3410	1/1	0.17	-1.47	51,51,51,51	0
86	OHX	1	3940	7/7	0.14	-1.47	127,127,127,127	0
86	OHX	7	224	7/7	0.09	-1.47	123,123,123,123	0
87	ZN	q0	3602	1/1	0.16	-1.47	38,38,38,38	0
86	OHX	6	2062	7/7	0.12	-1.47	109,109,109,109	0
86	OHX	D3	202	7/7	0.13	-1.48	114,114,114,114	0
85	MG	1	3578	1/1	0.13	-1.48	55,55,55,55	0
86	OHX	4	230	7/7	0.14	-1.48	136,136,136,136	0
86	OHX	6	2057	7/7	0.12	-1.48	111,111,111,111	0
85	MG	1	3763	1/1	0.17	-1.48	45,45,45,45	0
86	OHX	1	3950	7/7	0.13	-1.48	113,113,113,113	0
86	OHX	2	2039	7/7	0.15	-1.48	112,112,112,112	0
86	OHX	6	2059	7/7	0.12	-1.49	106,106,106,106	0
85	MG	5	3650	1/1	0.23	-1.49	63,63,63,63	0
86	OHX	1	3907	7/7	0.14	-1.49	110,110,110,110	0
86	OHX	1	3938	7/7	0.13	-1.49	120,120,120,120	0
86	OHX	1	4148	7/7	0.16	-1.49	157,157,157,157	0
85	MG	1	3443	1/1	0.34	-1.49	47,47,47,47	0
85	MG	m7	201	1/1	0.21	-1.50	39,39,39,39	0
86	OHX	1	3921	7/7	0.14	-1.50	114,114,114,114	0
86	OHX	6	2088	7/7	0.11	-1.50	142,142,142,142	0
86	OHX	5	4158	7/7	0.17	-1.50	141,141,141,141	0
86	OHX	5	3919	7/7	0.19	-1.50	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	1	3598	1/1	0.12	-1.51	36,36,36,36	0
86	OHX	1	3895	7/7	0.15	-1.51	85,85,85,85	0
86	OHX	1	4127	7/7	0.10	-1.51	176,176,176,176	0
86	OHX	2	2119	7/7	0.17	-1.51	161,161,161,161	0
86	OHX	5	3989	7/7	0.18	-1.51	122,122,122,122	0
86	OHX	5	3952	7/7	0.13	-1.51	88,88,88,88	0
86	OHX	O7	105	7/7	0.23	-1.52	107,107,107,107	0
86	OHX	5	3905	7/7	0.15	-1.53	77,77,77,77	0
86	OHX	6	2093	7/7	0.12	-1.53	145,145,145,145	0
86	OHX	2	2038	7/7	0.11	-1.53	114,114,114,114	0
86	OHX	1	3956	7/7	0.15	-1.54	112,112,112,112	0
85	MG	1	3537	1/1	0.23	-1.54	24,24,24,24	0
85	MG	L8	301	1/1	0.32	-1.54	69,69,69,69	0
86	OHX	2	2088	7/7	0.09	-1.54	135,135,135,135	0
85	MG	N3	203	1/1	0.47	-1.54	41,41,41,41	0
85	MG	2	1989	1/1	0.21	-1.55	61,61,61,61	0
86	OHX	2	2045	7/7	0.14	-1.55	127,127,127,127	0
85	MG	5	3463	1/1	0.19	-1.55	38,38,38,38	0
86	OHX	1	3935	7/7	0.29	-1.56	104,104,104,104	0
86	OHX	6	2099	7/7	0.10	-1.56	197,197,197,197	0
86	OHX	3	219	7/7	0.17	-1.56	131,131,131,131	0
86	OHX	5	4114	7/7	0.14	-1.56	142,142,142,142	0
85	MG	1	3741	1/1	0.17	-1.57	31,31,31,31	0
86	OHX	5	4084	7/7	0.10	-1.57	118,118,118,118	0
86	OHX	2	2076	7/7	0.13	-1.58	143,143,143,143	0
86	OHX	5	3923	7/7	0.16	-1.58	81,81,81,81	0
86	OHX	5	4247	7/7	0.12	-1.58	188,188,188,188	0
86	OHX	5	3947	7/7	0.12	-1.59	112,112,112,112	0
85	MG	1	3583	1/1	0.23	-1.59	33,33,33,33	0
86	OHX	1	4027	7/7	0.11	-1.59	121,121,121,121	0
85	MG	1	3573	1/1	0.16	-1.60	29,29,29,29	0
86	OHX	1	3941	7/7	0.10	-1.60	124,124,124,124	0
85	MG	1	3661	1/1	0.15	-1.61	60,60,60,60	0
86	OHX	6	2058	7/7	0.14	-1.61	105,105,105,105	0
85	MG	1	3742	1/1	0.14	-1.61	43,43,43,43	0
86	OHX	1	3965	7/7	0.17	-1.61	120,120,120,120	0
86	OHX	5	3975	7/7	0.08	-1.61	108,108,108,108	0
86	OHX	5	4078	7/7	0.11	-1.62	156,156,156,156	0
86	OHX	6	2149	7/7	0.15	-1.62	127,127,127,127	0
86	OHX	1	4032	7/7	0.11	-1.62	163,163,163,163	0
86	OHX	5	4065	7/7	0.18	-1.62	150,150,150,150	0
86	OHX	1	3881	7/7	0.14	-1.62	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3445	1/1	0.15	-1.63	47,47,47,47	0
85	MG	5	3829	1/1	0.15	-1.63	58,58,58,58	0
86	OHX	2	2062	7/7	0.10	-1.63	151,151,151,151	0
85	MG	1	3754	1/1	0.15	-1.63	56,56,56,56	0
86	OHX	1	4061	7/7	0.13	-1.63	164,164,164,164	0
85	MG	6	1957	1/1	0.25	-1.64	64,64,64,64	0
86	OHX	2	2087	7/7	0.10	-1.64	152,152,152,152	0
85	MG	M3	202	1/1	0.21	-1.64	108,108,108,108	0
85	MG	1	3548	1/1	0.17	-1.64	46,46,46,46	0
86	OHX	7	219	7/7	0.14	-1.64	101,101,101,101	0
85	MG	5	3427	1/1	0.19	-1.64	51,51,51,51	0
86	OHX	1	4103	7/7	0.17	-1.65	161,161,161,161	0
86	OHX	1	3882	7/7	0.15	-1.65	76,76,76,76	0
86	OHX	c5	201	7/7	0.11	-1.65	181,181,181,181	0
85	MG	1	3507	1/1	0.21	-1.65	20,20,20,20	0
85	MG	2	2011	1/1	0.22	-1.66	67,67,67,67	0
86	OHX	5	4019	7/7	0.10	-1.66	135,135,135,135	0
86	OHX	5	4016	7/7	0.10	-1.67	132,132,132,132	0
86	OHX	5	3962	7/7	0.11	-1.67	113,113,113,113	0
86	OHX	6	2105	7/7	0.10	-1.67	138,138,138,138	0
86	OHX	SR	401	7/7	0.15	-1.67	196,196,196,196	0
85	MG	5	3465	1/1	0.16	-1.68	60,60,60,60	0
86	OHX	5	3918	7/7	0.16	-1.68	68,68,68,68	0
87	ZN	D6	500	1/1	0.08	-1.69	84,84,84,84	0
86	OHX	1	4015	7/7	0.15	-1.69	140,140,140,140	0
86	OHX	6	2104	7/7	0.17	-1.69	141,141,141,141	0
86	OHX	6	2091	7/7	0.10	-1.69	140,140,140,140	0
85	MG	2	1991	1/1	0.06	-1.70	100,100,100,100	0
86	OHX	1	4020	7/7	0.12	-1.70	147,147,147,147	0
86	OHX	5	4032	7/7	0.12	-1.70	149,149,149,149	0
