



# wwPDB X-ray Structure Validation Summary Report

Oct 9, 2014 – 11:01 PM BST

PDB ID : 4U4Z  
Title : Crystal structure of Phyllanthoside bound to the yeast 80S ribosome  
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Deposited on : 2014-07-24  
Resolution : 3.10 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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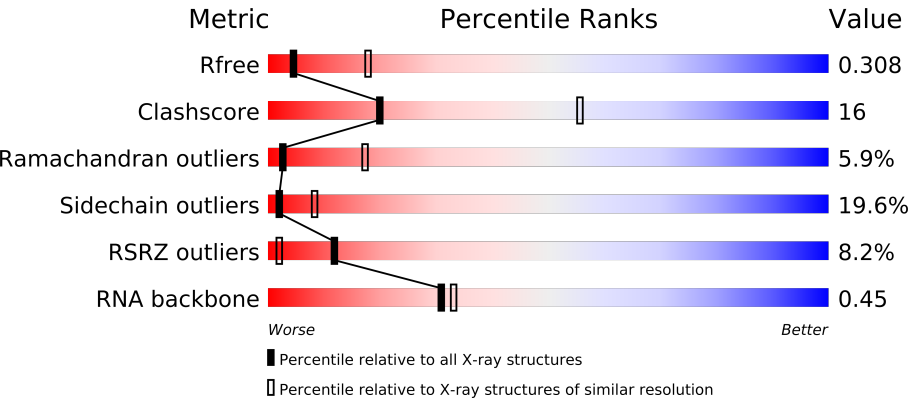
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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	119	

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

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

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3402	-	X
85	MG	1	3410	-	X
85	MG	1	3413	-	X
85	MG	1	3414	-	X
85	MG	1	3420	-	X
85	MG	1	3431	-	X
85	MG	1	3445	-	X
85	MG	1	3447	-	X
85	MG	1	3448	-	X
85	MG	1	3452	-	X
85	MG	1	3455	-	X
85	MG	1	3464	-	X
85	MG	1	3465	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3466	-	X
85	MG	1	3470	-	X
85	MG	1	3476	-	X
85	MG	1	3485	-	X
85	MG	1	3486	-	X
85	MG	1	3490	-	X
85	MG	1	3494	-	X
85	MG	1	3498	-	X
85	MG	1	3503	-	X
85	MG	1	3507	-	X
85	MG	1	3510	-	X
85	MG	1	3514	-	X
85	MG	1	3522	-	X
85	MG	1	3524	-	X
85	MG	1	3525	-	X
85	MG	1	3530	-	X
85	MG	1	3534	-	X
85	MG	1	3536	-	X
85	MG	1	3537	-	X
85	MG	1	3538	-	X
85	MG	1	3539	-	X
85	MG	1	3544	-	X
85	MG	1	3547	-	X
85	MG	1	3554	-	X
85	MG	1	3557	-	X
85	MG	1	3563	-	X
85	MG	1	3565	-	X
85	MG	1	3567	-	X
85	MG	1	3572	-	X
85	MG	1	3574	-	X
85	MG	1	3576	-	X
85	MG	1	3580	-	X
85	MG	1	3588	-	X
85	MG	1	3589	-	X
85	MG	1	3591	-	X
85	MG	1	3592	-	X
85	MG	1	3599	-	X
85	MG	1	3612	-	X
85	MG	1	3615	-	X
85	MG	1	3616	-	X
85	MG	1	3620	-	X
85	MG	1	3622	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3624	-	X
85	MG	1	3626	-	X
85	MG	1	3629	-	X
85	MG	1	3631	-	X
85	MG	1	3633	-	X
85	MG	1	3636	-	X
85	MG	1	3649	-	X
85	MG	1	3651	-	X
85	MG	1	3653	-	X
85	MG	1	3654	-	X
85	MG	1	3655	-	X
85	MG	1	3656	-	X
85	MG	1	3661	-	X
85	MG	1	3665	-	X
85	MG	1	3668	-	X
85	MG	1	3670	-	X
85	MG	1	3671	-	X
85	MG	1	3675	-	X
85	MG	1	3680	-	X
85	MG	1	3681	-	X
85	MG	1	3683	-	X
85	MG	1	3685	-	X
85	MG	1	3686	-	X
85	MG	1	3687	-	X
85	MG	1	3688	-	X
85	MG	1	3690	-	X
85	MG	1	3694	-	X
85	MG	1	3700	-	X
85	MG	1	3705	-	X
85	MG	1	3706	-	X
85	MG	1	3707	-	X
85	MG	1	3709	-	X
85	MG	1	3714	-	X
85	MG	1	3716	-	X
85	MG	1	3719	-	X
85	MG	1	3724	-	X
85	MG	1	3726	-	X
85	MG	1	3727	-	X
85	MG	1	3728	-	X
85	MG	1	3730	-	X
85	MG	1	3731	-	X
85	MG	1	3733	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3737	-	X
85	MG	1	3738	-	X
85	MG	1	3742	-	X
85	MG	1	3745	-	X
85	MG	1	3748	-	X
85	MG	1	3752	-	X
85	MG	1	3756	-	X
85	MG	1	3761	-	X
85	MG	1	3762	-	X
85	MG	1	3765	-	X
85	MG	1	3767	-	X
85	MG	1	3768	-	X
85	MG	1	3778	-	X
85	MG	1	3780	-	X
85	MG	1	3781	-	X
85	MG	1	3791	-	X
85	MG	1	3794	-	X
85	MG	1	3795	-	X
85	MG	1	3796	-	X
85	MG	1	3800	-	X
85	MG	1	3802	-	X
85	MG	1	3804	-	X
85	MG	1	3805	-	X
85	MG	1	3807	-	X
85	MG	1	3813	-	X
85	MG	1	3814	-	X
85	MG	1	3815	-	X
85	MG	1	3821	-	X
85	MG	1	3822	-	X
85	MG	1	3823	-	X
85	MG	1	3824	-	X
85	MG	1	3825	-	X
85	MG	1	3827	-	X
85	MG	1	3830	-	X
85	MG	1	3831	-	X
85	MG	1	3832	-	X
85	MG	1	3833	-	X
85	MG	1	3840	-	X
85	MG	1	3843	-	X
85	MG	1	3844	-	X
85	MG	1	3848	-	X
85	MG	1	3849	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3850	-	X
85	MG	1	3853	-	X
85	MG	1	3855	-	X
85	MG	1	3858	-	X
85	MG	1	3859	-	X
85	MG	1	3860	-	X
85	MG	1	3863	-	X
85	MG	1	3864	-	X
85	MG	1	3865	-	X
85	MG	1	3866	-	X
85	MG	1	3867	-	X
85	MG	1	3870	-	X
85	MG	2	1902	-	X
85	MG	2	1904	-	X
85	MG	2	1905	-	X
85	MG	2	1912	-	X
85	MG	2	1913	-	X
85	MG	2	1914	-	X
85	MG	2	1915	-	X
85	MG	2	1916	-	X
85	MG	2	1918	-	X
85	MG	2	1919	-	X
85	MG	2	1921	-	X
85	MG	2	1923	-	X
85	MG	2	1926	-	X
85	MG	2	1929	-	X
85	MG	2	1931	-	X
85	MG	2	1932	-	X
85	MG	2	1934	-	X
85	MG	2	1935	-	X
85	MG	2	1937	-	X
85	MG	2	1938	-	X
85	MG	2	1941	-	X
85	MG	2	1944	-	X
85	MG	2	1945	-	X
85	MG	2	1946	-	X
85	MG	2	1949	-	X
85	MG	2	1951	-	X
85	MG	2	1956	-	X
85	MG	2	1957	-	X
85	MG	2	1958	-	X
85	MG	2	1961	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1963	-	X
85	MG	2	1964	-	X
85	MG	2	1965	-	X
85	MG	2	1968	-	X
85	MG	2	1970	-	X
85	MG	2	1972	-	X
85	MG	2	1973	-	X
85	MG	2	1976	-	X
85	MG	2	1977	-	X
85	MG	2	1980	-	X
85	MG	2	1981	-	X
85	MG	2	1983	-	X
85	MG	2	1985	-	X
85	MG	2	1986	-	X
85	MG	2	1987	-	X
85	MG	2	1989	-	X
85	MG	2	1991	-	X
85	MG	2	1993	-	X
85	MG	2	1994	-	X
85	MG	2	1995	-	X
85	MG	2	1999	-	X
85	MG	2	2001	-	X
85	MG	2	2002	-	X
85	MG	2	2005	-	X
85	MG	2	2006	-	X
85	MG	2	2009	-	X
85	MG	2	2011	-	X
85	MG	2	2013	-	X
85	MG	2	2014	-	X
85	MG	2	2017	-	X
85	MG	3	201	-	X
85	MG	3	202	-	X
85	MG	3	203	-	X
85	MG	3	204	-	X
85	MG	3	205	-	X
85	MG	3	206	-	X
85	MG	3	207	-	X
85	MG	3	209	-	X
85	MG	3	212	-	X
85	MG	3	213	-	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	207	-	X
85	MG	4	211	-	X
85	MG	4	213	-	X
85	MG	4	216	-	X
85	MG	4	220	-	X
85	MG	4	221	-	X
85	MG	4	222	-	X
85	MG	4	223	-	X
85	MG	5	3403	-	X
85	MG	5	3405	-	X
85	MG	5	3410	-	X
85	MG	5	3414	-	X
85	MG	5	3420	-	X
85	MG	5	3421	-	X
85	MG	5	3432	-	X
85	MG	5	3433	-	X
85	MG	5	3435	-	X
85	MG	5	3440	-	X
85	MG	5	3444	-	X
85	MG	5	3446	-	X
85	MG	5	3449	-	X
85	MG	5	3450	-	X
85	MG	5	3451	-	X
85	MG	5	3455	-	X
85	MG	5	3464	-	X
85	MG	5	3467	-	X
85	MG	5	3468	-	X
85	MG	5	3473	-	X
85	MG	5	3476	-	X
85	MG	5	3479	-	X
85	MG	5	3480	-	X
85	MG	5	3481	-	X
85	MG	5	3483	-	X
85	MG	5	3487	-	X
85	MG	5	3488	-	X
85	MG	5	3491	-	X
85	MG	5	3495	-	X
85	MG	5	3499	-	X
85	MG	5	3505	-	X
85	MG	5	3506	-	X
85	MG	5	3508	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3514	-	X
85	MG	5	3521	-	X
85	MG	5	3526	-	X
85	MG	5	3527	-	X
85	MG	5	3532	-	X
85	MG	5	3533	-	X
85	MG	5	3534	-	X
85	MG	5	3538	-	X
85	MG	5	3539	-	X
85	MG	5	3542	-	X
85	MG	5	3543	-	X
85	MG	5	3547	-	X
85	MG	5	3551	-	X
85	MG	5	3554	-	X
85	MG	5	3562	-	X
85	MG	5	3563	-	X
85	MG	5	3565	-	X
85	MG	5	3571	-	X
85	MG	5	3572	-	X
85	MG	5	3574	-	X
85	MG	5	3576	-	X
85	MG	5	3577	-	X
85	MG	5	3578	-	X
85	MG	5	3580	-	X
85	MG	5	3581	-	X
85	MG	5	3583	-	X
85	MG	5	3585	-	X
85	MG	5	3586	-	X
85	MG	5	3589	-	X
85	MG	5	3595	-	X
85	MG	5	3597	-	X
85	MG	5	3599	-	X
85	MG	5	3601	-	X
85	MG	5	3607	-	X
85	MG	5	3608	-	X
85	MG	5	3609	-	X
85	MG	5	3615	-	X
85	MG	5	3619	-	X
85	MG	5	3624	-	X
85	MG	5	3631	-	X
85	MG	5	3633	-	X
85	MG	5	3636	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3640	-	X
85	MG	5	3646	-	X
85	MG	5	3647	-	X
85	MG	5	3648	-	X
85	MG	5	3649	-	X
85	MG	5	3650	-	X
85	MG	5	3651	-	X
85	MG	5	3652	-	X
85	MG	5	3654	-	X
85	MG	5	3657	-	X
85	MG	5	3659	-	X
85	MG	5	3660	-	X
85	MG	5	3664	-	X
85	MG	5	3667	-	X
85	MG	5	3671	-	X
85	MG	5	3675	-	X
85	MG	5	3676	-	X
85	MG	5	3680	-	X
85	MG	5	3683	-	X
85	MG	5	3684	-	X
85	MG	5	3685	-	X
85	MG	5	3686	-	X
85	MG	5	3687	-	X
85	MG	5	3689	-	X
85	MG	5	3690	-	X
85	MG	5	3695	-	X
85	MG	5	3700	-	X
85	MG	5	3705	-	X
85	MG	5	3708	-	X
85	MG	5	3709	-	X
85	MG	5	3710	-	X
85	MG	5	3711	-	X
85	MG	5	3712	-	X
85	MG	5	3713	-	X
85	MG	5	3716	-	X
85	MG	5	3720	-	X
85	MG	5	3722	-	X
85	MG	5	3728	-	X
85	MG	5	3731	-	X
85	MG	5	3732	-	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	3738	-	X
85	MG	5	3739	-	X
85	MG	5	3743	-	X
85	MG	5	3744	-	X
85	MG	5	3752	-	X
85	MG	5	3753	-	X
85	MG	5	3758	-	X
85	MG	5	3759	-	X
85	MG	5	3762	-	X
85	MG	5	3764	-	X
85	MG	5	3765	-	X
85	MG	5	3766	-	X
85	MG	5	3769	-	X
85	MG	5	3770	-	X
85	MG	5	3771	-	X
85	MG	5	3772	-	X
85	MG	5	3774	-	X
85	MG	5	3777	-	X
85	MG	5	3778	-	X
85	MG	5	3780	-	X
85	MG	5	3781	-	X
85	MG	5	3784	-	X
85	MG	5	3787	-	X
85	MG	5	3791	-	X
85	MG	5	3794	-	X
85	MG	5	3795	-	X
85	MG	5	3803	-	X
85	MG	5	3804	-	X
85	MG	5	3805	-	X
85	MG	5	3807	-	X
85	MG	5	3809	-	X
85	MG	5	3813	-	X
85	MG	5	3815	-	X
85	MG	5	3821	-	X
85	MG	5	3823	-	X
85	MG	5	3827	-	X
85	MG	5	3829	-	X
85	MG	5	3834	-	X
85	MG	5	3840	-	X
85	MG	5	3846	-	X
85	MG	5	3849	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3850	-	X
85	MG	5	3857	-	X
85	MG	5	3860	-	X
85	MG	5	3862	-	X
85	MG	5	3864	-	X
85	MG	5	3865	-	X
85	MG	5	3868	-	X
85	MG	5	3870	-	X
85	MG	5	3872	-	X
85	MG	5	3873	-	X
85	MG	5	3875	-	X
85	MG	5	3876	-	X
85	MG	5	3881	-	X
85	MG	5	3882	-	X
85	MG	5	3887	-	X
85	MG	5	3888	-	X
85	MG	5	3889	-	X
85	MG	5	3892	-	X
85	MG	5	3895	-	X
85	MG	5	3896	-	X
85	MG	6	1901	-	X
85	MG	6	1908	-	X
85	MG	6	1911	-	X
85	MG	6	1915	-	X
85	MG	6	1916	-	X
85	MG	6	1918	-	X
85	MG	6	1919	-	X
85	MG	6	1920	-	X
85	MG	6	1921	-	X
85	MG	6	1924	-	X
85	MG	6	1927	-	X
85	MG	6	1930	-	X
85	MG	6	1932	-	X
85	MG	6	1933	-	X
85	MG	6	1936	-	X
85	MG	6	1939	-	X
85	MG	6	1941	-	X
85	MG	6	1942	-	X
85	MG	6	1943	-	X
85	MG	6	1944	-	X
85	MG	6	1946	-	X
85	MG	6	1947	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1948	-	X
85	MG	6	1950	-	X
85	MG	6	1952	-	X
85	MG	6	1953	-	X
85	MG	6	1954	-	X
85	MG	6	1959	-	X
85	MG	6	1964	-	X
85	MG	6	1966	-	X
85	MG	6	1967	-	X
85	MG	6	1970	-	X
85	MG	6	1971	-	X
85	MG	6	1974	-	X
85	MG	6	1979	-	X
85	MG	6	1981	-	X
85	MG	6	1983	-	X
85	MG	6	1984	-	X
85	MG	6	1988	-	X
85	MG	6	1991	-	X
85	MG	6	1993	-	X
85	MG	6	1996	-	X
85	MG	6	2000	-	X
85	MG	6	2005	-	X
85	MG	6	2006	-	X
85	MG	6	2008	-	X
85	MG	6	2013	-	X
85	MG	6	2019	-	X
85	MG	6	2027	-	X
85	MG	6	2028	-	X
85	MG	6	2030	-	X
85	MG	6	2034	-	X
85	MG	6	2038	-	X
85	MG	6	2043	-	X
85	MG	6	2045	-	X
85	MG	7	201	-	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	216	-	X
85	MG	8	204	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	8	205	-	X
85	MG	8	207	-	X
85	MG	8	208	-	X
85	MG	8	209	-	X
85	MG	8	212	-	X
85	MG	8	214	-	X
85	MG	L7	301	-	X
85	MG	L7	302	-	X
85	MG	L7	303	-	X
85	MG	M0	303	-	X
85	MG	M7	204	-	X
85	MG	M9	201	-	X
85	MG	N3	201	-	X
85	MG	N5	201	-	X
85	MG	N8	201	-	X
85	MG	N8	203	-	X
85	MG	c7	201	-	X
85	MG	d3	202	-	X
85	MG	d6	102	-	X
85	MG	l3	401	-	X
85	MG	l3	402	-	X
85	MG	l3	403	-	X
85	MG	l5	301	-	X
85	MG	l7	301	-	X
85	MG	l7	303	-	X
85	MG	m4	201	-	X
85	MG	m6	202	-	X
85	MG	m7	205	-	X
85	MG	o3	202	-	X
85	MG	q3	502	-	X
86	OHX	1	3872	-	X
86	OHX	1	3894	-	X
86	OHX	1	3899	-	X
86	OHX	1	3902	-	X
86	OHX	1	3909	-	X
86	OHX	1	4022	-	X
86	OHX	1	4067	-	X
86	OHX	1	4117	-	X
86	OHX	1	4124	-	X
86	OHX	1	4130	-	X
86	OHX	1	4144	-	X
86	OHX	1	4145	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4146	-	X
86	OHX	1	4147	-	X
86	OHX	1	4182	-	X
86	OHX	1	4183	-	X
86	OHX	1	4190	-	X
86	OHX	1	4195	-	X
86	OHX	1	4201	-	X
86	OHX	1	4213	-	X
86	OHX	1	4217	-	X
86	OHX	1	4219	-	X
86	OHX	2	2029	-	X
86	OHX	2	2032	-	X
86	OHX	2	2142	-	X
86	OHX	2	2147	-	X
86	OHX	2	2158	-	X
86	OHX	2	2171	-	X
86	OHX	2	2172	-	X
86	OHX	5	3900	-	X
86	OHX	5	3906	-	X
86	OHX	5	3908	-	X
86	OHX	5	3912	-	X
86	OHX	5	3930	-	X
86	OHX	5	4010	-	X
86	OHX	5	4085	-	X
86	OHX	5	4150	-	X
86	OHX	5	4157	-	X
86	OHX	5	4172	-	X
86	OHX	5	4175	-	X
86	OHX	5	4184	-	X
86	OHX	5	4190	-	X
86	OHX	5	4203	-	X
86	OHX	5	4216	-	X
86	OHX	5	4218	-	X
86	OHX	5	4226	-	X
86	OHX	5	4229	-	X
86	OHX	5	4234	-	X
86	OHX	6	2052	-	X
86	OHX	6	2054	-	X
86	OHX	6	2065	-	X
86	OHX	6	2160	-	X
86	OHX	6	2181	-	X
86	OHX	6	2184	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	6	2187	-	X
86	OHX	6	2205	-	X
86	OHX	8	228	-	X
86	OHX	M7	205	-	X
86	OHX	l5	306	-	X
87	ZN	D7	101	-	X

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411276 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 22 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called Unknown protein m2.

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

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

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

- Molecule 83 is a protein called Unknown protein p1.

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

- Molecule 84 is a protein called Unknown protein p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	3	Total 3	Mg 3	0	0
85	m6	2	Total 2	Mg 2	0	0
85	n8	5	Total 5	Mg 5	0	0
85	q3	2	Total 2	Mg 2	0	0
85	o1	1	Total 1	Mg 1	0	0
85	N5	1	Total 1	Mg 1	0	0
85	6	145	Total 145	Mg 145	0	0
85	sM	2	Total 2	Mg 2	0	0
85	O4	1	Total 1	Mg 1	0	0
85	m5	3	Total 3	Mg 3	0	0
85	l3	3	Total 3	Mg 3	0	0
85	M1	2	Total 2	Mg 2	0	0
85	n0	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	121	Total 121	Mg 121	0	0
85	O3	1	Total 1	Mg 1	0	0
85	S6	1	Total 1	Mg 1	0	0
85	L4	2	Total 2	Mg 2	0	0
85	l7	3	Total 3	Mg 3	0	0
85	M5	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	2	Total 2	Mg 2	0	0
85	q0	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	497	Total 497	Mg 497	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
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	2	Total 2	Mg 2	0	0
85	d3	2	Total 2	Mg 2	0	0
85	o7	1	Total 1	Mg 1	0	0
85	o3	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	M3	3	Total 3	Mg 3	0	0
85	N3	3	Total 3	Mg 3	0	0
85	4	23	Total 23	Mg 23	0	0
85	n6	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	2	Total 2	Mg 2	0	0
85	m1	1	Total 1	Mg 1	0	0
85	l5	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	m4	1	Total 1	Mg 1	0	0
85	N8	3	Total 3	Mg 3	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	l8	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	16	Total 16	Mg 16	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	3	Total 3	Mg 3	0	0

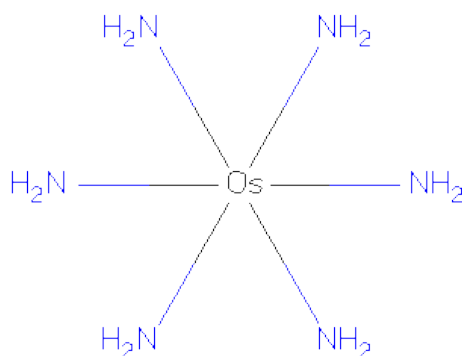
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	s4	1	Total 1	Mg 1	0	0
85	N6	1	Total 1	Mg 1	0	0
85	8	15	Total 15	Mg 15	0	0
85	l4	1	Total 1	Mg 1	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0
85	3	13	Total 13	Mg 13	0	0

- 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 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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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
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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			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	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
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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	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		
86	M5	1	Total	N	Os	0	0
			7	6	1		
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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	N9	1	Total	N	Os	0	0
			7	6	1		
86	O1	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	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
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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
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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
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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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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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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			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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			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

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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
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
			7	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	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	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	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	15	1	Total	N	Os	0	0
			7	6	1		
86	19	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	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	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	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	q1	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

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

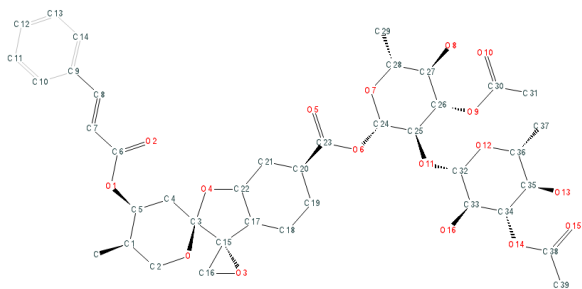
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		
87	q3	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		
87	D7	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
87	o7	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		

- Molecule 88 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-  
{[(2R,2'S,3a'R,4'S,5'R,6'S,7a'S)-5''-methyl-4''-{[(2E)-3-phenylprop-2-enoyl]oxy}decahy  
drodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose  
(three-letter code: 3K5) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>17</sub>).



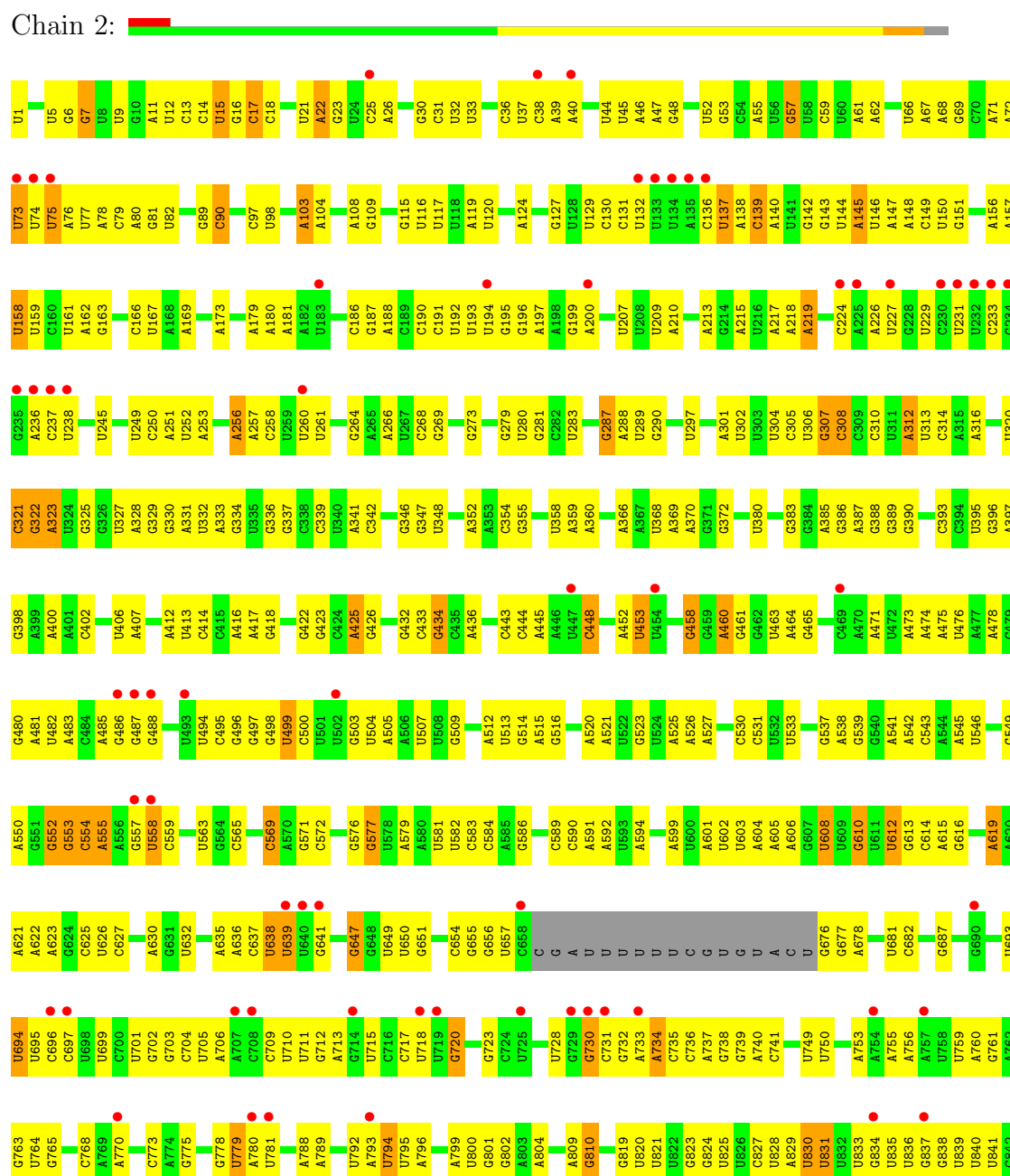


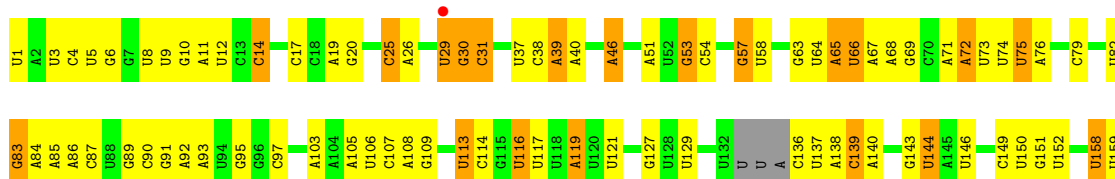
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			57	40	17		
88	5	1	Total	C	O	0	0
			57	40	17		

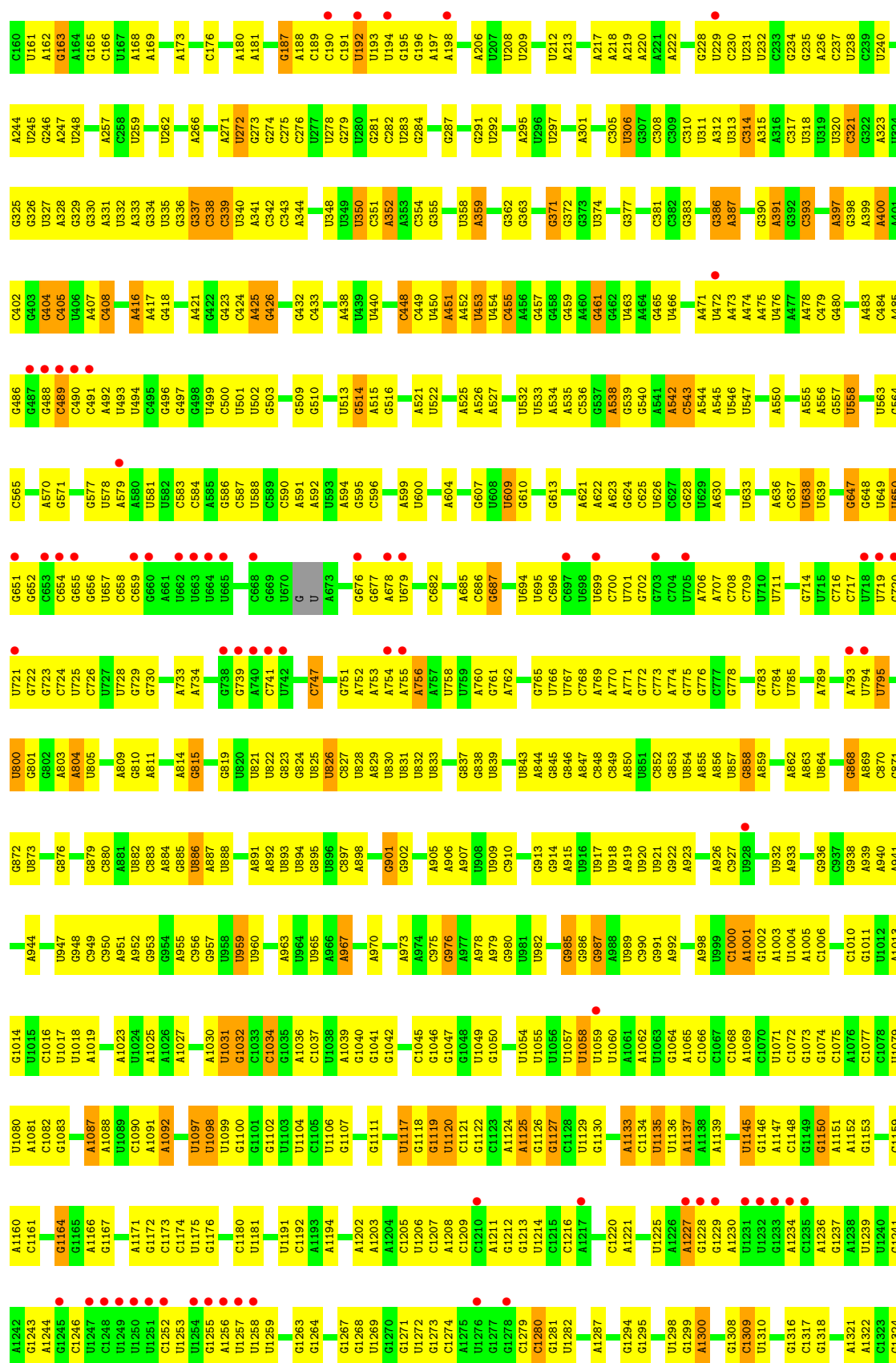
### 3 Residue-property plots

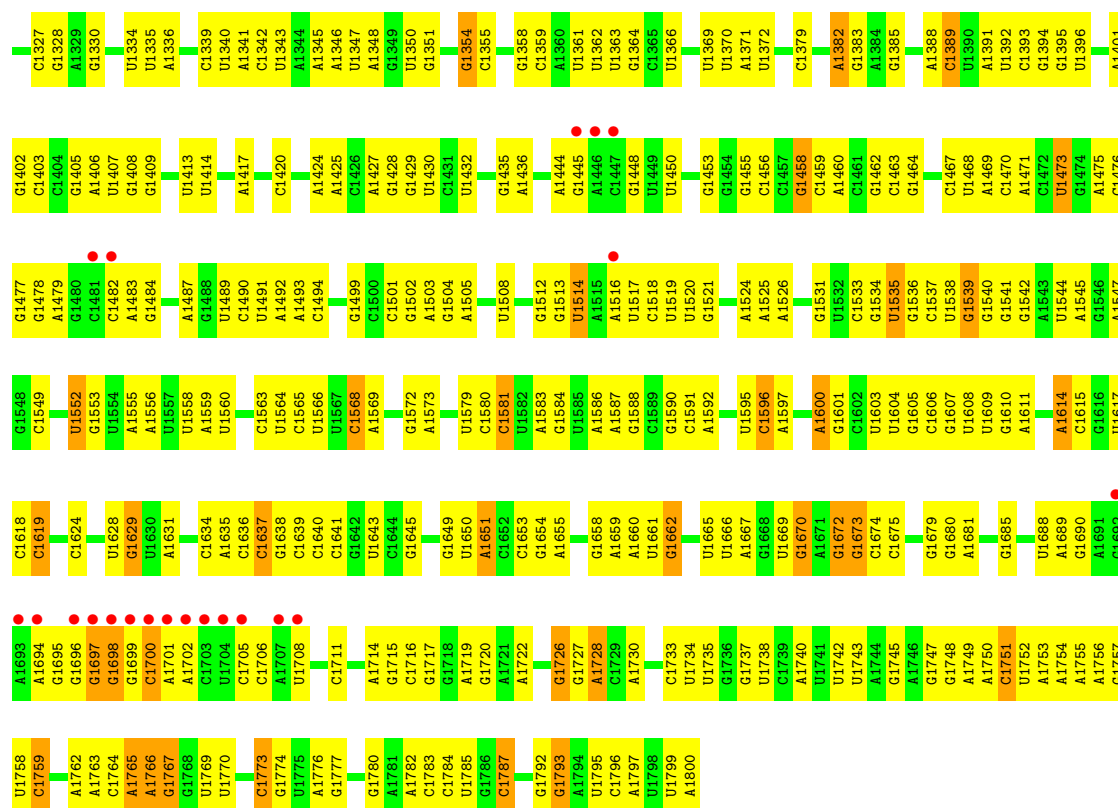
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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



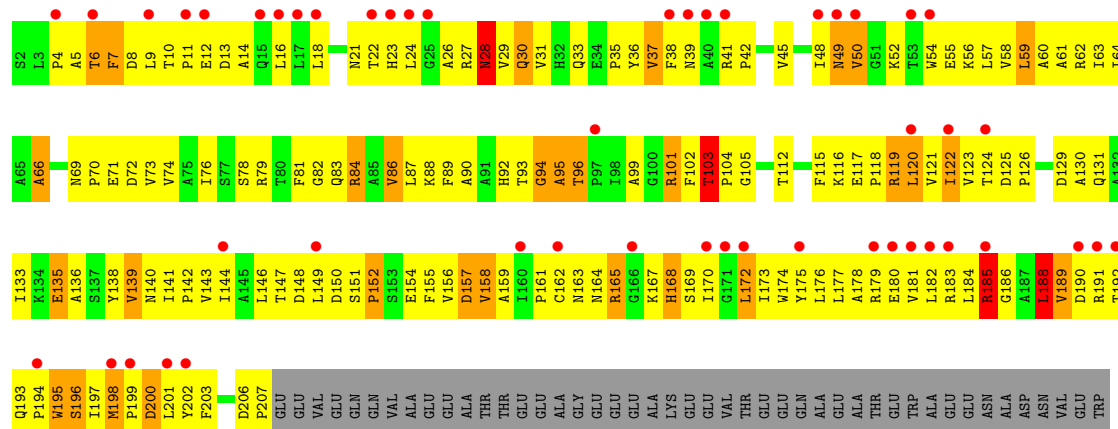






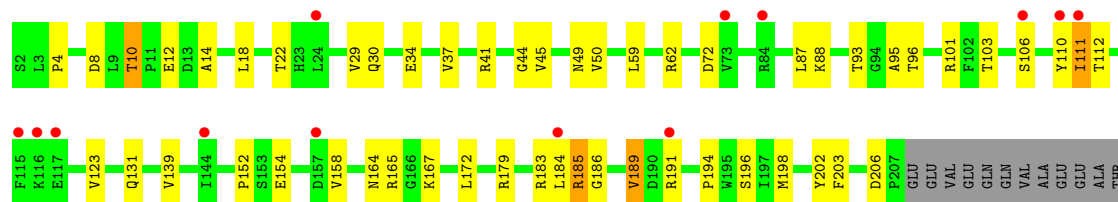
• Molecule 2: 40S ribosomal protein S0-A

Chain S0:

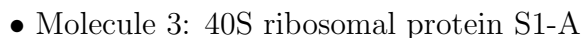


• Molecule 2: 40S ribosomal protein S0-A

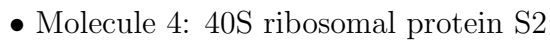
Chain s0:



