



# wwPDB X-ray Structure Validation Summary Report i

Oct 9, 2014 – 09:55 PM BST

PDB ID : 4U4Y  
Title : Crystal structure of Pactamycin bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-24  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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

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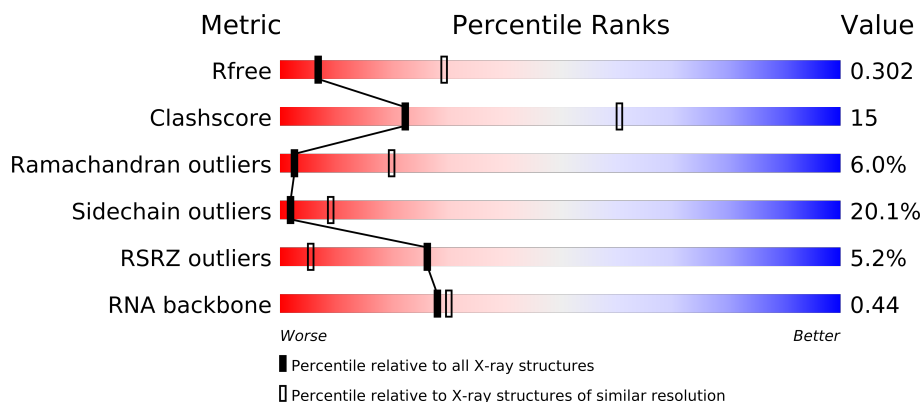
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	m2	160	
82	p0	311	
83	p1	47	
84	p2	46	

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

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3402	-	X
85	MG	1	3406	-	X
85	MG	1	3409	-	X
85	MG	1	3410	-	X
85	MG	1	3411	-	X
85	MG	1	3413	-	X
85	MG	1	3414	-	X
85	MG	1	3420	-	X
85	MG	1	3429	-	X
85	MG	1	3443	-	X
85	MG	1	3444	-	X
85	MG	1	3447	-	X
85	MG	1	3451	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3459	-	X
85	MG	1	3463	-	X
85	MG	1	3469	-	X
85	MG	1	3470	-	X
85	MG	1	3472	-	X
85	MG	1	3475	-	X
85	MG	1	3477	-	X
85	MG	1	3485	-	X
85	MG	1	3493	-	X
85	MG	1	3497	-	X
85	MG	1	3500	-	X
85	MG	1	3502	-	X
85	MG	1	3506	-	X
85	MG	1	3509	-	X
85	MG	1	3521	-	X
85	MG	1	3523	-	X
85	MG	1	3524	-	X
85	MG	1	3525	-	X
85	MG	1	3526	-	X
85	MG	1	3527	-	X
85	MG	1	3529	-	X
85	MG	1	3533	-	X
85	MG	1	3535	-	X
85	MG	1	3537	-	X
85	MG	1	3538	-	X
85	MG	1	3540	-	X
85	MG	1	3543	-	X
85	MG	1	3545	-	X
85	MG	1	3546	-	X
85	MG	1	3547	-	X
85	MG	1	3552	-	X
85	MG	1	3555	-	X
85	MG	1	3561	-	X
85	MG	1	3563	-	X
85	MG	1	3565	-	X
85	MG	1	3570	-	X
85	MG	1	3572	-	X
85	MG	1	3578	-	X
85	MG	1	3585	-	X
85	MG	1	3586	-	X
85	MG	1	3591	-	X
85	MG	1	3592	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3598	-	X
85	MG	1	3605	-	X
85	MG	1	3607	-	X
85	MG	1	3610	-	X
85	MG	1	3611	-	X
85	MG	1	3614	-	X
85	MG	1	3615	-	X
85	MG	1	3618	-	X
85	MG	1	3620	-	X
85	MG	1	3621	-	X
85	MG	1	3623	-	X
85	MG	1	3624	-	X
85	MG	1	3628	-	X
85	MG	1	3629	-	X
85	MG	1	3631	-	X
85	MG	1	3635	-	X
85	MG	1	3636	-	X
85	MG	1	3645	-	X
85	MG	1	3647	-	X
85	MG	1	3648	-	X
85	MG	1	3649	-	X
85	MG	1	3658	-	X
85	MG	1	3662	-	X
85	MG	1	3665	-	X
85	MG	1	3666	-	X
85	MG	1	3667	-	X
85	MG	1	3668	-	X
85	MG	1	3670	-	X
85	MG	1	3672	-	X
85	MG	1	3675	-	X
85	MG	1	3677	-	X
85	MG	1	3678	-	X
85	MG	1	3680	-	X
85	MG	1	3682	-	X
85	MG	1	3683	-	X
85	MG	1	3689	-	X
85	MG	1	3691	-	X
85	MG	1	3695	-	X
85	MG	1	3696	-	X
85	MG	1	3700	-	X
85	MG	1	3702	-	X
85	MG	1	3706	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3711	-	X
85	MG	1	3713	-	X
85	MG	1	3716	-	X
85	MG	1	3717	-	X
85	MG	1	3718	-	X
85	MG	1	3722	-	X
85	MG	1	3723	-	X
85	MG	1	3724	-	X
85	MG	1	3725	-	X
85	MG	1	3727	-	X
85	MG	1	3730	-	X
85	MG	1	3735	-	X
85	MG	1	3738	-	X
85	MG	1	3741	-	X
85	MG	1	3747	-	X
85	MG	1	3751	-	X
85	MG	1	3758	-	X
85	MG	1	3761	-	X
85	MG	1	3771	-	X
85	MG	1	3773	-	X
85	MG	1	3778	-	X
85	MG	1	3779	-	X
85	MG	1	3782	-	X
85	MG	1	3784	-	X
85	MG	1	3785	-	X
85	MG	1	3787	-	X
85	MG	1	3791	-	X
85	MG	1	3793	-	X
85	MG	1	3795	-	X
85	MG	1	3796	-	X
85	MG	1	3798	-	X
85	MG	1	3801	-	X
85	MG	1	3802	-	X
85	MG	1	3803	-	X
85	MG	1	3804	-	X
85	MG	1	3805	-	X
85	MG	1	3811	-	X
85	MG	1	3812	-	X
85	MG	1	3813	-	X
85	MG	1	3815	-	X
85	MG	1	3817	-	X
85	MG	1	3818	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3820	-	X
85	MG	1	3822	-	X
85	MG	1	3823	-	X
85	MG	1	3824	-	X
85	MG	1	3831	-	X
85	MG	1	3832	-	X
85	MG	1	3836	-	X
85	MG	1	3841	-	X
85	MG	1	3842	-	X
85	MG	1	3844	-	X
85	MG	1	3847	-	X
85	MG	1	3850	-	X
85	MG	1	3852	-	X
85	MG	1	3854	-	X
85	MG	1	3855	-	X
85	MG	1	3856	-	X
85	MG	1	3857	-	X
85	MG	1	3858	-	X
85	MG	1	3859	-	X
85	MG	1	3861	-	X
85	MG	1	4215	-	X
85	MG	1	4219	-	X
85	MG	2	1903	-	X
85	MG	2	1904	-	X
85	MG	2	1908	-	X
85	MG	2	1913	-	X
85	MG	2	1914	-	X
85	MG	2	1918	-	X
85	MG	2	1919	-	X
85	MG	2	1921	-	X
85	MG	2	1925	-	X
85	MG	2	1926	-	X
85	MG	2	1935	-	X
85	MG	2	1938	-	X
85	MG	2	1945	-	X
85	MG	2	1949	-	X
85	MG	2	1951	-	X
85	MG	2	1952	-	X
85	MG	2	1953	-	X
85	MG	2	1955	-	X
85	MG	2	1956	-	X
85	MG	2	1957	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1958	-	X
85	MG	2	1959	-	X
85	MG	2	1962	-	X
85	MG	2	1963	-	X
85	MG	2	1965	-	X
85	MG	2	1967	-	X
85	MG	2	1969	-	X
85	MG	2	1970	-	X
85	MG	2	1973	-	X
85	MG	2	1974	-	X
85	MG	2	1976	-	X
85	MG	2	1978	-	X
85	MG	2	1980	-	X
85	MG	2	1981	-	X
85	MG	2	1983	-	X
85	MG	2	1986	-	X
85	MG	2	1987	-	X
85	MG	2	1988	-	X
85	MG	2	1992	-	X
85	MG	2	1994	-	X
85	MG	2	1996	-	X
85	MG	2	2001	-	X
85	MG	2	2003	-	X
85	MG	2	2004	-	X
85	MG	2	2006	-	X
85	MG	2	2007	-	X
85	MG	2	2010	-	X
85	MG	2	2014	-	X
85	MG	2	2015	-	X
85	MG	2	2019	-	X
85	MG	2	2022	-	X
85	MG	3	201	-	X
85	MG	3	202	-	X
85	MG	3	204	-	X
85	MG	3	205	-	X
85	MG	3	206	-	X
85	MG	3	207	-	X
85	MG	3	209	-	X
85	MG	3	213	-	X
85	MG	3	214	-	X
85	MG	4	201	-	X
85	MG	4	202	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	4	203	-	X
85	MG	4	204	-	X
85	MG	4	209	-	X
85	MG	4	210	-	X
85	MG	4	214	-	X
85	MG	4	216	-	X
85	MG	4	218	-	X
85	MG	4	220	-	X
85	MG	5	3403	-	X
85	MG	5	3409	-	X
85	MG	5	3410	-	X
85	MG	5	3425	-	X
85	MG	5	3428	-	X
85	MG	5	3432	-	X
85	MG	5	3433	-	X
85	MG	5	3437	-	X
85	MG	5	3438	-	X
85	MG	5	3443	-	X
85	MG	5	3444	-	X
85	MG	5	3445	-	X
85	MG	5	3448	-	X
85	MG	5	3461	-	X
85	MG	5	3462	-	X
85	MG	5	3464	-	X
85	MG	5	3465	-	X
85	MG	5	3467	-	X
85	MG	5	3470	-	X
85	MG	5	3471	-	X
85	MG	5	3477	-	X
85	MG	5	3481	-	X
85	MG	5	3485	-	X
85	MG	5	3486	-	X
85	MG	5	3488	-	X
85	MG	5	3490	-	X
85	MG	5	3493	-	X
85	MG	5	3497	-	X
85	MG	5	3501	-	X
85	MG	5	3503	-	X
85	MG	5	3504	-	X
85	MG	5	3505	-	X
85	MG	5	3506	-	X
85	MG	5	3512	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3518	-	X
85	MG	5	3520	-	X
85	MG	5	3522	-	X
85	MG	5	3524	-	X
85	MG	5	3529	-	X
85	MG	5	3530	-	X
85	MG	5	3532	-	X
85	MG	5	3536	-	X
85	MG	5	3538	-	X
85	MG	5	3540	-	X
85	MG	5	3541	-	X
85	MG	5	3546	-	X
85	MG	5	3549	-	X
85	MG	5	3550	-	X
85	MG	5	3553	-	X
85	MG	5	3554	-	X
85	MG	5	3555	-	X
85	MG	5	3556	-	X
85	MG	5	3560	-	X
85	MG	5	3561	-	X
85	MG	5	3562	-	X
85	MG	5	3563	-	X
85	MG	5	3564	-	X
85	MG	5	3570	-	X
85	MG	5	3571	-	X
85	MG	5	3572	-	X
85	MG	5	3573	-	X
85	MG	5	3575	-	X
85	MG	5	3576	-	X
85	MG	5	3577	-	X
85	MG	5	3579	-	X
85	MG	5	3582	-	X
85	MG	5	3584	-	X
85	MG	5	3585	-	X
85	MG	5	3588	-	X
85	MG	5	3594	-	X
85	MG	5	3595	-	X
85	MG	5	3596	-	X
85	MG	5	3598	-	X
85	MG	5	3603	-	X
85	MG	5	3605	-	X
85	MG	5	3607	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3608	-	X
85	MG	5	3610	-	X
85	MG	5	3614	-	X
85	MG	5	3618	-	X
85	MG	5	3620	-	X
85	MG	5	3621	-	X
85	MG	5	3623	-	X
85	MG	5	3632	-	X
85	MG	5	3634	-	X
85	MG	5	3635	-	X
85	MG	5	3644	-	X
85	MG	5	3647	-	X
85	MG	5	3648	-	X
85	MG	5	3649	-	X
85	MG	5	3652	-	X
85	MG	5	3654	-	X
85	MG	5	3655	-	X
85	MG	5	3658	-	X
85	MG	5	3664	-	X
85	MG	5	3665	-	X
85	MG	5	3669	-	X
85	MG	5	3671	-	X
85	MG	5	3673	-	X
85	MG	5	3674	-	X
85	MG	5	3675	-	X
85	MG	5	3678	-	X
85	MG	5	3681	-	X
85	MG	5	3682	-	X
85	MG	5	3683	-	X
85	MG	5	3684	-	X
85	MG	5	3686	-	X
85	MG	5	3693	-	X
85	MG	5	3695	-	X
85	MG	5	3696	-	X
85	MG	5	3709	-	X
85	MG	5	3710	-	X
85	MG	5	3713	-	X
85	MG	5	3716	-	X
85	MG	5	3720	-	X
85	MG	5	3722	-	X
85	MG	5	3734	-	X
85	MG	5	3735	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3736	-	X
85	MG	5	3737	-	X
85	MG	5	3738	-	X
85	MG	5	3739	-	X
85	MG	5	3742	-	X
85	MG	5	3748	-	X
85	MG	5	3751	-	X
85	MG	5	3752	-	X
85	MG	5	3756	-	X
85	MG	5	3760	-	X
85	MG	5	3761	-	X
85	MG	5	3763	-	X
85	MG	5	3764	-	X
85	MG	5	3767	-	X
85	MG	5	3769	-	X
85	MG	5	3770	-	X
85	MG	5	3772	-	X
85	MG	5	3775	-	X
85	MG	5	3776	-	X
85	MG	5	3780	-	X
85	MG	5	3781	-	X
85	MG	5	3783	-	X
85	MG	5	3790	-	X
85	MG	5	3791	-	X
85	MG	5	3794	-	X
85	MG	5	3796	-	X
85	MG	5	3799	-	X
85	MG	5	3803	-	X
85	MG	5	3809	-	X
85	MG	5	3811	-	X
85	MG	5	3813	-	X
85	MG	5	3814	-	X
85	MG	5	3815	-	X
85	MG	5	3817	-	X
85	MG	5	3821	-	X
85	MG	5	3823	-	X
85	MG	5	3825	-	X
85	MG	5	3826	-	X
85	MG	5	3829	-	X
85	MG	5	3836	-	X
85	MG	5	3843	-	X
85	MG	5	3844	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3847	-	X
85	MG	5	3848	-	X
85	MG	5	3851	-	X
85	MG	5	3852	-	X
85	MG	5	3854	-	X
85	MG	5	3859	-	X
85	MG	5	3860	-	X
85	MG	5	3861	-	X
85	MG	5	3863	-	X
85	MG	5	3864	-	X
85	MG	5	3866	-	X
85	MG	5	3869	-	X
85	MG	5	3870	-	X
85	MG	5	3872	-	X
85	MG	5	3874	-	X
85	MG	5	3875	-	X
85	MG	5	3876	-	X
85	MG	5	3877	-	X
85	MG	5	3878	-	X
85	MG	5	3882	-	X
85	MG	5	3883	-	X
85	MG	5	3884	-	X
85	MG	5	3887	-	X
85	MG	5	3889	-	X
85	MG	5	3891	-	X
85	MG	5	3894	-	X
85	MG	5	3899	-	X
85	MG	5	4253	-	X
85	MG	5	4254	-	X
85	MG	6	1901	-	X
85	MG	6	1904	-	X
85	MG	6	1906	-	X
85	MG	6	1907	-	X
85	MG	6	1908	-	X
85	MG	6	1911	-	X
85	MG	6	1916	-	X
85	MG	6	1917	-	X
85	MG	6	1918	-	X
85	MG	6	1920	-	X
85	MG	6	1922	-	X
85	MG	6	1923	-	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	1928	-	X
85	MG	6	1929	-	X
85	MG	6	1931	-	X
85	MG	6	1933	-	X
85	MG	6	1934	-	X
85	MG	6	1936	-	X
85	MG	6	1937	-	X
85	MG	6	1940	-	X
85	MG	6	1942	-	X
85	MG	6	1943	-	X
85	MG	6	1944	-	X
85	MG	6	1945	-	X
85	MG	6	1946	-	X
85	MG	6	1947	-	X
85	MG	6	1948	-	X
85	MG	6	1953	-	X
85	MG	6	1954	-	X
85	MG	6	1959	-	X
85	MG	6	1965	-	X
85	MG	6	1966	-	X
85	MG	6	1967	-	X
85	MG	6	1968	-	X
85	MG	6	1971	-	X
85	MG	6	1981	-	X
85	MG	6	1987	-	X
85	MG	6	1991	-	X
85	MG	6	1994	-	X
85	MG	6	1997	-	X
85	MG	6	2001	-	X
85	MG	6	2007	-	X
85	MG	6	2008	-	X
85	MG	6	2009	-	X
85	MG	6	2010	-	X
85	MG	6	2011	-	X
85	MG	6	2012	-	X
85	MG	6	2013	-	X
85	MG	6	2016	-	X
85	MG	6	2017	-	X
85	MG	6	2018	-	X
85	MG	6	2020	-	X
85	MG	6	2024	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	2027	-	X
85	MG	6	2028	-	X
85	MG	6	2029	-	X
85	MG	6	2032	-	X
85	MG	6	2037	-	X
85	MG	6	2039	-	X
85	MG	6	2040	-	X
85	MG	6	2041	-	X
85	MG	6	2044	-	X
85	MG	6	2045	-	X
85	MG	7	201	-	X
85	MG	7	202	-	X
85	MG	7	203	-	X
85	MG	7	204	-	X
85	MG	7	205	-	X
85	MG	7	206	-	X
85	MG	7	207	-	X
85	MG	7	209	-	X
85	MG	7	214	-	X
85	MG	8	201	-	X
85	MG	8	202	-	X
85	MG	8	203	-	X
85	MG	8	206	-	X
85	MG	8	207	-	X
85	MG	8	210	-	X
85	MG	8	211	-	X
85	MG	L7	302	-	X
85	MG	L7	303	-	X
85	MG	M1	201	-	X
85	MG	M3	201	-	X
85	MG	M6	202	-	X
85	MG	M7	203	-	X
85	MG	M9	201	-	X
85	MG	N5	201	-	X
85	MG	N8	201	-	X
85	MG	N8	202	-	X
85	MG	N8	203	-	X
85	MG	N8	204	-	X
85	MG	Q2	502	-	X
85	MG	S2	301	-	X
85	MG	c7	201	-	X
85	MG	d3	201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	d3	202	-	X
85	MG	d6	102	-	X
85	MG	l3	401	-	X
85	MG	l3	402	-	X
85	MG	l5	301	-	X
85	MG	l7	302	-	X
85	MG	m1	202	-	X
85	MG	m5	302	-	X
85	MG	m7	203	-	X
85	MG	m7	205	-	X
85	MG	n0	201	-	X
85	MG	o1	201	-	X
85	MG	o3	201	-	X
85	MG	s2	301	-	X
85	MG	sM	302	-	X
86	OHX	1	3869	-	X
86	OHX	1	3876	-	X
86	OHX	1	3887	-	X
86	OHX	1	3890	-	X
86	OHX	1	3900	-	X
86	OHX	1	3917	-	X
86	OHX	1	4014	-	X
86	OHX	1	4061	-	X
86	OHX	1	4110	-	X
86	OHX	1	4111	-	X
86	OHX	1	4118	-	X
86	OHX	1	4124	-	X
86	OHX	1	4126	-	X
86	OHX	1	4138	-	X
86	OHX	1	4139	-	X
86	OHX	1	4140	-	X
86	OHX	1	4146	-	X
86	OHX	1	4161	-	X
86	OHX	1	4165	-	X
86	OHX	1	4169	-	X
86	OHX	1	4175	-	X
86	OHX	1	4176	-	X
86	OHX	1	4183	-	X
86	OHX	1	4185	-	X
86	OHX	1	4187	-	X
86	OHX	1	4188	-	X
86	OHX	1	4196	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4200	-	X
86	OHX	1	4206	-	X
86	OHX	1	4207	-	X
86	OHX	1	4208	-	X
86	OHX	1	4209	-	X
86	OHX	1	4210	-	X
86	OHX	1	4213	-	X
86	OHX	2	2135	-	X
86	OHX	2	2143	-	X
86	OHX	2	2147	-	X
86	OHX	2	2158	-	X
86	OHX	2	2162	-	X
86	OHX	2	2170	-	X
86	OHX	4	237	-	X
86	OHX	5	3901	-	X
86	OHX	5	3908	-	X
86	OHX	5	3915	-	X
86	OHX	5	3933	-	X
86	OHX	5	3940	-	X
86	OHX	5	3949	-	X
86	OHX	5	3952	-	X
86	OHX	5	3967	-	X
86	OHX	5	4013	-	X
86	OHX	5	4041	-	X
86	OHX	5	4153	-	X
86	OHX	5	4154	-	X
86	OHX	5	4160	-	X
86	OHX	5	4170	-	X
86	OHX	5	4176	-	X
86	OHX	5	4179	-	X
86	OHX	5	4180	-	X
86	OHX	5	4182	-	X
86	OHX	5	4187	-	X
86	OHX	5	4188	-	X
86	OHX	5	4206	-	X
86	OHX	5	4219	-	X
86	OHX	5	4221	-	X
86	OHX	5	4222	-	X
86	OHX	5	4228	-	X
86	OHX	5	4231	-	X
86	OHX	5	4235	-	X
86	OHX	5	4237	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4239	-	X
86	OHX	5	4245	-	X
86	OHX	5	4246	-	X
86	OHX	5	4247	-	X
86	OHX	6	2054	-	X
86	OHX	6	2126	-	X
86	OHX	6	2159	-	X
86	OHX	6	2164	-	X
86	OHX	6	2167	-	X
86	OHX	6	2170	-	X
86	OHX	6	2173	-	X
86	OHX	6	2179	-	X
86	OHX	6	2180	-	X
86	OHX	6	2182	-	X
86	OHX	6	2185	-	X
86	OHX	6	2188	-	X
86	OHX	6	2203	-	X
86	OHX	M7	205	-	X
86	OHX	M7	206	-	X
86	OHX	l4	403	-	X
86	OHX	s9	201	-	X

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411223 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 unknown protein chain m2.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	3	Total	Mg	0	0
			3	3		
85	N9	1	Total	Mg	0	0
			1	1		
85	n8	4	Total	Mg	0	0
			4	4		
85	o1	1	Total	Mg	0	0
			1	1		
85	N5	1	Total	Mg	0	0
			1	1		
85	6	147	Total	Mg	0	0
			147	147		
85	sM	2	Total	Mg	0	0
			2	2		
85	m5	4	Total	Mg	0	0
			4	4		
85	l3	2	Total	Mg	0	0
			2	2		
85	M1	1	Total	Mg	0	0
			1	1		
85	n0	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	d6	1	Total 1	Mg 1	0	0
85	2	124	Total 124	Mg 124	0	0
85	O3	1	Total 1	Mg 1	0	0
85	L4	2	Total 2	Mg 2	0	0
85	l7	2	Total 2	Mg 2	0	0
85	M5	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	S2	2	Total 2	Mg 2	0	0
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	o4	1	Total 1	Mg 1	0	0
85	M9	3	Total 3	Mg 3	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	504	Total 504	Mg 504	0	0
85	L5	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	1	471	Total 471	Mg 471	0	0
85	s2	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	1	Total 1	Mg 1	0	0
85	O2	1	Total 1	Mg 1	0	0
85	q3	2	Total 2	Mg 2	0	0
85	o3	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	2	Total 2	Mg 2	0	0
85	4	21	Total 21	Mg 21	0	0
85	n6	1	Total 1	Mg 1	0	0
85	L2	1	Total 1	Mg 1	0	0
85	m1	2	Total 2	Mg 2	0	0
85	l5	2	Total 2	Mg 2	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	4	Total 4	Mg 4	0	0
85	N8	4	Total 4	Mg 4	0	0
85	s1	1	Total 1	Mg 1	0	0
85	m6	2	Total 2	Mg 2	0	0

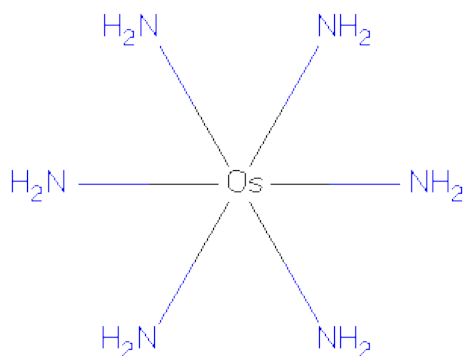
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	s8	2	Total 2	Mg 2	0	0
85	l8	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	14	Total 14	Mg 14	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	2	Total 2	Mg 2	0	0
85	N6	1	Total 1	Mg 1	0	0
85	8	16	Total 16	Mg 16	0	0
85	M6	2	Total 2	Mg 2	0	0
85	N0	1	Total 1	Mg 1	0	0
85	3	14	Total 14	Mg 14	0	0

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	C8	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			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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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
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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
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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
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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		
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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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
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86	1	1	Total	N	Os	0	0
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			7	6	1		
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
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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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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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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
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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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			7	6	1		
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
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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
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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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		
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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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
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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
			7	6	1		
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
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86	3	1	Total	N	Os	0	0
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			7	6	1		
86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L4	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	M5	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M9	1	Total	N	Os	0	0
			7	6	1		
86	N1	1	Total	N	Os	0	0
			7	6	1		
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		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	s1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	s4	1	Total	N	Os	0	0
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86	s8	1	Total	N	Os	0	0
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86	s9	1	Total	N	Os	0	0
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86	c3	1	Total	N	Os	0	0
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86	d4	1	Total	N	Os	0	0
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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	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			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	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	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	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		

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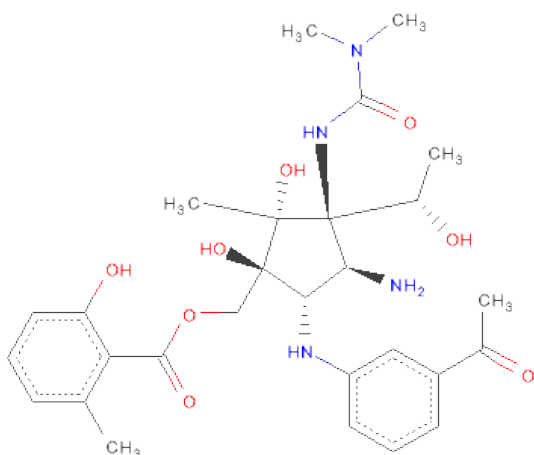
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	19	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q1	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is de-6-MSA-pactamycin (three-letter code: PCY) (formula:  $C_{28}H_{38}N_4O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
87	2	1	Total	C	N	O	0	0
			40	28	4	8		
87	6	1	Total	C	N	O	0	0
			40	28	4	8		

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

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

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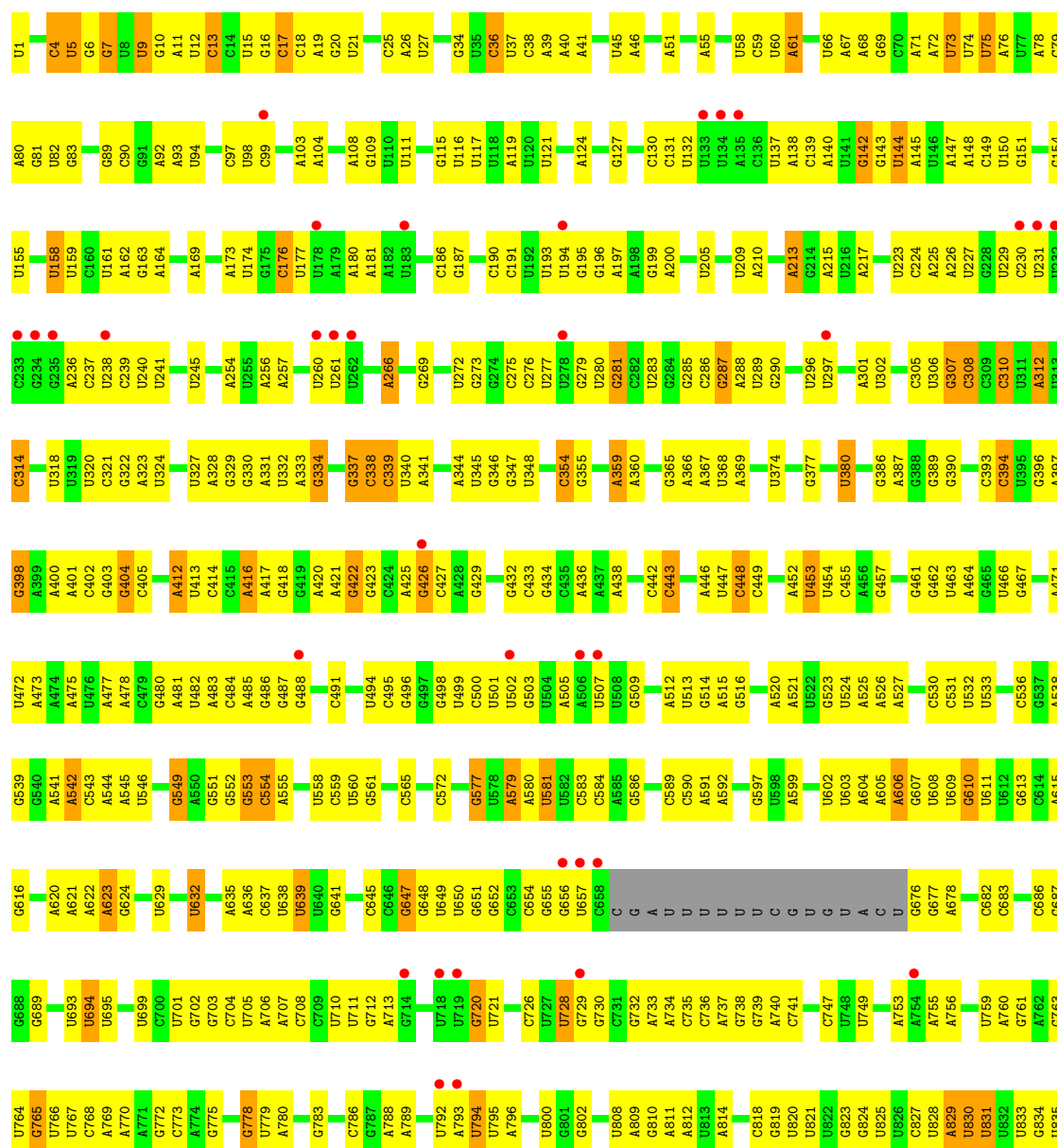
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	d9	1	Total 1	Zn 1	0	0
88	D7	1	Total 1	Zn 1	0	0
88	d6	1	Total 1	Zn 1	0	0
88	o7	1	Total 1	Zn 1	0	0
88	O7	1	Total 1	Zn 1	0	0
88	q2	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

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

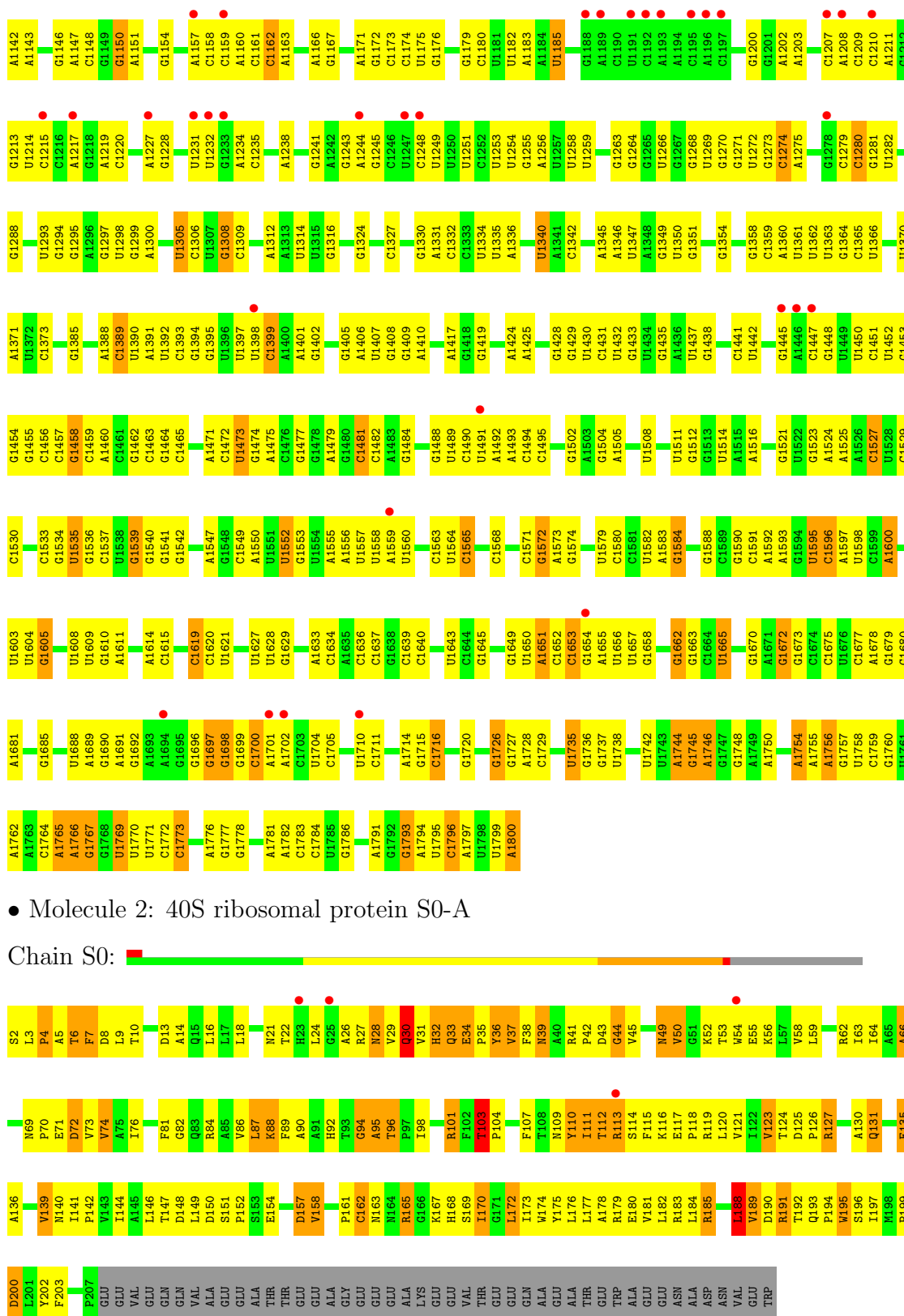
- Molecule 1: *Saccharomyces cerevisiae* chromosome XII cosmid 9634

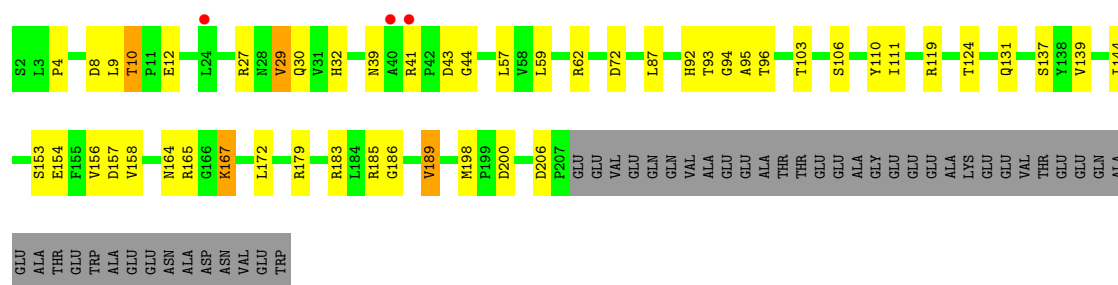
Chain 2: 





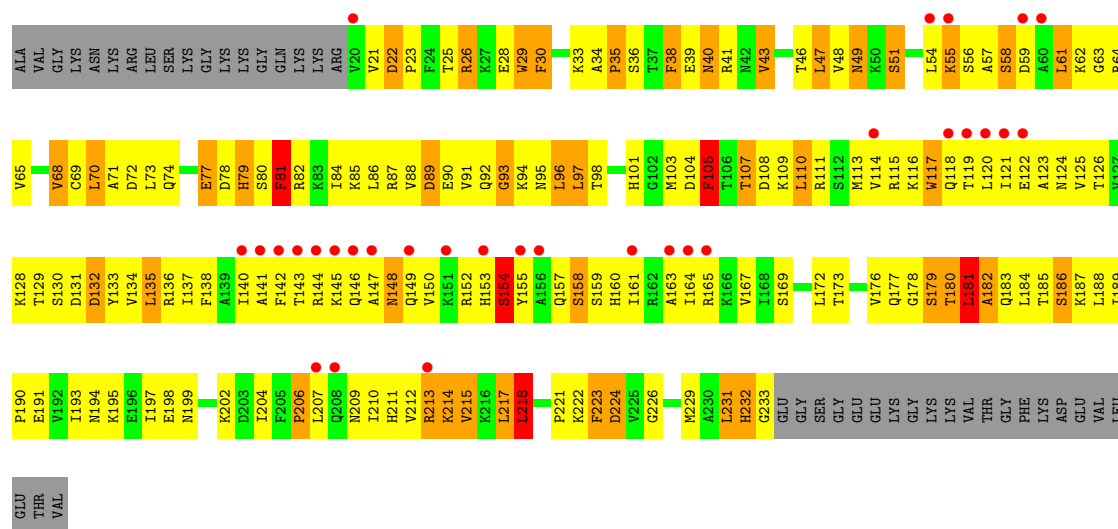
U1071	G994	G922	C852	U779	U890	A605	C530	C455	G377	G307	U223	C149	U1
C1072	A998	A923	C856	A780	U881	A606	C531	G459	A378	C308	C224	U150	A2
G1073	U999	A926	A856	U781	C686	G607	U532	A460	A379	C309	A225	U151	C3
G1074	C1000	C927	C857	G783	G687	U608	U533	G461	U609	C310	A226	U152	U4
C1077	A1001	G928	G858	C784	U694	G610	A534	G462	G584	U311	U227	G153	U5
C1078	G1002	A929	C859	U785	U695	G613	A535	U463	A385	U312	G228	G154	G6
U1079	A1003	A930	A862	U793	U696	G614	C536	G467	G386	U313	U229	U155	G7
U1080	U1004	A933	A863	A794	C696	G615	C537	G471	A387	C314	C230	A156	U8
C1081	A1005	C934	U864	U795	G697	G616	A538	U472	G390	U318	U232	U157	U9
C1082	C1006	G935	A865	U799	U698	A621	C539	A475	C393	U319	G235	U158	U10
A1087	U1007	G936	G866	A800	C700	A622	A540	U476	C394	U320	A236	U161	C14
A1088	C1010	C937	G867	U801	A706	A623	A541	A477	A397	U321	G239	A162	G16
A1091	G1011	G938	A868	A804	A707	A624	A542	U478	G398	U322	U240	G163	C17
A1092	U1014	A939	U869	A805	G716	U629	C543	U479	G399	U323	U241	A93	C18
A1093	A1015	A940	C870	A806	C717	A630	U546	C479	G398	U324	U242	U94	A19
G1094	C1016	A941	G871	U807	U711	G627	U547	C480	A400	U325	U243	G95	G20
U1095	U1017	A944	U873	A808	G712	G628	A550	C484	A401	G326	U245	A168	C25
C1096	U1018	U947	G876	U809	C718	U629	A555	A485	C402	U327	U246	A169	U98
U1097	A1019	G947	U877	A810	C719	A631	A556	G486	G403	A328	G246	U170	C99
U1098	A1020	U948	C879	G810	U720	A632	A557	G487	G404	G329	A247	A171	U29
U1099	C1021	C949	G880	A811	U721	G634	C557	G488	G405	G330	U248	C172	G30
G1100	C1022	C950	C881	A812	U722	U639	U558	C489	U406	A331	U249	G176	C36
C1101	A1025	A951	A881	U813	G720	U639	U558	C490	A407	U332	C250	C36	U87
G1102	U1103	A952	A884	U817	G721	C646	C561	C491	C408	A333	U259	A180	C38
U1103	C1028	A955	C818	A817	G722	C647	C562	C492	C409	U335	G263	A181	A39
C956	U1031	C956	U886	C819	G738	G648	U563	U493	A410	G337	C263	C37	A40
U1032	U1032	U958	A887	U820	G739	G649	C565	C495	A416	C338	A266	G187	A41
G1033	C1033	U959	U888	U821	A740	G651	C568	G496	A417	U340	G269	A188	G42
C1034	U1034	U960	G895	U822	C741	G652	C569	G497	G418	C339	C270	C189	A43
G1035	G1035	U961	U896	G823	U745	C653	C570	U499	G419	U341	A271	C190	U44
C962	A1036	C962	C897	G824	A746	A654	C571	U500	A420	U342	U271	U192	U45
A963	C1037	A963	U898	U825	C747	G655	G571	U501	A421	C343	U272	U193	A46
U1117	U1038	C967	G899	U826	C747	G656	C576	U502	G422	U344	G273	U194	A47
G1118	A1039	A967	A900	C827	U751	U657	C577	G503	G423	G346	C276	G195	G48
U1119	G1040	U968	G901	U828	A752	C658	C578	A506	C424	G347	U277	U122	C49
C1120	U1041	C969	U902	A829	A753	C659	U578	A507	A425	U348	G277	U123	G53
G1121	G1042	A970	U903	U830	A754	G660	A579	A511	G426	U349	G281	A124	C54
C1122	U1043	A971	G904	U831	A755	A661	C583	A512	G429	U350	C282	U125	A55
A1123	G1045	G972	A905	U832	A756	U662	C584	A513	A429	C351	A200	A126	U56
C1124	U1046	A973	A906	U833	A757	U663	C585	A514	G432	C352	G201	G127	G57
A1125	G1047	C975	U907	U834	U758	U664	C586	U515	C433	A353	A202	U128	U58
G1126	U1048	C976	U908	U835	C759	U665	C587	U516	G434	C354	C286	U129	C59
C1127	G1049	A977	C910	U836	G765	U666	C588	U517	A437	G357	G287	C130	G63
U1129	U1050	G977	U909	U837	U766	U667	C589	U518	A438	U358	U209	C131	U64
G1130	C1051	A978	U911	U838	U767	U668	C590	U519	A439	A359	U292	U132	A65
A1133	U1052	U982	U912	U839	C768	G669	C591	A510	A445	G362	U296	U133	U66
C1134	U1053	G987	G913	U840	A769	U670	C592	A511	A446	U363	U297	U134	A67
U1135	U1054	A988	G914	U841	A770	G	A592	A512	A447	G364	G291	U135	U68
C1136	U1055	U989	A915	C842	A771	U	A593	A513	U448	U365	U297	U136	A68
A1137	U1056	U990	U916	U843	A772	A673	A594	A514	C449	U366	A301	U137	G69
A1138	C1066	C990	U917	U844	G772	U674	C595	A515	U450	A369	U302	C138	A72
A1139	U1067	G991	U918	G845	G773	U675	C596	A516	A451	A370	U303	C139	U73
G1140	C1068	A992	U919	G846	G774	U676	U600	A517	A452	G371	U304	A140	U74
C1141	U1069	A993	U920	A847	C775	G677	A604	A518	A453	G372	U305	U144	U75
			U921	C848	C776	A678		A519	A454	U374	U306		A76
				C849	G778	U679		A520					
								A521					
								A522					
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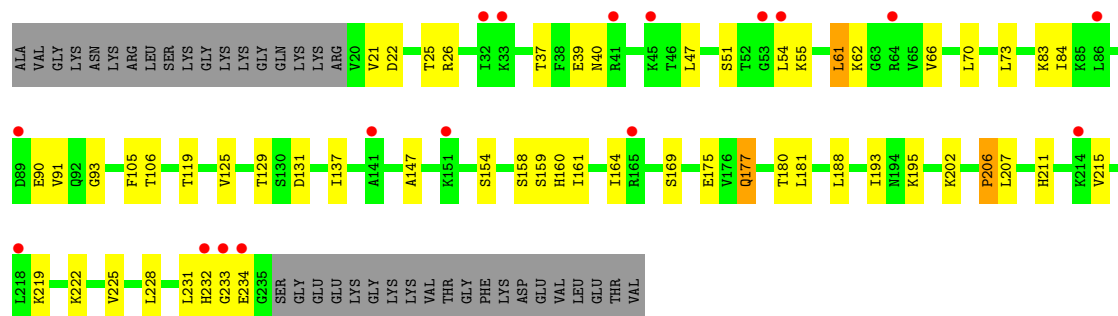
• Molecule 3: 40S ribosomal protein S1-A

Chain S1:



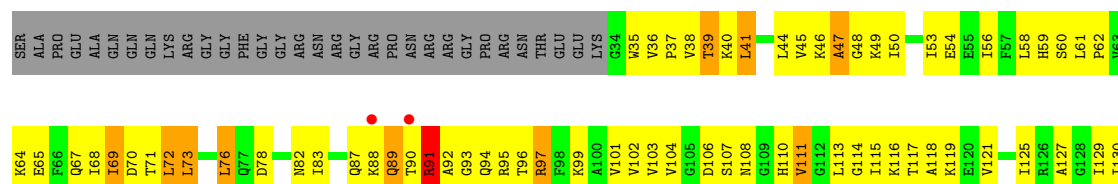
• Molecule 3: 40S ribosomal protein S1-A

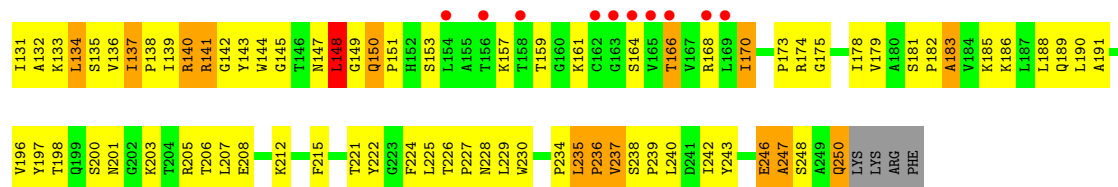
Chain s1:



• Molecule 4: 40S ribosomal protein S2

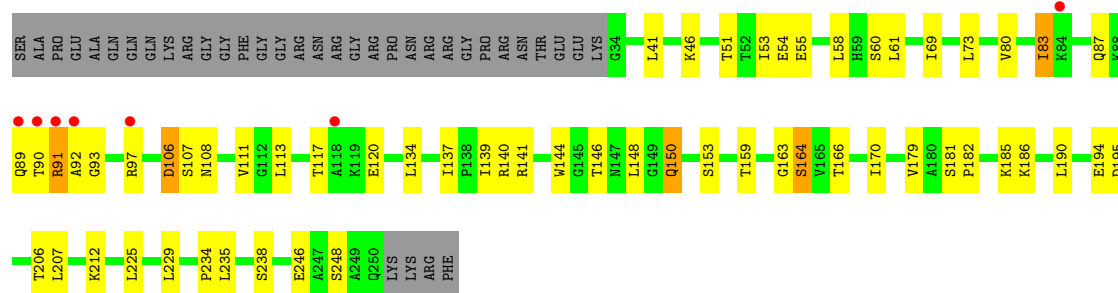
Chain S2:





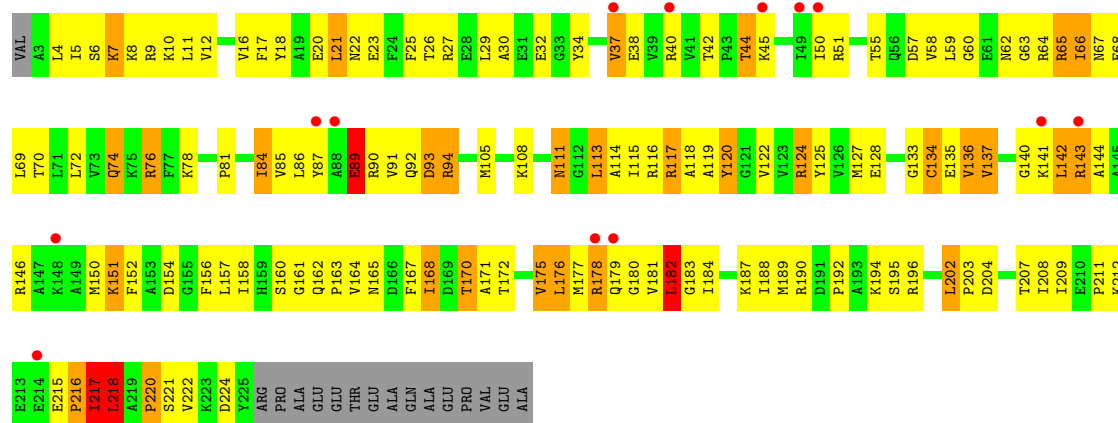
• Molecule 4: 40S ribosomal protein S2

Chain s2:



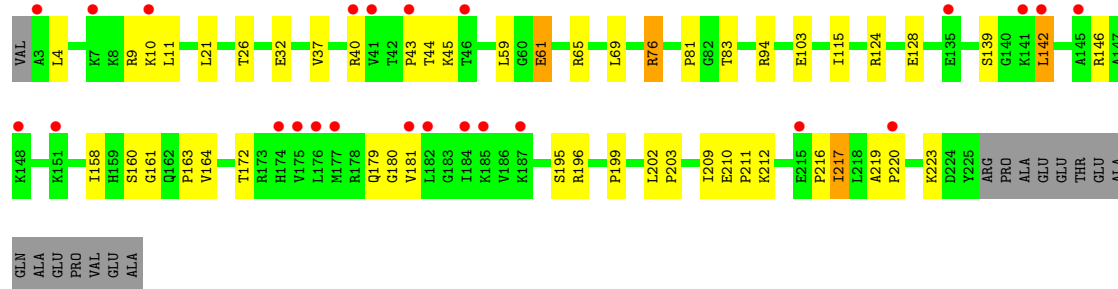
• Molecule 5: 40S ribosomal protein S3

Chain S3:



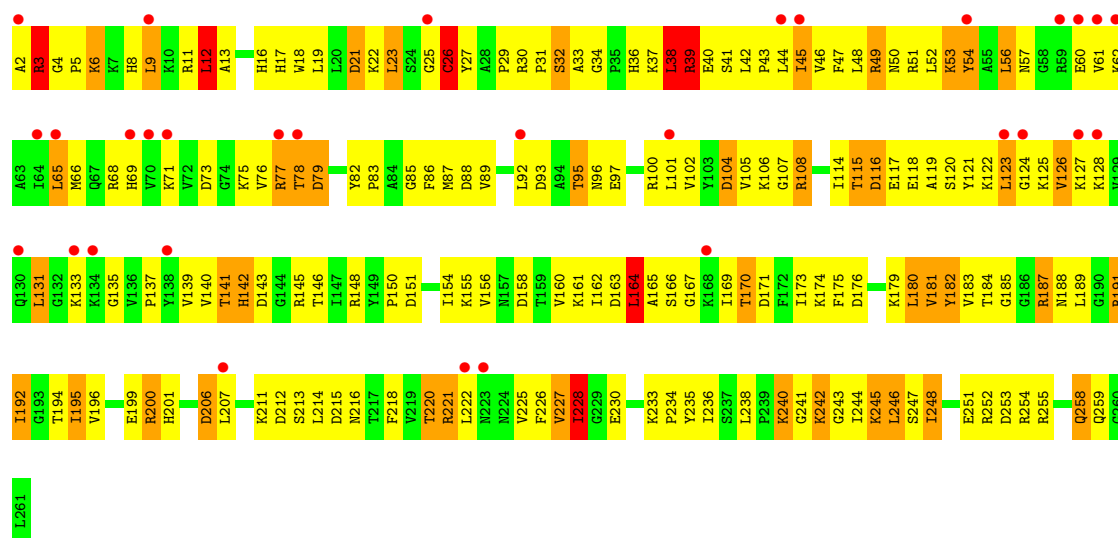
• Molecule 5: 40S ribosomal protein S3

Chain s3:



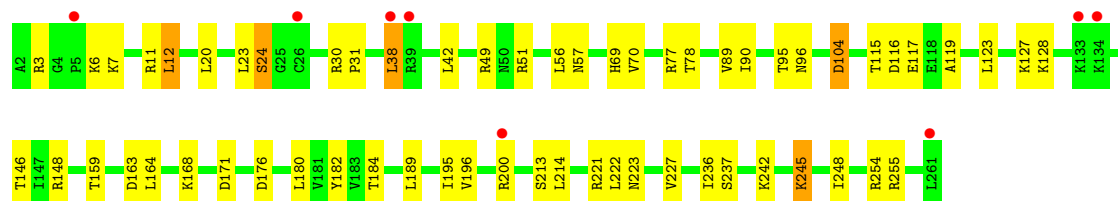
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



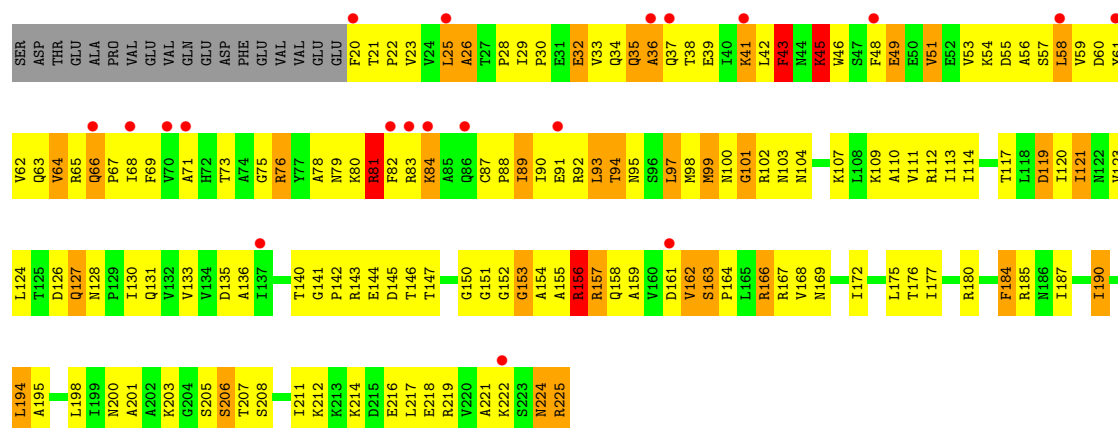
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



• Molecule 7: 40S ribosomal protein S5

Chain S5:

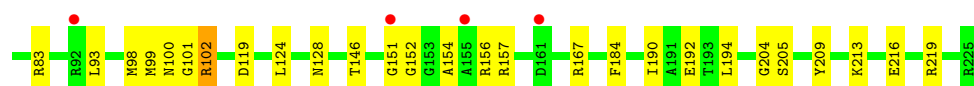


• Molecule 7: 40S ribosomal protein S5

Chain s5:

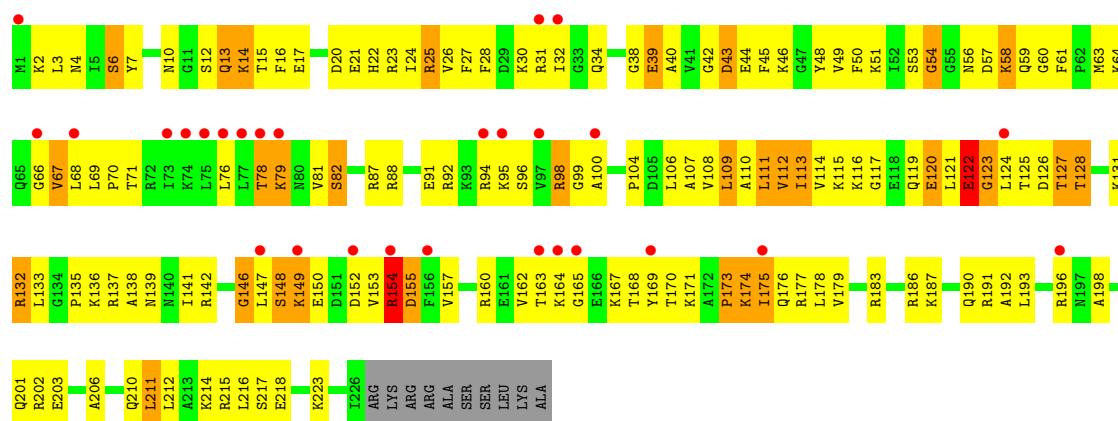






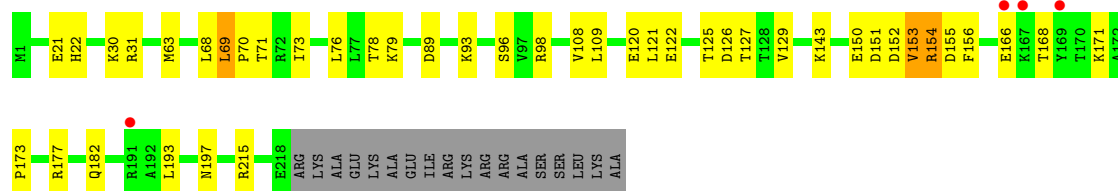
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



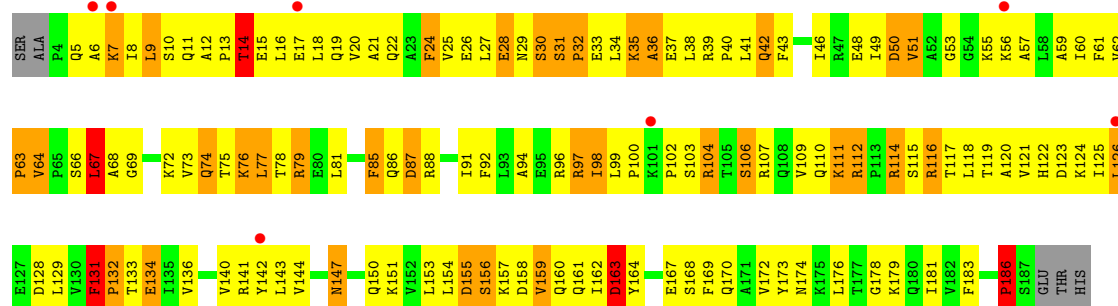
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



• Molecule 9: 40S ribosomal protein S7-A

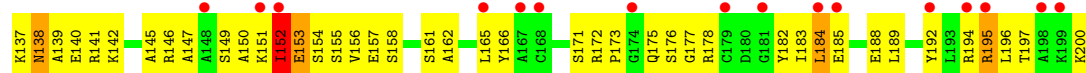
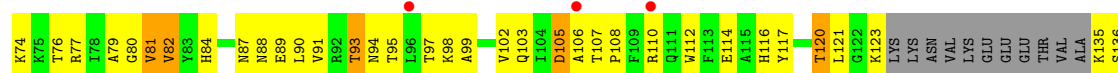
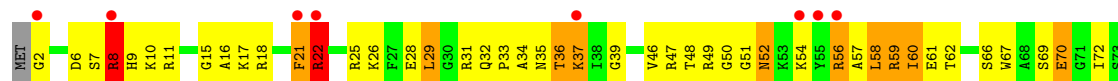
Chain s7:





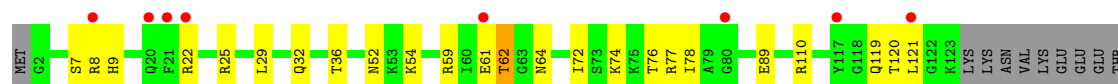
• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



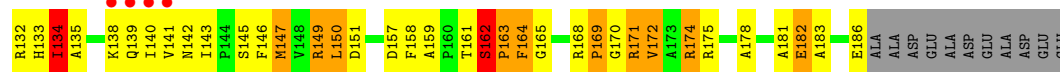
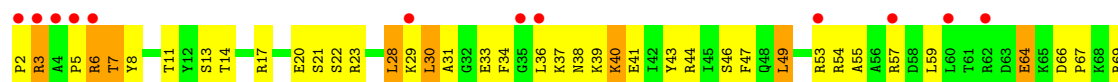
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



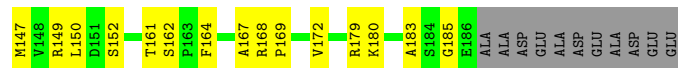
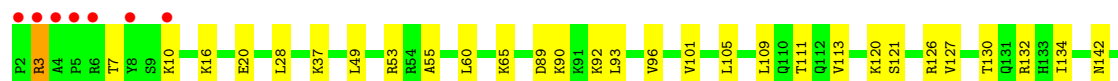
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



• Molecule 11: 40S ribosomal protein S9-A

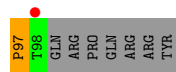
Chain s9:



• Molecule 12: 40S ribosomal protein S10-A

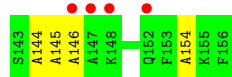


- Molecule 12: 40S ribosomal protein S10-A

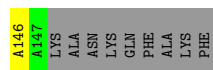


- Molecule 13: 40S ribosomal protein S11-A

Device Type	Percentage of Respondents
Smartphone	100%
Tablet	95%
Feature Phone	85%
Smartwatch	15%



- Molecule 13: 40S ribosomal protein S11-A



- Molecule 14: 40S ribosomal protein S12



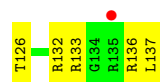
- Molecule 14: 40S ribosomal protein S12

- |      |      |     |  |
|------|------|-----|--|
| Y141 | V65  | G2  |  |
| E142 | I66  | R3  |  |
|      | T67  | M4  |  |
| T145 | G68  | H5  |  |
| A146 | N69  | S6  |  |
| S147 | K70  |     |  |
| A148 | I71  |     |  |
| L149 | M72  | K9  |  |
| V150 | R73  | G10 |  |
| N151 | I74  | I11 |  |
|      | L75  | S12 |  |
|      | K76  | A15 |  |
|      |      | I16 |  |
|      | L80  | P17 |  |
|      | E83  | Y18 |  |
|      | I84  | S19 |  |
|      |      | R20 |  |
|      |      | N21 |  |
|      | D87  | A22 |  |
|      | L88  | P23 |  |
|      | Y89  | A24 |  |
|      | L91  | W25 |  |
|      | T92  | F26 |  |
|      | K93  | K27 |  |
|      | K94  | L28 |  |
|      | A95  | S29 |  |
|      | Y96  | S30 |  |
|      | S97  | E31 |  |
|      | Y98  | S32 |  |
|      | K99  | V33 |  |
|      | K100 | I34 |  |
|      | H101 | E35 |  |
|      | L102 | Q36 |  |
|      | E103 | I37 |  |
|      | N105 | V38 |  |
|      | R106 | K39 |  |
|      |      | Y40 |  |
|      |      | A41 |  |
|      |      | R42 |  |
|      |      | K43 |  |
|      |      | L45 |  |
|      |      | T46 |  |
|      |      | P47 |  |
|      |      | S48 |  |
|      |      | Q49 |  |
|      |      | I50 |  |
|      |      | G51 |  |
|      |      | V52 |  |
|      |      | L53 |  |
|      |      | L54 |  |
|      |      | R55 |  |
|      |      | D56 |  |
|      |      | A57 |  |
|      |      | V60 |  |
|      |      | T61 |  |
|      |      | Q62 |  |
|      |      | A63 |  |
|      |      | R64 |  |

- 

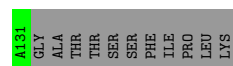
- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| I76 | I77 | A78 | V79 | H80 | K82 | I83 | H84 | A85 | T86 | G87 | G88 | T89 | R90 | T91 | K92 | F94 | G95 | G96 | P97 | G98 | Q99 | L102 | R103 | A104 | L105 | A106 | R107 | S108 | G109 | L110 | R111 | I112 | G113 | R114 | I115 | E116 | D117 | V118 | T119 | P120 | V121 | P122 | S123 | S125 | T126 | R127 | K128 | K129 | G130 | R131 | R132 | R133 | R136 | L137 |
| SER | ASN | VAL | GLN | ALA | ARG | ASP | ASN | S11 | Q12 | V13 | F14 | G15 | V16 | A17 | R18 | I19 | Z20 | A21 | S22 | F23 | N24 | D25  | T26  | F27  | V28  | H29  | T30  | T31  | S32  | L33  | G35  | E37  | T38  | I39  | A40  | R41  | V42  | T43  | M46  | K47  | V48  | K49  | A50  | D51  | B52  | D53  | E54  | S55  | M61  | L62  | A63  | A64  | C75  |      |

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|
| SER | ASN | VAL | VAL | GLN | ALA | ARG | ASP | N10 | R18 | I19 | Y20 | F23 | T26 | T31 | D32 | L33 | S34 | G35 | T43 | K49 | A50 | D51 | R52 | Y58 | L62 | K70 | V81 | T91 | K92 | G97 | G98 | Q99 | A100 | A101 | L102 | R107 | S108 | G109 | R114 | T119 | S123 | D124 | S125 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|



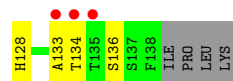
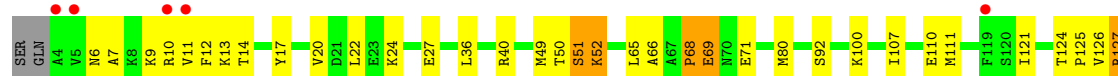
- Molecule 17: 40S ribosomal protein S15

Chain C5:



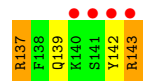
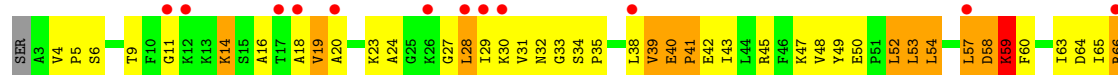
- Molecule 17: 40S ribosomal protein S15

Chain c5:



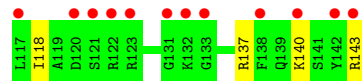
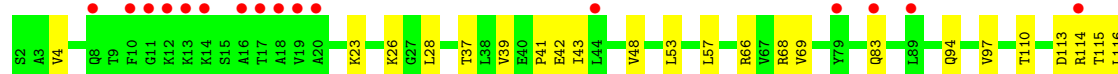
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:



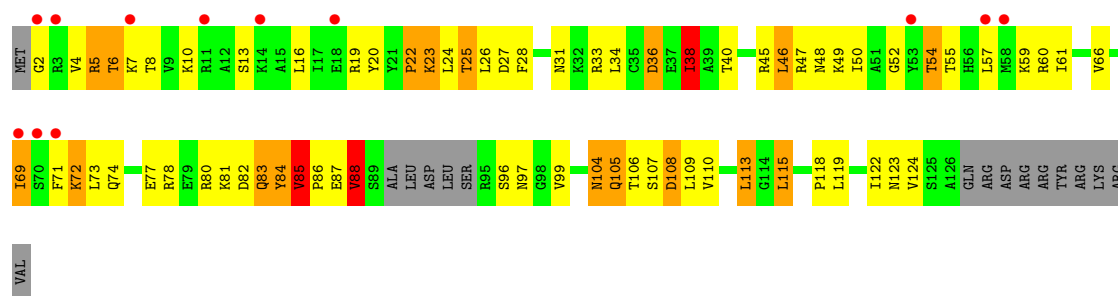
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:



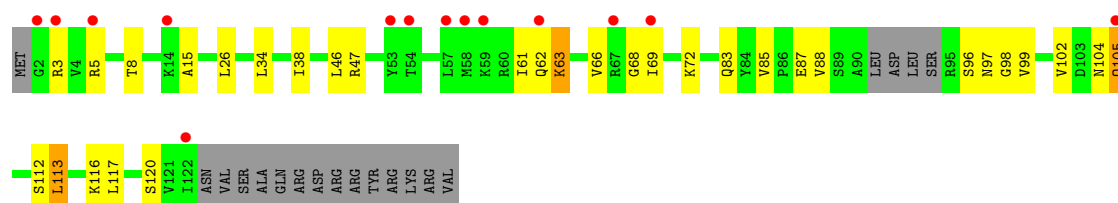
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:



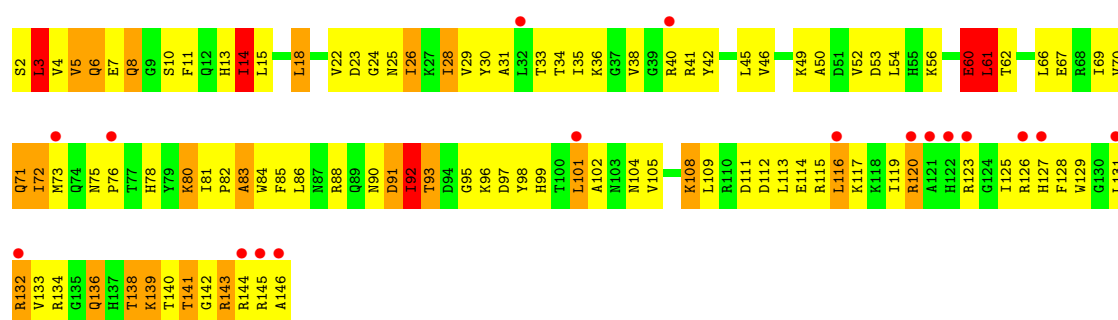
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:



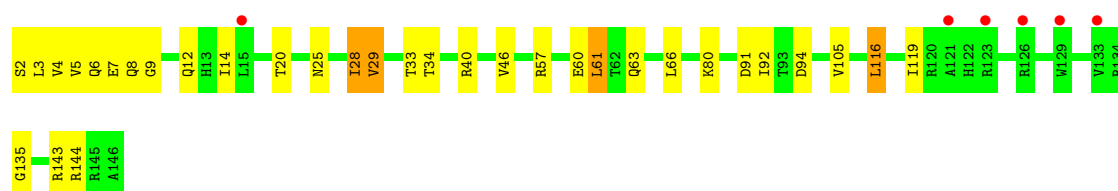
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:



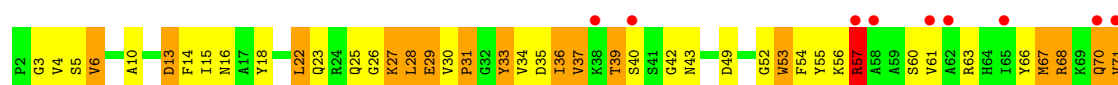
- Molecule 20: 40S ribosomal protein S18-A

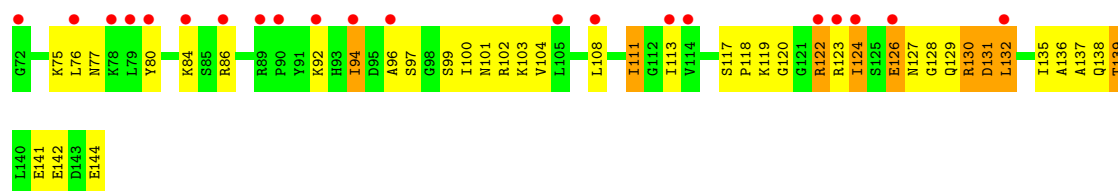
Chain c8:



- Molecule 21: 40S ribosomal protein S19-A

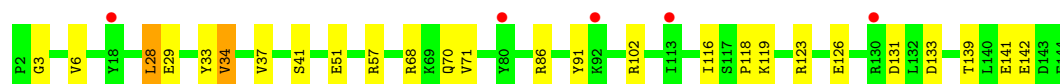
Chain C9:





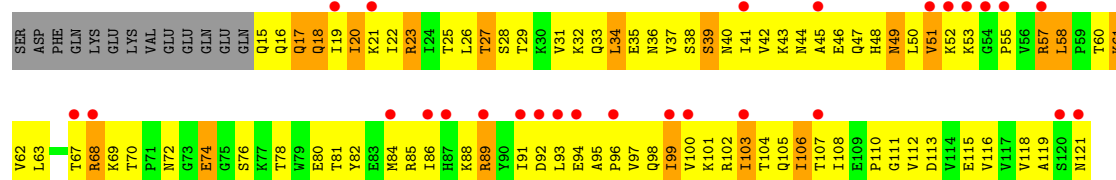
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



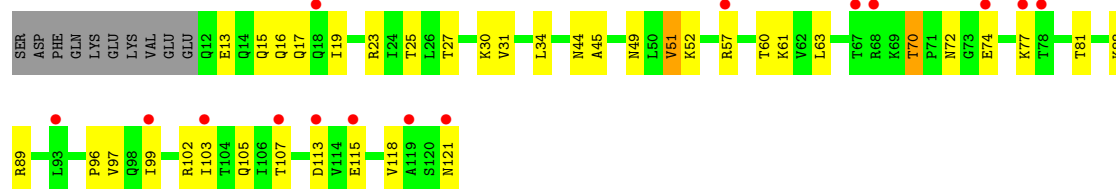
- Molecule 22: 40S ribosomal protein S20

Chain D0:



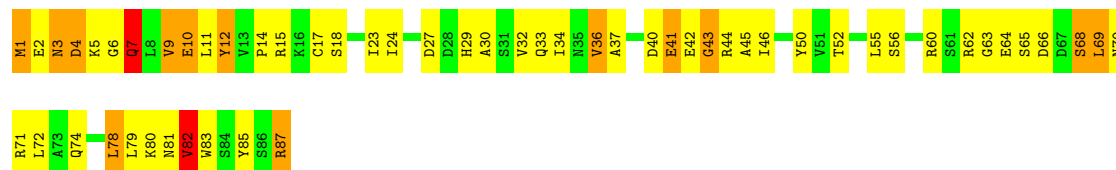
- Molecule 22: 40S ribosomal protein S20

Chain d0:



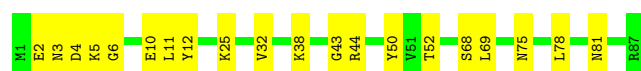
- Molecule 23: 40S ribosomal protein S21-A

Chain D1:



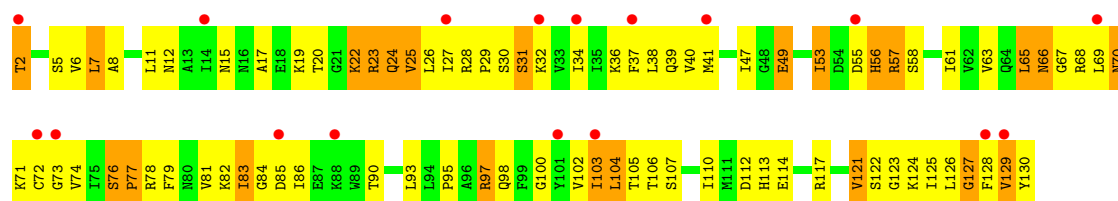
- Molecule 23: 40S ribosomal protein S21-A

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:



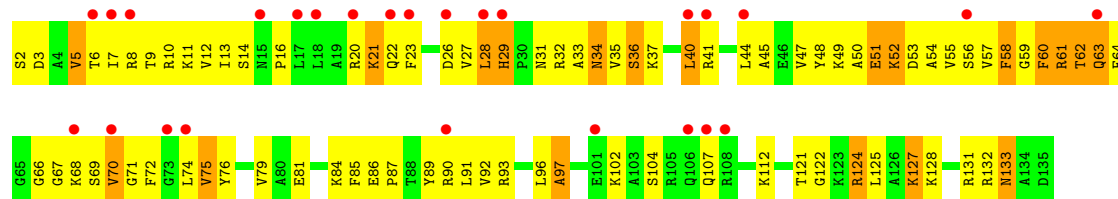
• Molecule 25: 40S ribosomal protein S23-A

Chain d3:



• Molecule 26: 40S ribosomal protein S24-A

Chain D4:



• Molecule 26: 40S ribosomal protein S24-A

Chain d4:

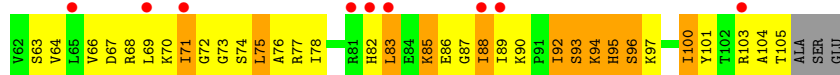
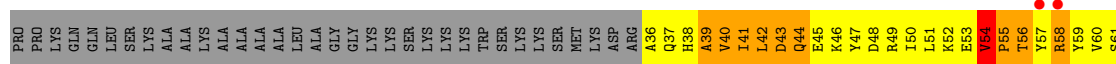






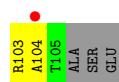
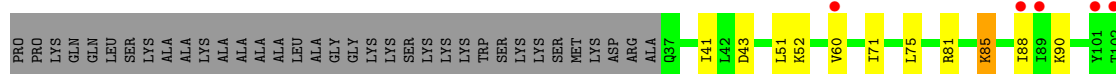
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:



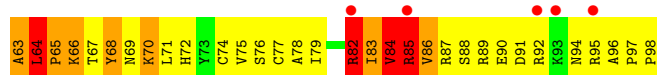
- Molecule 27: 40S ribosomal protein S25-A

Chain d5:



- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



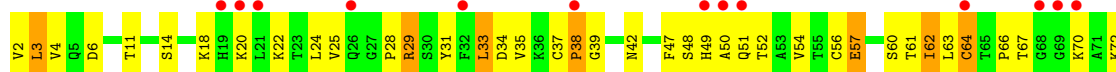
- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



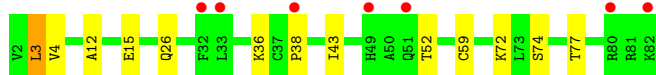
- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



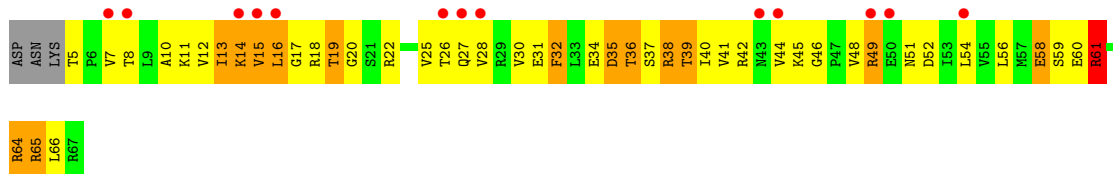
- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 



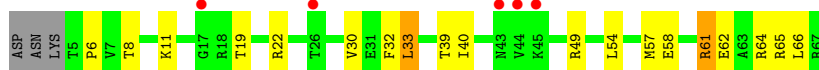
- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 



- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 



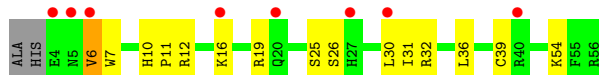
- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 



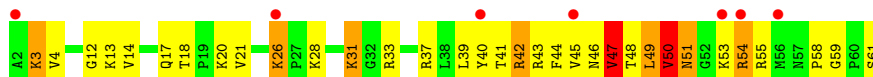
- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 



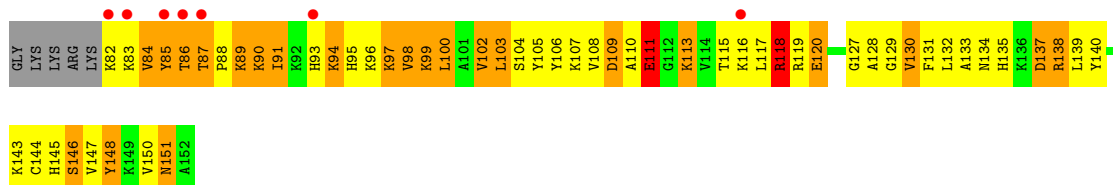
- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 

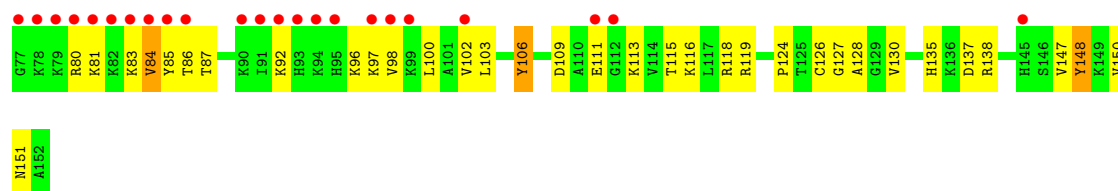


- Molecule 33: Ubiquitin-40S ribosomal protein S31

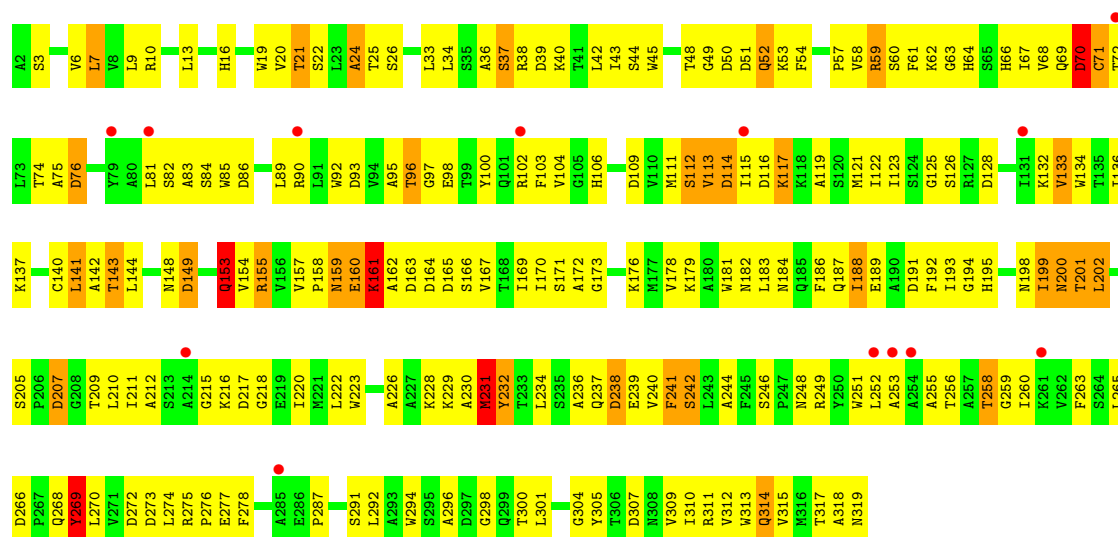
Chain E1: 



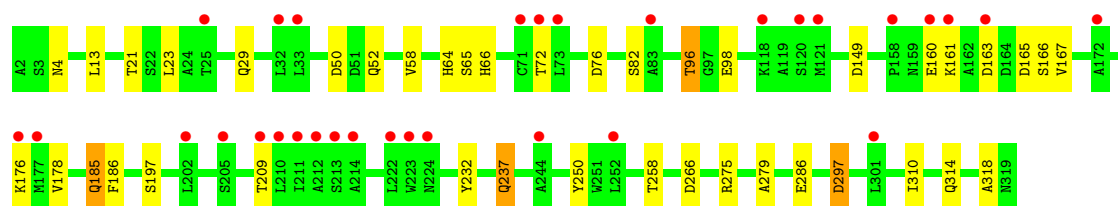
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 

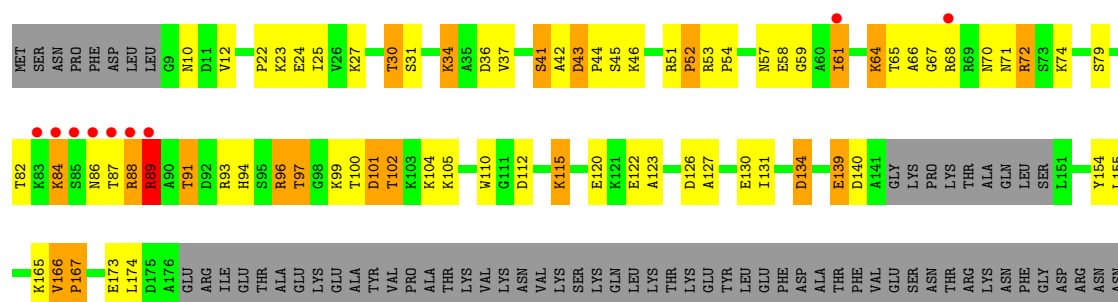
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR: 

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

Chain sR: 

- Molecule 35: Suppressor protein STM1

Chain SM: 

ASN	SER	ASN	ASN	PHE	ASN	ASN	GLY	GLY	GLY	ALA	ARG	LYS	GLY	ASN	ASN	THR	ALA	ASN	THR	ASN	THR	GLN	LYS	ASN	ARG	ASN	ILE	ASP	VAL	SER	ASN	LEU	PRO	SER	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 35: Suppressor protein STM1

Chain sM:

ASN	PHE	ASN	ASN	ARG	ARG	GLY	GLY	GLY	GLY	ALA	ARG	GLY	GLY	ASN	ASN	THR	ALA	ASN	THR	THR	ALA	ASN	THR	THR	LYS	VAL	ASN	ALA	ASN	THR	THR	GLN	LYS	ASN	ASN	ASN	ASP	VAL	SER	SER	ASN	LEU	LEU	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
K83	K84	S85	ASN	THR	ARG	ARG	ALA	THR	THR	ASP	HIS	SER	ARG	THR	GLY	LYS	THR	ASP	THR	LYS	LYS	LYS	VAL	VAL	ASN	GLN	GLY	TRP	GLY	ASP	LYS	GLN	LEU	TYR	LEU	GLU	ASP	ALA	THR	THR	ALA	THR	THR	VAL	GLY	PRO	SER	ASN	THR	THR	ALA	GLN	SER	LEU	GLY	ASP	ARG	ASN	ASN	ASN	SER	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
V172	E173	L174	ALA	GLU	ARG	ILE	THR	THR	ALA	ALA	ALA	GLU	GLY	ALA	TYR	VAL	PRO	ALA	THR	LYS	LYS	VAL	LYS	ASN	VAL	VAL	ASN	VAL	LYS	LYS	GLY	LYS	GLN	LEU	TYR	GLU	GLY	PHE	ASP	ALA	THR	THR	VAL	GLU	SER	ASN	THR	ASN	LEU	LEU	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN</

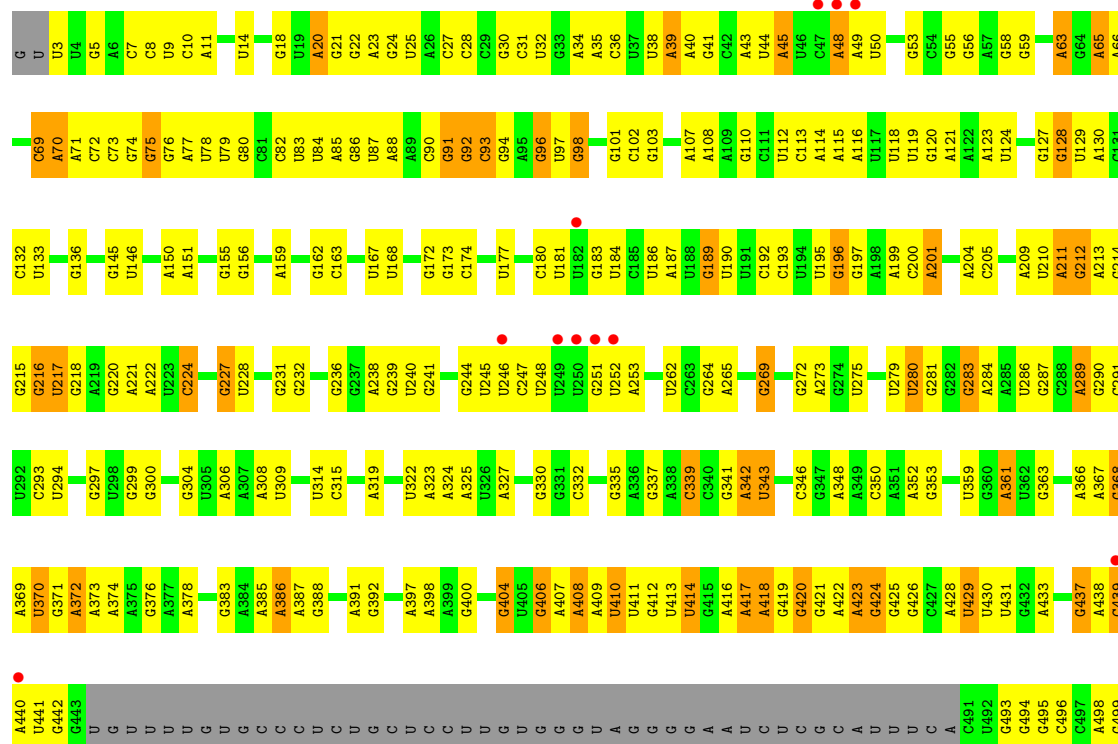
• Molecule 36: TPA\_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

Chain 1:

G	U	U3	C8	U9	A12	A13	U14	G18	U19	A20	G21	G22	U25	A26	C27	C28	C29	G30	C31	U32	G33	A34	A35	C36	U37	U38	A39	A40	G41	C42	A43	C47	A48	A49	U50	A51	A52	G53	G54	G55	G56	A57	G58	G59	A60	A61	A62	A63	G64	A65	A66	A67	C68	C69				
A70	A71	C72	C73	G74	G75	G76	A77	U78	U79	G80	C81	U84	A85	G86	A89	C90	G91	C92	G93	G94	A95	G96	U97	A100	G101	G104	C105	A106	A107	A108	A109	G110	G111	U112	A114	A115	A116	U117	U118	U119	G120	A121	A122	A123	U124	G127	G128	A209	U210	A285	A211	U286	G212	A213	G214	U133	G216	
G139	C140	C141	C142	G143	A144	G145	U146	U147	U148	U149	A150	U153	U154	G155	G156	U157	G158	A159	G160	U168	U169	G170	G171	G172	G173	C174	C175	G176	C185	U186	U187	U188	G189	U190	U191	C192	G196	G197	A198	C200	A201	C205	G206	U207	C208	A209	U210	A285	U286	G212	A213	G214	U133	G216				
U217	G218	A221	A222	U223	A224	C225	C226	U227	U228	G229	U230	G231	C232	C233	G239	U240	G241	G242	G243	G244	U245	U249	U250	G251	U252	A255	C256	U261	U262	C263	G264	G269	U270	C271	C272	G273	A274	U275	U278	U279	U280	G281	G282	G283	A284	G363	G364	U370	G371	C291	U292							
C293	U294	A295	A296	C297	U298	G299	G300	G304	U305	U314	C315	U316	A317	A318	A319	G320	A324	A325	U326	U329	G330	G331	C332	A336	G337	A338	C339	C340	G341	A342	U343	A344	G345	C350	G353	C356	A357	G358	U359	G360	A361	U362	G363	G364	G368	A369	U370	G371	A372									
A373	U380	U381	A385	A386	A387	G388	A391	G392	U393	G394	A395	A396	A397	A402	C403	G404	U405	G406	A407	A408	A409	U410	U411	G412	U413	U414	G415	A416	A417	G420	G421	A422	A423	G425	G426	C427	A428	U429	C435	A436	G437	A438	C439	A440	U	G	U	U	U	U								
U	G	U	G	C	C	U	C	U	C	U	C	C	C	U	G	U	G	G	A	G	G	G	G	A	U	C	U	C	U	C	A	C	U	G	G494	G495	C496	C497	A498	G499	C500	A501	U502	C503	A504	G505	U506	U507	G595									
G511	G514	A598	C599	G600	U601	A602	A603	G604	U628	A608	G609	G610	A611	A612	U613	U614	A619	U620	A621	U622	U623	G624	U627	U628	A629	U630	G631	U632	U633	U634	U635	U636	U637	U638	U639	U640	C641	U642	U643	G644	A645	A646	A647	C648	A649	G650	G651	G652	A653	G654	C655	A656	A657	G658	G659	U660	C734	A735
U662	C663	U664	A665	A666	C667	G668	U669	C670	U671	A672	U673	G674	C675	U676	U677	U678	G680	U681	G685	U686	U687	G688	U697	U698	A699	C700	G701	C702	A706	U707	G708	A709	A715	A716	C717	U718	U719	A720	G721	G725	U726	G727	U728	C729	C730	G733	C734	A735										

C1762	C1670	U1584	G1447	U1384	C1320	G1171	C1107	U1028	C958	G894	A736
U1763	C1671	C1585	U1448	C1385	G1321	G1174	C1108	C1032	C959	G895	A738
U1764	G1674	C1516	U1449	A1386	C1322	C1175	U1109	U1033	U960	A817	G739
U1765	C1675	C1517	C1452	G1389	U1324	C1176	U1110	U1034	A962	C818	
A1587	C1518	C1518	A1453	A1390	U1325	C1177	U1111	G1035	G953	C819	
A1588	C1519	C1519	A1454	C1391	A1326	C1178	U1112	A1036	G964	U819	G742
A1589	C1520	C1520	C1455	C1392	C1329	A1179	G1113	G1113	A965	A820	C743
G1590	C1521	C1521	U1456	A1393	C1330	U1180	G1114	U1039	U966	U821	C744
G1591	C1522	C1522	U1457	A1394	A1330	U1181	G1115	C1039	A906		C745
G1592	C1523	C1523	U1458	C1395	U1331	A1182	G1116	U1041	G907	C824	
U1595	C1525	C1525	C1459	C1396	A1332	C1183	G1117	U1042	U967	U822	
U1596	C1526	C1526	C1460	C1397	C1333	C1184	C1118	C1043	G908	U823	A751
C1597	C1528	C1597	A1461	C1398	C1334	C1185	C1119	U1044	C909	G826	
C1598	U1528	C1598	A1462	C1399	C1335	C1186	C1120	A1047	C911	U829	C758
G1599	U1530	C1530	A1463	A1399	C1336	G1187	A1120	A1048	C912	A830	
C1791	C1531	C1531	G1464	G1400	U1336	C1188	U1123	C1049	A914	C835	C765
C1792	C1532	C1532	G1465	A1401	A1337	U1267	U1124	U1050	C975	A836	
C1793	U1533	U1533	G1466	C1402	C1338	C1189	C1127	U1051	C976	A837	C768
C1794	C1540	C1540	A1468	C1403	C1339	A1190	G1128	U1052	U979	C838	
C1795	U1540	C1540	C1469	C1404	C1340	U1191	C1129	A1053	C981		C770
C1796	C1543	C1543	U1471	G1405	U1341	C1192	A1129	A1054	U980	A841	
U1702	G1544	G1544	U1472	A1406	C1342	C1193	A1130	U1055	U981	C842	U772
A1704	C1545	C1545	G1473	C1407	A1343	C1194	C1131	U1056	C982	A843	C773
U1705	A1613	C1546	C1474	G1408	G1344	C1195	C1132	C983	U992		
C1802	C1614	A1546	A1474	C1409	G1345	C1196	C1133	U1060	C984	A846	U776
C1803	C1615	C1547	A1475	U1410	C1346	A1197	A1134	A1061	C923	A847	U777
C1804	U1616	C1548	C1476	C1411	U1347	C1198	G1135	A1062	G924	A848	U778
A1804	C1617	C1549	A1477	G1412	C1348	C1201	A1136	G1063	C994	A849	U779
C1805	U1618	C1550	C1478	G1413	U1349	C1204	C1137	A1064	U995	C927	U780
C1806	U1619	C1551	U1479	C1414	A1350	C1205	U1138	U1065	A996	C928	G781
C1807	U1620	C1552	C1480	U1415	U1351	C1206	C1139	G1066	C997	U929	
C1808	U1621	C1553	A1481	C1416	A1352	C1207	G1140	U930	C998	C857	G785
A1809	C1634	U1553	C1482	C1417	U1353	U1210	C1141	C1069	C999	A858	A786
C1810	U1636	C1554	G1483	C1418	G1354	U1211	C1142	C1070	C999	C859	G787
C1811	U1637	C1555	U1484	A1419	A1355	U1212	G1143	U1074	C1000	C860	C788
C1812	U1638	C1556	C1485	C1420	C1360	C1213	A1143	A1075	C1001	C863	A791
C1813	C1646	C1557	C1486	U1421	C1361	U1214	C1144	C1078	C1002	C864	G792
C1814	U1647	C1558	C1487	C1422	U1362	C1215	G1145	U1079	C1003	U865	C793
C1815	U1648	C1559	C1488	U1423	C1363	C1216	C1146	A1150	C1004	C865	U794
C1816	U1649	C1560	C1489	C1424	C1364	C1217	C1147	C1080	U1007	C870	G795
C1817	U1650	C1561	C1490	C1425	C1365	C1218	U1151	G1083	C940	U871	U796
C1818	C1650	C1562	C1491	U1426	C1366	C1219	C1152	C1090	C941	U872	C797
C1819	C1651	C1563	C1492	C1427	C1367	C1220	C1153	A1011	C942	C873	G798
C1820	U1652	C1564	C1493	U1428	C1368	C1221	C1154	C1091	C943	U874	
U1821	C1653	C1565	C1494	C1429	C1369	C1222	C1155	C1092	C944	C877	G799
C1822	C1654	C1566	C1495	C1430	C1370	C1223	C1156	C1093	C945	C878	C800
A1828	U1740	C1655	C1496	G1431	C1371	C1224	C1157	C1094	C946	U879	A801
C1829	C1741	C1656	C1497	C1432	C1372	C1225	C1158	U1095	C947	C880	C802
C1830	U1742	C1657	C1498	C1433	C1373	C1226	C1159	C1096	C948	C881	C803
C1831	C1743	C1658	C1499	C1434	C1374	C1227	C1160	C1097	C949	C882	C804
C1832	C1744	C1659	G1500	U1435	C1375	C1228	C1161	C1098	C950	C883	G805
C1833	U1745	C1660	C1503	C1436	C1376	C1229	C1162	C1099	C951	A884	A806
C1834	C1746	C1661	C1504	C1437	C1377	C1230	C1163	C1100	A951	U885	A807
A1835	U1747	C1662	A1506	G1440	C1378	C1231	C1164	U1100	C952	C886	A808
C1836	C1748	C1663	C1507	G1441	U1378	C1232	C1165	C1101	C953	C887	G809
U1837	U1749	C1664	C1508	C1442	C1379	C1233	C1166	C1102	C954	C888	C810
C1838	C1758	C1665	C1509	U1443	C1380	C1234	C1167	A1103	U955	U889	C812
C1839	U1759	C1666	A1510	G1444	A1381	C1235	C1168	C1104	C956	C890	
C1840	C1760	C1667	C1511	C1445	C1382	C1236	C1169	C1105	C957		
C1841	U1761	C1668	C1512	U1446	C1383	C1237	C1170	C1106	C958		
C1842	C1762	C1669	C1513	C1447	C1384	C1238	C1171	C1107	C959		
C1843	U1763	C1670	C1514	C1448	C1385	C1239	C1172	C1108	C960		
C1844	C1764	C1671	C1515	U1449	C1386	C1240	C1173	C1109	C961		
C1845	U1765	C1672	C1516	C1450	C1387	C1241	C1174	C1110	C962		
C1846	C1766	C1673	C1517	C1451	C1388	C1242	C1175	C1111	C963		
C1847	U1767	C1674	C1518	C1452	C1389	C1243	C1176	C1112	C964		
C1848	C1768	C1675	C1519	A1453	A1389	C1244	C1177	C1113	C965		
C1849	U1769	C1676	C1520	C1454	C1390	C1245	C1178	C1114	U966		
C1850	C1770	G1592	C1521	C1455	C1391	C1246	C1179	C1115	A906		
C1851	U1681	C1592	C1522	U1456	C1392	C1247	U1180	C1116	G907		
C1852	U1682	C1593	C1523	C1457	A1393	C1248	U1181	C1117	U967		
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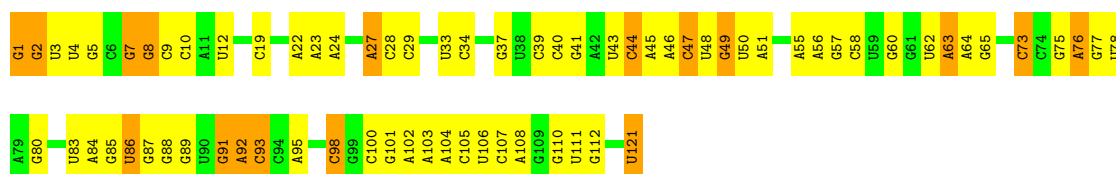


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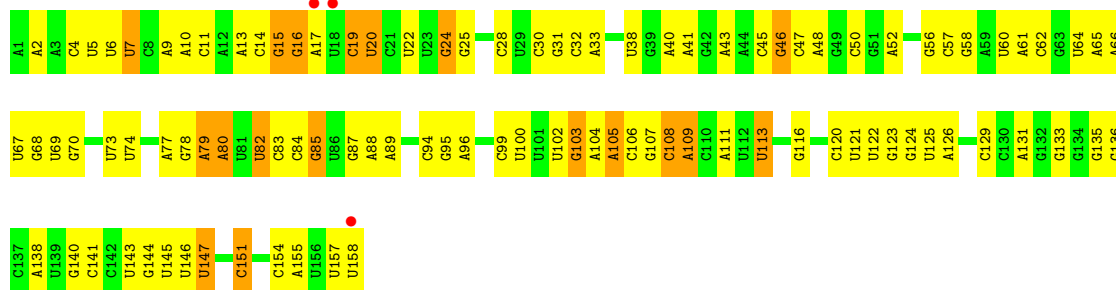
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C2399	C	U2336	A2271	U2203	C2137	C	U	U1877	A1723		
G2400	C	C2337	G2272	C2204	A2138	C	C	A1878	U1724	A1637	
A2401	U	C2338	G2273	U2205	A2139	G	U	U1880	C1725	A1638	
A2402	U	C2339	U2274	G2206	U2140	U	G	A1881		C1639	
G2403	C	U2340		A2207	U2141	C	U	U1882	A1729	G1640	
A2404	C	A2341	C2277	A2208	A2142	G	U	A1884	G1817	U1641	
C2405	C	U2342	C2278	U2209	A2143	U	A	U1885	G1730	A1731	
C2406	C	C2343	A2279	G2210	A2144	U	G	A1886	U1819	A1642	
C2407	G	U2344	A2280	U2211	A2145	U	G	A1887	U1820	U1732	A1643
U2408	C	C2345	A2281	C2212	A2146	G	G	U1888	G1733	C1644	
G2409	C	G2346	G2282	A2213	A2147	C	C	U1889	G1734	U1645	
U2410	A		G2283	A2214	U2148	U	G	U1890		G1646	
U2411	G	U2349	C2284			A	A	A1891	A1741		
G2412	U	C2350	C2285	U2217	C2151	C	C	U1892	U1742	G1650	
	G	U2351	U2286	G2218	A2152	A	U	A1893	G1829	U1851	
U2416	A	A2352	C2287	A2219		A	U	U1894	G1747	G1652	
A2419	A	G2353	G2288	G2220	G2155	U	A	A1895	G1749	A1656	
C2420	U	C2354	U2289	G2221	C2156	U	C	A1896	C1657	C1657	
G2425	A	G2355	C2290	A2223	G2157	A	U	G1897	A1750	U1658	
U2426	C	A2357	A2292	A2224	A2158	C	G	A1900	A1757	G1659	
U2427	C	U2358	U2293	U2225	U2159	C	A	G1901	G1758	C1660	
U2428	A	C2359	U2294	U2226	G2160	G	C	U1902		G1661	
G2429	U	A2361	A2295	C2227	C2163	G	U	U1903	U1764	C1662	
U2434	A	C2362	U2297	A2228	A2164	C	A	A1908	U1765	C1663	
G2435	C	A2363	U2298	C2230	G2165	C	C	U1909	G1766		
U2436	C	G2364	C2299	G2231	A2166	U	U	A1910	G1770	G1666	
U2439	U	C2365		A2232	A2167	G	G	U1911	C1771	A1667	
A2441	U	A2367	A2303	G2233	G2169	U	G	U1912	U1772	C1668	
U2442	A	G2370	G2305	C2234	U2170	C	C	A1913	C1773	C1669	
A2443	U	G2371	C2306	G2235	G2171	U	U	G1914	G1778	G1677	
G2503	A	G2372	C2307	G2236	A2172	U	U	A1915	C1779	G1680	
U2504	U	A2373	G2308	G2240	U2173	A	G	U1916	G1780	U1686	
			A2309	U2241	U2175	A	U	G1919	U1782	U1687	
C2507											
U2508											
U2509											
U2510											
A2511											
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A2580											
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U2599											
C2600											





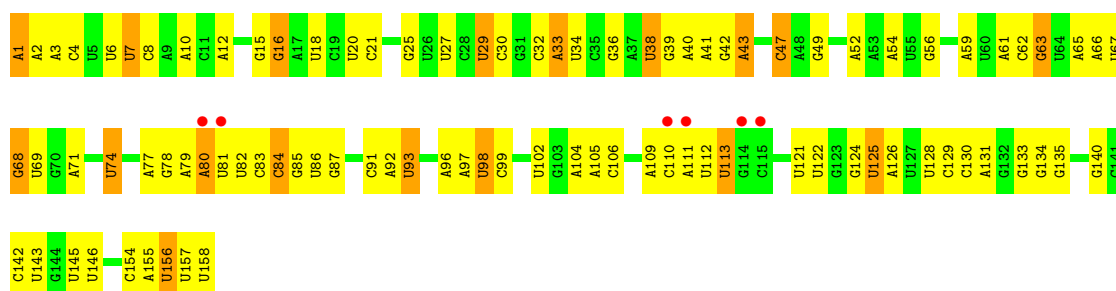
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 4:



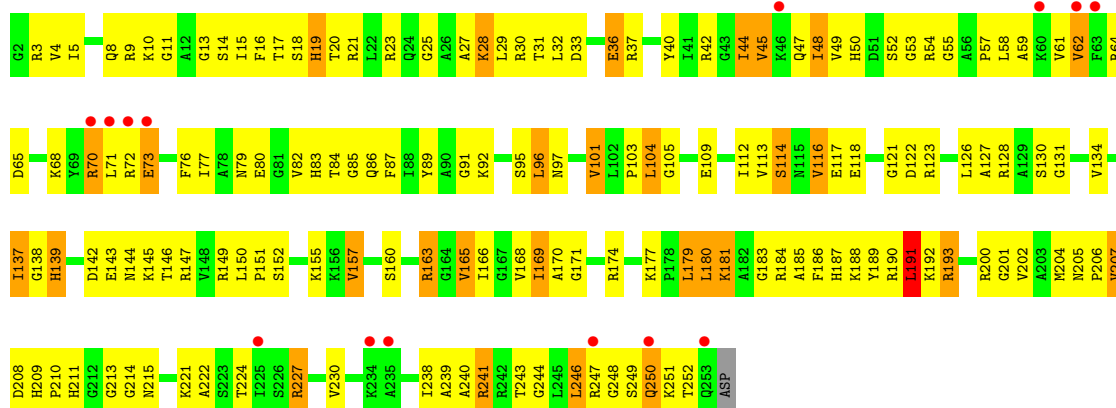
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 8:



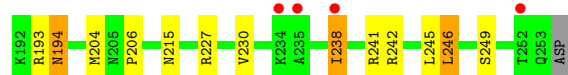
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



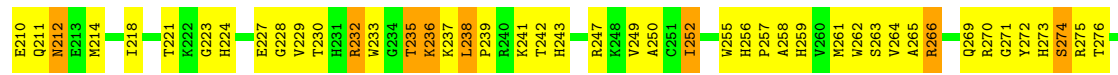
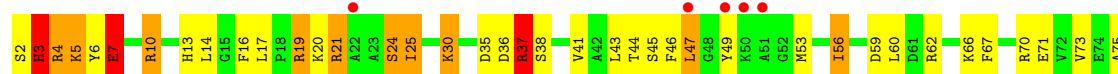
- Molecule 39: 60S ribosomal protein L2-A

Chain l2: 



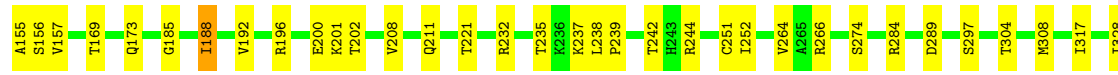
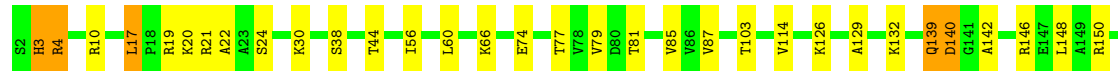
- Molecule 40: 60S ribosomal protein L3

Chain L3: 



- Molecule 40: 60S ribosomal protein L3

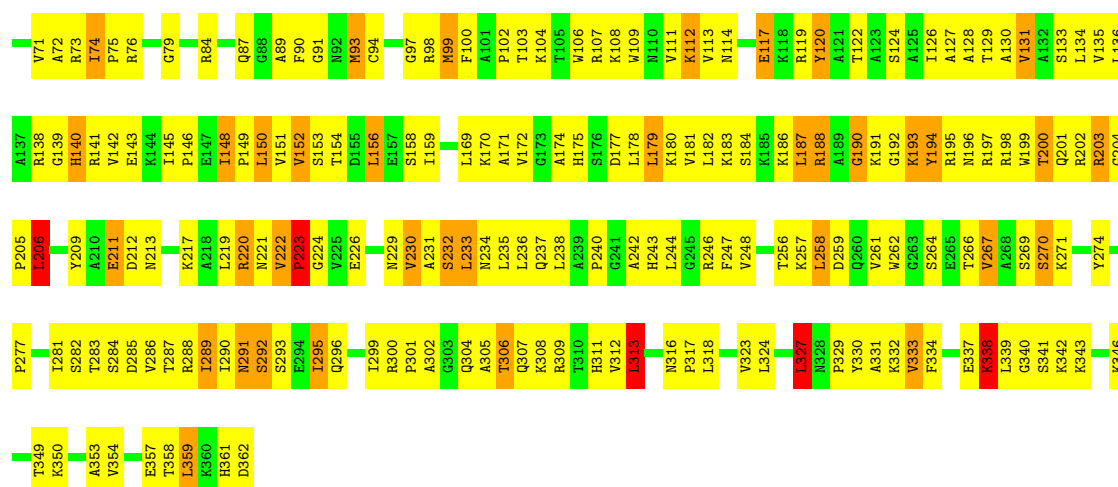
Chain l3: 



- Molecule 41: 60S ribosomal protein L4-A

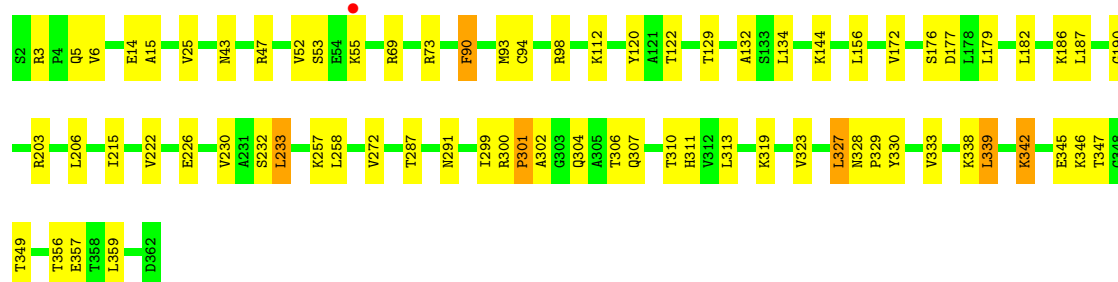
Chain L4: 





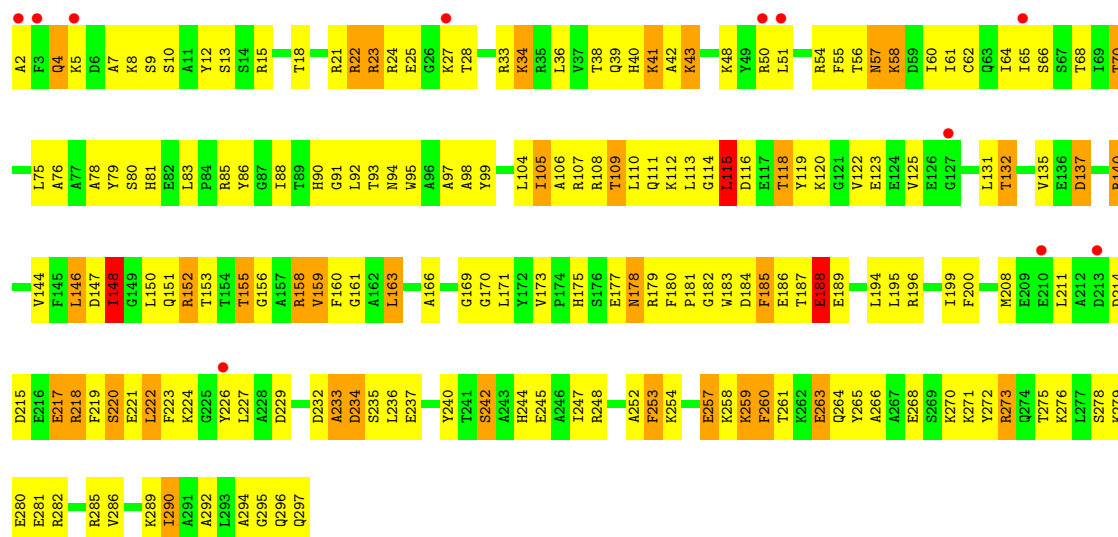
• Molecule 41: 60S ribosomal protein L4-A

Chain 14:



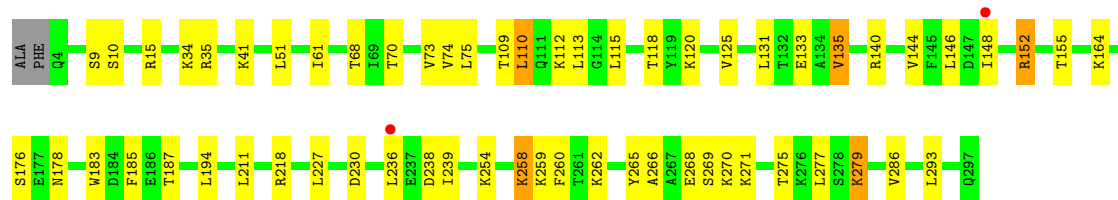
• Molecule 42: 60S ribosomal protein L5

Chain L5:



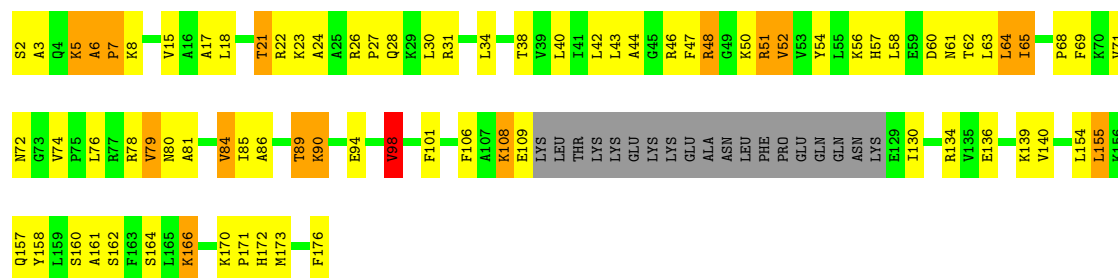
• Molecule 42: 60S ribosomal protein L5

Chain 15:



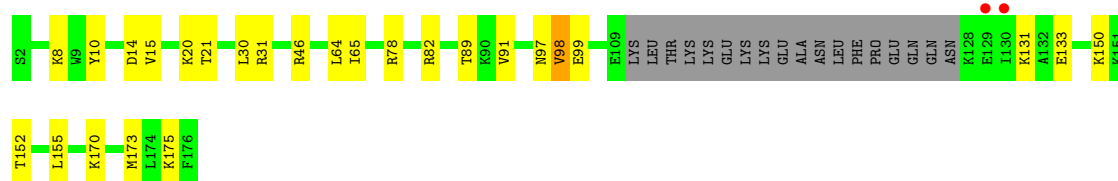
• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



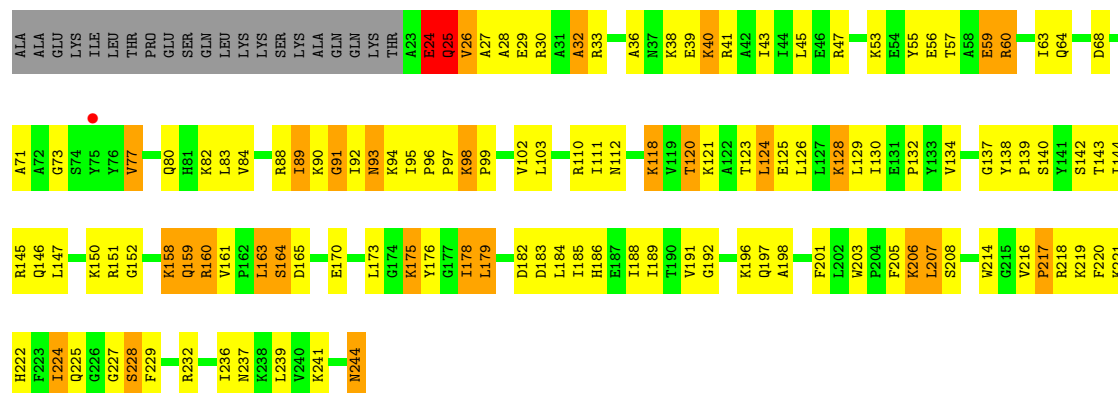
• Molecule 43: 60S ribosomal protein L6-A

Chain l6:



• Molecule 44: 60S ribosomal protein L7-A

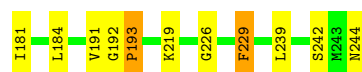
Chain L7:



• Molecule 44: 60S ribosomal protein L7-A

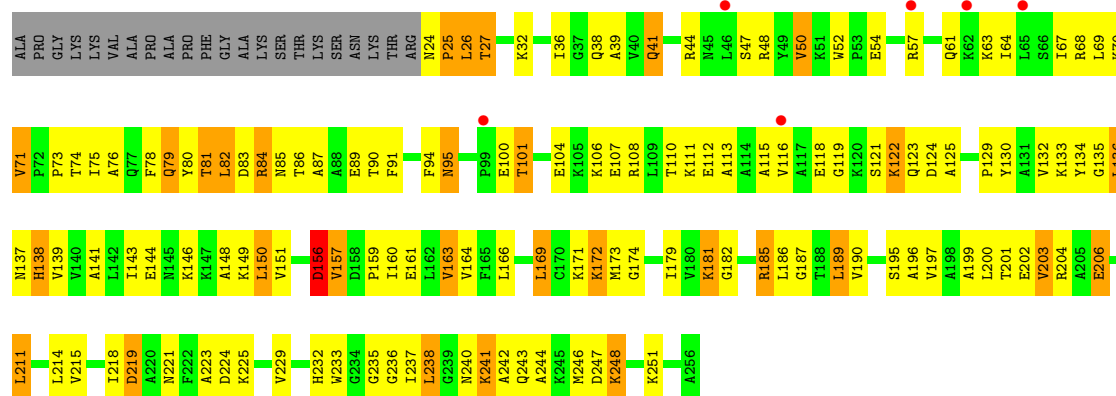
Chain l7:





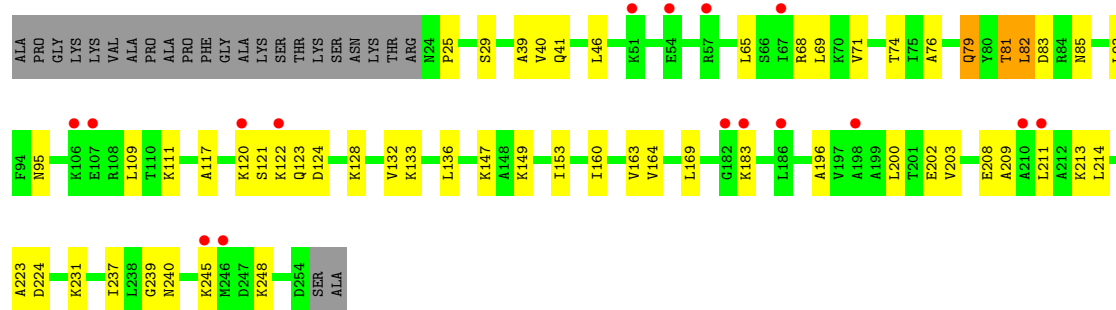
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



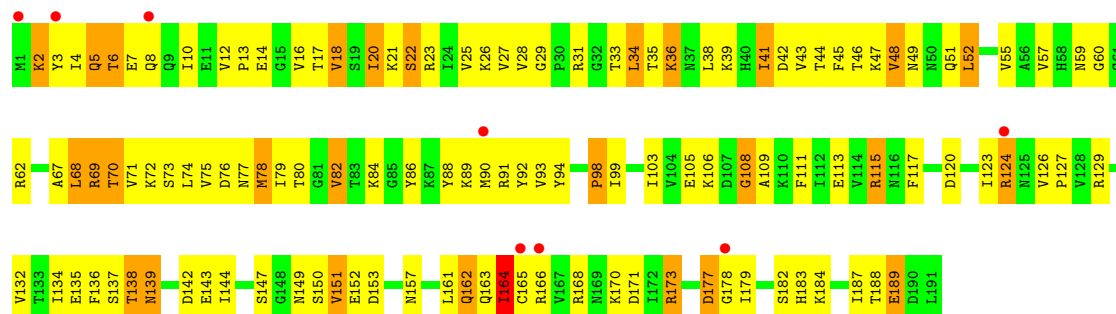
• Molecule 45: 60S ribosomal protein L8-A

Chain l8:



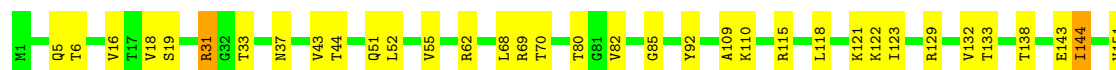
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



• Molecule 46: 60S ribosomal protein L9-A

Chain l9:

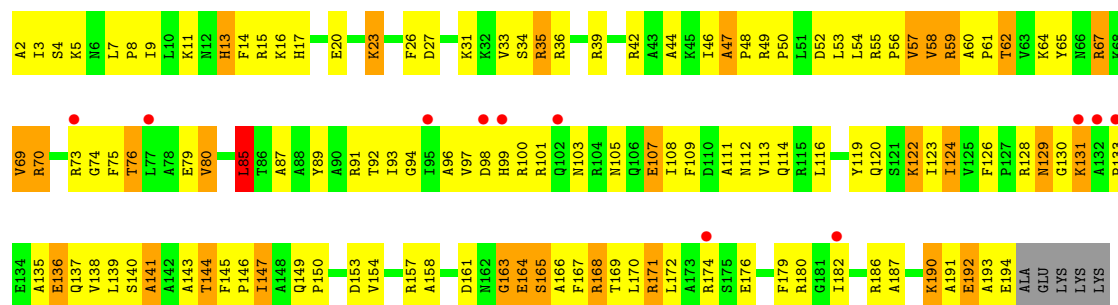






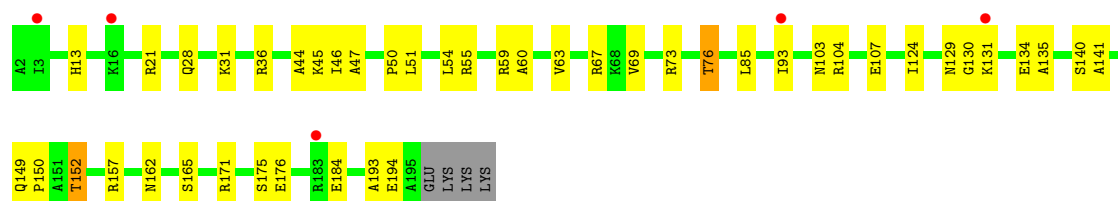
- Molecule 49: 60S ribosomal protein L13-A

Chain M3:



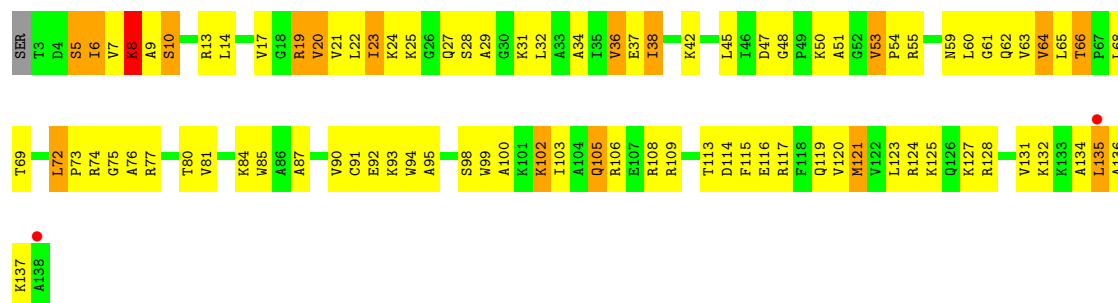
- Molecule 49: 60S ribosomal protein L13-A

Chain m3:



- Molecule 50: 60S ribosomal protein L14-A

Chain M4:



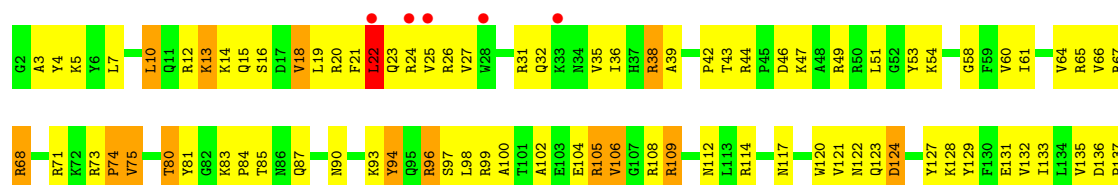
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:



- Molecule 51: 60S ribosomal protein L15-A

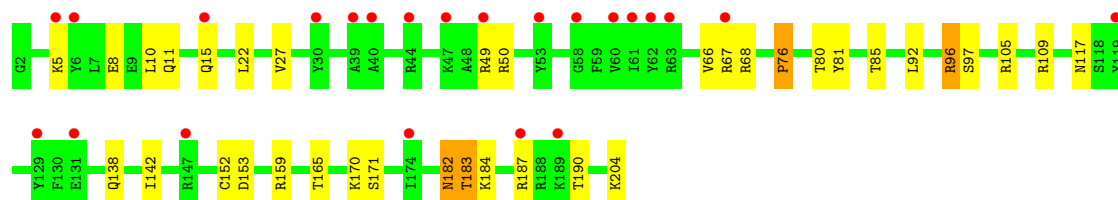
Chain M5:





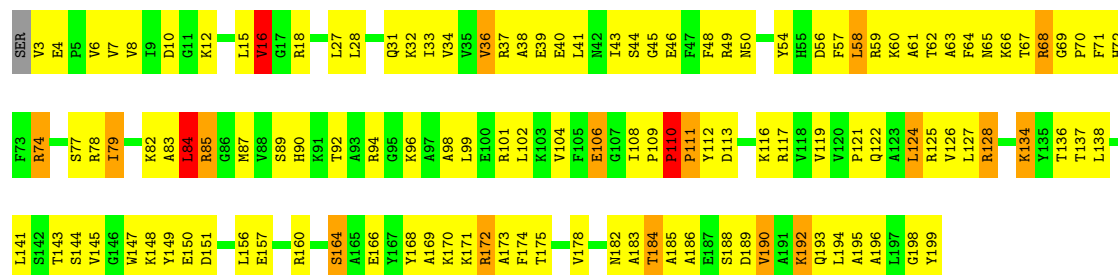
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



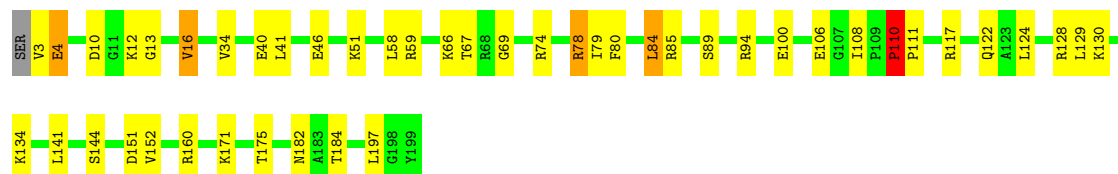
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



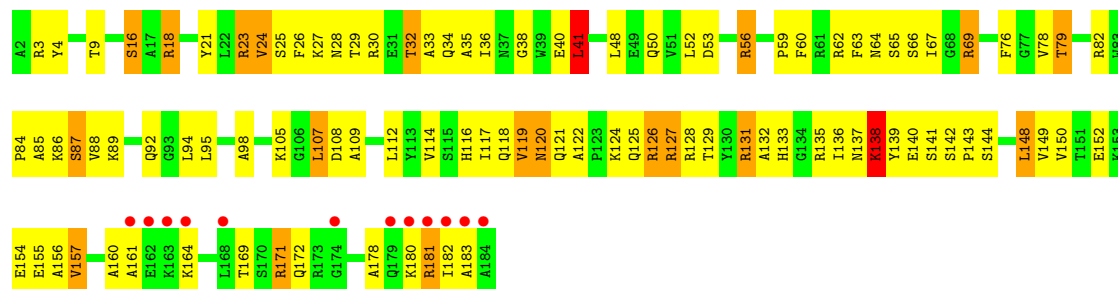
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



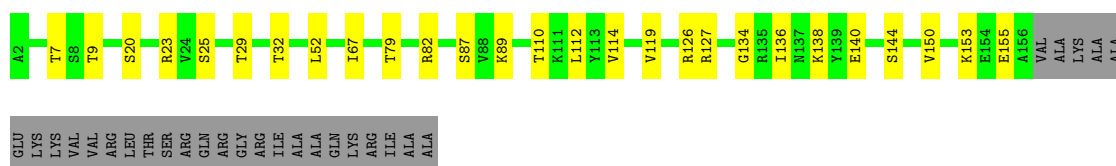
• Molecule 53: 60S ribosomal protein L17-A

Chain M7:



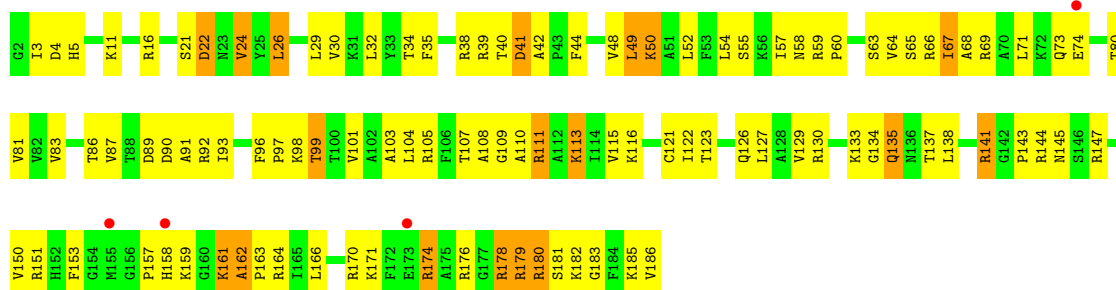
• Molecule 53: 60S ribosomal protein L17-A

Chain m7:



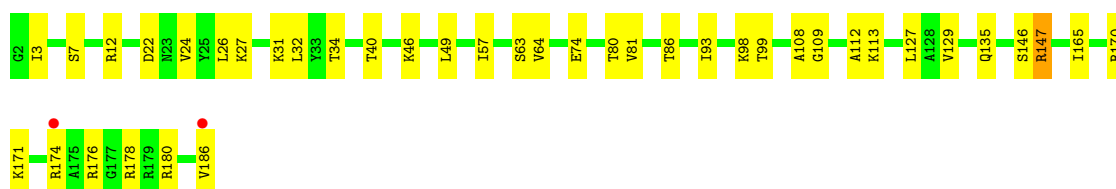
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



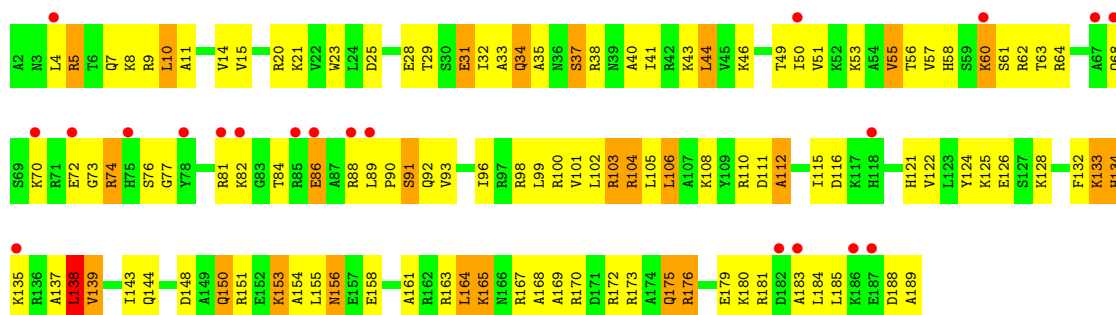
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



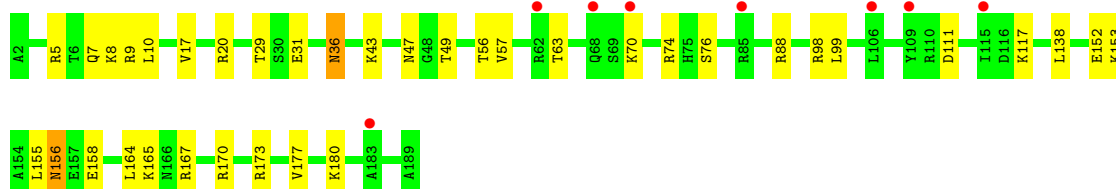
• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



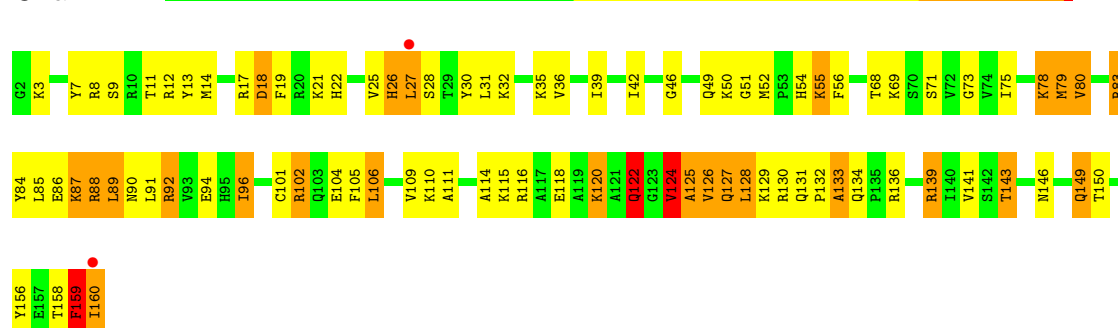
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:



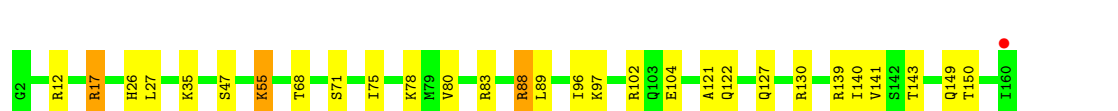
- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



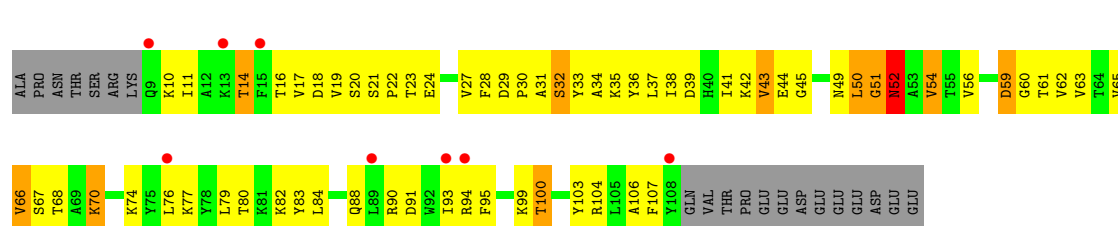
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:



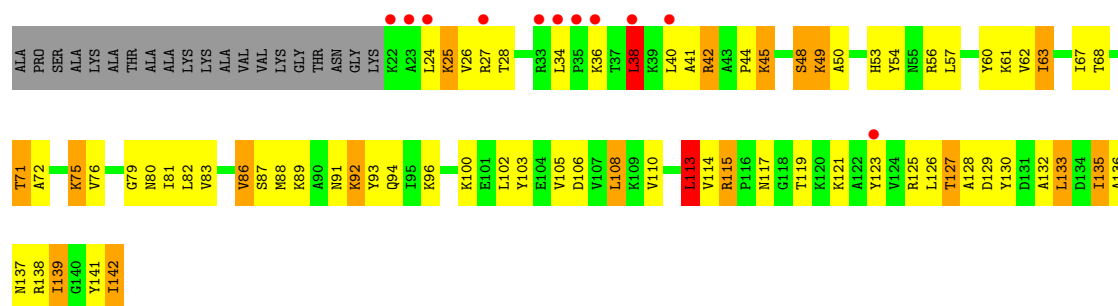
- Molecule 58: 60S ribosomal protein L22-A

Chain N2:



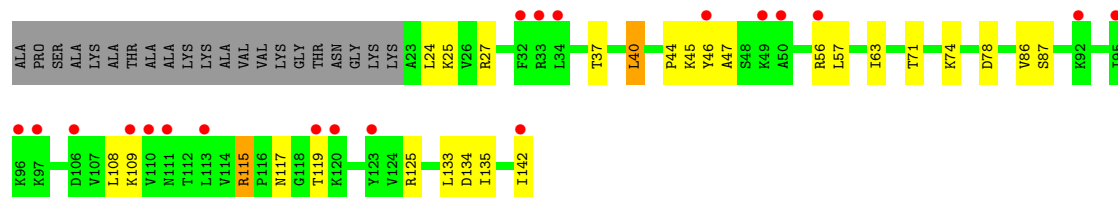
- Chain n2:





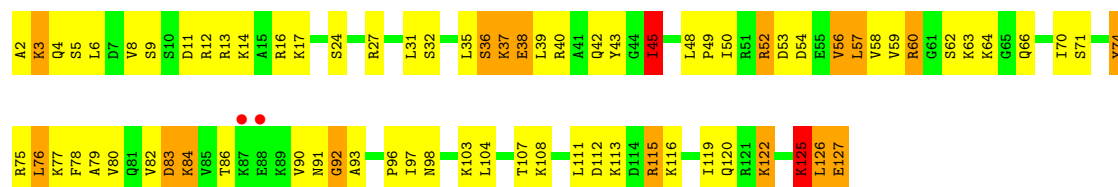
- Molecule 61: 60S ribosomal protein L25

Chain n5:



- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



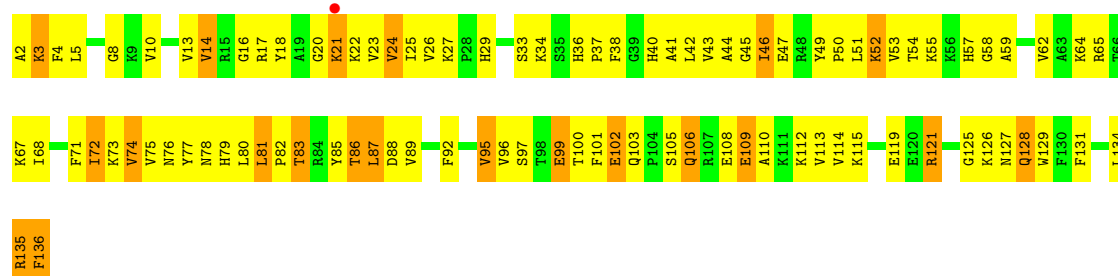
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



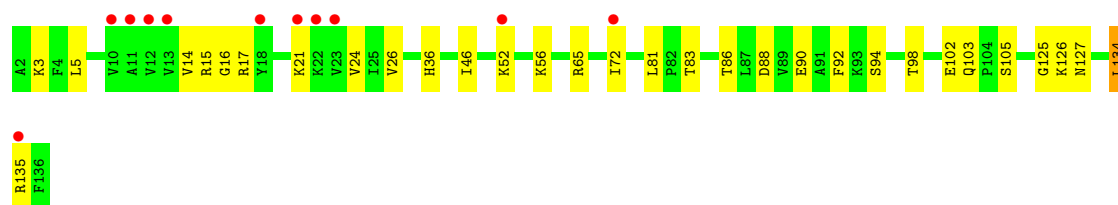
- Molecule 63: 60S ribosomal protein L27-A

Chain N7:



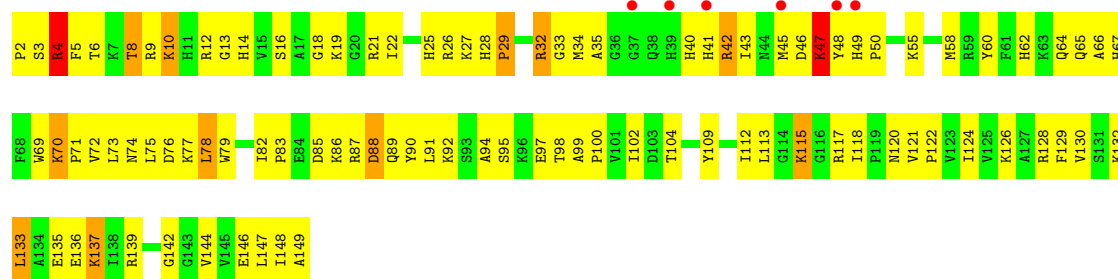
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:



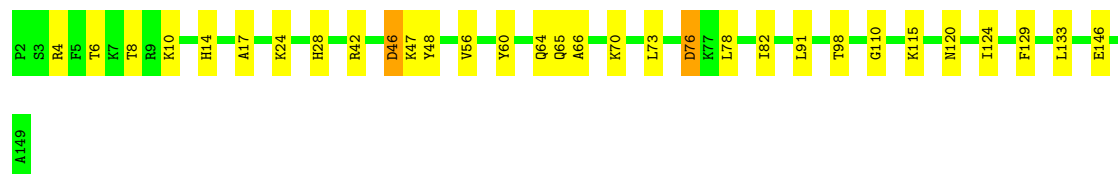
- Molecule 64: 60S ribosomal protein L28

Chain N8:



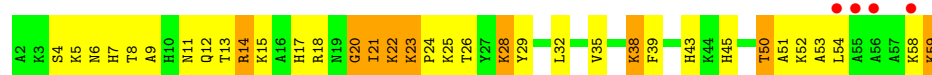
- Molecule 64: 60S ribosomal protein L28

Chain n8:



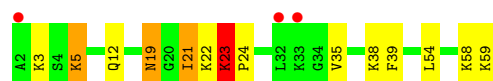
- Molecule 65: 60S ribosomal protein L29

Chain N9:



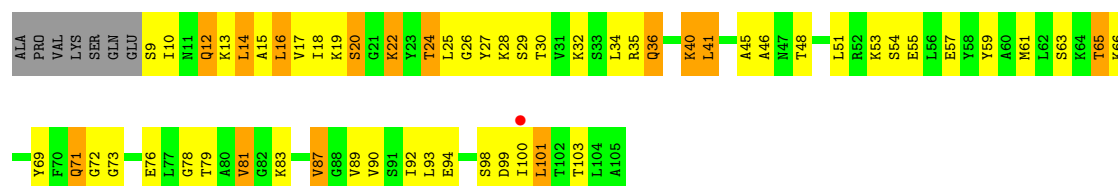
- Molecule 65: 60S ribosomal protein L29

Chain n9:



- Molecule 66: 60S ribosomal protein L30

Chain O0:



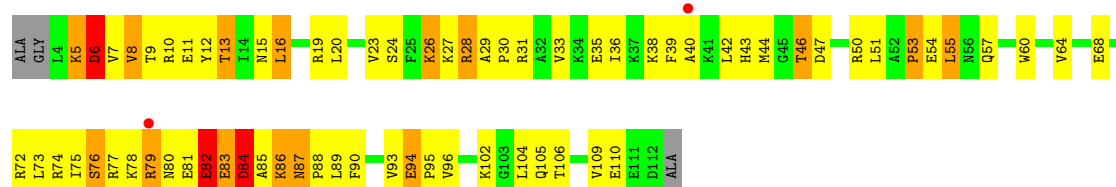
- Molecule 66: 60S ribosomal protein L30

Chain o0: 



- Molecule 67: 60S ribosomal protein L31-A

Chain O1: 



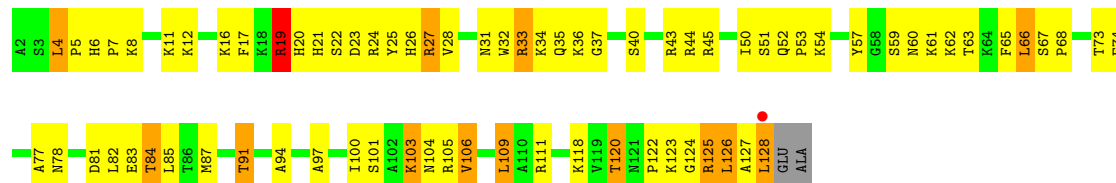
- Molecule 67: 60S ribosomal protein L31-A

Chain o1: 



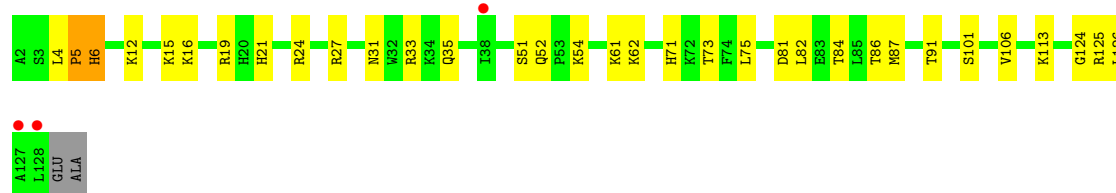
- Molecule 68: 60S ribosomal protein L32

Chain O2: 



- Molecule 68: 60S ribosomal protein L32

Chain o2: 

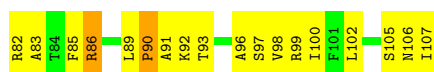


- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 

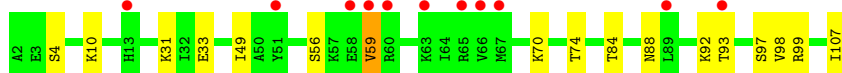






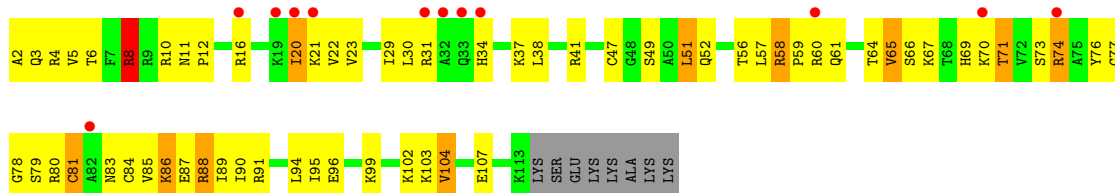
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



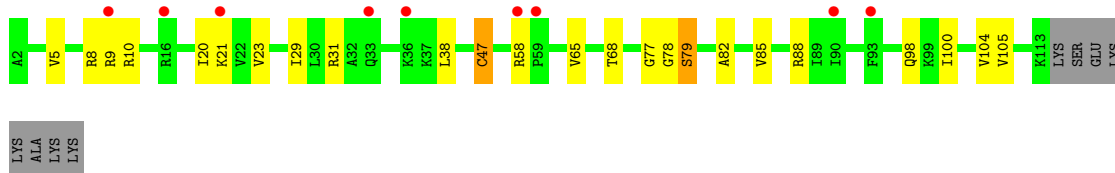
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



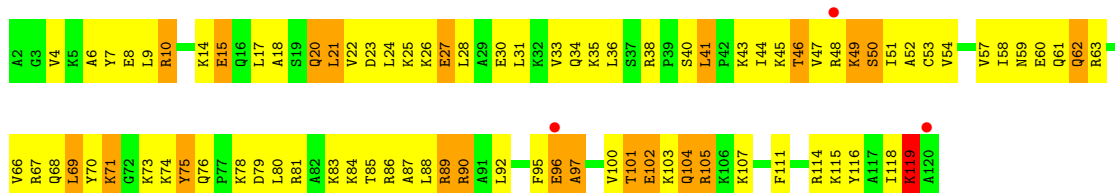
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



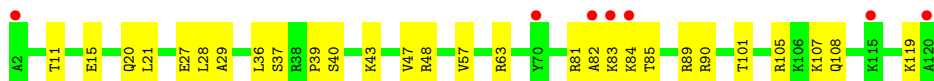
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



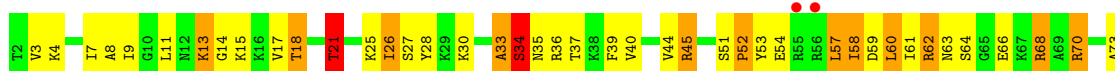
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:



- Molecule 72: 60S ribosomal protein L36-A

Chain O6:





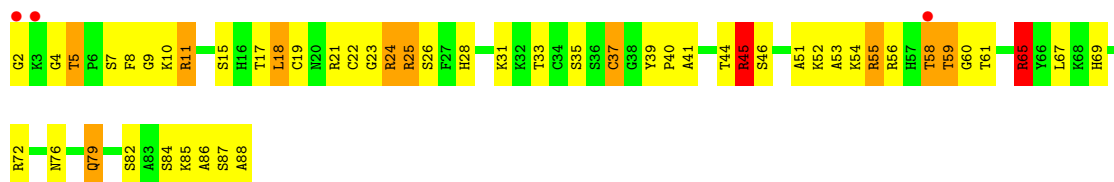
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



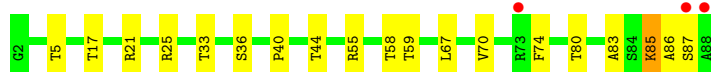
- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



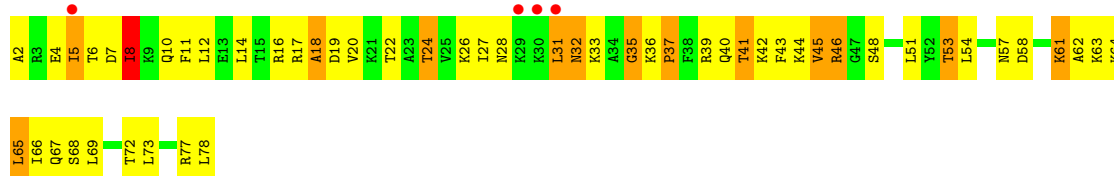
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



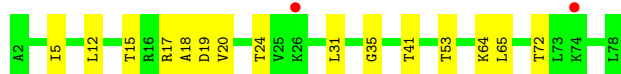
- Molecule 74: 60S ribosomal protein L38

Chain O8:



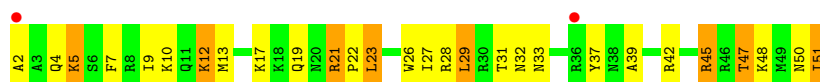
- Molecule 74: 60S ribosomal protein L38

Chain o8:



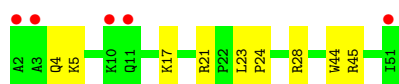
- Molecule 75: 60S ribosomal protein L39

Chain O9:



- Molecule 75: 60S ribosomal protein L39

Chain o9:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



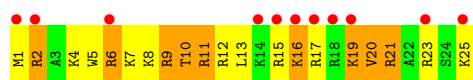
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



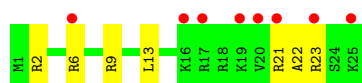
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



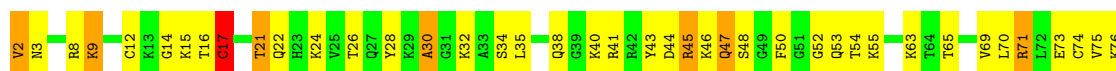
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:



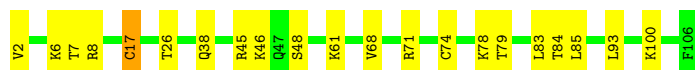
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



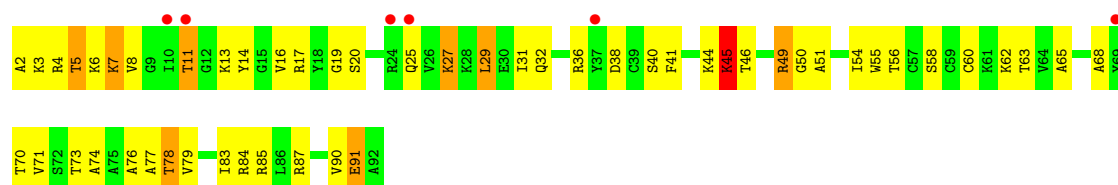
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:



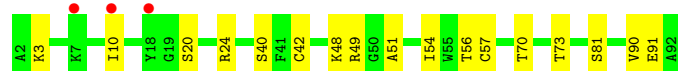
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



- Molecule 79: 60S ribosomal protein L43-A

Chain q3:



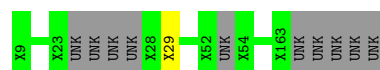
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:



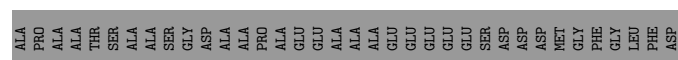
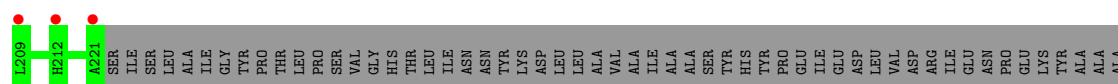
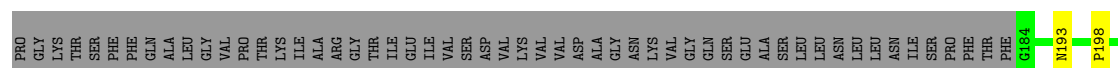
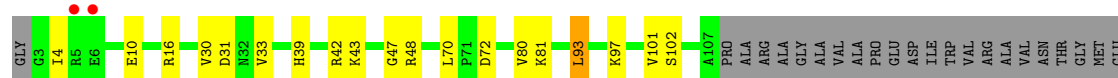
- Molecule 81: unknown protein chain m2

Chain m2:



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0:



- 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, $\alpha$ , $\beta$ , $\gamma$	436.92Å 288.52Å 305.75Å 90.00° 99.04° 90.00°	Depositor
Resolution (Å)	267.96 – 3.20 267.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (267.96-3.20) 99.9 (267.96-3.20)	Depositor EDS
$R_{merge}$	0.39	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.193 , 0.245 0.254 , 0.302	Depositor DCC
$R_{free}$ test set	17817 reflections (1.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.5	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 1226437 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	411223	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, PCY, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	2	0.79	6/41698 (0.0%)	1.36	368/64972 (0.6%)
1	6	0.95	31/42765 (0.1%)	1.47	608/66634 (0.9%)
2	S0	0.48	0/1617	0.69	0/2215
2	s0	0.53	0/1623	0.71	0/2222
3	S1	0.42	0/1735	0.70	1/2335 (0.0%)
3	s1	0.51	0/1748	0.70	1/2352 (0.0%)
4	S2	0.54	0/1665	0.69	0/2263
4	s2	0.64	0/1665	0.82	0/2263
5	S3	0.51	0/1759	0.71	1/2368 (0.0%)
5	s3	0.48	0/1759	0.63	0/2368
6	S4	0.51	0/2109	0.74	1/2839 (0.0%)
6	s4	0.60	0/2109	0.82	2/2839 (0.1%)
7	S5	0.43	0/1629	0.62	0/2202
7	s5	0.49	0/1629	0.67	0/2202
8	S6	0.49	0/1823	0.68	0/2439
8	s6	0.62	0/1779	0.74	0/2379
9	S7	0.46	0/1506	0.67	0/2028
9	s7	0.51	0/1516	0.71	2/2043 (0.1%)
10	S8	0.58	0/1514	0.77	1/2021 (0.0%)
10	s8	0.67	0/1514	0.80	1/2021 (0.0%)
11	S9	0.51	0/1519	0.68	0/2035
11	s9	0.62	0/1519	0.80	1/2035 (0.0%)
12	C0	0.45	0/790	0.65	1/1069 (0.1%)
12	c0	0.40	0/777	0.66	3/1049 (0.3%)
13	C1	0.64	0/1240	0.78	1/1675 (0.1%)
13	c1	0.70	1/1194 (0.1%)	0.81	0/1610
14	C2	0.38	0/900	0.61	0/1224
14	c2	0.29	0/900	0.58	1/1224 (0.1%)
15	C3	0.54	0/1215	0.71	1/1638 (0.1%)
15	c3	0.60	0/1215	0.74	0/1638
16	C4	0.46	0/901	0.69	0/1217
16	c4	0.55	0/960	0.77	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.48	0/998	0.69	0/1341
17	c5	0.51	0/1060	0.68	0/1426
18	C6	0.47	0/1125	0.71	2/1510 (0.1%)
18	c6	0.52	0/1131	0.73	0/1518
19	C7	0.46	0/935	0.67	0/1254
19	c7	0.53	0/914	0.73	0/1224
20	C8	0.48	0/1211	0.71	1/1628 (0.1%)
20	c8	0.52	0/1211	0.73	1/1628 (0.1%)
21	C9	0.47	0/1130	0.68	1/1517 (0.1%)
21	c9	0.56	0/1130	0.69	1/1517 (0.1%)
22	D0	0.48	0/865	0.68	0/1169
22	d0	0.53	0/892	0.68	0/1205
23	D1	0.51	0/693	0.67	0/935
23	d1	0.59	0/693	0.70	0/935
24	D2	0.53	0/1038	0.76	2/1395 (0.1%)
24	d2	0.66	0/1038	0.76	1/1395 (0.1%)
25	D3	0.65	0/1139	0.80	0/1518
25	d3	0.75	0/1139	0.87	1/1518 (0.1%)
26	D4	0.48	0/1087	0.67	0/1449
26	d4	0.59	0/1087	0.75	0/1449
27	D5	0.43	0/571	0.72	0/768
27	d5	0.49	0/566	0.75	0/761
28	D6	0.53	0/782	0.75	0/1047
28	d6	0.63	0/782	0.75	2/1047 (0.2%)
29	D7	0.47	0/620	0.71	0/838
29	d7	0.48	0/620	0.70	0/838
30	D8	0.40	0/499	0.64	0/670
30	d8	0.46	0/499	0.67	0/670
31	D9	0.55	0/452	0.80	1/600 (0.2%)
31	d9	0.57	0/452	0.68	0/600
32	E0	0.47	0/483	0.63	0/643
33	E1	0.47	0/577	0.76	0/770
33	e1	0.42	0/619	0.68	0/822
34	SR	0.44	0/2494	0.67	1/3393 (0.0%)
34	sR	0.42	0/2495	0.60	0/3395
35	SM	0.54	0/1113	0.76	2/1502 (0.1%)
35	sM	0.50	0/682	0.73	1/921 (0.1%)
36	1	1.21	245/75394 (0.3%)	1.71	2098/117545 (1.8%)
36	5	1.24	244/75414 (0.3%)	1.72	2161/117575 (1.8%)
37	3	1.00	5/2883 (0.2%)	1.48	35/4491 (0.8%)
37	7	1.20	3/2883 (0.1%)	1.74	84/4491 (1.9%)
38	4	1.17	3/3746 (0.1%)	1.66	91/5832 (1.6%)
38	8	1.05	3/3746 (0.1%)	1.57	70/5832 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L2	0.77	0/1948	0.86	2/2617 (0.1%)
39	l2	0.76	0/1946	0.91	4/2614 (0.2%)
40	L3	0.78	2/3146 (0.1%)	0.84	1/4228 (0.0%)
40	l3	0.90	1/3146 (0.0%)	0.94	5/4228 (0.1%)
41	L4	0.86	2/2800 (0.1%)	0.95	6/3790 (0.2%)
41	l4	0.77	1/2800 (0.0%)	0.89	3/3790 (0.1%)
42	L5	0.62	1/2425 (0.0%)	0.72	1/3271 (0.0%)
42	l5	0.77	0/2408	0.83	2/3248 (0.1%)
43	L6	0.79	0/1260	0.86	0/1694
43	l6	0.81	0/1269	0.88	1/1705 (0.1%)
44	L7	0.81	0/1821	0.91	4/2451 (0.2%)
44	l7	0.88	0/1828	0.91	3/2461 (0.1%)
45	L8	0.59	0/1836	0.68	0/2481
45	l8	0.55	0/1795	0.72	1/2429 (0.0%)
46	L9	0.66	0/1539	0.75	0/2073
46	l9	0.84	0/1539	0.83	0/2073
47	M0	0.77	1/1741 (0.1%)	0.82	2/2335 (0.1%)
47	m0	0.81	0/1758	0.88	2/2358 (0.1%)
48	M1	0.52	0/1374	0.73	1/1842 (0.1%)
48	m1	0.68	0/1374	0.85	3/1842 (0.2%)
49	M3	0.79	0/1568	0.91	4/2106 (0.2%)
49	m3	0.70	0/1573	0.87	2/2113 (0.1%)
50	M4	0.80	0/1068	0.81	0/1438
50	m4	0.88	0/1074	0.90	2/1446 (0.1%)
51	M5	0.79	0/1757	0.87	2/2354 (0.1%)
51	m5	0.67	0/1757	0.83	3/2354 (0.1%)
52	M6	0.86	0/1585	0.94	4/2128 (0.2%)
52	m6	1.08	3/1585 (0.2%)	1.03	7/2128 (0.3%)
53	M7	0.82	0/1443	0.86	4/1944 (0.2%)
53	m7	0.94	0/1250	0.89	0/1683
54	M8	0.81	0/1465	0.93	2/1965 (0.1%)
54	m8	0.77	0/1465	0.90	0/1965
55	M9	0.58	0/1538	0.72	1/2050 (0.0%)
55	m9	0.65	0/1538	0.71	1/2050 (0.0%)
56	N0	0.77	0/1481	0.86	5/1990 (0.3%)
56	n0	0.94	0/1481	0.96	4/1990 (0.2%)
57	N1	0.87	0/1300	0.85	0/1743
57	n1	0.87	1/1300 (0.1%)	0.88	4/1743 (0.2%)
58	N2	0.46	0/812	0.63	0/1099
58	n2	0.53	0/794	0.70	0/1076
59	N3	0.73	0/1018	0.80	0/1369
59	n3	0.90	0/1018	0.94	3/1369 (0.2%)
60	N4	0.61	0/712	0.70	0/958



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	n4	0.76	0/1052	0.77	0/1398
61	N5	0.67	0/979	0.88	4/1321 (0.3%)
61	n5	0.69	0/974	0.82	1/1314 (0.1%)
62	N6	0.73	0/1004	0.87	0/1341
62	n6	0.68	0/1004	0.84	0/1341
63	N7	0.56	0/1118	0.70	0/1497
63	n7	0.53	0/1118	0.66	0/1497
64	N8	0.86	0/1204	0.97	1/1612 (0.1%)
64	n8	0.78	0/1204	0.91	1/1612 (0.1%)
65	N9	0.75	0/473	0.84	0/629
65	n9	0.80	0/473	1.02	1/629 (0.2%)
66	O0	0.52	0/751	0.70	0/1008
66	o0	0.50	0/775	0.67	1/1040 (0.1%)
67	O1	0.69	0/890	0.78	0/1196
67	o1	0.83	0/897	0.89	2/1205 (0.2%)
68	O2	0.87	0/1041	0.94	1/1394 (0.1%)
68	o2	0.83	0/1041	0.91	0/1394
69	O3	0.91	0/868	0.87	1/1168 (0.1%)
69	o3	0.93	0/868	0.98	1/1168 (0.1%)
70	O4	0.72	1/890 (0.1%)	0.90	3/1189 (0.3%)
70	o4	0.61	0/890	0.84	1/1189 (0.1%)
71	O5	0.74	0/978	0.82	0/1301
71	o5	0.63	0/974	0.72	0/1297
72	O6	0.67	0/778	0.78	0/1034
72	o6	0.59	0/777	0.73	0/1033
73	O7	0.84	0/696	1.08	6/923 (0.7%)
73	o7	0.74	0/696	0.81	0/923
74	O8	0.51	0/618	0.70	0/826
74	o8	0.49	0/614	0.67	0/822
75	O9	0.82	0/443	0.87	0/588
75	o9	0.68	0/443	0.81	0/588
76	Q0	0.67	0/423	0.79	0/562
76	q0	0.96	1/423 (0.2%)	0.97	3/562 (0.5%)
77	Q1	0.66	0/234	0.81	0/300
77	q1	0.77	0/234	0.91	0/300
78	Q2	0.88	1/860 (0.1%)	0.86	0/1136
78	q2	0.80	1/860 (0.1%)	0.77	0/1136
79	Q3	0.75	0/701	0.86	1/934 (0.1%)
79	q3	0.72	0/701	0.80	0/934
80	e0	0.59	0/499	0.77	0/665
82	p0	0.49	0/1091	0.67	0/1472
All	All	0.95	557/430072 (0.1%)	1.36	5668/631360 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	2
9	S7	0	1
9	s7	0	2
10	S8	0	2
16	C4	0	2
16	c4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	2
22	d0	0	1
25	d3	0	1
26	d4	0	1
27	D5	0	2
27	d5	0	1
28	D6	0	1
31	D9	0	1
34	SR	0	1
39	L2	0	1
39	l2	0	2
43	L6	0	1
44	l7	0	2
47	m0	0	1
51	m5	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
68	o2	0	2
73	o7	0	1
81	m2	0	1
All	All	0	46

The worst 5 of 557 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	13.06	2.04	1.82
36	5	1152	G	N9-C4	-11.97	1.28	1.38
78	q2	17	CYS	CB-SG	11.57	2.02	1.82
36	5	1152	G	N3-C4	-10.20	1.28	1.35
36	5	2971	A	N9-C4	9.62	1.43	1.37

The worst 5 of 5668 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	C2-N3-C4	-24.18	99.81	111.90
36	5	1152	G	N3-C4-C5	20.67	138.94	128.60
36	5	1152	G	N3-C4-N9	-18.57	114.86	126.00
36	1	1902	G	N1-C6-O6	17.91	130.65	119.90
36	5	2893	C	N3-C4-C5	-17.30	114.98	121.90

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
9	S7	131	PHE	Peptide
10	S8	79	ALA	Peptide
10	S8	8	ARG	Peptide

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	960	1
1	6	38238	0	19240	859	0
2	S0	1577	0	1567	144	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	181	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	132	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	136	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	175	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	177	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1878	164	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	144	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	121	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	153	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	75	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	104	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	52	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	100	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	96	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	106	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	99	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	70	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	122	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	89	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	85	0
22	d0	882	0	939	0	0
23	D1	684	0	672	66	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	85	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	90	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	87	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	69	0
27	d5	558	0	598	0	0
28	D6	769	0	814	122	0
28	d6	769	0	814	0	0
29	D7	610	0	631	35	0
29	d7	610	0	632	0	0
30	D8	497	0	535	47	0
30	d8	497	0	535	0	0
31	D9	442	0	428	34	0
31	d9	442	0	428	0	0
32	E0	475	0	525	40	0
33	E1	566	0	602	61	0
33	e1	608	0	656	0	0
34	SR	2441	0	2397	182	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	80	0
35	sM	679	0	603	0	0
36	1	67355	0	33845	1215	0
36	5	67376	0	33856	1184	0
37	3	2579	0	1304	57	0
37	7	2579	0	1303	49	0
38	4	3353	0	1695	66	1
38	8	3353	0	1695	73	0
39	L2	1914	0	1981	162	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	232	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	224	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	190	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	77	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	123	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	122	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	143	0
46	l9	1518	0	1587	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	M0	1705	0	1735	145	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	111	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	147	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	90	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	134	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	122	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	91	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	97	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	118	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	92	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	99	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	40	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	73	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	20	0
60	n4	1038	0	1071	0	1
61	N5	964	0	1025	69	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	66	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	99	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	116	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	40	0
65	n9	462	0	491	0	0
66	O0	743	0	797	56	0
66	o0	767	0	816	0	0
67	O1	876	0	912	47	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	74	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	63	0
69	o3	850	0	880	0	0
70	O4	880	0	945	71	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	93	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	69	0
72	o6	770	0	846	0	0
73	O7	681	0	683	48	0
73	o7	681	0	683	0	0
74	O8	612	0	682	46	0
74	o8	608	0	671	0	0
75	O9	436	0	475	37	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	24	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	22	0
77	q1	233	0	284	0	0
78	Q2	847	0	917	55	0
78	q2	847	0	918	0	0
79	Q3	694	0	734	53	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	750	0	174	0	0
82	p0	1076	0	1040	0	1
83	p1	235	0	51	0	0
84	p2	230	0	54	0	0
85	1	471	0	0	0	0
85	2	124	0	0	0	0
85	3	14	0	0	0	0
85	4	21	0	0	0	0
85	5	504	0	0	0	0
85	6	147	0	0	0	0
85	7	14	0	0	0	0
85	8	16	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	L2	1	0	0	0	0
85	L3	2	0	0	0	0
85	L4	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L5	1	0	0	0	0
85	L7	3	0	0	0	0
85	L8	1	0	0	0	0
85	M0	2	0	0	0	0
85	M1	1	0	0	0	0
85	M3	3	0	0	0	0
85	M5	2	0	0	0	0
85	M6	2	0	0	0	0
85	M7	4	0	0	0	0
85	M9	3	0	0	0	0
85	N0	1	0	0	0	0
85	N3	2	0	0	0	0
85	N5	1	0	0	0	0
85	N6	1	0	0	0	0
85	N8	4	0	0	0	0
85	N9	1	0	0	0	0
85	O2	1	0	0	0	0
85	O3	1	0	0	0	0
85	O7	2	0	0	0	0
85	Q2	1	0	0	0	0
85	S2	2	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	2	0	0	0	0
85	d3	2	0	0	0	0
85	d6	1	0	0	0	0
85	l2	1	0	0	0	0
85	l3	2	0	0	0	0
85	l4	1	0	0	0	0
85	l5	2	0	0	0	0
85	l7	2	0	0	0	0
85	l8	1	0	0	0	0
85	m1	2	0	0	0	0
85	m5	4	0	0	0	0
85	m6	2	0	0	0	0
85	m7	5	0	0	0	0
85	n0	2	0	0	0	0
85	n3	2	0	0	0	0
85	n6	1	0	0	0	0
85	n8	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	o1	1	0	0	0	0
85	o3	1	0	0	0	0
85	o4	1	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	2	0	0	0	0
85	s1	1	0	0	0	0
85	s2	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2457	0	0	209	0
86	2	1078	0	0	113	0
86	3	84	0	0	2	0
86	4	119	0	0	13	0
86	5	2464	0	0	205	0
86	6	1106	0	0	111	0
86	7	84	0	0	8	0
86	8	112	0	0	15	0
86	C3	7	0	0	2	0
86	C5	7	0	0	3	0
86	C8	7	0	0	0	0
86	D3	7	0	0	0	0
86	D9	7	0	0	1	0
86	L3	21	0	0	1	0
86	L4	7	0	0	1	0
86	M0	7	0	0	0	0
86	M5	7	0	0	1	0
86	M7	14	0	0	3	0
86	M9	7	0	0	0	0
86	N1	7	0	0	1	0
86	N9	7	0	0	1	0
86	O3	7	0	0	2	0
86	O7	7	0	0	6	0
86	Q2	7	0	0	2	0
86	S6	7	0	0	0	0
86	S8	7	0	0	0	0
86	SR	7	0	0	0	0
86	c3	7	0	0	0	0
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	m8	7	0	0	0	0
86	n3	7	0	0	0	0
86	n9	14	0	0	0	0
86	o2	7	0	0	0	0
86	o3	7	0	0	0	0
86	o7	14	0	0	0	0
86	q1	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	0	0
86	sR	7	0	0	0	0
87	2	40	0	37	5	0
87	6	40	0	37	1	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	0	0
88	Q2	1	0	0	0	0
88	Q3	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
All	All	411223	0	297358	10229	2

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 15.

The worst 5 of 10229 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.04	1.48
40:L3:296:THR:HG22	40:L3:298:PHE:H	5.12	1.05
1:6:1011:G:OP2	86:6:2120:OHX:N3	1.90	1.03
1:2:1339:C:O2'	1:2:1341:A:N7	1.94	1.01
76:Q0:77:ILE:HG23	76:Q0:78:ILE:HG22	5.29	1.00

All (2) 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)
1:2:236:A:O2'	38:4:158:U:O2'[2.556]	2.13	0.07
60:n4:106:GLU:OE2	82:p0:16:ARG:NH2[2.657]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	148 (72%)	34 (17%)	22 (11%)	1	5
2	s0	204/251 (81%)	155 (76%)	31 (15%)	18 (9%)	1	8
3	S1	212/254 (84%)	143 (68%)	36 (17%)	33 (16%)	0	1
3	s1	214/254 (84%)	168 (78%)	30 (14%)	16 (8%)	2	12
4	S2	215/253 (85%)	176 (82%)	24 (11%)	15 (7%)	2	13
4	s2	215/253 (85%)	178 (83%)	24 (11%)	13 (6%)	2	20
5	S3	221/239 (92%)	182 (82%)	31 (14%)	8 (4%)	5	36
5	s3	221/239 (92%)	172 (78%)	31 (14%)	18 (8%)	1	10
6	S4	258/260 (99%)	208 (81%)	27 (10%)	23 (9%)	1	8
6	s4	258/260 (99%)	200 (78%)	36 (14%)	22 (8%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	S5	204/224 (91%)	154 (76%)	29 (14%)	21 (10%)	1	6
7	s5	204/224 (91%)	158 (78%)	26 (13%)	20 (10%)	1	7
8	S6	224/236 (95%)	185 (83%)	22 (10%)	17 (8%)	2	12
8	s6	216/236 (92%)	187 (87%)	19 (9%)	10 (5%)	4	28
9	S7	182/189 (96%)	134 (74%)	23 (13%)	25 (14%)	0	2
9	s7	184/189 (97%)	145 (79%)	27 (15%)	12 (6%)	2	17
10	S8	184/200 (92%)	149 (81%)	24 (13%)	11 (6%)	2	20
10	s8	184/200 (92%)	159 (86%)	19 (10%)	6 (3%)	6	38
11	S9	183/196 (93%)	143 (78%)	29 (16%)	11 (6%)	2	20
11	s9	183/196 (93%)	148 (81%)	25 (14%)	10 (6%)	3	23
12	C0	94/105 (90%)	74 (79%)	10 (11%)	10 (11%)	1	5
12	c0	92/105 (88%)	63 (68%)	15 (16%)	14 (15%)	0	1
13	C1	153/155 (99%)	118 (77%)	20 (13%)	15 (10%)	1	7
13	c1	144/155 (93%)	117 (81%)	19 (13%)	8 (6%)	3	23
14	C2	122/142 (86%)	75 (62%)	26 (21%)	21 (17%)	0	1
14	c2	122/142 (86%)	69 (57%)	34 (28%)	19 (16%)	0	1
15	C3	148/150 (99%)	120 (81%)	20 (14%)	8 (5%)	3	24
15	c3	148/150 (99%)	120 (81%)	18 (12%)	10 (7%)	2	15
16	C4	125/136 (92%)	94 (75%)	21 (17%)	10 (8%)	1	10
16	c4	126/136 (93%)	92 (73%)	22 (18%)	12 (10%)	1	7
17	C5	122/141 (86%)	90 (74%)	18 (15%)	14 (12%)	1	4
17	c5	133/141 (94%)	86 (65%)	23 (17%)	24 (18%)	0	1
18	C6	139/142 (98%)	116 (84%)	13 (9%)	10 (7%)	2	13
18	c6	140/142 (99%)	115 (82%)	18 (13%)	7 (5%)	3	26
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	1	6
19	c7	113/136 (83%)	87 (77%)	12 (11%)	14 (12%)	1	3
20	C8	143/145 (99%)	110 (77%)	22 (15%)	11 (8%)	1	11
20	c8	143/145 (99%)	111 (78%)	22 (15%)	10 (7%)	2	13
21	C9	141/143 (99%)	113 (80%)	25 (18%)	3 (2%)	11	55
21	c9	141/143 (99%)	116 (82%)	18 (13%)	7 (5%)	3	26
22	D0	105/120 (88%)	83 (79%)	19 (18%)	3 (3%)	7	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	1	8
23	D1	85/87 (98%)	65 (76%)	14 (16%)	6 (7%)	2	13
23	d1	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	4	27
24	D2	127/129 (98%)	108 (85%)	12 (9%)	7 (6%)	3	23
24	d2	127/129 (98%)	114 (90%)	9 (7%)	4 (3%)	7	41
25	D3	142/144 (99%)	107 (75%)	22 (16%)	13 (9%)	1	8
25	d3	142/144 (99%)	116 (82%)	19 (13%)	7 (5%)	3	26
26	D4	132/134 (98%)	102 (77%)	23 (17%)	7 (5%)	3	24
26	d4	132/134 (98%)	101 (76%)	21 (16%)	10 (8%)	2	12
27	D5	68/107 (64%)	43 (63%)	14 (21%)	11 (16%)	0	1
27	d5	67/107 (63%)	50 (75%)	14 (21%)	3 (4%)	4	29
28	D6	95/97 (98%)	56 (59%)	19 (20%)	20 (21%)	0	0
28	d6	95/97 (98%)	73 (77%)	13 (14%)	9 (10%)	1	7
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	5	34
29	d7	79/81 (98%)	60 (76%)	15 (19%)	4 (5%)	3	25
30	D8	61/66 (92%)	50 (82%)	7 (12%)	4 (7%)	2	16
30	d8	61/66 (92%)	44 (72%)	10 (16%)	7 (12%)	1	4
31	D9	51/55 (93%)	43 (84%)	7 (14%)	1 (2%)	11	56
31	d9	51/55 (93%)	39 (76%)	8 (16%)	4 (8%)	1	11
32	E0	58/60 (97%)	49 (84%)	6 (10%)	3 (5%)	3	25
33	E1	69/76 (91%)	33 (48%)	15 (22%)	21 (30%)	0	0
33	e1	74/76 (97%)	33 (45%)	24 (32%)	17 (23%)	0	0
34	SR	316/318 (99%)	244 (77%)	52 (16%)	20 (6%)	2	18
34	sR	316/318 (99%)	259 (82%)	43 (14%)	14 (4%)	4	29
35	SM	155/273 (57%)	114 (74%)	23 (15%)	18 (12%)	1	4
35	sM	98/273 (36%)	61 (62%)	21 (21%)	16 (16%)	0	1
39	L2	250/253 (99%)	218 (87%)	26 (10%)	6 (2%)	9	51
39	l2	250/253 (99%)	203 (81%)	36 (14%)	11 (4%)	4	29
40	L3	384/386 (100%)	336 (88%)	30 (8%)	18 (5%)	4	27
40	l3	384/386 (100%)	329 (86%)	42 (11%)	13 (3%)	6	38
41	L4	359/361 (99%)	303 (84%)	37 (10%)	19 (5%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	l4	359/361 (99%)	297 (83%)	43 (12%)	19 (5%)	3	24
42	L5	294/296 (99%)	244 (83%)	31 (10%)	19 (6%)	2	17
42	l5	292/296 (99%)	250 (86%)	30 (10%)	12 (4%)	4	32
43	L6	152/175 (87%)	129 (85%)	19 (12%)	4 (3%)	8	47
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	8	47
44	L7	220/243 (90%)	183 (83%)	28 (13%)	9 (4%)	4	32
44	l7	221/243 (91%)	191 (86%)	24 (11%)	6 (3%)	8	46
45	L8	231/255 (91%)	185 (80%)	37 (16%)	9 (4%)	5	33
45	l8	229/255 (90%)	175 (76%)	32 (14%)	22 (10%)	1	7
46	L9	189/191 (99%)	161 (85%)	24 (13%)	4 (2%)	11	55
46	l9	189/191 (99%)	165 (87%)	18 (10%)	6 (3%)	6	39
47	M0	207/220 (94%)	168 (81%)	33 (16%)	6 (3%)	7	43
47	m0	209/220 (95%)	175 (84%)	20 (10%)	14 (7%)	2	16
48	M1	167/173 (96%)	135 (81%)	18 (11%)	14 (8%)	1	9
48	m1	167/173 (96%)	132 (79%)	20 (12%)	15 (9%)	1	8
49	M3	191/198 (96%)	161 (84%)	21 (11%)	9 (5%)	4	27
49	m3	192/198 (97%)	154 (80%)	19 (10%)	19 (10%)	1	7
50	M4	134/137 (98%)	119 (89%)	8 (6%)	7 (5%)	3	25
50	m4	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	15	64
51	M5	201/203 (99%)	184 (92%)	11 (6%)	6 (3%)	7	42
51	m5	201/203 (99%)	181 (90%)	15 (8%)	5 (2%)	9	49
52	M6	195/198 (98%)	176 (90%)	16 (8%)	3 (2%)	15	64
52	m6	195/198 (98%)	175 (90%)	15 (8%)	5 (3%)	8	47
53	M7	181/183 (99%)	154 (85%)	22 (12%)	5 (3%)	8	44
53	m7	153/183 (84%)	131 (86%)	19 (12%)	3 (2%)	11	56
54	M8	183/185 (99%)	157 (86%)	19 (10%)	7 (4%)	5	34
54	m8	183/185 (99%)	148 (81%)	29 (16%)	6 (3%)	6	38
55	M9	186/188 (99%)	165 (89%)	17 (9%)	4 (2%)	10	53
55	m9	186/188 (99%)	162 (87%)	20 (11%)	4 (2%)	10	53
56	N0	170/172 (99%)	152 (89%)	15 (9%)	3 (2%)	13	60
56	n0	170/172 (99%)	154 (91%)	13 (8%)	3 (2%)	13	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	N1	157/159 (99%)	136 (87%)	13 (8%)	8 (5%)	3	25
57	n1	157/159 (99%)	139 (88%)	16 (10%)	2 (1%)	18	68
58	N2	98/120 (82%)	77 (79%)	15 (15%)	6 (6%)	2	19
58	n2	96/120 (80%)	75 (78%)	19 (20%)	2 (2%)	11	55
59	N3	134/136 (98%)	119 (89%)	15 (11%)	0	100	100
59	n3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	15	64
60	N4	96/155 (62%)	72 (75%)	18 (19%)	6 (6%)	2	18
60	n4	133/155 (86%)	111 (84%)	15 (11%)	7 (5%)	3	24
61	N5	119/141 (84%)	106 (89%)	9 (8%)	4 (3%)	6	38
61	n5	118/141 (84%)	96 (81%)	15 (13%)	7 (6%)	2	20
62	N6	124/126 (98%)	110 (89%)	8 (6%)	6 (5%)	4	27
62	n6	124/126 (98%)	108 (87%)	11 (9%)	5 (4%)	5	32
63	N7	133/135 (98%)	112 (84%)	14 (10%)	7 (5%)	3	24
63	n7	133/135 (98%)	108 (81%)	20 (15%)	5 (4%)	5	34
64	N8	146/148 (99%)	124 (85%)	18 (12%)	4 (3%)	8	46
64	n8	146/148 (99%)	120 (82%)	16 (11%)	10 (7%)	2	15
65	N9	56/58 (97%)	44 (79%)	10 (18%)	2 (4%)	5	36
65	n9	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	1	8
66	O0	95/104 (91%)	83 (87%)	10 (10%)	2 (2%)	11	55
66	o0	98/104 (94%)	86 (88%)	9 (9%)	3 (3%)	7	41
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	4	27
67	o1	107/112 (96%)	91 (85%)	12 (11%)	4 (4%)	5	34
68	O2	125/129 (97%)	109 (87%)	13 (10%)	3 (2%)	9	51
68	o2	125/129 (97%)	102 (82%)	18 (14%)	5 (4%)	5	32
69	O3	104/106 (98%)	93 (89%)	10 (10%)	1 (1%)	22	74
69	o3	104/106 (98%)	90 (86%)	11 (11%)	3 (3%)	7	43
70	O4	110/120 (92%)	92 (84%)	16 (14%)	2 (2%)	13	60
70	o4	110/120 (92%)	92 (84%)	12 (11%)	6 (6%)	3	23
71	O5	117/119 (98%)	103 (88%)	8 (7%)	6 (5%)	3	25
71	o5	117/119 (98%)	97 (83%)	13 (11%)	7 (6%)	2	20
72	O6	97/99 (98%)	76 (78%)	11 (11%)	10 (10%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	o6	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	2	13
73	O7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	9	51
73	o7	85/87 (98%)	69 (81%)	13 (15%)	3 (4%)	6	37
74	O8	75/77 (97%)	61 (81%)	9 (12%)	5 (7%)	2	16
74	o8	75/77 (97%)	59 (79%)	11 (15%)	5 (7%)	2	16
75	O9	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
75	o9	48/50 (96%)	41 (85%)	5 (10%)	2 (4%)	4	31
76	Q0	50/52 (96%)	43 (86%)	5 (10%)	2 (4%)	5	32
76	q0	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	11	56
77	Q1	23/25 (92%)	23 (100%)	0	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	4	30
78	Q2	103/105 (98%)	78 (76%)	16 (16%)	9 (9%)	1	8
78	q2	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	12	59
79	Q3	89/91 (98%)	75 (84%)	10 (11%)	4 (4%)	4	29
79	q3	89/91 (98%)	76 (85%)	12 (14%)	1 (1%)	21	72
80	e0	60/62 (97%)	48 (80%)	5 (8%)	7 (12%)	1	4
82	p0	139/311 (45%)	111 (80%)	23 (16%)	5 (4%)	5	36
All	All	22333/24143 (92%)	18179 (81%)	2816 (13%)	1338 (6%)	2	20

5 of 1338 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	66	ALA
2	S0	158	VAL
2	S0	191	ARG
2	S0	194	PRO
3	S1	40	ASN

### 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%)	129 (79%)	35 (21%)	1	7
2	s0	165/209 (79%)	129 (78%)	36 (22%)	1	7
3	S1	191/223 (86%)	150 (78%)	41 (22%)	1	7
3	s1	192/223 (86%)	150 (78%)	42 (22%)	1	7
4	S2	176/204 (86%)	142 (81%)	34 (19%)	2	10
4	s2	176/204 (86%)	124 (70%)	52 (30%)	0	1
5	S3	182/194 (94%)	140 (77%)	42 (23%)	1	5
5	s3	182/194 (94%)	146 (80%)	36 (20%)	2	9
6	S4	221/221 (100%)	167 (76%)	54 (24%)	1	3
6	s4	221/221 (100%)	180 (81%)	41 (19%)	2	11
7	S5	173/190 (91%)	141 (82%)	32 (18%)	2	11
7	s5	173/190 (91%)	142 (82%)	31 (18%)	2	12
8	S6	188/201 (94%)	156 (83%)	32 (17%)	3	14
8	s6	187/201 (93%)	151 (81%)	36 (19%)	2	10
9	S7	165/169 (98%)	137 (83%)	28 (17%)	3	14
9	s7	165/169 (98%)	137 (83%)	28 (17%)	3	14
10	S8	150/161 (93%)	125 (83%)	25 (17%)	3	14
10	s8	150/161 (93%)	119 (79%)	31 (21%)	2	8
11	S9	158/165 (96%)	122 (77%)	36 (23%)	1	6
11	s9	158/165 (96%)	123 (78%)	35 (22%)	1	6
12	C0	77/98 (79%)	61 (79%)	16 (21%)	2	8
12	c0	73/98 (74%)	64 (88%)	9 (12%)	7	31
13	C1	129/136 (95%)	108 (84%)	21 (16%)	3	15
13	c1	129/136 (95%)	104 (81%)	25 (19%)	2	10
14	C2	88/118 (75%)	64 (73%)	24 (27%)	0	2
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0	2
15	C3	127/127 (100%)	102 (80%)	25 (20%)	2	10
15	c3	127/127 (100%)	102 (80%)	25 (20%)	2	10
16	C4	81/104 (78%)	57 (70%)	24 (30%)	0	1
16	c4	97/104 (93%)	73 (75%)	24 (25%)	1	3
17	C5	101/117 (86%)	80 (79%)	21 (21%)	2	8
17	c5	103/117 (88%)	84 (82%)	19 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C6	117/118 (99%)	94 (80%)	23 (20%)	2	10
18	c6	118/118 (100%)	99 (84%)	19 (16%)	3	16
19	C7	94/124 (76%)	74 (79%)	20 (21%)	1	7
19	c7	92/124 (74%)	73 (79%)	19 (21%)	2	8
20	C8	128/128 (100%)	98 (77%)	30 (23%)	1	5
20	c8	128/128 (100%)	102 (80%)	26 (20%)	2	9
21	C9	115/115 (100%)	88 (76%)	27 (24%)	1	5
21	c9	115/115 (100%)	95 (83%)	20 (17%)	3	13
22	D0	100/113 (88%)	75 (75%)	25 (25%)	1	3
22	d0	103/113 (91%)	74 (72%)	29 (28%)	0	2
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	7
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	7
24	D2	110/110 (100%)	88 (80%)	22 (20%)	2	9
24	d2	110/110 (100%)	94 (86%)	16 (14%)	5	22
25	D3	119/119 (100%)	98 (82%)	21 (18%)	3	13
25	d3	119/119 (100%)	100 (84%)	19 (16%)	3	16
26	D4	112/112 (100%)	90 (80%)	22 (20%)	2	10
26	d4	112/112 (100%)	94 (84%)	18 (16%)	3	16
27	D5	61/88 (69%)	46 (75%)	15 (25%)	1	3
27	d5	61/88 (69%)	51 (84%)	10 (16%)	3	15
28	D6	83/83 (100%)	66 (80%)	17 (20%)	2	8
28	d6	83/83 (100%)	70 (84%)	13 (16%)	4	17
29	D7	70/70 (100%)	63 (90%)	7 (10%)	11	41
29	d7	70/70 (100%)	60 (86%)	10 (14%)	5	22
30	D8	56/59 (95%)	42 (75%)	14 (25%)	1	3
30	d8	56/59 (95%)	42 (75%)	14 (25%)	1	3
31	D9	47/48 (98%)	41 (87%)	6 (13%)	6	28
31	d9	47/48 (98%)	35 (74%)	12 (26%)	1	3
32	E0	51/51 (100%)	41 (80%)	10 (20%)	2	10
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	2
33	e1	66/66 (100%)	46 (70%)	20 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	SR	260/261 (100%)	219 (84%)	41 (16%)	4	16
34	sR	260/261 (100%)	229 (88%)	31 (12%)	8	33
35	SM	97/228 (42%)	77 (79%)	20 (21%)	2	8
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	2
39	L2	193/195 (99%)	154 (80%)	39 (20%)	2	9
39	l2	192/195 (98%)	161 (84%)	31 (16%)	3	16
40	L3	321/322 (100%)	245 (76%)	76 (24%)	1	4
40	l3	321/322 (100%)	257 (80%)	64 (20%)	2	9
41	L4	288/288 (100%)	231 (80%)	57 (20%)	2	9
41	l4	288/288 (100%)	232 (81%)	56 (19%)	2	10
42	L5	244/244 (100%)	199 (82%)	45 (18%)	2	11
42	l5	243/244 (100%)	192 (79%)	51 (21%)	1	8
43	L6	134/152 (88%)	116 (87%)	18 (13%)	6	26
43	l6	135/152 (89%)	113 (84%)	22 (16%)	3	15
44	L7	186/204 (91%)	156 (84%)	30 (16%)	3	16
44	l7	187/204 (92%)	159 (85%)	28 (15%)	4	19
45	L8	187/207 (90%)	150 (80%)	37 (20%)	2	9
45	l8	177/207 (86%)	141 (80%)	36 (20%)	2	9
46	L9	171/171 (100%)	138 (81%)	33 (19%)	2	10
46	l9	171/171 (100%)	131 (77%)	40 (23%)	1	5
47	M0	177/186 (95%)	142 (80%)	35 (20%)	2	9
47	m0	179/186 (96%)	138 (77%)	41 (23%)	1	5
48	M1	147/150 (98%)	112 (76%)	35 (24%)	1	4
48	m1	147/150 (98%)	114 (78%)	33 (22%)	1	6
49	M3	154/158 (98%)	129 (84%)	25 (16%)	3	15
49	m3	154/158 (98%)	128 (83%)	26 (17%)	3	14
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	13
50	m4	108/108 (100%)	81 (75%)	27 (25%)	1	3
51	M5	175/175 (100%)	146 (83%)	29 (17%)	3	14
51	m5	175/175 (100%)	144 (82%)	31 (18%)	3	13
52	M6	160/161 (99%)	134 (84%)	26 (16%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	m6	160/161 (99%)	123 (77%)	37 (23%)	1	5
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	7
53	m7	125/145 (86%)	101 (81%)	24 (19%)	2	10
54	M8	150/150 (100%)	126 (84%)	24 (16%)	3	16
54	m8	150/150 (100%)	115 (77%)	35 (23%)	1	5
55	M9	153/153 (100%)	123 (80%)	30 (20%)	2	10
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	6
56	N0	156/156 (100%)	127 (81%)	29 (19%)	2	11
56	n0	156/156 (100%)	118 (76%)	38 (24%)	1	3
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	5
57	n1	136/136 (100%)	110 (81%)	26 (19%)	2	11
58	N2	87/106 (82%)	69 (79%)	18 (21%)	2	8
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1	8
59	N3	104/104 (100%)	81 (78%)	23 (22%)	1	7
59	n3	104/104 (100%)	87 (84%)	17 (16%)	3	15
60	N4	57/129 (44%)	49 (86%)	8 (14%)	5	23
60	n4	100/129 (78%)	86 (86%)	14 (14%)	5	23
61	N5	104/117 (89%)	79 (76%)	25 (24%)	1	4
61	n5	104/117 (89%)	83 (80%)	21 (20%)	2	9
62	N6	109/109 (100%)	84 (77%)	25 (23%)	1	5
62	n6	109/109 (100%)	85 (78%)	24 (22%)	1	7
63	N7	115/115 (100%)	92 (80%)	23 (20%)	2	9
63	n7	115/115 (100%)	88 (76%)	27 (24%)	1	5
64	N8	118/118 (100%)	98 (83%)	20 (17%)	3	14
64	n8	118/118 (100%)	98 (83%)	20 (17%)	3	14
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1	7
65	n9	46/46 (100%)	34 (74%)	12 (26%)	1	2
66	O0	81/87 (93%)	64 (79%)	17 (21%)	1	8
66	o0	84/87 (97%)	65 (77%)	19 (23%)	1	6
67	O1	92/96 (96%)	65 (71%)	27 (29%)	0	1
67	o1	94/96 (98%)	70 (74%)	24 (26%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	O2	109/110 (99%)	90 (83%)	19 (17%)	3	13
68	o2	109/110 (99%)	81 (74%)	28 (26%)	1	2
69	O3	90/90 (100%)	76 (84%)	14 (16%)	4	17
69	o3	90/90 (100%)	76 (84%)	14 (16%)	4	17
70	O4	95/102 (93%)	80 (84%)	15 (16%)	4	16
70	o4	95/102 (93%)	76 (80%)	19 (20%)	2	9
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1	8
71	o5	103/104 (99%)	82 (80%)	21 (20%)	2	8
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1	8
72	o6	80/81 (99%)	53 (66%)	27 (34%)	0	0
73	O7	70/70 (100%)	53 (76%)	17 (24%)	1	3
73	o7	70/70 (100%)	54 (77%)	16 (23%)	1	5
74	O8	68/68 (100%)	51 (75%)	17 (25%)	1	3
74	o8	67/68 (98%)	57 (85%)	10 (15%)	4	20
75	O9	45/45 (100%)	34 (76%)	11 (24%)	1	3
75	o9	45/45 (100%)	38 (84%)	7 (16%)	4	17
76	Q0	47/47 (100%)	38 (81%)	9 (19%)	2	11
76	q0	47/47 (100%)	37 (79%)	10 (21%)	1	7
77	Q1	23/23 (100%)	12 (52%)	11 (48%)	0	0
77	q1	23/23 (100%)	17 (74%)	6 (26%)	1	2
78	Q2	90/90 (100%)	71 (79%)	19 (21%)	1	8
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1	8
79	Q3	71/71 (100%)	57 (80%)	14 (20%)	2	10
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	6
80	e0	53/53 (100%)	40 (76%)	13 (24%)	1	3
82	p0	105/253 (42%)	89 (85%)	16 (15%)	4	19
All	All	18730/20241 (92%)	14956 (80%)	3774 (20%)	2	9

5 of 3774 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	O2	128	LEU
8	s6	21	GLU

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Mol	Chain	Res	Type
63	n7	126	LYS
71	O5	107	LYS
3	s1	54	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
47	M0	144	ASN
61	N5	80	ASN
61	n5	111	ASN
49	M3	25	HIS
55	M9	34	GLN

### 5.3.3 RNA ⓘ

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

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
86	OHX	1	3863	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
86	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
86	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4213	-	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	-
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	-



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



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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	PCY	2	2178	-	42,42,42	0.48	0	65,65,65	1.77	11 (16%)
86	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

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



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



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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	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	-

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
87	PCY	6	2204	-	42,42,42	0.69	2 (4%)	65,65,65	2.34	10 (15%)
86	OHX	7	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
86	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	232	-	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	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S6	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	303	-	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	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	305	-	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	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q1	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4213	-	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
87	PCY	2	2178	-	-	0/33/67/67	0/3/3/3
86	OHX	3	215	-	-	0/0/0/0	0/0/0/0
86	OHX	3	216	-	-	0/0/0/0	0/0/0/0
86	OHX	3	217	-	-	0/0/0/0	0/0/0/0
86	OHX	3	218	-	-	0/0/0/0	0/0/0/0
86	OHX	3	219	-	-	0/0/0/0	0/0/0/0
86	OHX	3	220	-	-	0/0/0/0	0/0/0/0
86	OHX	3	221	-	-	0/0/0/0	0/0/0/0
86	OHX	3	222	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	3	223	-	-	0/0/0/0	0/0/0/0
86	OHX	3	224	-	-	0/0/0/0	0/0/0/0
86	OHX	3	225	-	-	0/0/0/0	0/0/0/0
86	OHX	3	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	222	-	-	0/0/0/0	0/0/0/0
86	OHX	4	223	-	-	0/0/0/0	0/0/0/0
86	OHX	4	224	-	-	0/0/0/0	0/0/0/0
86	OHX	4	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	227	-	-	0/0/0/0	0/0/0/0
86	OHX	4	228	-	-	0/0/0/0	0/0/0/0
86	OHX	4	229	-	-	0/0/0/0	0/0/0/0
86	OHX	4	230	-	-	0/0/0/0	0/0/0/0
86	OHX	4	231	-	-	0/0/0/0	0/0/0/0
86	OHX	4	232	-	-	0/0/0/0	0/0/0/0
86	OHX	4	233	-	-	0/0/0/0	0/0/0/0
86	OHX	4	234	-	-	0/0/0/0	0/0/0/0
86	OHX	4	235	-	-	0/0/0/0	0/0/0/0
86	OHX	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	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	86	-	0/0/0/0	0/0/0/0
86	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
86	OHX	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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
87	PCY	6	2204	-	-	0/33/67/67	0/3/3/3
86	OHX	7	215	-	-	0/0/0/0	0/0/0/0
86	OHX	7	216	-	-	0/0/0/0	0/0/0/0
86	OHX	7	217	-	-	0/0/0/0	0/0/0/0
86	OHX	7	218	-	-	0/0/0/0	0/0/0/0
86	OHX	7	219	-	-	0/0/0/0	0/0/0/0
86	OHX	7	220	-	-	0/0/0/0	0/0/0/0
86	OHX	7	221	-	-	0/0/0/0	0/0/0/0
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	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	8	219	-	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	-	-	0/0/0/0	0/0/0/0
86	OHX	8	222	-	-	0/0/0/0	0/0/0/0
86	OHX	8	223	-	-	0/0/0/0	0/0/0/0
86	OHX	8	224	-	-	0/0/0/0	0/0/0/0
86	OHX	8	225	-	-	0/0/0/0	0/0/0/0
86	OHX	8	226	-	-	0/0/0/0	0/0/0/0
86	OHX	8	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	229	-	-	0/0/0/0	0/0/0/0
86	OHX	8	230	-	-	0/0/0/0	0/0/0/0
86	OHX	8	231	-	-	0/0/0/0	0/0/0/0
86	OHX	8	232	-	-	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	403	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	205	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	204	-	-	0/0/0/0	0/0/0/0
86	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
86	OHX	S6	301	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	203	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	403	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	305	-	-	0/0/0/0	0/0/0/0
86	OHX	m6	203	-	-	0/0/0/0	0/0/0/0
86	OHX	m7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	503	-	-	0/0/0/0	0/0/0/0
86	OHX	q1	102	-	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	6	2204	PCY	C3-C7	-2.21	1.51	1.56
87	6	2204	PCY	C24-C28	2.06	1.42	1.39

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	6	2204	PCY	C6-C3-N2	12.82	118.47	107.39
87	2	2178	PCY	N2-C1-N4	-8.42	111.41	116.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	6	2204	PCY	N2-C1-N4	-8.07	111.64	116.83
87	6	2204	PCY	C18-C15-C7	-5.10	97.22	114.79
87	2	2178	PCY	C8-C17-N20	-4.72	104.32	112.80