86	OHX	5	4166	7/7	0.14	-1.70	184,184,184,184	0
85	MG	1	3704	1/1	0.17	-1.71	63,63,63,63	0
86	OHX	5	3934	7/7	0.17	-1.71	104,104,104,104	0
85	MG	1	3577	1/1	0.18	-1.72	39,39,39,39	0
86	OHX	l9	202	7/7	0.11	-1.72	138,138,138,138	0
86	OHX	1	3887	7/7	0.14	-1.72	88,88,88,88	0
86	OHX	Q2	503	7/7	0.12	-1.72	99,99,99,99	0
86	OHX	1	3986	7/7	0.15	-1.73	144,144,144,144	0
86	OHX	n3	202	7/7	0.11	-1.73	106,106,106,106	0
86	OHX	n9	103	7/7	0.14	-1.73	77,77,77,77	0
86	OHX	1	3992	7/7	0.12	-1.74	165,165,165,165	0
86	OHX	8	224	7/7	0.20	-1.74	172,172,172,172	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3496	1/1	0.22	-1.74	42,42,42,42	0
86	OHX	1	3970	7/7	0.13	-1.74	103,103,103,103	0
85	MG	6	1951	1/1	0.19	-1.75	64,64,64,64	0
86	OHX	2	2078	7/7	0.11	-1.75	145,145,145,145	0
86	OHX	5	3912	7/7	0.15	-1.75	92,92,92,92	0
86	OHX	2	2155	7/7	0.13	-1.75	164,164,164,164	0
86	OHX	2	2151	7/7	0.08	-1.75	201,201,201,201	0
86	OHX	c3	201	7/7	0.18	-1.76	182,182,182,182	0
85	MG	5	3557	1/1	0.16	-1.77	38,38,38,38	0
86	OHX	l3	404	7/7	0.10	-1.77	117,117,117,117	0
85	MG	1	3518	1/1	0.16	-1.77	40,40,40,40	0
86	OHX	2	2093	7/7	0.07	-1.78	173,173,173,173	0
85	MG	5	3556	1/1	0.47	-1.78	53,53,53,53	0
85	MG	5	3590	1/1	0.15	-1.79	30,30,30,30	0
86	OHX	2	2165	7/7	0.12	-1.79	197,197,197,197	0
85	MG	5	3419	1/1	0.12	-1.79	84,84,84,84	0
86	OHX	1	4153	7/7	0.13	-1.80	139,139,139,139	0
85	MG	1	3687	1/1	0.20	-1.80	28,28,28,28	0
86	OHX	6	2087	7/7	0.12	-1.80	146,146,146,146	0
86	OHX	sR	401	7/7	0.09	-1.80	182,182,182,182	0
86	OHX	1	4132	7/7	0.15	-1.81	122,122,122,122	0
86	OHX	5	4052	7/7	0.12	-1.81	161,161,161,161	0
86	OHX	1	3997	7/7	0.12	-1.81	135,135,135,135	0
86	OHX	1	3991	7/7	0.10	-1.81	171,171,171,171	0
86	OHX	5	3957	7/7	0.12	-1.81	101,101,101,101	0
85	MG	1	3593	1/1	0.28	-1.81	30,30,30,30	0
86	OHX	3	221	7/7	0.19	-1.82	145,145,145,145	0
85	MG	7	215	1/1	0.15	-1.82	44,44,44,44	0
86	OHX	6	2077	7/7	0.14	-1.82	111,111,111,111	0
85	MG	1	3697	1/1	0.19	-1.83	50,50,50,50	0
86	OHX	1	4110	7/7	0.16	-1.83	155,155,155,155	0
86	OHX	5	3935	7/7	0.12	-1.83	105,105,105,105	0
86	OHX	1	4034	7/7	0.06	-1.84	137,137,137,137	0
85	MG	2	1924	1/1	0.19	-1.84	83,83,83,83	0
86	OHX	1	4028	7/7	0.19	-1.84	130,130,130,130	0
86	OHX	1	4036	7/7	0.15	-1.85	152,152,152,152	0
86	OHX	1	3994	7/7	0.13	-1.85	113,113,113,113	0
85	MG	1	3566	1/1	0.15	-1.85	30,30,30,30	0
86	OHX	6	2112	7/7	0.13	-1.85	128,128,128,128	0
86	OHX	q2	502	7/7	0.11	-1.85	98,98,98,98	0
86	OHX	5	4109	7/7	0.10	-1.85	147,147,147,147	0
86	OHX	5	4213	7/7	0.14	-1.86	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3459	1/1	0.16	-1.86	74,74,74,74	0
86	OHX	1	4152	7/7	0.18	-1.86	123,123,123,123	0
86	OHX	1	3983	7/7	0.16	-1.87	131,131,131,131	0
85	MG	1	3556	1/1	0.18	-1.87	29,29,29,29	0
86	OHX	1	4004	7/7	0.14	-1.87	148,148,148,148	0
86	OHX	2	2061	7/7	0.11	-1.87	144,144,144,144	0
86	OHX	6	2056	7/7	0.14	-1.87	93,93,93,93	0
86	OHX	5	4071	7/7	0.11	-1.88	176,176,176,176	0
86	OHX	1	3900	7/7	0.14	-1.88	94,94,94,94	0
86	OHX	5	3993	7/7	0.12	-1.89	128,128,128,128	0
86	OHX	5	4021	7/7	0.16	-1.89	115,115,115,115	0
86	OHX	7	221	7/7	0.13	-1.89	109,109,109,109	0
85	MG	1	4216	1/1	0.15	-1.89	40,40,40,40	0
86	OHX	1	4164	7/7	0.15	-1.90	137,137,137,137	0
86	OHX	5	4044	7/7	0.08	-1.90	151,151,151,151	0
86	OHX	2	2175	7/7	0.12	-1.90	198,198,198,198	0
86	OHX	5	4177	7/7	0.15	-1.90	162,162,162,162	0
85	MG	1	3686	1/1	0.13	-1.90	46,46,46,46	0
85	MG	5	3736	1/1	0.18	-1.90	45,45,45,45	0
85	MG	5	3512	1/1	0.18	-1.90	51,51,51,51	0
86	OHX	6	2179	7/7	0.12	-1.91	174,174,174,174	0
86	OHX	2	2075	7/7	0.14	-1.91	151,151,151,151	0
85	MG	1	3506	1/1	0.14	-1.91	36,36,36,36	0
86	OHX	1	3952	7/7	0.08	-1.92	125,125,125,125	0
85	MG	5	3591	1/1	0.20	-1.92	34,34,34,34	0
86	OHX	1	4051	7/7	0.15	-1.92	121,121,121,121	0
86	OHX	6	2111	7/7	0.16	-1.92	152,152,152,152	0
86	OHX	1	3990	7/7	0.16	-1.92	121,121,121,121	0
86	OHX	4	234	7/7	0.17	-1.92	133,133,133,133	0
86	OHX	5	3984	7/7	0.33	-1.93	108,108,108,108	0
86	OHX	2	2077	7/7	0.11	-1.94	161,161,161,161	0
85	MG	1	3471	1/1	0.17	-1.94	37,37,37,37	0
86	OHX	m6	203	7/7	0.12	-1.95	113,113,113,113	0
86	OHX	1	3923	7/7	0.12	-1.96	104,104,104,104	0
86	OHX	5	3930	7/7	0.12	-1.96	86,86,86,86	0
86	OHX	5	3904	7/7	0.14	-1.96	81,81,81,81	0
85	MG	1	3502	1/1	0.23	-1.96	29,29,29,29	0
86	OHX	1	4086	7/7	0.14	-1.96	177,177,177,177	0
87	ZN	q2	501	1/1	0.10	-1.97	98,98,98,98	0
86	OHX	1	4092	7/7	0.20	-1.97	167,167,167,167	0