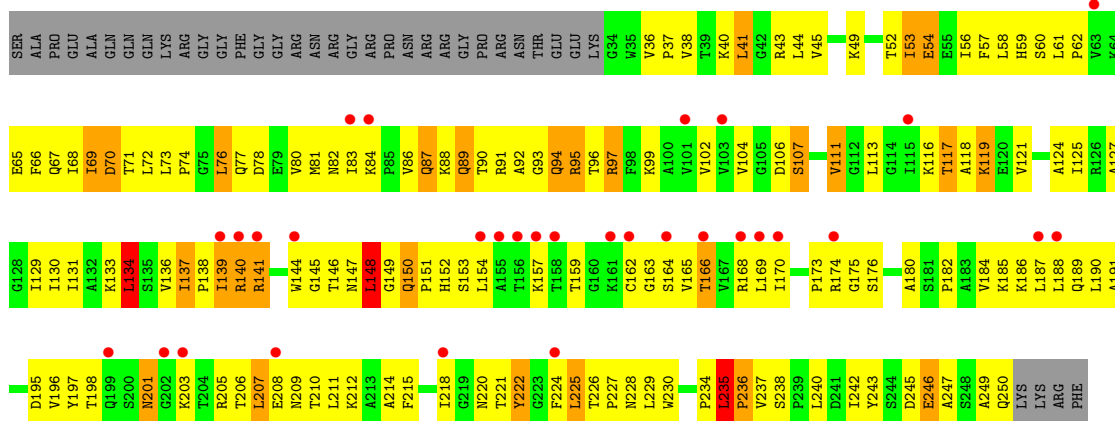
Chain S1:



## Chain s1:

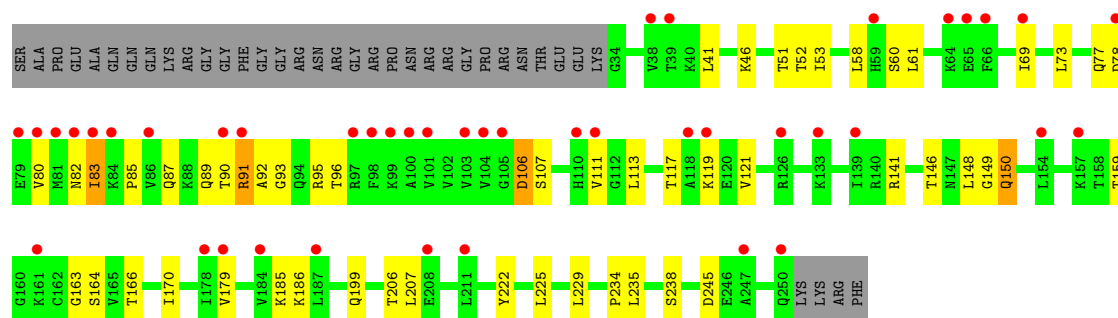


## Chain S2:



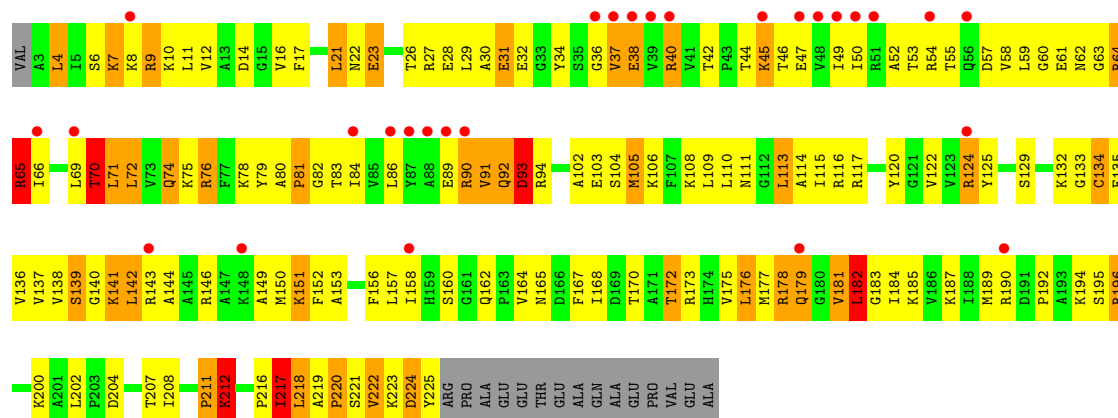
- Molecule 4: 40S ribosomal protein S2

Chain s2:



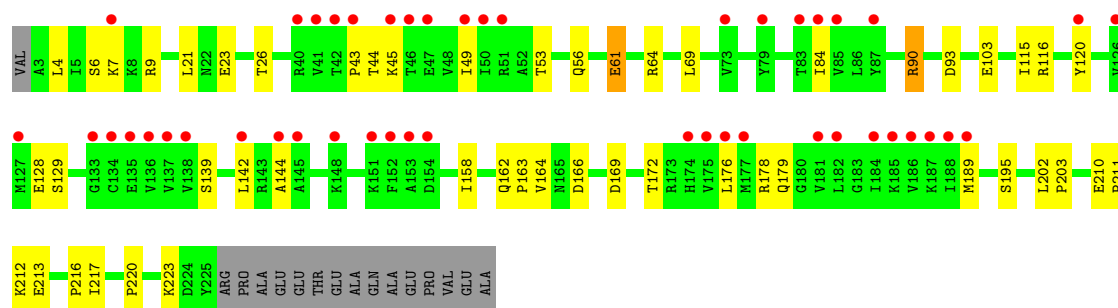
- Molecule 5: 40S ribosomal protein S3

Chain S3:



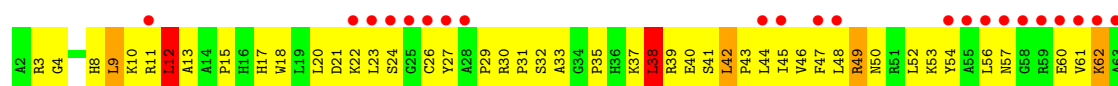
- Molecule 5: 40S ribosomal protein S3

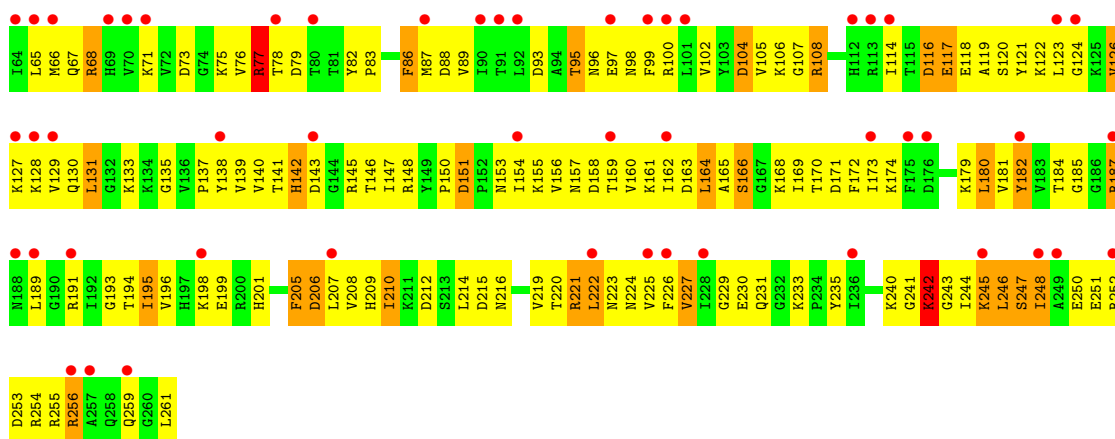
Chain s3:



- Molecule 6: 40S ribosomal protein S4-A

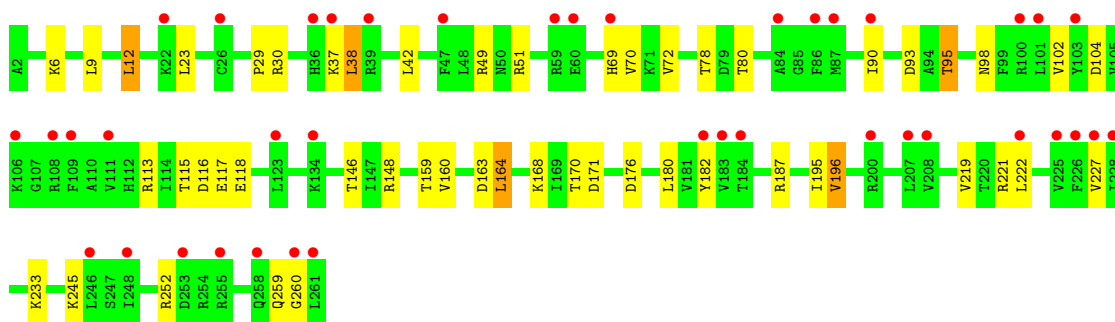
Chain S4:





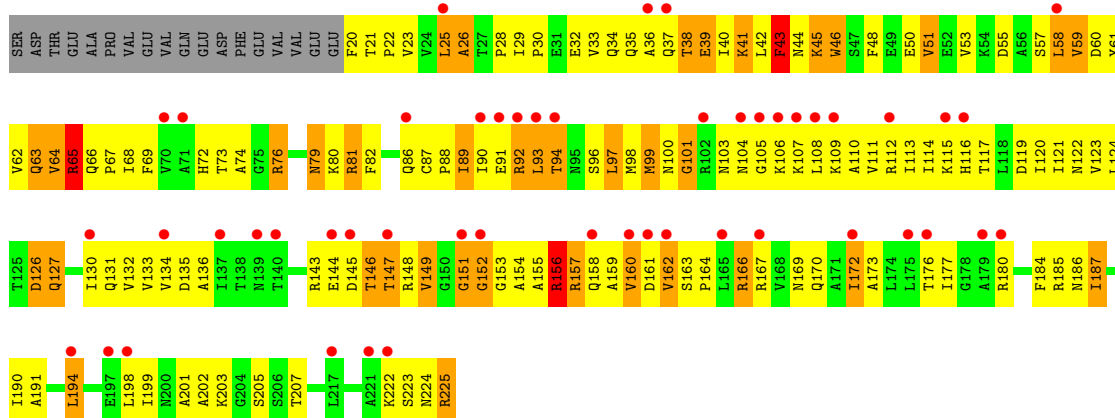
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



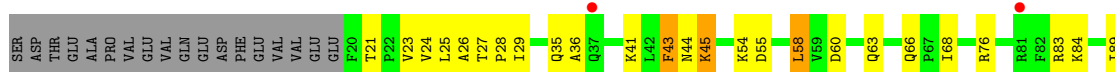
• Molecule 7: 40S ribosomal protein S5

Chain S5:



• Molecule 7: 40S ribosomal protein S5

Chain s5:

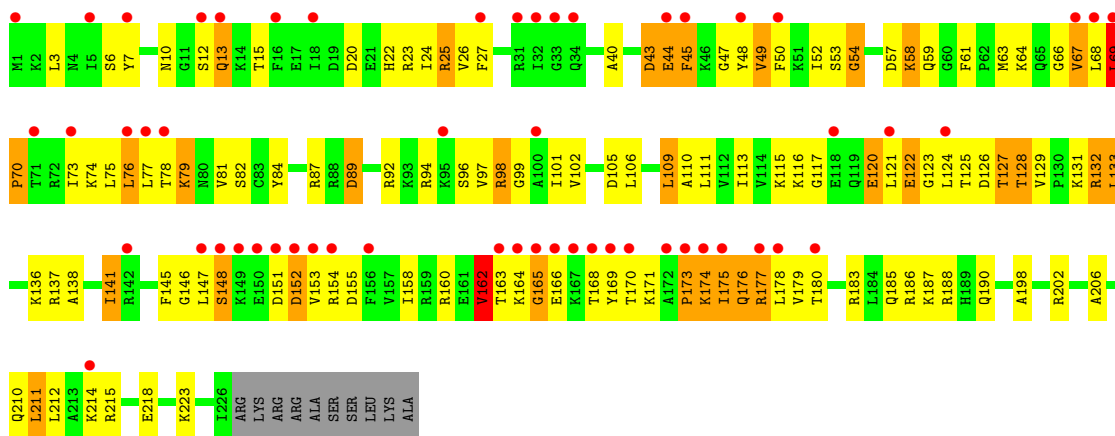






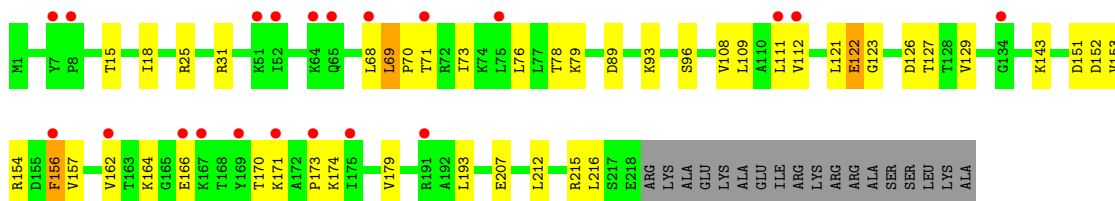
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



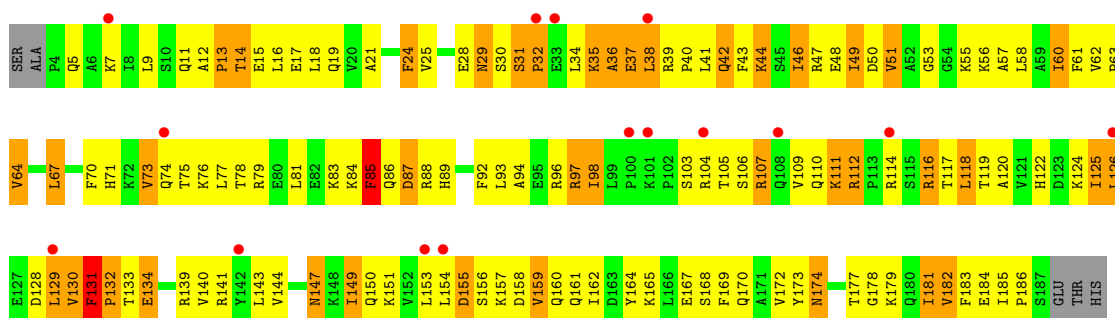
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



• Molecule 9: 40S ribosomal protein S7-A

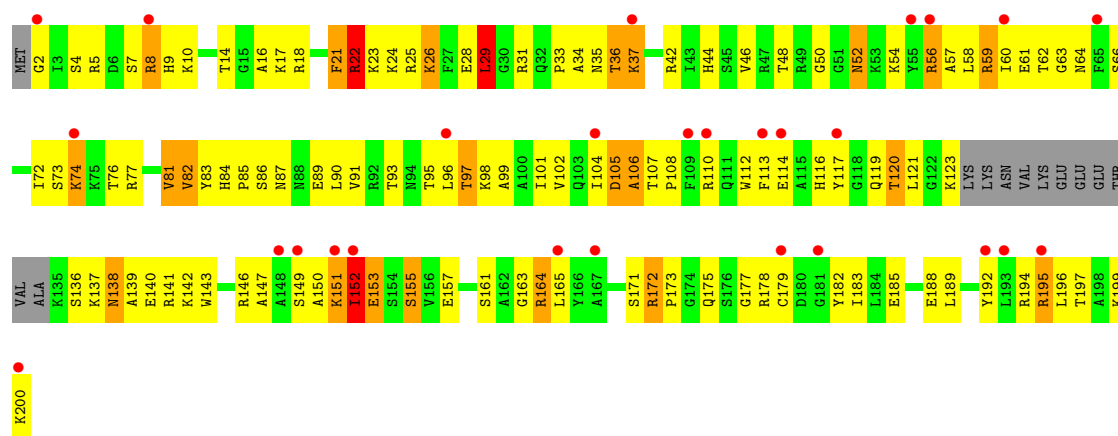
Chain s7:





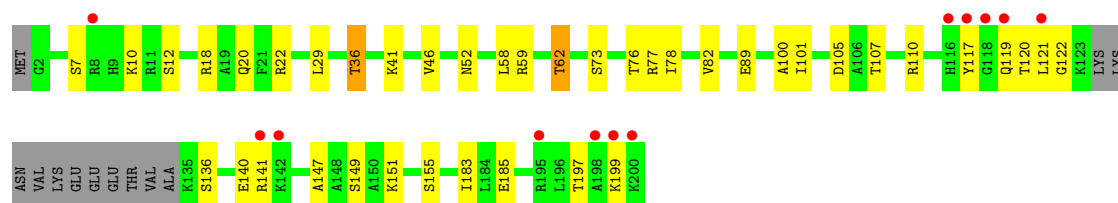
- Molecule 10: 40S ribosomal protein S8-A

Chain S8:



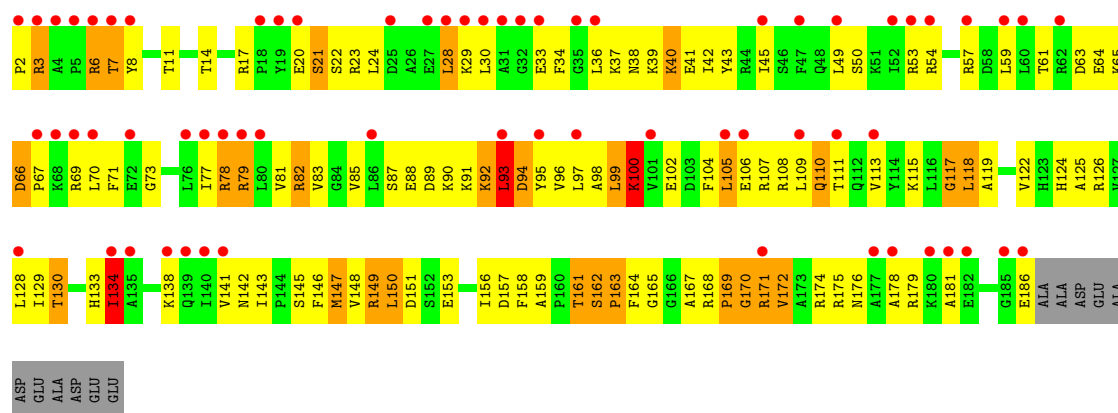
- Molecule 10: 40S ribosomal protein S8-A

Chain s8:



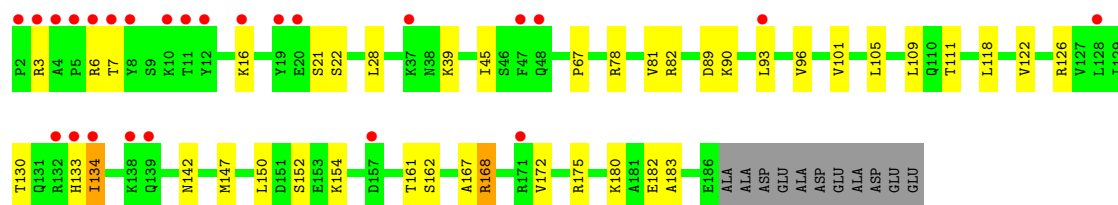
- Molecule 11: 40S ribosomal protein S9-A

Chain S9:



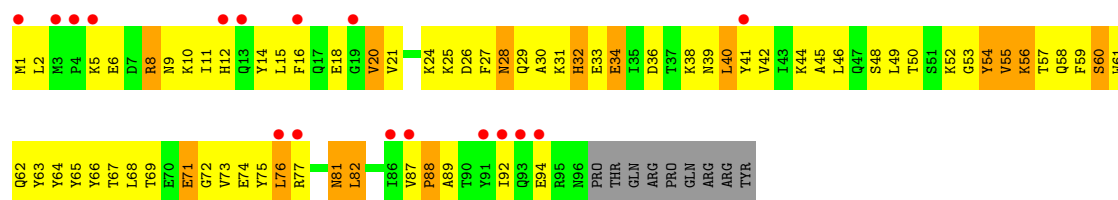
- Molecule 11: 40S ribosomal protein S9-A

Chain s9:



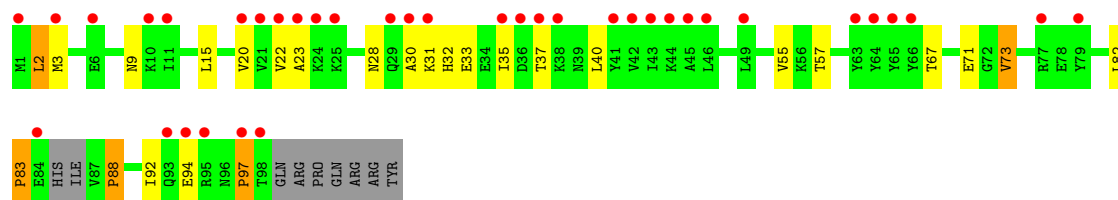
• Molecule 12: 40S ribosomal protein S10-A

Chain C0:



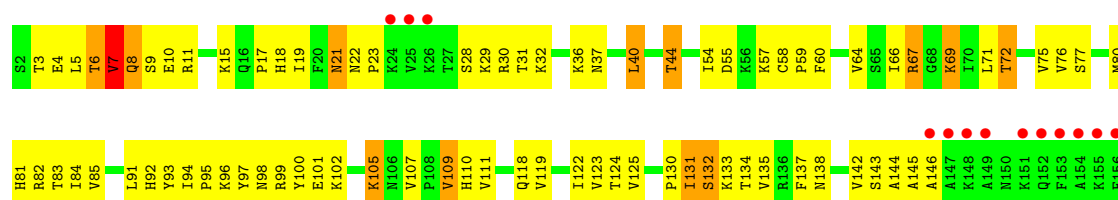
• Molecule 12: 40S ribosomal protein S10-A

Chain c0:



• Molecule 13: 40S ribosomal protein S11-A

Chain C1:



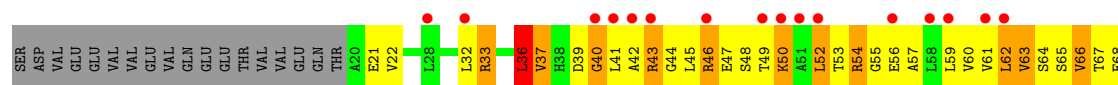
• Molecule 13: 40S ribosomal protein S11-A

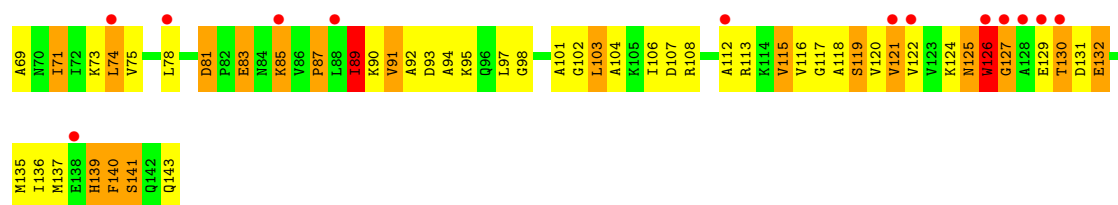
Chain c1:



• Molecule 14: 40S ribosomal protein S12

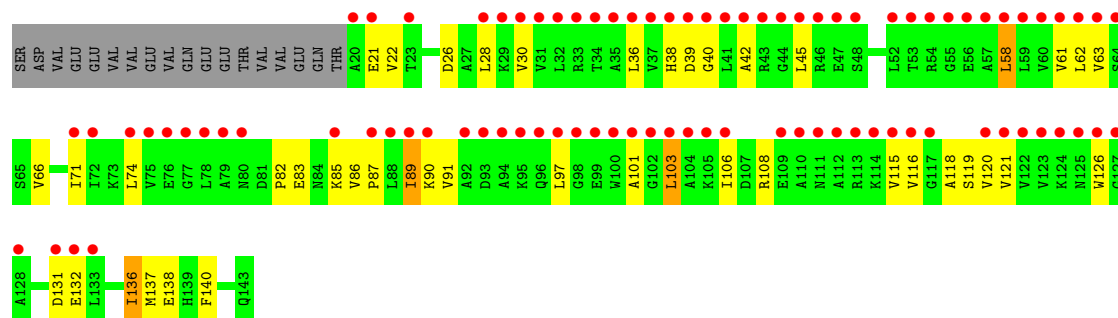
Chain C2:





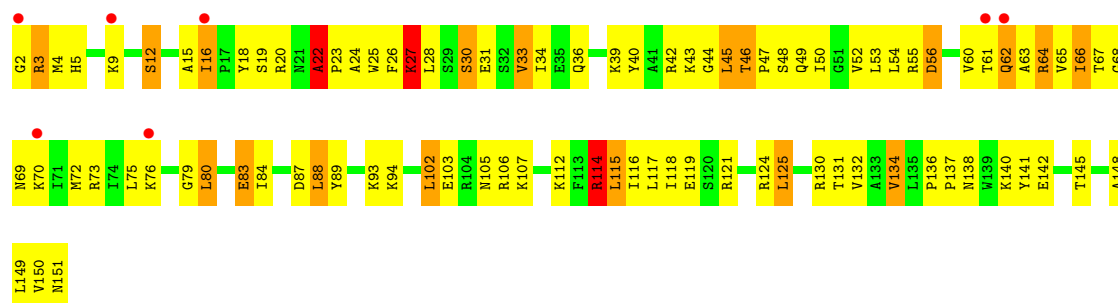
• Molecule 14: 40S ribosomal protein S12

Chain c2:



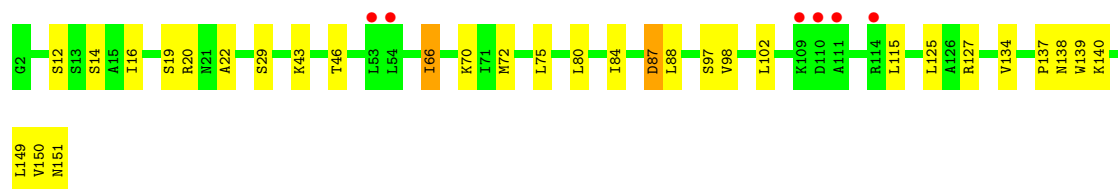
• Molecule 15: 40S ribosomal protein S13

Chain C3:



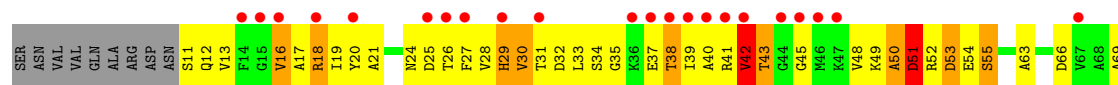
• Molecule 15: 40S ribosomal protein S13

Chain c3:



• Molecule 16: 40S ribosomal protein S14-A

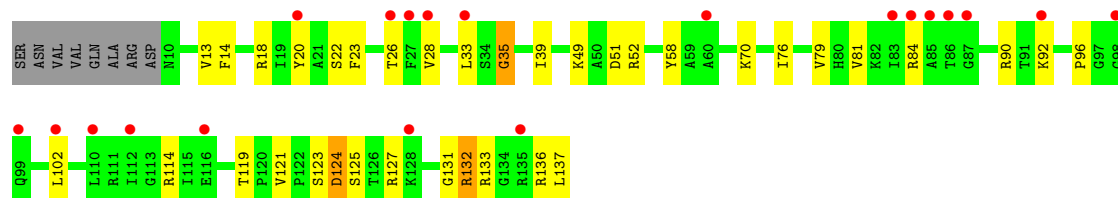
Chain C4:





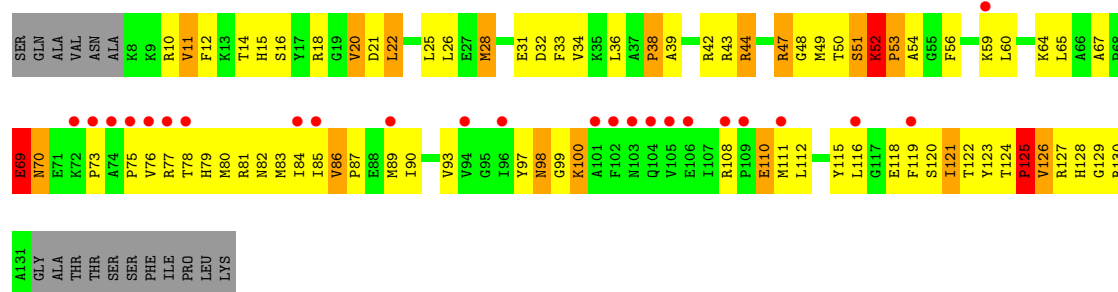
- Molecule 16: 40S ribosomal protein S14-A

Chain c4:



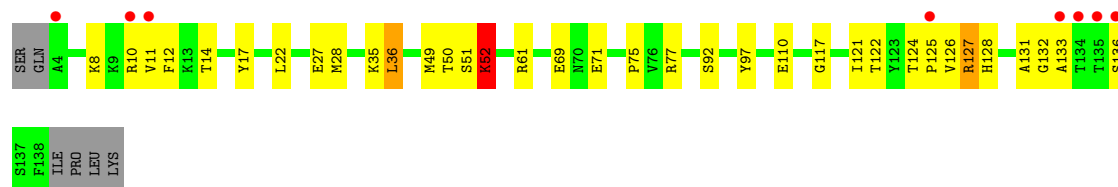
- Molecule 17: 40S ribosomal protein S15

Chain C5:



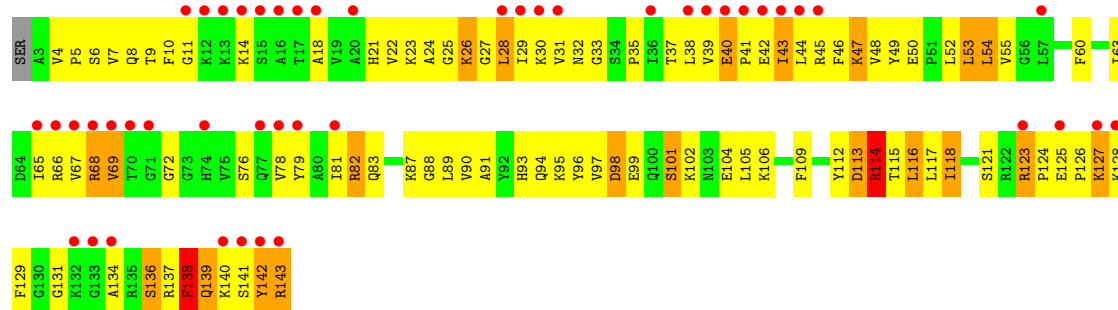
- Molecule 17: 40S ribosomal protein S15

Chain c5:



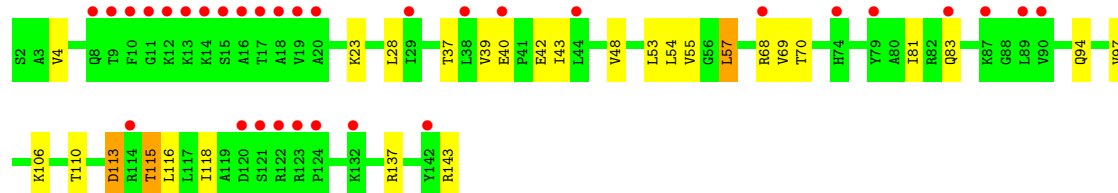
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:



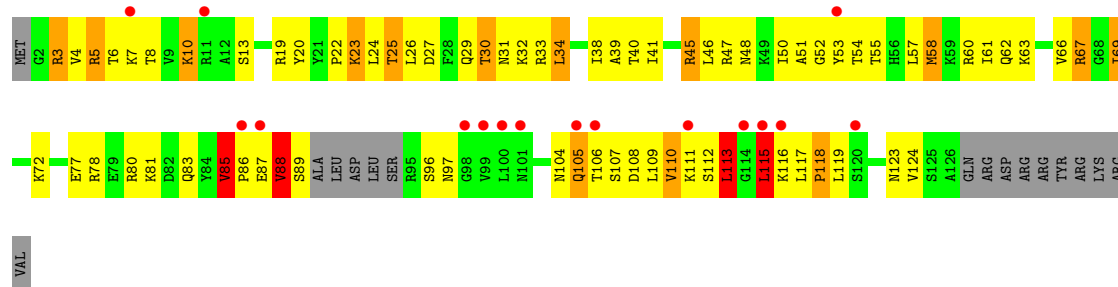
- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 



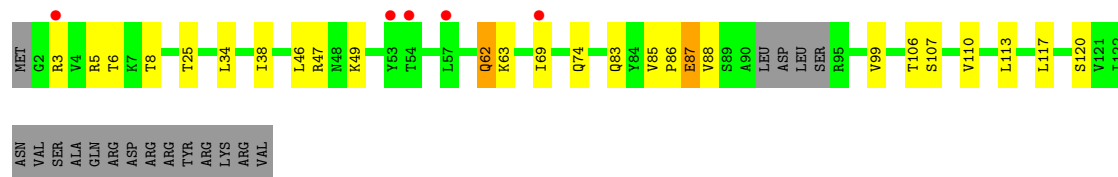
- Molecule 19: 40S ribosomal protein S17-A

Chain C7: 



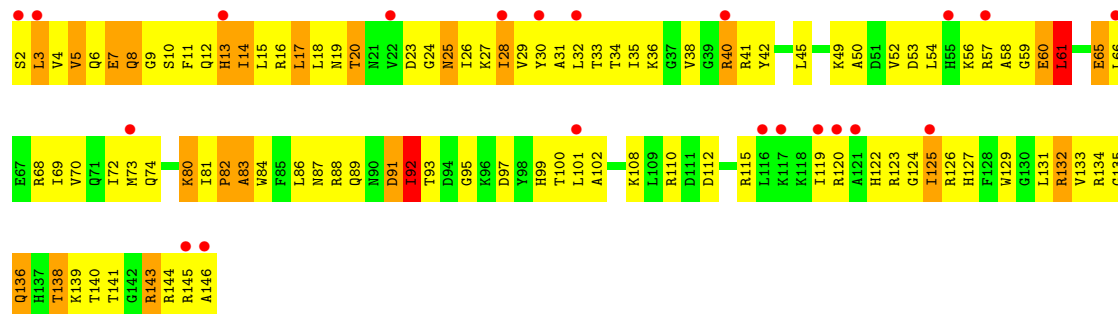
- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 



- Molecule 20: 40S ribosomal protein S18-A

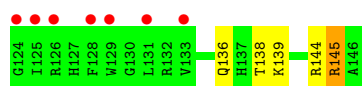
Chain C8: 



- Molecule 20: 40S ribosomal protein S18-A

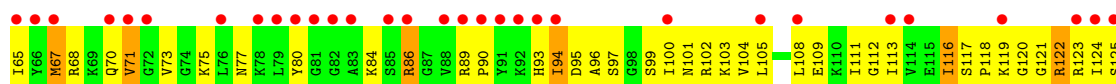
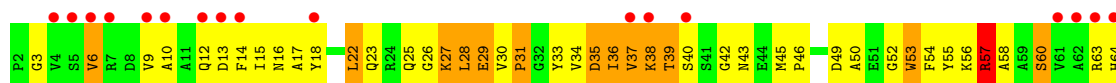
Chain c8: 





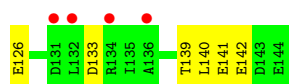
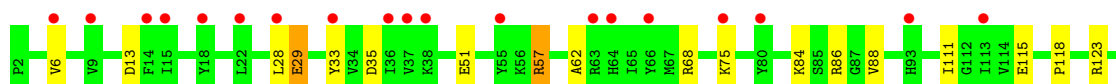
- Molecule 21: 40S ribosomal protein S19-A

Chain C9:



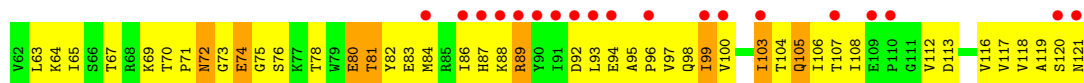
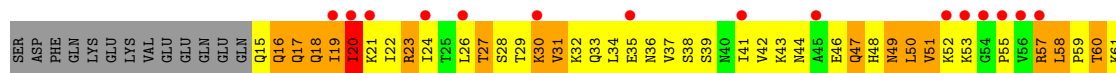
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



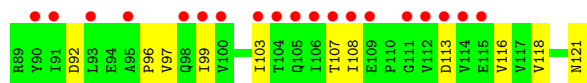
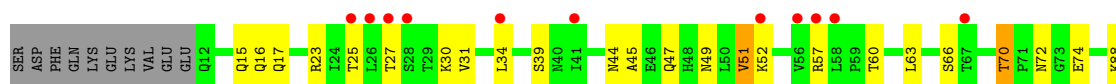
- Molecule 22: 40S ribosomal protein S20

Chain D0:



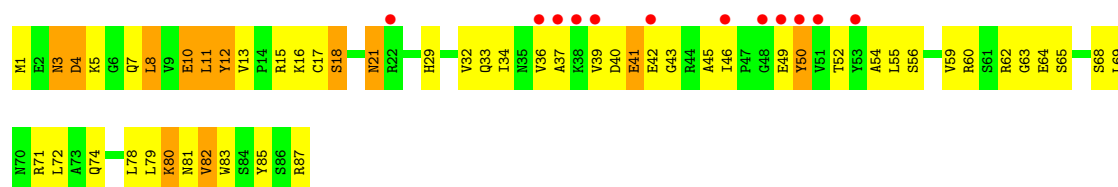
- Molecule 22: 40S ribosomal protein S20

Chain d0:



- Molecule 23: 40S ribosomal protein S21-A

Chain D1:



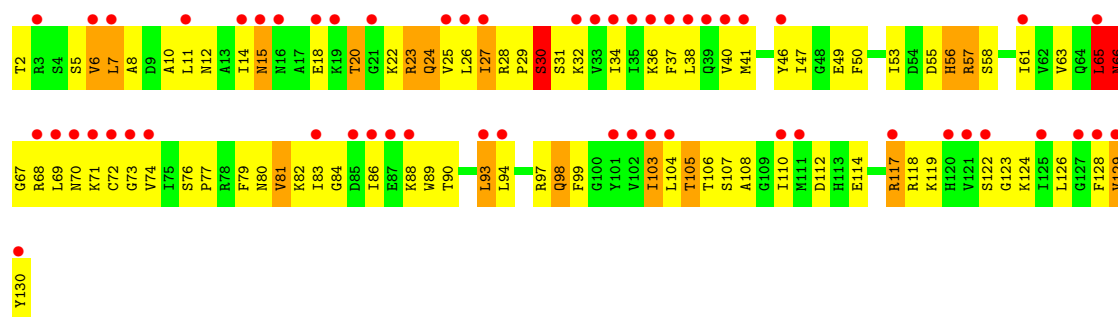
- Molecule 23: 40S ribosomal protein S21-A

Chain d1:



- Molecule 24: 40S ribosomal protein S22-A

Chain D2:



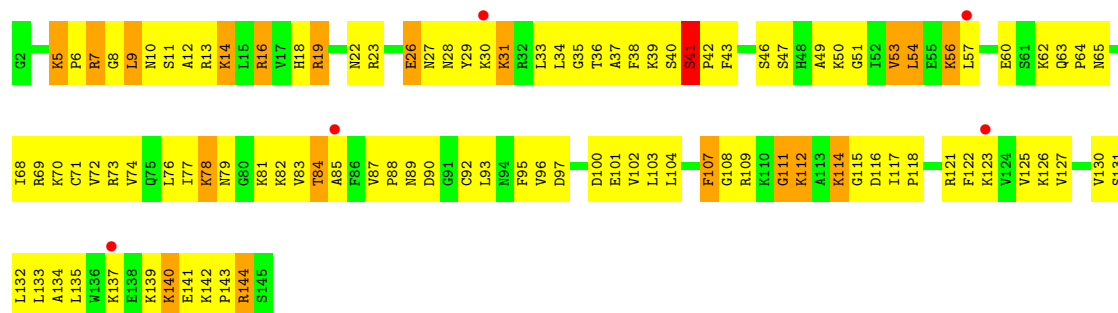
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:



- Molecule 25: 40S ribosomal protein S23-A

Chain D3:



- Molecule 25: 40S ribosomal protein S23-A

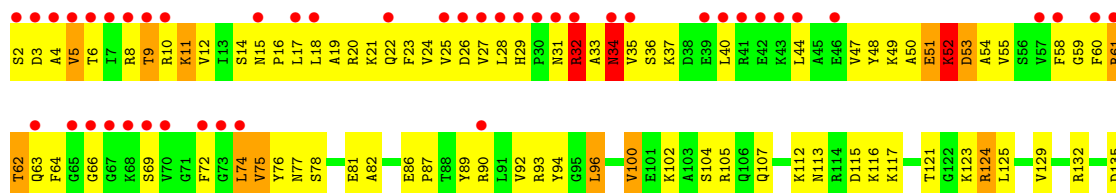
Chain d3:





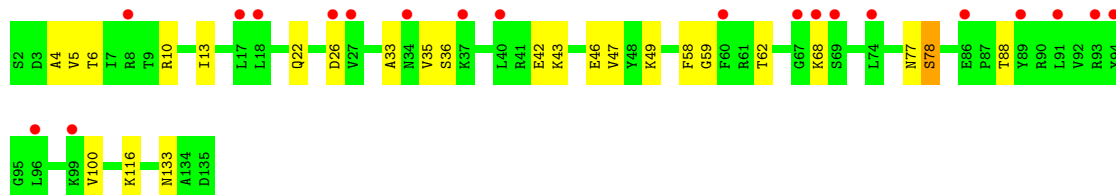
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:



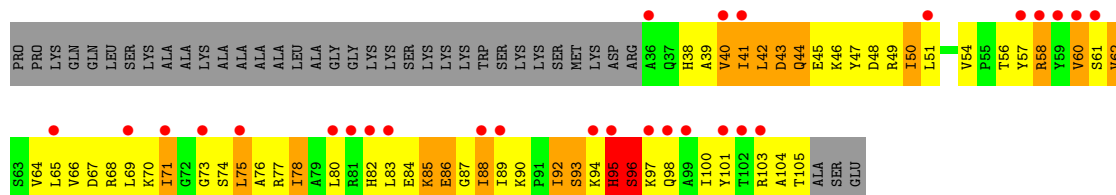
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:



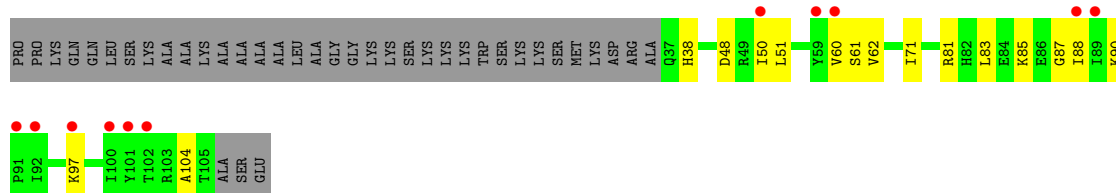
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:



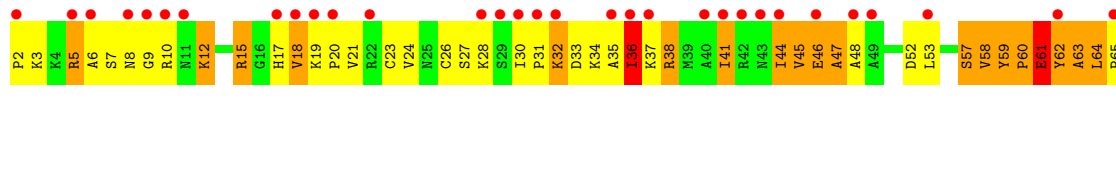
- Molecule 27: 40S ribosomal protein S25-A

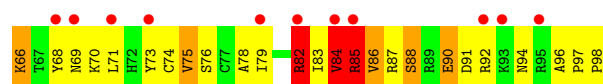
Chain d5:



- Molecule 28: 40S ribosomal protein S26-B

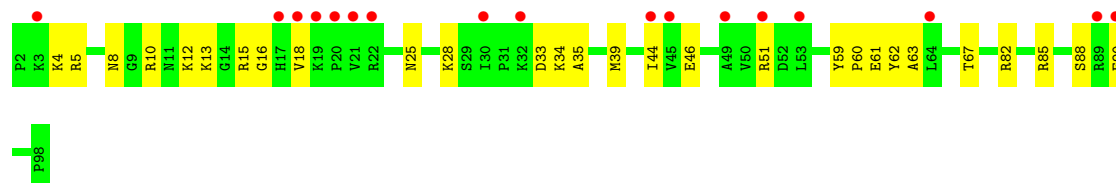
Chain D6:





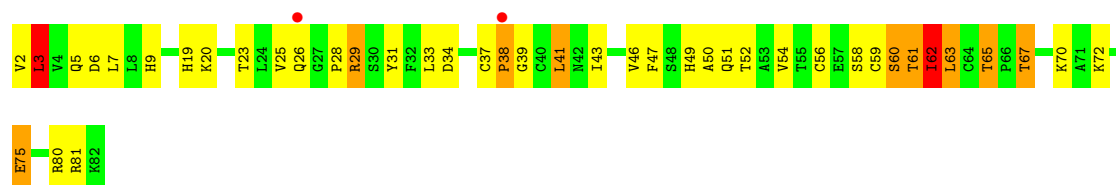
- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



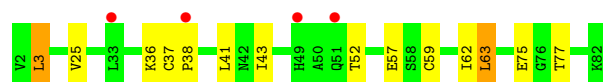
- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



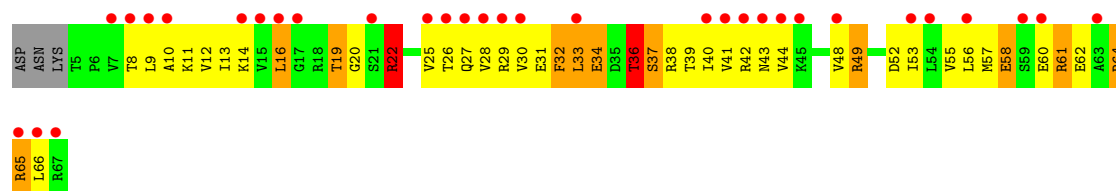
- Molecule 29: 40S ribosomal protein S27-A

Chain d7:



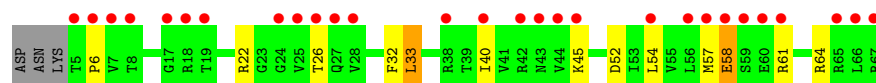
- Molecule 30: 40S ribosomal protein S28-A

Chain D8:



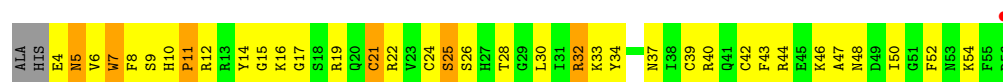
- Molecule 30: 40S ribosomal protein S28-A

Chain d8:



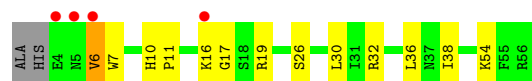
- Molecule 31: 40S ribosomal protein S29-A

Chain D9:



- Molecule 31: 40S ribosomal protein S29-A

Chain d9:



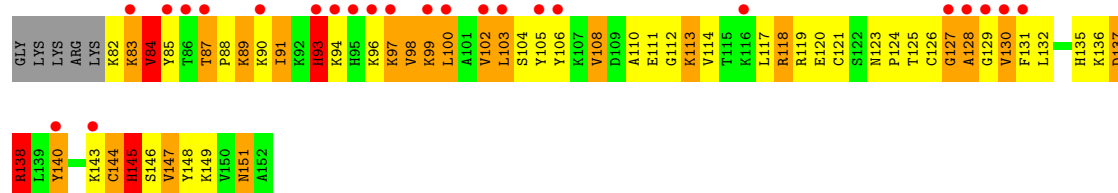
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:



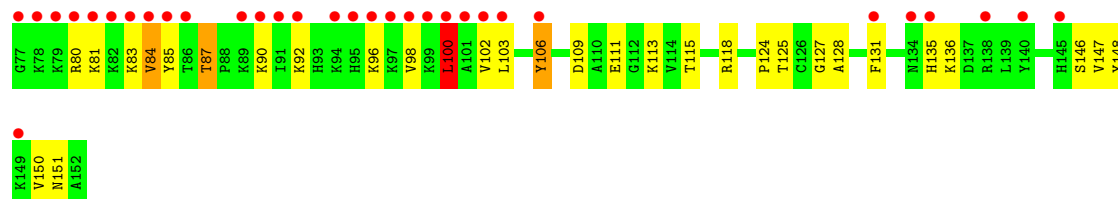
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



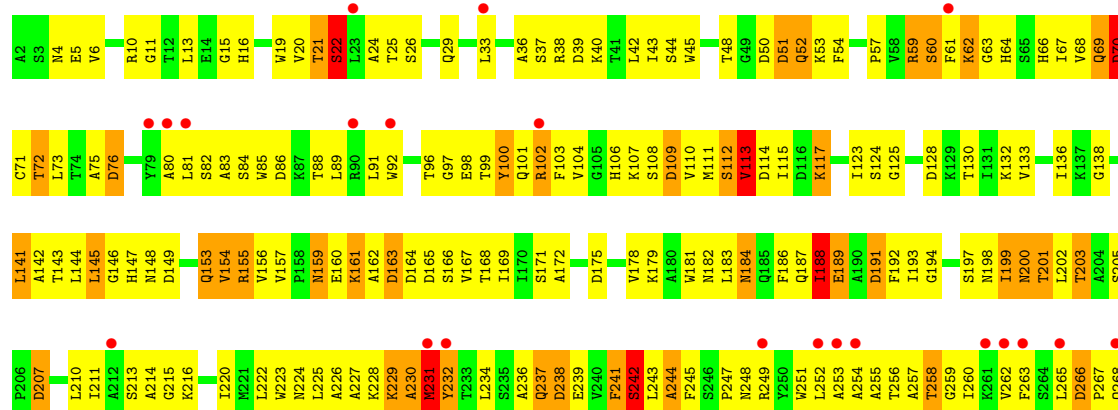
- Molecule 33: Ubiquitin-40S ribosomal protein S31

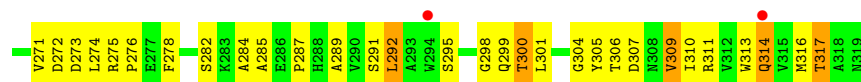
Chain e1:



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

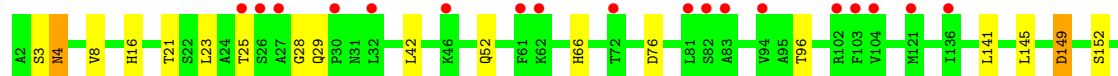
Chain SR:





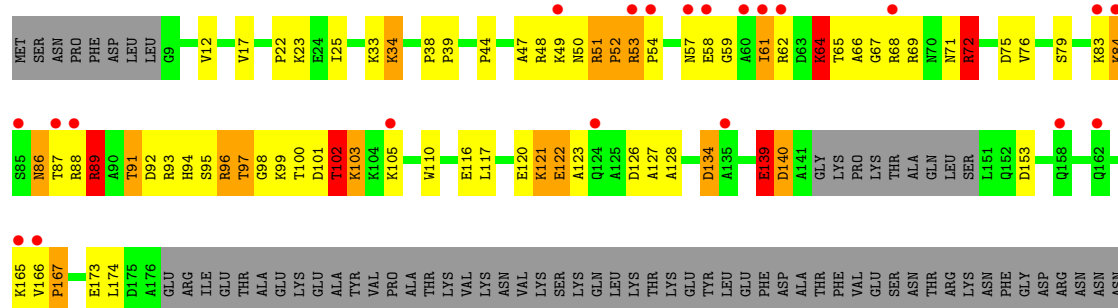
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



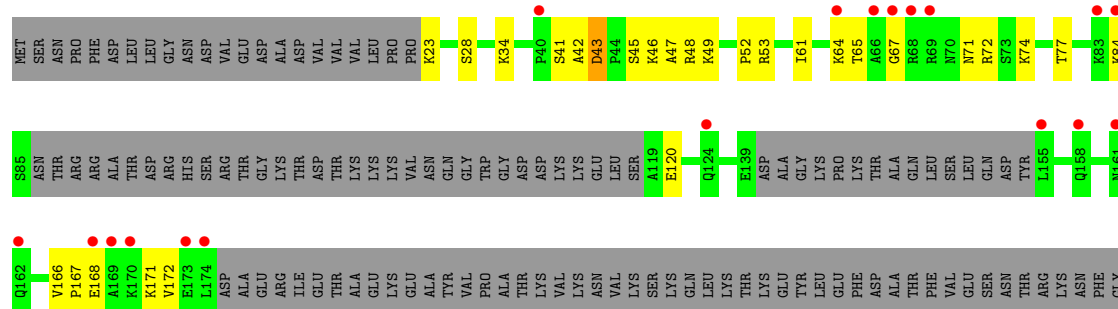
- Molecule 35: Suppressor protein STM1

Chain SM:



- Molecule 35: Suppressor protein STM1

Chain sM:



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

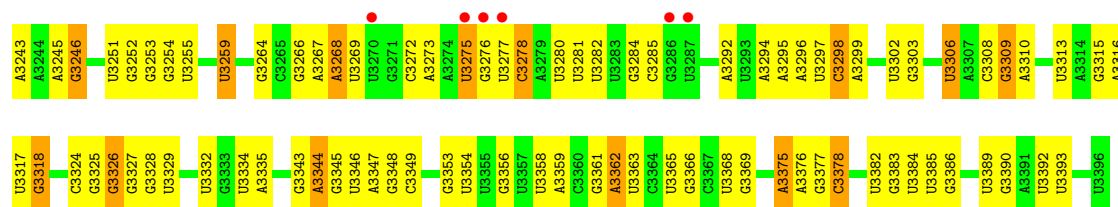
Chain 1:



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A150	U1078	G1005	G937	U871	G800	G718	G852	C578	C495	A436	G364	G297	G227	U154	C89
G151	U1087	A1006	C938	U872	A801	G719	A653	G579	C496	A437	A365	U298	U230	G155	C73
G152	U1088	C902	U939	C873	C903	A720	C554	G583	A501	A438	A366	U299	G231	G156	C74
A153	G1089	U1008	G940	U874	C904	G721	C555	U502	U502	C439	G368	G300	G232	A157	G75
A154	U1090	A1009	U942	U875	G805	G722	A656	C503	C503	A440	A369	G304	G233	G158	G76
C1155	A1093	G1010	U943	C877	G806	G723	G857	U587	U506	U	U370	G304	G234	A159	A77
C1156	U1094	U1014	C944	G878	A806	G724	G858	U588	U507	G	G371	A308	G239	U83	U83
C1157	U1095	U1015	C945	G879	A807	G725	G859	A589	U508	G	A372	A308	U240	U84	U84
A1158	U1096	C1016	U946	C881	G809	G726	A660	G590	U509	U	A373	A308	U241	A85	A85
A1159	G1097	U1017	C947	C882	A810	G727	U662	G591	U510	U	A374	A313	G242	G86	G86
C1160	A1098	G1018	C948	A883	U811	A735	C563	A592	G510	U	A375	A313	C242	A164	A164
G1161	U1099	G1019	G950	A884	G812	A736	U664	C593	G514	U	A376	U314	G243	A165	A165
A1162	U1100	U1020	A951	U885	G813	G737	A665	C594	G515	U	A377	U315	G244	U168	U168
A1163	G1101	G1021	A952	C886	U814	A738	A666	G595	A516	U	A378	U316	U245	G92	G92
G1164	A1102	G1022	G953	C887	G815	G739	C667	G596	A517	U	U382	U317	U246	C93	C93
A1165	A1025	A1025	U954	U854	A816	U748	G668	A598	G517	U	U383	A318	U247	G94	G94
G1166	A1026	A1026	U955	C880	A817	G742	U669	C599	U520	G	G383	A319	U248	G95	G95
A1170	A1105	A1027	U956	C889	C818	G743	C870	G600	A521	C	A384	G320	U249	G96	G96
G1171	G1106	U1028	C957	C893	A819	A744	U671	A608	A522	C	A385	C321	U250	G97	G97
A1172	C1107	G1029	C958	C894	A820	U745	A672	G609	A523	U	A386	C321	U251	U97	U97
A1173	U1108	A1030	C959	A895	U821	U746	C675	G610	U524	U	A391	A325	U252	G98	G98
G1174	U1109	U1033	U960	U886	G822	G749	G676	A611	U524	U	C392	U326	G256	A99	A99
C1175	U1110	U1034	C961	U889	C823	G750	G677	A612	A527	U	U393	A327	C180	A100	A100
G1176	U1111	U1035	A962	U890	C824	A751	A678	G613	U528	G	U394	U328	U181	G101	G101
G1177	A1112	U1036	G963	U900	U825	G752	G679	G614	A529	U	A395	U329	G182	C102	C102
A1178	G1113	G1037	G964	G901	G826	G754	U679	U615	A530	U	A396	G330	G183	G103	G103
A1179	U1114	A1040	A965	C902	U829	G755	G680	G616	G531	U	A397	G331	U188	G104	G104
A1180	G1115	U1041	U966	A906	U830	C765	U681	G617	A532	U	A398	G332	U189	C105	C105
U1181	U1116	U1042	A967	G907	G831	G766	G684	C618	A533	U	A399	G333	U190	A106	A106
A1182	C1117	C1043	G968	G908	G832	C768	G685	A619	U534	G	A400	A334	U191	A107	A107
C1185	C1118	U1044	C969	G909	G833	G769	G686	U620	U535	U	U401	G335	U192	A108	A108
G1186	U1120	C1045	A970	G910	G835	G770	U687	A621	G535	U	A402	A336	C193	A109	A109
C1187	A1047	A1047	G971	C911	G836	A771	U687	G624	U541	U	G403	G337	G267	G110	G110
U1188	U1048	A1048	A972	G912	A836	U772	A692	U627	C542	G	G404	A338	G268	C111	C111
C1189	C1049	U1050	C975	A913	A837	G773	A693	U628	C543	U	U405	A339	G269	U112	U112
A1190	U1051	U1051	U976	A914	G838	U774	C894	A629	C544	A	A406	C340	U270	C113	C113
C1191	G1126	U1052	C977	A915	C940	U776	C895	U629	U545	U	A407	G341	G271	A114	A114
C1192	G1127	U1053	G978	G916	C941	U777	C896	U630	C546	G	A408	G342	G272	A115	A115
A1193	U1128	A1053	U979	A917	A841	G779	A697	A630	G547	U	A409	U343	A273	A116	A116
G1194	U1129	U1054	A980	C918	A847	A780	U698	C633	C548	G	U410	G344	G274	U117	U117
A1195	A1130	A1055	U981	U919	A848	G781	A699	C634	U549	A	U411	G345	U275	U118	U118
C1196	G1131	U1056	C982	A920	C949	U782	A700	C635	A550	U	U412	C346	U276	U119	U119
A1197	A1132	U1057	A983	A921	U850	A784	G701	G636	A551	A	U413	G347	G277	G120	G120
C1198	G1133	U1058	G984	U922	C951	G785	C702	C637	C552	U	U414	A348	U278	A209	A209
C1199	A1134	U1059	G985	U923	C952	A786	G703	C638	C553	C	A416	A349	U279	U210	U210
A1200	A1135	A1061	G986	G924	U853	G787	U704	C639	A554	U	A417	C350	G280	A211	A211
C1201	A1136	G1063	A925	A925	G853	C788	A705	G640	U558	G	G420	A352	G281	U124	U124
A1202	C1137	A1064	G994	A926	G857	A789	U706	U640	A559	A	G421	G353	G282	C125	C125
A1203	U1138	A1065	U995	C927	A858	U790	U707	U641	A560	U	A418	G354	G283	C131	C131
A1204	G1139	G1066	A996	C928	G859	A791	G708	U643	C562	U	U419	A355	A284	U138	U138
A1205	A1140	U1071	A997	A929	G860	G792	A709	A644	C563	U	G425	C356	U286	G139	G139
G1207	C1141	U1072	G998	U930	G861	G793	A710	A645	U563	U	G426	A357	G287	C140	C140
U1211	G1142	G1073	G999	C931	U862	U794	A711	A646	C564	C	U429	G358	C288	U146	U146
A1212	A1143	U1074	U995	C932	G863	G795	G712	A647	U565	A	U430	U359	A289	U147	U147
G1213	G1145	A1075	G1001	A933	G864	U796	U712	C648	C566	U	U431	G360	G290	A222	A222
			A1002	G934	U865	U797	A715	A649		U		A361	C291	U223	U223

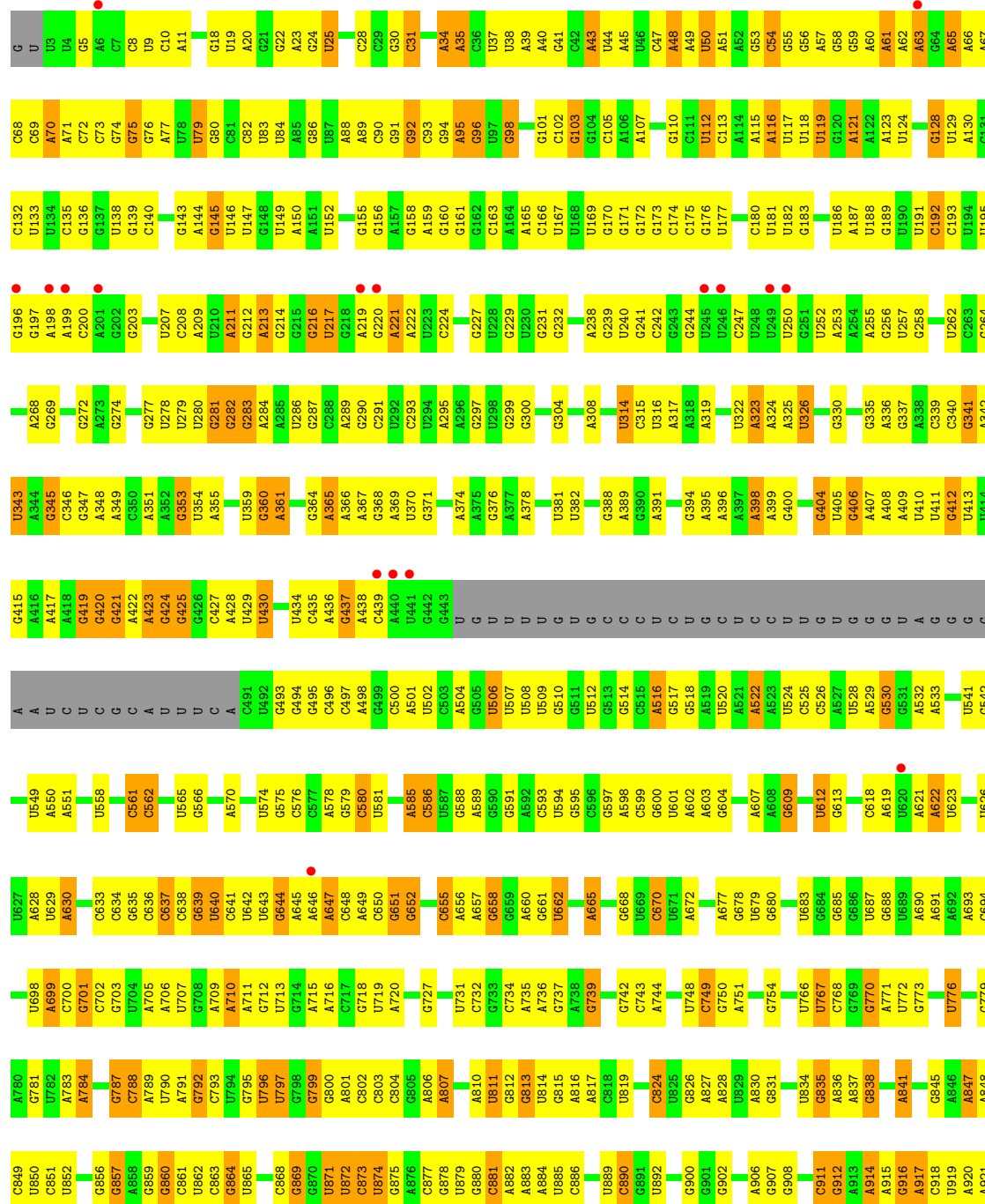


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G2273	U2274	A2275	C2276	C2277	C2278	A2281	U2282	U2283	C2284	U2285	U2286	U2287	U2288	U2289	C2293	U2294	A2295	A2296	A2297	U2298	U2301	G2302	A2303	C2304	C2305	G2306	G2307	C2308	A2309	U2310	G2311	A2312	A2313	U2314	G2315	A2316	U2317	U2318	U2319	A2320	A2321	C2322	G2323	U2324	U2325	A2326	C2329	C2333	U2334	U2335	U2336	C2337	C2339	U2340	A2341	C2342	C2343	U2351	A2352	G2353	C2354	A2355	A2356	A2357	U2358	C2359	C2360	C2361	C2362	A2363	C2366	A2367	A2368	G2369	G2370	G2371	A2372	A2373	C2374	G2375	G2376	G2377	C2378	U2379	U2380	G2381	A2382	A2383	A2384	G2385	A2386	A2387	A2390	C2391	C2392	G2393	A2394	U2395	G2396	G2397	A2398	U2399	G2400	A2401	A2402	U2403	U2404	C2405	C2406	U2407	U2408	G2409	U2410	U2411	G2412	G2413	G2414	U2417	U2418	A2419	U2420	U2421	C2422	U2423	U2424	U2425	U2426	U2427	U2428	U2429	U2433	U2434	G2437	A2438	A2439	G2442	A2443	C2444	A2445	U2450	A2451	G2452	U2453	U2454	U2455	U2456	U2457	U2458	U2459	U2460	U2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471	U2472	U2473	U2474	U2475	U2476	U2477	U2478	U2479	U2480	U2481	U2482	U2483	U2484	U2485	U2486	U2487	U2488	U2489	U2490	U2491	U2492	U2493	U2494	U2495	U2496	U2497	U2498	U2499	U2500	A2501	A2502	G2503	U2504	U2505	U2506	C2507	G2508	U2509	U2510	A2511	G2512	U2513	U2514	C2515	G2516	G2517	U2518	U2519	C2520	U2521	U2522	A2523	A2524	C2525	G2526	G2527	U2528	A2529	U2530	U2531	U2532	U2533	U2534	U2535	U2536	U2537	U2538	U2539	U2540	U2541	U2542	U2543	U2544	U2545	C2546	U2547	U2548	U2549	U2550	U2551	U2552	U2553	U2554	U2555	U2556	U2557	U2558	U2559	U2560	U2561	U2562	U2563	U2564	U2565	U2566	U2567	U2568	A2569	U2570	U2571	C2572	U2573	U2574	U2575	U2576	C2577	U2578	U2579	U2580	U2581	U2582	U2583	U2584	U2585	U2586	U2587	U2588	U2589	U2590	U2591	U2592	U2593	U2594	U2595	U2596	U2597	U2598	U2599	U2600	A2601	G2602	U2603	U2604	U2605	U2606	U2607	U2608	U2609	U2610	U2611	U2612	U2613	U2614	U2615	U2616	U2617	U2618	U2619	U2620	U2621	U2622	U2623	U2624	U2625	U2626	U2627	U2628	U2629	U2630	U2631	U2632	U2633	U2634	U2635	U2636	U2637	U2638	U2639	U2640	U2641	U2642	U2643	U2644	U2645	U2646	U2647	U2648	U2649	U2650	U2651	U2652	U2653	U2654	U2655	U2656	U2657	U2658	U2659	U2660	U2661	U2662	U2663	U2664	U2665	U2666	U2667	U2668	U2669	U2670	U2671	U2672	U2673	U2674	U2675	U2676	U2677	U2678	U2679	U2680	U2681	U2682	U2683	U2684	U2685	U2686	U2687	U2688	U2689	U2690	U2691	U2692	U2693	U2694	U2695	U2696	U2697	U2698	U2699	U2700	U2701	U2702	U2703	U2704	U2705	U2706	U2707	U2708	U2709	U2710	U2711	U2712	U2713	U2714	U2715	U2716	U2717	U2718	U2719	U2720	U2721	U2722	U2723	U2724	U2725	U2726	U2727	U2728	U2729	U2730	U2731	U2732	U2733	U2734	U2735	U2736	U2737	U2738	U2739	U2740	U2741	U2742	U2743	U2744	U2745	U2746	U2747	U2748	U2749	U2750	U2751	U2752	U2753	U2754	U2755	U2756	U2757	U2758	U2759	U2760	U2761	U2762	U2763	U2764	U2765	U2766	U2767	U2768	U2769	U2770	U2771	U2772	U2773	U2774	U2775	U2776	U2777	U2778	U2779	U2780	U2781	U2782	U2783	U2784	U2785	U2786	U2787	U2788	U2789	U2790	U2791	U2792	U2793	U2794	U2795	U2796	U2797	U2798	U2799	U2800	U2801	U2802	U2803	U2804	U2805	U2806	U2807	U2808	U2809	U2810	U2811	U2812	U2813	U2814	U2815	U2816	U2817	U2818	U2819	U2820	U2821	U2822	U2823	U2824	U2825	U2826	U2827	U2828	U2829	U2830	U2831	U2832	U2833	U2834	U2835	U2836	U2837	U2838	U2839	U2840	U2841	U2842	U2843	U2844	U2845	U2846	U2847	U2848	U2849	U2850	U2851	U2852	U2853	U2854	U2855	U2856	U2857	U2858	U2859	U2860	U2861	U2862	U2863	U2864	U2865	U2866	U2867	U2868	U2869	U2870	U2871	U2872	U2873	U2874	U2875	U2876	U2877	U2878	U2879	U2880	U2881	U2882	U2883	U2884	U2885	U2886	U2887	U2888	U2889	U2890	U2891	U2892	U2893	U2894	U2895	U2896	U2897	U2898	U2899	U2900	U2901	U2902	U2903	U2904	U2905	U2906	U2907	U2908	U2909	U2910	U2911	U2912	U2913	U2914	U2915	U2916	U2917	U2918	U2919	U2920	U2921	U2922	U2923	U2924	U2925	U2926	U2927	U2928	U2929	U2930	U2931	U2932	U2933	U2934	U2935	U2936	U2937	U2938	U2939	U2940	U2941	U2942	U2943	U2944	U2945	U2946	U2947	U2948	U2949	U2950	U2951	U2952	U2953	U2954	U2955	U2956	U2957	U2958	U2959	U2960	U2961	U2962	U2963	U2964	U2965	U2966	U2967	U2968	U2969	U2970	U2971	U2972	U2973	U2974	U2975	U2976	U2977	U2978	U2979	U2980	U2981	U2982	U2983	U2984	U2985	U2986	U2987	U2988	U2989	U2990	U2991	U2992	U2993	U2994	U2995	U2996	U2997	U2998	U2999	U3000	U3001	U3002	U3003	U3004	U3005	U3006	U3007	U3008	U3009	U3010	U3011	U3012	U3013	U3014	U3015	U3016	U3017	U3018	U3019	U3020	U3021	U3022	U3023	U3024	U3025	U3026	U3027	U3028	U3029	U3030	U3031	U3032	U3033	U3034	U3035	U3036	U3037	U3038	U3039	U3040	U3041	U3042	U3043	U3044	U3045	U3046	U3047	U3048	U3049	U3050	U3051	U3052	U3053	U3054	U3055	U3056	U3057	U3058	U3059	U3060	U3061	U3062	U3063	U3064	U3065	U3066	U3067	U3068	U3069	U3070	U3071	U3072	U3073	U3074	U3075	U3076	U3077	U3078	U3079	U3080	U3081	U3082	U3083	U3084	U3085	U3086	U3087	U3088	U3089	U3090	U3091	U3092	U3093	U3094	U3095	U3096	U3097	U3098	U3099	U3100	U3101	U3102	U3103	U3104	U3105	U3106	U3107	U3108	U3109	U3110	U3111	U3112	U3113	U3114	U3115	U3116	U3117	U3118	U3119	U3120	U3121	U3122	U3123	U3124	U3125	U3126	U3127	U3128	U3129	U3130	U3131	U3132	U3133	U3134	U3135	U3136	U3137	U3138	U3139	U3140	U3141	U3142	U3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● Molecule 36: TPA\_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

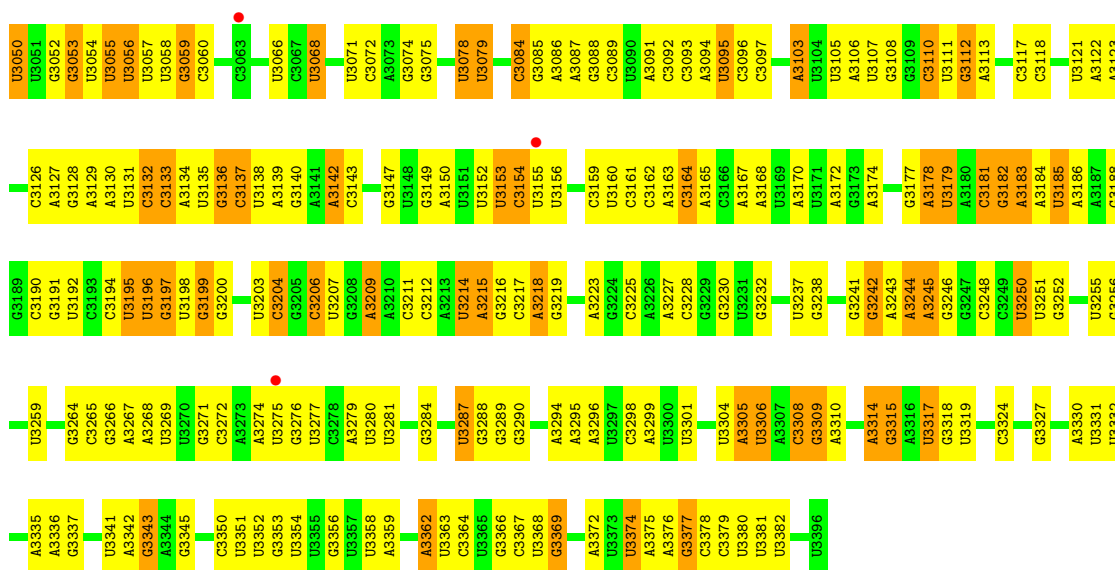
Chain 5:





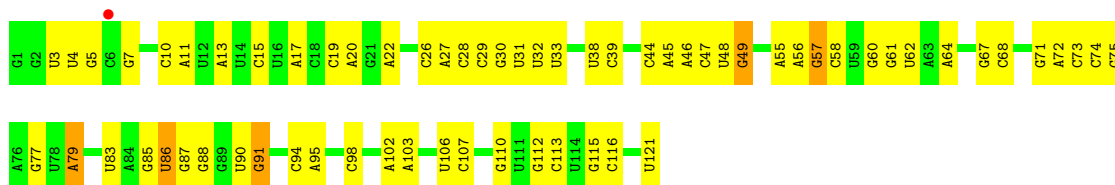
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A	G1718	G1807	G1561	A1491	G1349	U1277	A1191	U1126	U1056	U990	A925
U	A1873	A1808	C1633	G1492	A1350	C1277	C1192	G1127	A1057	G991	A926
G	G1874	G1809	G1634	G1493	U1351	A1278	A1193	U1128	U1060	A992	C927
C	G1875	A1810	G1635	U1494	A1352	C1279	G1194	U1129	U1061	G993	C928
U	U1876	G1811	U1636	U1495	A1355	U1282	A1195	A1130	A1062	G994	A929
U	G1725	C1812	A1637	C1496	U1356	C1283	C1196	G1131	U1063	U995	U930
A	A1813	A1813	A1638	U1500	U1357	U1284	A1197	U1132	G1064	A996	C931
G	G1878	A1814	C1639	U1501	A1362	A1286	C1198	U1133	U1065	A997	U932
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C	A1642	G1817	A1571	U1433	C1366	C1292	A1202	U1138	C1069	U1001	C938
U	A1643	U1572	U1573	A1433	A1367	U1293	A1203	U1139	A1070	A1002	
C	C1644	C1574	C1575	G1434	G1367	G1295	A1204	G1140	U1071	A1003	
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G	A1648	U1576	C1508	C1437	A1369	U1297	G1206	G1142	U1073	G1005	U942
G	U1649	G1577	U1511	U1438	G1370	G1300	U1208	A1143	U1074	A1006	U943
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G	G1658	C1582	C1516	U1445	U1378	G1306	C1219	G1149	A1079		C948
G	G1661	U1584	U1519	A1446	U1379	G1307	U1220	A1150	U1080	G1013	C949
C	G1662	C1585	G1520	G1447	U1380	A1308	A1221	U1151	U1081	U1014	G950
C	G1663	C1586	G1521	U1448	U1381	A1309	G1222	U1152	U1082	C1016	A951
G	U1664	A1587	G1522	A1449	G1382	G1310	A1223	A1153	C1017	C1017	A952
C	G1665	A1588	U1523	G1450	U1383	G1311		A1154	A1085	G1018	U954
C	G1666	A1589	U1524	C1451	U1384	C1312		C1155	C1086	G1019	U955
G	A1667	A1590	G1525	A1452	C1385	G1313	G1230	C1156	U1093	G1020	U956
G	G1668	G1591	G1526	U1460	A1386	C1314	U1235	A1157	U1094	U1021	C957
C	G1669	G1592	G1527	A1461	U1387	U1315	G1236	A1158	U1095	U1022	C958
U	C1670	U1595	A1529	A1462	U1388	C1316	G1237	U1159	U1096	C1023	C959
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C	G1675	C1597	C1531	G1464	C1391	G1319	C1239	G1161	A1098	A1025	C961
U	A1676	C1598	U1532	A1465	G1392	G1320	U1241	G1162	A1099	A1026	
U	G1677	G1599	U1533	G1466	A1393	G1321	G1242	U1167	U1100	U1027	G964
G	G1680	U1599	A1534	A1467	A1394		G1243	A1103	G1101	U1028	A965
G	U1681	G1602	A1535	U1468	C1395	U1324		U1168	A1102	G1029	U966
G	A1603	G1603	G1536	C1469	C1396		G1246	A1169	U1103	C1032	C969
A	G1604	A1605	A1537	U1470	C1397	C1328		A1170	G1104	U1033	A970
C	A1605	A1606	G1538	U1471	A1398	U1329	G1249	G1171	C1107	A1036	G971
C	U1606	U1607	A1539	A1475	A1399	A1330	G1250	U1108	C1037	A1037	A972
U	U1607	U1540	U1541	G1476	G1403	U1331	A1251	U1109	U1038	C1037	A973
C	C1608	G1542	G1543	A1477	G1404	A1332	A1252	C1175	U1110	U1039	C974
U	C1609	G1543		C1478	U1405	C1333		C1176	U1111	A1040	C975
U	A1613	U1547	G1548	U1479	A1406	U1334	G1261	G1177	A1112	U1044	U976
G	C1614	C1548	C1549	G1480	A1407	U1335	G1262	G1178	G1113	C1045	U979
U	C1615	C1549	C1550	A1481	G1408	U1336	A1263	A1179	U1114	A1046	A980
G	A1621	U1553	U1554	A1482	G1409	A1337	G1264	A1180	G1115	A1047	U981
U	U1622	U1554	U1555	G1483	U1410	C1338	U1265	A1181	G1116	A1047	C982
C	U1627	U1556	C1556	U1484	C1411	C1339	G1266	U1184	G1117	A1048	A983
C	U1627	U1557	C1557	G1485	G1412	U1340	U1267	A1184	C1118	C1049	G984
U	C1628	U1557	C1557	G1486	G1413	U1341	G1268	U1187	C1119	U1052	U985
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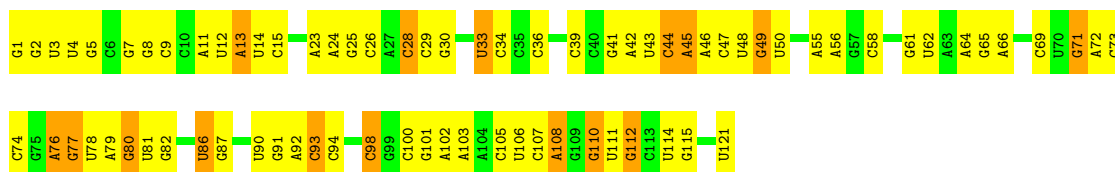
- Molecule 37: TPA\_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 3:



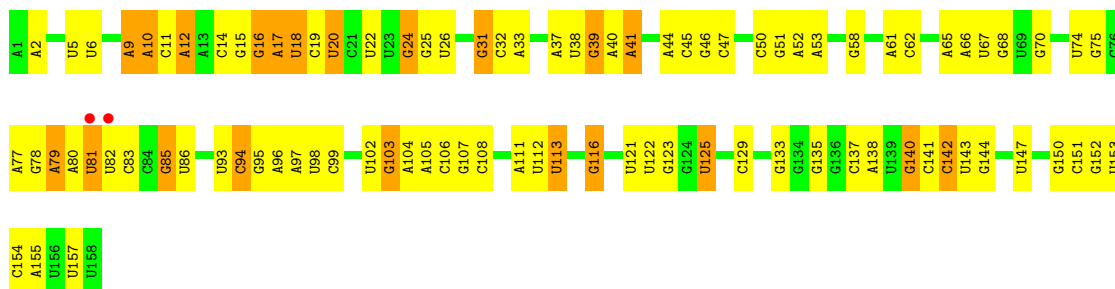
- Molecule 37: TPA\_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 7:

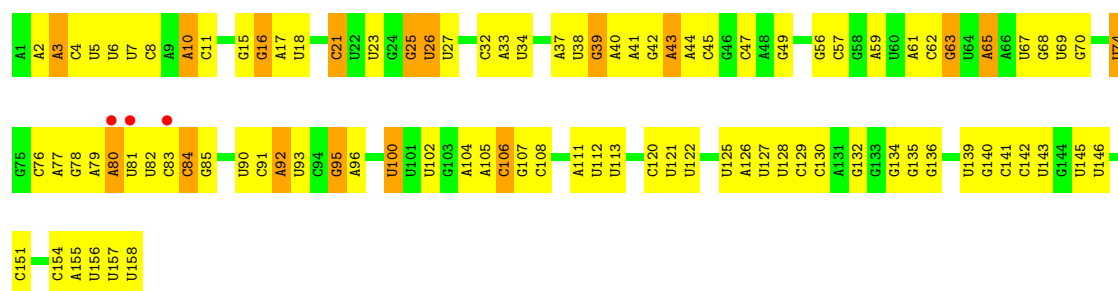


- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

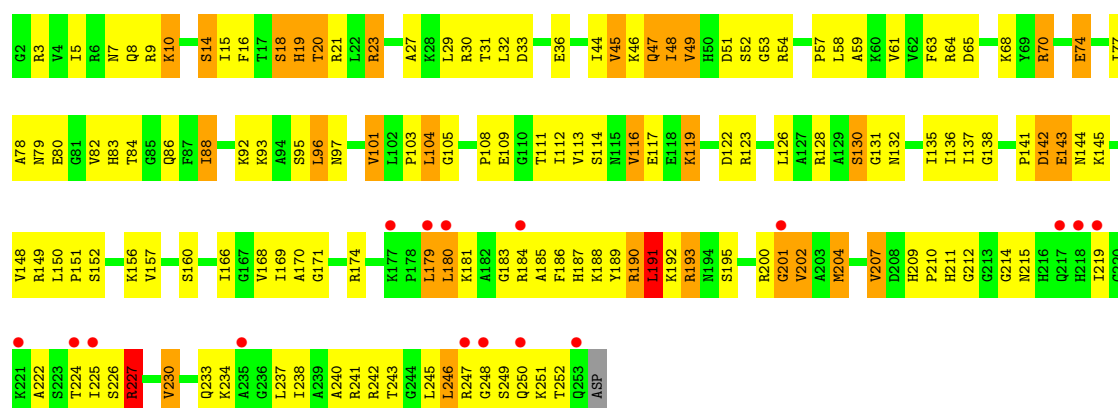
Chain 4:



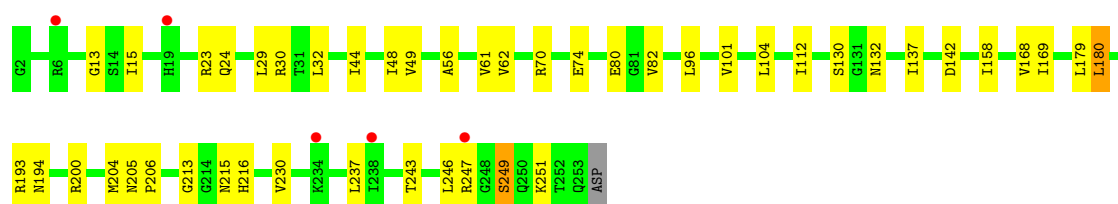
- Chain 8: 



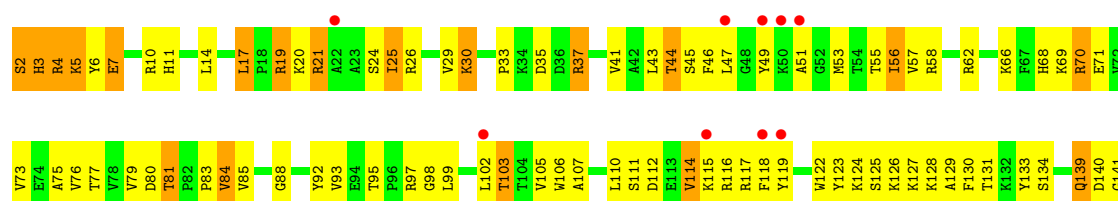
- Chain L2:

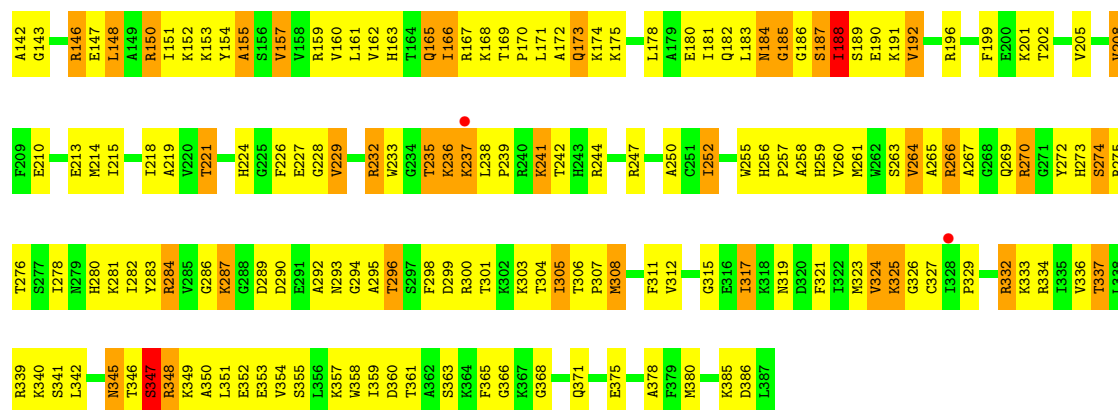


- Chain 12: 



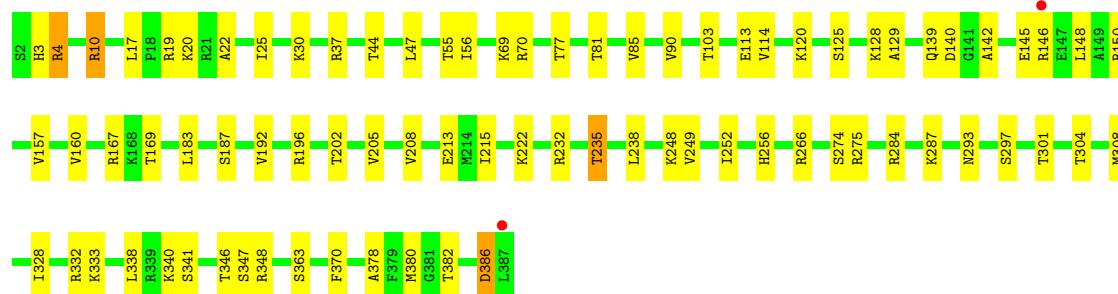
- Chain L3:





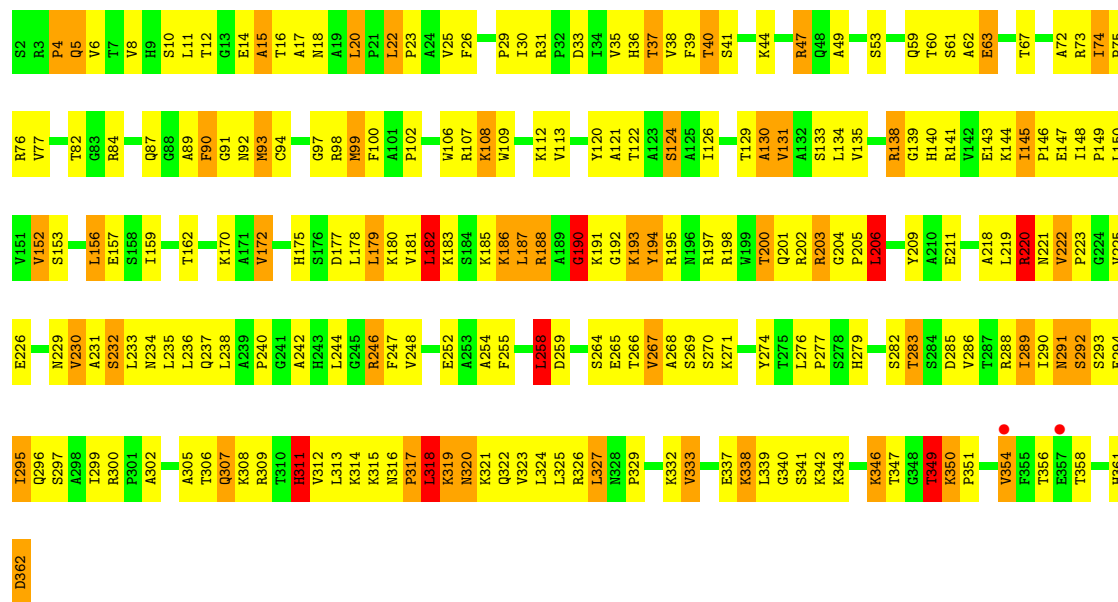
• Molecule 40: 60S ribosomal protein L3

Chain 13:



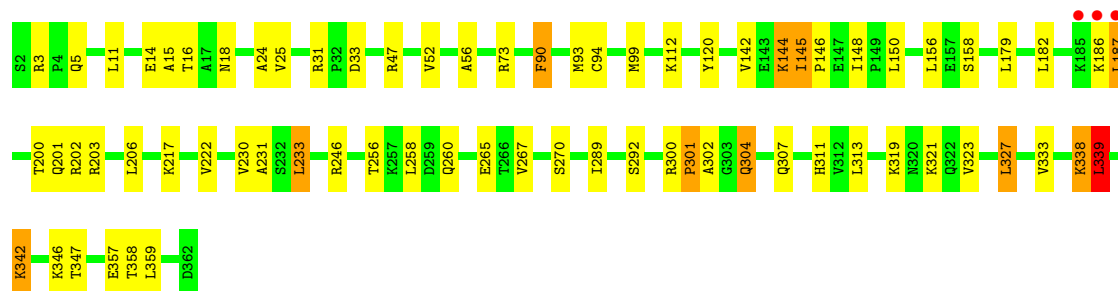
• Molecule 41: 60S ribosomal protein L4-A

Chain 14:



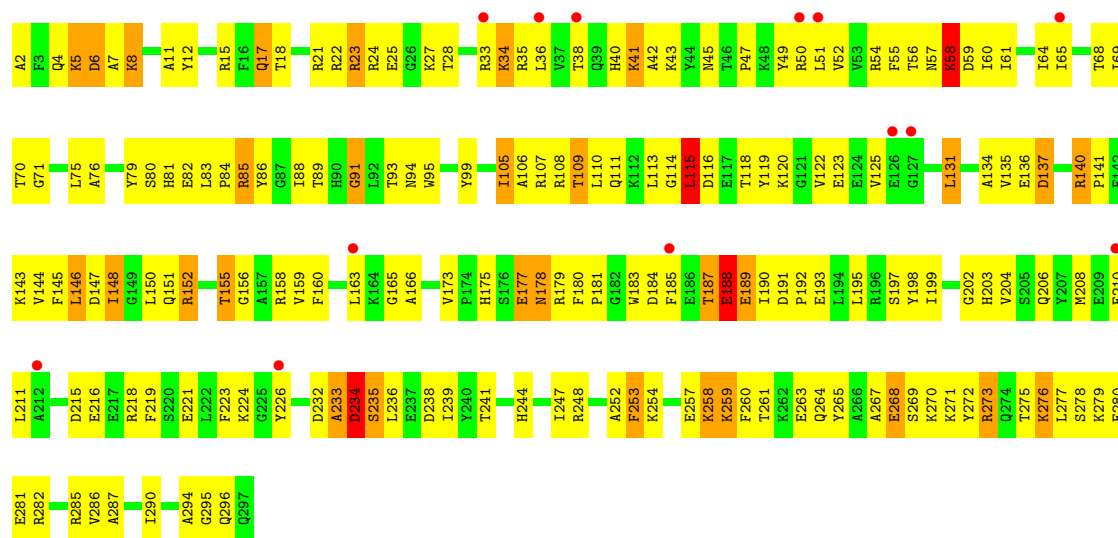
• Molecule 41: 60S ribosomal protein L4-A

Chain 14:



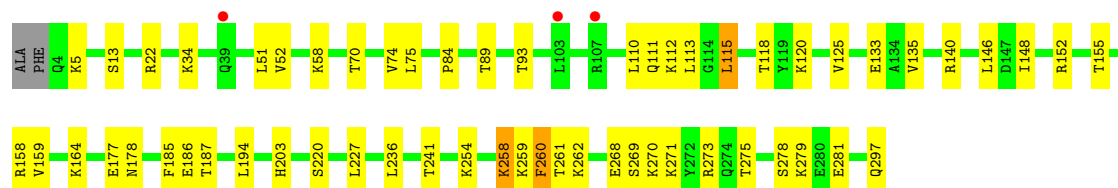
• Molecule 42: 60S ribosomal protein L5

Chain L5:



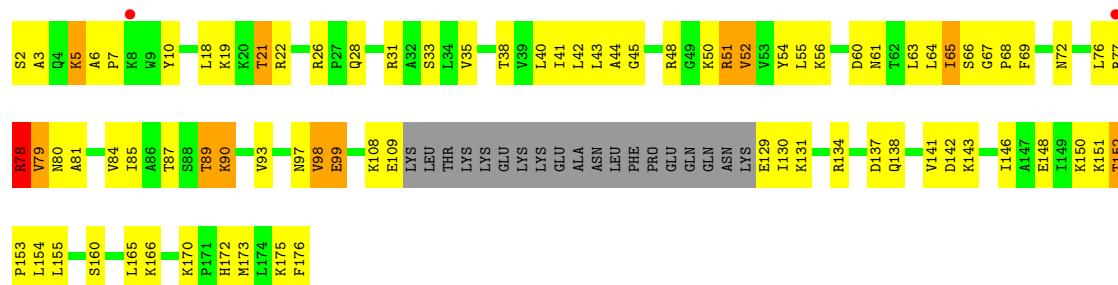
• Molecule 42: 60S ribosomal protein L5

Chain L5:



• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



- Chain 16:
- 
- S2  
 A3  
 Q4  
 K8  
 W9  
 Y10  
 T21  
 L30  
 R31  
 R46  
 L64  
 I65  
 L76  
 R77  
 R78  
 V79  
 M90  
 A81  
 V94  
 T99  
 V93  
 V98  
 E109  
 LYS  
 LEU  
 THR  
 LYS  
 LYS  
 LYS  
 LYS  
 LYS  
 ALA  
 ASN  
 LEU  
 PHE  
 PRO  
 GLU  
 GLN  
 GLN  
 ASN  
 K128  
 E129  
 I130  
 K131  
 S162  
 F163  
 S164  
 K170  
 R173  
 F176

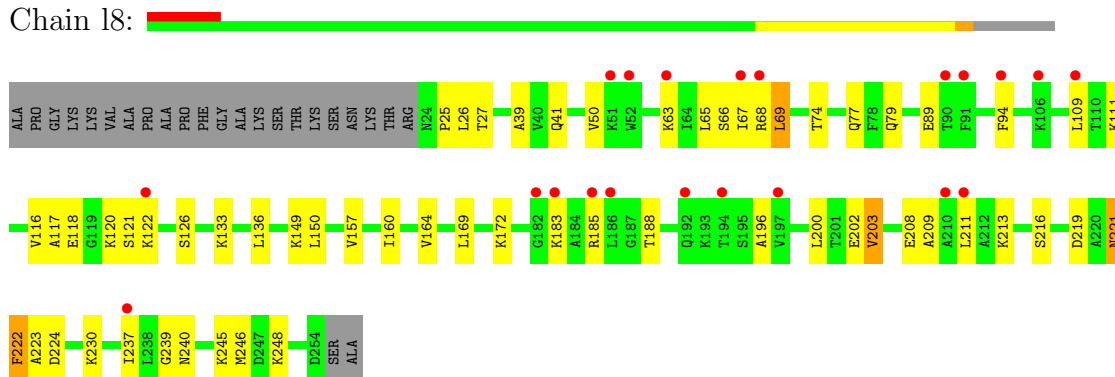
- ### Chain L7:

- Chain 17:
- 
- ALA  
ALA  
GLU  
LYS  
ILE  
LEU  
THR  
PRO  
GLU  
SER  
GLN  
LEU  
LYS  
LYS  
SER  
LYS  
ALA  
GLN  
GLN  
LYS  
T22  
A23  
E24  
A27  
A28  
E29  
K40  
R41  
L45  
E46  
E54  
Y55  
E56  
R60  
V77  
L83  
N93  
K98  
K101  
R110  
L124  
L129  
I130  
I156  
M157  
K159
- Q159  
L173  
I178  
L179  
S180  
L184  
V191  
G192  
M199  
G206  
F209  
E234  
L239  
K244

- ### Chain L8:

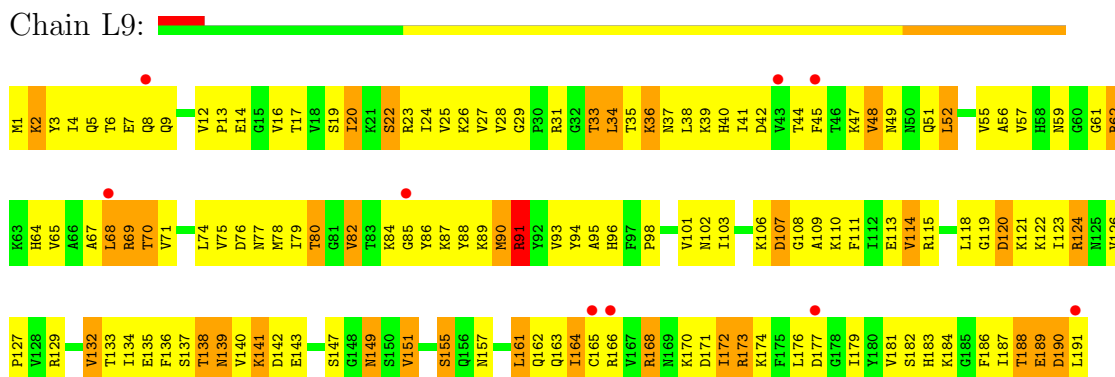
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:



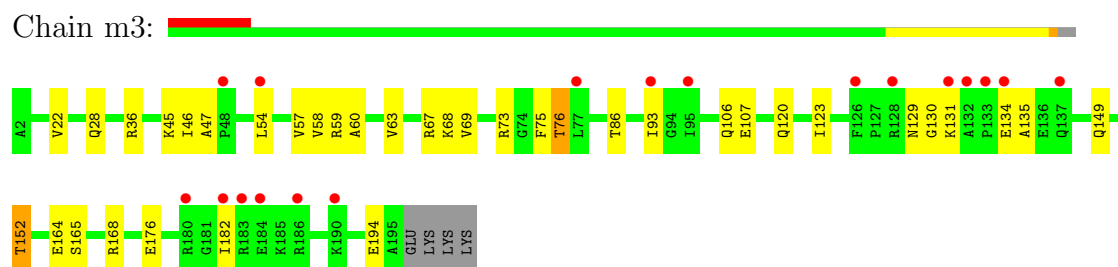
- Molecule 46: 60S ribosomal protein L9-A

Chain L9:

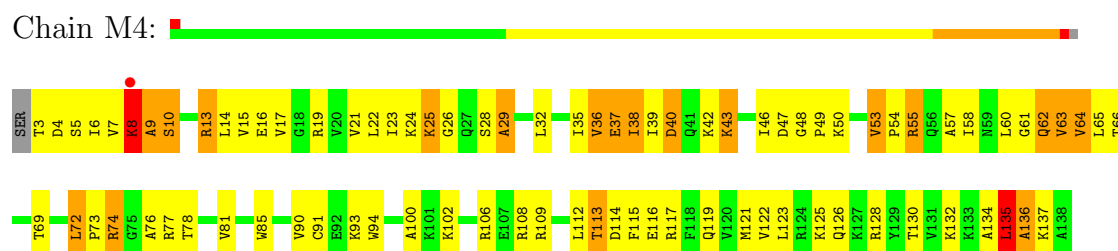




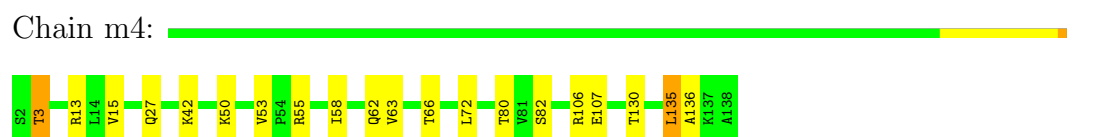




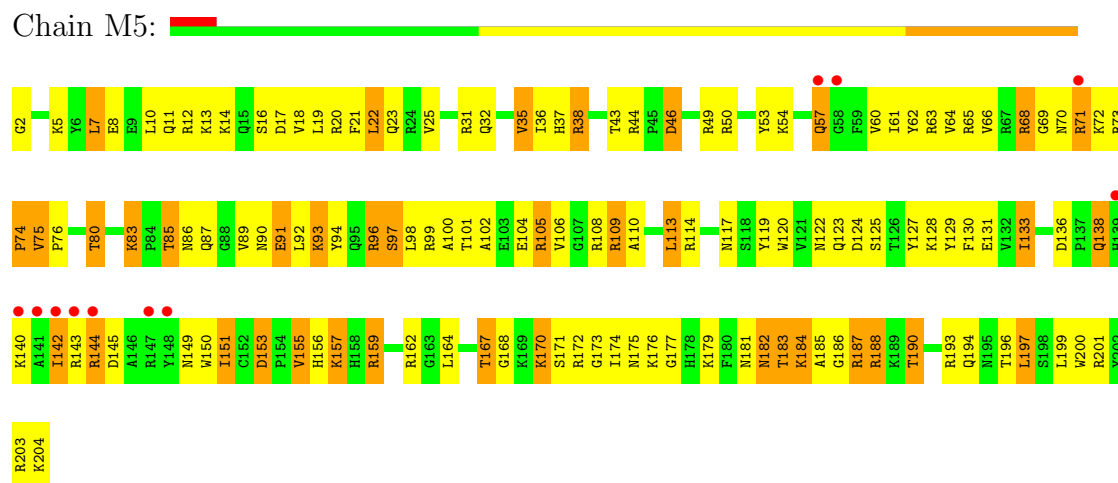
- Molecule 50: 60S ribosomal protein L14-A



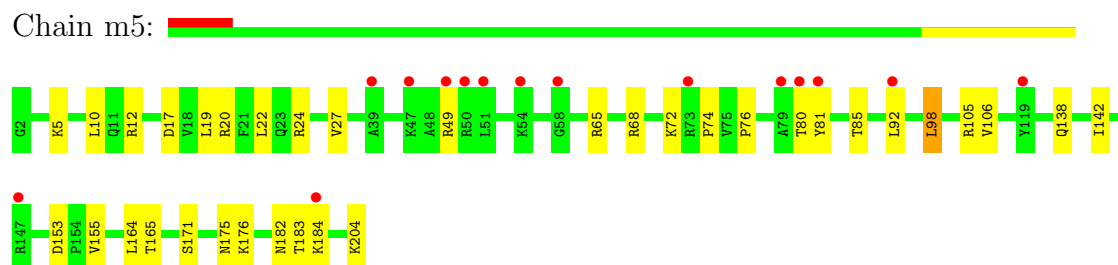
- Molecule 50: 60S ribosomal protein L14-A



- Molecule 51: 60S ribosomal protein L15-A

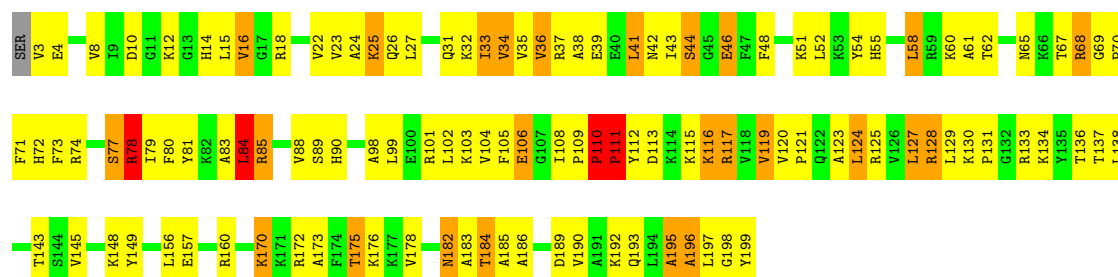


- Molecule 51: 60S ribosomal protein L15-A



- Molecule 52: 60S ribosomal protein L16-A

Chain M6:



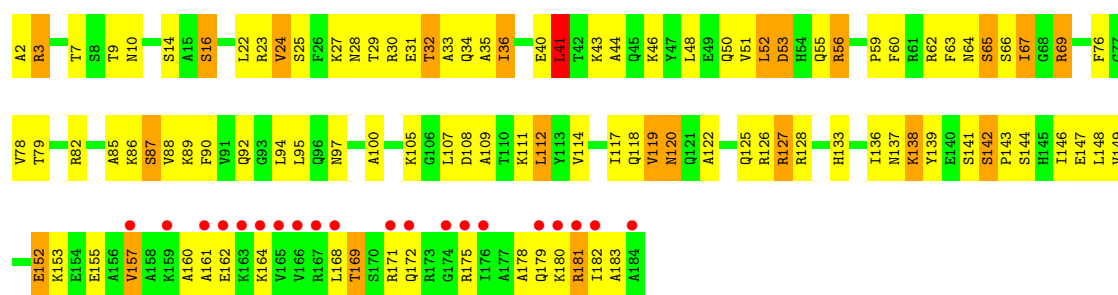
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:



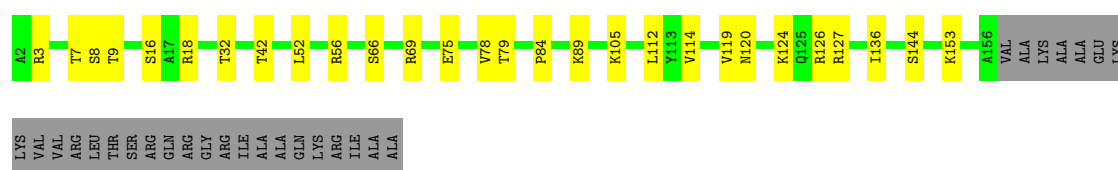
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:



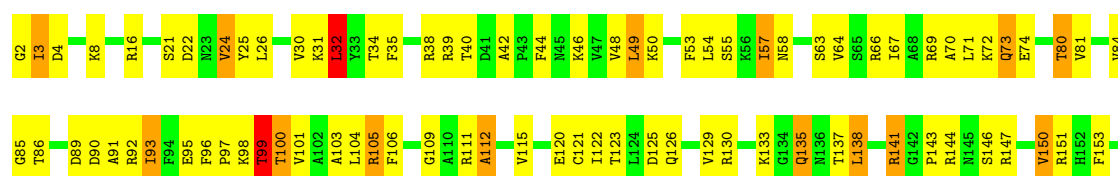
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:



- Molecule 54: 60S ribosomal protein L18-A

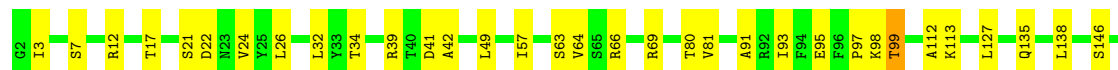
Chain M8:





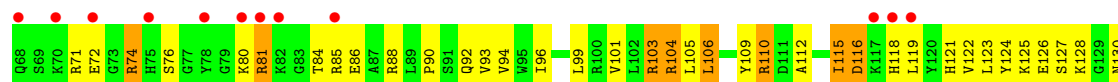
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



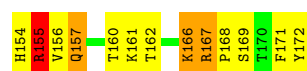
• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



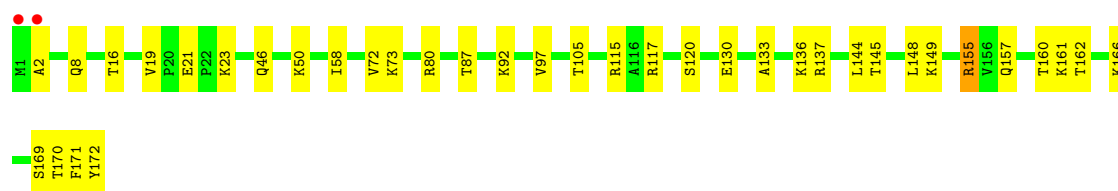
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



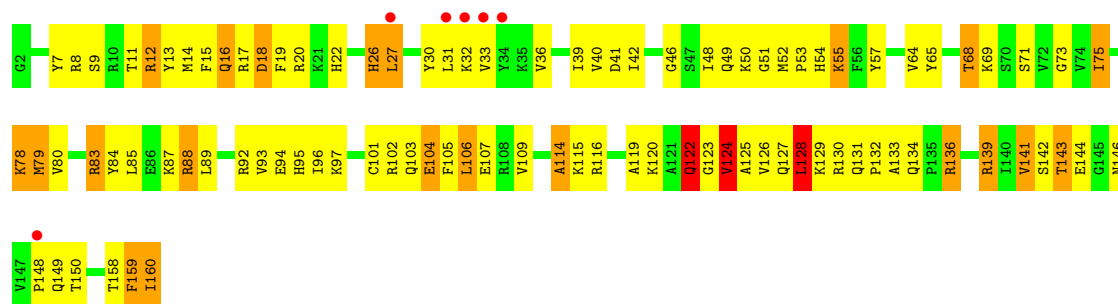
• Molecule 56: 60S ribosomal protein L20-A

Chain n0:



- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



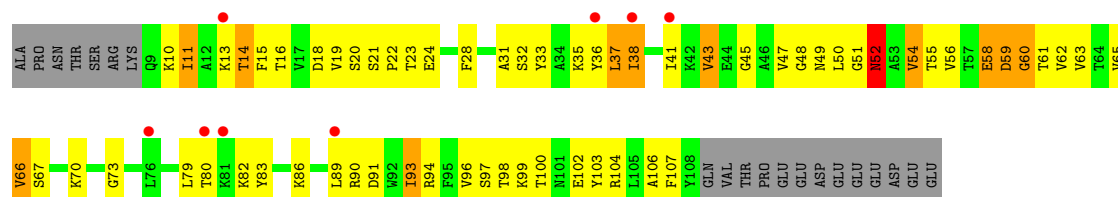
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:



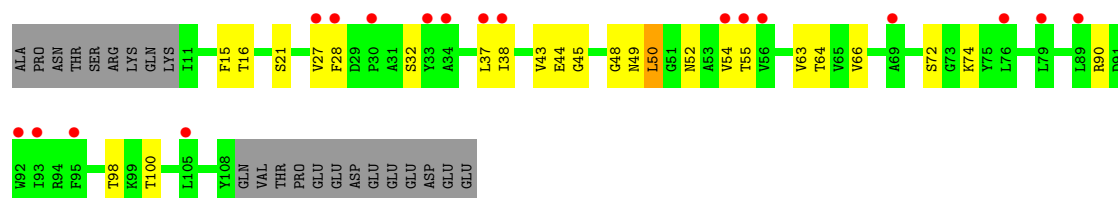
- Molecule 58: 60S ribosomal protein L22-A

Chain N2:



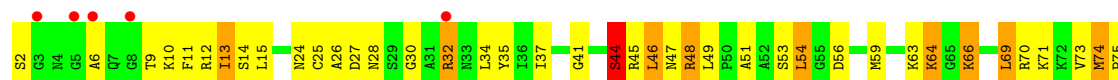
- Molecule 58: 60S ribosomal protein L22-A

Chain n2:



- Molecule 59: 60S ribosomal protein L23-A

Chain N3:





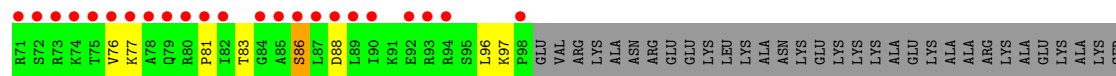
- Molecule 59: 60S ribosomal protein L23-A

Chain n3:



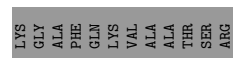
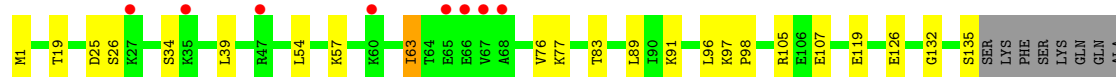
- Molecule 60: 60S ribosomal protein L24-A

Chain N4:



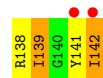
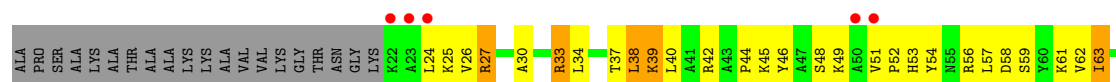
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:



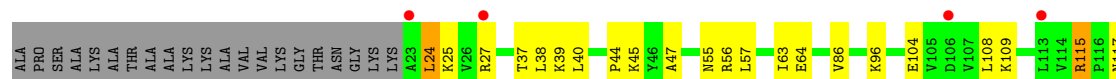
- Molecule 61: 60S ribosomal protein L25

Chain N5:



- Molecule 61: 60S ribosomal protein L25

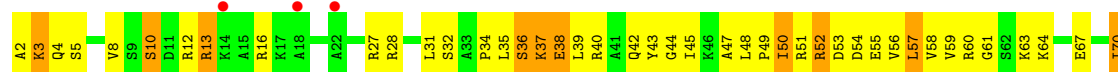
Chain n5:





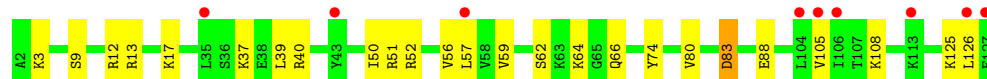
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