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	2	1750/1800 (97%)	0.39	62 (3%) 42 8	54, 88, 172, 274	0
1	6	1795/1800 (99%)	0.44	94 (5%) 26 5	41, 74, 181, 278	0
2	S0	206/251 (82%)	0.31	4 (1%) 64 18	90, 107, 123, 157	0
2	s0	206/251 (82%)	0.06	3 (1%) 70 21	71, 91, 109, 115	0
3	S1	214/254 (84%)	0.74	31 (14%) 3 1	92, 120, 146, 154	0
3	s1	216/254 (85%)	0.73	17 (7%) 13 3	67, 85, 111, 126	0
4	S2	217/253 (85%)	0.39	12 (5%) 24 5	68, 86, 104, 124	0
4	s2	217/253 (85%)	0.33	7 (3%) 45 9	54, 71, 92, 113	0
5	S3	223/239 (93%)	0.48	13 (5%) 22 5	77, 90, 128, 147	0
5	s3	223/239 (93%)	0.62	24 (10%) 6 2	73, 105, 129, 136	0
6	S4	260/260 (100%)	0.95	31 (11%) 5 1	63, 87, 102, 127	0
6	s4	260/260 (100%)	0.54	8 (3%) 47 10	54, 71, 90, 129	0
7	S5	206/224 (91%)	0.70	20 (9%) 8 2	94, 115, 135, 147	0
7	s5	206/224 (91%)	0.35	8 (3%) 37 7	65, 91, 121, 140	0
8	S6	226/236 (95%)	0.80	28 (12%) 5 1	64, 103, 123, 151	0
8	s6	218/236 (92%)	0.45	4 (1%) 65 18	50, 78, 105, 136	0
9	S7	184/189 (97%)	0.54	7 (3%) 38 7	86, 115, 149, 159	0
9	s7	186/189 (98%)	0.18	4 (2%) 59 14	68, 100, 138, 150	0
10	S8	188/200 (94%)	1.10	27 (14%) 3 1	56, 71, 112, 133	0
10	s8	188/200 (94%)	0.85	13 (6%) 17 4	45, 64, 107, 123	0
11	S9	185/196 (94%)	0.89	20 (10%) 6 2	80, 96, 132, 165	0
11	s9	185/196 (94%)	0.38	7 (3%) 38 7	63, 77, 116, 147	0
12	C0	96/105 (91%)	0.35	1 (1%) 79 29	82, 105, 138, 158	0
12	c0	96/105 (91%)	1.35	26 (27%) 1 1	96, 131, 153, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	C1	155/155 (100%)	1.02	13 (8%)	11	3	56, 70, 131, 141	0
13	c1	146/155 (94%)	0.40	2 (1%)	72	22	47, 61, 100, 114	0
14	C2	124/142 (87%)	0.43	5 (4%)	36	7	134, 149, 169, 186	0
14	c2	124/142 (87%)	2.39	69 (55%)	0	0	177, 199, 225, 235	0
15	C3	150/150 (100%)	0.50	10 (6%)	17	4	65, 84, 102, 111	0
15	c3	150/150 (100%)	0.36	4 (2%)	52	11	56, 72, 91, 114	0
16	C4	127/136 (93%)	0.69	17 (13%)	4	1	66, 109, 128, 132	0
16	c4	128/136 (94%)	0.34	1 (0%)	83	35	51, 80, 92, 103	0
17	C5	124/141 (87%)	0.81	12 (9%)	8	2	81, 100, 142, 154	0
17	c5	135/141 (95%)	0.66	8 (5%)	22	5	73, 102, 139, 202	0
18	C6	141/142 (99%)	0.95	23 (16%)	2	1	80, 104, 112, 117	0
18	c6	142/142 (100%)	1.02	28 (19%)	2	1	64, 85, 104, 132	0
19	C7	120/136 (88%)	0.65	12 (10%)	8	2	89, 106, 134, 140	0
19	c7	117/136 (86%)	0.61	14 (11%)	5	1	77, 93, 118, 122	0
20	C8	145/145 (100%)	0.79	17 (11%)	5	2	79, 106, 131, 142	0
20	c8	145/145 (100%)	0.46	6 (4%)	35	7	70, 85, 110, 129	0
21	C9	143/143 (100%)	1.16	30 (20%)	1	1	88, 106, 124, 137	0
21	c9	143/143 (100%)	0.59	5 (3%)	42	8	61, 77, 100, 124	0
22	D0	107/120 (89%)	1.15	27 (25%)	1	1	73, 108, 153, 160	0
22	d0	110/120 (91%)	1.03	15 (13%)	4	1	67, 107, 155, 192	0
23	D1	87/87 (100%)	0.07	0	100	100	87, 94, 114, 129	0
23	d1	87/87 (100%)	-0.17	0	100	100	65, 76, 101, 116	0
24	D2	129/129 (100%)	1.23	17 (13%)	4	1	67, 80, 88, 100	0
24	d2	129/129 (100%)	0.42	2 (1%)	68	20	52, 61, 69, 78	0
25	D3	144/144 (100%)	0.65	4 (2%)	50	11	57, 66, 77, 93	0
25	d3	144/144 (100%)	0.40	0	100	100	45, 50, 65, 83	0
26	D4	134/134 (100%)	1.14	26 (19%)	2	1	75, 104, 123, 135	0
26	d4	134/134 (100%)	0.61	9 (6%)	17	4	56, 81, 98, 127	0
27	D5	70/107 (65%)	1.06	11 (15%)	3	1	110, 127, 137, 141	0
27	d5	69/107 (64%)	0.59	6 (8%)	10	3	80, 107, 126, 134	0
28	D6	97/97 (100%)	1.06	19 (19%)	2	1	72, 88, 136, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	d6	97/97 (100%)	0.50	4 (4%) 35 7	56, 68, 99, 109	0
29	D7	81/81 (100%)	0.85	13 (16%) 3 1	81, 95, 140, 146	0
29	d7	81/81 (100%)	0.64	7 (8%) 11 3	66, 84, 135, 138	0
30	D8	63/66 (95%)	1.18	13 (20%) 1 1	105, 126, 146, 166	0
30	d8	63/66 (95%)	0.57	5 (7%) 13 3	83, 101, 121, 130	0
31	D9	53/55 (96%)	0.73	3 (5%) 23 5	74, 81, 107, 116	0
31	d9	53/55 (96%)	1.21	8 (15%) 3 1	73, 81, 128, 144	0
32	E0	60/60 (100%)	0.93	7 (11%) 5 2	64, 96, 136, 145	0
33	E1	71/76 (93%)	0.46	7 (9%) 8 2	108, 129, 150, 160	0
33	e1	76/76 (100%)	1.59	23 (30%) 1 1	134, 164, 176, 179	0
34	SR	318/318 (100%)	0.40	13 (4%) 35 7	69, 113, 140, 159	0
34	sR	318/318 (100%)	0.63	31 (9%) 8 2	91, 113, 135, 158	0
35	SM	159/273 (58%)	0.45	9 (5%) 23 5	63, 90, 144, 149	0
35	sM	104/273 (38%)	0.32	3 (2%) 49 10	71, 102, 185, 195	0
36	1	3149/3396 (92%)	0.45	130 (4%) 35 7	29, 53, 141, 267	0
36	5	3150/3396 (92%)	0.40	92 (2%) 49 10	28, 52, 128, 273	0
37	3	121/121 (100%)	0.15	1 (0%) 83 35	42, 72, 90, 96	0
37	7	121/121 (100%)	0.04	0 100 100	34, 55, 67, 75	0
38	4	158/158 (100%)	0.35	3 (1%) 64 18	37, 54, 98, 137	0
38	8	158/158 (100%)	0.38	6 (3%) 38 7	41, 64, 108, 133	0
39	L2	252/253 (99%)	0.69	14 (5%) 24 5	33, 48, 67, 74	0
39	l2	252/253 (99%)	0.57	6 (2%) 56 13	36, 54, 76, 89	0
40	L3	386/386 (100%)	0.32	7 (1%) 65 18	34, 57, 72, 117	0
40	l3	386/386 (100%)	0.16	1 (0%) 91 58	28, 41, 56, 99	0
41	L4	361/361 (100%)	0.16	0 100 100	30, 45, 63, 77	0
41	l4	361/361 (100%)	0.07	1 (0%) 91 58	36, 53, 74, 91	0
42	L5	296/296 (100%)	0.48	11 (3%) 39 8	52, 80, 102, 126	0
42	l5	294/296 (99%)	0.33	2 (0%) 84 38	42, 59, 88, 138	0
43	L6	156/175 (89%)	0.22	0 100 100	39, 48, 71, 93	0
43	l6	157/175 (89%)	0.15	2 (1%) 74 24	42, 51, 73, 90	0
44	L7	222/243 (91%)	0.23	1 (0%) 88 46	34, 42, 79, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	l7	223/243 (91%)	0.15	0 100 100	30, 40, 85, 136	0
45	L8	233/255 (91%)	0.40	6 (2%) 53 11	54, 70, 111, 124	0
45	l8	231/255 (90%)	0.58	16 (6%) 17 4	69, 84, 113, 121	0
46	L9	191/191 (100%)	0.54	8 (4%) 35 7	52, 66, 82, 100	0
46	l9	191/191 (100%)	0.20	0 100 100	38, 45, 69, 107	0
47	M0	211/220 (95%)	0.46	7 (3%) 44 9	41, 58, 93, 116	0
47	m0	213/220 (96%)	0.46	6 (2%) 50 11	36, 54, 82, 100	0
48	M1	169/173 (97%)	0.36	5 (2%) 48 10	61, 85, 101, 114	0
48	m1	169/173 (97%)	0.16	1 (0%) 86 41	44, 65, 77, 93	0
49	M3	193/198 (97%)	0.57	11 (5%) 23 5	34, 54, 100, 125	0
49	m3	194/198 (97%)	0.45	5 (2%) 53 11	45, 66, 110, 137	0
50	M4	136/137 (99%)	-0.03	2 (1%) 70 21	45, 53, 68, 80	0
50	m4	137/137 (100%)	-0.01	0 100 100	36, 44, 65, 79	0
51	M5	203/203 (100%)	0.66	8 (3%) 37 7	33, 46, 58, 65	0
51	m5	203/203 (100%)	1.06	23 (11%) 6 2	43, 59, 72, 77	0
52	M6	197/198 (99%)	0.23	0 100 100	35, 44, 65, 69	0
52	m6	197/198 (99%)	0.11	0 100 100	28, 33, 62, 70	0
53	M7	183/183 (100%)	0.53	12 (6%) 18 4	37, 45, 123, 148	0
53	m7	155/183 (84%)	0.35	0 100 100	32, 41, 57, 87	0
54	M8	185/185 (100%)	0.43	4 (2%) 59 14	36, 45, 59, 72	0
54	m8	185/185 (100%)	0.37	2 (1%) 77 27	39, 51, 60, 67	0
55	M9	188/188 (100%)	0.75	21 (11%) 6 2	50, 67, 157, 165	0
55	m9	188/188 (100%)	0.46	8 (4%) 34 7	46, 62, 130, 144	0
56	N0	172/172 (100%)	0.25	2 (1%) 75 26	43, 51, 66, 73	0
56	n0	172/172 (100%)	0.12	1 (0%) 86 41	32, 40, 50, 67	0
57	N1	159/159 (100%)	0.41	2 (1%) 74 24	41, 51, 93, 101	0
57	n1	159/159 (100%)	0.39	1 (0%) 86 41	36, 44, 86, 97	0
58	N2	100/120 (83%)	0.64	8 (8%) 12 3	81, 100, 116, 131	0
58	n2	98/120 (81%)	1.16	17 (17%) 2 1	72, 88, 103, 109	0
59	N3	136/136 (100%)	0.49	5 (3%) 39 8	40, 51, 67, 82	0
59	n3	136/136 (100%)	0.39	2 (1%) 70 21	28, 40, 56, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
60	N4	98/155 (63%)	1.81	30 (30%)	1 1	52, 68, 167, 180	0
60	n4	135/155 (87%)	0.52	7 (5%)	26 5	40, 87, 138, 158	0
61	N5	121/141 (85%)	0.60	11 (9%)	9 2	46, 61, 81, 115	0
61	n5	120/141 (85%)	1.12	20 (16%)	2 1	52, 67, 89, 96	0
62	N6	126/126 (100%)	0.25	2 (1%)	68 20	40, 55, 68, 85	0
62	n6	126/126 (100%)	0.83	3 (2%)	56 13	49, 64, 81, 89	0
63	N7	135/135 (100%)	0.24	1 (0%)	84 38	70, 85, 99, 108	0
63	n7	135/135 (100%)	0.58	11 (8%)	12 3	78, 96, 117, 126	0
64	N8	148/148 (100%)	0.50	6 (4%)	35 7	27, 44, 72, 84	0
64	n8	148/148 (100%)	0.58	0	100 100	33, 53, 76, 80	0
65	N9	58/58 (100%)	0.58	4 (6%)	17 4	39, 55, 105, 116	0
65	n9	58/58 (100%)	0.63	3 (5%)	26 5	37, 56, 83, 92	0
66	O0	97/104 (93%)	0.11	1 (1%)	79 29	68, 78, 111, 117	0
66	o0	100/104 (96%)	0.49	4 (4%)	36 7	74, 85, 115, 124	0
67	O1	109/112 (97%)	0.38	2 (1%)	65 18	47, 61, 102, 118	0
67	o1	109/112 (97%)	0.10	1 (0%)	81 32	39, 52, 94, 118	0
68	O2	127/129 (98%)	0.41	1 (0%)	83 35	28, 42, 55, 76	0
68	o2	127/129 (98%)	0.55	3 (2%)	56 13	30, 49, 66, 88	0
69	O3	106/106 (100%)	0.49	1 (0%)	81 32	34, 41, 67, 78	0
69	o3	106/106 (100%)	0.81	11 (10%)	7 2	31, 39, 71, 87	0
70	O4	112/120 (93%)	0.90	12 (10%)	6 2	47, 66, 111, 123	0
70	o4	112/120 (93%)	0.84	9 (8%)	12 3	46, 70, 116, 128	0
71	O5	119/119 (100%)	0.49	3 (2%)	54 12	43, 65, 71, 75	0
71	o5	119/119 (100%)	0.58	7 (5%)	22 5	56, 71, 83, 88	0
72	O6	99/99 (100%)	0.50	2 (2%)	62 17	49, 63, 97, 118	0
72	o6	99/99 (100%)	0.63	4 (4%)	36 7	61, 75, 99, 124	0
73	O7	87/87 (100%)	0.67	3 (3%)	43 9	33, 41, 79, 106	0
73	o7	87/87 (100%)	0.65	3 (3%)	43 9	41, 46, 85, 122	0
74	O8	77/77 (100%)	0.71	4 (5%)	26 5	72, 88, 110, 122	0
74	o8	77/77 (100%)	0.32	2 (2%)	53 11	75, 92, 108, 113	0
75	O9	50/50 (100%)	0.62	2 (4%)	36 7	43, 49, 55, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
75	o9	50/50 (100%)	0.82	5 (10%) 8 2	51, 54, 66, 72	0
76	Q0	52/52 (100%)	0.31	1 (1%) 64 18	49, 59, 85, 96	0
76	q0	52/52 (100%)	0.25	1 (1%) 64 18	34, 40, 54, 66	0
77	Q1	25/25 (100%)	1.80	11 (44%) 1 0	52, 55, 59, 67	0
77	q1	25/25 (100%)	1.75	8 (32%) 1 1	43, 48, 62, 69	0
78	Q2	105/105 (100%)	0.27	0 100 100	39, 56, 86, 124	0
78	q2	105/105 (100%)	0.32	0 100 100	45, 57, 87, 120	0
79	Q3	91/91 (100%)	0.56	6 (6%) 18 4	42, 54, 74, 89	0
79	q3	91/91 (100%)	0.43	3 (3%) 44 9	40, 55, 74, 84	0
80	e0	62/62 (100%)	0.14	2 (3%) 45 9	59, 77, 119, 141	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	0.38	5 (3%) 42 8	88, 107, 193, 202	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35346 (93%)	0.50	1704 (5%) 26 5	27, 68, 134, 278	0

The worst 5 of 1704 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	76	VAL	13.7
60	N4	69	LYS	12.5
36	1	1572	U	11.1
33	e1	77	GLY	11.0
1	6	493	U	10.7