86	OHX	1	4050	7/7	0.11	-1.97	164,164,164,164	0
86	OHX	5	4197	7/7	0.12	-1.98	166,166,166,166	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	6	2121	7/7	0.09	-1.98	163,163,163,163	0
86	OHX	5	4003	7/7	0.11	-1.98	127,127,127,127	0
85	MG	1	3439	1/1	0.29	-1.98	31,31,31,31	0
85	MG	1	3683	1/1	0.13	-1.98	103,103,103,103	0
86	OHX	1	3929	7/7	0.12	-1.98	112,112,112,112	0
87	ZN	Q3	501	1/1	0.07	-1.99	72,72,72,72	0
86	OHX	1	3982	7/7	0.13	-1.99	116,116,116,116	0
86	OHX	6	2158	7/7	0.13	-1.99	163,163,163,163	0
86	OHX	1	4054	7/7	0.11	-2.00	183,183,183,183	0
86	OHX	5	4043	7/7	0.14	-2.00	121,121,121,121	0
86	OHX	2	2108	7/7	0.09	-2.01	170,170,170,170	0
86	OHX	5	3928	7/7	0.13	-2.01	93,93,93,93	0
86	OHX	1	4039	7/7	0.07	-2.01	125,125,125,125	0
86	OHX	6	2107	7/7	0.11	-2.01	130,130,130,130	0
85	MG	1	3722	1/1	0.15	-2.02	68,68,68,68	0
86	OHX	1	4079	7/7	0.09	-2.02	161,161,161,161	0
86	OHX	2	2141	7/7	0.08	-2.03	202,202,202,202	0
86	OHX	o3	203	7/7	0.20	-2.03	124,124,124,124	0
86	OHX	5	4027	7/7	0.13	-2.03	126,126,126,126	0
85	MG	5	3844	1/1	0.16	-2.03	54,54,54,54	0
86	OHX	1	4080	7/7	0.10	-2.03	150,150,150,150	0
85	MG	1	3569	1/1	0.22	-2.04	41,41,41,41	0
86	OHX	1	3946	7/7	0.14	-2.04	112,112,112,112	0
86	OHX	6	2129	7/7	0.10	-2.04	160,160,160,160	0
86	OHX	1	3979	7/7	0.10	-2.04	136,136,136,136	0
85	MG	5	3623	1/1	0.17	-2.04	59,59,59,59	0
86	OHX	2	2125	7/7	0.12	-2.05	155,155,155,155	0
86	OHX	5	4175	7/7	0.12	-2.05	183,183,183,183	0
86	OHX	2	2100	7/7	0.12	-2.05	165,165,165,165	0
86	OHX	1	3904	7/7	0.12	-2.06	103,103,103,103	0
86	OHX	6	2134	7/7	0.14	-2.07	153,153,153,153	0
85	MG	5	3595	1/1	0.20	-2.07	41,41,41,41	0
86	OHX	1	4005	7/7	0.12	-2.07	148,148,148,148	0
85	MG	1	3547	1/1	0.18	-2.07	36,36,36,36	0
86	OHX	5	3913	7/7	0.17	-2.08	78,78,78,78	0
86	OHX	5	4024	7/7	0.12	-2.08	138,138,138,138	0
85	MG	1	3494	1/1	0.16	-2.08	50,50,50,50	0
85	MG	1	3699	1/1	0.17	-2.10	48,48,48,48	0
86	OHX	2	2171	7/7	0.09	-2.10	167,167,167,167	0
86	OHX	6	2049	7/7	0.18	-2.11	79,79,79,79	0
86	OHX	5	4099	7/7	0.10	-2.12	163,163,163,163	0
86	OHX	6	2098	7/7	0.07	-2.13	181,181,181,181	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4070	7/7	0.12	-2.13	133,133,133,133	0
86	OHX	1	3959	7/7	0.13	-2.13	134,134,134,134	0
85	MG	1	3809	1/1	0.13	-2.14	53,53,53,53	0
86	OHX	6	2101	7/7	0.12	-2.14	124,124,124,124	0
86	OHX	1	3906	7/7	0.14	-2.14	94,94,94,94	0
86	OHX	5	4156	7/7	0.12	-2.15	151,151,151,151	0
86	OHX	1	4107	7/7	0.17	-2.15	167,167,167,167	0
86	OHX	5	4140	7/7	0.08	-2.15	160,160,160,160	0
86	OHX	2	2089	7/7	0.10	-2.15	141,141,141,141	0
86	OHX	2	2048	7/7	0.11	-2.16	139,139,139,139	0
85	MG	5	3524	1/1	0.23	-2.16	22,22,22,22	0
86	OHX	N9	101	7/7	0.16	-2.16	72,72,72,72	0
85	MG	5	3437	1/1	0.10	-2.16	58,58,58,58	0
86	OHX	5	4082	7/7	0.13	-2.16	138,138,138,138	0
86	OHX	6	2060	7/7	0.13	-2.16	103,103,103,103	0
85	MG	1	3824	1/1	0.16	-2.17	43,43,43,43	0
86	OHX	2	2053	7/7	0.14	-2.17	140,140,140,140	0
85	MG	12	302	1/1	0.19	-2.17	36,36,36,36	0
86	OHX	2	2055	7/7	0.11	-2.18	143,143,143,143	0
85	MG	5	3610	1/1	0.18	-2.18	35,35,35,35	0
86	OHX	1	4038	7/7	0.10	-2.18	122,122,122,122	0
86	OHX	M0	304	7/7	0.13	-2.18	118,118,118,118	0
86	OHX	1	3868	7/7	0.15	-2.18	78,78,78,78	0
85	MG	1	3802	1/1	0.12	-2.19	47,47,47,47	0
86	OHX	5	4000	7/7	0.12	-2.19	146,146,146,146	0
86	OHX	1	3864	7/7	0.17	-2.20	63,63,63,63	0
86	OHX	2	2094	7/7	0.10	-2.20	170,170,170,170	0
85	MG	1	3794	1/1	0.10	-2.20	63,63,63,63	0
86	OHX	2	2025	7/7	0.17	-2.21	97,97,97,97	0
86	OHX	1	3984	7/7	0.14	-2.21	127,127,127,127	0
86	OHX	1	4145	7/7	0.12	-2.22	173,173,173,173	0
85	MG	6	1975	1/1	0.14	-2.22	68,68,68,68	0
86	OHX	1	3903	7/7	0.15	-2.23	103,103,103,103	0
87	ZN	Q2	501	1/1	0.06	-2.24	87,87,87,87	0
85	MG	1	3423	1/1	0.17	-2.24	48,48,48,48	0
86	OHX	3	220	7/7	0.16	-2.25	144,144,144,144	0
86	OHX	5	4150	7/7	0.15	-2.25	132,132,132,132	0
86	OHX	1	4197	7/7	0.14	-2.25	162,162,162,162	0
86	OHX	6	2138	7/7	0.13	-2.26	138,138,138,138	0
86	OHX	2	2162	7/7	0.14	-2.27	190,190,190,190	0
86	OHX	5	3965	7/7	0.11	-2.27	98,98,98,98	0
86	OHX	5	3953	7/7	0.15	-2.27	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3750	1/1	0.17	-2.27	36,36,36,36	0
85	MG	5	3414	1/1	0.20	-2.27	36,36,36,36	0
86	OHX	2	2166	7/7	0.12	-2.28	177,177,177,177	0
86	OHX	1	3908	7/7	0.11	-2.28	118,118,118,118	0
86	OHX	6	2130	7/7	0.11	-2.29	133,133,133,133	0
86	OHX	5	4013	7/7	0.19	-2.30	138,138,138,138	0
85	MG	5	3550	1/1	0.33	-2.31	49,49,49,49	0
85	MG	1	3540	1/1	0.18	-2.31	34,34,34,34	0