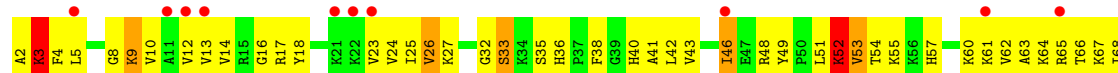
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



- Molecule 63: 60S ribosomal protein L27-A

Chain N7:



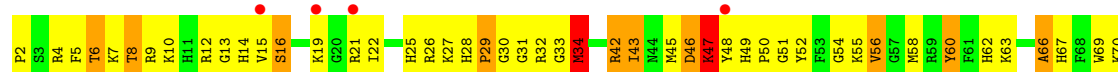
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:



- Molecule 64: 60S ribosomal protein L28

Chain N8:



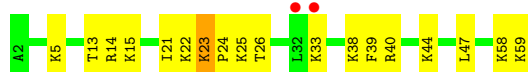
- Molecule 64: 60S ribosomal protein L28

Chain n8: 

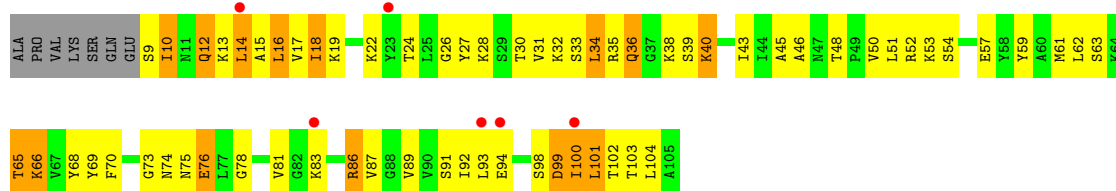
- Molecule 65: 60S ribosomal protein L29

Chain N9: 

- Molecule 65: 60S ribosomal protein L29

Chain n9: 

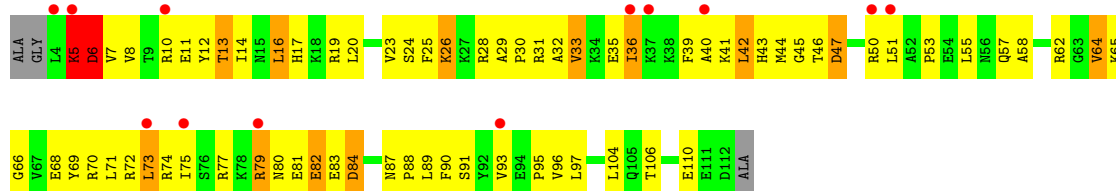
- Molecule 66: 60S ribosomal protein L30

Chain O0: 

- Molecule 66: 60S ribosomal protein L30

Chain o0: 

- Molecule 67: 60S ribosomal protein L31-A

Chain O1: 

- Molecule 67: 60S ribosomal protein L31-A

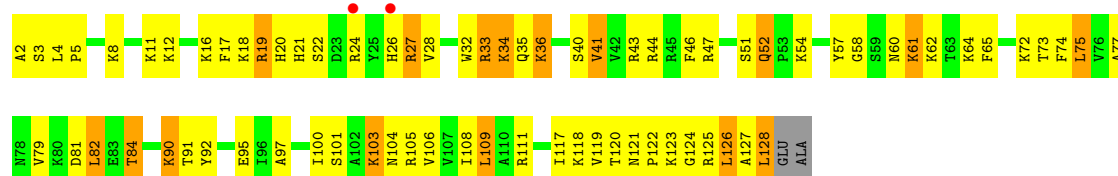
Chain o1: 





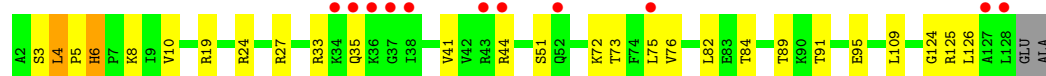
- Molecule 68: 60S ribosomal protein L32

Chain O2:



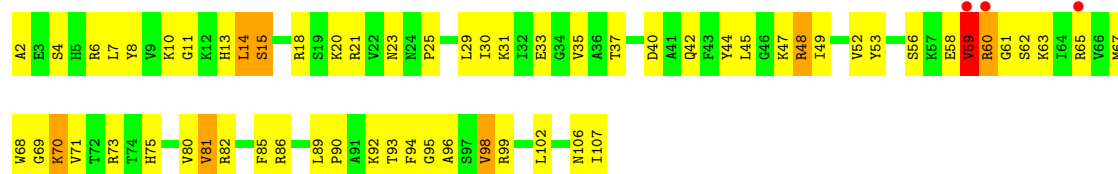
- Molecule 68: 60S ribosomal protein L32

Chain o2:



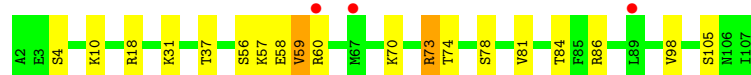
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



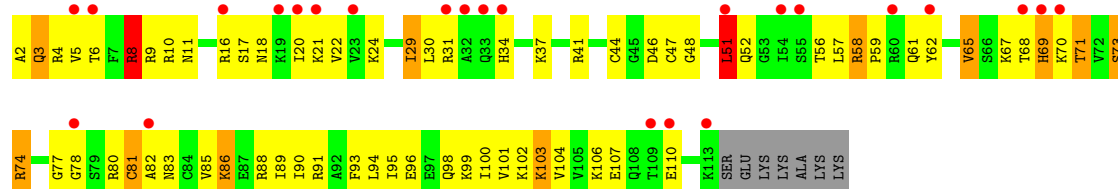
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



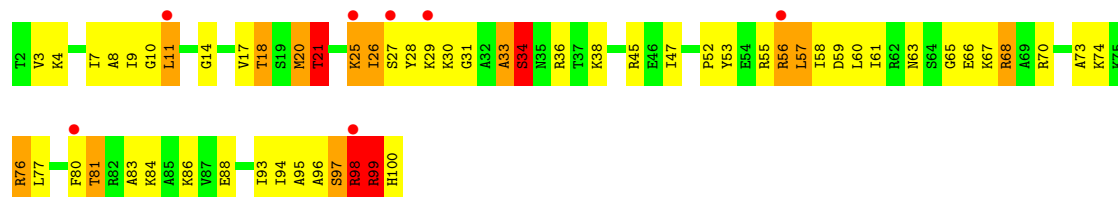
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:



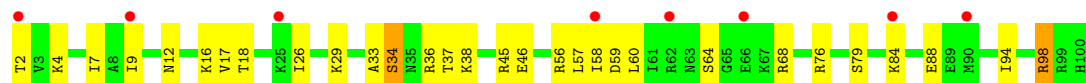
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:



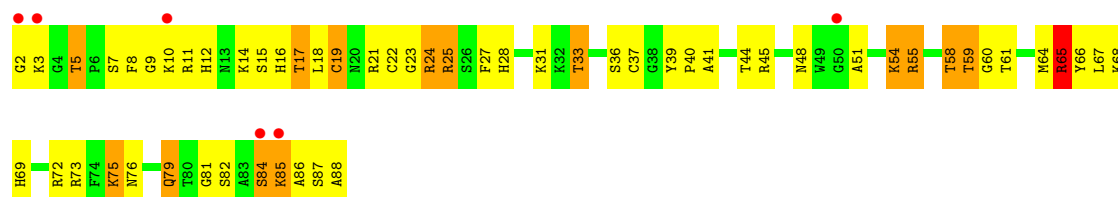
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



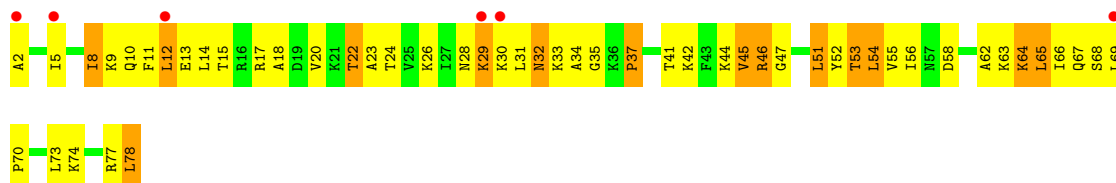
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



- Molecule 74: 60S ribosomal protein L38

Chain O8:



- Molecule 74: 60S ribosomal protein L38

Chain o8:



- Molecule 75: 60S ribosomal protein L39

Chain O9:



- Molecule 75: 60S ribosomal protein L39

Chain o9:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



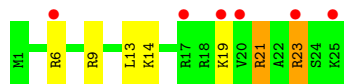
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



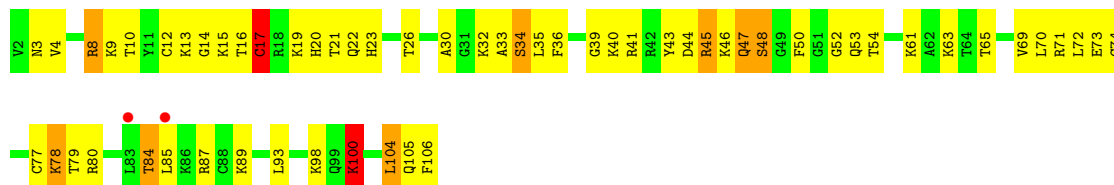
- Molecule 77: 60S ribosomal protein L41-A

Chain q1: 



- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 



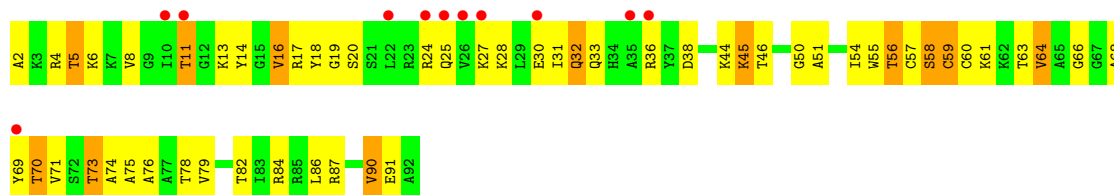
- Molecule 78: 60S ribosomal protein L42-A

Chain q2: 



- Molecule 79: 60S ribosomal protein L43-A

Chain Q3: 



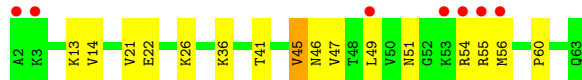
- Molecule 79: 60S ribosomal protein L43-A

Chain q3: 



- Molecule 80: 40S ribosomal protein S30-A

Chain e0: 



- Molecule 81: Unknown protein m2

Chain m2: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	434.98Å 287.50Å 303.22Å 90.00° 98.85° 90.00°	Depositor
Resolution (Å)	299.60 – 3.10 299.61 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (299.60-3.10) 99.9 (299.61-3.10)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.202 , 0.252 0.263 , 0.308	Depositor DCC
$R_{free}$ test set	19718 reflections (1.49%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.2	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 1327406 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	411276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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: 3K5, ZN, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	2	0.73	5/41698 (0.0%)	1.28	279/64972 (0.4%)
1	6	0.89	29/42765 (0.1%)	1.39	455/66634 (0.7%)
2	S0	0.48	0/1617	0.67	0/2215
2	s0	0.50	0/1623	0.68	0/2222
3	S1	0.37	0/1735	0.68	1/2335 (0.0%)
3	s1	0.53	0/1748	0.70	0/2352
4	S2	0.51	0/1665	0.66	0/2263
4	s2	0.59	0/1665	0.77	0/2263
5	S3	0.51	0/1759	0.70	1/2368 (0.0%)
5	s3	0.47	0/1759	0.61	0/2368
6	S4	0.50	0/2109	0.72	0/2839
6	s4	0.56	0/2109	0.76	1/2839 (0.0%)
7	S5	0.41	0/1629	0.61	0/2202
7	s5	0.47	0/1629	0.66	0/2202
8	S6	0.49	0/1823	0.67	0/2439
8	s6	0.57	0/1779	0.71	0/2379
9	S7	0.44	0/1506	0.67	0/2028
9	s7	0.49	0/1516	0.72	1/2043 (0.0%)
10	S8	0.56	0/1514	0.74	2/2021 (0.1%)
10	s8	0.65	0/1514	0.78	0/2021
11	S9	0.49	0/1519	0.68	1/2035 (0.0%)
11	s9	0.59	0/1519	0.74	0/2035
12	C0	0.42	0/790	0.64	1/1069 (0.1%)
12	c0	0.40	0/777	0.64	3/1049 (0.3%)
13	C1	0.61	0/1240	0.75	0/1675
13	c1	0.65	0/1194	0.77	0/1610
14	C2	0.38	0/900	0.64	0/1224
14	c2	0.30	0/900	0.59	1/1224 (0.1%)
15	C3	0.51	0/1215	0.72	3/1638 (0.2%)
15	c3	0.60	0/1215	0.73	0/1638
16	C4	0.38	0/901	0.63	0/1217
16	c4	0.54	0/960	0.78	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.46	0/998	0.71	0/1341
17	c5	0.52	0/1060	0.69	1/1426 (0.1%)
18	C6	0.46	0/1125	0.67	0/1510
18	c6	0.50	0/1131	0.72	1/1518 (0.1%)
19	C7	0.44	0/935	0.63	0/1254
19	c7	0.50	0/914	0.71	0/1224
20	C8	0.45	0/1211	0.65	1/1628 (0.1%)
20	c8	0.50	0/1211	0.70	1/1628 (0.1%)
21	C9	0.46	0/1130	0.68	1/1517 (0.1%)
21	c9	0.50	0/1130	0.67	1/1517 (0.1%)
22	D0	0.48	0/865	0.66	0/1169
22	d0	0.50	0/892	0.66	0/1205
23	D1	0.45	0/693	0.62	1/935 (0.1%)
23	d1	0.57	0/693	0.73	0/935
24	D2	0.52	0/1038	0.73	1/1395 (0.1%)
24	d2	0.63	0/1038	0.75	1/1395 (0.1%)
25	D3	0.62	0/1139	0.76	1/1518 (0.1%)
25	d3	0.74	0/1139	0.87	3/1518 (0.2%)
26	D4	0.46	0/1087	0.62	0/1449
26	d4	0.57	0/1087	0.74	0/1449
27	D5	0.40	0/571	0.73	1/768 (0.1%)
27	d5	0.41	0/566	0.64	0/761
28	D6	0.47	0/782	0.68	0/1047
28	d6	0.57	0/782	0.70	0/1047
29	D7	0.43	0/620	0.67	0/838
29	d7	0.49	0/620	0.71	0/838
30	D8	0.36	0/499	0.59	0/670
30	d8	0.45	0/499	0.66	0/670
31	D9	0.55	0/452	0.74	0/600
31	d9	0.57	0/452	0.69	0/600
32	E0	0.48	0/483	0.62	0/643
33	E1	0.46	0/577	0.78	0/770
33	e1	0.42	0/619	0.73	1/822 (0.1%)
34	SR	0.41	0/2494	0.64	0/3393
34	sR	0.40	0/2495	0.60	0/3395
35	SM	0.52	0/1113	0.73	2/1502 (0.1%)
35	sM	0.48	0/682	0.68	1/921 (0.1%)
36	1	1.17	163/75394 (0.2%)	1.66	1841/117545 (1.6%)
36	5	1.20	181/75414 (0.2%)	1.67	1895/117575 (1.6%)
37	3	0.96	1/2883 (0.0%)	1.41	24/4491 (0.5%)
37	7	1.17	3/2883 (0.1%)	1.66	57/4491 (1.3%)
38	4	1.15	2/3746 (0.1%)	1.64	82/5832 (1.4%)
38	8	1.04	3/3746 (0.1%)	1.50	53/5832 (0.9%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L2	0.74	0/1948	0.86	3/2617 (0.1%)
39	l2	0.74	0/1946	0.89	3/2614 (0.1%)
40	L3	0.72	0/3146	0.81	0/4228
40	l3	0.86	0/3146	0.90	5/4228 (0.1%)
41	L4	0.84	2/2800 (0.1%)	0.95	6/3790 (0.2%)
41	l4	0.75	1/2800 (0.0%)	0.92	6/3790 (0.2%)
42	L5	0.60	0/2425	0.71	1/3271 (0.0%)
42	l5	0.70	0/2408	0.79	1/3248 (0.0%)
43	L6	0.76	0/1260	0.84	1/1694 (0.1%)
43	l6	0.78	0/1269	0.85	3/1705 (0.2%)
44	L7	0.82	0/1821	0.94	3/2451 (0.1%)
44	l7	0.85	1/1828 (0.1%)	0.89	2/2461 (0.1%)
45	L8	0.60	0/1836	0.69	1/2481 (0.0%)
45	l8	0.57	0/1795	0.70	1/2429 (0.0%)
46	L9	0.67	0/1539	0.78	1/2073 (0.0%)
46	l9	0.79	0/1539	0.81	0/2073
47	M0	0.77	2/1741 (0.1%)	0.87	2/2335 (0.1%)
47	m0	0.78	1/1758 (0.1%)	0.87	3/2358 (0.1%)
48	M1	0.55	0/1374	0.74	1/1842 (0.1%)
48	m1	0.65	0/1374	0.78	1/1842 (0.1%)
49	M3	0.77	0/1568	0.88	2/2106 (0.1%)
49	m3	0.67	0/1573	0.79	1/2113 (0.0%)
50	M4	0.72	0/1068	0.80	1/1438 (0.1%)
50	m4	0.85	0/1074	0.87	2/1446 (0.1%)
51	M5	0.80	0/1757	0.87	3/2354 (0.1%)
51	m5	0.69	0/1757	0.82	2/2354 (0.1%)
52	M6	0.85	0/1585	0.91	5/2128 (0.2%)
52	m6	1.03	4/1585 (0.3%)	0.98	3/2128 (0.1%)
53	M7	0.77	0/1443	0.86	2/1944 (0.1%)
53	m7	0.90	0/1250	0.84	0/1683
54	M8	0.79	0/1465	0.90	4/1965 (0.2%)
54	m8	0.76	0/1465	0.91	2/1965 (0.1%)
55	M9	0.55	0/1538	0.69	0/2050
55	m9	0.63	0/1538	0.71	0/2050
56	N0	0.82	0/1481	0.87	0/1990
56	n0	0.88	0/1481	0.88	2/1990 (0.1%)
57	N1	0.77	0/1300	0.84	2/1743 (0.1%)
57	n1	0.83	1/1300 (0.1%)	0.81	0/1743
58	N2	0.48	0/812	0.64	0/1099
58	n2	0.51	0/794	0.69	0/1076
59	N3	0.73	0/1018	0.81	0/1369
59	n3	0.88	0/1018	0.90	3/1369 (0.2%)
60	N4	0.57	0/712	0.71	1/958 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	n4	0.71	0/1052	0.76	0/1398
61	N5	0.64	0/979	0.81	1/1321 (0.1%)
61	n5	0.68	0/974	0.85	1/1314 (0.1%)
62	N6	0.73	0/1004	0.91	0/1341
62	n6	0.68	0/1004	0.84	0/1341
63	N7	0.52	0/1118	0.66	0/1497
63	n7	0.49	0/1118	0.72	3/1497 (0.2%)
64	N8	0.80	0/1204	0.90	2/1612 (0.1%)
64	n8	0.78	0/1204	0.87	0/1612
65	N9	0.72	0/473	0.79	0/629
65	n9	0.80	0/473	0.87	0/629
66	O0	0.50	0/751	0.72	0/1008
66	o0	0.52	0/775	0.68	1/1040 (0.1%)
67	O1	0.63	0/890	0.78	0/1196
67	o1	0.79	0/897	0.89	0/1205
68	O2	0.86	0/1041	0.90	1/1394 (0.1%)
68	o2	0.85	0/1041	0.92	2/1394 (0.1%)
69	O3	0.90	0/868	0.89	0/1168
69	o3	0.92	0/868	0.90	3/1168 (0.3%)
70	O4	0.63	0/890	0.83	2/1189 (0.2%)
70	o4	0.65	0/890	0.83	0/1189
71	O5	0.73	0/978	0.76	1/1301 (0.1%)
71	o5	0.62	0/974	0.74	1/1297 (0.1%)
72	O6	0.67	0/778	0.78	0/1034
72	o6	0.63	0/777	0.71	0/1033
73	O7	0.80	0/696	0.93	2/923 (0.2%)
73	o7	0.77	0/696	0.88	1/923 (0.1%)
74	O8	0.53	0/618	0.64	0/826
74	o8	0.50	0/614	0.66	0/822
75	O9	0.76	0/443	0.98	1/588 (0.2%)
75	o9	0.71	0/443	0.79	0/588
76	Q0	0.71	0/423	0.80	0/562
76	q0	0.94	0/423	0.94	0/562
77	Q1	0.74	0/234	0.89	0/300
77	q1	0.76	0/234	0.94	1/300 (0.3%)
78	Q2	0.89	1/860 (0.1%)	0.88	1/1136 (0.1%)
78	q2	0.80	1/860 (0.1%)	0.82	0/1136
79	Q3	0.76	0/701	0.83	0/934
79	q3	0.75	0/701	0.80	1/934 (0.1%)
80	e0	0.56	0/499	0.81	0/665
82	p0	0.47	0/1091	0.63	0/1472
All	All	0.92	401/430072 (0.1%)	1.31	4824/631360 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	s0	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
12	c0	0	1
16	c4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	1
22	d0	0	1
25	D3	0	1
26	d4	0	1
27	D5	0	2
33	E1	0	1
39	L2	0	2
41	L4	0	1
43	L6	0	1
44	l7	0	2
45	l8	0	1
48	M1	0	1
49	M3	0	1
50	M4	0	1
52	M6	0	2
52	m6	0	1
53	M7	0	1
56	n0	0	2
57	N1	0	1
63	N7	0	1
64	N8	0	1
64	n8	0	3
65	N9	0	1
67	O1	0	1
All	All	0	43

The worst 5 of 401 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-12.58	1.27	1.38
78	Q2	17	CYS	CB-SG	11.86	2.02	1.82
36	5	960	U	N1-C2	10.74	1.48	1.38
36	5	2971	A	N9-C4	9.52	1.43	1.37
78	q2	17	CYS	CB-SG	8.98	1.97	1.82

The worst 5 of 4824 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	C2-N3-C4	-23.10	100.35	111.90
36	5	1152	G	N3-C4-C5	23.05	140.12	128.60
36	5	1152	G	N3-C4-N9	-22.76	112.34	126.00
36	1	2714	G	N3-C4-C5	15.18	136.19	128.60
36	1	1308	A	O5'-P-OP2	-14.90	92.29	105.70

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	C6	113	ASP	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
25	D3	78	LYS	Peptide
9	S7	131	PHE	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	944	0
1	6	38238	0	19241	917	0
2	S0	1577	0	1567	175	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	175	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	147	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	168	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	175	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	132	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	130	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	150	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	148	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	77	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	77	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	67	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	110	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	97	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	109	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	105	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	73	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	129	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	105	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	98	0
22	d0	882	0	939	0	0
23	D1	684	0	672	62	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	99	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	103	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	94	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	62	0
27	d5	558	0	598	0	0
28	D6	769	0	814	91	0
28	d6	769	0	814	0	0
29	D7	610	0	631	47	0
29	d7	610	0	633	0	0
30	D8	497	0	535	47	0
30	d8	497	0	535	0	0
31	D9	442	0	428	45	0
31	d9	442	0	428	0	0
32	E0	475	0	525	42	0
33	E1	566	0	602	67	0
33	e1	608	0	656	0	0
34	SR	2441	0	2397	197	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	83	0
35	sM	679	0	603	0	0
36	1	67355	0	33846	1397	0
36	5	67376	0	33860	1385	0
37	3	2579	0	1303	58	0
37	7	2579	0	1303	49	0
38	4	3353	0	1695	74	0
38	8	3353	0	1695	80	0
39	L2	1914	0	1981	147	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	281	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	209	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	208	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	84	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	155	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	151	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	162	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	112	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	145	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	83	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	157	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	140	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	114	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	105	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	116	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	112	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	111	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	52	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	83	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	29	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	74	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	77	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	102	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	113	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	43	0
65	n9	462	0	491	0	0
66	O0	743	0	797	61	0
66	o0	767	0	816	0	0
67	O1	876	0	912	68	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	72	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	59	0
69	o3	850	0	880	0	0
70	O4	880	0	945	76	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	97	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	54	0
72	o6	770	0	846	0	0
73	O7	681	0	682	65	0
73	o7	681	0	683	0	0
74	O8	612	0	682	51	0
74	o8	608	0	671	0	0
75	O9	436	0	475	45	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	25	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	26	0
77	q1	233	0	284	0	0
78	Q2	847	0	917	63	0
78	q2	847	0	917	0	0
79	Q3	694	0	734	50	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	750	0	175	0	0
82	p0	1076	0	1040	0	0
83	p1	235	0	52	0	0
84	p2	230	0	51	0	0
85	1	471	0	0	0	0
85	2	121	0	0	0	0
85	3	13	0	0	0	0
85	4	23	0	0	0	0
85	5	497	0	0	0	0
85	6	145	0	0	0	0
85	7	16	0	0	0	0
85	8	15	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	L2	2	0	0	0	0
85	L3	3	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	3	0	0	0	0
85	M1	2	0	0	0	0
85	M3	3	0	0	0	0
85	M5	1	0	0	0	0
85	M6	1	0	0	0	0
85	M7	4	0	0	0	0
85	M9	2	0	0	0	0
85	N0	1	0	0	0	0
85	N3	3	0	0	0	0
85	N5	1	0	0	0	0
85	N6	1	0	0	0	0
85	N8	3	0	0	0	0
85	O3	1	0	0	0	0
85	O4	1	0	0	0	0
85	O7	2	0	0	0	0
85	Q2	1	0	0	0	0
85	S2	2	0	0	0	0
85	S4	1	0	0	0	0
85	S6	1	0	0	0	0
85	S8	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	c9	1	0	0	0	0
85	d3	2	0	0	0	0
85	d6	1	0	0	0	0
85	l2	2	0	0	0	0
85	l3	3	0	0	0	0
85	l4	1	0	0	0	0
85	l5	2	0	0	0	0
85	l7	3	0	0	0	0
85	l8	1	0	0	0	0
85	l9	1	0	0	0	0
85	m1	1	0	0	0	0
85	m4	1	0	0	0	0
85	m5	3	0	0	0	0
85	m6	2	0	0	0	0
85	m7	5	0	0	0	0
85	n0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	n3	2	0	0	0	0
85	n6	1	0	0	0	0
85	n8	5	0	0	0	0
85	o1	1	0	0	0	0
85	o3	2	0	0	0	0
85	o4	1	0	0	0	0
85	o7	1	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	2	0	0	0	0
85	s1	1	0	0	0	0
85	s2	1	0	0	0	0
85	s4	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2443	0	0	239	0
86	2	1106	0	0	115	0
86	3	77	0	0	3	0
86	4	112	0	0	10	0
86	5	2457	0	0	240	0
86	6	1120	0	0	118	0
86	7	77	0	0	11	0
86	8	119	0	0	19	0
86	C3	7	0	0	2	0
86	C5	7	0	0	4	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	2	0
86	L4	7	0	0	2	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	O1	7	0	0	6	0
86	O2	7	0	0	0	0
86	O3	7	0	0	1	0
86	O7	14	0	0	6	0
86	Q2	7	0	0	2	0
86	S8	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	SR	7	0	0	0	0
86	c3	7	0	0	0	0
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	21	0	0	0	0
86	l4	14	0	0	0	0
86	l5	28	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	14	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	7	0	0	0	0
86	o2	7	0	0	0	0
86	o3	7	0	0	0	0
86	o7	7	0	0	0	0
86	q1	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	sR	7	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	0	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
88	1	57	0	0	1	0
88	5	57	0	0	3	0
All	All	411276	0	297288	10974	0

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

The worst 5 of 10974 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	2.02	1.47
7:S5:94:THR:HG22	7:S5:114:ILE:HG13	2.36	1.08
36:5:3274:A:H3'	36:5:3275:U:H5''	1.36	1.07
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.39	1.05
36:5:2273:G:O6	86:5:4195:OHX:N5	1.91	1.03

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	142 (70%)	40 (20%)	22 (11%)	1	5
2	s0	204/251 (81%)	155 (76%)	28 (14%)	21 (10%)	1	6
3	S1	212/254 (84%)	144 (68%)	35 (16%)	33 (16%)	0	1
3	s1	214/254 (84%)	174 (81%)	27 (13%)	13 (6%)	2	16
4	S2	215/253 (85%)	182 (85%)	22 (10%)	11 (5%)	3	22
4	s2	215/253 (85%)	178 (83%)	22 (10%)	15 (7%)	2	13
5	S3	221/239 (92%)	177 (80%)	25 (11%)	19 (9%)	1	9
5	s3	221/239 (92%)	179 (81%)	28 (13%)	14 (6%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S4	258/260 (99%)	205 (80%)	36 (14%)	17 (7%)	2	15
6	s4	258/260 (99%)	212 (82%)	29 (11%)	17 (7%)	2	15
7	S5	204/224 (91%)	155 (76%)	33 (16%)	16 (8%)	1	11
7	s5	204/224 (91%)	160 (78%)	23 (11%)	21 (10%)	1	6
8	S6	224/236 (95%)	195 (87%)	17 (8%)	12 (5%)	3	20
8	s6	216/236 (92%)	181 (84%)	22 (10%)	13 (6%)	2	17
9	S7	182/189 (96%)	128 (70%)	28 (15%)	26 (14%)	0	2
9	s7	184/189 (97%)	148 (80%)	26 (14%)	10 (5%)	3	20
10	S8	184/200 (92%)	152 (83%)	21 (11%)	11 (6%)	2	17
10	s8	184/200 (92%)	155 (84%)	17 (9%)	12 (6%)	2	15
11	S9	183/196 (93%)	149 (81%)	24 (13%)	10 (6%)	3	19
11	s9	183/196 (93%)	152 (83%)	22 (12%)	9 (5%)	3	23
12	C0	94/105 (90%)	77 (82%)	10 (11%)	7 (7%)	2	11
12	c0	92/105 (88%)	58 (63%)	19 (21%)	15 (16%)	0	0
13	C1	153/155 (99%)	121 (79%)	23 (15%)	9 (6%)	2	17
13	c1	144/155 (93%)	122 (85%)	15 (10%)	7 (5%)	3	23
14	C2	122/142 (86%)	66 (54%)	30 (25%)	26 (21%)	0	0
14	c2	122/142 (86%)	62 (51%)	37 (30%)	23 (19%)	0	0
15	C3	148/150 (99%)	124 (84%)	19 (13%)	5 (3%)	6	32
15	c3	148/150 (99%)	116 (78%)	22 (15%)	10 (7%)	2	14
16	C4	125/136 (92%)	90 (72%)	25 (20%)	10 (8%)	1	10
16	c4	126/136 (93%)	100 (79%)	16 (13%)	10 (8%)	1	11
17	C5	122/141 (86%)	85 (70%)	26 (21%)	11 (9%)	1	8
17	c5	133/141 (94%)	93 (70%)	23 (17%)	17 (13%)	0	3
18	C6	139/142 (98%)	114 (82%)	19 (14%)	6 (4%)	4	26
18	c6	140/142 (99%)	120 (86%)	13 (9%)	7 (5%)	3	22
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	1	6
19	c7	113/136 (83%)	89 (79%)	17 (15%)	7 (6%)	2	16
20	C8	143/145 (99%)	106 (74%)	25 (18%)	12 (8%)	1	9
20	c8	143/145 (99%)	116 (81%)	16 (11%)	11 (8%)	1	11
21	C9	141/143 (99%)	116 (82%)	18 (13%)	7 (5%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	c9	141/143 (99%)	119 (84%)	18 (13%)	4 (3%)	8	39
22	D0	105/120 (88%)	84 (80%)	16 (15%)	5 (5%)	4	23
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	1	7
23	D1	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	2	17
23	d1	85/87 (98%)	70 (82%)	9 (11%)	6 (7%)	2	12
24	D2	127/129 (98%)	102 (80%)	19 (15%)	6 (5%)	4	23
24	d2	127/129 (98%)	114 (90%)	10 (8%)	3 (2%)	9	43
25	D3	142/144 (99%)	114 (80%)	22 (16%)	6 (4%)	4	27
25	d3	142/144 (99%)	125 (88%)	13 (9%)	4 (3%)	8	39
26	D4	132/134 (98%)	104 (79%)	17 (13%)	11 (8%)	1	9
26	d4	132/134 (98%)	111 (84%)	15 (11%)	6 (4%)	4	24
27	D5	68/107 (64%)	48 (71%)	12 (18%)	8 (12%)	1	4
27	d5	67/107 (63%)	51 (76%)	10 (15%)	6 (9%)	1	8
28	D6	95/97 (98%)	59 (62%)	18 (19%)	18 (19%)	0	0
28	d6	95/97 (98%)	74 (78%)	10 (10%)	11 (12%)	1	4
29	D7	79/81 (98%)	65 (82%)	8 (10%)	6 (8%)	2	11
29	d7	79/81 (98%)	59 (75%)	14 (18%)	6 (8%)	2	11
30	D8	61/66 (92%)	49 (80%)	6 (10%)	6 (10%)	1	6
30	d8	61/66 (92%)	42 (69%)	14 (23%)	5 (8%)	1	10
31	D9	51/55 (93%)	40 (78%)	9 (18%)	2 (4%)	5	29
31	d9	51/55 (93%)	40 (78%)	6 (12%)	5 (10%)	1	6
32	E0	58/60 (97%)	43 (74%)	12 (21%)	3 (5%)	3	21
33	E1	69/76 (91%)	36 (52%)	14 (20%)	19 (28%)	0	0
33	e1	74/76 (97%)	35 (47%)	20 (27%)	19 (26%)	0	0
34	SR	316/318 (99%)	242 (77%)	50 (16%)	24 (8%)	2	11
34	sR	316/318 (99%)	253 (80%)	48 (15%)	15 (5%)	4	23
35	SM	155/273 (57%)	103 (66%)	30 (19%)	22 (14%)	0	2
35	sM	98/273 (36%)	65 (66%)	18 (18%)	15 (15%)	0	1
39	L2	250/253 (99%)	224 (90%)	20 (8%)	6 (2%)	9	43
39	l2	250/253 (99%)	215 (86%)	24 (10%)	11 (4%)	4	25
40	L3	384/386 (100%)	328 (85%)	38 (10%)	18 (5%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	l3	384/386 (100%)	338 (88%)	35 (9%)	11 (3%)	7	38
41	L4	359/361 (99%)	299 (83%)	36 (10%)	24 (7%)	2	14
41	l4	359/361 (99%)	287 (80%)	51 (14%)	21 (6%)	3	18
42	L5	294/296 (99%)	241 (82%)	37 (13%)	16 (5%)	3	20
42	l5	292/296 (99%)	247 (85%)	37 (13%)	8 (3%)	8	39
43	L6	152/175 (87%)	128 (84%)	21 (14%)	3 (2%)	11	49
43	l6	153/175 (87%)	131 (86%)	17 (11%)	5 (3%)	6	33
44	L7	220/243 (90%)	186 (84%)	23 (10%)	11 (5%)	3	22
44	l7	221/243 (91%)	194 (88%)	23 (10%)	4 (2%)	13	52
45	L8	231/255 (91%)	190 (82%)	32 (14%)	9 (4%)	5	29
45	l8	229/255 (90%)	177 (77%)	30 (13%)	22 (10%)	1	7
46	L9	189/191 (99%)	164 (87%)	21 (11%)	4 (2%)	11	48
46	l9	189/191 (99%)	172 (91%)	14 (7%)	3 (2%)	14	55
47	M0	207/220 (94%)	172 (83%)	24 (12%)	11 (5%)	3	21
47	m0	209/220 (95%)	168 (80%)	28 (13%)	13 (6%)	2	16
48	M1	167/173 (96%)	126 (75%)	28 (17%)	13 (8%)	1	11
48	m1	167/173 (96%)	137 (82%)	16 (10%)	14 (8%)	1	9
49	M3	191/198 (96%)	161 (84%)	22 (12%)	8 (4%)	4	27
49	m3	192/198 (97%)	162 (84%)	21 (11%)	9 (5%)	4	23
50	M4	134/137 (98%)	113 (84%)	11 (8%)	10 (8%)	2	11
50	m4	135/137 (98%)	119 (88%)	13 (10%)	3 (2%)	10	46
51	M5	201/203 (99%)	182 (90%)	15 (8%)	4 (2%)	11	49
51	m5	201/203 (99%)	179 (89%)	17 (8%)	5 (2%)	9	42
52	M6	195/198 (98%)	173 (89%)	14 (7%)	8 (4%)	4	27
52	m6	195/198 (98%)	178 (91%)	11 (6%)	6 (3%)	7	36
53	M7	181/183 (99%)	146 (81%)	30 (17%)	5 (3%)	8	39
53	m7	153/183 (84%)	138 (90%)	11 (7%)	4 (3%)	8	41
54	M8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	6	33
54	m8	183/185 (99%)	154 (84%)	19 (10%)	10 (6%)	3	19
55	M9	186/188 (99%)	164 (88%)	18 (10%)	4 (2%)	10	46
55	m9	186/188 (99%)	162 (87%)	18 (10%)	6 (3%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	N0	170/172 (99%)	149 (88%)	16 (9%)	5 (3%)	7	38
56	n0	170/172 (99%)	156 (92%)	13 (8%)	1 (1%)	33	78
57	N1	157/159 (99%)	134 (85%)	16 (10%)	7 (4%)	4	24
57	n1	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	18	60
58	N2	98/120 (82%)	77 (79%)	15 (15%)	6 (6%)	2	16
58	n2	96/120 (80%)	76 (79%)	14 (15%)	6 (6%)	2	16
59	N3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	15	57
59	n3	134/136 (98%)	125 (93%)	6 (4%)	3 (2%)	10	46
60	N4	96/155 (62%)	65 (68%)	20 (21%)	11 (12%)	1	4
60	n4	133/155 (86%)	108 (81%)	17 (13%)	8 (6%)	2	17
61	N5	119/141 (84%)	103 (87%)	15 (13%)	1 (1%)	27	74
61	n5	118/141 (84%)	99 (84%)	10 (8%)	9 (8%)	2	11
62	N6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	5	28
62	n6	124/126 (98%)	110 (89%)	11 (9%)	3 (2%)	9	43
63	N7	133/135 (98%)	114 (86%)	12 (9%)	7 (5%)	3	21
63	n7	133/135 (98%)	109 (82%)	13 (10%)	11 (8%)	1	9
64	N8	146/148 (99%)	125 (86%)	16 (11%)	5 (3%)	6	32
64	n8	146/148 (99%)	121 (83%)	19 (13%)	6 (4%)	4	27
65	N9	56/58 (97%)	48 (86%)	7 (12%)	1 (2%)	13	52
65	n9	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	1	8
66	O0	95/104 (91%)	82 (86%)	12 (13%)	1 (1%)	21	65
66	o0	98/104 (94%)	81 (83%)	14 (14%)	3 (3%)	7	36
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	3	19
67	o1	107/112 (96%)	88 (82%)	12 (11%)	7 (6%)	2	15
68	O2	125/129 (97%)	114 (91%)	10 (8%)	1 (1%)	27	74
68	o2	125/129 (97%)	101 (81%)	18 (14%)	6 (5%)	4	23
69	O3	104/106 (98%)	93 (89%)	9 (9%)	2 (2%)	12	51
69	o3	104/106 (98%)	94 (90%)	9 (9%)	1 (1%)	22	68
70	O4	110/119 (92%)	91 (83%)	16 (14%)	3 (3%)	8	39
70	o4	110/119 (92%)	92 (84%)	15 (14%)	3 (3%)	8	39
71	O5	117/119 (98%)	96 (82%)	17 (14%)	4 (3%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	o5	117/119 (98%)	96 (82%)	14 (12%)	7 (6%)	2	17
72	O6	97/99 (98%)	77 (79%)	12 (12%)	8 (8%)	1	10
72	o6	97/99 (98%)	77 (79%)	14 (14%)	6 (6%)	2	16
73	O7	85/87 (98%)	76 (89%)	7 (8%)	2 (2%)	9	43
73	o7	85/87 (98%)	73 (86%)	9 (11%)	3 (4%)	6	32
74	O8	75/77 (97%)	63 (84%)	10 (13%)	2 (3%)	8	39
74	o8	75/77 (97%)	62 (83%)	11 (15%)	2 (3%)	8	39
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	11	48
75	o9	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	4	27
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	5	28
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	11	49
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	3 (13%)	1 (4%)	4	26
78	Q2	103/105 (98%)	82 (80%)	15 (15%)	6 (6%)	3	18
78	q2	103/105 (98%)	92 (89%)	7 (7%)	4 (4%)	5	29
79	Q3	89/91 (98%)	73 (82%)	15 (17%)	1 (1%)	21	65
79	q3	89/91 (98%)	78 (88%)	10 (11%)	1 (1%)	21	65
80	e0	60/62 (97%)	46 (77%)	9 (15%)	5 (8%)	1	9
82	p0	139/311 (45%)	109 (78%)	20 (14%)	10 (7%)	2	12
All	All	22333/24141 (92%)	18272 (82%)	2751 (12%)	1310 (6%)	2	17