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
85	MG	5	3861	1/1	0.54	663.00	60,60,60,60	0
85	MG	2	2003	1/1	0.39	503.00	118,118,118,118	0
85	MG	5	3501	1/1	0.29	235.00	44,44,44,44	0
85	MG	2	1952	1/1	0.54	208.00	95,95,95,95	0
85	MG	1	3859	1/1	0.64	193.00	131,131,131,131	0
85	MG	7	214	1/1	0.49	187.00	51,51,51,51	0
85	MG	5	3485	1/1	0.37	178.00	47,47,47,47	0
85	MG	5	3769	1/1	0.81	164.43	111,111,111,111	0
85	MG	1	3500	1/1	0.34	157.00	75,75,75,75	0
85	MG	5	3410	1/1	0.41	133.95	54,54,54,54	0
85	MG	1	3578	1/1	0.58	129.85	34,34,34,34	0
85	MG	6	1944	1/1	0.51	120.90	59,59,59,59	0
85	MG	6	2013	1/1	0.51	120.60	150,150,150,150	0
85	MG	6	1924	1/1	0.44	119.50	95,95,95,95	0
85	MG	5	3852	1/1	0.51	102.00	59,59,59,59	0
85	MG	1	3785	1/1	1.60	99.84	43,43,43,43	0
85	MG	5	3632	1/1	0.43	98.11	86,86,86,86	0
85	MG	5	3859	1/1	0.44	96.00	77,77,77,77	0
85	MG	1	3852	1/1	0.46	76.77	60,60,60,60	0
85	MG	6	2028	1/1	0.55	75.35	80,80,80,80	0
85	MG	5	3851	1/1	0.52	72.80	58,58,58,58	0
85	MG	1	3725	1/1	1.39	70.29	40,40,40,40	0
85	MG	1	3696	1/1	0.34	66.50	64,64,64,64	0
85	MG	5	3481	1/1	0.41	62.25	57,57,57,57	0
85	MG	6	2018	1/1	0.67	62.07	59,59,59,59	0
85	MG	5	3780	1/1	0.49	57.10	83,83,83,83	0
85	MG	6	2045	1/1	0.28	55.50	78,78,78,78	0
85	MG	1	3665	1/1	0.40	54.07	75,75,75,75	0
85	MG	1	3854	1/1	1.11	53.97	93,93,93,93	0
86	OHX	6	2182	7/7	0.51	53.77	154,154,154,154	0
85	MG	6	1994	1/1	0.72	51.84	46,46,46,46	0
85	MG	1	3493	1/1	0.39	51.67	74,74,74,74	0
85	MG	5	3756	1/1	0.56	49.62	49,49,49,49	0
85	MG	6	1945	1/1	0.47	49.00	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3804	1/1	0.83	44.02	42,42,42,42	0
85	MG	1	3815	1/1	0.80	43.00	128,128,128,128	0
85	MG	5	3648	1/1	0.34	42.71	54,54,54,54	0
85	MG	5	3764	1/1	1.60	42.32	45,45,45,45	0
85	MG	5	3734	1/1	0.36	41.60	71,71,71,71	0
85	MG	6	1920	1/1	0.40	39.60	61,61,61,61	0
85	MG	2	1904	1/1	0.56	37.48	74,74,74,74	0
85	MG	5	3576	1/1	0.43	37.44	42,42,42,42	0
85	MG	2	1994	1/1	0.34	37.22	98,98,98,98	0
85	MG	3	202	1/1	0.33	36.75	46,46,46,46	0
85	MG	5	3683	1/1	0.50	36.06	36,36,36,36	0
85	MG	5	3658	1/1	0.35	36.00	47,47,47,47	0
85	MG	2	1957	1/1	0.47	35.84	80,80,80,80	0
85	MG	1	3727	1/1	0.84	35.31	35,35,35,35	0
85	MG	5	3874	1/1	0.54	33.94	54,54,54,54	0
85	MG	6	1940	1/1	0.57	32.23	85,85,85,85	0
85	MG	1	3861	1/1	0.38	31.31	53,53,53,53	0
85	MG	3	204	1/1	0.60	30.66	57,57,57,57	0
85	MG	7	207	1/1	0.23	30.33	56,56,56,56	0
85	MG	5	3618	1/1	0.38	29.74	52,52,52,52	0
85	MG	1	3773	1/1	0.46	27.99	57,57,57,57	0
85	MG	5	3823	1/1	1.21	27.94	45,45,45,45	0
85	MG	5	3791	1/1	1.20	26.72	55,55,55,55	0
85	MG	6	2039	1/1	0.55	26.60	94,94,94,94	0
85	MG	1	3796	1/1	1.11	26.34	39,39,39,39	0
85	MG	1	3758	1/1	0.59	26.31	61,61,61,61	0
85	MG	1	3546	1/1	0.33	25.75	68,68,68,68	0
85	MG	6	2040	1/1	0.46	25.57	53,53,53,53	0
85	MG	5	3582	1/1	0.29	25.35	34,34,34,34	0
85	MG	5	3433	1/1	0.39	23.42	85,85,85,85	0
85	MG	1	3444	1/1	0.49	23.18	67,67,67,67	0
85	MG	5	3760	1/1	0.50	23.01	57,57,57,57	0
85	MG	7	206	1/1	0.30	22.86	43,43,43,43	0
85	MG	5	3763	1/1	0.86	22.79	41,41,41,41	0
85	MG	5	3811	1/1	0.56	22.59	45,45,45,45	0
85	MG	1	3823	1/1	0.94	22.57	45,45,45,45	0
85	MG	1	3858	1/1	1.12	22.51	74,74,74,74	0
85	MG	5	3444	1/1	0.31	22.27	40,40,40,40	0
85	MG	1	3670	1/1	0.86	22.24	54,54,54,54	0
85	MG	L7	303	1/1	0.51	22.23	56,56,56,56	0
85	MG	1	4219	1/1	1.25	21.49	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	2	1978	1/1	0.29	21.13	93,93,93,93	0
85	MG	2	1981	1/1	0.47	21.07	62,62,62,62	0
85	MG	1	3592	1/1	0.27	21.00	53,53,53,53	0
85	MG	6	2008	1/1	0.63	20.99	49,49,49,49	0
85	MG	1	3813	1/1	0.25	20.41	52,52,52,52	0
85	MG	5	3877	1/1	0.53	20.18	46,46,46,46	0
85	MG	5	3443	1/1	0.58	19.99	37,37,37,37	0
85	MG	1	4215	1/1	0.94	19.79	42,42,42,42	0
85	MG	1	3856	1/1	0.70	19.67	67,67,67,67	0
85	MG	5	3520	1/1	0.34	19.67	42,42,42,42	0
85	MG	1	3735	1/1	0.39	19.60	64,64,64,64	0
85	MG	7	205	1/1	0.43	19.57	30,30,30,30	0
85	MG	1	3645	1/1	0.31	19.55	42,42,42,42	0
85	MG	o1	201	1/1	2.80	19.43	85,85,85,85	0
85	MG	1	3803	1/1	0.93	19.31	38,38,38,38	0
85	MG	2	1962	1/1	0.37	19.19	130,130,130,130	0
85	MG	5	3790	1/1	1.34	19.09	58,58,58,58	0
85	MG	5	3796	1/1	1.04	19.05	50,50,50,50	0
85	MG	4	201	1/1	0.40	19.00	43,43,43,43	0
85	MG	5	3722	1/1	0.91	18.87	49,49,49,49	0
85	MG	5	3556	1/1	0.31	18.60	42,42,42,42	0
85	MG	6	1931	1/1	0.54	18.55	65,65,65,65	0
85	MG	2	1913	1/1	0.47	18.45	79,79,79,79	0
85	MG	1	3533	1/1	0.59	18.34	38,38,38,38	0
85	MG	5	3678	1/1	0.46	18.32	97,97,97,97	0
85	MG	3	207	1/1	0.34	18.32	70,70,70,70	0
85	MG	3	209	1/1	0.40	18.20	69,69,69,69	0
85	MG	17	302	1/1	0.42	18.12	40,40,40,40	0
85	MG	2	1926	1/1	0.46	17.98	91,91,91,91	0
85	MG	5	3847	1/1	0.34	17.90	42,42,42,42	0
85	MG	5	3403	1/1	0.43	17.59	54,54,54,54	0
85	MG	1	3706	1/1	0.36	17.53	63,63,63,63	0
85	MG	1	3572	1/1	0.53	17.14	27,27,27,27	0
85	MG	8	211	1/1	0.58	17.11	68,68,68,68	0
85	MG	5	3621	1/1	0.37	17.06	49,49,49,49	0
85	MG	1	3702	1/1	0.27	17.00	51,51,51,51	0
85	MG	5	3887	1/1	0.45	16.82	58,58,58,58	0
85	MG	8	210	1/1	0.97	16.69	54,54,54,54	0
85	MG	5	3588	1/1	0.52	16.49	51,51,51,51	0
85	MG	1	3695	1/1	0.30	16.48	47,47,47,47	0
85	MG	5	3883	1/1	0.50	16.43	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3811	1/1	0.23	16.39	51,51,51,51	0
85	MG	6	1953	1/1	0.54	16.35	62,62,62,62	0
85	MG	2	1965	1/1	0.30	16.04	86,86,86,86	0
85	MG	5	3848	1/1	0.89	15.96	37,37,37,37	0
85	MG	1	3817	1/1	0.63	15.85	50,50,50,50	0
85	MG	c7	201	1/1	0.49	15.77	73,73,73,73	0
85	MG	1	3502	1/1	0.50	15.47	41,41,41,41	0
85	MG	5	3584	1/1	0.44	15.44	29,29,29,29	0
85	MG	5	3761	1/1	0.35	15.25	77,77,77,77	0
85	MG	1	3771	1/1	0.29	15.19	52,52,52,52	0
85	MG	5	3713	1/1	1.21	15.15	43,43,43,43	0
86	OHX	2	2158	7/7	0.36	15.08	167,167,167,167	0
85	MG	5	3532	1/1	0.34	15.07	36,36,36,36	0
85	MG	1	3610	1/1	0.31	15.05	41,41,41,41	0
86	OHX	1	4161	7/7	0.29	14.99	160,160,160,160	0
85	MG	5	3817	1/1	0.34	14.94	65,65,65,65	0
85	MG	5	3596	1/1	0.46	14.90	21,21,21,21	0
85	MG	5	3751	1/1	0.41	14.79	48,48,48,48	0
85	MG	l3	402	1/1	1.24	14.76	37,37,37,37	0
85	MG	5	3575	1/1	0.40	14.72	26,26,26,26	0
85	MG	6	1971	1/1	0.45	14.68	65,65,65,65	0
85	MG	2	1949	1/1	0.56	14.65	82,82,82,82	0
85	MG	1	3509	1/1	0.43	14.62	44,44,44,44	0
85	MG	N5	201	1/1	0.33	14.62	70,70,70,70	0
85	MG	8	203	1/1	0.32	14.25	40,40,40,40	0
85	MG	1	3540	1/1	0.35	14.20	54,54,54,54	0
85	MG	l5	301	1/1	0.42	14.17	67,67,67,67	0
85	MG	7	204	1/1	0.36	13.95	63,63,63,63	0
85	MG	5	3477	1/1	0.30	13.84	56,56,56,56	0
85	MG	4	220	1/1	0.53	13.67	82,82,82,82	0
85	MG	6	1934	1/1	0.34	13.60	72,72,72,72	0
85	MG	5	3884	1/1	0.38	13.46	83,83,83,83	0
85	MG	2	1918	1/1	0.47	13.32	55,55,55,55	0
85	MG	5	3655	1/1	0.41	13.22	66,66,66,66	0
85	MG	6	1966	1/1	0.37	13.04	82,82,82,82	0
85	MG	5	3506	1/1	0.33	13.03	36,36,36,36	0
85	MG	5	3497	1/1	0.60	13.01	43,43,43,43	0
85	MG	1	3713	1/1	0.56	12.81	46,46,46,46	0
85	MG	2	1970	1/1	0.35	12.78	69,69,69,69	0
85	MG	5	3854	1/1	0.41	12.73	66,66,66,66	0
85	MG	5	3536	1/1	0.46	12.66	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3812	1/1	0.41	12.60	49,49,49,49	0
85	MG	5	3471	1/1	0.49	12.53	39,39,39,39	0
85	MG	2	1914	1/1	0.38	12.44	71,71,71,71	0
85	MG	1	3591	1/1	0.47	12.34	53,53,53,53	0
85	MG	1	3485	1/1	0.37	12.23	43,43,43,43	0
85	MG	2	1980	1/1	0.59	12.23	68,68,68,68	0
85	MG	6	2012	1/1	0.50	12.14	70,70,70,70	0
85	MG	1	3409	1/1	0.38	12.09	31,31,31,31	0
85	MG	1	3683	1/1	0.30	11.98	52,52,52,52	0
85	MG	6	2017	1/1	0.33	11.94	47,47,47,47	0
85	MG	5	3876	1/1	0.45	11.88	63,63,63,63	0
85	MG	5	3767	1/1	0.50	11.88	45,45,45,45	0
85	MG	1	3682	1/1	0.41	11.81	40,40,40,40	0
85	MG	6	1943	1/1	0.39	11.73	38,38,38,38	0
85	MG	5	3709	1/1	0.48	11.73	45,45,45,45	0
85	MG	2	1983	1/1	0.30	11.63	71,71,71,71	0
85	MG	5	3720	1/1	0.39	11.53	63,63,63,63	0
85	MG	1	3565	1/1	0.40	11.49	29,29,29,29	0
85	MG	4	214	1/1	0.69	11.40	47,47,47,47	0
85	MG	1	3607	1/1	0.35	11.35	78,78,78,78	0
85	MG	5	3644	1/1	0.28	11.31	57,57,57,57	0
85	MG	2	1956	1/1	0.44	11.29	65,65,65,65	0
85	MG	5	3577	1/1	0.29	11.24	38,38,38,38	0
85	MG	8	202	1/1	0.33	11.22	71,71,71,71	0
85	MG	6	1954	1/1	0.34	11.22	45,45,45,45	0
85	MG	1	3470	1/1	0.42	11.11	51,51,51,51	0
85	MG	1	3700	1/1	0.50	11.10	50,50,50,50	0
85	MG	6	1933	1/1	0.41	10.95	65,65,65,65	0
85	MG	5	4254	1/1	1.20	10.94	29,29,29,29	0
85	MG	1	3402	1/1	0.42	10.90	56,56,56,56	0
85	MG	1	3841	1/1	0.39	10.89	45,45,45,45	0
85	MG	5	3836	1/1	0.35	10.86	39,39,39,39	0
85	MG	7	201	1/1	0.47	10.85	40,40,40,40	0
85	MG	1	3722	1/1	0.39	10.76	48,48,48,48	0
85	MG	1	3711	1/1	0.36	10.53	81,81,81,81	0
85	MG	1	3820	1/1	0.25	10.52	53,53,53,53	0
85	MG	5	3562	1/1	0.36	10.45	20,20,20,20	0
85	MG	6	1918	1/1	0.40	10.38	64,64,64,64	0
85	MG	6	2044	1/1	0.47	10.32	81,81,81,81	0
85	MG	5	3553	1/1	0.39	10.31	47,47,47,47	0
85	MG	1	3537	1/1	0.37	10.29	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3541	1/1	0.36	10.24	34,34,34,34	0
86	OHX	1	4175	7/7	0.45	10.23	134,134,134,134	0
85	MG	5	3737	1/1	0.33	10.06	36,36,36,36	0
85	MG	5	4253	1/1	1.28	10.05	45,45,45,45	0
85	MG	n0	201	1/1	0.59	10.03	42,42,42,42	0
85	MG	1	3647	1/1	0.45	10.01	51,51,51,51	0
85	MG	2	1969	1/1	0.36	9.92	66,66,66,66	0
85	MG	6	2016	1/1	0.63	9.88	30,30,30,30	0
85	MG	1	3857	1/1	0.30	9.69	46,46,46,46	0
85	MG	5	3571	1/1	0.40	9.68	21,21,21,21	0
85	MG	1	3847	1/1	0.30	9.61	54,54,54,54	0
85	MG	5	3686	1/1	0.46	9.59	63,63,63,63	0
85	MG	2	1958	1/1	0.43	9.55	98,98,98,98	0
85	MG	5	3448	1/1	0.36	9.51	52,52,52,52	0
85	MG	1	3447	1/1	0.28	9.47	47,47,47,47	0
85	MG	5	3882	1/1	0.33	9.46	32,32,32,32	0
85	MG	5	3649	1/1	0.60	9.44	43,43,43,43	0
85	MG	5	3736	1/1	0.23	9.39	53,53,53,53	0
85	MG	5	3607	1/1	0.33	9.37	51,51,51,51	0
85	MG	5	3783	1/1	0.35	9.37	60,60,60,60	0
85	MG	6	2020	1/1	0.58	9.23	91,91,91,91	0
85	MG	5	3546	1/1	0.35	9.22	45,45,45,45	0
85	MG	1	3598	1/1	0.48	9.22	14,14,14,14	0
85	MG	5	3445	1/1	0.26	9.18	40,40,40,40	0
86	OHX	1	4206	7/7	0.55	9.17	137,137,137,137	0
85	MG	6	2024	1/1	0.62	9.11	66,66,66,66	0
85	MG	5	3634	1/1	0.29	9.11	36,36,36,36	0
85	MG	5	3863	1/1	0.42	9.10	42,42,42,42	0
85	MG	5	3673	1/1	0.71	9.08	32,32,32,32	0
85	MG	5	3488	1/1	0.41	9.04	33,33,33,33	0
85	MG	6	1947	1/1	0.44	9.03	52,52,52,52	0
85	MG	5	3735	1/1	0.56	8.95	42,42,42,42	0
85	MG	6	1987	1/1	0.30	8.90	48,48,48,48	0
85	MG	1	3648	1/1	0.51	8.81	46,46,46,46	0
85	MG	3	213	1/1	0.41	8.77	58,58,58,58	0
85	MG	1	3635	1/1	0.40	8.72	72,72,72,72	0
85	MG	2	2019	1/1	0.42	8.72	73,73,73,73	0
85	MG	1	3538	1/1	0.24	8.66	40,40,40,40	0
85	MG	2	1959	1/1	0.49	8.57	66,66,66,66	0
85	MG	d3	202	1/1	1.21	8.49	54,54,54,54	0
85	MG	6	1991	1/1	0.37	8.46	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3775	1/1	0.61	8.45	30,30,30,30	0
85	MG	8	206	1/1	0.33	8.43	51,51,51,51	0
85	MG	1	3477	1/1	0.39	8.32	52,52,52,52	0
85	MG	1	3716	1/1	0.42	8.30	36,36,36,36	0
85	MG	5	3598	1/1	0.48	8.26	28,28,28,28	0
86	OHX	5	4228	7/7	0.36	8.26	130,130,130,130	0
86	OHX	1	4185	7/7	0.25	8.25	190,190,190,190	0
85	MG	1	3561	1/1	0.35	8.24	25,25,25,25	0
85	MG	1	3818	1/1	0.29	8.21	64,64,64,64	0
85	MG	1	3662	1/1	0.70	8.17	53,53,53,53	0
85	MG	6	1928	1/1	0.43	8.17	74,74,74,74	0
85	MG	1	3724	1/1	0.41	8.06	65,65,65,65	0
85	MG	1	3463	1/1	0.41	8.04	25,25,25,25	0
85	MG	5	3684	1/1	0.61	8.02	35,35,35,35	0
85	MG	6	1908	1/1	0.35	7.86	49,49,49,49	0
85	MG	6	2041	1/1	0.39	7.85	68,68,68,68	0
85	MG	6	2027	1/1	0.43	7.77	55,55,55,55	0
85	MG	3	214	1/1	0.47	7.76	64,64,64,64	0
85	MG	5	3524	1/1	0.34	7.70	31,31,31,31	0
85	MG	6	1917	1/1	0.33	7.69	57,57,57,57	0
85	MG	2	2022	1/1	0.78	7.65	102,102,102,102	0
85	MG	5	3860	1/1	0.39	7.60	88,88,88,88	0
85	MG	6	2032	1/1	0.49	7.54	51,51,51,51	0
85	MG	5	3875	1/1	0.35	7.51	45,45,45,45	0
85	MG	2	1992	1/1	0.71	7.45	56,56,56,56	0
86	OHX	14	403	7/7	0.37	7.42	156,156,156,156	0
85	MG	2	1919	1/1	0.42	7.34	76,76,76,76	0
85	MG	5	3675	1/1	0.30	7.29	39,39,39,39	0
85	MG	1	3524	1/1	0.53	7.24	43,43,43,43	0
86	OHX	1	4176	7/7	0.34	7.15	163,163,163,163	0
85	MG	1	3802	1/1	0.57	7.14	64,64,64,64	0
85	MG	6	1936	1/1	0.29	7.10	72,72,72,72	0
86	OHX	5	4160	7/7	0.40	7.10	137,137,137,137	0
85	MG	5	3608	1/1	0.27	7.02	31,31,31,31	0
85	MG	5	3866	1/1	0.25	7.00	54,54,54,54	0
85	MG	1	3795	1/1	0.26	6.98	54,54,54,54	0
85	MG	6	2010	1/1	0.25	6.97	56,56,56,56	0
85	MG	5	3518	1/1	0.43	6.89	26,26,26,26	0
85	MG	1	3831	1/1	0.32	6.88	24,24,24,24	0
85	MG	3	206	1/1	0.31	6.88	36,36,36,36	0
85	MG	4	204	1/1	0.30	6.87	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3672	1/1	0.25	6.85	49,49,49,49	0
85	MG	2	1986	1/1	0.37	6.81	103,103,103,103	0
86	OHX	5	4219	7/7	0.43	6.79	140,140,140,140	0
85	MG	6	1901	1/1	0.35	6.76	42,42,42,42	0
86	OHX	1	4188	7/7	0.40	6.73	146,146,146,146	0
85	MG	8	201	1/1	0.31	6.67	52,52,52,52	0
85	MG	1	3555	1/1	0.35	6.65	36,36,36,36	0
85	MG	7	203	1/1	0.33	6.61	57,57,57,57	0
85	MG	1	3747	1/1	0.30	6.56	50,50,50,50	0
85	MG	5	3647	1/1	0.33	6.53	38,38,38,38	0
85	MG	4	216	1/1	0.23	6.51	61,61,61,61	0
85	MG	5	3654	1/1	0.77	6.49	43,43,43,43	0
86	OHX	5	4239	7/7	0.30	6.47	158,158,158,158	0
85	MG	5	3635	1/1	0.42	6.46	81,81,81,81	0
85	MG	1	3787	1/1	0.81	6.44	28,28,28,28	0
85	MG	1	3691	1/1	0.49	6.43	42,42,42,42	0
85	MG	2	2014	1/1	0.40	6.43	61,61,61,61	0
85	MG	6	1942	1/1	0.46	6.41	32,32,32,32	0
85	MG	1	3618	1/1	0.28	6.27	59,59,59,59	0
85	MG	5	3710	1/1	0.32	6.25	91,91,91,91	0
86	OHX	1	4187	7/7	0.28	6.24	138,138,138,138	0
85	MG	5	3512	1/1	0.35	6.24	58,58,58,58	0
85	MG	6	1916	1/1	0.31	6.20	52,52,52,52	0
85	MG	2	1945	1/1	0.27	6.19	89,89,89,89	0
86	OHX	5	4188	7/7	0.45	6.14	126,126,126,126	0
85	MG	5	3464	1/1	0.34	6.12	88,88,88,88	0
85	MG	1	3631	1/1	0.29	6.03	40,40,40,40	0
85	MG	5	3889	1/1	0.28	6.02	65,65,65,65	0
85	MG	5	3781	1/1	0.30	6.00	82,82,82,82	0
85	MG	1	3420	1/1	0.23	5.99	83,83,83,83	0
86	OHX	6	2126	7/7	0.40	5.97	116,116,116,116	0
85	MG	3	201	1/1	0.35	5.94	78,78,78,78	0
85	MG	1	3668	1/1	0.27	5.92	82,82,82,82	0
85	MG	1	3836	1/1	0.30	5.92	34,34,34,34	0
85	MG	5	3815	1/1	0.24	5.90	89,89,89,89	0
85	MG	1	3469	1/1	0.32	5.90	56,56,56,56	0
85	MG	1	3793	1/1	0.66	5.88	41,41,41,41	0
85	MG	5	3561	1/1	0.35	5.85	26,26,26,26	0
86	OHX	1	4207	7/7	0.43	5.81	144,144,144,144	0
85	MG	1	3611	1/1	0.22	5.78	43,43,43,43	0
85	MG	1	3784	1/1	0.32	5.74	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	2	1973	1/1	0.35	5.66	73,73,73,73	0
85	MG	m7	203	1/1	0.73	5.66	51,51,51,51	0
85	MG	5	3770	1/1	0.37	5.64	71,71,71,71	0
85	MG	1	3723	1/1	0.21	5.60	43,43,43,43	0
85	MG	1	3850	1/1	0.28	5.56	45,45,45,45	0
85	MG	1	3778	1/1	0.36	5.55	46,46,46,46	0
85	MG	1	3545	1/1	0.27	5.50	52,52,52,52	0
85	MG	2	1976	1/1	0.32	5.47	88,88,88,88	0
85	MG	5	3878	1/1	0.26	5.44	51,51,51,51	0
85	MG	5	3409	1/1	0.33	5.43	44,44,44,44	0
85	MG	1	3615	1/1	0.42	5.40	36,36,36,36	0
85	MG	2	1925	1/1	0.43	5.38	65,65,65,65	0
85	MG	2	2007	1/1	0.44	5.35	74,74,74,74	0
85	MG	5	3742	1/1	0.31	5.34	35,35,35,35	0
85	MG	1	3411	1/1	0.28	5.30	44,44,44,44	0
85	MG	1	3718	1/1	0.26	5.27	56,56,56,56	0
85	MG	2	2001	1/1	0.31	5.27	78,78,78,78	0
85	MG	N8	202	1/1	0.38	5.27	32,32,32,32	0
85	MG	5	3652	1/1	0.39	5.24	63,63,63,63	0
85	MG	N8	204	1/1	1.08	5.22	38,38,38,38	0
85	MG	1	3506	1/1	0.36	5.21	32,32,32,32	0
85	MG	2	1921	1/1	0.41	5.20	54,54,54,54	0
86	OHX	5	4170	7/7	0.33	5.20	142,142,142,142	0
85	MG	1	3475	1/1	0.28	5.20	74,74,74,74	0
85	MG	1	3529	1/1	0.33	5.18	33,33,33,33	0
86	OHX	4	237	7/7	0.40	5.16	144,144,144,144	0
85	MG	2	1903	1/1	0.32	5.16	41,41,41,41	0
85	MG	6	1965	1/1	0.43	5.16	66,66,66,66	0
85	MG	1	3844	1/1	0.37	5.10	59,59,59,59	0
85	MG	L7	302	1/1	0.52	5.10	42,42,42,42	0
85	MG	5	3465	1/1	0.27	5.09	36,36,36,36	0
85	MG	5	3738	1/1	0.33	5.08	67,67,67,67	0
85	MG	1	3535	1/1	0.34	5.07	45,45,45,45	0
85	MG	1	3628	1/1	0.32	5.05	70,70,70,70	0
85	MG	5	3681	1/1	0.34	5.02	39,39,39,39	0
85	MG	1	3414	1/1	0.27	4.99	59,59,59,59	0
86	OHX	5	4235	7/7	0.31	4.95	154,154,154,154	0
85	MG	1	3526	1/1	0.31	4.91	26,26,26,26	0
85	MG	1	3779	1/1	0.31	4.90	50,50,50,50	0
85	MG	5	3623	1/1	0.34	4.87	66,66,66,66	0
85	MG	1	3523	1/1	0.33	4.87	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	3887	7/7	0.23	4.86	79,79,79,79	0
85	MG	5	3594	1/1	0.29	4.83	41,41,41,41	0
85	MG	6	1968	1/1	0.41	4.80	58,58,58,58	0
85	MG	5	3872	1/1	0.37	4.79	40,40,40,40	0
85	MG	1	3543	1/1	0.35	4.76	39,39,39,39	0
85	MG	5	3560	1/1	0.30	4.76	36,36,36,36	0
86	OHX	2	2143	7/7	0.29	4.75	138,138,138,138	0
85	MG	1	3614	1/1	0.35	4.75	43,43,43,43	0
85	MG	5	3437	1/1	0.34	4.73	61,61,61,61	0
85	MG	2	1953	1/1	0.29	4.72	104,104,104,104	0
85	MG	1	3822	1/1	0.17	4.68	58,58,58,58	0
85	MG	1	3563	1/1	0.32	4.68	42,42,42,42	0
85	MG	5	3470	1/1	0.26	4.60	44,44,44,44	0
85	MG	5	3825	1/1	0.23	4.59	63,63,63,63	0
85	MG	5	3529	1/1	0.31	4.57	29,29,29,29	0
85	MG	6	1925	1/1	0.40	4.57	36,36,36,36	0
85	MG	1	3805	1/1	0.63	4.56	190,190,190,190	0
86	OHX	5	3933	7/7	0.20	4.53	94,94,94,94	0
86	OHX	5	4176	7/7	0.34	4.53	148,148,148,148	0
86	OHX	1	4210	7/7	0.50	4.51	135,135,135,135	0
85	MG	2	2010	1/1	0.34	4.49	73,73,73,73	0
85	MG	1	3667	1/1	0.28	4.48	53,53,53,53	0
86	OHX	6	2054	7/7	0.23	4.48	85,85,85,85	0
85	MG	1	3689	1/1	0.25	4.48	60,60,60,60	0
85	MG	1	3658	1/1	0.35	4.47	47,47,47,47	0
85	MG	5	3530	1/1	0.34	4.45	28,28,28,28	0
85	MG	5	3620	1/1	0.22	4.39	41,41,41,41	0
85	MG	6	1906	1/1	0.38	4.37	47,47,47,47	0
85	MG	6	2029	1/1	0.26	4.37	105,105,105,105	0
86	OHX	1	3917	7/7	0.25	4.37	118,118,118,118	0
85	MG	4	210	1/1	0.22	4.35	58,58,58,58	0
85	MG	8	207	1/1	0.41	4.35	44,44,44,44	0
85	MG	2	1967	1/1	0.60	4.32	106,106,106,106	0
86	OHX	1	4140	7/7	0.26	4.30	147,147,147,147	0
85	MG	5	3505	1/1	0.33	4.30	26,26,26,26	0
85	MG	1	3624	1/1	0.58	4.30	82,82,82,82	0
85	MG	1	3525	1/1	0.30	4.27	26,26,26,26	0
85	MG	1	3552	1/1	0.40	4.27	31,31,31,31	0
85	MG	1	3649	1/1	0.30	4.21	69,69,69,69	0
85	MG	7	202	1/1	0.28	4.19	27,27,27,27	0
86	OHX	5	4221	7/7	0.26	4.18	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	1959	1/1	0.27	4.18	51,51,51,51	0
85	MG	5	3674	1/1	0.22	4.16	69,69,69,69	0
85	MG	1	3429	1/1	0.37	4.12	42,42,42,42	0
85	MG	1	3761	1/1	0.47	4.11	51,51,51,51	0
86	OHX	1	4014	7/7	0.25	4.10	165,165,165,165	0
85	MG	5	3864	1/1	0.27	4.10	47,47,47,47	0
85	MG	1	3570	1/1	0.33	4.09	42,42,42,42	0
85	MG	2	1955	1/1	0.34	4.08	54,54,54,54	0
86	OHX	2	2170	7/7	0.29	4.08	154,154,154,154	0
86	OHX	6	2185	7/7	0.34	4.06	152,152,152,152	0
85	MG	5	3538	1/1	0.35	4.06	42,42,42,42	0
85	MG	5	3776	1/1	0.27	4.05	66,66,66,66	0
85	MG	1	3547	1/1	0.37	4.03	50,50,50,50	0
85	MG	5	3564	1/1	0.29	4.01	31,31,31,31	0
85	MG	5	3585	1/1	0.41	4.01	31,31,31,31	0
85	MG	M1	201	1/1	0.38	3.99	78,78,78,78	0
86	OHX	1	4124	7/7	0.44	3.98	127,127,127,127	0
86	OHX	5	4182	7/7	0.26	3.96	145,145,145,145	0
86	OHX	1	4061	7/7	0.27	3.95	141,141,141,141	0
85	MG	5	3748	1/1	0.31	3.94	48,48,48,48	0
85	MG	5	3605	1/1	0.53	3.92	31,31,31,31	0
85	MG	1	3832	1/1	0.36	3.91	62,62,62,62	0
85	MG	2	1988	1/1	0.26	3.90	96,96,96,96	0
85	MG	1	3751	1/1	0.38	3.89	44,44,44,44	0
85	MG	l3	401	1/1	0.46	3.89	27,27,27,27	0
85	MG	6	2001	1/1	0.70	3.82	82,82,82,82	0
85	MG	1	3459	1/1	0.26	3.82	62,62,62,62	0
85	MG	5	3503	1/1	0.34	3.82	32,32,32,32	0
85	MG	1	3680	1/1	0.48	3.81	58,58,58,58	0
85	MG	5	3803	1/1	0.39	3.80	40,40,40,40	0
85	MG	1	3675	1/1	0.31	3.80	60,60,60,60	0
85	MG	3	205	1/1	0.29	3.80	37,37,37,37	0
86	OHX	1	3890	7/7	0.22	3.79	74,74,74,74	0
85	MG	5	3821	1/1	0.49	3.79	60,60,60,60	0
85	MG	5	3603	1/1	0.28	3.78	42,42,42,42	0
85	MG	5	3579	1/1	0.30	3.76	32,32,32,32	0
85	MG	1	3636	1/1	0.51	3.75	46,46,46,46	0
85	MG	5	3522	1/1	0.33	3.74	41,41,41,41	0
85	MG	5	3555	1/1	0.36	3.74	46,46,46,46	0
85	MG	6	1997	1/1	0.27	3.73	59,59,59,59	0
86	OHX	5	4231	7/7	0.31	3.73	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	2	1996	1/1	0.21	3.72	96,96,96,96	0
85	MG	5	3504	1/1	0.30	3.72	52,52,52,52	0
86	OHX	1	4200	7/7	0.25	3.71	148,148,148,148	0
85	MG	4	218	1/1	0.24	3.71	40,40,40,40	0
85	MG	2	1938	1/1	0.32	3.70	66,66,66,66	0
85	MG	2	1963	1/1	0.30	3.68	94,94,94,94	0
85	MG	5	3490	1/1	0.68	3.68	50,50,50,50	0
85	MG	1	3741	1/1	0.36	3.67	44,44,44,44	0
85	MG	5	3772	1/1	0.61	3.64	31,31,31,31	0
86	OHX	5	4153	7/7	0.31	3.63	124,124,124,124	0
85	MG	5	3716	1/1	0.26	3.59	51,51,51,51	0
85	MG	m5	302	1/1	0.57	3.56	60,60,60,60	0
85	MG	1	3730	1/1	0.22	3.53	86,86,86,86	0
85	MG	5	3570	1/1	0.36	3.53	29,29,29,29	0
85	MG	m7	205	1/1	0.73	3.52	34,34,34,34	0
85	MG	5	3669	1/1	0.34	3.52	33,33,33,33	0
85	MG	1	3406	1/1	0.57	3.51	96,96,96,96	0
85	MG	5	3540	1/1	0.36	3.51	28,28,28,28	0
85	MG	S2	301	1/1	0.41	3.50	52,52,52,52	0
86	OHX	6	2203	7/7	0.26	3.50	157,157,157,157	0
86	OHX	5	4179	7/7	0.47	3.50	119,119,119,119	0
85	MG	1	3521	1/1	0.34	3.49	74,74,74,74	0
85	MG	1	3605	1/1	0.45	3.48	57,57,57,57	0
85	MG	1	3410	1/1	0.29	3.46	22,22,22,22	0
85	MG	6	1946	1/1	0.32	3.44	64,64,64,64	0
86	OHX	5	3908	7/7	0.23	3.42	62,62,62,62	0
85	MG	5	3572	1/1	0.32	3.39	41,41,41,41	0
85	MG	5	3682	1/1	0.39	3.38	81,81,81,81	0
85	MG	5	3554	1/1	0.36	3.37	35,35,35,35	0
85	MG	1	3855	1/1	0.30	3.36	44,44,44,44	0
85	MG	5	3665	1/1	0.38	3.35	58,58,58,58	0
85	MG	5	3573	1/1	0.27	3.33	31,31,31,31	0
85	MG	N8	201	1/1	0.39	3.33	31,31,31,31	0
85	MG	5	3614	1/1	0.21	3.32	34,34,34,34	0
85	MG	1	3824	1/1	0.23	3.31	45,45,45,45	0
85	MG	4	209	1/1	0.28	3.30	53,53,53,53	0
85	MG	1	3677	1/1	0.29	3.29	46,46,46,46	0
86	OHX	1	4165	7/7	0.25	3.29	127,127,127,127	0
86	OHX	2	2162	7/7	0.27	3.25	159,159,159,159	0
85	MG	5	3696	1/1	0.28	3.24	76,76,76,76	0
85	MG	1	3621	1/1	0.26	3.24	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3717	1/1	0.43	3.21	57,57,57,57	0
85	MG	5	3486	1/1	0.28	3.20	56,56,56,56	0
85	MG	5	3425	1/1	0.30	3.20	46,46,46,46	0
86	OHX	M7	205	7/7	0.52	3.16	124,124,124,124	0
85	MG	s2	301	1/1	0.58	3.12	53,53,53,53	0
85	MG	6	2011	1/1	0.34	3.11	51,51,51,51	0
85	MG	1	3629	1/1	0.38	3.10	41,41,41,41	0
86	OHX	1	4169	7/7	0.36	3.10	181,181,181,181	0
85	MG	5	3550	1/1	0.33	3.08	50,50,50,50	0
85	MG	6	2037	1/1	0.59	3.08	58,58,58,58	0
85	MG	5	3438	1/1	0.26	3.07	32,32,32,32	0
85	MG	5	3549	1/1	0.40	3.07	44,44,44,44	0
85	MG	4	203	1/1	0.28	3.07	45,45,45,45	0
86	OHX	6	2159	7/7	0.40	3.06	140,140,140,140	0
85	MG	6	2009	1/1	0.24	3.05	55,55,55,55	0
86	OHX	M7	206	7/7	0.33	3.04	142,142,142,142	0
86	OHX	1	4183	7/7	0.26	3.03	140,140,140,140	0
85	MG	o3	201	1/1	0.46	3.02	37,37,37,37	0
85	MG	7	209	1/1	0.27	3.01	42,42,42,42	0
85	MG	1	3413	1/1	0.29	2.98	47,47,47,47	0
85	MG	2	2006	1/1	0.43	2.96	64,64,64,64	0
86	OHX	5	3940	7/7	0.24	2.96	88,88,88,88	0
85	MG	6	1967	1/1	0.32	2.94	81,81,81,81	0
85	MG	M6	202	1/1	0.49	2.93	65,65,65,65	0
85	MG	5	3894	1/1	0.25	2.92	61,61,61,61	0
85	MG	2	1935	1/1	0.35	2.91	50,50,50,50	0
86	OHX	6	2180	7/7	0.33	2.91	147,147,147,147	0
85	MG	6	1904	1/1	0.33	2.91	68,68,68,68	0
85	MG	5	3844	1/1	0.48	2.90	59,59,59,59	0
85	MG	5	3493	1/1	0.30	2.89	45,45,45,45	0
85	MG	2	2004	1/1	0.29	2.88	87,87,87,87	0
85	MG	1	3782	1/1	0.26	2.87	64,64,64,64	0
85	MG	6	1929	1/1	0.28	2.86	57,57,57,57	0
85	MG	5	3664	1/1	0.40	2.85	57,57,57,57	0
86	OHX	1	4139	7/7	0.25	2.85	137,137,137,137	0
85	MG	5	3695	1/1	0.26	2.84	42,42,42,42	0
85	MG	6	1948	1/1	0.34	2.84	41,41,41,41	0
85	MG	5	3809	1/1	0.24	2.83	100,100,100,100	0
85	MG	5	3829	1/1	0.68	2.82	36,36,36,36	0
85	MG	5	3752	1/1	0.23	2.82	41,41,41,41	0
86	OHX	6	2179	7/7	0.39	2.81	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4237	7/7	0.24	2.81	168,168,168,168	0
85	MG	2	1951	1/1	0.24	2.79	97,97,97,97	0
86	OHX	1	4196	7/7	0.32	2.78	139,139,139,139	0
85	MG	5	3693	1/1	0.25	2.77	44,44,44,44	0
85	MG	2	1974	1/1	0.44	2.76	86,86,86,86	0
86	OHX	2	2147	7/7	0.34	2.74	130,130,130,130	0
85	MG	1	3451	1/1	0.29	2.73	47,47,47,47	0
85	MG	5	3671	1/1	0.40	2.73	34,34,34,34	0
86	OHX	1	4208	7/7	0.30	2.73	137,137,137,137	0
85	MG	1	3842	1/1	0.26	2.72	59,59,59,59	0
85	MG	2	2015	1/1	0.36	2.72	61,61,61,61	0
85	MG	1	3791	1/1	0.41	2.71	31,31,31,31	0
86	OHX	5	3952	7/7	0.21	2.69	109,109,109,109	0
85	MG	5	3467	1/1	0.25	2.68	114,114,114,114	0
86	OHX	1	4138	7/7	0.38	2.68	124,124,124,124	0
85	MG	d3	201	1/1	0.37	2.67	48,48,48,48	0
85	MG	5	3462	1/1	0.39	2.67	42,42,42,42	0
85	MG	M9	201	1/1	0.31	2.67	68,68,68,68	0
86	OHX	6	2167	7/7	0.39	2.64	128,128,128,128	0
85	MG	5	3843	1/1	0.41	2.64	42,42,42,42	0
85	MG	5	3461	1/1	0.34	2.63	53,53,53,53	0
85	MG	1	3678	1/1	0.26	2.63	36,36,36,36	0
85	MG	N8	203	1/1	0.65	2.63	50,50,50,50	0
86	OHX	5	3967	7/7	0.21	2.62	106,106,106,106	0
85	MG	5	3899	1/1	0.31	2.61	47,47,47,47	0
85	MG	6	2007	1/1	0.30	2.60	55,55,55,55	0
85	MG	6	1911	1/1	0.33	2.59	82,82,82,82	0
85	MG	6	1937	1/1	0.28	2.56	41,41,41,41	0
85	MG	5	3432	1/1	0.27	2.55	42,42,42,42	0
86	OHX	1	4213	7/7	0.33	2.52	159,159,159,159	0
86	OHX	5	4246	7/7	0.24	2.51	154,154,154,154	0
85	MG	m1	202	1/1	0.27	2.48	64,64,64,64	0
85	MG	1	3798	1/1	0.32	2.47	60,60,60,60	0
85	MG	5	3563	1/1	0.43	2.45	35,35,35,35	0
85	MG	5	3794	1/1	0.27	2.44	36,36,36,36	0
85	MG	sM	302	1/1	0.51	2.43	51,51,51,51	0
86	OHX	1	4209	7/7	0.39	2.42	133,133,133,133	0
85	MG	1	3527	1/1	0.39	2.40	32,32,32,32	0
85	MG	6	1922	1/1	0.34	2.37	52,52,52,52	0
86	OHX	5	3915	7/7	0.24	2.37	66,66,66,66	0
85	MG	1	3738	1/1	0.30	2.37	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3891	1/1	0.32	2.36	38,38,38,38	0
85	MG	5	3799	1/1	0.29	2.36	42,42,42,42	0
85	MG	1	3585	1/1	0.34	2.33	51,51,51,51	0
86	OHX	5	4245	7/7	0.32	2.32	167,167,167,167	0
85	MG	4	202	1/1	0.38	2.32	49,49,49,49	0
85	MG	1	3666	1/1	0.40	2.32	56,56,56,56	0
85	MG	2	1908	1/1	0.26	2.31	73,73,73,73	0
86	OHX	1	4126	7/7	0.28	2.31	155,155,155,155	0
86	OHX	1	4146	7/7	0.26	2.29	144,144,144,144	0
86	OHX	1	4110	7/7	0.27	2.29	155,155,155,155	0
86	OHX	6	2164	7/7	0.25	2.28	160,160,160,160	0
85	MG	1	3497	1/1	0.24	2.26	41,41,41,41	0
85	MG	1	3586	1/1	0.33	2.25	38,38,38,38	0
86	OHX	5	4247	7/7	0.35	2.24	152,152,152,152	0
86	OHX	5	4013	7/7	0.18	2.23	149,149,149,149	0
85	MG	5	3870	1/1	0.99	2.22	39,39,39,39	0
85	MG	5	3428	1/1	0.27	2.21	29,29,29,29	0
85	MG	5	3610	1/1	0.29	2.21	31,31,31,31	0
86	OHX	5	3901	7/7	0.24	2.20	49,49,49,49	0
86	OHX	5	4154	7/7	0.47	2.19	130,130,130,130	0
85	MG	6	1923	1/1	0.21	2.19	68,68,68,68	0
85	MG	1	3443	1/1	0.23	2.18	82,82,82,82	0
85	MG	5	3826	1/1	0.39	2.17	46,46,46,46	0
86	OHX	6	2173	7/7	0.33	2.16	138,138,138,138	0
86	OHX	5	3949	7/7	0.24	2.16	100,100,100,100	0
85	MG	5	3595	1/1	0.36	2.15	37,37,37,37	0
85	MG	1	3801	1/1	0.28	2.13	62,62,62,62	0
86	OHX	5	4187	7/7	0.26	2.12	133,133,133,133	0
86	OHX	1	3869	7/7	0.23	2.11	60,60,60,60	0
86	OHX	5	4222	7/7	0.25	2.10	186,186,186,186	0
86	OHX	1	3900	7/7	0.21	2.10	84,84,84,84	0
85	MG	1	3623	1/1	0.23	2.10	56,56,56,56	0
86	OHX	6	2188	7/7	0.29	2.08	148,148,148,148	0
85	MG	6	1907	1/1	0.29	2.08	70,70,70,70	0
85	MG	Q2	502	1/1	0.28	2.07	75,75,75,75	0
85	MG	5	3739	1/1	0.28	2.07	29,29,29,29	0
86	OHX	1	4111	7/7	0.43	2.07	128,128,128,128	0
86	OHX	5	4180	7/7	0.25	2.07	161,161,161,161	0
85	MG	5	3814	1/1	0.20	2.06	50,50,50,50	0
86	OHX	5	4041	7/7	0.21	2.04	164,164,164,164	0
85	MG	1	3620	1/1	0.26	2.02	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	6	2170	7/7	0.32	2.01	119,119,119,119	0
86	OHX	2	2135	7/7	0.31	2.01	147,147,147,147	0
86	OHX	1	4118	7/7	0.42	2.01	123,123,123,123	0
86	OHX	1	3876	7/7	0.20	2.00	67,67,67,67	0
85	MG	5	3441	1/1	0.26	2.00	33,33,33,33	0
86	OHX	5	3950	7/7	0.19	2.00	103,103,103,103	0
85	MG	5	3631	1/1	0.25	1.98	47,47,47,47	0
85	MG	1	3697	1/1	0.33	1.98	74,74,74,74	0
85	MG	1	3458	1/1	0.27	1.94	40,40,40,40	0
85	MG	5	3704	1/1	0.19	1.94	64,64,64,64	0
85	MG	1	3472	1/1	0.60	1.94	38,38,38,38	0
85	MG	2	1936	1/1	0.29	1.93	55,55,55,55	0
85	MG	1	3637	1/1	0.31	1.93	62,62,62,62	0
85	MG	5	3831	1/1	0.28	1.91	49,49,49,49	0
86	OHX	2	2092	7/7	0.27	1.91	150,150,150,150	0
85	MG	2	1977	1/1	0.48	1.90	72,72,72,72	0
86	OHX	5	4249	7/7	0.23	1.89	163,163,163,163	0
86	OHX	1	4194	7/7	0.18	1.88	146,146,146,146	0
86	OHX	5	3902	7/7	0.23	1.88	47,47,47,47	0
85	MG	5	3601	1/1	0.23	1.88	42,42,42,42	0
86	OHX	5	4162	7/7	0.26	1.86	121,121,121,121	0
85	MG	2	1961	1/1	0.28	1.85	81,81,81,81	0
85	MG	M3	201	1/1	0.58	1.83	48,48,48,48	0
85	MG	1	3602	1/1	0.41	1.83	39,39,39,39	0
85	MG	1	3560	1/1	0.27	1.82	36,36,36,36	0
86	OHX	5	3913	7/7	0.20	1.81	65,65,65,65	0
85	MG	1	3431	1/1	0.27	1.80	43,43,43,43	0
85	MG	1	3515	1/1	0.33	1.78	34,34,34,34	0
86	OHX	5	4206	7/7	0.52	1.78	158,158,158,158	0
85	MG	5	3697	1/1	0.30	1.78	45,45,45,45	0
85	MG	2	1905	1/1	0.31	1.78	62,62,62,62	0
85	MG	2	2017	1/1	0.36	1.77	85,85,85,85	0
85	MG	1	3517	1/1	0.30	1.77	33,33,33,33	0
86	OHX	1	3871	7/7	0.24	1.76	68,68,68,68	0
85	MG	8	204	1/1	0.31	1.73	40,40,40,40	0
85	MG	2	1979	1/1	0.35	1.73	53,53,53,53	0
85	MG	2	1931	1/1	0.36	1.73	59,59,59,59	0
85	MG	5	3755	1/1	0.21	1.72	58,58,58,58	0
85	MG	5	3606	1/1	0.22	1.72	38,38,38,38	0
85	MG	1	3715	1/1	0.23	1.71	70,70,70,70	0
86	OHX	5	4017	7/7	0.19	1.69	161,161,161,161	0
86	OHX	5	4196	7/7	0.30	1.69	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	N6	201	1/1	0.28	1.69	51,51,51,51	0
85	MG	6	1985	1/1	0.42	1.67	48,48,48,48	0
86	OHX	5	4211	7/7	0.30	1.66	124,124,124,124	0
85	MG	1	3430	1/1	0.31	1.66	47,47,47,47	0
86	OHX	5	4111	7/7	0.23	1.65	145,145,145,145	0
85	MG	5	3646	1/1	0.28	1.65	55,55,55,55	0
85	MG	5	3574	1/1	0.31	1.64	35,35,35,35	0
85	MG	l5	302	1/1	0.30	1.63	64,64,64,64	0
85	MG	1	3481	1/1	0.27	1.62	41,41,41,41	0
86	OHX	8	229	7/7	0.20	1.61	138,138,138,138	0
85	MG	2	2011	1/1	0.38	1.60	63,63,63,63	0
85	MG	5	3757	1/1	0.22	1.60	60,60,60,60	0
85	MG	1	3764	1/1	0.23	1.60	58,58,58,58	0
85	MG	5	3813	1/1	0.85	1.60	42,42,42,42	0
85	MG	5	3435	1/1	0.26	1.60	35,35,35,35	0
85	MG	5	3566	1/1	0.38	1.60	37,37,37,37	0
86	OHX	1	3863	7/7	0.24	1.57	47,47,47,47	0
85	MG	6	2030	1/1	0.28	1.56	73,73,73,73	0
85	MG	1	3513	1/1	0.32	1.56	26,26,26,26	0
85	MG	1	3617	1/1	0.28	1.56	45,45,45,45	0
85	MG	2	1972	1/1	0.27	1.55	72,72,72,72	0
85	MG	1	3712	1/1	0.31	1.55	36,36,36,36	0
85	MG	M7	203	1/1	0.66	1.54	40,40,40,40	0
86	OHX	5	3900	7/7	0.24	1.54	51,51,51,51	0
85	MG	2	1937	1/1	0.32	1.53	61,61,61,61	0
85	MG	1	3632	1/1	0.35	1.53	75,75,75,75	0
85	MG	1	3657	1/1	0.28	1.52	47,47,47,47	0
86	OHX	1	4141	7/7	0.35	1.51	133,133,133,133	0
86	OHX	4	223	7/7	0.23	1.51	67,67,67,67	0
85	MG	5	3778	1/1	0.32	1.51	81,81,81,81	0
85	MG	1	3539	1/1	0.34	1.50	25,25,25,25	0
85	MG	5	3466	1/1	0.27	1.49	37,37,37,37	0
85	MG	1	3710	1/1	0.47	1.48	53,53,53,53	0
85	MG	5	3523	1/1	0.28	1.47	38,38,38,38	0
85	MG	5	3531	1/1	0.32	1.47	33,33,33,33	0
85	MG	2	1987	1/1	0.76	1.46	72,72,72,72	0
85	MG	2	1934	1/1	0.34	1.46	58,58,58,58	0
85	MG	5	3568	1/1	0.26	1.46	30,30,30,30	0
85	MG	6	1919	1/1	0.36	1.45	43,43,43,43	0
85	MG	1	3849	1/1	0.24	1.45	58,58,58,58	0
85	MG	1	3456	1/1	0.32	1.45	62,62,62,62	0
85	MG	5	3551	1/1	0.28	1.44	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3766	1/1	0.25	1.43	61,61,61,61	0
85	MG	1	3640	1/1	0.22	1.42	42,42,42,42	0
85	MG	6	1903	1/1	0.29	1.42	47,47,47,47	0
85	MG	5	3414	1/1	0.29	1.42	31,31,31,31	0
85	MG	1	3650	1/1	0.37	1.42	100,100,100,100	0
85	MG	5	3416	1/1	0.35	1.41	36,36,36,36	0
85	MG	5	3578	1/1	0.37	1.40	37,37,37,37	0
85	MG	7	210	1/1	0.22	1.39	64,64,64,64	0
86	OHX	1	4093	7/7	0.20	1.38	138,138,138,138	0
86	OHX	2	2156	7/7	0.32	1.38	129,129,129,129	0
85	MG	4	215	1/1	0.26	1.38	70,70,70,70	0
86	OHX	1	4170	7/7	0.29	1.38	151,151,151,151	0
86	OHX	1	4202	7/7	0.31	1.36	144,144,144,144	0
86	OHX	6	2120	7/7	0.24	1.36	122,122,122,122	0
85	MG	2	1909	1/1	0.35	1.35	65,65,65,65	0
85	MG	1	3568	1/1	0.29	1.35	27,27,27,27	0
85	MG	5	3569	1/1	0.33	1.35	32,32,32,32	0
85	MG	5	3897	1/1	0.30	1.35	66,66,66,66	0
86	OHX	o7	503	7/7	0.29	1.34	142,142,142,142	0
85	MG	1	3418	1/1	0.25	1.34	44,44,44,44	0
86	OHX	1	3947	7/7	0.21	1.34	118,118,118,118	0
85	MG	n3	201	1/1	0.35	1.33	26,26,26,26	0
86	OHX	6	2202	7/7	0.42	1.33	155,155,155,155	0
86	OHX	1	3866	7/7	0.26	1.32	59,59,59,59	0
85	MG	2	1968	1/1	0.27	1.31	79,79,79,79	0
85	MG	5	3724	1/1	0.30	1.31	40,40,40,40	0
86	OHX	5	3904	7/7	0.26	1.28	58,58,58,58	0
86	OHX	4	238	7/7	0.31	1.27	145,145,145,145	0
85	MG	4	217	1/1	0.33	1.27	41,41,41,41	0
85	MG	L7	301	1/1	0.25	1.26	39,39,39,39	0
85	MG	1	3749	1/1	0.22	1.26	55,55,55,55	0
85	MG	1	3687	1/1	0.22	1.25	53,53,53,53	0
86	OHX	5	4139	7/7	0.34	1.25	137,137,137,137	0
86	OHX	8	232	7/7	0.36	1.25	152,152,152,152	0
86	OHX	1	3912	7/7	0.18	1.25	105,105,105,105	0
85	MG	5	3558	1/1	0.44	1.25	53,53,53,53	0
85	MG	5	3474	1/1	0.24	1.25	79,79,79,79	0
85	MG	5	3723	1/1	0.22	1.24	53,53,53,53	0
86	OHX	1	4201	7/7	0.50	1.24	148,148,148,148	0
86	OHX	5	4113	7/7	0.32	1.23	117,117,117,117	0
86	OHX	6	2189	7/7	0.21	1.22	150,150,150,150	0
85	MG	1	3486	1/1	0.27	1.21	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3403	1/1	0.28	1.21	37,37,37,37	0
85	MG	1	3455	1/1	0.47	1.21	55,55,55,55	0
85	MG	5	3893	1/1	0.21	1.20	73,73,73,73	0
85	MG	5	3537	1/1	0.31	1.19	36,36,36,36	0
85	MG	1	3471	1/1	0.27	1.18	40,40,40,40	0
86	OHX	5	3910	7/7	0.24	1.18	71,71,71,71	0
85	MG	6	1981	1/1	0.66	1.17	50,50,50,50	0
85	MG	1	3551	1/1	0.30	1.17	35,35,35,35	0
85	MG	5	3698	1/1	0.28	1.16	51,51,51,51	0
86	OHX	1	4044	7/7	0.37	1.16	120,120,120,120	0
86	OHX	1	4068	7/7	0.34	1.15	127,127,127,127	0
85	MG	1	3685	1/1	0.43	1.12	38,38,38,38	0
86	OHX	1	3946	7/7	0.19	1.11	127,127,127,127	0
85	MG	2	2013	1/1	0.26	1.11	58,58,58,58	0
86	OHX	1	4071	7/7	0.45	1.10	113,113,113,113	0
86	OHX	8	231	7/7	0.27	1.10	138,138,138,138	0
86	OHX	5	4220	7/7	0.18	1.10	185,185,185,185	0
86	OHX	2	2159	7/7	0.42	1.09	145,145,145,145	0
85	MG	2	1999	1/1	0.28	1.09	71,71,71,71	0
85	MG	q0	202	1/1	0.27	1.09	52,52,52,52	0
85	MG	2	1946	1/1	0.45	1.09	60,60,60,60	0
85	MG	s8	301	1/1	0.43	1.09	50,50,50,50	0
86	OHX	1	4212	7/7	0.30	1.08	146,146,146,146	0
85	MG	5	3597	1/1	0.31	1.08	32,32,32,32	0
86	OHX	5	3989	7/7	0.20	1.07	121,121,121,121	0
86	OHX	1	4137	7/7	0.30	1.05	146,146,146,146	0
85	MG	1	3816	1/1	0.20	1.05	38,38,38,38	0
85	MG	1	3582	1/1	0.26	1.05	32,32,32,32	0
86	OHX	6	2084	7/7	0.19	1.04	131,131,131,131	0
85	MG	1	3653	1/1	0.34	1.03	47,47,47,47	0
85	MG	m7	201	1/1	0.33	1.02	32,32,32,32	0
85	MG	5	3865	1/1	0.39	1.02	38,38,38,38	0
85	MG	1	3579	1/1	0.28	1.01	40,40,40,40	0
85	MG	l8	301	1/1	0.35	1.01	73,73,73,73	0
85	MG	1	3853	1/1	0.30	1.01	28,28,28,28	0
85	MG	5	3690	1/1	0.26	0.99	62,62,62,62	0
86	OHX	5	4204	7/7	0.21	0.98	151,151,151,151	0
86	OHX	6	2190	7/7	0.33	0.98	179,179,179,179	0
86	OHX	2	2104	7/7	0.24	0.97	156,156,156,156	0
86	OHX	1	4198	7/7	0.23	0.96	137,137,137,137	0
85	MG	1	3556	1/1	0.24	0.96	53,53,53,53	0
85	MG	5	3430	1/1	0.24	0.96	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2000	1/1	0.25	0.96	57,57,57,57	0
85	MG	7	212	1/1	0.19	0.94	51,51,51,51	0
86	OHX	5	3998	7/7	0.19	0.94	120,120,120,120	0
85	MG	1	3809	1/1	0.23	0.94	49,49,49,49	0
85	MG	8	212	1/1	0.41	0.94	43,43,43,43	0
85	MG	4	212	1/1	0.29	0.93	39,39,39,39	0
86	OHX	4	235	7/7	0.20	0.93	161,161,161,161	0
85	MG	d6	102	1/1	0.53	0.93	53,53,53,53	0
85	MG	5	3840	1/1	0.24	0.92	47,47,47,47	0
85	MG	1	3731	1/1	0.23	0.92	59,59,59,59	0
86	OHX	5	4105	7/7	0.38	0.92	111,111,111,111	0
85	MG	6	1909	1/1	0.36	0.92	107,107,107,107	0
85	MG	1	3721	1/1	0.29	0.90	55,55,55,55	0
85	MG	5	3663	1/1	0.23	0.90	48,48,48,48	0
86	OHX	5	4142	7/7	0.24	0.89	142,142,142,142	0
85	MG	1	3655	1/1	0.27	0.88	41,41,41,41	0
85	MG	1	3587	1/1	0.28	0.88	25,25,25,25	0
85	MG	5	3685	1/1	0.48	0.88	52,52,52,52	0
85	MG	1	3613	1/1	0.28	0.88	35,35,35,35	0
85	MG	1	3714	1/1	0.39	0.88	49,49,49,49	0
85	MG	2	1943	1/1	0.23	0.87	67,67,67,67	0
85	MG	1	3830	1/1	0.26	0.86	37,37,37,37	0
85	MG	5	3715	1/1	0.21	0.86	52,52,52,52	0
85	MG	5	3547	1/1	0.32	0.86	46,46,46,46	0
86	OHX	1	3877	7/7	0.21	0.83	70,70,70,70	0
85	MG	5	3499	1/1	0.29	0.82	40,40,40,40	0
85	MG	5	3662	1/1	0.23	0.82	36,36,36,36	0
85	MG	1	3595	1/1	0.32	0.82	25,25,25,25	0
86	OHX	6	2177	7/7	0.25	0.81	149,149,149,149	0
85	MG	5	3731	1/1	0.24	0.81	47,47,47,47	0
85	MG	1	3760	1/1	0.22	0.81	47,47,47,47	0
85	MG	1	3757	1/1	0.22	0.81	39,39,39,39	0
85	MG	2	1928	1/1	0.27	0.79	79,79,79,79	0
85	MG	5	3402	1/1	0.32	0.78	30,30,30,30	0
85	MG	1	3755	1/1	0.39	0.78	33,33,33,33	0
85	MG	1	3516	1/1	0.35	0.77	39,39,39,39	0
85	MG	2	2016	1/1	0.30	0.77	63,63,63,63	0
86	OHX	1	4168	7/7	0.25	0.77	165,165,165,165	0
85	MG	5	3645	1/1	0.21	0.76	40,40,40,40	0
85	MG	5	3839	1/1	0.28	0.76	39,39,39,39	0
85	MG	14	401	1/1	0.43	0.75	38,38,38,38	0
85	MG	5	3726	1/1	0.26	0.75	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	8	215	1/1	0.33	0.75	51,51,51,51	0
85	MG	1	3562	1/1	0.24	0.75	48,48,48,48	0
85	MG	n3	202	1/1	0.37	0.74	45,45,45,45	0
85	MG	1	3588	1/1	0.27	0.73	31,31,31,31	0
86	OHX	1	4158	7/7	0.18	0.73	162,162,162,162	0
85	MG	5	3869	1/1	0.62	0.72	40,40,40,40	0
86	OHX	6	2156	7/7	0.24	0.72	144,144,144,144	0
85	MG	5	3659	1/1	0.23	0.72	49,49,49,49	0
86	OHX	1	3940	7/7	0.20	0.72	112,112,112,112	0
85	MG	5	3613	1/1	0.35	0.71	34,34,34,34	0
86	OHX	1	4163	7/7	0.27	0.71	137,137,137,137	0
85	MG	5	3758	1/1	0.37	0.70	56,56,56,56	0
85	MG	5	4255	1/1	0.32	0.69	28,28,28,28	0
85	MG	6	2036	1/1	0.26	0.68	56,56,56,56	0
85	MG	2	2002	1/1	0.21	0.68	80,80,80,80	0
85	MG	1	3499	1/1	0.26	0.67	63,63,63,63	0
85	MG	M5	302	1/1	0.46	0.67	54,54,54,54	0
85	MG	2	2179	1/1	0.47	0.67	69,69,69,69	0
85	MG	1	3422	1/1	0.29	0.67	32,32,32,32	0
85	MG	5	3496	1/1	0.27	0.66	32,32,32,32	0
86	OHX	6	2070	7/7	0.18	0.66	111,111,111,111	0
85	MG	1	3594	1/1	0.28	0.66	24,24,24,24	0
85	MG	M6	201	1/1	0.27	0.66	47,47,47,47	0
86	OHX	1	4131	7/7	0.26	0.65	132,132,132,132	0
86	OHX	5	4133	7/7	0.23	0.64	132,132,132,132	0
86	OHX	2	2085	7/7	0.27	0.64	130,130,130,130	0
85	MG	6	1927	1/1	0.24	0.64	47,47,47,47	0
86	OHX	3	225	7/7	0.22	0.63	139,139,139,139	0
86	OHX	5	4092	7/7	0.28	0.63	125,125,125,125	0
85	MG	1	3573	1/1	0.24	0.63	39,39,39,39	0
85	MG	1	3478	1/1	0.24	0.62	47,47,47,47	0
85	MG	6	1972	1/1	0.23	0.62	53,53,53,53	0
85	MG	1	3704	1/1	0.23	0.62	63,63,63,63	0
85	MG	5	3801	1/1	0.25	0.62	78,78,78,78	0
85	MG	SM	301	1/1	0.24	0.60	57,57,57,57	0
85	MG	1	3729	1/1	0.30	0.60	57,57,57,57	0
85	MG	1	3676	1/1	0.24	0.59	43,43,43,43	0
85	MG	1	3606	1/1	0.33	0.59	52,52,52,52	0
86	OHX	1	4167	7/7	0.23	0.59	124,124,124,124	0
85	MG	5	3835	1/1	0.26	0.58	42,42,42,42	0
85	MG	5	3782	1/1	0.32	0.58	84,84,84,84	0
86	OHX	1	4181	7/7	0.26	0.58	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	5	3519	1/1	0.30	0.57	31,31,31,31	0
85	MG	6	1982	1/1	0.41	0.57	54,54,54,54	0
86	OHX	5	4216	7/7	0.28	0.57	152,152,152,152	0
85	MG	1	3554	1/1	0.35	0.55	25,25,25,25	0
85	MG	1	3404	1/1	0.45	0.55	54,54,54,54	0
85	MG	5	3845	1/1	0.22	0.54	50,50,50,50	0
85	MG	1	3609	1/1	0.20	0.54	45,45,45,45	0
85	MG	1	3501	1/1	0.29	0.54	27,27,27,27	0
85	MG	5	3721	1/1	0.23	0.54	56,56,56,56	0
86	OHX	2	2069	7/7	0.16	0.53	150,150,150,150	0
85	MG	5	3830	1/1	0.24	0.52	26,26,26,26	0
86	OHX	m7	206	7/7	0.40	0.52	131,131,131,131	0
85	MG	1	3596	1/1	0.29	0.52	23,23,23,23	0
85	MG	5	3858	1/1	0.34	0.52	53,53,53,53	0
85	MG	M7	204	1/1	0.36	0.51	66,66,66,66	0
85	MG	1	3644	1/1	0.26	0.51	70,70,70,70	0
85	MG	1	3522	1/1	0.30	0.50	33,33,33,33	0
86	OHX	1	3893	7/7	0.25	0.49	81,81,81,81	0
85	MG	5	3689	1/1	0.18	0.49	48,48,48,48	0
86	OHX	2	2172	7/7	0.23	0.49	172,172,172,172	0
85	MG	1	3597	1/1	0.31	0.48	44,44,44,44	0