86	OHX	2	2107	7/7	0.15	-2.31	154,154,154,154	0
85	MG	5	3587	1/1	0.19	-2.31	26,26,26,26	0
85	MG	1	3458	1/1	0.17	-2.31	34,34,34,34	0
86	OHX	1	4048	7/7	0.10	-2.31	161,161,161,161	0
86	OHX	5	3979	7/7	0.13	-2.32	107,107,107,107	0
86	OHX	6	2073	7/7	0.10	-2.32	157,157,157,157	0
86	OHX	1	3951	7/7	0.10	-2.32	87,87,87,87	0
86	OHX	1	3902	7/7	0.16	-2.33	92,92,92,92	0
85	MG	1	3601	1/1	0.14	-2.33	46,46,46,46	0
86	OHX	2	2074	7/7	0.14	-2.33	162,162,162,162	0
86	OHX	5	4056	7/7	0.13	-2.33	142,142,142,142	0
86	OHX	1	3927	7/7	0.11	-2.33	94,94,94,94	0
86	OHX	1	3870	7/7	0.12	-2.34	85,85,85,85	0
85	MG	1	3477	1/1	0.10	-2.36	98,98,98,98	0
85	MG	1	3831	1/1	0.20	-2.36	34,34,34,34	0
86	OHX	1	4104	7/7	0.10	-2.36	142,142,142,142	0
86	OHX	5	4165	7/7	0.11	-2.37	203,203,203,203	0
86	OHX	5	3945	7/7	0.14	-2.38	116,116,116,116	0
86	OHX	5	4203	7/7	0.12	-2.38	192,192,192,192	0
86	OHX	5	3946	7/7	0.13	-2.40	84,84,84,84	0
86	OHX	1	4014	7/7	0.14	-2.40	131,131,131,131	0
85	MG	1	3825	1/1	0.26	-2.42	23,23,23,23	0
86	OHX	5	4193	7/7	0.13	-2.42	103,103,103,103	0
86	OHX	1	3939	7/7	0.12	-2.42	104,104,104,104	0
86	OHX	5	4049	7/7	0.09	-2.42	124,124,124,124	0
86	OHX	5	3943	7/7	0.15	-2.42	100,100,100,100	0
86	OHX	6	2122	7/7	0.09	-2.43	164,164,164,164	0
85	MG	5	4252	1/1	0.14	-2.43	40,40,40,40	0
86	OHX	5	3956	7/7	0.11	-2.43	113,113,113,113	0
86	OHX	6	2190	7/7	0.13	-2.43	174,174,174,174	0
86	OHX	15	305	7/7	0.11	-2.43	166,166,166,166	0
85	MG	1	3771	1/1	0.12	-2.43	40,40,40,40	0
85	MG	5	3597	1/1	0.15	-2.44	44,44,44,44	0
85	MG	5	3884	1/1	0.14	-2.44	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	6	2068	7/7	0.12	-2.44	118,118,118,118	0
86	OHX	5	3922	7/7	0.13	-2.46	93,93,93,93	0
85	MG	5	3566	1/1	0.13	-2.47	30,30,30,30	0
85	MG	1	3435	1/1	0.14	-2.47	51,51,51,51	0
86	OHX	5	4227	7/7	0.11	-2.48	216,216,216,216	0
86	OHX	5	4005	7/7	0.08	-2.48	120,120,120,120	0
85	MG	6	2016	1/1	0.11	-2.48	82,82,82,82	0
86	OHX	2	2064	7/7	0.10	-2.49	130,130,130,130	0
86	OHX	5	4135	7/7	0.13	-2.49	173,173,173,173	0
85	MG	6	2026	1/1	0.10	-2.49	88,88,88,88	0
85	MG	1	3446	1/1	0.23	-2.49	32,32,32,32	0
86	OHX	1	4163	7/7	0.16	-2.49	136,136,136,136	0
85	MG	1	3511	1/1	0.20	-2.49	25,25,25,25	0
85	MG	1	3426	1/1	0.16	-2.49	44,44,44,44	0
86	OHX	5	4120	7/7	0.07	-2.51	175,175,175,175	0
85	MG	5	3779	1/1	0.14	-2.51	56,56,56,56	0
86	OHX	5	3920	7/7	0.13	-2.51	95,95,95,95	0
85	MG	1	3847	1/1	0.16	-2.52	77,77,77,77	0
86	OHX	4	226	7/7	0.12	-2.52	112,112,112,112	0
86	OHX	2	2124	7/7	0.09	-2.53	172,172,172,172	0
86	OHX	L3	406	7/7	0.12	-2.54	175,175,175,175	0
86	OHX	c8	202	7/7	0.10	-2.54	163,163,163,163	0
85	MG	1	3486	1/1	0.16	-2.54	35,35,35,35	0
86	OHX	1	4208	7/7	0.09	-2.55	185,185,185,185	0
86	OHX	5	3915	7/7	0.16	-2.56	83,83,83,83	0
86	OHX	3	225	7/7	0.15	-2.56	165,165,165,165	0
85	MG	1	3455	1/1	0.14	-2.56	26,26,26,26	0
86	OHX	5	3909	7/7	0.14	-2.56	74,74,74,74	0
85	MG	5	3495	1/1	0.19	-2.57	41,41,41,41	0
86	OHX	7	220	7/7	0.12	-2.57	115,115,115,115	0
85	MG	sM	301	1/1	0.11	-2.57	51,51,51,51	0
85	MG	1	3519	1/1	0.11	-2.58	39,39,39,39	0
86	OHX	6	2074	7/7	0.12	-2.58	110,110,110,110	0
86	OHX	2	2081	7/7	0.07	-2.58	167,167,167,167	0
86	OHX	2	2057	7/7	0.11	-2.58	126,126,126,126	0
86	OHX	m5	306	7/7	0.27	-2.59	145,145,145,145	0
86	OHX	1	4085	7/7	0.11	-2.60	146,146,146,146	0
85	MG	1	3404	1/1	0.21	-2.60	73,73,73,73	0
85	MG	5	3423	1/1	0.14	-2.62	74,74,74,74	0
86	OHX	1	4129	7/7	0.12	-2.62	157,157,157,157	0
86	OHX	6	2110	7/7	0.15	-2.62	144,144,144,144	0
85	MG	5	3876	1/1	0.17	-2.63	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	1	3752	1/1	0.12	-2.63	106,106,106,106	0
86	OHX	1	4045	7/7	0.12	-2.63	136,136,136,136	0
85	MG	1	3625	1/1	0.17	-2.63	41,41,41,41	0
86	OHX	1	4096	7/7	0.10	-2.63	181,181,181,181	0
86	OHX	5	4029	7/7	0.09	-2.64	138,138,138,138	0
86	OHX	5	4041	7/7	0.11	-2.65	149,149,149,149	0
85	MG	1	3706	1/1	0.19	-2.65	36,36,36,36	0
86	OHX	2	2070	7/7	0.09	-2.65	152,152,152,152	0
86	OHX	1	4069	7/7	0.10	-2.66	133,133,133,133	0
85	MG	1	3450	1/1	0.10	-2.66	42,42,42,42	0
86	OHX	1	4147	7/7	0.09	-2.68	128,128,128,128	0
86	OHX	1	3954	7/7	0.11	-2.68	116,116,116,116	0
85	MG	1	3437	1/1	0.07	-2.69	50,50,50,50	0
86	OHX	1	3937	7/7	0.12	-2.70	112,112,112,112	0
87	ZN	q3	501	1/1	0.05	-2.70	78,78,78,78	0
86	OHX	5	4042	7/7	0.11	-2.70	133,133,133,133	0
86	OHX	l5	304	7/7	0.06	-2.71	166,166,166,166	0
86	OHX	6	2155	7/7	0.05	-2.71	133,133,133,133	0
86	OHX	1	4126	7/7	0.09	-2.71	169,169,169,169	0