5 of 1310 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	66	ALA
2	S0	158	VAL
2	S0	191	ARG

### 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%)	136 (83%)	28 (17%)	3	11
2	s0	165/209 (79%)	130 (79%)	35 (21%)	1	7
3	S1	191/223 (86%)	150 (78%)	41 (22%)	1	6
3	s1	192/223 (86%)	151 (79%)	41 (21%)	1	7
4	S2	176/204 (86%)	137 (78%)	39 (22%)	1	6
4	s2	176/204 (86%)	133 (76%)	43 (24%)	1	4
5	S3	182/194 (94%)	138 (76%)	44 (24%)	1	4
5	s3	182/194 (94%)	144 (79%)	38 (21%)	1	7
6	S4	221/221 (100%)	175 (79%)	46 (21%)	2	7
6	s4	221/221 (100%)	183 (83%)	38 (17%)	3	11
7	S5	173/190 (91%)	137 (79%)	36 (21%)	2	7
7	s5	173/190 (91%)	140 (81%)	33 (19%)	2	9
8	S6	188/201 (94%)	152 (81%)	36 (19%)	2	9
8	s6	187/201 (93%)	152 (81%)	35 (19%)	2	9
9	S7	165/169 (98%)	140 (85%)	25 (15%)	4	16
9	s7	165/169 (98%)	135 (82%)	30 (18%)	2	10
10	S8	150/161 (93%)	128 (85%)	22 (15%)	4	18
10	s8	150/161 (93%)	119 (79%)	31 (21%)	2	8
11	S9	158/165 (96%)	126 (80%)	32 (20%)	2	8
11	s9	158/165 (96%)	124 (78%)	34 (22%)	1	6
12	C0	77/98 (79%)	64 (83%)	13 (17%)	3	11
12	c0	73/98 (74%)	61 (84%)	12 (16%)	3	12
13	C1	129/136 (95%)	115 (89%)	14 (11%)	9	34
13	c1	129/136 (95%)	109 (84%)	20 (16%)	4	14
14	C2	88/118 (75%)	62 (70%)	26 (30%)	0	1
14	c2	88/118 (75%)	64 (73%)	24 (27%)	0	2
15	C3	127/127 (100%)	102 (80%)	25 (20%)	2	8
15	c3	127/127 (100%)	104 (82%)	23 (18%)	2	10
16	C4	81/104 (78%)	57 (70%)	24 (30%)	0	1
16	c4	97/104 (93%)	70 (72%)	27 (28%)	0	1
17	C5	101/117 (86%)	82 (81%)	19 (19%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	c5	103/117 (88%)	83 (81%)	20 (19%)	2	8
18	C6	117/118 (99%)	90 (77%)	27 (23%)	1	5
18	c6	118/118 (100%)	96 (81%)	22 (19%)	2	9
19	C7	94/124 (76%)	74 (79%)	20 (21%)	1	7
19	c7	92/124 (74%)	72 (78%)	20 (22%)	1	6
20	C8	128/128 (100%)	107 (84%)	21 (16%)	3	12
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	5
21	C9	115/115 (100%)	92 (80%)	23 (20%)	2	8
21	c9	115/115 (100%)	94 (82%)	21 (18%)	2	10
22	D0	100/113 (88%)	72 (72%)	28 (28%)	0	1
22	d0	103/113 (91%)	77 (75%)	26 (25%)	1	3
23	D1	74/74 (100%)	61 (82%)	13 (18%)	3	10
23	d1	74/74 (100%)	62 (84%)	12 (16%)	3	13
24	D2	110/110 (100%)	91 (83%)	19 (17%)	3	11
24	d2	110/110 (100%)	94 (86%)	16 (14%)	5	18
25	D3	119/119 (100%)	97 (82%)	22 (18%)	2	9
25	d3	119/119 (100%)	98 (82%)	21 (18%)	3	10
26	D4	112/112 (100%)	98 (88%)	14 (12%)	7	25
26	d4	112/112 (100%)	93 (83%)	19 (17%)	3	11
27	D5	61/88 (69%)	43 (70%)	18 (30%)	0	1
27	d5	61/88 (69%)	51 (84%)	10 (16%)	3	12
28	D6	83/83 (100%)	63 (76%)	20 (24%)	1	4
28	d6	83/83 (100%)	66 (80%)	17 (20%)	2	8
29	D7	70/70 (100%)	59 (84%)	11 (16%)	4	14
29	d7	70/70 (100%)	60 (86%)	10 (14%)	5	19
30	D8	56/59 (95%)	43 (77%)	13 (23%)	1	5
30	d8	56/59 (95%)	46 (82%)	10 (18%)	2	10
31	D9	47/48 (98%)	39 (83%)	8 (17%)	3	11
31	d9	47/48 (98%)	38 (81%)	9 (19%)	2	9
32	E0	51/51 (100%)	39 (76%)	12 (24%)	1	5
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	e1	66/66 (100%)	50 (76%)	16 (24%)	1	4
34	SR	260/261 (100%)	211 (81%)	49 (19%)	2	9
34	sR	260/261 (100%)	231 (89%)	29 (11%)	9	33
35	SM	97/228 (42%)	80 (82%)	17 (18%)	3	11
35	sM	54/228 (24%)	41 (76%)	13 (24%)	1	4
39	L2	193/195 (99%)	157 (81%)	36 (19%)	2	9
39	l2	192/195 (98%)	158 (82%)	34 (18%)	3	10
40	L3	320/322 (99%)	252 (79%)	68 (21%)	1	7
40	l3	321/322 (100%)	252 (78%)	69 (22%)	1	6
41	L4	288/288 (100%)	230 (80%)	58 (20%)	2	8
41	l4	288/288 (100%)	231 (80%)	57 (20%)	2	8
42	L5	244/244 (100%)	206 (84%)	38 (16%)	4	14
42	l5	243/244 (100%)	191 (79%)	52 (21%)	1	7
43	L6	134/152 (88%)	114 (85%)	20 (15%)	4	17
43	l6	135/152 (89%)	114 (84%)	21 (16%)	4	14
44	L7	186/204 (91%)	160 (86%)	26 (14%)	5	21
44	l7	187/204 (92%)	157 (84%)	30 (16%)	3	13
45	L8	187/207 (90%)	157 (84%)	30 (16%)	3	13
45	l8	177/207 (86%)	138 (78%)	39 (22%)	1	6
46	L9	171/171 (100%)	128 (75%)	43 (25%)	1	3
46	l9	171/171 (100%)	136 (80%)	35 (20%)	2	8
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	6
47	m0	179/186 (96%)	149 (83%)	30 (17%)	3	11
48	M1	147/150 (98%)	109 (74%)	38 (26%)	1	2
48	m1	147/150 (98%)	117 (80%)	30 (20%)	2	8
49	M3	154/158 (98%)	124 (80%)	30 (20%)	2	8
49	m3	154/158 (98%)	125 (81%)	29 (19%)	2	9
50	M4	107/108 (99%)	87 (81%)	20 (19%)	2	9
50	m4	108/108 (100%)	91 (84%)	17 (16%)	4	14
51	M5	175/175 (100%)	139 (79%)	36 (21%)	2	8
51	m5	175/175 (100%)	146 (83%)	29 (17%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	M6	160/161 (99%)	132 (82%)	28 (18%)	3	11
52	m6	160/161 (99%)	134 (84%)	26 (16%)	3	12
53	M7	140/145 (97%)	106 (76%)	34 (24%)	1	4
53	m7	125/145 (86%)	101 (81%)	24 (19%)	2	9
54	M8	150/150 (100%)	121 (81%)	29 (19%)	2	8
54	m8	150/150 (100%)	121 (81%)	29 (19%)	2	8
55	M9	153/153 (100%)	131 (86%)	22 (14%)	5	19
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	6
56	N0	156/156 (100%)	127 (81%)	29 (19%)	2	9
56	n0	156/156 (100%)	123 (79%)	33 (21%)	1	7
57	N1	136/136 (100%)	111 (82%)	25 (18%)	2	9
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	7
58	N2	87/106 (82%)	72 (83%)	15 (17%)	3	11
58	n2	85/106 (80%)	65 (76%)	20 (24%)	1	5
59	N3	104/104 (100%)	84 (81%)	20 (19%)	2	9
59	n3	104/104 (100%)	91 (88%)	13 (12%)	7	25
60	N4	57/129 (44%)	50 (88%)	7 (12%)	7	26
60	n4	100/129 (78%)	84 (84%)	16 (16%)	3	13
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	6
61	n5	104/117 (89%)	86 (83%)	18 (17%)	3	11
62	N6	109/109 (100%)	88 (81%)	21 (19%)	2	8
62	n6	109/109 (100%)	86 (79%)	23 (21%)	1	7
63	N7	115/115 (100%)	92 (80%)	23 (20%)	2	8
63	n7	115/115 (100%)	90 (78%)	25 (22%)	1	6
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	10
64	n8	118/118 (100%)	103 (87%)	15 (13%)	6	24
65	N9	46/46 (100%)	38 (83%)	8 (17%)	3	11
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0	1
66	O0	81/87 (93%)	63 (78%)	18 (22%)	1	6
66	o0	84/87 (97%)	63 (75%)	21 (25%)	1	3
67	O1	92/96 (96%)	76 (83%)	16 (17%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	o1	94/96 (98%)	68 (72%)	26 (28%)	0	1
68	O2	109/110 (99%)	87 (80%)	22 (20%)	2	8
68	o2	109/110 (99%)	87 (80%)	22 (20%)	2	8
69	O3	90/90 (100%)	80 (89%)	10 (11%)	9	33
69	o3	90/90 (100%)	72 (80%)	18 (20%)	2	8
70	O4	95/101 (94%)	77 (81%)	18 (19%)	2	9
70	o4	95/101 (94%)	76 (80%)	19 (20%)	2	8
71	O5	104/104 (100%)	78 (75%)	26 (25%)	1	3
71	o5	103/104 (99%)	84 (82%)	19 (18%)	2	9
72	O6	81/81 (100%)	61 (75%)	20 (25%)	1	3
72	o6	80/81 (99%)	54 (68%)	26 (32%)	0	0
73	O7	70/70 (100%)	52 (74%)	18 (26%)	1	2
73	o7	70/70 (100%)	56 (80%)	14 (20%)	2	8
74	O8	68/68 (100%)	49 (72%)	19 (28%)	0	1
74	o8	67/68 (98%)	51 (76%)	16 (24%)	1	4
75	O9	45/45 (100%)	37 (82%)	8 (18%)	2	10
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	10
76	Q0	47/47 (100%)	41 (87%)	6 (13%)	6	24
76	q0	47/47 (100%)	40 (85%)	7 (15%)	4	17
77	Q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2	10
78	q2	90/90 (100%)	67 (74%)	23 (26%)	1	2
79	Q3	71/71 (100%)	55 (78%)	16 (22%)	1	6
79	q3	71/71 (100%)	57 (80%)	14 (20%)	2	8
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	5
82	p0	105/253 (42%)	87 (83%)	18 (17%)	3	11
All	All	18729/20239 (92%)	15053 (80%)	3676 (20%)	2	8

5 of 3676 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	O2	126	LEU

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Mol	Chain	Res	Type
7	s5	216	GLU
64	n8	60	TYR
71	O5	100	VAL
3	s1	25	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
57	N1	26	HIS
3	s1	74	GLN
61	n5	111	ASN
59	N3	98	ASN
64	N8	64	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 2559 ligands modelled in this entry, 1424 are monoatomic - leaving 1135 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	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-



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

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

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

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

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

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

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3K5	1	4221	-	63,63,63	1.06	1 (1%)	95,95,95	1.83	17 (17%)
86	OHX	2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-



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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	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	4	239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

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



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



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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3K5	5	4249	-	63,63,63	0.58	1 (1%)	95,95,95	1.70	15 (15%)
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	-
86	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	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	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	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	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	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	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	l3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	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	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	304	-	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	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	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	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3878	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	1	4214	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4220	-	-	0/0/0/0	0/0/0/0
88	3K5	1	4221	-	-	0/29/121/121	0/6/7/7
86	OHX	2	2022	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	3	214	-	-	0/0/0/0	0/0/0/0
86	OHX	3	215	-	-	0/0/0/0	0/0/0/0
86	OHX	3	216	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	3	217	-	-	0/0/0/0	0/0/0/0
86	OHX	3	218	-	-	0/0/0/0	0/0/0/0
86	OHX	3	219	-	-	0/0/0/0	0/0/0/0
86	OHX	3	220	-	-	0/0/0/0	0/0/0/0
86	OHX	3	221	-	-	0/0/0/0	0/0/0/0
86	OHX	3	222	-	-	0/0/0/0	0/0/0/0
86	OHX	3	223	-	-	0/0/0/0	0/0/0/0
86	OHX	3	224	-	-	0/0/0/0	0/0/0/0
86	OHX	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	4	239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
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
88	3K5	5	4249	-	-	0/29/121/121	0/6/7/7
86	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2047	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2089	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2131	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2173	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2205	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	-	-	0/0/0/0	0/0/0/0
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0
86	OHX	8	219	-	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	-	-	0/0/0/0	0/0/0/0
86	OHX	8	222	-	-	0/0/0/0	0/0/0/0
86	OHX	8	223	-	-	0/0/0/0	0/0/0/0
86	OHX	8	224	-	-	0/0/0/0	0/0/0/0
86	OHX	8	225	-	-	0/0/0/0	0/0/0/0
86	OHX	8	226	-	-	0/0/0/0	0/0/0/0
86	OHX	8	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	229	-	-	0/0/0/0	0/0/0/0
86	OHX	8	230	-	-	0/0/0/0	0/0/0/0
86	OHX	8	231	-	-	0/0/0/0	0/0/0/0
86	OHX	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	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	406	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	304	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	302	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	205	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	203	-	-	0/0/0/0	0/0/0/0
86	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	105	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	503	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	404	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	406	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	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	l5	306	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	304	-	-	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	o2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	203	-	-	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	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4221	3K5	O3-C15	7.76	1.60	1.44
88	5	4249	3K5	O3-C15	-2.98	1.38	1.44

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4221	3K5	O3-C15-C17	-8.96	91.61	118.82
88	1	4221	3K5	O3-C16-C15	6.85	67.35	59.24
88	5	4249	3K5	C16-C15-C17	-6.28	112.79	124.96
88	5	4249	3K5	O14-C34-C35	5.46	120.52	107.83
88	5	4249	3K5	C16-C15-C3	-5.26	111.05	125.13

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%)	0.44	98 (5%) 24 3	56, 92, 171, 265	0
1	6	1795/1800 (99%)	0.43	91 (5%) 27 4	43, 76, 180, 301	0
2	S0	206/251 (82%)	1.31	49 (23%) 1 0	94, 110, 125, 156	0
2	s0	206/251 (82%)	0.57	13 (6%) 19 3	73, 93, 110, 119	0
3	S1	214/254 (84%)	0.60	26 (12%) 5 1	100, 132, 158, 166	0
3	s1	216/254 (85%)	0.31	3 (1%) 72 17	66, 83, 109, 119	0
4	S2	217/253 (85%)	0.85	31 (14%) 3 1	72, 89, 106, 122	0
4	s2	217/253 (85%)	1.18	43 (19%) 2 0	56, 74, 98, 119	0
5	S3	223/239 (93%)	0.86	28 (12%) 4 1	79, 93, 131, 147	0
5	s3	223/239 (93%)	1.05	46 (20%) 1 0	74, 105, 131, 146	0
6	S4	260/260 (100%)	1.36	73 (28%) 1 0	68, 90, 104, 129	0
6	s4	260/260 (100%)	1.04	40 (15%) 3 1	54, 73, 92, 130	0
7	S5	206/224 (91%)	1.25	49 (23%) 1 0	97, 118, 136, 149	0
7	s5	206/224 (91%)	0.44	11 (5%) 25 4	70, 94, 125, 139	0
8	S6	226/236 (95%)	1.22	55 (24%) 1 0	65, 105, 126, 151	0
8	s6	218/236 (92%)	0.75	21 (9%) 8 2	53, 80, 105, 133	0
9	S7	184/189 (97%)	0.80	15 (8%) 12 2	89, 117, 148, 159	0
9	s7	186/189 (98%)	0.75	20 (10%) 6 1	67, 103, 136, 144	0
10	S8	188/200 (94%)	0.90	27 (14%) 3 1	58, 75, 115, 137	0
10	s8	188/200 (94%)	0.53	12 (6%) 19 3	47, 65, 114, 129	0
11	S9	185/196 (94%)	1.76	65 (35%) 1 0	83, 101, 136, 162	0
11	s9	185/196 (94%)	1.04	25 (13%) 4 1	63, 78, 117, 150	0
12	C0	96/105 (91%)	0.95	17 (17%) 2 0	82, 106, 140, 160	0
12	c0	96/105 (91%)	1.88	37 (38%) 1 0	97, 131, 158, 190	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	C1	155/155 (100%)	0.68	13 (8%)	11	2	60, 74, 134, 145	0
13	c1	146/155 (94%)	0.20	4 (2%)	52	8	47, 63, 99, 116	0
14	C2	124/142 (87%)	1.24	29 (23%)	1	0	129, 146, 167, 187	0
14	c2	124/142 (87%)	3.57	87 (70%)	0	0	172, 191, 208, 219	0
15	C3	150/150 (100%)	0.65	7 (4%)	30	4	69, 89, 108, 116	0
15	c3	150/150 (100%)	0.44	6 (4%)	36	5	57, 72, 93, 111	0
16	C4	127/136 (93%)	1.46	40 (31%)	1	0	71, 130, 147, 150	0
16	c4	128/136 (94%)	1.11	20 (15%)	3	1	53, 84, 94, 102	0
17	C5	124/141 (87%)	0.92	24 (19%)	2	0	79, 97, 136, 160	0
17	c5	135/141 (95%)	0.34	8 (5%)	22	3	76, 101, 136, 181	0
18	C6	141/142 (99%)	1.54	46 (32%)	1	0	83, 108, 115, 118	0
18	c6	142/142 (100%)	1.18	32 (22%)	1	0	66, 87, 106, 134	0
19	C7	120/136 (88%)	0.80	16 (13%)	4	1	92, 107, 138, 141	0
19	c7	117/136 (86%)	0.43	5 (4%)	34	5	78, 95, 122, 132	0
20	C8	145/145 (100%)	0.77	21 (14%)	3	1	80, 106, 132, 141	0
20	c8	145/145 (100%)	0.70	16 (11%)	6	1	72, 87, 117, 136	0
21	C9	143/143 (100%)	1.51	55 (38%)	1	0	90, 107, 127, 142	0
21	c9	143/143 (100%)	1.01	23 (16%)	2	1	66, 79, 100, 120	0
22	D0	107/120 (89%)	1.42	34 (31%)	1	0	73, 112, 152, 158	0
22	d0	110/120 (91%)	1.63	30 (27%)	1	0	68, 109, 156, 199	0
23	D1	87/87 (100%)	0.76	12 (13%)	4	1	92, 98, 116, 132	0
23	d1	87/87 (100%)	0.46	5 (5%)	23	3	67, 78, 102, 117	0
24	D2	129/129 (100%)	1.82	55 (42%)	1	0	70, 83, 90, 100	0
24	d2	129/129 (100%)	0.49	1 (0%)	83	28	52, 63, 71, 82	0
25	D3	144/144 (100%)	0.41	5 (3%)	42	6	61, 67, 79, 97	0
25	d3	144/144 (100%)	0.46	1 (0%)	84	32	45, 52, 66, 79	0
26	D4	134/134 (100%)	1.66	45 (33%)	1	0	79, 109, 128, 138	0
26	d4	134/134 (100%)	0.92	20 (14%)	3	1	60, 83, 101, 127	0
27	D5	70/107 (65%)	1.82	28 (40%)	1	0	113, 129, 139, 142	0
27	d5	69/107 (64%)	0.92	11 (15%)	3	1	85, 111, 128, 135	0
28	D6	97/97 (100%)	1.78	42 (43%)	1	0	79, 96, 149, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	d6	97/97 (100%)	1.20	17 (17%) 2 0	57, 73, 100, 109	0
29	D7	81/81 (100%)	0.18	2 (2%) 54 9	84, 103, 146, 152	0
29	d7	81/81 (100%)	0.43	4 (4%) 28 4	66, 85, 132, 137	0
30	D8	63/66 (95%)	2.18	32 (50%) 0 0	108, 129, 143, 159	0
30	d8	63/66 (95%)	1.84	28 (44%) 1 0	86, 105, 128, 135	0
31	D9	53/55 (96%)	0.42	1 (1%) 64 13	74, 82, 101, 114	0
31	d9	53/55 (96%)	0.86	4 (7%) 14 2	75, 82, 126, 139	0
32	E0	60/60 (100%)	1.89	19 (31%) 1 0	64, 98, 141, 153	0
33	E1	71/76 (93%)	1.63	24 (33%) 1 0	103, 126, 142, 150	0
33	e1	76/76 (100%)	2.26	32 (42%) 1 0	129, 159, 171, 175	0
34	SR	318/318 (100%)	0.56	23 (7%) 15 2	69, 115, 139, 157	0
34	sR	318/318 (100%)	0.54	25 (7%) 13 2	94, 116, 137, 155	0
35	SM	159/273 (58%)	0.93	21 (13%) 4 1	64, 92, 142, 149	0
35	sM	104/273 (38%)	0.77	18 (17%) 2 0	64, 101, 189, 194	0
36	1	3149/3396 (92%)	0.49	147 (4%) 30 4	29, 53, 142, 278	0
36	5	3150/3396 (92%)	0.42	72 (2%) 57 9	29, 52, 126, 288	0
37	3	121/121 (100%)	0.15	1 (0%) 83 28	44, 71, 87, 93	0
37	7	121/121 (100%)	0.18	0 100 100	36, 56, 69, 78	0
38	4	158/158 (100%)	0.37	2 (1%) 74 19	35, 54, 96, 136	0
38	8	158/158 (100%)	0.30	3 (1%) 64 13	40, 63, 102, 133	0
39	L2	252/253 (99%)	0.57	16 (6%) 19 3	34, 49, 69, 79	0
39	l2	252/253 (99%)	0.63	5 (1%) 62 12	35, 54, 74, 87	0
40	L3	386/386 (100%)	0.42	11 (2%) 50 8	35, 59, 74, 110	0
40	l3	386/386 (100%)	0.26	2 (0%) 88 39	28, 42, 57, 96	0
41	L4	361/361 (100%)	0.33	2 (0%) 86 36	31, 46, 65, 78	0
41	l4	361/361 (100%)	0.27	3 (0%) 83 28	35, 52, 72, 86	0
42	L5	296/296 (100%)	0.52	13 (4%) 33 5	53, 78, 98, 128	0
42	l5	294/296 (99%)	0.32	3 (1%) 79 23	44, 59, 88, 136	0
43	L6	156/175 (89%)	0.51	2 (1%) 74 19	41, 49, 73, 101	0
43	l6	157/175 (89%)	0.19	3 (1%) 64 13	43, 53, 75, 90	0
44	L7	222/243 (91%)	0.06	1 (0%) 88 39	34, 42, 75, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	l7	223/243 (91%)	0.29	1 (0%) 90 45	31, 41, 84, 129	0
45	L8	233/255 (91%)	0.17	3 (1%) 74 19	56, 71, 108, 122	0
45	l8	231/255 (90%)	0.65	21 (9%) 9 2	69, 83, 110, 117	0
46	L9	191/191 (100%)	0.57	9 (4%) 30 4	52, 67, 83, 103	0
46	l9	191/191 (100%)	0.03	0 100 100	38, 48, 71, 103	0
47	M0	211/220 (95%)	0.59	9 (4%) 34 5	39, 56, 94, 130	0
47	m0	213/220 (96%)	0.34	5 (2%) 57 9	34, 53, 83, 102	0
48	M1	169/173 (97%)	0.31	6 (3%) 41 6	61, 82, 95, 103	0
48	m1	169/173 (97%)	0.11	1 (0%) 86 36	46, 65, 80, 92	0
49	M3	193/198 (97%)	0.77	13 (6%) 17 3	34, 54, 102, 130	0
49	m3	194/198 (97%)	0.82	18 (9%) 9 2	41, 65, 108, 136	0
50	M4	136/137 (99%)	0.07	1 (0%) 84 32	44, 54, 68, 79	0
50	m4	137/137 (100%)	0.09	0 100 100	38, 45, 65, 77	0
51	M5	203/203 (100%)	0.57	11 (5%) 25 4	32, 47, 59, 64	0
51	m5	203/203 (100%)	0.93	15 (7%) 14 2	40, 58, 70, 75	0
52	M6	197/198 (99%)	0.06	0 100 100	35, 44, 67, 72	0
52	m6	197/198 (99%)	0.28	0 100 100	29, 34, 62, 70	0
53	M7	183/183 (100%)	0.68	20 (10%) 6 1	39, 46, 120, 144	0
53	m7	155/183 (84%)	0.33	0 100 100	32, 41, 54, 89	0
54	M8	185/185 (100%)	0.25	0 100 100	36, 45, 61, 81	0
54	m8	185/185 (100%)	0.15	1 (0%) 88 39	40, 51, 61, 67	0
55	M9	188/188 (100%)	0.78	23 (12%) 5 1	53, 70, 157, 171	0
55	m9	188/188 (100%)	0.54	5 (2%) 52 8	47, 60, 130, 144	0
56	N0	172/172 (100%)	0.20	2 (1%) 75 20	44, 52, 66, 74	0
56	n0	172/172 (100%)	0.26	2 (1%) 75 20	34, 42, 54, 67	0
57	N1	159/159 (100%)	0.68	6 (3%) 38 5	40, 51, 95, 103	0
57	n1	159/159 (100%)	0.42	0 100 100	37, 45, 89, 96	0
58	N2	100/120 (83%)	0.57	8 (8%) 12 2	83, 102, 119, 132	0
58	n2	98/120 (81%)	1.13	18 (18%) 2 0	72, 87, 102, 107	0
59	N3	136/136 (100%)	0.55	7 (5%) 27 4	41, 53, 70, 87	0
59	n3	136/136 (100%)	0.40	2 (1%) 70 16	30, 41, 59, 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%)	2.58	34 (34%)	1 0	52, 68, 162, 167	0
60	n4	135/155 (87%)	0.64	8 (5%)	22 3	41, 90, 134, 156	0
61	N5	121/141 (85%)	0.75	14 (11%)	5 1	49, 62, 83, 105	0
61	n5	120/141 (85%)	0.80	5 (4%)	35 5	50, 65, 86, 93	0
62	N6	126/126 (100%)	0.44	3 (2%)	56 9	40, 55, 68, 81	0
62	n6	126/126 (100%)	0.90	9 (7%)	16 3	47, 61, 80, 91	0
63	N7	135/135 (100%)	0.73	13 (9%)	8 2	70, 85, 101, 114	0
63	n7	135/135 (100%)	0.48	4 (2%)	48 7	75, 92, 116, 128	0
64	N8	148/148 (100%)	0.28	4 (2%)	52 8	27, 46, 74, 86	0
64	n8	148/148 (100%)	0.50	1 (0%)	84 32	32, 53, 76, 81	0
65	N9	58/58 (100%)	0.78	5 (8%)	11 2	36, 56, 107, 121	0
65	n9	58/58 (100%)	0.70	2 (3%)	43 6	35, 57, 89, 106	0
66	O0	97/104 (93%)	0.49	6 (6%)	20 3	68, 80, 107, 120	0
66	o0	100/104 (96%)	0.50	4 (4%)	36 5	72, 83, 115, 126	0
67	O1	109/112 (97%)	0.79	12 (11%)	6 1	50, 64, 107, 121	0
67	o1	109/112 (97%)	0.70	7 (6%)	19 3	40, 53, 96, 123	0
68	O2	127/129 (98%)	0.46	2 (1%)	68 15	28, 43, 56, 71	0
68	o2	127/129 (98%)	0.74	11 (8%)	10 2	30, 48, 65, 86	0
69	O3	106/106 (100%)	0.61	3 (2%)	50 8	35, 42, 65, 77	0
69	o3	106/106 (100%)	0.64	3 (2%)	50 8	33, 41, 70, 85	0
70	O4	112/119 (94%)	1.20	24 (21%)	1 0	49, 67, 112, 129	0
70	o4	112/119 (94%)	0.74	12 (10%)	6 1	49, 69, 114, 127	0
71	O5	119/119 (100%)	1.61	34 (28%)	1 0	45, 65, 73, 76	0
71	o5	119/119 (100%)	0.56	7 (5%)	22 3	54, 70, 82, 89	0
72	O6	99/99 (100%)	0.69	7 (7%)	16 3	53, 65, 101, 123	0
72	o6	99/99 (100%)	0.87	8 (8%)	12 2	58, 73, 99, 120	0
73	O7	87/87 (100%)	0.74	6 (6%)	17 3	35, 43, 75, 102	0
73	o7	87/87 (100%)	0.63	5 (5%)	23 3	39, 46, 82, 120	0
74	O8	77/77 (100%)	1.05	6 (7%)	13 2	73, 89, 113, 124	0
74	o8	77/77 (100%)	0.54	4 (5%)	26 4	73, 90, 105, 109	0
75	O9	50/50 (100%)	0.20	0	100 100	44, 50, 58, 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%)	0.69	3 (6%) 21 3	50, 54, 64, 75	0
76	Q0	52/52 (100%)	0.31	2 (3%) 38 5	49, 59, 84, 94	0
76	q0	52/52 (100%)	-0.10	0 100 100	34, 40, 54, 65	0
77	Q1	25/25 (100%)	2.08	13 (52%) 0 0	54, 59, 63, 73	0
77	q1	25/25 (100%)	1.09	6 (24%) 1 0	44, 48, 63, 70	0
78	Q2	105/105 (100%)	0.46	2 (1%) 64 13	36, 54, 84, 116	0
78	q2	105/105 (100%)	0.43	5 (4%) 29 4	43, 55, 84, 115	0
79	Q3	91/91 (100%)	0.71	11 (12%) 5 1	44, 54, 74, 87	0
79	q3	91/91 (100%)	0.80	6 (6%) 18 3	41, 55, 71, 84	0
80	e0	62/62 (100%)	0.56	7 (11%) 6 1	58, 81, 120, 139	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	0.92	19 (13%) 4 1	86, 105, 187, 197	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35344 (93%)	0.63	2716 (8%) 12 2	27, 69, 136, 301	0

The worst 5 of 2716 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	76	VAL	11.8
14	c2	112	ALA	11.6
14	c2	40	GLY	11.0
60	N4	69	LYS	11.0
60	N4	68	ALA	10.9