85	MG	5	3548	1/1	0.23	0.48	50,50,50,50	0
85	MG	1	3821	1/1	0.28	0.47	40,40,40,40	0
86	OHX	7	215	7/7	0.22	0.46	91,91,91,91	0
86	OHX	6	2146	7/7	0.22	0.46	119,119,119,119	0
85	MG	1	3783	1/1	0.24	0.46	51,51,51,51	0
86	OHX	5	4234	7/7	0.38	0.45	162,162,162,162	0
85	MG	5	3407	1/1	0.19	0.45	39,39,39,39	0
86	OHX	5	4224	7/7	0.26	0.44	136,136,136,136	0
85	MG	M7	202	1/1	0.36	0.44	35,35,35,35	0
85	MG	1	3619	1/1	0.19	0.44	70,70,70,70	0
86	OHX	1	4192	7/7	0.18	0.43	178,178,178,178	0
85	MG	1	3432	1/1	0.26	0.42	39,39,39,39	0
85	MG	1	3759	1/1	0.22	0.42	37,37,37,37	0
86	OHX	2	2176	7/7	0.35	0.42	153,153,153,153	0
86	OHX	1	3965	7/7	0.19	0.42	131,131,131,131	0
85	MG	1	3720	1/1	0.25	0.42	61,61,61,61	0
85	MG	5	3807	1/1	0.20	0.41	163,163,163,163	0
85	MG	1	3460	1/1	0.26	0.41	35,35,35,35	0
85	MG	6	1980	1/1	0.23	0.41	71,71,71,71	0
85	MG	5	3517	1/1	0.28	0.41	23,23,23,23	0
85	MG	2	1923	1/1	0.28	0.40	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3770	1/1	0.19	0.40	53,53,53,53	0
85	MG	2	1929	1/1	0.31	0.40	66,66,66,66	0
85	MG	1	3671	1/1	0.36	0.39	50,50,50,50	0
85	MG	1	3416	1/1	0.35	0.39	51,51,51,51	0
85	MG	2	1917	1/1	0.33	0.39	55,55,55,55	0
86	OHX	5	4194	7/7	0.26	0.39	132,132,132,132	0
85	MG	5	3463	1/1	0.29	0.39	62,62,62,62	0
85	MG	6	1949	1/1	0.31	0.39	56,56,56,56	0
85	MG	5	3717	1/1	0.24	0.38	52,52,52,52	0
86	OHX	6	2047	7/7	0.22	0.37	75,75,75,75	0
85	MG	1	3833	1/1	0.26	0.37	30,30,30,30	0
86	OHX	1	3894	7/7	0.21	0.37	81,81,81,81	0
85	MG	1	3745	1/1	0.29	0.36	56,56,56,56	0
86	OHX	8	217	7/7	0.21	0.36	60,60,60,60	0
85	MG	2	2020	1/1	0.34	0.35	65,65,65,65	0
85	MG	m5	303	1/1	0.38	0.35	57,57,57,57	0
85	MG	2	2008	1/1	0.36	0.34	48,48,48,48	0
85	MG	5	3436	1/1	0.25	0.33	48,48,48,48	0
85	MG	1	3421	1/1	0.44	0.33	77,77,77,77	0
85	MG	4	206	1/1	0.28	0.33	36,36,36,36	0
86	OHX	1	4056	7/7	0.23	0.32	125,125,125,125	0
86	OHX	n9	102	7/7	0.24	0.32	173,173,173,173	0
86	OHX	1	4193	7/7	0.27	0.32	150,150,150,150	0
86	OHX	5	4202	7/7	0.23	0.32	129,129,129,129	0
85	MG	1	3608	1/1	0.30	0.31	67,67,67,67	0
86	OHX	6	2049	7/7	0.21	0.31	75,75,75,75	0
85	MG	5	3629	1/1	0.24	0.31	66,66,66,66	0
85	MG	6	1932	1/1	0.24	0.31	46,46,46,46	0
86	OHX	6	2174	7/7	0.24	0.31	168,168,168,168	0
85	MG	L4	402	1/1	0.33	0.30	36,36,36,36	0
86	OHX	5	4076	7/7	0.22	0.30	131,131,131,131	0
86	OHX	1	3937	7/7	0.20	0.29	106,106,106,106	0
85	MG	m6	201	1/1	0.24	0.27	36,36,36,36	0
85	MG	m5	301	1/1	0.42	0.27	43,43,43,43	0
86	OHX	1	3932	7/7	0.19	0.27	108,108,108,108	0
85	MG	5	3583	1/1	0.24	0.27	45,45,45,45	0
85	MG	5	3469	1/1	0.27	0.26	37,37,37,37	0
85	MG	5	3708	1/1	0.26	0.26	48,48,48,48	0
85	MG	m1	201	1/1	0.30	0.25	64,64,64,64	0
85	MG	6	1930	1/1	0.25	0.25	56,56,56,56	0
85	MG	O7	102	1/1	0.30	0.25	81,81,81,81	0
85	MG	5	3786	1/1	0.28	0.25	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4230	7/7	0.27	0.25	165,165,165,165	0
85	MG	5	3612	1/1	0.23	0.24	51,51,51,51	0
86	OHX	5	3905	7/7	0.23	0.23	58,58,58,58	0
86	OHX	5	4248	7/7	0.22	0.23	142,142,142,142	0
85	MG	1	3584	1/1	0.29	0.22	51,51,51,51	0
86	OHX	1	4205	7/7	0.38	0.21	155,155,155,155	0
86	OHX	6	2183	7/7	0.27	0.21	147,147,147,147	0
85	MG	6	1956	1/1	0.28	0.21	43,43,43,43	0
85	MG	1	3553	1/1	0.26	0.21	36,36,36,36	0
85	MG	6	1955	1/1	0.34	0.20	40,40,40,40	0
86	OHX	s9	201	7/7	0.51	0.20	138,138,138,138	0
86	OHX	3	222	7/7	0.27	0.20	131,131,131,131	0
85	MG	5	3521	1/1	0.24	0.19	35,35,35,35	0
85	MG	1	3703	1/1	0.25	0.19	64,64,64,64	0
85	MG	2	1964	1/1	0.28	0.19	56,56,56,56	0
86	OHX	2	2137	7/7	0.20	0.19	176,176,176,176	0
85	MG	c8	201	1/1	0.27	0.19	69,69,69,69	0
85	MG	5	3421	1/1	0.26	0.18	35,35,35,35	0
85	MG	2	1927	1/1	0.28	0.17	51,51,51,51	0
85	MG	1	3434	1/1	0.21	0.17	49,49,49,49	0
86	OHX	5	4038	7/7	0.14	0.17	135,135,135,135	0
85	MG	6	2023	1/1	0.33	0.17	48,48,48,48	0
86	OHX	5	4209	7/7	0.29	0.17	131,131,131,131	0
86	OHX	s1	303	7/7	0.38	0.16	184,184,184,184	0
86	OHX	1	4195	7/7	0.18	0.16	174,174,174,174	0
85	MG	1	3828	1/1	0.37	0.16	37,37,37,37	0
86	OHX	6	2155	7/7	0.28	0.15	187,187,187,187	0
86	OHX	1	3907	7/7	0.22	0.15	90,90,90,90	0
86	OHX	6	2197	7/7	0.28	0.14	148,148,148,148	0
86	OHX	6	2200	7/7	0.40	0.14	156,156,156,156	0
85	MG	1	3504	1/1	0.29	0.14	36,36,36,36	0
86	OHX	1	3994	7/7	0.17	0.14	171,171,171,171	0
86	OHX	1	3864	7/7	0.22	0.14	50,50,50,50	0
85	MG	5	3804	1/1	0.21	0.14	42,42,42,42	0
86	OHX	1	3998	7/7	0.30	0.13	120,120,120,120	0
86	OHX	6	2172	7/7	0.25	0.13	155,155,155,155	0
85	MG	1	3641	1/1	0.27	0.13	44,44,44,44	0
85	MG	5	3657	1/1	0.23	0.13	47,47,47,47	0
85	MG	5	3478	1/1	0.27	0.12	64,64,64,64	0
85	MG	1	3520	1/1	0.25	0.12	39,39,39,39	0
85	MG	5	3896	1/1	0.31	0.12	54,54,54,54	0
85	MG	1	3581	1/1	0.31	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
87	PCY	2	2178	40/40	0.37	0.12	77,77,77,77	0
86	OHX	5	4109	7/7	0.23	0.12	128,128,128,128	0
85	MG	2	1950	1/1	0.24	0.11	97,97,97,97	0
86	OHX	1	4081	7/7	0.27	0.11	136,136,136,136	0
86	OHX	1	4134	7/7	0.23	0.10	121,121,121,121	0
85	MG	5	3816	1/1	0.21	0.10	57,57,57,57	0
85	MG	5	3639	1/1	0.21	0.09	55,55,55,55	0
86	OHX	M9	204	7/7	0.24	0.09	175,175,175,175	0
85	MG	5	3642	1/1	0.23	0.08	54,54,54,54	0
86	OHX	6	2065	7/7	0.19	0.08	112,112,112,112	0
85	MG	S8	301	1/1	0.29	0.07	56,56,56,56	0
86	OHX	5	4193	7/7	0.19	0.07	135,135,135,135	0
85	MG	5	3593	1/1	0.26	0.06	29,29,29,29	0
85	MG	5	3855	1/1	0.29	0.06	54,54,54,54	0
85	MG	5	3495	1/1	0.27	0.06	36,36,36,36	0
85	MG	5	3472	1/1	0.20	0.06	47,47,47,47	0
85	MG	1	3679	1/1	0.24	0.06	65,65,65,65	0
85	MG	7	208	1/1	0.31	0.06	52,52,52,52	0
85	MG	5	3413	1/1	0.28	0.06	39,39,39,39	0
86	OHX	5	4062	7/7	0.24	0.05	132,132,132,132	0
85	MG	5	3800	1/1	0.33	0.04	40,40,40,40	0
85	MG	1	3642	1/1	0.18	0.04	44,44,44,44	0
85	MG	5	3468	1/1	0.32	0.03	46,46,46,46	0
85	MG	5	3849	1/1	0.32	0.03	54,54,54,54	0
85	MG	5	3535	1/1	0.30	0.02	33,33,33,33	0
86	OHX	6	2176	7/7	0.23	0.02	127,127,127,127	0
86	OHX	5	4244	7/7	0.29	0.02	143,143,143,143	0
86	OHX	5	4172	7/7	0.28	0.02	179,179,179,179	0
85	MG	n8	203	1/1	0.27	0.02	47,47,47,47	0
85	MG	1	3571	1/1	0.29	0.01	32,32,32,32	0
86	OHX	1	3867	7/7	0.23	0.01	62,62,62,62	0
85	MG	5	3890	1/1	0.22	0.00	53,53,53,53	0
86	OHX	1	4159	7/7	0.22	0.00	164,164,164,164	0
86	OHX	1	4157	7/7	0.23	-0.01	143,143,143,143	0
86	OHX	1	4178	7/7	0.31	-0.01	145,145,145,145	0
88	ZN	d7	101	1/1	0.25	-0.02	156,156,156,156	0
85	MG	5	3457	1/1	0.25	-0.03	31,31,31,31	0
85	MG	1	3544	1/1	0.28	-0.04	34,34,34,34	0
85	MG	N0	201	1/1	0.26	-0.04	45,45,45,45	0
85	MG	M9	203	1/1	0.34	-0.04	61,61,61,61	0
86	OHX	7	225	7/7	0.20	-0.04	127,127,127,127	0
86	OHX	5	4197	7/7	0.17	-0.05	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4225	7/7	0.36	-0.05	157,157,157,157	0
86	OHX	5	4135	7/7	0.25	-0.06	128,128,128,128	0
86	OHX	6	2132	7/7	0.33	-0.06	133,133,133,133	0
86	OHX	5	4183	7/7	0.21	-0.07	153,153,153,153	0
86	OHX	1	3930	7/7	0.20	-0.07	107,107,107,107	0
86	OHX	2	2148	7/7	0.20	-0.07	166,166,166,166	0
86	OHX	5	3939	7/7	0.21	-0.07	86,86,86,86	0
86	OHX	6	2116	7/7	0.21	-0.08	145,145,145,145	0
85	MG	6	1902	1/1	0.24	-0.08	55,55,55,55	0
85	MG	2	1901	1/1	0.34	-0.09	82,82,82,82	0
85	MG	s8	302	1/1	0.30	-0.10	45,45,45,45	0
85	MG	5	3440	1/1	0.26	-0.10	34,34,34,34	0
85	MG	17	301	1/1	0.21	-0.11	47,47,47,47	0
85	MG	5	3774	1/1	0.23	-0.11	39,39,39,39	0
86	OHX	5	4243	7/7	0.21	-0.12	178,178,178,178	0
85	MG	1	3566	1/1	0.28	-0.12	30,30,30,30	0
85	MG	5	3824	1/1	0.29	-0.13	94,94,94,94	0
85	MG	5	3509	1/1	0.27	-0.14	27,27,27,27	0
85	MG	5	3768	1/1	0.23	-0.14	55,55,55,55	0
86	OHX	1	4179	7/7	0.22	-0.14	144,144,144,144	0
88	ZN	D7	101	1/1	0.15	-0.14	162,162,162,162	0
85	MG	1	3446	1/1	0.24	-0.14	45,45,45,45	0
86	OHX	5	3927	7/7	0.22	-0.15	72,72,72,72	0
86	OHX	1	4114	7/7	0.18	-0.15	138,138,138,138	0
85	MG	2	1932	1/1	0.24	-0.16	59,59,59,59	0
86	OHX	15	305	7/7	0.26	-0.16	149,149,149,149	0
86	OHX	2	2054	7/7	0.17	-0.16	134,134,134,134	0
86	OHX	6	2187	7/7	0.24	-0.16	161,161,161,161	0
86	OHX	6	2196	7/7	0.26	-0.17	149,149,149,149	0
85	MG	2	1933	1/1	0.24	-0.17	75,75,75,75	0
85	MG	5	3633	1/1	0.24	-0.17	39,39,39,39	0
85	MG	5	3679	1/1	0.28	-0.18	43,43,43,43	0
86	OHX	1	4045	7/7	0.24	-0.18	119,119,119,119	0
85	MG	6	2004	1/1	0.30	-0.18	69,69,69,69	0
86	OHX	5	4226	7/7	0.25	-0.19	155,155,155,155	0
85	MG	L3	401	1/1	0.27	-0.20	39,39,39,39	0
85	MG	5	3846	1/1	0.22	-0.20	55,55,55,55	0
85	MG	6	1912	1/1	0.27	-0.20	52,52,52,52	0
86	OHX	2	2038	7/7	0.18	-0.21	120,120,120,120	0
85	MG	5	3743	1/1	0.20	-0.21	35,35,35,35	0
85	MG	5	3527	1/1	0.31	-0.22	55,55,55,55	0
85	MG	1	3467	1/1	0.19	-0.23	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4240	7/7	0.24	-0.23	194,194,194,194	0
86	OHX	2	2029	7/7	0.19	-0.23	98,98,98,98	0
85	MG	1	3415	1/1	0.26	-0.23	37,37,37,37	0
85	MG	5	3892	1/1	0.31	-0.23	31,31,31,31	0
85	MG	6	1957	1/1	0.31	-0.23	49,49,49,49	0
85	MG	6	1988	1/1	0.26	-0.23	84,84,84,84	0
85	MG	6	1977	1/1	0.26	-0.23	48,48,48,48	0
85	MG	5	3810	1/1	0.23	-0.23	43,43,43,43	0
86	OHX	5	3959	7/7	0.18	-0.24	89,89,89,89	0
86	OHX	5	4108	7/7	0.28	-0.24	135,135,135,135	0
85	MG	5	3701	1/1	0.28	-0.24	63,63,63,63	0
85	MG	1	3401	1/1	0.26	-0.24	38,38,38,38	0
86	OHX	2	2130	7/7	0.15	-0.24	207,207,207,207	0
85	MG	1	3750	1/1	0.20	-0.25	60,60,60,60	0
85	MG	N3	201	1/1	0.25	-0.25	33,33,33,33	0
86	OHX	2	2131	7/7	0.26	-0.26	125,125,125,125	0
86	OHX	5	3948	7/7	0.20	-0.26	92,92,92,92	0
86	OHX	1	3915	7/7	0.18	-0.26	98,98,98,98	0
86	OHX	5	4137	7/7	0.24	-0.27	135,135,135,135	0
85	MG	O3	201	1/1	0.22	-0.28	74,74,74,74	0
86	OHX	2	2134	7/7	0.33	-0.28	148,148,148,148	0
86	OHX	N9	102	7/7	0.21	-0.28	68,68,68,68	0
85	MG	5	3513	1/1	0.30	-0.29	34,34,34,34	0
85	MG	5	3833	1/1	0.20	-0.29	52,52,52,52	0
86	OHX	2	2149	7/7	0.21	-0.29	181,181,181,181	0
86	OHX	5	3941	7/7	0.18	-0.30	85,85,85,85	0
86	OHX	2	2151	7/7	0.17	-0.30	154,154,154,154	0
85	MG	M5	301	1/1	0.28	-0.30	48,48,48,48	0
86	OHX	1	3959	7/7	0.17	-0.30	123,123,123,123	0
86	OHX	6	2175	7/7	0.25	-0.30	119,119,119,119	0
86	OHX	1	4189	7/7	0.18	-0.31	151,151,151,151	0
86	OHX	6	2191	7/7	0.19	-0.32	165,165,165,165	0
85	MG	5	3415	1/1	0.22	-0.32	55,55,55,55	0
85	MG	6	1935	1/1	0.24	-0.32	52,52,52,52	0
85	MG	1	3746	1/1	0.31	-0.32	49,49,49,49	0
86	OHX	6	2052	7/7	0.21	-0.32	78,78,78,78	0
86	OHX	5	3914	7/7	0.21	-0.33	67,67,67,67	0
86	OHX	2	2025	7/7	0.20	-0.33	82,82,82,82	0
86	OHX	14	402	7/7	0.23	-0.34	155,155,155,155	0
85	MG	1	3800	1/1	0.23	-0.34	56,56,56,56	0
85	MG	1	3439	1/1	0.27	-0.34	34,34,34,34	0
85	MG	6	1963	1/1	0.22	-0.34	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2145	7/7	0.19	-0.34	127,127,127,127	0
86	OHX	1	3872	7/7	0.21	-0.35	61,61,61,61	0
85	MG	5	3508	1/1	0.24	-0.35	41,41,41,41	0
85	MG	5	3725	1/1	0.25	-0.36	37,37,37,37	0
85	MG	2	1998	1/1	0.22	-0.36	109,109,109,109	0
85	MG	1	3692	1/1	0.23	-0.37	43,43,43,43	0
86	OHX	1	4097	7/7	0.26	-0.37	120,120,120,120	0
85	MG	5	3482	1/1	0.26	-0.37	29,29,29,29	0
85	MG	1	3507	1/1	0.25	-0.37	33,33,33,33	0
86	OHX	6	2181	7/7	0.24	-0.37	143,143,143,143	0
85	MG	1	3708	1/1	0.23	-0.37	35,35,35,35	0
85	MG	5	3711	1/1	0.26	-0.37	47,47,47,47	0
87	PCY	6	2204	40/40	0.21	-0.37	59,59,59,59	0
85	MG	6	1958	1/1	0.25	-0.37	61,61,61,61	0
85	MG	6	1995	1/1	0.21	-0.38	72,72,72,72	0
85	MG	6	1960	1/1	0.24	-0.38	40,40,40,40	0
86	OHX	6	2095	7/7	0.18	-0.38	129,129,129,129	0
85	MG	5	3487	1/1	0.31	-0.38	28,28,28,28	0
86	OHX	5	4173	7/7	0.20	-0.39	111,111,111,111	0
86	OHX	2	2117	7/7	0.23	-0.39	148,148,148,148	0
86	OHX	2	2081	7/7	0.15	-0.39	161,161,161,161	0
85	MG	5	3534	1/1	0.24	-0.40	36,36,36,36	0
85	MG	1	3440	1/1	0.24	-0.40	41,41,41,41	0
86	OHX	1	4199	7/7	0.25	-0.41	150,150,150,150	0
86	OHX	5	3975	7/7	0.20	-0.41	112,112,112,112	0
86	OHX	2	2146	7/7	0.18	-0.41	183,183,183,183	0
85	MG	5	3853	1/1	0.25	-0.42	51,51,51,51	0
86	OHX	2	2136	7/7	0.19	-0.43	140,140,140,140	0
86	OHX	6	2063	7/7	0.18	-0.44	101,101,101,101	0
86	OHX	5	4238	7/7	0.17	-0.44	154,154,154,154	0
85	MG	1	3835	1/1	0.28	-0.44	52,52,52,52	0
86	OHX	5	3907	7/7	0.20	-0.44	65,65,65,65	0
86	OHX	1	4203	7/7	0.22	-0.45	150,150,150,150	0
86	OHX	6	2098	7/7	0.13	-0.45	157,157,157,157	0
85	MG	1	3684	1/1	0.28	-0.45	49,49,49,49	0
86	OHX	5	4145	7/7	0.25	-0.46	142,142,142,142	0
85	MG	5	3885	1/1	0.22	-0.46	34,34,34,34	0
85	MG	5	3419	1/1	0.32	-0.46	39,39,39,39	0
85	MG	5	3827	1/1	0.19	-0.47	36,36,36,36	0
85	MG	n0	202	1/1	0.18	-0.47	41,41,41,41	0
85	MG	M0	302	1/1	0.33	-0.47	55,55,55,55	0
86	OHX	L4	403	7/7	0.17	-0.48	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	4186	7/7	0.24	-0.48	146,146,146,146	0
86	OHX	1	4174	7/7	0.16	-0.48	162,162,162,162	0
85	MG	5	3600	1/1	0.20	-0.48	44,44,44,44	0
85	MG	6	1989	1/1	0.20	-0.49	68,68,68,68	0
85	MG	4	207	1/1	0.23	-0.49	41,41,41,41	0
86	OHX	2	2163	7/7	0.14	-0.49	180,180,180,180	0
85	MG	5	3533	1/1	0.17	-0.50	54,54,54,54	0
85	MG	5	3699	1/1	0.21	-0.50	50,50,50,50	0
86	OHX	5	4242	7/7	0.32	-0.50	116,116,116,116	0
85	MG	1	3479	1/1	0.22	-0.50	84,84,84,84	0
85	MG	6	2021	1/1	0.23	-0.50	62,62,62,62	0
86	OHX	1	4133	7/7	0.26	-0.50	125,125,125,125	0
86	OHX	2	2160	7/7	0.24	-0.51	181,181,181,181	0
85	MG	3	210	1/1	0.20	-0.51	60,60,60,60	0
85	MG	5	3677	1/1	0.22	-0.51	43,43,43,43	0
85	MG	5	3423	1/1	0.22	-0.51	60,60,60,60	0
85	MG	5	3707	1/1	0.22	-0.52	57,57,57,57	0
85	MG	2	1907	1/1	0.25	-0.52	61,61,61,61	0
86	OHX	5	4031	7/7	0.14	-0.52	143,143,143,143	0
86	OHX	5	4149	7/7	0.21	-0.52	136,136,136,136	0
85	MG	n8	202	1/1	0.28	-0.53	33,33,33,33	0
85	MG	2	1915	1/1	0.26	-0.53	74,74,74,74	0
86	OHX	S6	301	7/7	0.21	-0.53	164,164,164,164	0
86	OHX	5	4075	7/7	0.27	-0.54	128,128,128,128	0
85	MG	6	1969	1/1	0.20	-0.54	54,54,54,54	0
86	OHX	5	4128	7/7	0.24	-0.54	136,136,136,136	0
85	MG	1	3732	1/1	0.21	-0.54	36,36,36,36	0
85	MG	2	1966	1/1	0.29	-0.55	52,52,52,52	0
85	MG	1	4214	1/1	0.20	-0.55	30,30,30,30	0
85	MG	2	1920	1/1	0.25	-0.55	56,56,56,56	0
85	MG	L3	402	1/1	0.21	-0.55	43,43,43,43	0
85	MG	n8	204	1/1	0.20	-0.55	43,43,43,43	0
85	MG	1	3622	1/1	0.20	-0.55	49,49,49,49	0
85	MG	D3	201	1/1	0.29	-0.56	55,55,55,55	0
86	OHX	1	4184	7/7	0.20	-0.56	158,158,158,158	0
85	MG	1	4218	1/1	0.20	-0.57	74,74,74,74	0
85	MG	2	1984	1/1	0.21	-0.57	60,60,60,60	0
85	MG	6	2034	1/1	0.25	-0.57	73,73,73,73	0
86	OHX	6	2112	7/7	0.24	-0.58	110,110,110,110	0
86	OHX	5	3906	7/7	0.22	-0.58	62,62,62,62	0
85	MG	5	3543	1/1	0.21	-0.58	66,66,66,66	0
85	MG	2	1982	1/1	0.21	-0.58	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4151	7/7	0.23	-0.58	125,125,125,125	0
86	OHX	5	4141	7/7	0.22	-0.58	139,139,139,139	0
85	MG	1	3550	1/1	0.24	-0.58	43,43,43,43	0
85	MG	8	205	1/1	0.23	-0.59	54,54,54,54	0
88	ZN	e1	501	1/1	0.14	-0.59	169,169,169,169	0
86	OHX	5	4103	7/7	0.17	-0.60	158,158,158,158	0
86	OHX	5	4147	7/7	0.22	-0.60	126,126,126,126	0
86	OHX	2	2048	7/7	0.13	-0.60	136,136,136,136	0
86	OHX	5	4000	7/7	0.18	-0.61	117,117,117,117	0
85	MG	5	3688	1/1	0.19	-0.61	46,46,46,46	0
86	OHX	5	3935	7/7	0.19	-0.61	83,83,83,83	0
85	MG	5	3492	1/1	0.18	-0.61	47,47,47,47	0
86	OHX	1	4211	7/7	0.18	-0.61	169,169,169,169	0
86	OHX	1	4153	7/7	0.22	-0.61	139,139,139,139	0
86	OHX	5	4089	7/7	0.24	-0.62	120,120,120,120	0
85	MG	1	3534	1/1	0.29	-0.62	29,29,29,29	0
86	OHX	1	3868	7/7	0.22	-0.63	55,55,55,55	0
85	MG	2	1924	1/1	0.27	-0.63	83,83,83,83	0
85	MG	N9	101	1/1	0.26	-0.63	31,31,31,31	0
85	MG	1	3659	1/1	0.25	-0.63	63,63,63,63	0
86	OHX	5	4178	7/7	0.23	-0.63	136,136,136,136	0
85	MG	8	208	1/1	0.28	-0.64	45,45,45,45	0
86	OHX	6	2128	7/7	0.26	-0.64	157,157,157,157	0
86	OHX	1	4132	7/7	0.20	-0.64	148,148,148,148	0
85	MG	5	3630	1/1	0.28	-0.65	41,41,41,41	0
86	OHX	C8	201	7/7	0.18	-0.65	117,117,117,117	0
85	MG	O7	103	1/1	0.28	-0.65	41,41,41,41	0
86	OHX	m0	301	7/7	0.16	-0.65	126,126,126,126	0
85	MG	q3	502	1/1	0.24	-0.66	62,62,62,62	0
85	MG	5	3729	1/1	0.22	-0.66	31,31,31,31	0
86	OHX	2	2177	7/7	0.27	-0.66	184,184,184,184	0
85	MG	2	1990	1/1	0.16	-0.66	106,106,106,106	0
86	OHX	1	4078	7/7	0.30	-0.66	138,138,138,138	0
86	OHX	1	3926	7/7	0.15	-0.67	111,111,111,111	0
85	MG	2	2012	1/1	0.26	-0.67	67,67,67,67	0
85	MG	6	1921	1/1	0.24	-0.68	43,43,43,43	0
85	MG	5	3694	1/1	0.23	-0.68	51,51,51,51	0
86	OHX	1	4120	7/7	0.25	-0.68	161,161,161,161	0
86	OHX	5	3956	7/7	0.18	-0.68	102,102,102,102	0
85	MG	5	3714	1/1	0.21	-0.68	61,61,61,61	0
85	MG	1	3492	1/1	0.24	-0.68	69,69,69,69	0
86	OHX	5	3966	7/7	0.20	-0.69	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2118	7/7	0.18	-0.69	149,149,149,149	0
85	MG	1	3737	1/1	0.19	-0.70	52,52,52,52	0
86	OHX	2	2093	7/7	0.23	-0.70	123,123,123,123	0
86	OHX	1	4076	7/7	0.25	-0.70	129,129,129,129	0
86	OHX	5	4189	7/7	0.23	-0.71	164,164,164,164	0
86	OHX	2	2157	7/7	0.14	-0.71	289,289,289,289	0
85	MG	5	3500	1/1	0.22	-0.72	31,31,31,31	0
86	OHX	5	4083	7/7	0.21	-0.72	117,117,117,117	0
85	MG	5	3619	1/1	0.20	-0.72	46,46,46,46	0
86	OHX	6	2104	7/7	0.17	-0.72	123,123,123,123	0
85	MG	1	3583	1/1	0.22	-0.72	43,43,43,43	0
86	OHX	6	2199	7/7	0.21	-0.72	160,160,160,160	0
86	OHX	5	4184	7/7	0.18	-0.72	140,140,140,140	0
86	OHX	d9	102	7/7	0.25	-0.72	181,181,181,181	0
86	OHX	6	2046	7/7	0.21	-0.72	61,61,61,61	0
85	MG	6	2005	1/1	0.17	-0.72	62,62,62,62	0
85	MG	5	3750	1/1	0.20	-0.73	43,43,43,43	0
86	OHX	5	4099	7/7	0.22	-0.73	129,129,129,129	0
86	OHX	6	2106	7/7	0.20	-0.74	139,139,139,139	0
85	MG	5	3789	1/1	0.31	-0.74	36,36,36,36	0
86	OHX	5	4169	7/7	0.18	-0.74	148,148,148,148	0
85	MG	q3	503	1/1	0.38	-0.74	63,63,63,63	0
86	OHX	5	3969	7/7	0.20	-0.74	93,93,93,93	0
85	MG	5	4252	1/1	0.16	-0.75	40,40,40,40	0
85	MG	1	3518	1/1	0.27	-0.75	29,29,29,29	0
86	OHX	2	2174	7/7	0.19	-0.75	187,187,187,187	0
86	OHX	5	3922	7/7	0.19	-0.75	69,69,69,69	0
86	OHX	1	3902	7/7	0.19	-0.76	88,88,88,88	0
86	OHX	2	2041	7/7	0.20	-0.76	103,103,103,103	0
86	OHX	6	2137	7/7	0.28	-0.76	129,129,129,129	0
85	MG	6	1964	1/1	0.19	-0.77	55,55,55,55	0
86	OHX	6	2056	7/7	0.19	-0.77	77,77,77,77	0
86	OHX	6	2124	7/7	0.11	-0.77	141,141,141,141	0
85	MG	2	1910	1/1	0.23	-0.78	60,60,60,60	0
86	OHX	8	227	7/7	0.15	-0.78	134,134,134,134	0
86	OHX	2	2125	7/7	0.18	-0.79	151,151,151,151	0
86	OHX	6	2073	7/7	0.16	-0.79	131,131,131,131	0
86	OHX	1	4191	7/7	0.15	-0.79	154,154,154,154	0
85	MG	3	208	1/1	0.20	-0.80	60,60,60,60	0
86	OHX	2	2086	7/7	0.12	-0.80	146,146,146,146	0
85	MG	5	3746	1/1	0.24	-0.80	66,66,66,66	0
85	MG	1	3484	1/1	0.19	-0.81	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2025	1/1	0.16	-0.81	88,88,88,88	0
86	OHX	1	3885	7/7	0.21	-0.81	80,80,80,80	0
85	MG	5	3581	1/1	0.24	-0.82	36,36,36,36	0
86	OHX	2	2139	7/7	0.19	-0.82	171,171,171,171	0
85	MG	2	2018	1/1	0.17	-0.82	80,80,80,80	0
85	MG	5	3591	1/1	0.25	-0.82	44,44,44,44	0
85	MG	5	3798	1/1	0.19	-0.82	59,59,59,59	0
86	OHX	5	4190	7/7	0.18	-0.82	134,134,134,134	0
86	OHX	6	2161	7/7	0.20	-0.82	129,129,129,129	0
85	MG	1	3834	1/1	0.21	-0.83	43,43,43,43	0
85	MG	5	3706	1/1	0.17	-0.83	37,37,37,37	0
86	OHX	1	4025	7/7	0.22	-0.84	125,125,125,125	0
85	MG	5	3494	1/1	0.23	-0.85	29,29,29,29	0
86	OHX	5	4159	7/7	0.19	-0.85	125,125,125,125	0
86	OHX	1	4100	7/7	0.19	-0.85	145,145,145,145	0
86	OHX	1	3878	7/7	0.16	-0.86	69,69,69,69	0
86	OHX	6	2192	7/7	0.19	-0.86	188,188,188,188	0
86	OHX	6	2147	7/7	0.25	-0.86	147,147,147,147	0
85	MG	5	3637	1/1	0.23	-0.86	49,49,49,49	0
86	OHX	5	4101	7/7	0.13	-0.87	150,150,150,150	0
86	OHX	6	2136	7/7	0.22	-0.87	138,138,138,138	0
86	OHX	1	4121	7/7	0.19	-0.87	117,117,117,117	0
86	OHX	1	4117	7/7	0.19	-0.88	138,138,138,138	0
85	MG	1	3768	1/1	0.27	-0.88	43,43,43,43	0
85	MG	2	2000	1/1	0.16	-0.88	91,91,91,91	0
85	MG	1	3781	1/1	0.24	-0.88	42,42,42,42	0
85	MG	5	3431	1/1	0.23	-0.89	35,35,35,35	0
86	OHX	1	4033	7/7	0.18	-0.89	104,104,104,104	0
85	MG	5	3719	1/1	0.24	-0.89	52,52,52,52	0
85	MG	2	1939	1/1	0.15	-0.90	68,68,68,68	0
85	MG	D0	201	1/1	0.24	-0.90	68,68,68,68	0
85	MG	5	3640	1/1	0.19	-0.90	49,49,49,49	0
85	MG	o4	201	1/1	0.22	-0.90	69,69,69,69	0
85	MG	5	3539	1/1	0.25	-0.90	23,23,23,23	0
86	OHX	8	218	7/7	0.21	-0.91	60,60,60,60	0
85	MG	6	2033	1/1	0.27	-0.91	64,64,64,64	0
86	OHX	5	4156	7/7	0.19	-0.91	142,142,142,142	0
85	MG	4	205	1/1	0.23	-0.92	29,29,29,29	0
85	MG	N3	202	1/1	0.16	-0.92	46,46,46,46	0
85	MG	5	4256	1/1	0.21	-0.92	35,35,35,35	0
86	OHX	5	4084	7/7	0.14	-0.93	144,144,144,144	0
86	OHX	1	3882	7/7	0.18	-0.93	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	3994	7/7	0.22	-0.93	105,105,105,105	0
86	OHX	2	2122	7/7	0.14	-0.93	156,156,156,156	0
86	OHX	1	4164	7/7	0.10	-0.93	219,219,219,219	0
86	OHX	D9	102	7/7	0.20	-0.94	153,153,153,153	0
85	MG	1	3862	1/1	0.21	-0.94	55,55,55,55	0
85	MG	c1	201	1/1	0.21	-0.94	47,47,47,47	0
85	MG	1	3810	1/1	0.22	-0.94	44,44,44,44	0
86	OHX	2	2097	7/7	0.19	-0.94	138,138,138,138	0
85	MG	5	3429	1/1	0.22	-0.94	33,33,33,33	0
86	OHX	2	2100	7/7	0.18	-0.94	128,128,128,128	0
86	OHX	2	2128	7/7	0.22	-0.95	143,143,143,143	0
86	OHX	5	4203	7/7	0.16	-0.95	147,147,147,147	0
86	OHX	2	2108	7/7	0.12	-0.95	123,123,123,123	0
85	MG	5	3703	1/1	0.19	-0.95	65,65,65,65	0
86	OHX	5	4251	7/7	0.14	-0.96	168,168,168,168	0
85	MG	1	3777	1/1	0.21	-0.96	66,66,66,66	0
86	OHX	5	4090	7/7	0.25	-0.96	109,109,109,109	0
86	OHX	6	2145	7/7	0.10	-0.96	139,139,139,139	0
86	OHX	2	2031	7/7	0.21	-0.97	97,97,97,97	0
86	OHX	5	4177	7/7	0.19	-0.97	144,144,144,144	0
86	OHX	5	4146	7/7	0.23	-0.97	126,126,126,126	0
86	OHX	1	3897	7/7	0.18	-0.97	88,88,88,88	0
86	OHX	1	4148	7/7	0.14	-0.97	148,148,148,148	0
86	OHX	1	3968	7/7	0.23	-0.97	118,118,118,118	0
86	OHX	5	3974	7/7	0.16	-0.97	87,87,87,87	0
86	OHX	2	2044	7/7	0.15	-0.98	118,118,118,118	0
86	OHX	1	4032	7/7	0.09	-0.98	150,150,150,150	0
88	ZN	Q3	501	1/1	0.12	-0.98	68,68,68,68	0
85	MG	1	3541	1/1	0.20	-0.98	27,27,27,27	0
85	MG	1	3510	1/1	0.25	-0.99	34,34,34,34	0
86	OHX	1	4065	7/7	0.17	-0.99	123,123,123,123	0
86	OHX	1	3923	7/7	0.15	-1.00	111,111,111,111	0
86	OHX	1	3913	7/7	0.16	-1.00	92,92,92,92	0
86	OHX	m0	302	7/7	0.23	-1.00	139,139,139,139	0
85	MG	S2	302	1/1	0.25	-1.01	66,66,66,66	0
85	MG	2	1991	1/1	0.17	-1.01	101,101,101,101	0
86	OHX	m8	201	7/7	0.20	-1.01	145,145,145,145	0
85	MG	6	1984	1/1	0.14	-1.01	78,78,78,78	0
86	OHX	5	4003	7/7	0.16	-1.01	122,122,122,122	0
85	MG	6	2003	1/1	0.14	-1.01	96,96,96,96	0
86	OHX	2	2090	7/7	0.17	-1.02	117,117,117,117	0
86	OHX	5	4102	7/7	0.22	-1.02	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	L5	301	1/1	0.27	-1.02	56,56,56,56	0
86	OHX	5	3903	7/7	0.21	-1.02	55,55,55,55	0
86	OHX	1	4144	7/7	0.16	-1.03	166,166,166,166	0
88	ZN	d6	101	1/1	0.15	-1.03	62,62,62,62	0
85	MG	5	3771	1/1	0.14	-1.03	71,71,71,71	0
88	ZN	Q0	500	1/1	0.17	-1.03	56,56,56,56	0
85	MG	5	3604	1/1	0.22	-1.03	38,38,38,38	0
86	OHX	8	219	7/7	0.09	-1.04	119,119,119,119	0
85	MG	5	3745	1/1	0.16	-1.04	64,64,64,64	0
85	MG	5	3411	1/1	0.24	-1.04	42,42,42,42	0
85	MG	1	3630	1/1	0.18	-1.05	36,36,36,36	0
86	OHX	2	2144	7/7	0.14	-1.05	179,179,179,179	0
88	ZN	d9	101	1/1	0.14	-1.05	78,78,78,78	0
86	OHX	6	2123	7/7	0.17	-1.05	111,111,111,111	0
86	OHX	2	2168	7/7	0.17	-1.05	145,145,145,145	0
85	MG	1	3601	1/1	0.21	-1.05	31,31,31,31	0
85	MG	5	3754	1/1	0.18	-1.05	56,56,56,56	0
86	OHX	s8	303	7/7	0.16	-1.06	167,167,167,167	0
86	OHX	1	3954	7/7	0.22	-1.07	99,99,99,99	0
86	OHX	2	2116	7/7	0.22	-1.07	125,125,125,125	0
85	MG	1	3428	1/1	0.14	-1.07	57,57,57,57	0
86	OHX	5	4122	7/7	0.19	-1.07	150,150,150,150	0
85	MG	5	3818	1/1	0.13	-1.07	45,45,45,45	0
86	OHX	1	4204	7/7	0.20	-1.07	148,148,148,148	0
85	MG	5	3871	1/1	0.32	-1.07	48,48,48,48	0
88	ZN	E1	501	1/1	0.12	-1.07	123,123,123,123	0
86	OHX	1	3963	7/7	0.16	-1.07	124,124,124,124	0
86	OHX	2	2161	7/7	0.15	-1.07	181,181,181,181	0
85	MG	1	3754	1/1	0.16	-1.08	44,44,44,44	0
85	MG	2	1948	1/1	0.19	-1.08	62,62,62,62	0
85	MG	1	3487	1/1	0.19	-1.08	45,45,45,45	0
85	MG	1	3776	1/1	0.20	-1.08	35,35,35,35	0
86	OHX	5	3970	7/7	0.14	-1.09	100,100,100,100	0
86	OHX	4	224	7/7	0.14	-1.09	81,81,81,81	0
86	OHX	5	4233	7/7	0.18	-1.10	109,109,109,109	0
86	OHX	5	4195	7/7	0.12	-1.11	176,176,176,176	0
85	MG	1	3408	1/1	0.22	-1.11	44,44,44,44	0
86	OHX	m1	203	7/7	0.15	-1.12	162,162,162,162	0
85	MG	6	1913	1/1	0.24	-1.12	36,36,36,36	0
85	MG	1	3673	1/1	0.18	-1.12	28,28,28,28	0
86	OHX	2	2153	7/7	0.16	-1.13	157,157,157,157	0
86	OHX	1	4113	7/7	0.22	-1.13	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2149	7/7	0.17	-1.14	149,149,149,149	0
86	OHX	1	3873	7/7	0.19	-1.14	66,66,66,66	0
86	OHX	2	2141	7/7	0.09	-1.14	169,169,169,169	0
86	OHX	L3	403	7/7	0.20	-1.14	126,126,126,126	0
85	MG	1	3508	1/1	0.25	-1.14	20,20,20,20	0
85	MG	5	3762	1/1	0.17	-1.15	39,39,39,39	0
85	MG	2	1902	1/1	0.23	-1.15	39,39,39,39	0
85	MG	O2	201	1/1	0.25	-1.15	34,34,34,34	0
86	OHX	1	3865	7/7	0.20	-1.15	52,52,52,52	0
86	OHX	6	2072	7/7	0.13	-1.15	135,135,135,135	0
86	OHX	n9	101	7/7	0.18	-1.15	70,70,70,70	0
86	OHX	1	3953	7/7	0.18	-1.16	102,102,102,102	0
85	MG	5	3700	1/1	0.20	-1.16	40,40,40,40	0
86	OHX	5	3980	7/7	0.15	-1.16	100,100,100,100	0
85	MG	6	2035	1/1	0.20	-1.16	71,71,71,71	0
85	MG	6	1952	1/1	0.22	-1.17	62,62,62,62	0
86	OHX	2	2035	7/7	0.18	-1.17	103,103,103,103	0
86	OHX	1	3874	7/7	0.18	-1.17	64,64,64,64	0
86	OHX	5	3909	7/7	0.20	-1.17	52,52,52,52	0
86	OHX	5	4132	7/7	0.11	-1.17	192,192,192,192	0
85	MG	5	3837	1/1	0.18	-1.17	50,50,50,50	0
85	MG	1	3705	1/1	0.19	-1.17	43,43,43,43	0
85	MG	5	3424	1/1	0.20	-1.17	41,41,41,41	0
86	OHX	1	4077	7/7	0.20	-1.18	130,130,130,130	0
85	MG	1	3445	1/1	0.21	-1.18	46,46,46,46	0
86	OHX	O7	104	7/7	0.12	-1.18	102,102,102,102	0
86	OHX	5	3976	7/7	0.17	-1.18	100,100,100,100	0
86	OHX	5	4024	7/7	0.13	-1.19	119,119,119,119	0
85	MG	5	3832	1/1	0.17	-1.19	73,73,73,73	0
85	MG	1	3739	1/1	0.18	-1.20	49,49,49,49	0
85	MG	1	3786	1/1	0.17	-1.20	36,36,36,36	0
85	MG	M3	202	1/1	0.29	-1.21	91,91,91,91	0
85	MG	5	3480	1/1	0.22	-1.21	41,41,41,41	0
85	MG	1	3480	1/1	0.25	-1.21	78,78,78,78	0
86	OHX	4	229	7/7	0.10	-1.21	125,125,125,125	0
88	ZN	Q2	501	1/1	0.12	-1.22	92,92,92,92	0
86	OHX	6	2050	7/7	0.21	-1.22	73,73,73,73	0
85	MG	1	3709	1/1	0.27	-1.22	66,66,66,66	0
86	OHX	1	4062	7/7	0.18	-1.22	130,130,130,130	0
85	MG	n6	201	1/1	0.23	-1.22	49,49,49,49	0
85	MG	L2	301	1/1	0.17	-1.22	38,38,38,38	0
85	MG	5	3515	1/1	0.24	-1.23	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3483	1/1	0.18	-1.23	53,53,53,53	0
86	OHX	5	4241	7/7	0.14	-1.23	239,239,239,239	0
86	OHX	1	4036	7/7	0.12	-1.23	122,122,122,122	0
86	OHX	7	221	7/7	0.11	-1.24	112,112,112,112	0
86	OHX	4	236	7/7	0.20	-1.24	153,153,153,153	0
85	MG	1	3453	1/1	0.21	-1.24	45,45,45,45	0
85	MG	5	3627	1/1	0.16	-1.24	64,64,64,64	0
86	OHX	2	2169	7/7	0.17	-1.24	150,150,150,150	0
86	OHX	q1	102	7/7	0.20	-1.25	103,103,103,103	0
86	OHX	1	3921	7/7	0.17	-1.25	94,94,94,94	0
85	MG	5	3766	1/1	0.23	-1.25	42,42,42,42	0
86	OHX	2	2152	7/7	0.14	-1.25	178,178,178,178	0
85	MG	5	3451	1/1	0.17	-1.26	33,33,33,33	0
86	OHX	5	3962	7/7	0.15	-1.26	98,98,98,98	0
86	OHX	5	4152	7/7	0.19	-1.26	158,158,158,158	0
85	MG	5	3753	1/1	0.16	-1.27	52,52,52,52	0
86	OHX	6	2096	7/7	0.12	-1.27	157,157,157,157	0
86	OHX	l3	404	7/7	0.15	-1.28	143,143,143,143	0
86	OHX	5	4077	7/7	0.12	-1.28	163,163,163,163	0
86	OHX	5	4115	7/7	0.18	-1.28	125,125,125,125	0
86	OHX	5	3963	7/7	0.14	-1.28	92,92,92,92	0
86	OHX	5	3920	7/7	0.18	-1.28	70,70,70,70	0
85	MG	6	1905	1/1	0.18	-1.28	54,54,54,54	0
86	OHX	5	4205	7/7	0.23	-1.29	145,145,145,145	0
86	OHX	6	2082	7/7	0.17	-1.29	119,119,119,119	0
86	OHX	5	3918	7/7	0.20	-1.29	63,63,63,63	0
86	OHX	1	4180	7/7	0.17	-1.30	114,114,114,114	0
86	OHX	5	4001	7/7	0.15	-1.30	119,119,119,119	0
86	OHX	2	2095	7/7	0.12	-1.31	140,140,140,140	0
85	MG	1	3845	1/1	0.21	-1.31	53,53,53,53	0
86	OHX	5	4125	7/7	0.09	-1.31	154,154,154,154	0
85	MG	1	3643	1/1	0.18	-1.32	44,44,44,44	0
85	MG	1	3774	1/1	0.15	-1.32	66,66,66,66	0
86	OHX	5	3971	7/7	0.15	-1.32	103,103,103,103	0
85	MG	5	3473	1/1	0.15	-1.32	43,43,43,43	0
86	OHX	1	3899	7/7	0.15	-1.33	85,85,85,85	0
85	MG	5	3460	1/1	0.19	-1.33	33,33,33,33	0
85	MG	2	2009	1/1	0.19	-1.33	50,50,50,50	0
86	OHX	5	3911	7/7	0.20	-1.33	62,62,62,62	0
86	OHX	2	2032	7/7	0.17	-1.33	117,117,117,117	0
86	OHX	5	3938	7/7	0.16	-1.33	78,78,78,78	0
86	OHX	5	3944	7/7	0.18	-1.34	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4107	7/7	0.18	-1.34	130,130,130,130	0
85	MG	1	3633	1/1	0.18	-1.34	59,59,59,59	0
86	OHX	1	4160	7/7	0.19	-1.34	147,147,147,147	0
86	OHX	6	2093	7/7	0.13	-1.34	135,135,135,135	0
86	OHX	5	3937	7/7	0.14	-1.35	76,76,76,76	0
88	ZN	q3	501	1/1	0.11	-1.35	75,75,75,75	0
86	OHX	2	2101	7/7	0.17	-1.35	159,159,159,159	0
86	OHX	5	4046	7/7	0.18	-1.35	110,110,110,110	0
85	MG	1	3819	1/1	0.15	-1.35	45,45,45,45	0
85	MG	M0	301	1/1	0.23	-1.35	48,48,48,48	0
85	MG	2	1985	1/1	0.20	-1.35	67,67,67,67	0
86	OHX	5	4120	7/7	0.17	-1.36	133,133,133,133	0
85	MG	6	2206	1/1	0.14	-1.36	68,68,68,68	0
86	OHX	1	4173	7/7	0.16	-1.37	151,151,151,151	0
86	OHX	5	3981	7/7	0.14	-1.37	112,112,112,112	0
86	OHX	2	2132	7/7	0.11	-1.37	159,159,159,159	0
86	OHX	2	2111	7/7	0.07	-1.37	147,147,147,147	0
86	OHX	6	2135	7/7	0.13	-1.37	145,145,145,145	0
85	MG	2	1954	1/1	0.19	-1.37	64,64,64,64	0
85	MG	1	3575	1/1	0.21	-1.37	28,28,28,28	0
85	MG	5	3881	1/1	0.19	-1.38	34,34,34,34	0
86	OHX	5	4060	7/7	0.14	-1.38	154,154,154,154	0
86	OHX	2	2028	7/7	0.17	-1.39	78,78,78,78	0
85	MG	5	3458	1/1	0.24	-1.39	35,35,35,35	0
86	OHX	1	4027	7/7	0.09	-1.39	141,141,141,141	0
86	OHX	c3	201	7/7	0.11	-1.39	162,162,162,162	0
86	OHX	1	3950	7/7	0.19	-1.40	109,109,109,109	0
85	MG	1	3664	1/1	0.18	-1.40	45,45,45,45	0
86	OHX	5	4186	7/7	0.17	-1.40	131,131,131,131	0
86	OHX	2	2026	7/7	0.20	-1.41	86,86,86,86	0
85	MG	8	214	1/1	0.25	-1.41	50,50,50,50	0
85	MG	2	1947	1/1	0.14	-1.41	88,88,88,88	0
85	MG	M7	201	1/1	0.19	-1.41	36,36,36,36	0
85	MG	6	2002	1/1	0.17	-1.41	75,75,75,75	0
85	MG	2	1941	1/1	0.30	-1.41	68,68,68,68	0
85	MG	6	1970	1/1	0.18	-1.41	65,65,65,65	0
86	OHX	1	3870	7/7	0.21	-1.42	59,59,59,59	0
86	OHX	6	2051	7/7	0.18	-1.42	70,70,70,70	0
85	MG	1	3530	1/1	0.20	-1.43	61,61,61,61	0
86	OHX	5	4071	7/7	0.21	-1.43	137,137,137,137	0
85	MG	5	3666	1/1	0.15	-1.43	46,46,46,46	0
86	OHX	6	2100	7/7	0.11	-1.43	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4207	7/7	0.20	-1.43	146,146,146,146	0
85	MG	5	3792	1/1	0.19	-1.43	36,36,36,36	0
86	OHX	6	2083	7/7	0.12	-1.44	119,119,119,119	0
86	OHX	6	2088	7/7	0.13	-1.44	133,133,133,133	0
86	OHX	6	2140	7/7	0.19	-1.44	138,138,138,138	0
85	MG	5	3718	1/1	0.20	-1.44	61,61,61,61	0
86	OHX	1	4136	7/7	0.20	-1.45	133,133,133,133	0
86	OHX	1	4109	7/7	0.22	-1.45	123,123,123,123	0
86	OHX	6	2169	7/7	0.16	-1.46	163,163,163,163	0
85	MG	5	3777	1/1	0.15	-1.46	61,61,61,61	0
86	OHX	2	2105	7/7	0.13	-1.47	206,206,206,206	0
86	OHX	1	4063	7/7	0.18	-1.47	111,111,111,111	0
85	MG	5	3426	1/1	0.23	-1.48	38,38,38,38	0
86	OHX	1	4105	7/7	0.16	-1.48	126,126,126,126	0
86	OHX	2	2063	7/7	0.19	-1.48	135,135,135,135	0
85	MG	5	3828	1/1	0.20	-1.49	43,43,43,43	0
86	OHX	6	2153	7/7	0.15	-1.49	145,145,145,145	0
86	OHX	1	3936	7/7	0.16	-1.49	116,116,116,116	0
85	MG	5	3567	1/1	0.23	-1.49	28,28,28,28	0
85	MG	1	3589	1/1	0.23	-1.50	40,40,40,40	0
86	OHX	2	2033	7/7	0.14	-1.50	104,104,104,104	0
85	MG	1	3686	1/1	0.15	-1.50	96,96,96,96	0
85	MG	3	203	1/1	0.20	-1.50	97,97,97,97	0
86	OHX	6	2068	7/7	0.15	-1.50	102,102,102,102	0
86	OHX	2	2034	7/7	0.18	-1.51	110,110,110,110	0
86	OHX	1	4000	7/7	0.14	-1.51	133,133,133,133	0
86	OHX	1	3919	7/7	0.15	-1.52	98,98,98,98	0
86	OHX	1	3920	7/7	0.15	-1.52	85,85,85,85	0
88	ZN	D6	500	1/1	0.12	-1.52	80,80,80,80	0
88	ZN	D9	101	1/1	0.12	-1.52	81,81,81,81	0
85	MG	1	3564	1/1	0.23	-1.52	38,38,38,38	0
86	OHX	2	2129	7/7	0.12	-1.52	149,149,149,149	0
85	MG	1	3616	1/1	0.12	-1.52	67,67,67,67	0
85	MG	5	3498	1/1	0.20	-1.52	36,36,36,36	0
85	MG	5	3676	1/1	0.19	-1.53	47,47,47,47	0
85	MG	1	3593	1/1	0.23	-1.53	29,29,29,29	0
86	OHX	5	3957	7/7	0.16	-1.53	96,96,96,96	0
85	MG	5	3741	1/1	0.13	-1.54	40,40,40,40	0
86	OHX	6	2163	7/7	0.15	-1.54	198,198,198,198	0
86	OHX	2	2071	7/7	0.14	-1.54	130,130,130,130	0
86	OHX	6	2119	7/7	0.09	-1.54	127,127,127,127	0
86	OHX	2	2075	7/7	0.23	-1.54	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2148	7/7	0.19	-1.54	115,115,115,115	0
86	OHX	4	234	7/7	0.20	-1.55	126,126,126,126	0
86	OHX	1	4087	7/7	0.21	-1.55	94,94,94,94	0
86	OHX	2	2155	7/7	0.14	-1.55	247,247,247,247	0
86	OHX	5	4114	7/7	0.15	-1.55	124,124,124,124	0
85	MG	1	3417	1/1	0.15	-1.55	35,35,35,35	0
86	OHX	2	2087	7/7	0.18	-1.56	122,122,122,122	0
86	OHX	6	2081	7/7	0.12	-1.56	109,109,109,109	0
86	OHX	1	3929	7/7	0.16	-1.56	106,106,106,106	0
86	OHX	5	4002	7/7	0.15	-1.56	80,80,80,80	0
86	OHX	1	3888	7/7	0.17	-1.56	75,75,75,75	0
86	OHX	2	2102	7/7	0.11	-1.56	148,148,148,148	0
85	MG	5	3484	1/1	0.18	-1.56	51,51,51,51	0
85	MG	12	301	1/1	0.18	-1.57	38,38,38,38	0
86	OHX	1	4064	7/7	0.14	-1.57	151,151,151,151	0
86	OHX	5	3988	7/7	0.13	-1.58	107,107,107,107	0
85	MG	8	213	1/1	0.18	-1.58	59,59,59,59	0
86	OHX	S8	302	7/7	0.16	-1.59	173,173,173,173	0
86	OHX	1	4135	7/7	0.19	-1.59	115,115,115,115	0
85	MG	6	1951	1/1	0.23	-1.60	68,68,68,68	0
86	OHX	6	2150	7/7	0.16	-1.60	125,125,125,125	0
85	MG	5	3599	1/1	0.21	-1.60	46,46,46,46	0
85	MG	1	3424	1/1	0.21	-1.61	45,45,45,45	0
85	MG	1	3829	1/1	0.28	-1.61	37,37,37,37	0
86	OHX	2	2154	7/7	0.14	-1.61	149,149,149,149	0
85	MG	5	3834	1/1	0.13	-1.61	68,68,68,68	0
85	MG	1	3756	1/1	0.17	-1.62	52,52,52,52	0
85	MG	m7	202	1/1	0.23	-1.62	32,32,32,32	0
85	MG	1	3652	1/1	0.19	-1.62	50,50,50,50	0
85	MG	6	2015	1/1	0.18	-1.63	78,78,78,78	0
85	MG	1	3634	1/1	0.18	-1.63	48,48,48,48	0
86	OHX	5	4020	7/7	0.15	-1.63	125,125,125,125	0
85	MG	5	3483	1/1	0.13	-1.64	69,69,69,69	0
86	OHX	1	4010	7/7	0.11	-1.64	140,140,140,140	0
86	OHX	1	3989	7/7	0.16	-1.64	135,135,135,135	0
86	OHX	c8	203	7/7	0.10	-1.64	153,153,153,153	0
86	OHX	6	2121	7/7	0.09	-1.64	147,147,147,147	0
85	MG	5	3856	1/1	0.27	-1.64	76,76,76,76	0
86	OHX	1	3898	7/7	0.15	-1.65	72,72,72,72	0
86	OHX	2	2098	7/7	0.11	-1.65	174,174,174,174	0
85	MG	2	2005	1/1	0.15	-1.65	64,64,64,64	0
86	OHX	5	3932	7/7	0.19	-1.65	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2048	7/7	0.20	-1.66	69,69,69,69	0
85	MG	1	3806	1/1	0.21	-1.66	56,56,56,56	0
85	MG	5	3842	1/1	0.19	-1.66	68,68,68,68	0
85	MG	1	3843	1/1	0.22	-1.66	37,37,37,37	0
85	MG	5	3446	1/1	0.18	-1.67	43,43,43,43	0
86	OHX	5	3993	7/7	0.15	-1.67	108,108,108,108	0
86	OHX	5	3954	7/7	0.14	-1.67	78,78,78,78	0
86	OHX	6	2074	7/7	0.13	-1.67	90,90,90,90	0
86	OHX	6	2067	7/7	0.16	-1.68	94,94,94,94	0
86	OHX	5	4064	7/7	0.12	-1.68	160,160,160,160	0
86	OHX	2	2112	7/7	0.18	-1.68	128,128,128,128	0
85	MG	1	4220	1/1	0.17	-1.68	48,48,48,48	0
86	OHX	5	4191	7/7	0.12	-1.68	148,148,148,148	0
86	OHX	1	3967	7/7	0.14	-1.68	109,109,109,109	0
86	OHX	7	216	7/7	0.17	-1.69	97,97,97,97	0
86	OHX	4	228	7/7	0.14	-1.69	123,123,123,123	0
86	OHX	2	2068	7/7	0.10	-1.69	146,146,146,146	0
85	MG	1	3734	1/1	0.20	-1.70	34,34,34,34	0
86	OHX	4	222	7/7	0.22	-1.70	59,59,59,59	0
86	OHX	1	3975	7/7	0.19	-1.70	100,100,100,100	0
86	OHX	1	4016	7/7	0.15	-1.71	140,140,140,140	0
86	OHX	O3	202	7/7	0.19	-1.71	126,126,126,126	0
86	OHX	1	4082	7/7	0.12	-1.71	144,144,144,144	0
85	MG	5	3557	1/1	0.23	-1.71	28,28,28,28	0
86	OHX	1	4129	7/7	0.19	-1.71	158,158,158,158	0
85	MG	6	1973	1/1	0.22	-1.71	50,50,50,50	0
86	OHX	2	2099	7/7	0.09	-1.71	156,156,156,156	0
86	OHX	2	2040	7/7	0.14	-1.72	103,103,103,103	0
85	MG	6	1914	1/1	0.21	-1.72	70,70,70,70	0
86	OHX	1	3909	7/7	0.15	-1.72	86,86,86,86	0
86	OHX	5	4201	7/7	0.14	-1.72	130,130,130,130	0
86	OHX	1	3925	7/7	0.19	-1.72	104,104,104,104	0
85	MG	1	3454	1/1	0.20	-1.72	43,43,43,43	0
85	MG	1	3437	1/1	0.15	-1.73	35,35,35,35	0
85	MG	1	3569	1/1	0.18	-1.73	26,26,26,26	0
86	OHX	6	2064	7/7	0.15	-1.73	104,104,104,104	0
85	MG	1	3489	1/1	0.20	-1.73	54,54,54,54	0
86	OHX	5	4214	7/7	0.20	-1.73	133,133,133,133	0
86	OHX	4	227	7/7	0.18	-1.73	108,108,108,108	0
86	OHX	1	4079	7/7	0.12	-1.74	126,126,126,126	0
86	OHX	1	3982	7/7	0.17	-1.74	113,113,113,113	0
86	OHX	6	2066	7/7	0.13	-1.74	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4223	7/7	0.13	-1.74	153,153,153,153	0
85	MG	1	3574	1/1	0.25	-1.75	24,24,24,24	0
86	OHX	2	2175	7/7	0.14	-1.75	178,178,178,178	0
86	OHX	2	2133	7/7	0.11	-1.76	163,163,163,163	0
85	MG	5	3502	1/1	0.17	-1.76	45,45,45,45	0
86	OHX	5	3945	7/7	0.19	-1.77	90,90,90,90	0
85	MG	6	1938	1/1	0.15	-1.77	45,45,45,45	0
86	OHX	5	4025	7/7	0.12	-1.77	113,113,113,113	0
85	MG	5	3857	1/1	0.17	-1.78	65,65,65,65	0
86	OHX	6	2062	7/7	0.15	-1.78	86,86,86,86	0
86	OHX	5	3934	7/7	0.18	-1.78	73,73,73,73	0
85	MG	5	3820	1/1	0.10	-1.78	75,75,75,75	0
85	MG	1	4217	1/1	0.12	-1.78	32,32,32,32	0
85	MG	m5	304	1/1	0.27	-1.79	108,108,108,108	0
86	OHX	Q2	503	7/7	0.17	-1.79	86,86,86,86	0
86	OHX	5	4029	7/7	0.16	-1.79	101,101,101,101	0
86	OHX	5	3912	7/7	0.19	-1.79	59,59,59,59	0
86	OHX	6	2058	7/7	0.19	-1.79	94,94,94,94	0
86	OHX	2	2067	7/7	0.12	-1.79	140,140,140,140	0
86	OHX	1	3980	7/7	0.14	-1.79	112,112,112,112	0
86	OHX	6	2057	7/7	0.15	-1.79	89,89,89,89	0
85	MG	5	3412	1/1	0.18	-1.79	33,33,33,33	0
85	MG	5	3667	1/1	0.17	-1.80	51,51,51,51	0
86	OHX	5	4035	7/7	0.12	-1.80	130,130,130,130	0
86	OHX	5	3916	7/7	0.17	-1.80	70,70,70,70	0
86	OHX	2	2050	7/7	0.13	-1.81	127,127,127,127	0
85	MG	5	3805	1/1	0.14	-1.81	65,65,65,65	0
86	OHX	6	2085	7/7	0.14	-1.81	109,109,109,109	0
86	OHX	5	4008	7/7	0.13	-1.82	80,80,80,80	0
88	ZN	q0	201	1/1	0.15	-1.82	37,37,37,37	0
86	OHX	L3	405	7/7	0.10	-1.82	162,162,162,162	0
85	MG	5	3747	1/1	0.21	-1.83	39,39,39,39	0
86	OHX	N1	201	7/7	0.18	-1.83	70,70,70,70	0
85	MG	1	3557	1/1	0.17	-1.83	49,49,49,49	0
86	OHX	1	3944	7/7	0.14	-1.83	112,112,112,112	0
86	OHX	5	4037	7/7	0.13	-1.84	125,125,125,125	0
86	OHX	o2	201	7/7	0.13	-1.84	105,105,105,105	0
85	MG	5	3611	1/1	0.16	-1.84	39,39,39,39	0
86	OHX	1	4003	7/7	0.17	-1.85	124,124,124,124	0
85	MG	c8	202	1/1	0.18	-1.85	66,66,66,66	0
86	OHX	1	4088	7/7	0.10	-1.85	141,141,141,141	0
85	MG	2	2023	1/1	0.14	-1.86	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4018	7/7	0.12	-1.86	128,128,128,128	0
86	OHX	1	3941	7/7	0.13	-1.86	99,99,99,99	0
86	OHX	2	2036	7/7	0.18	-1.86	103,103,103,103	0
85	MG	1	3438	1/1	0.17	-1.87	43,43,43,43	0
85	MG	1	3577	1/1	0.23	-1.87	25,25,25,25	0
86	OHX	7	224	7/7	0.16	-1.87	150,150,150,150	0
85	MG	6	1983	1/1	0.15	-1.87	80,80,80,80	0
86	OHX	5	3923	7/7	0.18	-1.88	66,66,66,66	0
86	OHX	5	4229	7/7	0.12	-1.88	194,194,194,194	0
86	OHX	2	2127	7/7	0.16	-1.88	142,142,142,142	0
86	OHX	2	2030	7/7	0.15	-1.88	107,107,107,107	0
86	OHX	6	2130	7/7	0.17	-1.89	128,128,128,128	0
85	MG	5	3624	1/1	0.17	-1.89	46,46,46,46	0
86	OHX	1	4009	7/7	0.14	-1.89	136,136,136,136	0
86	OHX	1	3942	7/7	0.15	-1.89	106,106,106,106	0
86	OHX	L3	404	7/7	0.13	-1.90	118,118,118,118	0
85	MG	1	3532	1/1	0.20	-1.90	37,37,37,37	0
85	MG	5	3417	1/1	0.15	-1.90	29,29,29,29	0
85	MG	1	3846	1/1	0.20	-1.90	45,45,45,45	0
85	MG	2	1993	1/1	0.14	-1.91	67,67,67,67	0
86	OHX	5	4091	7/7	0.17	-1.91	117,117,117,117	0
85	MG	2	1930	1/1	0.14	-1.91	64,64,64,64	0
86	OHX	sR	401	7/7	0.10	-1.91	169,169,169,169	0
86	OHX	5	4227	7/7	0.18	-1.91	142,142,142,142	0
86	OHX	4	232	7/7	0.14	-1.91	147,147,147,147	0
86	OHX	6	2094	7/7	0.10	-1.91	135,135,135,135	0