86	OHX	5	4034	7/7	0.09	-2.73	151,151,151,151	0
86	OHX	2	2024	7/7	0.16	-2.73	94,94,94,94	0
86	OHX	1	4042	7/7	0.10	-2.74	140,140,140,140	0
87	ZN	o7	102	1/1	0.08	-2.75	53,53,53,53	0
85	MG	5	3601	1/1	0.14	-2.75	33,33,33,33	0
86	OHX	5	3917	7/7	0.12	-2.76	83,83,83,83	0
86	OHX	1	3933	7/7	0.12	-2.76	112,112,112,112	0
86	OHX	1	3897	7/7	0.14	-2.77	78,78,78,78	0
85	MG	5	3513	1/1	0.18	-2.77	34,34,34,34	0
86	OHX	2	2112	7/7	0.09	-2.78	158,158,158,158	0
86	OHX	2	2128	7/7	0.08	-2.79	172,172,172,172	0
86	OHX	5	4126	7/7	0.17	-2.79	127,127,127,127	0
86	OHX	1	3989	7/7	0.10	-2.79	149,149,149,149	0
85	MG	1	3822	1/1	0.12	-2.80	56,56,56,56	0
86	OHX	6	2142	7/7	0.06	-2.80	150,150,150,150	0
85	MG	2	1948	1/1	0.15	-2.82	91,91,91,91	0
85	MG	5	3584	1/1	0.25	-2.82	20,20,20,20	0
86	OHX	5	4231	7/7	0.14	-2.82	157,157,157,157	0
85	MG	5	3412	1/1	0.21	-2.83	45,45,45,45	0
86	OHX	6	2164	7/7	0.11	-2.83	214,214,214,214	0
85	MG	1	3557	1/1	0.10	-2.83	39,39,39,39	0
85	MG	1	3433	1/1	0.11	-2.83	49,49,49,49	0
85	MG	5	4250	1/1	0.19	-2.83	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3947	7/7	0.12	-2.84	113,113,113,113	0
86	OHX	4	227	7/7	0.10	-2.84	135,135,135,135	0
85	MG	7	205	1/1	0.14	-2.86	75,75,75,75	0
85	MG	5	3480	1/1	0.10	-2.86	49,49,49,49	0
86	OHX	1	3987	7/7	0.10	-2.86	145,145,145,145	0
86	OHX	5	3976	7/7	0.11	-2.87	116,116,116,116	0
85	MG	5	3744	1/1	0.18	-2.87	54,54,54,54	0
86	OHX	2	2109	7/7	0.06	-2.88	152,152,152,152	0
85	MG	5	3403	1/1	0.14	-2.90	34,34,34,34	0
85	MG	5	3675	1/1	0.10	-2.91	54,54,54,54	0
86	OHX	1	3885	7/7	0.15	-2.91	83,83,83,83	0
86	OHX	1	4013	7/7	0.09	-2.91	146,146,146,146	0
86	OHX	2	2058	7/7	0.12	-2.92	141,141,141,141	0
86	OHX	5	4116	7/7	0.09	-2.92	157,157,157,157	0
86	OHX	1	3993	7/7	0.10	-2.93	127,127,127,127	0
86	OHX	2	2082	7/7	0.08	-2.93	159,159,159,159	0
85	MG	1	3738	1/1	0.12	-2.94	40,40,40,40	0
86	OHX	2	2105	7/7	0.10	-2.95	158,158,158,158	0
86	OHX	5	4093	7/7	0.08	-2.95	166,166,166,166	0
86	OHX	5	4074	7/7	0.09	-2.96	141,141,141,141	0
86	OHX	5	3939	7/7	0.14	-2.96	89,89,89,89	0
86	OHX	1	4091	7/7	0.13	-2.97	165,165,165,165	0
86	OHX	1	3879	7/7	0.15	-2.97	81,81,81,81	0
85	MG	1	3854	1/1	0.18	-2.98	56,56,56,56	0
86	OHX	5	4186	7/7	0.09	-3.00	147,147,147,147	0
86	OHX	6	2080	7/7	0.11	-3.00	117,117,117,117	0
86	OHX	5	3999	7/7	0.14	-3.02	135,135,135,135	0
86	OHX	1	3874	7/7	0.13	-3.03	87,87,87,87	0
86	OHX	O1	202	7/7	0.14	-3.03	135,135,135,135	0
86	OHX	5	4123	7/7	0.19	-3.04	159,159,159,159	0
86	OHX	2	2103	7/7	0.12	-3.04	204,204,204,204	0
85	MG	1	3803	1/1	0.10	-3.05	42,42,42,42	0
86	OHX	5	4051	7/7	0.08	-3.05	148,148,148,148	0
85	MG	1	3572	1/1	0.23	-3.06	15,15,15,15	0
86	OHX	6	2075	7/7	0.14	-3.06	125,125,125,125	0
85	MG	1	3645	1/1	0.14	-3.07	37,37,37,37	0
86	OHX	5	4075	7/7	0.09	-3.07	125,125,125,125	0
86	OHX	6	2197	7/7	0.13	-3.08	163,163,163,163	0
86	OHX	4	228	7/7	0.06	-3.09	141,141,141,141	0
86	OHX	5	3974	7/7	0.11	-3.11	107,107,107,107	0
86	OHX	6	2176	7/7	0.12	-3.11	132,132,132,132	0
85	MG	1	3602	1/1	0.10	-3.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2071	7/7	0.08	-3.12	137,137,137,137	0
86	OHX	1	4055	7/7	0.11	-3.13	147,147,147,147	0
86	OHX	5	4015	7/7	0.10	-3.13	144,144,144,144	0
86	OHX	5	4037	7/7	0.12	-3.15	140,140,140,140	0
86	OHX	1	3969	7/7	0.08	-3.15	111,111,111,111	0
86	OHX	1	4003	7/7	0.11	-3.15	142,142,142,142	0
86	OHX	1	4046	7/7	0.08	-3.16	159,159,159,159	0
85	MG	1	3460	1/1	0.22	-3.17	28,28,28,28	0
86	OHX	1	4112	7/7	0.08	-3.18	147,147,147,147	0
86	OHX	5	4105	7/7	0.09	-3.19	110,110,110,110	0
85	MG	5	3711	1/1	0.13	-3.19	72,72,72,72	0
86	OHX	1	4088	7/7	0.12	-3.19	165,165,165,165	0
86	OHX	6	2196	7/7	0.09	-3.20	183,183,183,183	0
86	OHX	6	2145	7/7	0.10	-3.20	154,154,154,154	0
87	ZN	O7	101	1/1	0.07	-3.20	50,50,50,50	0
85	MG	6	2004	1/1	0.10	-3.20	101,101,101,101	0
86	OHX	1	3934	7/7	0.14	-3.21	109,109,109,109	0
86	OHX	1	3974	7/7	0.15	-3.22	98,98,98,98	0
85	MG	2	1940	1/1	0.09	-3.22	74,74,74,74	0
86	OHX	2	2117	7/7	0.09	-3.23	171,171,171,171	0
85	MG	5	3500	1/1	0.15	-3.23	48,48,48,48	0
86	OHX	1	3893	7/7	0.12	-3.24	97,97,97,97	0
86	OHX	2	2060	7/7	0.10	-3.24	138,138,138,138	0
86	OHX	3	224	7/7	0.13	-3.24	157,157,157,157	0
86	OHX	5	4139	7/7	0.09	-3.25	134,134,134,134	0
86	OHX	5	4068	7/7	0.08	-3.28	141,141,141,141	0
86	OHX	5	4064	7/7	0.14	-3.28	141,141,141,141	0
86	OHX	2	2041	7/7	0.14	-3.28	113,113,113,113	0
85	MG	1	3431	1/1	0.14	-3.29	33,33,33,33	0
85	MG	6	1987	1/1	0.11	-3.29	76,76,76,76	0