## 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	3857	1/1	0.38	449.00	68,68,68,68	0
85	MG	5	3781	1/1	0.49	355.00	80,80,80,80	0
85	MG	17	303	1/1	0.30	217.00	47,47,47,47	0
85	MG	1	3821	1/1	0.26	194.45	52,52,52,52	0
85	MG	1	3707	1/1	0.29	185.00	49,49,49,49	0
85	MG	5	3585	1/1	0.51	177.78	28,28,28,28	0
85	MG	5	3410	1/1	0.47	177.49	48,48,48,48	0
85	MG	5	3420	1/1	0.34	157.00	69,69,69,69	0
85	MG	6	2019	1/1	0.38	133.67	108,108,108,108	0
85	MG	5	3479	1/1	0.31	133.00	68,68,68,68	0
85	MG	1	3870	1/1	0.48	127.40	57,57,57,57	0
85	MG	5	3487	1/1	0.31	113.00	51,51,51,51	0
85	MG	1	3591	1/1	0.34	107.71	33,33,33,33	0
85	MG	2	1949	1/1	0.60	102.78	88,88,88,88	0
85	MG	2	2013	1/1	0.39	98.00	62,62,62,62	0
85	MG	6	1919	1/1	0.29	91.00	54,54,54,54	0
85	MG	2	1957	1/1	0.37	84.33	81,81,81,81	0
85	MG	2	1904	1/1	0.51	81.75	77,77,77,77	0
85	MG	1	3860	1/1	0.30	78.00	99,99,99,99	0
85	MG	1	3686	1/1	0.31	75.70	49,49,49,49	0
85	MG	3	209	1/1	0.46	65.32	62,62,62,62	0
85	MG	5	3882	1/1	0.55	61.80	86,86,86,86	0
85	MG	2	2001	1/1	0.52	55.15	109,109,109,109	0
85	MG	1	3580	1/1	0.57	54.88	38,38,38,38	0
85	MG	1	3731	1/1	0.88	54.58	41,41,41,41	0
85	MG	1	3843	1/1	0.31	54.00	50,50,50,50	0
85	MG	3	204	1/1	0.59	53.94	56,56,56,56	0
85	MG	1	3733	1/1	1.04	47.24	35,35,35,35	0
85	MG	5	3860	1/1	1.12	39.59	62,62,62,62	0
85	MG	5	3657	1/1	0.37	37.43	68,68,68,68	0
85	MG	8	209	1/1	0.42	35.85	61,61,61,61	0
85	MG	7	216	1/1	0.43	35.33	57,57,57,57	0
85	MG	6	1970	1/1	0.45	34.87	73,73,73,73	0
85	MG	6	1943	1/1	0.49	34.29	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3574	1/1	0.47	34.27	32,32,32,32	0
85	MG	1	3832	1/1	2.12	33.27	52,52,52,52	0
85	MG	5	3758	1/1	0.44	32.83	48,48,48,48	0
85	MG	5	3809	1/1	0.65	32.49	41,41,41,41	0
85	MG	6	1942	1/1	0.44	30.60	39,39,39,39	0
85	MG	1	3859	1/1	0.40	30.17	70,70,70,70	0
85	MG	5	3766	1/1	1.23	30.15	44,44,44,44	0
85	MG	5	3872	1/1	0.50	29.73	51,51,51,51	0
85	MG	5	3722	1/1	1.74	29.57	48,48,48,48	0
85	MG	1	3765	1/1	0.51	28.79	64,64,64,64	0
85	MG	1	3685	1/1	0.31	28.43	45,45,45,45	0
85	MG	2	1932	1/1	0.43	27.40	61,61,61,61	0
85	MG	5	3667	1/1	0.85	27.15	60,60,60,60	0
85	MG	2	1994	1/1	0.45	26.65	63,63,63,63	0
85	MG	1	3620	1/1	0.31	26.56	59,59,59,59	0
85	MG	5	3728	1/1	0.35	26.31	43,43,43,43	0
85	MG	5	3864	1/1	0.32	26.27	45,45,45,45	0
85	MG	5	3687	1/1	0.40	26.20	69,69,69,69	0
85	MG	5	3738	1/1	0.33	25.91	49,49,49,49	0
85	MG	5	3660	1/1	0.29	25.71	47,47,47,47	0
85	MG	5	3680	1/1	0.56	25.70	94,94,94,94	0
85	MG	6	1954	1/1	0.46	25.30	40,40,40,40	0
85	MG	4	213	1/1	0.40	25.00	53,53,53,53	0
85	MG	2	1987	1/1	0.35	24.86	85,85,85,85	0
85	MG	1	3794	1/1	0.70	24.76	46,46,46,46	0
85	MG	7	209	1/1	0.38	24.53	45,45,45,45	0
85	MG	5	3765	1/1	1.01	24.36	40,40,40,40	0
85	MG	1	3719	1/1	0.87	23.98	45,45,45,45	0
85	MG	3	207	1/1	0.44	23.01	64,64,64,64	0
85	MG	5	3578	1/1	0.35	22.98	30,30,30,30	0
85	MG	5	3650	1/1	0.31	22.87	62,62,62,62	0
85	MG	1	3724	1/1	0.40	22.73	55,55,55,55	0
85	MG	6	1936	1/1	0.38	22.16	46,46,46,46	0
85	MG	5	3651	1/1	0.82	22.09	47,47,47,47	0
85	MG	5	3619	1/1	0.43	22.05	53,53,53,53	0
85	MG	c7	201	1/1	0.43	21.98	72,72,72,72	0
85	MG	1	3420	1/1	0.36	21.37	82,82,82,82	0
85	MG	5	3762	1/1	1.14	21.34	54,54,54,54	0
85	MG	6	2006	1/1	0.37	21.21	53,53,53,53	0
85	MG	5	3473	1/1	1.05	21.07	41,41,41,41	0
85	MG	1	3567	1/1	0.47	21.02	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	4	207	1/1	0.36	20.95	34,34,34,34	0
85	MG	5	3633	1/1	0.50	20.78	82,82,82,82	0
85	MG	N5	201	1/1	0.31	20.56	69,69,69,69	0
85	MG	5	3538	1/1	0.52	20.20	48,48,48,48	0
85	MG	6	1939	1/1	0.48	20.00	90,90,90,90	0
86	OHX	5	4234	7/7	0.29	19.90	165,165,165,165	0
85	MG	6	1920	1/1	0.38	19.67	43,43,43,43	0
85	MG	1	3714	1/1	1.07	19.63	45,45,45,45	0
85	MG	1	3866	1/1	1.25	19.55	70,70,70,70	0
85	MG	5	3739	1/1	0.29	19.35	65,65,65,65	0
85	MG	1	3470	1/1	0.33	19.33	54,54,54,54	0
85	MG	1	3534	1/1	0.81	18.95	38,38,38,38	0
85	MG	6	1918	1/1	0.47	18.94	41,41,41,41	0
85	MG	5	3467	1/1	0.42	18.92	87,87,87,87	0
85	MG	1	3670	1/1	0.28	18.17	41,41,41,41	0
86	OHX	1	4195	7/7	0.48	17.77	145,145,145,145	0
85	MG	5	3483	1/1	0.44	17.22	58,58,58,58	0
85	MG	3	201	1/1	0.39	17.06	73,73,73,73	0
85	MG	5	3753	1/1	0.37	16.97	52,52,52,52	0
85	MG	1	3802	1/1	0.86	16.94	46,46,46,46	0
86	OHX	5	4226	7/7	0.42	16.76	132,132,132,132	0
85	MG	1	3700	1/1	0.33	16.59	51,51,51,51	0
85	MG	1	3728	1/1	0.53	16.22	52,52,52,52	0
85	MG	5	3676	1/1	0.36	16.12	76,76,76,76	0
85	MG	4	201	1/1	0.40	15.96	49,49,49,49	0
85	MG	1	3864	1/1	0.87	15.93	81,81,81,81	0
85	MG	2	2011	1/1	0.36	15.86	58,58,58,58	0
85	MG	5	3709	1/1	0.39	15.83	48,48,48,48	0
85	MG	5	3778	1/1	0.38	15.80	71,71,71,71	0
85	MG	5	3805	1/1	0.24	15.67	155,155,155,155	0
85	MG	6	1944	1/1	0.47	15.61	37,37,37,37	0
85	MG	5	3875	1/1	0.54	15.26	40,40,40,40	0
85	MG	5	3794	1/1	0.63	15.26	49,49,49,49	0
85	MG	1	3781	1/1	0.49	15.25	59,59,59,59	0
85	MG	5	3771	1/1	0.71	15.23	106,106,106,106	0
85	MG	3	213	1/1	0.37	14.98	61,61,61,61	0
85	MG	6	1959	1/1	0.37	14.97	44,44,44,44	0
86	OHX	1	4182	7/7	0.50	14.93	130,130,130,130	0
85	MG	3	212	1/1	0.38	14.92	57,57,57,57	0
85	MG	5	3881	1/1	0.39	14.90	49,49,49,49	0
85	MG	1	3827	1/1	0.57	14.83	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	4	223	1/1	0.37	14.55	64,64,64,64	0
85	MG	2	1951	1/1	0.41	14.51	99,99,99,99	0
85	MG	5	3451	1/1	0.38	14.38	57,57,57,57	0
85	MG	q3	502	1/1	0.33	14.16	62,62,62,62	0
85	MG	5	3870	1/1	0.45	14.15	43,43,43,43	0
85	MG	8	204	1/1	0.34	13.89	53,53,53,53	0
85	MG	5	3562	1/1	0.35	13.63	30,30,30,30	0
85	MG	7	203	1/1	0.35	13.49	58,58,58,58	0
85	MG	5	3534	1/1	0.37	13.43	35,35,35,35	0
85	MG	1	3651	1/1	0.96	13.37	51,51,51,51	0
85	MG	5	3846	1/1	0.55	13.36	38,38,38,38	0
85	MG	5	3686	1/1	1.09	13.34	36,36,36,36	0
85	MG	6	1953	1/1	0.41	13.28	51,51,51,51	0
85	MG	2	1902	1/1	0.28	13.16	48,48,48,48	0
85	MG	7	205	1/1	0.37	13.09	28,28,28,28	0
85	MG	1	3507	1/1	0.39	13.07	35,35,35,35	0
85	MG	5	3784	1/1	0.73	12.95	62,62,62,62	0
85	MG	1	3848	1/1	0.42	12.84	59,59,59,59	0
85	MG	5	3403	1/1	0.38	12.84	49,49,49,49	0
85	MG	5	3577	1/1	0.40	12.51	57,57,57,57	0
85	MG	1	3485	1/1	0.61	12.20	46,46,46,46	0
85	MG	1	3823	1/1	0.34	12.17	47,47,47,47	0
85	MG	4	220	1/1	0.51	12.14	40,40,40,40	0
85	MG	1	3804	1/1	0.45	12.12	56,56,56,56	0
85	MG	1	3825	1/1	0.65	12.10	121,121,121,121	0
85	MG	5	3440	1/1	0.43	12.09	62,62,62,62	0
85	MG	1	3402	1/1	0.49	12.07	55,55,55,55	0
85	MG	1	3807	1/1	0.31	11.95	63,63,63,63	0
85	MG	1	3814	1/1	0.63	11.90	44,44,44,44	0
85	MG	5	3624	1/1	0.47	11.77	58,58,58,58	0
85	MG	5	3615	1/1	0.28	11.77	41,41,41,41	0
85	MG	7	201	1/1	0.52	11.71	42,42,42,42	0
85	MG	6	2045	1/1	0.35	11.69	79,79,79,79	0
85	MG	5	3815	1/1	0.30	11.43	64,64,64,64	0
85	MG	2	1935	1/1	0.37	11.40	55,55,55,55	0
85	MG	3	202	1/1	0.35	11.39	51,51,51,51	0
85	MG	5	3849	1/1	0.48	11.34	61,61,61,61	0
85	MG	1	3653	1/1	0.53	11.31	101,101,101,101	0
85	MG	2	1944	1/1	0.27	11.27	69,69,69,69	0
85	MG	1	3822	1/1	0.27	11.21	50,50,50,50	0
85	MG	5	3597	1/1	0.42	11.17	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3445	1/1	0.39	11.11	63,63,63,63	0
85	MG	5	3777	1/1	0.63	11.06	32,32,32,32	0
85	MG	2	1938	1/1	0.41	10.94	72,72,72,72	0
85	MG	1	3671	1/1	0.29	10.92	80,80,80,80	0
85	MG	2	2017	1/1	0.40	10.91	80,80,80,80	0
85	MG	6	1991	1/1	0.27	10.91	55,55,55,55	0
85	MG	2	1972	1/1	0.42	10.90	72,72,72,72	0
86	OHX	1	4183	7/7	0.34	10.86	159,159,159,159	0
85	MG	1	3675	1/1	0.33	10.75	43,43,43,43	0
85	MG	5	3583	1/1	0.40	10.68	49,49,49,49	0
85	MG	1	3649	1/1	0.34	10.67	53,53,53,53	0
85	MG	5	3563	1/1	0.36	10.50	27,27,27,27	0
85	MG	1	3538	1/1	0.38	10.47	35,35,35,35	0
85	MG	5	3421	1/1	0.21	10.43	96,96,96,96	0
85	MG	2	1923	1/1	0.37	10.42	61,61,61,61	0
85	MG	5	3495	1/1	0.26	10.40	45,45,45,45	0
85	MG	5	3759	1/1	0.32	10.28	62,62,62,62	0
85	MG	6	2005	1/1	0.26	10.14	59,59,59,59	0
85	MG	1	3536	1/1	0.40	10.09	48,48,48,48	0
85	MG	1	3414	1/1	0.39	9.97	57,57,57,57	0
85	MG	6	2013	1/1	0.62	9.79	150,150,150,150	0
85	MG	1	3547	1/1	0.27	9.75	66,66,66,66	0
85	MG	1	3858	1/1	0.26	9.64	45,45,45,45	0
85	MG	6	1971	1/1	0.32	9.57	52,52,52,52	0
85	MG	13	402	1/1	1.04	9.44	31,31,31,31	0
85	MG	1	3742	1/1	0.36	9.37	70,70,70,70	0
85	MG	2	1985	1/1	0.45	9.31	106,106,106,106	0
85	MG	5	3607	1/1	0.28	9.28	45,45,45,45	0
85	MG	15	301	1/1	0.41	9.19	65,65,65,65	0
85	MG	5	3764	1/1	0.29	9.19	44,44,44,44	0
85	MG	5	3521	1/1	0.35	9.15	34,34,34,34	0
85	MG	4	221	1/1	0.32	9.14	53,53,53,53	0
85	MG	1	3730	1/1	0.54	9.02	64,64,64,64	0
85	MG	6	1924	1/1	0.37	8.94	38,38,38,38	0
85	MG	1	3539	1/1	0.39	8.94	41,41,41,41	0
85	MG	8	212	1/1	1.18	8.93	43,43,43,43	0
85	MG	5	3636	1/1	0.43	8.93	79,79,79,79	0
85	MG	1	3636	1/1	0.41	8.88	80,80,80,80	0
85	MG	3	205	1/1	0.31	8.78	45,45,45,45	0
85	MG	1	3813	1/1	0.66	8.78	39,39,39,39	0
85	MG	6	1993	1/1	0.36	8.78	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3599	1/1	0.39	8.75	23,23,23,23	0
85	MG	6	1933	1/1	0.33	8.69	77,77,77,77	0
85	MG	1	3752	1/1	0.26	8.67	61,61,61,61	0
85	MG	L7	302	1/1	0.68	8.62	51,51,51,51	0
85	MG	6	2030	1/1	0.39	8.61	74,74,74,74	0
85	MG	6	2028	1/1	0.51	8.60	83,83,83,83	0
85	MG	5	3690	1/1	0.32	8.55	43,43,43,43	0
85	MG	5	3705	1/1	0.21	8.52	67,67,67,67	0
85	MG	2	1983	1/1	0.51	8.50	63,63,63,63	0
85	MG	5	3732	1/1	0.21	8.50	45,45,45,45	0
85	MG	1	3768	1/1	0.76	8.49	52,52,52,52	0
85	MG	N8	203	1/1	0.97	8.45	43,43,43,43	0
85	MG	5	3834	1/1	0.35	8.33	42,42,42,42	0
85	MG	1	3452	1/1	0.34	8.25	44,44,44,44	0
85	MG	5	3432	1/1	0.42	8.22	44,44,44,44	0
86	OHX	6	2184	7/7	0.40	8.20	147,147,147,147	0
85	MG	2	1993	1/1	0.41	8.17	114,114,114,114	0
85	MG	l3	403	1/1	0.88	8.16	36,36,36,36	0
85	MG	1	3791	1/1	1.12	8.13	42,42,42,42	0
85	MG	1	3448	1/1	0.34	8.02	44,44,44,44	0
85	MG	5	3695	1/1	0.33	7.92	55,55,55,55	0
85	MG	5	3649	1/1	0.38	7.89	38,38,38,38	0
85	MG	5	3865	1/1	0.30	7.80	58,58,58,58	0
85	MG	1	3840	1/1	0.35	7.79	49,49,49,49	0
85	MG	7	206	1/1	0.61	7.77	48,48,48,48	0
85	MG	5	3433	1/1	0.33	7.77	43,43,43,43	0
85	MG	5	3675	1/1	0.56	7.74	31,31,31,31	0
85	MG	1	3656	1/1	0.84	7.71	35,35,35,35	0
85	MG	5	3532	1/1	0.37	7.69	23,23,23,23	0
85	MG	o3	202	1/1	0.95	7.57	37,37,37,37	0
85	MG	8	214	1/1	0.39	7.55	57,57,57,57	0
85	MG	6	1901	1/1	0.34	7.53	44,44,44,44	0
85	MG	2	1958	1/1	0.46	7.51	101,101,101,101	0
85	MG	1	3525	1/1	0.52	7.51	43,43,43,43	0
85	MG	5	3743	1/1	0.30	7.46	36,36,36,36	0
86	OHX	5	4184	7/7	0.50	7.45	124,124,124,124	0
85	MG	L7	303	1/1	0.37	7.41	46,46,46,46	0
85	MG	2	1995	1/1	0.35	7.39	92,92,92,92	0
85	MG	1	3486	1/1	0.40	7.38	44,44,44,44	0
85	MG	1	3410	1/1	0.32	7.34	27,27,27,27	0
86	OHX	1	4217	7/7	0.52	7.27	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3705	1/1	0.41	7.23	44,44,44,44	0
85	MG	6	1950	1/1	0.36	7.21	72,72,72,72	0
85	MG	1	3612	1/1	0.25	7.10	45,45,45,45	0
86	OHX	1	4022	7/7	0.22	7.06	159,159,159,159	0
85	MG	1	3756	1/1	0.33	7.05	47,47,47,47	0
85	MG	2	1945	1/1	0.29	7.04	84,84,84,84	0
85	MG	1	3863	1/1	0.34	7.01	46,46,46,46	0
85	MG	5	3444	1/1	0.28	7.00	39,39,39,39	0
85	MG	2	1981	1/1	0.26	6.95	77,77,77,77	0
85	MG	6	1915	1/1	0.43	6.92	62,62,62,62	0
85	MG	5	3506	1/1	0.35	6.91	46,46,46,46	0
85	MG	5	3813	1/1	0.25	6.90	88,88,88,88	0
85	MG	1	3431	1/1	0.31	6.89	52,52,52,52	0
86	OHX	2	2158	7/7	0.29	6.89	167,167,167,167	0
85	MG	2	1916	1/1	0.28	6.87	51,51,51,51	0
85	MG	5	3664	1/1	0.32	6.81	36,36,36,36	0
86	OHX	1	4144	7/7	0.47	6.80	123,123,123,123	0
85	MG	17	301	1/1	0.38	6.76	39,39,39,39	0
85	MG	5	3648	1/1	0.50	6.74	54,54,54,54	0
85	MG	5	3435	1/1	0.34	6.72	75,75,75,75	0
85	MG	d3	202	1/1	0.99	6.68	55,55,55,55	0
85	MG	5	3514	1/1	0.29	6.66	57,57,57,57	0
85	MG	1	3796	1/1	1.01	6.64	29,29,29,29	0
85	MG	1	3665	1/1	0.57	6.63	50,50,50,50	0
85	MG	1	3849	1/1	0.37	6.62	50,50,50,50	0
85	MG	6	1927	1/1	0.40	6.56	71,71,71,71	0
85	MG	1	3476	1/1	0.31	6.56	85,85,85,85	0
85	MG	6	1983	1/1	0.44	6.55	84,84,84,84	0
85	MG	5	3774	1/1	1.02	6.54	36,36,36,36	0
85	MG	1	3865	1/1	0.30	6.53	47,47,47,47	0
86	OHX	1	4213	7/7	0.49	6.49	134,134,134,134	0
85	MG	6	1952	1/1	0.41	6.46	60,60,60,60	0
85	MG	2	2014	1/1	0.39	6.44	52,52,52,52	0
85	MG	1	3745	1/1	0.35	6.44	63,63,63,63	0
85	MG	3	206	1/1	0.33	6.42	34,34,34,34	0
85	MG	1	3503	1/1	0.45	6.38	45,45,45,45	0
85	MG	5	3554	1/1	0.33	6.33	43,43,43,43	0
85	MG	5	3829	1/1	0.30	6.28	54,54,54,54	0
85	MG	2	1973	1/1	0.35	6.27	74,74,74,74	0
86	OHX	2	2142	7/7	0.37	6.27	134,134,134,134	0
85	MG	6	1966	1/1	0.42	6.23	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3595	1/1	0.32	6.16	40,40,40,40	0
85	MG	5	3572	1/1	0.35	6.16	30,30,30,30	0
85	MG	2	1968	1/1	0.36	6.14	83,83,83,83	0
85	MG	7	207	1/1	0.23	6.10	61,61,61,61	0
85	MG	6	1974	1/1	0.25	6.09	73,73,73,73	0
85	MG	5	3654	1/1	0.48	6.07	72,72,72,72	0
86	OHX	15	306	7/7	0.33	6.05	153,153,153,153	0
85	MG	2	1921	1/1	0.41	6.02	55,55,55,55	0
85	MG	5	3647	1/1	0.37	6.01	43,43,43,43	0
85	MG	1	3844	1/1	0.33	6.00	37,37,37,37	0
85	MG	2	1914	1/1	0.37	6.00	71,71,71,71	0
85	MG	2	1956	1/1	0.33	6.00	63,63,63,63	0
85	MG	1	3466	1/1	0.33	5.96	48,48,48,48	0
85	MG	6	1967	1/1	0.34	5.95	71,71,71,71	0
85	MG	5	3876	1/1	0.29	5.91	46,46,46,46	0
86	OHX	2	2032	7/7	0.24	5.88	111,111,111,111	0
85	MG	1	3557	1/1	0.38	5.87	39,39,39,39	0
85	MG	5	3685	1/1	0.44	5.86	35,35,35,35	0
85	MG	5	3736	1/1	0.34	5.84	47,47,47,47	0
85	MG	5	3769	1/1	0.36	5.81	44,44,44,44	0
85	MG	5	3772	1/1	0.35	5.79	68,68,68,68	0
85	MG	5	3795	1/1	0.30	5.79	63,63,63,63	0
85	MG	5	3889	1/1	0.46	5.77	38,38,38,38	0
85	MG	5	3542	1/1	0.35	5.74	30,30,30,30	0
85	MG	2	1991	1/1	0.66	5.74	65,65,65,65	0
85	MG	1	3654	1/1	0.35	5.73	70,70,70,70	0
85	MG	1	3494	1/1	0.30	5.71	79,79,79,79	0
85	MG	1	3522	1/1	0.33	5.71	77,77,77,77	0
85	MG	1	3738	1/1	0.35	5.59	65,65,65,65	0
85	MG	1	3748	1/1	0.48	5.56	48,48,48,48	0
85	MG	2	1913	1/1	0.44	5.53	84,84,84,84	0
85	MG	1	3716	1/1	0.68	5.49	54,54,54,54	0
85	MG	1	3537	1/1	0.34	5.47	45,45,45,45	0
85	MG	6	1988	1/1	0.26	5.44	73,73,73,73	0
85	MG	5	3712	1/1	0.25	5.43	89,89,89,89	0
85	MG	5	3887	1/1	0.33	5.43	64,64,64,64	0
85	MG	5	3640	1/1	0.32	5.42	62,62,62,62	0
86	OHX	6	2205	7/7	0.36	5.42	157,157,157,157	0
85	MG	5	3896	1/1	0.37	5.42	87,87,87,87	0
85	MG	5	3543	1/1	0.35	5.41	35,35,35,35	0
85	MG	5	3468	1/1	0.29	5.39	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	2	1926	1/1	0.41	5.38	99,99,99,99	0
85	MG	1	3510	1/1	0.31	5.37	53,53,53,53	0
85	MG	6	1932	1/1	0.28	5.33	63,63,63,63	0
85	MG	5	3508	1/1	0.35	5.29	37,37,37,37	0
85	MG	1	3624	1/1	0.29	5.26	58,58,58,58	0
85	MG	2	1999	1/1	0.27	5.24	83,83,83,83	0
85	MG	5	3683	1/1	0.31	5.22	42,42,42,42	0
85	MG	6	2043	1/1	0.23	5.17	54,54,54,54	0
85	MG	2	1918	1/1	0.46	5.16	55,55,55,55	0
85	MG	2	2005	1/1	0.43	5.14	78,78,78,78	0
85	MG	5	3731	1/1	0.23	5.08	53,53,53,53	0
85	MG	1	3855	1/1	0.29	5.08	53,53,53,53	0
85	MG	4	222	1/1	0.44	5.07	76,76,76,76	0
85	MG	1	3572	1/1	0.32	5.05	46,46,46,46	0
85	MG	1	3683	1/1	0.53	5.02	67,67,67,67	0
85	MG	1	3867	1/1	0.37	4.97	56,56,56,56	0
85	MG	6	1930	1/1	0.44	4.97	61,61,61,61	0
85	MG	5	3735	1/1	0.25	4.95	69,69,69,69	0
85	MG	1	3737	1/1	0.31	4.93	83,83,83,83	0
85	MG	5	3752	1/1	0.41	4.89	44,44,44,44	0
85	MG	8	207	1/1	0.19	4.88	70,70,70,70	0
85	MG	5	3488	1/1	0.35	4.86	55,55,55,55	0
85	MG	1	3616	1/1	0.56	4.82	46,46,46,46	0
85	MG	1	3680	1/1	0.26	4.82	51,51,51,51	0
85	MG	2	2009	1/1	0.29	4.78	66,66,66,66	0
85	MG	5	3586	1/1	0.40	4.77	28,28,28,28	0
85	MG	1	3706	1/1	0.54	4.76	53,53,53,53	0
85	MG	4	211	1/1	0.71	4.75	54,54,54,54	0
85	MG	5	3873	1/1	0.33	4.74	48,48,48,48	0
85	MG	5	3720	1/1	0.39	4.73	61,61,61,61	0
85	MG	6	1921	1/1	0.40	4.71	55,55,55,55	0
85	MG	6	1946	1/1	0.44	4.69	53,53,53,53	0
85	MG	6	1981	1/1	0.34	4.66	58,58,58,58	0
85	MG	2	1905	1/1	0.45	4.66	66,66,66,66	0
85	MG	5	3780	1/1	0.42	4.64	54,54,54,54	0
85	MG	2	1976	1/1	0.34	4.63	93,93,93,93	0
85	MG	M9	201	1/1	0.59	4.62	67,67,67,67	0
85	MG	1	3544	1/1	0.33	4.60	38,38,38,38	0
85	MG	1	3850	1/1	0.28	4.56	60,60,60,60	0
85	MG	1	3795	1/1	0.36	4.55	38,38,38,38	0
85	MG	5	3491	1/1	0.32	4.55	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	1	3805	1/1	0.39	4.54	35,35,35,35	0
85	MG	6	1984	1/1	0.58	4.54	49,49,49,49	0
86	OHX	1	4201	7/7	0.25	4.48	147,147,147,147	0
85	MG	2	2002	1/1	0.36	4.48	85,85,85,85	0
86	OHX	2	2147	7/7	0.42	4.42	127,127,127,127	0
85	MG	5	3526	1/1	0.32	4.40	30,30,30,30	0
85	MG	5	3581	1/1	0.28	4.39	34,34,34,34	0
85	MG	5	3450	1/1	0.24	4.38	61,61,61,61	0
85	MG	1	3464	1/1	0.36	4.37	28,28,28,28	0
85	MG	2	1970	1/1	0.34	4.35	71,71,71,71	0
85	MG	4	203	1/1	0.34	4.35	52,52,52,52	0
85	MG	2	1977	1/1	0.37	4.34	101,101,101,101	0
86	OHX	1	4146	7/7	0.24	4.34	151,151,151,151	0
85	MG	1	3413	1/1	0.30	4.33	42,42,42,42	0
85	MG	6	1941	1/1	0.45	4.29	34,34,34,34	0
86	OHX	5	4150	7/7	0.49	4.27	120,120,120,120	0
85	MG	1	3780	1/1	0.46	4.26	58,58,58,58	0
85	MG	1	3709	1/1	0.25	4.25	61,61,61,61	0
85	MG	m4	201	1/1	0.36	4.23	46,46,46,46	0
85	MG	1	3633	1/1	0.65	4.17	37,37,37,37	0
85	MG	5	3476	1/1	0.37	4.16	81,81,81,81	0
86	OHX	1	4067	7/7	0.25	4.13	136,136,136,136	0
85	MG	5	3840	1/1	0.27	4.12	78,78,78,78	0
85	MG	N8	201	1/1	0.35	4.11	33,33,33,33	0
85	MG	2	1964	1/1	0.39	4.11	63,63,63,63	0
86	OHX	6	2052	7/7	0.24	4.10	79,79,79,79	0
85	MG	5	3716	1/1	0.28	4.09	56,56,56,56	0
85	MG	6	1979	1/1	0.32	4.06	72,72,72,72	0
85	MG	5	3821	1/1	0.35	4.05	45,45,45,45	0
85	MG	5	3580	1/1	0.30	4.03	35,35,35,35	0
85	MG	6	1916	1/1	0.32	4.02	55,55,55,55	0
85	MG	5	3888	1/1	0.27	4.01	45,45,45,45	0
85	MG	5	3659	1/1	0.23	4.00	46,46,46,46	0
85	MG	1	3576	1/1	0.32	3.98	21,21,21,21	0
85	MG	6	1964	1/1	0.45	3.94	73,73,73,73	0
86	OHX	1	4219	7/7	0.42	3.83	140,140,140,140	0
85	MG	1	3778	1/1	0.29	3.80	59,59,59,59	0
86	OHX	6	2187	7/7	0.32	3.79	156,156,156,156	0
85	MG	5	3892	1/1	0.23	3.78	69,69,69,69	0
85	MG	5	3684	1/1	0.45	3.76	78,78,78,78	0
86	OHX	5	4218	7/7	0.23	3.76	150,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3527	1/1	0.46	3.76	49,49,49,49	0
85	MG	1	3514	1/1	0.41	3.71	26,26,26,26	0
85	MG	3	203	1/1	0.29	3.69	94,94,94,94	0
86	OHX	1	3872	7/7	0.25	3.68	47,47,47,47	0
85	MG	5	3700	1/1	0.30	3.68	48,48,48,48	0
85	MG	1	3465	1/1	0.29	3.67	41,41,41,41	0
86	OHX	5	4229	7/7	0.31	3.65	130,130,130,130	0
85	MG	1	3589	1/1	0.28	3.62	34,34,34,34	0
85	MG	1	3530	1/1	0.32	3.62	34,34,34,34	0
86	OHX	5	3900	7/7	0.25	3.62	49,49,49,49	0
85	MG	1	3767	1/1	0.34	3.61	50,50,50,50	0
85	MG	5	3599	1/1	0.43	3.59	30,30,30,30	0
86	OHX	1	4117	7/7	0.49	3.57	123,123,123,123	0
86	OHX	1	4130	7/7	0.40	3.55	128,128,128,128	0
85	MG	1	3800	1/1	0.82	3.52	32,32,32,32	0
85	MG	2	1980	1/1	0.29	3.52	56,56,56,56	0
85	MG	6	1911	1/1	0.36	3.51	87,87,87,87	0
85	MG	5	3827	1/1	0.73	3.50	40,40,40,40	0
85	MG	5	3547	1/1	0.37	3.49	55,55,55,55	0
85	MG	2	1915	1/1	0.34	3.49	74,74,74,74	0
85	MG	4	202	1/1	0.39	3.48	49,49,49,49	0
85	MG	1	3563	1/1	0.33	3.46	27,27,27,27	0
85	MG	6	1948	1/1	0.41	3.42	52,52,52,52	0
85	MG	1	3498	1/1	0.27	3.42	44,44,44,44	0
85	MG	4	216	1/1	0.75	3.41	48,48,48,48	0
85	MG	1	3615	1/1	0.30	3.38	40,40,40,40	0
85	MG	1	3655	1/1	0.28	3.35	47,47,47,47	0
85	MG	2	1946	1/1	0.28	3.31	65,65,65,65	0
86	OHX	1	4190	7/7	0.21	3.30	143,143,143,143	0
85	MG	5	3787	1/1	0.33	3.29	87,87,87,87	0
85	MG	5	3601	1/1	0.26	3.27	47,47,47,47	0
86	OHX	5	4172	7/7	0.30	3.24	149,149,149,149	0
85	MG	6	1996	1/1	0.27	3.23	57,57,57,57	0
85	MG	M7	204	1/1	0.87	3.23	38,38,38,38	0
85	MG	6	1947	1/1	0.36	3.22	44,44,44,44	0
85	MG	5	3446	1/1	0.29	3.22	35,35,35,35	0
85	MG	1	3762	1/1	0.68	3.22	36,36,36,36	0
86	OHX	2	2171	7/7	0.41	3.21	157,157,157,157	0
86	OHX	8	228	7/7	0.25	3.20	136,136,136,136	0
85	MG	1	3681	1/1	0.26	3.19	42,42,42,42	0
85	MG	1	3455	1/1	0.30	3.19	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3902	7/7	0.25	3.13	84,84,84,84	0
85	MG	5	3505	1/1	0.35	3.12	34,34,34,34	0
85	MG	1	3668	1/1	0.34	3.12	75,75,75,75	0
85	MG	1	3592	1/1	0.32	3.12	55,55,55,55	0
86	OHX	6	2054	7/7	0.24	3.11	87,87,87,87	0
85	MG	2	2006	1/1	0.36	3.10	52,52,52,52	0
85	MG	5	3708	1/1	0.29	3.10	52,52,52,52	0
86	OHX	5	4085	7/7	0.43	3.09	119,119,119,119	0
86	OHX	6	2181	7/7	0.42	3.08	141,141,141,141	0
85	MG	5	3539	1/1	0.32	3.04	35,35,35,35	0
85	MG	5	3464	1/1	0.33	3.03	54,54,54,54	0
85	MG	8	205	1/1	0.36	3.03	41,41,41,41	0
85	MG	2	1934	1/1	0.41	3.02	61,61,61,61	0
85	MG	2	1931	1/1	0.38	3.02	62,62,62,62	0
86	OHX	5	4216	7/7	0.35	3.02	143,143,143,143	0
85	MG	8	208	1/1	0.52	3.01	55,55,55,55	0
85	MG	6	2038	1/1	0.28	3.00	59,59,59,59	0
85	MG	5	3744	1/1	0.26	3.00	36,36,36,36	0
86	OHX	5	3906	7/7	0.23	3.00	60,60,60,60	0
85	MG	5	3574	1/1	0.29	2.99	33,33,33,33	0
85	MG	5	3481	1/1	0.34	2.97	61,61,61,61	0
86	OHX	5	3930	7/7	0.19	2.93	89,89,89,89	0
86	OHX	6	2065	7/7	0.22	2.91	114,114,114,114	0
85	MG	1	3830	1/1	0.60	2.89	45,45,45,45	0
86	OHX	5	4203	7/7	0.49	2.88	152,152,152,152	0
86	OHX	5	3908	7/7	0.25	2.87	73,73,73,73	0
85	MG	1	3631	1/1	0.35	2.85	40,40,40,40	0
85	MG	1	3833	1/1	0.23	2.83	50,50,50,50	0
85	MG	6	2027	1/1	0.36	2.83	59,59,59,59	0
85	MG	2	1965	1/1	0.26	2.82	87,87,87,87	0
87	ZN	D7	101	1/1	0.23	2.82	167,167,167,167	0
86	OHX	1	4145	7/7	0.30	2.82	134,134,134,134	0
86	OHX	1	3899	7/7	0.22	2.81	77,77,77,77	0
85	MG	5	3823	1/1	0.24	2.80	65,65,65,65	0
85	MG	2	1963	1/1	0.26	2.80	99,99,99,99	0
85	MG	5	3609	1/1	0.27	2.77	33,33,33,33	0
85	MG	5	3414	1/1	0.31	2.76	31,31,31,31	0
85	MG	5	3646	1/1	0.31	2.76	50,50,50,50	0
85	MG	5	3711	1/1	0.49	2.75	46,46,46,46	0
85	MG	6	2000	1/1	0.42	2.73	77,77,77,77	0
86	OHX	5	4190	7/7	0.28	2.72	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	6	2160	7/7	0.28	2.70	138,138,138,138	0
85	MG	2	1919	1/1	0.46	2.70	71,71,71,71	0
86	OHX	1	4124	7/7	0.43	2.69	122,122,122,122	0
86	OHX	5	3912	7/7	0.24	2.68	68,68,68,68	0
85	MG	5	3807	1/1	0.28	2.67	97,97,97,97	0
85	MG	5	3576	1/1	0.34	2.66	33,33,33,33	0
86	OHX	M7	205	7/7	0.55	2.63	118,118,118,118	0
85	MG	5	3804	1/1	0.39	2.61	52,52,52,52	0
86	OHX	2	2029	7/7	0.21	2.59	101,101,101,101	0
85	MG	2	1937	1/1	0.38	2.59	63,63,63,63	0
85	MG	5	3405	1/1	0.25	2.59	32,32,32,32	0
85	MG	1	3661	1/1	0.28	2.58	48,48,48,48	0
85	MG	5	3803	1/1	0.20	2.57	65,65,65,65	0
86	OHX	5	4010	7/7	0.19	2.57	149,149,149,149	0
85	MG	1	3565	1/1	0.31	2.57	40,40,40,40	0
85	MG	2	1941	1/1	0.29	2.56	77,77,77,77	0
85	MG	5	3455	1/1	0.28	2.55	38,38,38,38	0
85	MG	2	1961	1/1	0.31	2.55	77,77,77,77	0
85	MG	5	3862	1/1	0.47	2.55	45,45,45,45	0
85	MG	1	3761	1/1	0.28	2.52	51,51,51,51	0
85	MG	5	3734	1/1	0.32	2.50	45,45,45,45	0
85	MG	6	2034	1/1	0.41	2.49	87,87,87,87	0
85	MG	1	3688	1/1	0.41	2.49	41,41,41,41	0
85	MG	1	3524	1/1	0.26	2.48	27,27,27,27	0
85	MG	L7	301	1/1	0.25	2.47	40,40,40,40	0
85	MG	1	3629	1/1	0.40	2.45	47,47,47,47	0
85	MG	1	3853	1/1	0.23	2.44	56,56,56,56	0
85	MG	1	3726	1/1	0.32	2.44	64,64,64,64	0
85	MG	2	1929	1/1	0.34	2.44	69,69,69,69	0
85	MG	5	3533	1/1	0.31	2.42	39,39,39,39	0
86	OHX	5	4157	7/7	0.39	2.41	134,134,134,134	0
85	MG	5	3571	1/1	0.36	2.41	35,35,35,35	0
85	MG	5	3565	1/1	0.30	2.40	32,32,32,32	0
85	MG	1	3727	1/1	0.38	2.39	57,57,57,57	0
85	MG	1	3694	1/1	0.58	2.38	41,41,41,41	0
85	MG	5	3480	1/1	0.33	2.38	67,67,67,67	0
85	MG	1	3831	1/1	0.20	2.36	59,59,59,59	0
85	MG	7	204	1/1	0.29	2.35	68,68,68,68	0
85	MG	N3	201	1/1	0.30	2.35	37,37,37,37	0
86	OHX	5	4175	7/7	0.44	2.35	119,119,119,119	0
85	MG	5	3608	1/1	0.28	2.35	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	2	1989	1/1	0.25	2.34	105,105,105,105	0
85	MG	5	3631	1/1	0.43	2.33	42,42,42,42	0
85	MG	5	3710	1/1	0.29	2.31	77,77,77,77	0
85	MG	5	3551	1/1	0.34	2.31	51,51,51,51	0
85	MG	5	3671	1/1	0.40	2.30	31,31,31,31	0
85	MG	1	3824	1/1	0.22	2.30	53,53,53,53	0
85	MG	2	1912	1/1	0.24	2.27	68,68,68,68	0