86	OHX	1	4143	7/7	0.15	-1.91	122,122,122,122	0
86	OHX	6	2198	7/7	0.20	-1.91	153,153,153,153	0
86	OHX	5	4007	7/7	0.12	-1.91	126,126,126,126	0
86	OHX	1	3880	7/7	0.19	-1.92	68,68,68,68	0
86	OHX	1	4123	7/7	0.09	-1.92	153,153,153,153	0
85	MG	1	3528	1/1	0.19	-1.93	46,46,46,46	0
86	OHX	5	4098	7/7	0.16	-1.93	144,144,144,144	0
86	OHX	1	4012	7/7	0.17	-1.93	125,125,125,125	0
86	OHX	5	4192	7/7	0.12	-1.93	132,132,132,132	0
86	OHX	1	3908	7/7	0.14	-1.93	100,100,100,100	0
85	MG	5	3692	1/1	0.20	-1.94	52,52,52,52	0
86	OHX	5	4236	7/7	0.15	-1.94	144,144,144,144	0
85	MG	1	3733	1/1	0.20	-1.95	52,52,52,52	0
86	OHX	2	2058	7/7	0.08	-1.95	144,144,144,144	0
86	OHX	1	3905	7/7	0.19	-1.95	91,91,91,91	0
85	MG	5	3552	1/1	0.19	-1.95	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	s4	301	7/7	0.14	-1.95	149,149,149,149	0
85	MG	5	3453	1/1	0.11	-1.95	102,102,102,102	0
86	OHX	1	4042	7/7	0.09	-1.96	117,117,117,117	0
86	OHX	1	4030	7/7	0.12	-1.97	106,106,106,106	0
86	OHX	1	3993	7/7	0.14	-1.97	103,103,103,103	0
85	MG	5	3638	1/1	0.21	-1.97	50,50,50,50	0
86	OHX	5	4161	7/7	0.15	-1.97	134,134,134,134	0
86	OHX	6	2125	7/7	0.13	-1.98	142,142,142,142	0
86	OHX	1	3974	7/7	0.15	-1.98	99,99,99,99	0
86	OHX	2	2164	7/7	0.11	-1.98	172,172,172,172	0
86	OHX	2	2078	7/7	0.12	-1.99	119,119,119,119	0
85	MG	5	3542	1/1	0.19	-1.99	31,31,31,31	0
86	OHX	2	2120	7/7	0.14	-1.99	158,158,158,158	0
86	OHX	5	4005	7/7	0.16	-1.99	111,111,111,111	0
86	OHX	5	4118	7/7	0.13	-1.99	139,139,139,139	0
86	OHX	1	4108	7/7	0.17	-1.99	148,148,148,148	0
85	MG	2	1960	1/1	0.21	-2.00	57,57,57,57	0
86	OHX	2	2037	7/7	0.12	-2.00	97,97,97,97	0
85	MG	6	2042	1/1	0.20	-2.01	52,52,52,52	0
86	OHX	2	2173	7/7	0.15	-2.01	151,151,151,151	0
86	OHX	s1	302	7/7	0.19	-2.01	86,86,86,86	0
86	OHX	1	4155	7/7	0.13	-2.01	120,120,120,120	0
86	OHX	1	3904	7/7	0.16	-2.02	87,87,87,87	0
86	OHX	2	2114	7/7	0.16	-2.02	138,138,138,138	0
85	MG	1	3580	1/1	0.14	-2.02	43,43,43,43	0
86	OHX	2	2140	7/7	0.12	-2.02	167,167,167,167	0
86	OHX	c5	201	7/7	0.11	-2.03	176,176,176,176	0
85	MG	6	1978	1/1	0.15	-2.03	77,77,77,77	0
86	OHX	5	4250	7/7	0.12	-2.03	143,143,143,143	0
86	OHX	1	3945	7/7	0.11	-2.04	110,110,110,110	0
85	MG	6	2205	1/1	0.12	-2.04	54,54,54,54	0
85	MG	6	1993	1/1	0.12	-2.04	57,57,57,57	0
85	MG	1	3654	1/1	0.19	-2.04	34,34,34,34	0
86	OHX	1	3914	7/7	0.18	-2.05	100,100,100,100	0
86	OHX	6	2053	7/7	0.18	-2.05	89,89,89,89	0
86	OHX	2	2049	7/7	0.11	-2.05	118,118,118,118	0
85	MG	5	3450	1/1	0.19	-2.06	38,38,38,38	0
86	OHX	5	4061	7/7	0.13	-2.06	116,116,116,116	0
86	OHX	5	4110	7/7	0.15	-2.06	98,98,98,98	0
86	OHX	1	4182	7/7	0.13	-2.06	153,153,153,153	0
88	ZN	O7	101	1/1	0.14	-2.06	41,41,41,41	0
85	MG	5	3439	1/1	0.21	-2.06	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	sM	301	1/1	0.12	-2.07	48,48,48,48	0
85	MG	5	3733	1/1	0.15	-2.07	43,43,43,43	0
86	OHX	5	3924	7/7	0.20	-2.07	74,74,74,74	0
86	OHX	1	4094	7/7	0.14	-2.08	152,152,152,152	0
85	MG	1	3772	1/1	0.23	-2.08	62,62,62,62	0
86	OHX	1	3949	7/7	0.16	-2.09	115,115,115,115	0
85	MG	5	3616	1/1	0.16	-2.09	49,49,49,49	0
86	OHX	5	4068	7/7	0.16	-2.09	117,117,117,117	0
85	MG	2	1942	1/1	0.12	-2.09	64,64,64,64	0
85	MG	1	3663	1/1	0.12	-2.10	53,53,53,53	0
85	MG	3	211	1/1	0.15	-2.10	85,85,85,85	0
86	OHX	5	3931	7/7	0.15	-2.10	68,68,68,68	0
86	OHX	1	4035	7/7	0.12	-2.11	149,149,149,149	0
86	OHX	6	2171	7/7	0.11	-2.11	149,149,149,149	0
85	MG	1	3701	1/1	0.25	-2.11	50,50,50,50	0
86	OHX	5	3955	7/7	0.13	-2.11	99,99,99,99	0
85	MG	1	3789	1/1	0.11	-2.11	84,84,84,84	0
86	OHX	1	3883	7/7	0.18	-2.11	70,70,70,70	0
85	MG	5	3880	1/1	0.15	-2.11	26,26,26,26	0
86	OHX	n3	203	7/7	0.12	-2.12	92,92,92,92	0
86	OHX	2	2123	7/7	0.14	-2.12	151,151,151,151	0
86	OHX	l3	403	7/7	0.10	-2.12	106,106,106,106	0
86	OHX	1	3991	7/7	0.12	-2.13	108,108,108,108	0
86	OHX	SR	401	7/7	0.09	-2.13	175,175,175,175	0
86	OHX	6	2099	7/7	0.13	-2.13	164,164,164,164	0
86	OHX	l5	303	7/7	0.09	-2.13	147,147,147,147	0
85	MG	1	3656	1/1	0.19	-2.13	45,45,45,45	0
86	OHX	4	231	7/7	0.12	-2.15	124,124,124,124	0
85	MG	1	3699	1/1	0.23	-2.15	46,46,46,46	0
85	MG	M3	203	1/1	0.15	-2.16	33,33,33,33	0
86	OHX	5	4163	7/7	0.15	-2.16	123,123,123,123	0
86	OHX	2	2077	7/7	0.16	-2.16	141,141,141,141	0
85	MG	5	3822	1/1	0.18	-2.16	55,55,55,55	0
85	MG	5	3886	1/1	0.19	-2.16	57,57,57,57	0
86	OHX	6	2201	7/7	0.06	-2.16	193,193,193,193	0
86	OHX	5	4117	7/7	0.14	-2.17	110,110,110,110	0
85	MG	5	3626	1/1	0.18	-2.17	34,34,34,34	0
86	OHX	5	4165	7/7	0.17	-2.17	194,194,194,194	0
85	MG	1	3448	1/1	0.22	-2.17	27,27,27,27	0
86	OHX	6	2151	7/7	0.14	-2.18	169,169,169,169	0
85	MG	5	3491	1/1	0.26	-2.18	62,62,62,62	0
86	OHX	1	4130	7/7	0.11	-2.19	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3987	7/7	0.19	-2.20	122,122,122,122	0
86	OHX	1	3983	7/7	0.13	-2.20	125,125,125,125	0
85	MG	1	3514	1/1	0.21	-2.20	37,37,37,37	0
86	OHX	1	4059	7/7	0.12	-2.21	156,156,156,156	0
86	OHX	1	4149	7/7	0.14	-2.21	155,155,155,155	0
88	ZN	q2	501	1/1	0.11	-2.22	95,95,95,95	0
86	OHX	6	2158	7/7	0.10	-2.22	119,119,119,119	0
85	MG	5	3580	1/1	0.22	-2.22	38,38,38,38	0
86	OHX	5	4036	7/7	0.16	-2.23	135,135,135,135	0
86	OHX	2	2115	7/7	0.09	-2.23	164,164,164,164	0
86	OHX	1	4116	7/7	0.10	-2.25	132,132,132,132	0
86	OHX	1	3995	7/7	0.09	-2.25	148,148,148,148	0
86	OHX	6	2105	7/7	0.15	-2.26	121,121,121,121	0
85	MG	5	3590	1/1	0.23	-2.26	32,32,32,32	0
86	OHX	2	2057	7/7	0.12	-2.26	135,135,135,135	0
86	OHX	5	3958	7/7	0.13	-2.27	91,91,91,91	0
85	MG	6	1941	1/1	0.20	-2.27	53,53,53,53	0
86	OHX	m4	201	7/7	0.12	-2.27	219,219,219,219	0
85	MG	q1	101	1/1	0.15	-2.27	40,40,40,40	0
86	OHX	1	4112	7/7	0.09	-2.27	181,181,181,181	0
86	OHX	2	2047	7/7	0.13	-2.28	117,117,117,117	0
86	OHX	1	3910	7/7	0.15	-2.28	87,87,87,87	0
85	MG	5	3475	1/1	0.16	-2.28	37,37,37,37	0
86	OHX	3	218	7/7	0.11	-2.28	123,123,123,123	0
85	MG	1	3840	1/1	0.17	-2.28	66,66,66,66	0
85	MG	1	3780	1/1	0.17	-2.28	48,48,48,48	0
85	MG	5	3643	1/1	0.19	-2.30	46,46,46,46	0
86	OHX	1	3901	7/7	0.15	-2.30	77,77,77,77	0
85	MG	1	3531	1/1	0.21	-2.30	24,24,24,24	0
86	OHX	8	222	7/7	0.11	-2.31	129,129,129,129	0
85	MG	1	3496	1/1	0.18	-2.31	38,38,38,38	0
86	OHX	1	4004	7/7	0.14	-2.31	111,111,111,111	0
85	MG	5	3559	1/1	0.15	-2.31	34,34,34,34	0
86	OHX	5	4040	7/7	0.13	-2.31	132,132,132,132	0
85	MG	5	3653	1/1	0.19	-2.31	31,31,31,31	0
86	OHX	6	2152	7/7	0.13	-2.32	151,151,151,151	0
85	MG	M9	202	1/1	0.20	-2.33	68,68,68,68	0
85	MG	5	3615	1/1	0.11	-2.33	53,53,53,53	0
85	MG	5	3628	1/1	0.19	-2.34	58,58,58,58	0
86	OHX	2	2072	7/7	0.11	-2.34	132,132,132,132	0
86	OHX	2	2150	7/7	0.13	-2.34	197,197,197,197	0
88	ZN	o7	501	1/1	0.13	-2.35	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3850	1/1	0.21	-2.35	47,47,47,47	0
86	OHX	6	2061	7/7	0.14	-2.36	88,88,88,88	0
85	MG	6	2031	1/1	0.18	-2.36	70,70,70,70	0
86	OHX	6	2134	7/7	0.19	-2.36	134,134,134,134	0
85	MG	5	3660	1/1	0.18	-2.36	30,30,30,30	0
85	MG	L4	401	1/1	0.18	-2.37	68,68,68,68	0
86	OHX	5	4054	7/7	0.16	-2.37	115,115,115,115	0
86	OHX	1	4127	7/7	0.13	-2.38	135,135,135,135	0
86	OHX	5	3926	7/7	0.17	-2.38	63,63,63,63	0
86	OHX	5	4140	7/7	0.13	-2.38	146,146,146,146	0
86	OHX	1	4090	7/7	0.19	-2.39	128,128,128,128	0
86	OHX	5	3946	7/7	0.16	-2.39	80,80,80,80	0
86	OHX	3	221	7/7	0.11	-2.40	150,150,150,150	0
86	OHX	7	226	7/7	0.14	-2.40	157,157,157,157	0
86	OHX	5	4011	7/7	0.13	-2.40	113,113,113,113	0
86	OHX	6	2193	7/7	0.10	-2.40	195,195,195,195	0
86	OHX	5	4053	7/7	0.18	-2.40	108,108,108,108	0
86	OHX	1	3896	7/7	0.18	-2.40	89,89,89,89	0
86	OHX	1	3971	7/7	0.13	-2.40	132,132,132,132	0
85	MG	s1	301	1/1	0.17	-2.40	78,78,78,78	0
86	OHX	5	4048	7/7	0.11	-2.41	120,120,120,120	0
86	OHX	5	3999	7/7	0.14	-2.41	108,108,108,108	0
85	MG	m6	202	1/1	0.15	-2.41	32,32,32,32	0
86	OHX	7	220	7/7	0.14	-2.41	106,106,106,106	0
86	OHX	1	3956	7/7	0.13	-2.41	111,111,111,111	0
85	MG	2	1912	1/1	0.17	-2.42	66,66,66,66	0
86	OHX	5	3942	7/7	0.15	-2.42	87,87,87,87	0
86	OHX	1	3979	7/7	0.09	-2.44	119,119,119,119	0
86	OHX	2	2138	7/7	0.09	-2.44	147,147,147,147	0
86	OHX	2	2062	7/7	0.12	-2.44	133,133,133,133	0
86	OHX	8	224	7/7	0.11	-2.44	126,126,126,126	0
85	MG	1	3762	1/1	0.14	-2.45	51,51,51,51	0
86	OHX	1	4053	7/7	0.18	-2.45	119,119,119,119	0
86	OHX	5	4130	7/7	0.10	-2.45	145,145,145,145	0
86	OHX	6	2076	7/7	0.17	-2.45	115,115,115,115	0
85	MG	5	3687	1/1	0.11	-2.46	79,79,79,79	0
85	MG	6	1939	1/1	0.18	-2.46	62,62,62,62	0
86	OHX	q2	502	7/7	0.13	-2.46	87,87,87,87	0
86	OHX	1	4060	7/7	0.14	-2.46	158,158,158,158	0
86	OHX	1	4046	7/7	0.11	-2.46	126,126,126,126	0
85	MG	n8	201	1/1	0.13	-2.46	37,37,37,37	0
85	MG	5	3586	1/1	0.25	-2.46	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	o3	202	7/7	0.14	-2.46	111,111,111,111	0
86	OHX	2	2091	7/7	0.12	-2.46	124,124,124,124	0
85	MG	1	3651	1/1	0.22	-2.46	74,74,74,74	0
85	MG	5	3622	1/1	0.17	-2.46	37,37,37,37	0
86	OHX	6	2133	7/7	0.13	-2.47	161,161,161,161	0
85	MG	5	3592	1/1	0.15	-2.47	27,27,27,27	0
86	OHX	8	223	7/7	0.13	-2.47	128,128,128,128	0
86	OHX	1	3881	7/7	0.17	-2.48	64,64,64,64	0
86	OHX	6	2107	7/7	0.12	-2.49	120,120,120,120	0
86	OHX	2	2027	7/7	0.17	-2.49	86,86,86,86	0
85	MG	1	3669	1/1	0.11	-2.49	63,63,63,63	0
86	OHX	6	2108	7/7	0.08	-2.50	128,128,128,128	0
86	OHX	1	4122	7/7	0.09	-2.50	146,146,146,146	0
86	OHX	5	4027	7/7	0.16	-2.51	112,112,112,112	0
85	MG	6	1986	1/1	0.13	-2.51	69,69,69,69	0
86	OHX	2	2024	7/7	0.21	-2.52	76,76,76,76	0
86	OHX	M5	303	7/7	0.17	-2.52	116,116,116,116	0
86	OHX	1	3924	7/7	0.13	-2.53	92,92,92,92	0
86	OHX	1	3943	7/7	0.15	-2.53	95,95,95,95	0
86	OHX	4	225	7/7	0.16	-2.53	94,94,94,94	0
86	OHX	1	4039	7/7	0.07	-2.53	137,137,137,137	0
86	OHX	2	2171	7/7	0.20	-2.53	177,177,177,177	0
86	OHX	5	4087	7/7	0.10	-2.54	131,131,131,131	0
86	OHX	2	2070	7/7	0.11	-2.55	117,117,117,117	0
86	OHX	5	4150	7/7	0.21	-2.55	153,153,153,153	0
85	MG	m7	204	1/1	0.16	-2.55	32,32,32,32	0
86	OHX	6	2077	7/7	0.12	-2.56	99,99,99,99	0
86	OHX	6	2117	7/7	0.09	-2.56	115,115,115,115	0
86	OHX	6	2086	7/7	0.09	-2.56	118,118,118,118	0
86	OHX	2	2110	7/7	0.11	-2.56	161,161,161,161	0
86	OHX	3	226	7/7	0.11	-2.56	149,149,149,149	0
85	MG	1	3639	1/1	0.16	-2.57	70,70,70,70	0
86	OHX	l5	304	7/7	0.09	-2.57	148,148,148,148	0
86	OHX	5	4080	7/7	0.13	-2.57	122,122,122,122	0
86	OHX	1	4029	7/7	0.15	-2.58	138,138,138,138	0
85	MG	1	3827	1/1	0.20	-2.58	52,52,52,52	0
86	OHX	5	4093	7/7	0.15	-2.59	119,119,119,119	0
86	OHX	2	2074	7/7	0.09	-2.59	148,148,148,148	0
85	MG	1	3826	1/1	0.19	-2.59	29,29,29,29	0
85	MG	1	3567	1/1	0.14	-2.59	35,35,35,35	0
86	OHX	2	2167	7/7	0.12	-2.59	163,163,163,163	0
85	MG	5	3787	1/1	0.13	-2.60	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	3961	7/7	0.18	-2.60	79,79,79,79	0
86	OHX	5	4044	7/7	0.16	-2.60	106,106,106,106	0
86	OHX	2	2166	7/7	0.09	-2.61	129,129,129,129	0
86	OHX	2	2089	7/7	0.13	-2.61	138,138,138,138	0
86	OHX	1	4055	7/7	0.13	-2.61	106,106,106,106	0
86	OHX	1	3933	7/7	0.16	-2.62	101,101,101,101	0
85	MG	1	3748	1/1	0.19	-2.62	57,57,57,57	0
86	OHX	2	2039	7/7	0.14	-2.62	106,106,106,106	0
85	MG	1	3825	1/1	0.15	-2.63	62,62,62,62	0
85	MG	1	3794	1/1	0.21	-2.63	29,29,29,29	0
85	MG	1	3494	1/1	0.16	-2.63	45,45,45,45	0
86	OHX	1	4047	7/7	0.09	-2.64	144,144,144,144	0
86	OHX	6	2195	7/7	0.10	-2.64	186,186,186,186	0
86	OHX	5	4106	7/7	0.13	-2.64	120,120,120,120	0
85	MG	1	3512	1/1	0.21	-2.64	25,25,25,25	0
86	OHX	1	4086	7/7	0.14	-2.64	133,133,133,133	0
86	OHX	8	220	7/7	0.11	-2.64	116,116,116,116	0
86	OHX	6	2118	7/7	0.12	-2.64	143,143,143,143	0
86	OHX	2	2142	7/7	0.16	-2.65	140,140,140,140	0
85	MG	2	1975	1/1	0.16	-2.65	62,62,62,62	0
86	OHX	6	2138	7/7	0.10	-2.65	130,130,130,130	0
86	OHX	6	2111	7/7	0.19	-2.65	128,128,128,128	0
85	MG	1	3491	1/1	0.16	-2.66	34,34,34,34	0
86	OHX	2	2094	7/7	0.12	-2.66	151,151,151,151	0
86	OHX	5	4121	7/7	0.10	-2.66	154,154,154,154	0
86	OHX	2	2046	7/7	0.13	-2.66	107,107,107,107	0
86	OHX	1	4145	7/7	0.15	-2.66	154,154,154,154	0
86	OHX	1	3969	7/7	0.14	-2.66	108,108,108,108	0
86	OHX	6	2115	7/7	0.14	-2.67	130,130,130,130	0
86	OHX	5	4232	7/7	0.12	-2.68	179,179,179,179	0
85	MG	5	3454	1/1	0.15	-2.68	30,30,30,30	0
85	MG	1	4222	1/1	0.15	-2.68	34,34,34,34	0
86	OHX	5	4218	7/7	0.12	-2.69	145,145,145,145	0
86	OHX	5	4208	7/7	0.10	-2.69	160,160,160,160	0
86	OHX	D3	202	7/7	0.14	-2.70	145,145,145,145	0
86	OHX	1	4041	7/7	0.11	-2.70	112,112,112,112	0
86	OHX	1	4092	7/7	0.12	-2.71	145,145,145,145	0
86	OHX	5	3977	7/7	0.13	-2.71	102,102,102,102	0
86	OHX	1	4103	7/7	0.15	-2.71	133,133,133,133	0
85	MG	1	4221	1/1	0.11	-2.72	40,40,40,40	0
86	OHX	1	4106	7/7	0.15	-2.73	142,142,142,142	0
85	MG	1	3495	1/1	0.16	-2.73	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	L8	301	1/1	0.24	-2.73	63,63,63,63	0
85	MG	1	3474	1/1	0.20	-2.74	23,23,23,23	0
85	MG	5	3641	1/1	0.17	-2.75	37,37,37,37	0
86	OHX	6	2059	7/7	0.15	-2.75	87,87,87,87	0
86	OHX	7	223	7/7	0.17	-2.75	122,122,122,122	0
85	MG	5	3507	1/1	0.22	-2.75	27,27,27,27	0
85	MG	1	3558	1/1	0.19	-2.75	27,27,27,27	0
86	OHX	1	3992	7/7	0.10	-2.76	137,137,137,137	0
86	OHX	6	2087	7/7	0.12	-2.76	126,126,126,126	0
85	MG	6	1961	1/1	0.16	-2.76	80,80,80,80	0
86	OHX	1	4067	7/7	0.16	-2.76	126,126,126,126	0
85	MG	1	3450	1/1	0.18	-2.76	39,39,39,39	0
86	OHX	5	4164	7/7	0.15	-2.78	159,159,159,159	0
86	OHX	5	3996	7/7	0.14	-2.79	115,115,115,115	0
86	OHX	8	221	7/7	0.10	-2.79	119,119,119,119	0
85	MG	5	3793	1/1	0.19	-2.79	89,89,89,89	0
86	OHX	1	4084	7/7	0.09	-2.80	195,195,195,195	0
85	MG	1	3441	1/1	0.15	-2.80	46,46,46,46	0
86	OHX	2	2106	7/7	0.21	-2.80	127,127,127,127	0
86	OHX	5	4032	7/7	0.16	-2.80	119,119,119,119	0
86	OHX	m6	203	7/7	0.12	-2.81	100,100,100,100	0
86	OHX	C5	201	7/7	0.09	-2.81	179,179,179,179	0
86	OHX	5	3983	7/7	0.11	-2.82	91,91,91,91	0
86	OHX	2	2042	7/7	0.15	-2.83	99,99,99,99	0
86	OHX	1	3916	7/7	0.15	-2.83	92,92,92,92	0
85	MG	6	1950	1/1	0.17	-2.83	44,44,44,44	0
86	OHX	1	3957	7/7	0.12	-2.83	113,113,113,113	0
85	MG	5	3422	1/1	0.13	-2.84	43,43,43,43	0
86	OHX	1	4028	7/7	0.12	-2.84	116,116,116,116	0
86	OHX	5	4059	7/7	0.17	-2.84	119,119,119,119	0
86	OHX	1	3999	7/7	0.13	-2.84	106,106,106,106	0
85	MG	1	3790	1/1	0.17	-2.84	60,60,60,60	0
86	OHX	1	3931	7/7	0.14	-2.85	84,84,84,84	0
85	MG	1	3433	1/1	0.17	-2.85	37,37,37,37	0
86	OHX	6	2166	7/7	0.11	-2.85	189,189,189,189	0
86	OHX	6	2194	7/7	0.11	-2.86	173,173,173,173	0
85	MG	5	3749	1/1	0.13	-2.86	52,52,52,52	0
86	OHX	5	4079	7/7	0.16	-2.87	139,139,139,139	0
86	OHX	1	3935	7/7	0.15	-2.87	98,98,98,98	0
85	MG	5	3670	1/1	0.13	-2.87	49,49,49,49	0
86	OHX	5	4199	7/7	0.14	-2.88	94,94,94,94	0
86	OHX	2	2109	7/7	0.15	-2.88	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	5	3427	1/1	0.20	-2.89	48,48,48,48	0
86	OHX	2	2043	7/7	0.15	-2.89	104,104,104,104	0
85	MG	5	3808	1/1	0.14	-2.89	29,29,29,29	0
85	MG	2	1922	1/1	0.22	-2.89	55,55,55,55	0
86	OHX	1	3884	7/7	0.19	-2.89	74,74,74,74	0
85	MG	5	3806	1/1	0.18	-2.90	53,53,53,53	0
86	OHX	5	3919	7/7	0.17	-2.90	72,72,72,72	0
85	MG	1	3627	1/1	0.21	-2.90	41,41,41,41	0
86	OHX	5	3928	7/7	0.16	-2.91	78,78,78,78	0
86	OHX	5	4138	7/7	0.13	-2.94	135,135,135,135	0
86	OHX	6	2144	7/7	0.10	-2.94	133,133,133,133	0
86	OHX	5	3960	7/7	0.17	-2.94	75,75,75,75	0
86	OHX	1	4102	7/7	0.12	-2.94	130,130,130,130	0
86	OHX	5	4078	7/7	0.11	-2.94	100,100,100,100	0
85	MG	5	3587	1/1	0.16	-2.95	26,26,26,26	0
86	OHX	C3	201	7/7	0.08	-2.95	179,179,179,179	0
86	OHX	5	3985	7/7	0.17	-2.95	98,98,98,98	0
86	OHX	1	4075	7/7	0.09	-2.98	143,143,143,143	0
85	MG	5	3526	1/1	0.22	-2.98	32,32,32,32	0
85	MG	5	3625	1/1	0.21	-2.98	39,39,39,39	0
86	OHX	2	2088	7/7	0.10	-2.98	130,130,130,130	0
85	MG	1	3698	1/1	0.12	-2.98	42,42,42,42	0
86	OHX	5	3990	7/7	0.13	-2.98	88,88,88,88	0
86	OHX	5	4010	7/7	0.11	-2.99	112,112,112,112	0
85	MG	5	3511	1/1	0.13	-2.99	34,34,34,34	0
86	OHX	1	4051	7/7	0.09	-3.00	149,149,149,149	0
86	OHX	5	3961	7/7	0.17	-3.01	77,77,77,77	0
86	OHX	2	2103	7/7	0.09	-3.01	147,147,147,147	0
85	MG	2	1971	1/1	0.19	-3.01	81,81,81,81	0
86	OHX	m5	305	7/7	0.10	-3.02	133,133,133,133	0
86	OHX	6	2142	7/7	0.17	-3.02	132,132,132,132	0
86	OHX	8	225	7/7	0.09	-3.03	129,129,129,129	0
85	MG	1	3425	1/1	0.17	-3.03	49,49,49,49	0
86	OHX	5	4074	7/7	0.07	-3.05	125,125,125,125	0
86	OHX	1	3891	7/7	0.13	-3.05	75,75,75,75	0
85	MG	1	3519	1/1	0.12	-3.06	41,41,41,41	0
85	MG	1	3808	1/1	0.15	-3.07	43,43,43,43	0
85	MG	4	219	1/1	0.17	-3.07	50,50,50,50	0
86	OHX	1	4147	7/7	0.18	-3.07	152,152,152,152	0
85	MG	1	3753	1/1	0.10	-3.07	100,100,100,100	0
86	OHX	1	3875	7/7	0.18	-3.08	60,60,60,60	0
86	OHX	1	4177	7/7	0.11	-3.08	238,238,238,238	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	2	2165	7/7	0.07	-3.09	167,167,167,167	0
86	OHX	2	2083	7/7	0.06	-3.09	157,157,157,157	0
86	OHX	1	3892	7/7	0.15	-3.09	83,83,83,83	0
85	MG	1	3707	1/1	0.14	-3.09	55,55,55,55	0
85	MG	1	3590	1/1	0.15	-3.09	38,38,38,38	0
86	OHX	1	4066	7/7	0.19	-3.10	143,143,143,143	0
86	OHX	5	4198	7/7	0.15	-3.10	128,128,128,128	0
86	OHX	5	4050	7/7	0.10	-3.10	133,133,133,133	0
85	MG	5	3785	1/1	0.17	-3.11	35,35,35,35	0
86	OHX	6	2102	7/7	0.12	-3.11	126,126,126,126	0
86	OHX	5	4119	7/7	0.14	-3.11	125,125,125,125	0
85	MG	1	3436	1/1	0.14	-3.11	43,43,43,43	0
86	OHX	o7	502	7/7	0.10	-3.11	110,110,110,110	0
86	OHX	1	4099	7/7	0.08	-3.11	170,170,170,170	0
86	OHX	2	2082	7/7	0.12	-3.12	138,138,138,138	0
85	MG	1	3426	1/1	0.27	-3.13	59,59,59,59	0
85	MG	6	1910	1/1	0.20	-3.13	46,46,46,46	0
86	OHX	1	4119	7/7	0.13	-3.13	142,142,142,142	0
86	OHX	5	4039	7/7	0.18	-3.13	103,103,103,103	0
86	OHX	5	4104	7/7	0.09	-3.15	140,140,140,140	0
86	OHX	1	4052	7/7	0.11	-3.15	142,142,142,142	0
86	OHX	6	2091	7/7	0.11	-3.15	116,116,116,116	0
86	OHX	5	4185	7/7	0.14	-3.16	132,132,132,132	0
86	OHX	5	3951	7/7	0.16	-3.16	85,85,85,85	0
86	OHX	5	3973	7/7	0.14	-3.17	87,87,87,87	0
85	MG	1	3744	1/1	0.14	-3.17	39,39,39,39	0
85	MG	6	2026	1/1	0.12	-3.17	86,86,86,86	0
85	MG	1	3498	1/1	0.20	-3.18	36,36,36,36	0
86	OHX	1	4048	7/7	0.16	-3.19	125,125,125,125	0
85	MG	5	3514	1/1	0.12	-3.19	39,39,39,39	0
85	MG	5	3408	1/1	0.15	-3.19	33,33,33,33	0
86	OHX	2	2060	7/7	0.11	-3.20	124,124,124,124	0
85	MG	1	3807	1/1	0.17	-3.20	41,41,41,41	0
86	OHX	1	4074	7/7	0.11	-3.20	134,134,134,134	0
86	OHX	5	4082	7/7	0.16	-3.20	114,114,114,114	0
86	OHX	5	4157	7/7	0.10	-3.20	143,143,143,143	0
86	OHX	5	4014	7/7	0.11	-3.21	100,100,100,100	0
86	OHX	5	4174	7/7	0.12	-3.22	93,93,93,93	0
85	MG	5	3841	1/1	0.11	-3.22	59,59,59,59	0
85	MG	5	3759	1/1	0.13	-3.22	46,46,46,46	0
86	OHX	1	4098	7/7	0.15	-3.22	128,128,128,128	0
86	OHX	7	222	7/7	0.15	-3.23	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3740	1/1	0.14	-3.23	40,40,40,40	0
85	MG	6	1962	1/1	0.11	-3.23	41,41,41,41	0
85	MG	5	3545	1/1	0.22	-3.24	51,51,51,51	0
86	OHX	1	4021	7/7	0.12	-3.24	153,153,153,153	0
86	OHX	5	3965	7/7	0.14	-3.24	88,88,88,88	0
86	OHX	5	4181	7/7	0.09	-3.25	163,163,163,163	0
85	MG	1	3405	1/1	0.17	-3.25	70,70,70,70	0
86	OHX	1	4156	7/7	0.16	-3.25	150,150,150,150	0
85	MG	6	2006	1/1	0.12	-3.25	54,54,54,54	0
86	OHX	1	4069	7/7	0.13	-3.26	140,140,140,140	0
85	MG	1	3542	1/1	0.18	-3.26	35,35,35,35	0
85	MG	2	1997	1/1	0.23	-3.26	80,80,80,80	0
85	MG	5	3680	1/1	0.13	-3.27	52,52,52,52	0
86	OHX	1	4023	7/7	0.10	-3.27	138,138,138,138	0
86	OHX	5	4043	7/7	0.12	-3.27	122,122,122,122	0
86	OHX	1	4072	7/7	0.11	-3.27	131,131,131,131	0
85	MG	2	1944	1/1	0.13	-3.28	67,67,67,67	0
85	MG	6	1976	1/1	0.12	-3.28	48,48,48,48	0
86	OHX	1	4037	7/7	0.05	-3.28	128,128,128,128	0
85	MG	1	3442	1/1	0.19	-3.28	30,30,30,30	0
86	OHX	5	4171	7/7	0.06	-3.30	190,190,190,190	0
86	OHX	5	4131	7/7	0.13	-3.30	121,121,121,121	0
86	OHX	6	2129	7/7	0.08	-3.30	141,141,141,141	0
86	OHX	2	2061	7/7	0.09	-3.32	108,108,108,108	0
86	OHX	M0	303	7/7	0.13	-3.33	124,124,124,124	0
86	OHX	1	3955	7/7	0.12	-3.33	81,81,81,81	0
86	OHX	1	3889	7/7	0.17	-3.33	70,70,70,70	0
86	OHX	1	4017	7/7	0.10	-3.34	120,120,120,120	0
86	OHX	8	226	7/7	0.11	-3.34	145,145,145,145	0
85	MG	5	3873	1/1	0.15	-3.34	38,38,38,38	0
86	OHX	5	4166	7/7	0.14	-3.36	149,149,149,149	0
86	OHX	2	2055	7/7	0.10	-3.37	135,135,135,135	0
86	OHX	6	2184	7/7	0.11	-3.37	179,179,179,179	0
86	OHX	2	2079	7/7	0.11	-3.37	135,135,135,135	0
86	OHX	5	4123	7/7	0.10	-3.37	141,141,141,141	0
86	OHX	6	2141	7/7	0.09	-3.38	174,174,174,174	0
86	OHX	5	4033	7/7	0.11	-3.38	114,114,114,114	0
85	MG	5	3516	1/1	0.17	-3.39	42,42,42,42	0
85	MG	2	1916	1/1	0.22	-3.40	54,54,54,54	0
86	OHX	1	3997	7/7	0.12	-3.40	95,95,95,95	0
85	MG	1	3419	1/1	0.19	-3.40	48,48,48,48	0
85	MG	1	3690	1/1	0.17	-3.42	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	2	1940	1/1	0.10	-3.42	69,69,69,69	0
85	MG	5	3867	1/1	0.26	-3.43	67,67,67,67	0
85	MG	1	3681	1/1	0.17	-3.44	50,50,50,50	0
86	OHX	5	4085	7/7	0.11	-3.44	121,121,121,121	0
86	OHX	1	4054	7/7	0.08	-3.45	154,154,154,154	0
85	MG	1	3626	1/1	0.17	-3.45	34,34,34,34	0
86	OHX	6	2071	7/7	0.13	-3.48	94,94,94,94	0
85	MG	5	3702	1/1	0.17	-3.48	32,32,32,32	0
86	OHX	5	3925	7/7	0.16	-3.49	72,72,72,72	0
86	OHX	5	4143	7/7	0.13	-3.49	140,140,140,140	0
86	OHX	5	3991	7/7	0.12	-3.50	115,115,115,115	0
86	OHX	1	3964	7/7	0.11	-3.50	106,106,106,106	0
86	OHX	1	4040	7/7	0.07	-3.51	123,123,123,123	0
86	OHX	1	4034	7/7	0.14	-3.52	134,134,134,134	0
86	OHX	2	2126	7/7	0.10	-3.53	135,135,135,135	0
85	MG	1	3775	1/1	0.20	-3.54	55,55,55,55	0
85	MG	1	3728	1/1	0.12	-3.54	38,38,38,38	0
86	OHX	1	3918	7/7	0.13	-3.55	92,92,92,92	0
86	OHX	6	2186	7/7	0.19	-3.58	172,172,172,172	0
86	OHX	5	3930	7/7	0.15	-3.58	84,84,84,84	0
85	MG	5	3525	1/1	0.15	-3.60	47,47,47,47	0
85	MG	1	3407	1/1	0.16	-3.60	39,39,39,39	0
86	OHX	1	4057	7/7	0.08	-3.60	189,189,189,189	0
85	MG	1	3660	1/1	0.10	-3.61	34,34,34,34	0
85	MG	1	3600	1/1	0.11	-3.61	30,30,30,30	0
85	MG	2	1911	1/1	0.18	-3.62	55,55,55,55	0
86	OHX	5	3964	7/7	0.15	-3.62	99,99,99,99	0
86	OHX	6	2114	7/7	0.10	-3.63	129,129,129,129	0
86	OHX	6	2110	7/7	0.14	-3.64	134,134,134,134	0
86	OHX	5	4088	7/7	0.14	-3.64	123,123,123,123	0
85	MG	1	3646	1/1	0.20	-3.66	40,40,40,40	0
85	MG	5	3727	1/1	0.21	-3.66	36,36,36,36	0
85	MG	1	3468	1/1	0.16	-3.67	48,48,48,48	0
85	MG	1	3452	1/1	0.16	-3.67	36,36,36,36	0
86	OHX	5	3917	7/7	0.16	-3.69	67,67,67,67	0
85	MG	5	3895	1/1	0.10	-3.69	119,119,119,119	0
86	OHX	5	4055	7/7	0.10	-3.69	107,107,107,107	0
86	OHX	1	3938	7/7	0.14	-3.70	102,102,102,102	0
86	OHX	1	4095	7/7	0.08	-3.70	153,153,153,153	0
86	OHX	1	3972	7/7	0.11	-3.70	112,112,112,112	0
86	OHX	1	3948	7/7	0.12	-3.71	103,103,103,103	0
86	OHX	5	3992	7/7	0.18	-3.72	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	7	217	7/7	0.14	-3.72	105,105,105,105	0
85	MG	1	3559	1/1	0.17	-3.74	39,39,39,39	0
86	OHX	5	3953	7/7	0.16	-3.76	104,104,104,104	0
85	MG	5	3744	1/1	0.18	-3.76	42,42,42,42	0
85	MG	1	3719	1/1	0.15	-3.78	47,47,47,47	0
86	OHX	2	2096	7/7	0.09	-3.78	156,156,156,156	0
86	OHX	1	4024	7/7	0.10	-3.79	132,132,132,132	0
85	MG	1	3449	1/1	0.09	-3.79	43,43,43,43	0
86	OHX	4	226	7/7	0.11	-3.80	104,104,104,104	0
86	OHX	5	4047	7/7	0.14	-3.80	128,128,128,128	0
86	OHX	5	3968	7/7	0.12	-3.81	97,97,97,97	0
85	MG	5	3449	1/1	0.21	-3.82	33,33,33,33	0
86	OHX	3	219	7/7	0.08	-3.83	130,130,130,130	0
86	OHX	5	3921	7/7	0.17	-3.83	65,65,65,65	0
86	OHX	1	3973	7/7	0.11	-3.84	107,107,107,107	0
85	MG	4	213	1/1	0.14	-3.84	63,63,63,63	0
86	OHX	6	2139	7/7	0.10	-3.84	140,140,140,140	0
86	OHX	1	3911	7/7	0.14	-3.84	91,91,91,91	0
85	MG	5	3404	1/1	0.08	-3.85	52,52,52,52	0
85	MG	6	1915	1/1	0.15	-3.85	53,53,53,53	0
86	OHX	5	4045	7/7	0.16	-3.86	130,130,130,130	0
85	MG	5	3418	1/1	0.24	-3.86	28,28,28,28	0
85	MG	1	3693	1/1	0.13	-3.86	39,39,39,39	0
86	OHX	2	2084	7/7	0.09	-3.87	138,138,138,138	0
86	OHX	6	2178	7/7	0.11	-3.87	163,163,163,163	0
86	OHX	5	4212	7/7	0.15	-3.87	146,146,146,146	0
86	OHX	1	4104	7/7	0.10	-3.89	147,147,147,147	0
86	OHX	2	2119	7/7	0.14	-3.89	165,165,165,165	0
86	OHX	8	230	7/7	0.09	-3.90	150,150,150,150	0
85	MG	5	3459	1/1	0.15	-3.90	41,41,41,41	0
86	OHX	6	2075	7/7	0.13	-3.96	115,115,115,115	0
85	MG	5	3609	1/1	0.18	-3.97	31,31,31,31	0
86	OHX	6	2090	7/7	0.17	-3.98	125,125,125,125	0
86	OHX	5	4066	7/7	0.08	-3.98	120,120,120,120	0
85	MG	1	3461	1/1	0.15	-3.99	25,25,25,25	0
85	MG	5	3476	1/1	0.14	-4.00	32,32,32,32	0
85	MG	5	3728	1/1	0.16	-4.00	102,102,102,102	0
85	MG	5	3442	1/1	0.13	-4.00	30,30,30,30	0
86	OHX	1	3927	7/7	0.14	-4.01	92,92,92,92	0
86	OHX	1	3966	7/7	0.12	-4.01	104,104,104,104	0
86	OHX	5	4056	7/7	0.12	-4.02	111,111,111,111	0
86	OHX	1	4197	7/7	0.14	-4.02	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	3934	7/7	0.17	-4.02	96,96,96,96	0
86	OHX	2	2076	7/7	0.15	-4.03	152,152,152,152	0
86	OHX	3	220	7/7	0.10	-4.03	138,138,138,138	0
86	OHX	5	3943	7/7	0.12	-4.04	98,98,98,98	0
86	OHX	3	216	7/7	0.12	-4.06	117,117,117,117	0
85	MG	6	1926	1/1	0.17	-4.08	52,52,52,52	0
86	OHX	5	3997	7/7	0.15	-4.09	99,99,99,99	0
85	MG	5	3528	1/1	0.17	-4.09	33,33,33,33	0
86	OHX	1	4190	7/7	0.09	-4.10	157,157,157,157	0
86	OHX	1	4043	7/7	0.15	-4.10	117,117,117,117	0
86	OHX	1	3984	7/7	0.14	-4.11	119,119,119,119	0
85	MG	1	3427	1/1	0.13	-4.11	43,43,43,43	0
86	OHX	5	4129	7/7	0.06	-4.11	150,150,150,150	0
86	OHX	1	3886	7/7	0.17	-4.12	73,73,73,73	0
86	OHX	1	3958	7/7	0.11	-4.13	102,102,102,102	0
86	OHX	5	4065	7/7	0.09	-4.16	121,121,121,121	0
86	OHX	6	2154	7/7	0.09	-4.16	121,121,121,121	0
86	OHX	5	4019	7/7	0.11	-4.18	114,114,114,114	0
86	OHX	2	2073	7/7	0.08	-4.18	128,128,128,128	0
86	OHX	6	2097	7/7	0.11	-4.19	126,126,126,126	0
86	OHX	5	4028	7/7	0.14	-4.22	94,94,94,94	0
86	OHX	1	3939	7/7	0.11	-4.22	102,102,102,102	0
86	OHX	5	4030	7/7	0.11	-4.24	124,124,124,124	0
86	OHX	6	2055	7/7	0.18	-4.25	76,76,76,76	0
86	OHX	5	4006	7/7	0.16	-4.25	121,121,121,121	0
85	MG	1	3814	1/1	0.12	-4.25	53,53,53,53	0
86	OHX	7	219	7/7	0.10	-4.27	104,104,104,104	0
86	OHX	5	4215	7/7	0.07	-4.29	204,204,204,204	0
85	MG	5	3819	1/1	0.14	-4.30	36,36,36,36	0
85	MG	5	3602	1/1	0.13	-4.31	64,64,64,64	0
86	OHX	6	2157	7/7	0.10	-4.31	145,145,145,145	0
85	MG	1	3482	1/1	0.12	-4.31	34,34,34,34	0
85	MG	1	3505	1/1	0.11	-4.32	35,35,35,35	0
86	OHX	1	3895	7/7	0.15	-4.32	79,79,79,79	0
86	OHX	1	3960	7/7	0.16	-4.32	103,103,103,103	0
86	OHX	5	3978	7/7	0.15	-4.33	100,100,100,100	0
86	OHX	3	224	7/7	0.16	-4.33	148,148,148,148	0
86	OHX	1	3976	7/7	0.11	-4.33	116,116,116,116	0
85	MG	5	3565	1/1	0.23	-4.34	28,28,28,28	0
85	MG	5	3405	1/1	0.14	-4.34	32,32,32,32	0
85	MG	1	3839	1/1	0.18	-4.38	31,31,31,31	0
86	OHX	1	4022	7/7	0.15	-4.39	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4081	7/7	0.11	-4.39	115,115,115,115	0
86	OHX	1	4049	7/7	0.12	-4.40	126,126,126,126	0
85	MG	1	3694	1/1	0.16	-4.41	52,52,52,52	0
86	OHX	4	230	7/7	0.12	-4.41	115,115,115,115	0
85	MG	1	3763	1/1	0.15	-4.42	43,43,43,43	0
86	OHX	1	3879	7/7	0.19	-4.42	75,75,75,75	0
86	OHX	5	3984	7/7	0.14	-4.43	103,103,103,103	0
86	OHX	5	4058	7/7	0.08	-4.45	143,143,143,143	0
86	OHX	4	233	7/7	0.08	-4.47	136,136,136,136	0
86	OHX	1	4085	7/7	0.12	-4.48	142,142,142,142	0
85	MG	5	3452	1/1	0.09	-4.48	47,47,47,47	0
85	MG	1	3511	1/1	0.22	-4.48	38,38,38,38	0
85	MG	1	3549	1/1	0.15	-4.48	29,29,29,29	0
86	OHX	6	2101	7/7	0.12	-4.49	116,116,116,116	0
86	OHX	8	228	7/7	0.15	-4.50	156,156,156,156	0
85	MG	5	3650	1/1	0.20	-4.50	43,43,43,43	0
85	MG	1	3466	1/1	0.14	-4.50	48,48,48,48	0
86	OHX	1	4080	7/7	0.10	-4.51	144,144,144,144	0
86	OHX	2	2052	7/7	0.13	-4.53	109,109,109,109	0
86	OHX	5	4057	7/7	0.09	-4.54	137,137,137,137	0
86	OHX	3	215	7/7	0.18	-4.54	108,108,108,108	0
85	MG	1	3423	1/1	0.14	-4.54	35,35,35,35	0
85	MG	3	212	1/1	0.14	-4.55	80,80,80,80	0
86	OHX	1	4096	7/7	0.07	-4.56	159,159,159,159	0
86	OHX	2	2080	7/7	0.17	-4.56	130,130,130,130	0
85	MG	1	3473	1/1	0.14	-4.57	32,32,32,32	0
86	OHX	d4	201	7/7	0.12	-4.58	162,162,162,162	0
86	OHX	6	2168	7/7	0.12	-4.58	162,162,162,162	0
86	OHX	1	3922	7/7	0.14	-4.59	80,80,80,80	0
86	OHX	1	3988	7/7	0.10	-4.59	112,112,112,112	0
86	OHX	5	4112	7/7	0.15	-4.60	135,135,135,135	0
86	OHX	5	3936	7/7	0.13	-4.60	81,81,81,81	0
85	MG	5	3434	1/1	0.12	-4.62	36,36,36,36	0
86	OHX	5	4051	7/7	0.11	-4.62	117,117,117,117	0
86	OHX	2	2059	7/7	0.09	-4.64	115,115,115,115	0
86	OHX	5	4052	7/7	0.12	-4.66	115,115,115,115	0
86	OHX	1	3986	7/7	0.10	-4.67	112,112,112,112	0
86	OHX	6	2078	7/7	0.11	-4.68	107,107,107,107	0
86	OHX	1	3906	7/7	0.16	-4.70	78,78,78,78	0
86	OHX	3	223	7/7	0.10	-4.72	175,175,175,175	0
86	OHX	5	4070	7/7	0.12	-4.72	135,135,135,135	0
86	OHX	5	4124	7/7	0.11	-4.74	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3947	7/7	0.18	-4.80	75,75,75,75	0
86	OHX	6	2122	7/7	0.09	-4.80	138,138,138,138	0
86	OHX	1	3951	7/7	0.15	-4.82	103,103,103,103	0
86	OHX	5	4063	7/7	0.15	-4.82	136,136,136,136	0
85	MG	5	3589	1/1	0.19	-4.83	28,28,28,28	0
86	OHX	6	2160	7/7	0.14	-4.84	133,133,133,133	0
86	OHX	5	4026	7/7	0.17	-4.85	116,116,116,116	0
86	OHX	5	4042	7/7	0.14	-4.86	138,138,138,138	0
86	OHX	5	4022	7/7	0.08	-4.88	123,123,123,123	0
86	OHX	5	3987	7/7	0.14	-4.88	95,95,95,95	0
86	OHX	1	3928	7/7	0.14	-4.89	87,87,87,87	0
86	OHX	5	3986	7/7	0.12	-4.89	91,91,91,91	0
85	MG	1	3488	1/1	0.12	-4.89	35,35,35,35	0
86	OHX	1	4073	7/7	0.10	-4.89	135,135,135,135	0
86	OHX	1	3978	7/7	0.12	-4.91	86,86,86,86	0
86	OHX	5	4034	7/7	0.12	-4.91	114,114,114,114	0
85	MG	5	3456	1/1	0.13	-4.92	61,61,61,61	0
85	MG	6	1992	1/1	0.12	-4.95	54,54,54,54	0
86	OHX	1	3985	7/7	0.09	-4.97	124,124,124,124	0
86	OHX	6	2162	7/7	0.16	-4.97	137,137,137,137	0
85	MG	1	3674	1/1	0.12	-4.97	76,76,76,76	0
85	MG	5	3740	1/1	0.16	-4.97	57,57,57,57	0
86	OHX	6	2092	7/7	0.14	-4.99	113,113,113,113	0
86	OHX	5	4086	7/7	0.12	-4.99	132,132,132,132	0
86	OHX	1	3996	7/7	0.13	-5.01	121,121,121,121	0
86	OHX	1	3952	7/7	0.12	-5.02	104,104,104,104	0
86	OHX	5	3982	7/7	0.15	-5.03	95,95,95,95	0
85	MG	5	3668	1/1	0.12	-5.03	34,34,34,34	0
85	MG	1	3462	1/1	0.20	-5.03	28,28,28,28	0
85	MG	1	3688	1/1	0.17	-5.05	39,39,39,39	0
86	OHX	1	4058	7/7	0.10	-5.10	135,135,135,135	0
85	MG	5	3510	1/1	0.18	-5.10	26,26,26,26	0
85	MG	6	1990	1/1	0.17	-5.10	74,74,74,74	0
85	MG	1	3503	1/1	0.19	-5.14	30,30,30,30	0
85	MG	1	3752	1/1	0.12	-5.14	31,31,31,31	0
86	OHX	6	2109	7/7	0.13	-5.15	116,116,116,116	0
86	OHX	1	4151	7/7	0.07	-5.15	139,139,139,139	0
85	MG	5	3838	1/1	0.11	-5.16	74,74,74,74	0
85	MG	5	3812	1/1	0.13	-5.19	90,90,90,90	0
85	MG	1	3638	1/1	0.17	-5.20	64,64,64,64	0
86	OHX	1	4038	7/7	0.15	-5.21	120,120,120,120	0
86	OHX	5	4094	7/7	0.08	-5.22	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2065	7/7	0.13	-5.22	118,118,118,118	0
85	MG	1	3625	1/1	0.13	-5.25	37,37,37,37	0
86	OHX	5	3979	7/7	0.11	-5.27	86,86,86,86	0
85	MG	8	209	1/1	0.11	-5.27	70,70,70,70	0
85	MG	6	2019	1/1	0.15	-5.29	110,110,110,110	0
86	OHX	5	4072	7/7	0.16	-5.31	122,122,122,122	0
85	MG	5	3544	1/1	0.11	-5.31	37,37,37,37	0
86	OHX	5	3972	7/7	0.10	-5.32	91,91,91,91	0
86	OHX	5	4009	7/7	0.13	-5.33	105,105,105,105	0
86	OHX	6	2143	7/7	0.07	-5.33	154,154,154,154	0
85	MG	1	3797	1/1	0.15	-5.35	54,54,54,54	0
86	OHX	1	4083	7/7	0.07	-5.36	137,137,137,137	0
86	OHX	1	4005	7/7	0.09	-5.36	112,112,112,112	0
85	MG	2	1906	1/1	0.13	-5.36	53,53,53,53	0
86	OHX	6	2113	7/7	0.10	-5.37	130,130,130,130	0
86	OHX	5	4134	7/7	0.12	-5.38	136,136,136,136	0
85	MG	5	3784	1/1	0.12	-5.39	33,33,33,33	0
86	OHX	1	4107	7/7	0.07	-5.43	132,132,132,132	0
86	OHX	5	4200	7/7	0.13	-5.43	124,124,124,124	0
86	OHX	5	4148	7/7	0.16	-5.43	137,137,137,137	0
85	MG	1	3457	1/1	0.10	-5.44	27,27,27,27	0
86	OHX	1	4026	7/7	0.10	-5.46	137,137,137,137	0
86	OHX	1	4152	7/7	0.12	-5.46	137,137,137,137	0
86	OHX	1	4089	7/7	0.07	-5.47	162,162,162,162	0
85	MG	6	2022	1/1	0.09	-5.47	57,57,57,57	0
86	OHX	1	3903	7/7	0.15	-5.49	94,94,94,94	0
86	OHX	6	2165	7/7	0.11	-5.51	157,157,157,157	0
85	MG	2	1989	1/1	0.14	-5.52	57,57,57,57	0
86	OHX	1	3981	7/7	0.10	-5.53	100,100,100,100	0
85	MG	1	3743	1/1	0.11	-5.54	32,32,32,32	0
86	OHX	2	2121	7/7	0.09	-5.57	146,146,146,146	0
86	OHX	1	4125	7/7	0.09	-5.58	156,156,156,156	0
86	OHX	1	4019	7/7	0.10	-5.59	121,121,121,121	0
86	OHX	5	4175	7/7	0.13	-5.62	133,133,133,133	0
86	OHX	5	3929	7/7	0.15	-5.62	77,77,77,77	0
86	OHX	2	2056	7/7	0.12	-5.65	124,124,124,124	0
86	OHX	1	4050	7/7	0.10	-5.65	147,147,147,147	0
86	OHX	2	2045	7/7	0.11	-5.69	109,109,109,109	0
85	MG	5	3672	1/1	0.18	-5.69	48,48,48,48	0
85	MG	5	3401	1/1	0.13	-5.71	63,63,63,63	0
86	OHX	1	4128	7/7	0.08	-5.73	179,179,179,179	0
86	OHX	1	4115	7/7	0.08	-5.73	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3604	1/1	0.14	-5.73	42,42,42,42	0
86	OHX	1	4166	7/7	0.13	-5.78	132,132,132,132	0
85	MG	1	3476	1/1	0.13	-5.78	37,37,37,37	0
86	OHX	2	2051	7/7	0.11	-5.83	121,121,121,121	0
86	OHX	1	4002	7/7	0.12	-5.86	128,128,128,128	0
85	MG	1	3742	1/1	0.15	-5.90	51,51,51,51	0
86	OHX	5	4127	7/7	0.10	-5.93	134,134,134,134	0
85	MG	1	3412	1/1	0.14	-5.95	36,36,36,36	0
86	OHX	5	4012	7/7	0.10	-6.01	119,119,119,119	0
86	OHX	6	2089	7/7	0.09	-6.06	113,113,113,113	0
86	OHX	1	4142	7/7	0.12	-6.17	153,153,153,153	0
86	OHX	1	4070	7/7	0.10	-6.21	152,152,152,152	0
86	OHX	2	2064	7/7	0.09	-6.23	137,137,137,137	0
86	OHX	19	600	7/7	0.09	-6.24	134,134,134,134	0
86	OHX	6	2060	7/7	0.14	-6.25	87,87,87,87	0
86	OHX	6	2131	7/7	0.16	-6.34	149,149,149,149	0
86	OHX	6	2080	7/7	0.16	-6.36	107,107,107,107	0
86	OHX	1	4171	7/7	0.09	-6.37	112,112,112,112	0
85	MG	5	3489	1/1	0.12	-6.41	56,56,56,56	0
86	OHX	1	4031	7/7	0.14	-6.44	115,115,115,115	0
85	MG	5	3636	1/1	0.09	-6.53	54,54,54,54	0
86	OHX	1	4020	7/7	0.07	-6.54	143,143,143,143	0
86	OHX	2	2066	7/7	0.11	-6.58	114,114,114,114	0
85	MG	5	3779	1/1	0.10	-6.61	53,53,53,53	0
86	OHX	6	2079	7/7	0.10	-6.66	106,106,106,106	0
86	OHX	1	4008	7/7	0.15	-6.68	134,134,134,134	0
85	MG	5	3406	1/1	0.15	-6.72	41,41,41,41	0
85	MG	1	3851	1/1	0.15	-6.81	66,66,66,66	0
86	OHX	1	4013	7/7	0.11	-6.85	123,123,123,123	0
86	OHX	3	217	7/7	0.12	-6.87	113,113,113,113	0
86	OHX	1	4011	7/7	0.10	-6.88	126,126,126,126	0
86	OHX	6	2103	7/7	0.09	-6.88	129,129,129,129	0
86	OHX	5	4158	7/7	0.16	-6.89	144,144,144,144	0
86	OHX	7	218	7/7	0.10	-6.89	101,101,101,101	0
85	MG	5	3788	1/1	0.14	-6.92	45,45,45,45	0
86	OHX	5	4100	7/7	0.09	-6.93	136,136,136,136	0
85	MG	5	3691	1/1	0.15	-6.93	40,40,40,40	0
85	MG	5	3661	1/1	0.16	-7.00	46,46,46,46	0
86	OHX	5	4015	7/7	0.08	-7.01	111,111,111,111	0
86	OHX	1	3977	7/7	0.14	-7.03	117,117,117,117	0
86	OHX	5	4144	7/7	0.10	-7.04	123,123,123,123	0
85	MG	6	1974	1/1	0.16	-7.05	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4155	7/7	0.10	-7.11	128,128,128,128	0
86	OHX	2	2053	7/7	0.16	-7.12	116,116,116,116	0
86	OHX	1	4150	7/7	0.07	-7.15	120,120,120,120	0
85	MG	1	3726	1/1	0.08	-7.20	70,70,70,70	0
86	OHX	2	2107	7/7	0.09	-7.22	140,140,140,140	0
86	OHX	5	4021	7/7	0.08	-7.23	107,107,107,107	0
86	OHX	5	4217	7/7	0.08	-7.34	109,109,109,109	0
85	MG	1	3435	1/1	0.10	-7.41	50,50,50,50	0
86	OHX	1	4006	7/7	0.13	-7.47	128,128,128,128	0
86	OHX	6	2127	7/7	0.18	-7.49	132,132,132,132	0
86	OHX	5	4067	7/7	0.08	-7.54	135,135,135,135	0
85	MG	7	211	1/1	0.12	-7.68	72,72,72,72	0
86	OHX	5	4168	7/7	0.09	-7.85	159,159,159,159	0
86	OHX	1	3962	7/7	0.10	-7.88	103,103,103,103	0
85	MG	1	3860	1/1	0.14	-7.95	43,43,43,43	0
86	OHX	5	4049	7/7	0.09	-7.97	116,116,116,116	0
85	MG	5	3730	1/1	0.16	-7.98	52,52,52,52	0
86	OHX	5	4004	7/7	0.10	-8.09	102,102,102,102	0
85	MG	6	2014	1/1	0.17	-8.23	48,48,48,48	0
86	OHX	5	4136	7/7	0.11	-8.23	140,140,140,140	0
86	OHX	5	4167	7/7	0.11	-8.28	134,134,134,134	0
85	MG	5	3420	1/1	0.13	-8.30	96,96,96,96	0
86	OHX	1	4172	7/7	0.10	-8.30	174,174,174,174	0
86	OHX	5	3995	7/7	0.08	-8.33	132,132,132,132	0
86	OHX	5	4096	7/7	0.15	-8.40	152,152,152,152	0
86	OHX	5	4097	7/7	0.08	-8.45	132,132,132,132	0
85	MG	1	4216	1/1	0.11	-8.82	48,48,48,48	0
85	MG	1	3599	1/1	0.11	-9.08	39,39,39,39	0
85	MG	5	3455	1/1	0.18	-9.09	43,43,43,43	0
85	MG	5	3479	1/1	0.26	-9.25	70,70,70,70	0
86	OHX	5	4023	7/7	0.07	-9.60	115,115,115,115	0
85	MG	4	208	1/1	0.14	-9.61	46,46,46,46	0
85	MG	6	1996	1/1	0.11	-9.62	53,53,53,53	0
85	MG	1	3767	1/1	0.14	-9.70	89,89,89,89	0
85	MG	6	1975	1/1	0.18	-9.87	59,59,59,59	0
85	MG	5	3765	1/1	0.17	-9.88	60,60,60,60	0
86	OHX	1	4007	7/7	0.09	-10.08	140,140,140,140	0
86	OHX	1	4091	7/7	0.10	-10.16	160,160,160,160	0
86	OHX	1	3990	7/7	0.09	-10.19	131,131,131,131	0
86	OHX	1	3970	7/7	0.07	-10.29	110,110,110,110	0
86	OHX	6	2069	7/7	0.14	-10.30	90,90,90,90	0
85	MG	5	3447	1/1	0.17	-10.38	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4154	7/7	0.09	-10.54	110,110,110,110	0
85	MG	5	3656	1/1	0.17	-10.87	59,59,59,59	0
85	MG	1	3769	1/1	0.18	-11.00	69,69,69,69	0
86	OHX	1	4101	7/7	0.09	-11.08	149,149,149,149	0
86	OHX	2	2113	7/7	0.06	-11.10	167,167,167,167	0
85	MG	1	3603	1/1	0.12	-11.20	39,39,39,39	0
86	OHX	5	4213	7/7	0.11	-11.58	152,152,152,152	0
85	MG	5	3712	1/1	0.18	-11.62	90,90,90,90	0
86	OHX	1	4001	7/7	0.08	-11.66	115,115,115,115	0
86	OHX	5	4073	7/7	0.08	-13.28	122,122,122,122	0
85	MG	5	3862	1/1	0.18	-13.67	63,63,63,63	0
86	OHX	5	4116	7/7	0.11	-13.73	159,159,159,159	0
85	MG	4	211	1/1	0.23	-14.33	54,54,54,54	0
86	OHX	5	4069	7/7	0.07	-14.43	143,143,143,143	0
85	MG	5	3795	1/1	0.19	-14.53	43,43,43,43	0
85	MG	5	3797	1/1	0.14	-15.73	93,93,93,93	0
86	OHX	5	4095	7/7	0.09	-17.03	128,128,128,128	0
85	MG	1	3661	1/1	0.16	-19.11	50,50,50,50	0
86	OHX	5	4210	7/7	0.13	-19.64	157,157,157,157	0
86	OHX	5	4126	7/7	0.10	-20.53	146,146,146,146	0
86	OHX	1	4015	7/7	0.10	-23.13	128,128,128,128	0
86	OHX	2	2124	7/7	0.13	-27.46	145,145,145,145	0
85	MG	1	3736	1/1	0.08	-27.56	56,56,56,56	0
85	MG	1	3576	1/1	0.16	-28.13	28,28,28,28	0
85	MG	5	3705	1/1	0.19	-29.00	41,41,41,41	0
85	MG	4	221	1/1	0.19	-31.00	67,67,67,67	0
86	OHX	1	4018	7/7	0.16	-34.26	129,129,129,129	0
86	OHX	5	4016	7/7	0.14	-51.58	111,111,111,111	0
86	OHX	1	4162	7/7	0.10	-51.67	166,166,166,166	0
85	MG	1	3464	1/1	0.19	-77.00	37,37,37,37	0
85	MG	2	2021	1/1	0.36	-	66,66,66,66	0
85	MG	1	3788	1/1	0.25	-	68,68,68,68	0
85	MG	5	3879	1/1	0.13	-	42,42,42,42	0
85	MG	5	3868	1/1	0.29	-	49,49,49,49	0
85	MG	5	3888	1/1	0.66	-	90,90,90,90	0
85	MG	1	3536	1/1	0.31	-	55,55,55,55	0
85	MG	1	3490	1/1	0.25	-	47,47,47,47	0
85	MG	6	1999	1/1	0.11	-	102,102,102,102	0
85	MG	1	3848	1/1	0.14	-	52,52,52,52	0
85	MG	1	3548	1/1	0.34	-	54,54,54,54	0
85	MG	2	1995	1/1	0.40	-	49,49,49,49	0
85	MG	1	3838	1/1	0.29	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3732	1/1	0.38	-	69,69,69,69	0
85	MG	1	3612	1/1	0.31	-	46,46,46,46	0
85	MG	6	2038	1/1	0.47	-	81,81,81,81	0
85	MG	5	3802	1/1	0.14	-	47,47,47,47	0
85	MG	1	3465	1/1	0.47	-	57,57,57,57	0
85	MG	5	3773	1/1	0.27	-	111,111,111,111	0
85	MG	1	3765	1/1	0.20	-	54,54,54,54	0
85	MG	6	2043	1/1	0.38	-	50,50,50,50	0
85	MG	5	3651	1/1	0.32	-	111,111,111,111	0
85	MG	5	3617	1/1	0.31	-	35,35,35,35	0
85	MG	6	1998	1/1	0.33	-	95,95,95,95	0
85	MG	6	1979	1/1	0.45	-	63,63,63,63	0
85	MG	1	3837	1/1	0.28	-	44,44,44,44	0
85	MG	1	3799	1/1	0.14	-	86,86,86,86	0
85	MG	7	213	1/1	0.39	-	52,52,52,52	0
85	MG	8	216	1/1	0.28	-	33,33,33,33	0
85	MG	1	3792	1/1	0.27	-	67,67,67,67	0
85	MG	5	3898	1/1	0.36	-	154,154,154,154	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.