85	MG	5	3802	1/1	0.13	-3.29	82,82,82,82	0
86	OHX	1	4192	7/7	0.12	-3.29	183,183,183,183	0
86	OHX	7	229	7/7	0.11	-3.31	156,156,156,156	0
86	OHX	2	2026	7/7	0.12	-3.31	98,98,98,98	0
85	MG	1	3596	1/1	0.14	-3.31	43,43,43,43	0
85	MG	1	3652	1/1	0.09	-3.31	40,40,40,40	0
86	OHX	5	4095	7/7	0.11	-3.32	152,152,152,152	0
86	OHX	2	2122	7/7	0.13	-3.32	170,170,170,170	0
86	OHX	5	4112	7/7	0.11	-3.32	120,120,120,120	0
86	OHX	2	2063	7/7	0.10	-3.32	128,128,128,128	0
85	MG	1	3474	1/1	0.12	-3.32	41,41,41,41	0
86	OHX	2	2050	7/7	0.11	-3.33	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	1928	1/1	0.20	-3.33	61,61,61,61	0
85	MG	5	3443	1/1	0.14	-3.33	33,33,33,33	0
85	MG	5	3532	1/1	0.16	-3.33	44,44,44,44	0
86	OHX	3	222	7/7	0.10	-3.34	160,160,160,160	0
86	OHX	6	2078	7/7	0.09	-3.35	126,126,126,126	0
86	OHX	1	3918	7/7	0.16	-3.35	94,94,94,94	0
86	OHX	1	4063	7/7	0.13	-3.35	155,155,155,155	0
86	OHX	1	3876	7/7	0.13	-3.36	73,73,73,73	0
86	OHX	2	2111	7/7	0.10	-3.37	179,179,179,179	0
86	OHX	5	3970	7/7	0.14	-3.39	110,110,110,110	0
85	MG	5	3753	1/1	0.12	-3.39	46,46,46,46	0
86	OHX	2	2036	7/7	0.12	-3.40	110,110,110,110	0
86	OHX	6	2152	7/7	0.10	-3.40	177,177,177,177	0
86	OHX	1	3888	7/7	0.12	-3.41	94,94,94,94	0
86	OHX	3	223	7/7	0.10	-3.41	173,173,173,173	0
86	OHX	2	2044	7/7	0.11	-3.43	120,120,120,120	0
86	OHX	6	2120	7/7	0.13	-3.43	134,134,134,134	0
85	MG	1	3407	1/1	0.20	-3.44	51,51,51,51	0
86	OHX	5	4185	7/7	0.07	-3.44	157,157,157,157	0
85	MG	5	3543	1/1	0.29	-3.45	53,53,53,53	0
86	OHX	3	217	7/7	0.09	-3.46	127,127,127,127	0
85	MG	5	3447	1/1	0.12	-3.46	50,50,50,50	0
85	MG	1	3497	1/1	0.10	-3.50	39,39,39,39	0
86	OHX	5	4208	7/7	0.12	-3.50	175,175,175,175	0
85	MG	1	3441	1/1	0.21	-3.51	24,24,24,24	0
86	OHX	1	3914	7/7	0.14	-3.55	103,103,103,103	0
85	MG	5	3864	1/1	0.20	-3.55	46,46,46,46	0
86	OHX	5	4159	7/7	0.10	-3.56	172,172,172,172	0
86	OHX	1	3953	7/7	0.10	-3.56	123,123,123,123	0
86	OHX	2	2154	7/7	0.10	-3.58	172,172,172,172	0
86	OHX	1	3931	7/7	0.14	-3.60	104,104,104,104	0
86	OHX	6	2103	7/7	0.11	-3.63	144,144,144,144	0
86	OHX	2	2079	7/7	0.07	-3.63	193,193,193,193	0
86	OHX	1	4194	7/7	0.11	-3.64	152,152,152,152	0
86	OHX	1	4035	7/7	0.10	-3.64	133,133,133,133	0
86	OHX	5	4020	7/7	0.17	-3.65	118,118,118,118	0
86	OHX	5	4207	7/7	0.11	-3.66	164,164,164,164	0
86	OHX	5	4026	7/7	0.10	-3.66	125,125,125,125	0
85	MG	L4	402	1/1	0.26	-3.66	74,74,74,74	0
86	OHX	5	3971	7/7	0.08	-3.67	101,101,101,101	0
85	MG	2	1906	1/1	0.14	-3.67	62,62,62,62	0
86	OHX	6	2161	7/7	0.10	-3.68	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4048	7/7	0.09	-3.69	126,126,126,126	0
86	OHX	5	3983	7/7	0.09	-3.69	120,120,120,120	0
85	MG	1	3751	1/1	0.15	-3.70	29,29,29,29	0
86	OHX	2	2065	7/7	0.09	-3.70	142,142,142,142	0
86	OHX	5	4092	7/7	0.10	-3.70	147,147,147,147	0
86	OHX	2	2086	7/7	0.09	-3.73	148,148,148,148	0
86	OHX	5	4236	7/7	0.13	-3.73	250,250,250,250	0
86	OHX	6	2151	7/7	0.09	-3.74	144,144,144,144	0
86	OHX	5	4009	7/7	0.09	-3.76	134,134,134,134	0
86	OHX	1	4130	7/7	0.13	-3.76	134,134,134,134	0
85	MG	5	3460	1/1	0.21	-3.76	33,33,33,33	0
85	MG	5	3647	1/1	0.09	-3.78	39,39,39,39	0
85	MG	6	1991	1/1	0.10	-3.80	79,79,79,79	0
86	OHX	5	4180	7/7	0.08	-3.80	147,147,147,147	0
86	OHX	6	2067	7/7	0.10	-3.81	108,108,108,108	0
86	OHX	1	4160	7/7	0.12	-3.81	185,185,185,185	0
86	OHX	2	2169	7/7	0.12	-3.82	182,182,182,182	0
86	OHX	6	2108	7/7	0.08	-3.82	144,144,144,144	0
86	OHX	3	218	7/7	0.12	-3.82	119,119,119,119	0
86	OHX	1	3899	7/7	0.12	-3.83	101,101,101,101	0
86	OHX	5	3937	7/7	0.18	-3.83	102,102,102,102	0
86	OHX	6	2184	7/7	0.10	-3.87	164,164,164,164	0
85	MG	1	3571	1/1	0.18	-3.87	38,38,38,38	0
86	OHX	1	3924	7/7	0.11	-3.92	96,96,96,96	0
86	OHX	2	2051	7/7	0.10	-3.93	127,127,127,127	0
86	OHX	2	2168	7/7	0.09	-3.94	144,144,144,144	0
86	OHX	5	4002	7/7	0.10	-3.95	104,104,104,104	0
86	OHX	5	4022	7/7	0.10	-3.95	108,108,108,108	0
86	OHX	6	2169	7/7	0.07	-3.97	176,176,176,176	0
86	OHX	7	222	7/7	0.12	-3.97	114,114,114,114	0
86	OHX	1	4037	7/7	0.07	-3.97	154,154,154,154	0
86	OHX	5	4046	7/7	0.10	-3.99	124,124,124,124	0
86	OHX	2	2101	7/7	0.09	-3.99	158,158,158,158	0
86	OHX	6	2186	7/7	0.14	-4.00	166,166,166,166	0
86	OHX	5	4133	7/7	0.11	-4.02	151,151,151,151	0
86	OHX	5	3987	7/7	0.09	-4.02	150,150,150,150	0
86	OHX	1	4017	7/7	0.08	-4.04	162,162,162,162	0
86	OHX	1	4047	7/7	0.07	-4.04	155,155,155,155	0
85	MG	1	3575	1/1	0.13	-4.05	24,24,24,24	0
86	OHX	6	2115	7/7	0.10	-4.06	147,147,147,147	0
86	OHX	5	4163	7/7	0.09	-4.07	162,162,162,162	0
85	MG	5	3482	1/1	0.11	-4.07	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	1988	1/1	0.16	-4.07	58,58,58,58	0
86	OHX	5	4053	7/7	0.12	-4.08	134,134,134,134	0
85	MG	5	3640	1/1	0.11	-4.10	64,64,64,64	0
86	OHX	5	3960	7/7	0.15	-4.13	108,108,108,108	0
86	OHX	2	2043	7/7	0.08	-4.14	120,120,120,120	0
85	MG	1	3586	1/1	0.18	-4.14	51,51,51,51	0
86	OHX	1	4010	7/7	0.09	-4.15	131,131,131,131	0
86	OHX	5	3982	7/7	0.12	-4.16	100,100,100,100	0
86	OHX	5	4121	7/7	0.08	-4.17	160,160,160,160	0
86	OHX	1	4064	7/7	0.07	-4.17	140,140,140,140	0
86	OHX	5	4119	7/7	0.07	-4.18	176,176,176,176	0
86	OHX	6	2118	7/7	0.10	-4.20	164,164,164,164	0
86	OHX	5	3950	7/7	0.13	-4.20	96,96,96,96	0
86	OHX	5	3964	7/7	0.11	-4.21	105,105,105,105	0
86	OHX	5	4122	7/7	0.12	-4.21	150,150,150,150	0
85	MG	6	2023	1/1	0.12	-4.25	62,62,62,62	0
86	OHX	6	2143	7/7	0.09	-4.27	166,166,166,166	0
85	MG	1	3551	1/1	0.14	-4.27	40,40,40,40	0
85	MG	5	3450	1/1	0.21	-4.27	38,38,38,38	0
86	OHX	2	2167	7/7	0.08	-4.33	172,172,172,172	0
86	OHX	1	4109	7/7	0.07	-4.34	181,181,181,181	0
86	OHX	5	4187	7/7	0.13	-4.35	146,146,146,146	0
86	OHX	6	2086	7/7	0.08	-4.35	138,138,138,138	0
86	OHX	5	4162	7/7	0.11	-4.36	161,161,161,161	0
86	OHX	5	4125	7/7	0.07	-4.36	169,169,169,169	0
86	OHX	5	4073	7/7	0.08	-4.38	152,152,152,152	0
86	OHX	6	2139	7/7	0.10	-4.40	161,161,161,161	0
86	OHX	2	2080	7/7	0.08	-4.42	165,165,165,165	0
86	OHX	1	4057	7/7	0.09	-4.47	165,165,165,165	0
86	OHX	1	4006	7/7	0.09	-4.54	148,148,148,148	0
86	OHX	1	4044	7/7	0.11	-4.55	136,136,136,136	0
86	OHX	2	2178	7/7	0.10	-4.55	192,192,192,192	0
86	OHX	2	2059	7/7	0.10	-4.56	130,130,130,130	0
85	MG	1	3529	1/1	0.18	-4.56	29,29,29,29	0
86	OHX	1	3973	7/7	0.14	-4.62	131,131,131,131	0
86	OHX	5	4061	7/7	0.09	-4.64	139,139,139,139	0
86	OHX	1	3944	7/7	0.14	-4.64	114,114,114,114	0
85	MG	5	3507	1/1	0.19	-4.65	38,38,38,38	0
86	OHX	5	4039	7/7	0.09	-4.66	148,148,148,148	0
86	OHX	5	3978	7/7	0.10	-4.67	110,110,110,110	0
85	MG	5	3887	1/1	0.11	-4.67	135,135,135,135	0
86	OHX	6	2069	7/7	0.12	-4.70	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3967	7/7	0.11	-4.75	135,135,135,135	0
86	OHX	1	3998	7/7	0.11	-4.75	131,131,131,131	0
86	OHX	5	4045	7/7	0.08	-4.78	126,126,126,126	0
86	OHX	5	4212	7/7	0.08	-4.82	119,119,119,119	0
86	OHX	5	4008	7/7	0.11	-4.83	117,117,117,117	0
86	OHX	1	4043	7/7	0.06	-4.84	153,153,153,153	0
85	MG	5	3662	1/1	0.11	-4.84	40,40,40,40	0
86	OHX	5	4104	7/7	0.13	-4.84	137,137,137,137	0
86	OHX	1	4187	7/7	0.08	-4.87	171,171,171,171	0
86	OHX	6	2089	7/7	0.07	-4.91	121,121,121,121	0
85	MG	5	3645	1/1	0.12	-4.92	103,103,103,103	0
86	OHX	8	221	7/7	0.09	-4.93	147,147,147,147	0
86	OHX	5	4014	7/7	0.07	-4.93	122,122,122,122	0
86	OHX	5	4246	7/7	0.10	-4.96	166,166,166,166	0
86	OHX	1	4002	7/7	0.09	-4.97	127,127,127,127	0
86	OHX	5	4169	7/7	0.14	-4.99	157,157,157,157	0
85	MG	1	3734	1/1	0.14	-4.99	54,54,54,54	0
85	MG	5	3672	1/1	0.14	-5.03	44,44,44,44	0
86	OHX	5	4063	7/7	0.09	-5.04	160,160,160,160	0
86	OHX	1	3968	7/7	0.09	-5.04	124,124,124,124	0
86	OHX	6	2071	7/7	0.09	-5.06	108,108,108,108	0
86	OHX	5	4131	7/7	0.11	-5.08	157,157,157,157	0
86	OHX	5	4060	7/7	0.09	-5.20	130,130,130,130	0
85	MG	1	3724	1/1	0.12	-5.20	70,70,70,70	0
86	OHX	2	2170	7/7	0.10	-5.21	162,162,162,162	0
86	OHX	5	4012	7/7	0.07	-5.24	129,129,129,129	0
86	OHX	C5	201	7/7	0.08	-5.26	178,178,178,178	0
86	OHX	5	4205	7/7	0.12	-5.30	167,167,167,167	0
85	MG	6	2000	1/1	0.09	-5.30	108,108,108,108	0
86	OHX	1	4019	7/7	0.09	-5.30	128,128,128,128	0
86	OHX	6	2199	7/7	0.15	-5.31	178,178,178,178	0
86	OHX	1	4169	7/7	0.09	-5.33	125,125,125,125	0
85	MG	1	3589	1/1	0.15	-5.43	83,83,83,83	0
86	OHX	6	2166	7/7	0.09	-5.46	169,169,169,169	0
86	OHX	1	3958	7/7	0.10	-5.47	115,115,115,115	0
85	MG	5	3537	1/1	0.16	-5.48	21,21,21,21	0
86	OHX	2	2049	7/7	0.09	-5.60	136,136,136,136	0
86	OHX	1	4171	7/7	0.07	-5.63	155,155,155,155	0
86	OHX	2	2129	7/7	0.12	-5.66	218,218,218,218	0
85	MG	1	3478	1/1	0.12	-5.73	79,79,79,79	0
86	OHX	6	2090	7/7	0.08	-5.76	137,137,137,137	0
86	OHX	5	4234	7/7	0.15	-5.77	171,171,171,171	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3584	1/1	0.22	-5.80	24,24,24,24	0
86	OHX	5	3938	7/7	0.11	-5.80	93,93,93,93	0
86	OHX	5	4174	7/7	0.14	-5.84	177,177,177,177	0
86	OHX	2	2072	7/7	0.07	-5.88	157,157,157,157	0
86	OHX	1	4143	7/7	0.11	-5.90	155,155,155,155	0
86	OHX	5	4036	7/7	0.11	-5.95	157,157,157,157	0
86	OHX	1	3966	7/7	0.08	-5.97	129,129,129,129	0
85	MG	5	3542	1/1	0.13	-5.99	43,43,43,43	0
85	MG	5	3740	1/1	0.07	-6.00	73,73,73,73	0
86	OHX	4	233	7/7	0.10	-6.03	152,152,152,152	0
86	OHX	5	4017	7/7	0.08	-6.04	125,125,125,125	0
86	OHX	1	3981	7/7	0.10	-6.09	136,136,136,136	0
86	OHX	1	4012	7/7	0.08	-6.12	142,142,142,142	0
86	OHX	5	4007	7/7	0.12	-6.24	122,122,122,122	0
85	MG	5	3689	1/1	0.14	-6.28	55,55,55,55	0
86	OHX	1	4101	7/7	0.10	-6.29	163,163,163,163	0
85	MG	2	1934	1/1	0.26	-6.31	53,53,53,53	0
86	OHX	2	2110	7/7	0.07	-6.35	128,128,128,128	0
85	MG	6	2017	1/1	0.14	-6.36	33,33,33,33	0
86	OHX	2	2113	7/7	0.08	-6.42	179,179,179,179	0
86	OHX	2	2090	7/7	0.06	-6.45	159,159,159,159	0
86	OHX	6	2092	7/7	0.07	-6.56	126,126,126,126	0
85	MG	5	3671	1/1	0.13	-6.66	52,52,52,52	0
86	OHX	1	3999	7/7	0.08	-6.68	140,140,140,140	0
86	OHX	5	4218	7/7	0.10	-6.70	170,170,170,170	0
86	OHX	1	4150	7/7	0.09	-6.73	159,159,159,159	0
86	OHX	5	4059	7/7	0.08	-6.78	137,137,137,137	0
86	OHX	1	4125	7/7	0.08	-6.94	165,165,165,165	0
85	MG	5	3872	1/1	0.14	-7.13	40,40,40,40	0
86	OHX	4	232	7/7	0.13	-7.13	166,166,166,166	0
86	OHX	5	4241	7/7	0.15	-7.17	177,177,177,177	0
86	OHX	1	3980	7/7	0.07	-7.19	138,138,138,138	0
85	MG	5	3859	1/1	0.17	-7.28	51,51,51,51	0
86	OHX	1	3930	7/7	0.13	-7.32	108,108,108,108	0
86	OHX	5	4086	7/7	0.11	-7.48	133,133,133,133	0
86	OHX	1	4023	7/7	0.08	-7.56	154,154,154,154	0
86	OHX	6	2140	7/7	0.07	-7.58	165,165,165,165	0
86	OHX	5	4129	7/7	0.09	-7.64	156,156,156,156	0
85	MG	6	2003	1/1	0.14	-7.67	74,74,74,74	0
86	OHX	5	3997	7/7	0.08	-7.81	114,114,114,114	0
86	OHX	6	2114	7/7	0.06	-7.89	146,146,146,146	0
86	OHX	2	2118	7/7	0.08	-8.02	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2144	7/7	0.08	-8.03	159,159,159,159	0
86	OHX	5	4067	7/7	0.06	-8.15	126,126,126,126	0
85	MG	2	1998	1/1	0.09	-8.20	117,117,117,117	0
86	OHX	6	2113	7/7	0.13	-8.49	148,148,148,148	0
86	OHX	1	4082	7/7	0.08	-8.69	151,151,151,151	0
86	OHX	1	4021	7/7	0.10	-8.82	140,140,140,140	0
86	OHX	1	3948	7/7	0.09	-8.92	111,111,111,111	0
86	OHX	6	2150	7/7	0.09	-9.31	172,172,172,172	0
86	OHX	5	4089	7/7	0.06	-9.54	155,155,155,155	0
86	OHX	6	2131	7/7	0.07	-9.61	172,172,172,172	0
86	OHX	1	3912	7/7	0.11	-9.77	109,109,109,109	0
85	MG	3	203	1/1	0.07	-10.35	73,73,73,73	0
86	OHX	5	4152	7/7	0.09	-10.40	156,156,156,156	0
85	MG	5	3776	1/1	0.06	-10.56	39,39,39,39	0
86	OHX	1	4100	7/7	0.09	-11.27	143,143,143,143	0
86	OHX	1	4172	7/7	0.13	-11.28	177,177,177,177	0
85	MG	1	3762	1/1	0.09	-11.31	102,102,102,102	0
86	OHX	1	4116	7/7	0.10	-11.35	164,164,164,164	0
85	MG	4	223	1/1	0.17	-11.40	86,86,86,86	0
86	OHX	6	2079	7/7	0.09	-11.41	120,120,120,120	0
86	OHX	5	4138	7/7	0.07	-11.64	151,151,151,151	0
86	OHX	1	4008	7/7	0.10	-11.66	149,149,149,149	0
86	OHX	5	4066	7/7	0.10	-12.02	148,148,148,148	0
86	OHX	5	4224	7/7	0.09	-12.12	212,212,212,212	0
86	OHX	5	4111	7/7	0.12	-12.20	172,172,172,172	0
85	MG	5	3479	1/1	0.16	-12.24	46,46,46,46	0
85	MG	1	3667	1/1	0.18	-12.33	49,49,49,49	0
86	OHX	5	4079	7/7	0.11	-12.36	135,135,135,135	0
85	MG	5	3527	1/1	0.19	-13.64	33,33,33,33	0
86	OHX	1	4142	7/7	0.10	-14.27	171,171,171,171	0
85	MG	5	3759	1/1	0.09	-22.95	73,73,73,73	0
85	MG	5	3789	1/1	0.10	-54.91	82,82,82,82	0
85	MG	1	3671	1/1	0.10	-	83,83,83,83	0
85	MG	4	219	1/1	0.25	-	43,43,43,43	0
85	MG	5	3854	1/1	0.17	-	73,73,73,73	0
85	MG	7	212	1/1	0.54	-	63,63,63,63	0
85	MG	5	3794	1/1	0.26	-	36,36,36,36	0
85	MG	1	3833	1/1	0.27	-	31,31,31,31	0
85	MG	5	3433	1/1	0.26	-	86,86,86,86	0
85	MG	L3	404	1/1	0.21	-	57,57,57,57	0
85	MG	2	2020	1/1	0.32	-	50,50,50,50	0
85	MG	6	2031	1/1	0.16	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3845	1/1	0.50	-	115,115,115,115	0
85	MG	6	2015	1/1	0.32	-	51,51,51,51	0
85	MG	2	1953	1/1	0.74	-	107,107,107,107	0
85	MG	3	215	1/1	0.48	-	46,46,46,46	0
85	MG	5	3867	1/1	0.43	-	43,43,43,43	0
85	MG	6	2043	1/1	0.28	-	52,52,52,52	0
85	MG	5	3766	1/1	0.45	-	102,102,102,102	0
85	MG	1	3468	1/1	0.20	-	29,29,29,29	0
85	MG	1	3830	1/1	0.39	-	64,64,64,64	0
86	OHX	2	2158	7/7	0.15	-	278,278,278,278	0
85	MG	5	3411	1/1	0.49	-	45,45,45,45	0
85	MG	6	1923	1/1	0.62	-	115,115,115,115	0
85	MG	5	3420	1/1	0.25	-	124,124,124,124	0
85	MG	1	3843	1/1	0.21	-	49,49,49,49	0
85	MG	5	3885	1/1	0.26	-	89,89,89,89	0
85	MG	5	3870	1/1	0.15	-	49,49,49,49	0
85	MG	5	3879	1/1	0.59	-	79,79,79,79	0
85	MG	1	3778	1/1	0.26	-	37,37,37,37	0
85	MG	1	3786	1/1	0.18	-	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.