86	OHX	1	4147	7/7	0.27	2.27	133,133,133,133	0
85	MG	1	3588	1/1	0.29	2.26	28,28,28,28	0
85	MG	5	3499	1/1	0.33	2.25	56,56,56,56	0
85	MG	5	3791	1/1	0.32	2.24	56,56,56,56	0
85	MG	M0	303	1/1	0.28	2.23	38,38,38,38	0
86	OHX	1	3894	7/7	0.24	2.22	82,82,82,82	0
85	MG	6	2008	1/1	0.24	2.21	57,57,57,57	0
85	MG	1	3447	1/1	0.54	2.17	45,45,45,45	0
85	MG	5	3713	1/1	0.36	2.17	43,43,43,43	0
86	OHX	1	3909	7/7	0.20	2.15	81,81,81,81	0
85	MG	6	1908	1/1	0.22	2.13	50,50,50,50	0
85	MG	5	3850	1/1	0.26	2.13	52,52,52,52	0
85	MG	5	3589	1/1	0.37	2.12	56,56,56,56	0
85	MG	5	3895	1/1	0.28	2.12	69,69,69,69	0
85	MG	5	3868	1/1	0.66	2.11	40,40,40,40	0
85	MG	1	3554	1/1	0.26	2.11	53,53,53,53	0
85	MG	l3	401	1/1	0.42	2.11	26,26,26,26	0
85	MG	m6	202	1/1	0.45	2.10	36,36,36,36	0
85	MG	5	3689	1/1	0.30	2.09	46,46,46,46	0
85	MG	5	3449	1/1	0.24	2.07	45,45,45,45	0
85	MG	5	3652	1/1	0.23	2.06	43,43,43,43	0
86	OHX	2	2172	7/7	0.30	2.05	157,157,157,157	0
85	MG	1	3690	1/1	0.21	2.03	57,57,57,57	0
85	MG	1	3626	1/1	0.48	2.02	72,72,72,72	0
86	OHX	1	4194	7/7	0.21	1.99	140,140,140,140	0
85	MG	m7	205	1/1	0.58	1.99	38,38,38,38	0
86	OHX	1	3880	7/7	0.24	1.99	66,66,66,66	0
85	MG	6	1903	1/1	0.26	1.98	47,47,47,47	0
85	MG	5	3564	1/1	0.39	1.98	28,28,28,28	0
85	MG	6	1945	1/1	0.31	1.98	65,65,65,65	0
85	MG	1	3695	1/1	0.25	1.97	47,47,47,47	0
85	MG	5	3666	1/1	0.36	1.97	65,65,65,65	0
85	MG	5	3596	1/1	0.37	1.96	41,41,41,41	0
85	MG	6	1931	1/1	0.26	1.96	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3802	1/1	0.22	1.95	46,46,46,46	0
85	MG	5	3841	1/1	0.28	1.93	43,43,43,43	0
86	OHX	1	4099	7/7	0.27	1.92	135,135,135,135	0
85	MG	1	3815	1/1	0.56	1.92	193,193,193,193	0
86	OHX	1	4176	7/7	0.37	1.91	185,185,185,185	0
86	OHX	5	4178	7/7	0.27	1.91	142,142,142,142	0
85	MG	1	3516	1/1	0.34	1.90	39,39,39,39	0
85	MG	1	3696	1/1	0.29	1.90	50,50,50,50	0
86	OHX	1	4077	7/7	0.47	1.88	114,114,114,114	0
85	MG	1	3490	1/1	0.75	1.88	57,57,57,57	0
85	MG	5	3623	1/1	0.45	1.88	41,41,41,41	0
85	MG	5	3792	1/1	0.25	1.84	93,93,93,93	0
85	MG	5	3500	1/1	0.25	1.84	36,36,36,36	0
86	OHX	5	3937	7/7	0.25	1.83	91,91,91,91	0
86	OHX	1	4220	7/7	0.36	1.83	158,158,158,158	0
85	MG	6	1913	1/1	0.29	1.83	37,37,37,37	0
85	MG	1	3639	1/1	0.28	1.81	61,61,61,61	0
85	MG	4	206	1/1	0.30	1.80	32,32,32,32	0
85	MG	2	1925	1/1	0.30	1.80	67,67,67,67	0
85	MG	sM	302	1/1	0.45	1.79	50,50,50,50	0
85	MG	2	1907	1/1	0.32	1.78	62,62,62,62	0
86	OHX	C8	201	7/7	0.22	1.74	120,120,120,120	0
86	OHX	2	2134	7/7	0.38	1.73	142,142,142,142	0
85	MG	5	3519	1/1	0.32	1.73	27,27,27,27	0
85	MG	1	3540	1/1	0.30	1.73	26,26,26,26	0
85	MG	2	2007	1/1	0.34	1.71	51,51,51,51	0
85	MG	1	3432	1/1	0.33	1.70	54,54,54,54	0
85	MG	5	3725	1/1	0.30	1.70	41,41,41,41	0
85	MG	5	3727	1/1	0.36	1.69	58,58,58,58	0
85	MG	M3	203	1/1	0.41	1.65	35,35,35,35	0
85	MG	s1	301	1/1	0.31	1.65	75,75,75,75	0
85	MG	1	3618	1/1	0.35	1.65	57,57,57,57	0
85	MG	5	3796	1/1	0.28	1.64	60,60,60,60	0
86	OHX	M7	206	7/7	0.33	1.64	145,145,145,145	0
85	MG	6	1904	1/1	0.36	1.63	75,75,75,75	0
85	MG	6	2039	1/1	0.43	1.63	91,91,91,91	0
85	MG	O3	201	1/1	0.21	1.62	40,40,40,40	0
86	OHX	8	216	7/7	0.23	1.61	61,61,61,61	0
86	OHX	5	4148	7/7	0.35	1.59	126,126,126,126	0
86	OHX	5	4221	7/7	0.41	1.59	136,136,136,136	0
85	MG	1	3622	1/1	0.50	1.58	37,37,37,37	0
86	OHX	5	3898	7/7	0.24	1.57	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3853	1/1	0.24	1.56	56,56,56,56	0
86	OHX	4	233	7/7	0.37	1.56	119,119,119,119	0
85	MG	2	1959	1/1	0.33	1.55	63,63,63,63	0
85	MG	N3	202	1/1	0.31	1.55	68,68,68,68	0
85	MG	2	2015	1/1	0.40	1.54	74,74,74,74	0
85	MG	5	3757	1/1	0.21	1.52	62,62,62,62	0
86	OHX	5	4139	7/7	0.28	1.51	135,135,135,135	0
85	MG	6	1906	1/1	0.38	1.51	48,48,48,48	0
85	MG	n3	202	1/1	0.47	1.50	47,47,47,47	0
86	OHX	5	4244	7/7	0.32	1.50	147,147,147,147	0
86	OHX	2	2156	7/7	0.30	1.50	125,125,125,125	0
85	MG	1	3606	1/1	0.24	1.50	59,59,59,59	0
86	OHX	5	4246	7/7	0.24	1.49	158,158,158,158	0
85	MG	5	3418	1/1	0.31	1.49	27,27,27,27	0
85	MG	2	1986	1/1	0.61	1.48	79,79,79,79	0
85	MG	1	3422	1/1	0.26	1.48	38,38,38,38	0
85	MG	1	3497	1/1	0.30	1.48	34,34,34,34	0
85	MG	6	1955	1/1	0.31	1.47	46,46,46,46	0
86	OHX	1	4148	7/7	0.21	1.47	147,147,147,147	0
85	MG	6	1987	1/1	0.35	1.47	86,86,86,86	0
85	MG	1	3678	1/1	0.29	1.46	66,66,66,66	0
85	MG	1	3597	1/1	0.30	1.46	27,27,27,27	0
85	MG	5	3782	1/1	0.21	1.46	97,97,97,97	0
85	MG	2	1933	1/1	0.29	1.44	77,77,77,77	0
85	MG	1	3790	1/1	0.25	1.42	71,71,71,71	0
86	OHX	5	4192	7/7	0.34	1.41	140,140,140,140	0
85	MG	1	3673	1/1	0.22	1.40	50,50,50,50	0
85	MG	5	3893	1/1	0.19	1.39	125,125,125,125	0
85	MG	5	3673	1/1	0.36	1.39	35,35,35,35	0
85	MG	5	3569	1/1	0.25	1.38	28,28,28,28	0
86	OHX	5	4208	7/7	0.36	1.38	122,122,122,122	0
86	OHX	2	2163	7/7	0.28	1.37	154,154,154,154	0
85	MG	5	3770	1/1	0.52	1.37	52,52,52,52	0
85	MG	1	3773	1/1	0.31	1.37	65,65,65,65	0
86	OHX	5	4108	7/7	0.23	1.37	146,146,146,146	0
85	MG	5	3549	1/1	0.26	1.37	54,54,54,54	0
86	OHX	5	4151	7/7	0.35	1.37	131,131,131,131	0
86	OHX	5	3949	7/7	0.22	1.36	108,108,108,108	0
85	MG	4	205	1/1	0.24	1.36	43,43,43,43	0
86	OHX	5	3946	7/7	0.22	1.35	99,99,99,99	0
85	MG	1	3401	1/1	0.32	1.35	43,43,43,43	0
87	ZN	d7	101	1/1	0.44	1.35	161,161,161,161	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2156	7/7	0.27	1.35	181,181,181,181	0
85	MG	1	3723	1/1	0.30	1.34	60,60,60,60	0
85	MG	5	3880	1/1	0.27	1.33	39,39,39,39	0
85	MG	1	3443	1/1	0.28	1.32	30,30,30,30	0
85	MG	2	1967	1/1	0.49	1.32	121,121,121,121	0
85	MG	5	3621	1/1	0.20	1.32	46,46,46,46	0
85	MG	1	3786	1/1	0.18	1.31	48,48,48,48	0
86	OHX	4	237	7/7	0.29	1.30	150,150,150,150	0
86	OHX	1	3878	7/7	0.23	1.30	60,60,60,60	0
85	MG	1	3715	1/1	0.34	1.29	61,61,61,61	0
85	MG	5	3517	1/1	0.28	1.29	32,32,32,32	0
85	MG	1	3652	1/1	0.24	1.28	70,70,70,70	0
85	MG	1	3717	1/1	0.26	1.28	85,85,85,85	0
85	MG	n3	201	1/1	0.30	1.27	27,27,27,27	0
86	OHX	5	4037	7/7	0.21	1.27	159,159,159,159	0
86	OHX	2	2027	7/7	0.20	1.26	97,97,97,97	0
85	MG	1	3406	1/1	0.47	1.26	105,105,105,105	0
85	MG	l8	301	1/1	0.28	1.26	70,70,70,70	0
85	MG	1	3722	1/1	0.33	1.26	38,38,38,38	0
85	MG	5	3417	1/1	0.21	1.25	30,30,30,30	0
85	MG	s8	301	1/1	0.35	1.24	53,53,53,53	0
86	OHX	5	4200	7/7	0.29	1.23	138,138,138,138	0
86	OHX	6	2190	7/7	0.28	1.22	147,147,147,147	0
85	MG	1	3603	1/1	0.43	1.22	36,36,36,36	0
85	MG	1	3517	1/1	0.36	1.22	43,43,43,43	0
85	MG	6	1917	1/1	0.28	1.21	69,69,69,69	0
86	OHX	1	4192	7/7	0.34	1.20	190,190,190,190	0
86	OHX	1	4205	7/7	0.24	1.20	133,133,133,133	0
86	OHX	5	4183	7/7	0.21	1.20	135,135,135,135	0
86	OHX	5	3938	7/7	0.23	1.20	89,89,89,89	0
85	MG	1	3746	1/1	0.23	1.19	47,47,47,47	0
86	OHX	5	3901	7/7	0.23	1.19	54,54,54,54	0
86	OHX	1	4083	7/7	0.27	1.19	128,128,128,128	0
85	MG	M1	201	1/1	0.32	1.18	74,74,74,74	0
85	MG	1	3430	1/1	0.31	1.18	49,49,49,49	0
85	MG	1	3428	1/1	0.23	1.17	42,42,42,42	0
85	MG	6	2020	1/1	0.25	1.16	89,89,89,89	0
86	OHX	5	3941	7/7	0.22	1.16	85,85,85,85	0
85	MG	1	3403	1/1	0.31	1.16	39,39,39,39	0
85	MG	5	3641	1/1	0.23	1.16	46,46,46,46	0
85	MG	1	3409	1/1	0.27	1.16	33,33,33,33	0
85	MG	1	3548	1/1	0.33	1.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4116	7/7	0.22	1.14	145,145,145,145	0
86	OHX	4	239	7/7	0.30	1.12	144,144,144,144	0
86	OHX	1	4210	7/7	0.22	1.12	139,139,139,139	0
85	MG	1	3650	1/1	0.45	1.11	32,32,32,32	0
86	OHX	1	4214	7/7	0.20	1.11	138,138,138,138	0
86	OHX	1	4175	7/7	0.30	1.11	167,167,167,167	0
86	OHX	1	4202	7/7	0.19	1.09	173,173,173,173	0
85	MG	6	1909	1/1	0.35	1.09	108,108,108,108	0
86	OHX	1	4177	7/7	0.33	1.08	148,148,148,148	0
85	MG	5	3750	1/1	0.24	1.05	51,51,51,51	0
85	MG	5	3544	1/1	0.24	1.04	29,29,29,29	0
85	MG	6	2036	1/1	0.19	1.03	68,68,68,68	0
86	OHX	5	3903	7/7	0.23	1.03	60,60,60,60	0
86	OHX	5	4245	7/7	0.26	1.03	139,139,139,139	0
85	MG	2	1955	1/1	0.38	1.01	56,56,56,56	0
85	MG	1	3691	1/1	0.40	1.01	41,41,41,41	0
86	OHX	5	4199	7/7	0.19	1.01	145,145,145,145	0
85	MG	1	3772	1/1	0.21	1.00	57,57,57,57	0
85	MG	6	2024	1/1	0.35	0.98	65,65,65,65	0
85	MG	1	3562	1/1	0.31	0.97	35,35,35,35	0
86	OHX	6	2179	7/7	0.30	0.96	147,147,147,147	0
86	OHX	1	3881	7/7	0.23	0.96	61,61,61,61	0
85	MG	6	1949	1/1	0.26	0.95	47,47,47,47	0
85	MG	1	3854	1/1	0.23	0.95	49,49,49,49	0
85	MG	5	3606	1/1	0.38	0.94	31,31,31,31	0
86	OHX	1	3903	7/7	0.23	0.93	82,82,82,82	0
85	MG	1	3607	1/1	0.29	0.92	51,51,51,51	0
86	OHX	1	4165	7/7	0.24	0.91	156,156,156,156	0
86	OHX	5	4146	7/7	0.25	0.91	132,132,132,132	0
85	MG	2	1910	1/1	0.26	0.90	57,57,57,57	0
86	OHX	6	2056	7/7	0.20	0.89	79,79,79,79	0
85	MG	5	3788	1/1	0.20	0.89	47,47,47,47	0
85	MG	5	3761	1/1	0.20	0.89	45,45,45,45	0
85	MG	5	3617	1/1	0.30	0.89	44,44,44,44	0
85	MG	2	1974	1/1	0.28	0.89	80,80,80,80	0
85	MG	5	3573	1/1	0.26	0.88	40,40,40,40	0
86	OHX	5	4219	7/7	0.24	0.87	173,173,173,173	0
86	OHX	1	3905	7/7	0.21	0.87	92,92,92,92	0
85	MG	5	3470	1/1	0.20	0.87	110,110,110,110	0
85	MG	5	3837	1/1	0.41	0.86	37,37,37,37	0
85	MG	2	1903	1/1	0.28	0.86	40,40,40,40	0
86	OHX	5	3899	7/7	0.24	0.86	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3644	1/1	0.18	0.85	49,49,49,49	0
85	MG	d3	201	1/1	0.31	0.85	55,55,55,55	0
86	OHX	1	3955	7/7	0.19	0.85	119,119,119,119	0
85	MG	19	201	1/1	0.25	0.83	43,43,43,43	0
85	MG	1	3871	1/1	0.23	0.83	69,69,69,69	0
86	OHX	6	2192	7/7	0.30	0.80	176,176,176,176	0
85	MG	1	3713	1/1	0.27	0.80	38,38,38,38	0
85	MG	5	3811	1/1	0.47	0.79	42,42,42,42	0
85	MG	5	3630	1/1	0.27	0.79	65,65,65,65	0
85	MG	4	212	1/1	0.25	0.77	57,57,57,57	0
85	MG	5	3611	1/1	0.24	0.77	33,33,33,33	0
85	MG	2	1936	1/1	0.25	0.77	56,56,56,56	0
86	OHX	5	4228	7/7	0.30	0.76	168,168,168,168	0
85	MG	2	1928	1/1	0.27	0.76	86,86,86,86	0
86	OHX	6	2165	7/7	0.22	0.75	156,156,156,156	0
86	OHX	1	4132	7/7	0.27	0.75	151,151,151,151	0
85	MG	6	1957	1/1	0.32	0.75	52,52,52,52	0
85	MG	6	1958	1/1	0.23	0.74	53,53,53,53	0
85	MG	5	3775	1/1	0.24	0.74	101,101,101,101	0
86	OHX	1	4174	7/7	0.22	0.74	126,126,126,126	0
85	MG	5	3412	1/1	0.33	0.74	36,36,36,36	0
85	MG	2	1978	1/1	0.28	0.73	60,60,60,60	0
85	MG	5	3525	1/1	0.27	0.73	37,37,37,37	0
86	OHX	1	3973	7/7	0.19	0.72	132,132,132,132	0
86	OHX	1	3873	7/7	0.24	0.71	53,53,53,53	0
85	MG	6	1965	1/1	0.25	0.71	86,86,86,86	0
85	MG	5	3830	1/1	0.20	0.71	76,76,76,76	0
86	OHX	2	2174	7/7	0.26	0.68	178,178,178,178	0
85	MG	5	3568	1/1	0.27	0.67	31,31,31,31	0
86	OHX	1	4123	7/7	0.31	0.67	138,138,138,138	0
86	OHX	1	3874	7/7	0.21	0.67	52,52,52,52	0
85	MG	5	3635	1/1	0.25	0.67	40,40,40,40	0
85	MG	5	3693	1/1	0.23	0.67	50,50,50,50	0
86	OHX	5	4136	7/7	0.29	0.66	134,134,134,134	0
86	OHX	6	2126	7/7	0.25	0.66	109,109,109,109	0
85	MG	6	2037	1/1	0.28	0.65	53,53,53,53	0
86	OHX	5	4110	7/7	0.38	0.65	111,111,111,111	0
86	OHX	m7	206	7/7	0.41	0.64	125,125,125,125	0
85	MG	2	1927	1/1	0.30	0.64	57,57,57,57	0
86	OHX	1	3876	7/7	0.25	0.64	63,63,63,63	0
86	OHX	6	2047	7/7	0.24	0.64	77,77,77,77	0
85	MG	1	3518	1/1	0.30	0.63	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3693	1/1	0.30	0.63	37,37,37,37	0
85	MG	d6	102	1/1	0.57	0.63	60,60,60,60	0
86	OHX	1	4203	7/7	0.26	0.62	149,149,149,149	0
85	MG	5	3501	1/1	0.27	0.62	40,40,40,40	0
85	MG	1	3787	1/1	0.20	0.61	56,56,56,56	0
86	OHX	4	225	7/7	0.22	0.60	66,66,66,66	0
86	OHX	1	3885	7/7	0.19	0.60	70,70,70,70	0
86	OHX	1	4198	7/7	0.18	0.59	158,158,158,158	0
86	OHX	6	2204	7/7	0.28	0.59	154,154,154,154	0
85	MG	1	3829	1/1	0.20	0.59	53,53,53,53	0
86	OHX	1	4208	7/7	0.31	0.58	150,150,150,150	0
86	OHX	2	2083	7/7	0.37	0.58	133,133,133,133	0
85	MG	1	3527	1/1	0.27	0.58	26,26,26,26	0
85	MG	6	1938	1/1	0.29	0.57	67,67,67,67	0
86	OHX	5	4169	7/7	0.24	0.57	109,109,109,109	0
85	MG	5	3612	1/1	0.42	0.57	38,38,38,38	0
85	MG	1	3725	1/1	0.28	0.57	47,47,47,47	0
86	OHX	6	2171	7/7	0.31	0.55	121,121,121,121	0
85	MG	5	3489	1/1	0.29	0.55	31,31,31,31	0
86	OHX	1	3875	7/7	0.26	0.54	57,57,57,57	0
85	MG	5	3498	1/1	0.27	0.54	34,34,34,34	0
85	MG	s2	301	1/1	0.37	0.53	55,55,55,55	0
86	OHX	1	4062	7/7	0.18	0.53	122,122,122,122	0
85	MG	5	3522	1/1	0.24	0.52	36,36,36,36	0
86	OHX	5	3916	7/7	0.21	0.51	67,67,67,67	0
86	OHX	2	2159	7/7	0.49	0.51	148,148,148,148	0
85	MG	L5	301	1/1	0.35	0.51	68,68,68,68	0
85	MG	N0	201	1/1	0.28	0.50	49,49,49,49	0
85	MG	5	3856	1/1	0.28	0.49	52,52,52,52	0
85	MG	5	3718	1/1	0.20	0.48	65,65,65,65	0
85	MG	1	3779	1/1	0.39	0.48	62,62,62,62	0
85	MG	q0	202	1/1	0.22	0.47	47,47,47,47	0
85	MG	6	2011	1/1	0.25	0.47	52,52,52,52	0
85	MG	5	3867	1/1	0.43	0.46	45,45,45,45	0
85	MG	S8	301	1/1	0.28	0.46	57,57,57,57	0
88	3K5	1	4221	57/57	0.30	0.45	44,44,44,44	0
85	MG	1	3701	1/1	0.19	0.45	64,64,64,64	0
85	MG	5	3656	1/1	0.31	0.45	43,43,43,43	0
85	MG	5	3824	1/1	0.32	0.45	47,47,47,47	0
85	MG	L3	403	1/1	0.23	0.44	40,40,40,40	0
86	OHX	5	3947	7/7	0.19	0.44	101,101,101,101	0
85	MG	5	3844	1/1	0.29	0.44	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	5	3492	1/1	0.38	0.44	48,48,48,48	0
85	MG	7	208	1/1	0.25	0.43	52,52,52,52	0
85	MG	2	1917	1/1	0.32	0.42	59,59,59,59	0
85	MG	s8	302	1/1	0.21	0.42	50,50,50,50	0
85	MG	2	1960	1/1	0.27	0.41	60,60,60,60	0
85	MG	5	3838	1/1	0.27	0.40	42,42,42,42	0
85	MG	6	1907	1/1	0.27	0.40	68,68,68,68	0
86	OHX	1	4216	7/7	0.24	0.40	146,146,146,146	0
86	OHX	2	2178	7/7	0.20	0.39	154,154,154,154	0
85	MG	1	3720	1/1	0.30	0.39	51,51,51,51	0
85	MG	1	3646	1/1	0.19	0.39	68,68,68,68	0
86	OHX	1	3886	7/7	0.22	0.39	66,66,66,66	0
85	MG	5	3413	1/1	0.29	0.39	43,43,43,43	0
86	OHX	2	2133	7/7	0.27	0.38	148,148,148,148	0
85	MG	1	3418	1/1	0.24	0.36	44,44,44,44	0
85	MG	6	1962	1/1	0.26	0.36	92,92,92,92	0
86	OHX	5	4232	7/7	0.32	0.36	162,162,162,162	0
86	OHX	2	2033	7/7	0.21	0.35	107,107,107,107	0
85	MG	5	3663	1/1	0.26	0.35	49,49,49,49	0
85	MG	6	2022	1/1	0.30	0.35	62,62,62,62	0
85	MG	o3	201	1/1	0.40	0.34	53,53,53,53	0
86	OHX	1	3941	7/7	0.20	0.34	108,108,108,108	0
85	MG	1	3594	1/1	0.26	0.33	30,30,30,30	0
85	MG	2	1998	1/1	0.36	0.33	74,74,74,74	0
86	OHX	2	2042	7/7	0.19	0.32	118,118,118,118	0
86	OHX	1	4166	7/7	0.24	0.32	170,170,170,170	0
85	MG	1	3679	1/1	0.22	0.31	48,48,48,48	0
85	MG	1	3541	1/1	0.19	0.31	60,60,60,60	0
86	OHX	1	3914	7/7	0.20	0.30	91,91,91,91	0
86	OHX	1	4185	7/7	0.38	0.30	143,143,143,143	0
86	OHX	5	3913	7/7	0.22	0.30	63,63,63,63	0
86	OHX	5	4079	7/7	0.29	0.29	113,113,113,113	0
88	3K5	5	4249	57/57	0.27	0.29	52,52,52,52	0
85	MG	1	3611	1/1	0.23	0.28	44,44,44,44	0
85	MG	6	1926	1/1	0.22	0.28	46,46,46,46	0
85	MG	5	3570	1/1	0.28	0.28	34,34,34,34	0
86	OHX	5	3964	7/7	0.19	0.28	105,105,105,105	0
85	MG	1	3619	1/1	0.26	0.27	51,51,51,51	0
85	MG	1	3736	1/1	0.25	0.25	63,63,63,63	0
86	OHX	6	2202	7/7	0.36	0.25	155,155,155,155	0
85	MG	1	3687	1/1	0.53	0.25	52,52,52,52	0
86	OHX	1	3924	7/7	0.19	0.24	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3567	1/1	0.33	0.24	48,48,48,48	0
85	MG	L8	301	1/1	0.25	0.24	50,50,50,50	0
86	OHX	5	4211	7/7	0.28	0.22	130,130,130,130	0
85	MG	5	3747	1/1	0.33	0.21	30,30,30,30	0
85	MG	5	3798	1/1	0.30	0.21	44,44,44,44	0
85	MG	5	3437	1/1	0.25	0.20	35,35,35,35	0
85	MG	6	1912	1/1	0.28	0.20	48,48,48,48	0
85	MG	1	3585	1/1	0.29	0.19	50,50,50,50	0
85	MG	5	3706	1/1	0.20	0.19	51,51,51,51	0
86	OHX	2	2102	7/7	0.23	0.19	146,146,146,146	0
85	MG	5	3425	1/1	0.24	0.19	41,41,41,41	0
85	MG	5	3799	1/1	0.24	0.19	78,78,78,78	0
85	MG	2	1943	1/1	0.21	0.18	69,69,69,69	0
86	OHX	1	3939	7/7	0.21	0.18	107,107,107,107	0
85	MG	L2	302	1/1	0.29	0.18	42,42,42,42	0
85	MG	2	1982	1/1	0.20	0.18	72,72,72,72	0
85	MG	1	3628	1/1	0.20	0.17	40,40,40,40	0
86	OHX	5	4170	7/7	0.24	0.17	98,98,98,98	0
85	MG	5	3737	1/1	0.20	0.16	51,51,51,51	0
86	OHX	5	3995	7/7	0.17	0.15	116,116,116,116	0
86	OHX	6	2063	7/7	0.20	0.15	100,100,100,100	0
86	OHX	1	3926	7/7	0.21	0.15	118,118,118,118	0
85	MG	l5	302	1/1	0.24	0.15	67,67,67,67	0
85	MG	5	3550	1/1	0.30	0.14	43,43,43,43	0
85	MG	5	3822	1/1	0.33	0.14	99,99,99,99	0
85	MG	2	2004	1/1	0.22	0.14	68,68,68,68	0
86	OHX	1	4140	7/7	0.24	0.14	123,123,123,123	0
86	OHX	5	3936	7/7	0.22	0.13	84,84,84,84	0
85	MG	5	3416	1/1	0.24	0.13	42,42,42,42	0
85	MG	5	3556	1/1	0.31	0.13	44,44,44,44	0
86	OHX	5	3963	7/7	0.23	0.12	97,97,97,97	0
85	MG	1	3471	1/1	0.22	0.12	49,49,49,49	0
85	MG	1	3632	1/1	0.25	0.11	38,38,38,38	0
86	OHX	5	3986	7/7	0.19	0.10	121,121,121,121	0
86	OHX	2	2136	7/7	0.21	0.10	175,175,175,175	0
85	MG	1	3456	1/1	0.37	0.10	55,55,55,55	0
85	MG	6	2042	1/1	0.26	0.09	53,53,53,53	0
86	OHX	6	2199	7/7	0.21	0.08	147,147,147,147	0
85	MG	1	3472	1/1	0.22	0.08	43,43,43,43	0
86	OHX	1	4152	7/7	0.18	0.07	141,141,141,141	0
85	MG	n8	203	1/1	0.24	0.07	46,46,46,46	0
86	OHX	5	4222	7/7	0.34	0.07	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4115	7/7	0.26	0.07	119,119,119,119	0
85	MG	8	202	1/1	0.27	0.06	38,38,38,38	0
86	OHX	1	3930	7/7	0.19	0.06	93,93,93,93	0
85	MG	5	3471	1/1	0.26	0.06	39,39,39,39	0
86	OHX	5	4243	7/7	0.23	0.06	148,148,148,148	0
85	MG	2	2016	1/1	0.21	0.05	81,81,81,81	0
86	OHX	1	3896	7/7	0.21	0.05	82,82,82,82	0
85	MG	m6	201	1/1	0.38	0.05	77,77,77,77	0
86	OHX	2	2026	7/7	0.20	0.04	81,81,81,81	0
85	MG	1	3553	1/1	0.33	0.04	36,36,36,36	0
86	OHX	5	4134	7/7	0.21	0.04	135,135,135,135	0
86	OHX	6	2147	7/7	0.19	0.04	117,117,117,117	0
85	MG	5	3717	1/1	0.28	0.04	52,52,52,52	0
85	MG	5	3694	1/1	0.20	0.03	47,47,47,47	0
85	MG	3	211	1/1	0.20	0.03	75,75,75,75	0
85	MG	2	1901	1/1	0.37	0.03	81,81,81,81	0
86	OHX	1	4137	7/7	0.24	0.03	126,126,126,126	0
85	MG	5	3469	1/1	0.25	0.02	41,41,41,41	0
85	MG	5	3443	1/1	0.25	0.02	33,33,33,33	0
85	MG	L4	401	1/1	0.34	0.02	67,67,67,67	0
85	MG	5	3603	1/1	0.20	0.01	62,62,62,62	0
85	MG	m7	203	1/1	0.29	0.01	57,57,57,57	0
86	OHX	2	2041	7/7	0.18	-0.00	104,104,104,104	0
85	MG	1	3785	1/1	0.18	0.00	63,63,63,63	0
86	OHX	1	4051	7/7	0.26	-0.01	119,119,119,119	0
85	MG	1	3482	1/1	0.25	-0.01	44,44,44,44	0
86	OHX	5	4130	7/7	0.20	-0.01	127,127,127,127	0
86	OHX	1	4186	7/7	0.23	-0.02	141,141,141,141	0
85	MG	5	3515	1/1	0.30	-0.02	31,31,31,31	0
85	MG	1	3450	1/1	0.17	-0.02	49,49,49,49	0
85	MG	1	3811	1/1	0.26	-0.03	59,59,59,59	0
85	MG	1	3718	1/1	0.26	-0.04	34,34,34,34	0
86	OHX	1	4179	7/7	0.19	-0.04	169,169,169,169	0
86	OHX	6	2100	7/7	0.14	-0.04	159,159,159,159	0
85	MG	D3	201	1/1	0.35	-0.04	65,65,65,65	0
85	MG	1	3551	1/1	0.28	-0.04	44,44,44,44	0
86	OHX	2	2116	7/7	0.27	-0.05	150,150,150,150	0
85	MG	8	213	1/1	0.20	-0.05	59,59,59,59	0
85	MG	7	202	1/1	0.23	-0.06	31,31,31,31	0
86	OHX	1	3948	7/7	0.17	-0.06	108,108,108,108	0
85	MG	1	3479	1/1	0.25	-0.07	42,42,42,42	0
86	OHX	6	2168	7/7	0.27	-0.08	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3997	7/7	0.18	-0.08	114,114,114,114	0
85	MG	n8	205	1/1	0.23	-0.08	40,40,40,40	0
86	OHX	5	4096	7/7	0.23	-0.08	127,127,127,127	0
85	MG	1	3674	1/1	0.30	-0.08	68,68,68,68	0
86	OHX	5	4086	7/7	0.35	-0.09	109,109,109,109	0
86	OHX	5	4217	7/7	0.28	-0.10	181,181,181,181	0
85	MG	S2	302	1/1	0.32	-0.10	76,76,76,76	0
85	MG	m5	303	1/1	0.40	-0.10	98,98,98,98	0
85	MG	1	3404	1/1	0.42	-0.11	57,57,57,57	0
85	MG	6	1976	1/1	0.26	-0.12	51,51,51,51	0
85	MG	5	3697	1/1	0.26	-0.13	69,69,69,69	0
86	OHX	M9	203	7/7	0.20	-0.13	181,181,181,181	0
85	MG	5	3814	1/1	0.23	-0.14	62,62,62,62	0
85	MG	5	3474	1/1	0.20	-0.14	52,52,52,52	0
86	OHX	2	2090	7/7	0.19	-0.14	146,146,146,146	0
85	MG	6	1969	1/1	0.20	-0.14	64,64,64,64	0
86	OHX	5	4248	7/7	0.16	-0.14	169,169,169,169	0
85	MG	5	3842	1/1	0.25	-0.14	59,59,59,59	0
85	MG	1	3545	1/1	0.26	-0.15	35,35,35,35	0
85	MG	1	3697	1/1	0.24	-0.15	55,55,55,55	0
86	OHX	4	238	7/7	0.26	-0.15	149,149,149,149	0
86	OHX	6	2185	7/7	0.22	-0.15	145,145,145,145	0
85	MG	1	3609	1/1	0.25	-0.15	65,65,65,65	0
85	MG	5	3724	1/1	0.17	-0.15	51,51,51,51	0
85	MG	5	3509	1/1	0.25	-0.15	26,26,26,26	0
86	OHX	6	2178	7/7	0.42	-0.16	139,139,139,139	0
85	MG	1	3408	1/1	0.24	-0.16	45,45,45,45	0
86	OHX	1	4172	7/7	0.22	-0.16	122,122,122,122	0
86	OHX	l5	305	7/7	0.19	-0.16	151,151,151,151	0
85	MG	1	3508	1/1	0.27	-0.17	32,32,32,32	0
85	MG	5	3428	1/1	0.28	-0.17	45,45,45,45	0
85	MG	c8	201	1/1	0.27	-0.17	73,73,73,73	0
85	MG	6	2004	1/1	0.25	-0.17	60,60,60,60	0
85	MG	2	1988	1/1	0.26	-0.17	64,64,64,64	0
85	MG	1	3729	1/1	0.18	-0.17	47,47,47,47	0
86	OHX	2	2139	7/7	0.24	-0.18	170,170,170,170	0
85	MG	5	3672	1/1	0.24	-0.18	42,42,42,42	0
85	MG	5	3644	1/1	0.30	-0.18	67,67,67,67	0
85	MG	M7	203	1/1	0.26	-0.18	36,36,36,36	0
85	MG	m1	201	1/1	0.22	-0.18	62,62,62,62	0
85	MG	5	3812	1/1	0.19	-0.19	45,45,45,45	0
85	MG	5	3634	1/1	0.29	-0.19	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	2	2000	1/1	0.20	-0.19	104,104,104,104	0
85	MG	1	3828	1/1	0.23	-0.20	45,45,45,45	0
86	OHX	s1	303	7/7	0.30	-0.20	168,168,168,168	0
86	OHX	5	4235	7/7	0.18	-0.20	151,151,151,151	0
85	MG	5	3783	1/1	0.22	-0.20	84,84,84,84	0
85	MG	o4	201	1/1	0.35	-0.21	72,72,72,72	0
85	MG	8	215	1/1	0.26	-0.21	38,38,38,38	0
85	MG	5	3797	1/1	0.21	-0.22	44,44,44,44	0
86	OHX	8	231	7/7	0.18	-0.23	133,133,133,133	0
85	MG	5	3528	1/1	0.26	-0.23	27,27,27,27	0
85	MG	1	3770	1/1	0.20	-0.23	45,45,45,45	0
85	MG	2	1948	1/1	0.22	-0.24	62,62,62,62	0
85	MG	2	1906	1/1	0.18	-0.24	58,58,58,58	0
86	OHX	1	4215	7/7	0.23	-0.24	131,131,131,131	0
86	OHX	6	2084	7/7	0.17	-0.24	131,131,131,131	0
86	OHX	5	3932	7/7	0.20	-0.24	82,82,82,82	0
86	OHX	1	4127	7/7	0.24	-0.24	115,115,115,115	0
85	MG	2	1911	1/1	0.33	-0.24	66,66,66,66	0
85	MG	1	3500	1/1	0.22	-0.26	73,73,73,73	0
85	MG	n0	201	1/1	0.21	-0.26	46,46,46,46	0
86	OHX	2	2145	7/7	0.18	-0.26	128,128,128,128	0
85	MG	2	2008	1/1	0.24	-0.26	77,77,77,77	0
86	OHX	6	2051	7/7	0.20	-0.26	72,72,72,72	0
86	OHX	2	2039	7/7	0.20	-0.26	106,106,106,106	0
86	OHX	1	4170	7/7	0.28	-0.26	132,132,132,132	0
85	MG	5	3756	1/1	0.22	-0.27	53,53,53,53	0
85	MG	4	208	1/1	0.25	-0.27	38,38,38,38	0
85	MG	5	3407	1/1	0.20	-0.28	41,41,41,41	0
85	MG	5	3520	1/1	0.26	-0.28	28,28,28,28	0
86	OHX	1	4164	7/7	0.23	-0.29	138,138,138,138	0
85	MG	1	3782	1/1	0.26	-0.29	77,77,77,77	0
85	MG	c9	201	1/1	0.20	-0.29	74,74,74,74	0
85	MG	5	3622	1/1	0.22	-0.29	52,52,52,52	0
85	MG	1	3523	1/1	0.27	-0.29	38,38,38,38	0
86	OHX	5	4014	7/7	0.18	-0.29	149,149,149,149	0
86	OHX	5	4223	7/7	0.23	-0.30	156,156,156,156	0
86	OHX	5	4227	7/7	0.14	-0.30	191,191,191,191	0
85	MG	6	1902	1/1	0.22	-0.30	59,59,59,59	0
85	MG	2	1920	1/1	0.26	-0.30	63,63,63,63	0
86	OHX	2	2148	7/7	0.18	-0.30	173,173,173,173	0
85	MG	M1	202	1/1	0.17	-0.30	78,78,78,78	0
85	MG	1	3480	1/1	0.24	-0.31	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	2	2038	7/7	0.16	-0.31	103,103,103,103	0
86	OHX	6	2201	7/7	0.23	-0.31	167,167,167,167	0
85	MG	1	3435	1/1	0.21	-0.31	51,51,51,51	0
85	MG	5	3409	1/1	0.23	-0.31	44,44,44,44	0
85	MG	5	3510	1/1	0.24	-0.32	41,41,41,41	0
86	OHX	5	4071	7/7	0.30	-0.32	121,121,121,121	0
86	OHX	2	2162	7/7	0.20	-0.32	181,181,181,181	0
85	MG	5	3610	1/1	0.21	-0.32	33,33,33,33	0
86	OHX	5	4162	7/7	0.23	-0.33	187,187,187,187	0
85	MG	1	3610	1/1	0.18	-0.33	46,46,46,46	0
86	OHX	1	3923	7/7	0.22	-0.34	101,101,101,101	0
86	OHX	5	4240	7/7	0.26	-0.34	166,166,166,166	0
85	MG	5	3723	1/1	0.27	-0.35	38,38,38,38	0
85	MG	5	3426	1/1	0.24	-0.36	41,41,41,41	0
85	MG	4	204	1/1	0.28	-0.36	71,71,71,71	0
86	OHX	1	4070	7/7	0.18	-0.36	156,156,156,156	0
85	MG	2	1969	1/1	0.25	-0.36	73,73,73,73	0
86	OHX	6	2193	7/7	0.18	-0.36	169,169,169,169	0
86	OHX	s1	302	7/7	0.20	-0.36	85,85,85,85	0
85	MG	1	3769	1/1	0.28	-0.36	49,49,49,49	0
86	OHX	5	3956	7/7	0.18	-0.37	90,90,90,90	0
86	OHX	5	3921	7/7	0.21	-0.37	72,72,72,72	0
85	MG	5	3548	1/1	0.21	-0.37	50,50,50,50	0
85	MG	6	2009	1/1	0.22	-0.38	65,65,65,65	0
85	MG	5	3453	1/1	0.24	-0.38	44,44,44,44	0
86	OHX	14	403	7/7	0.20	-0.38	154,154,154,154	0
86	OHX	5	4144	7/7	0.26	-0.38	122,122,122,122	0
85	MG	M6	201	1/1	0.24	-0.38	46,46,46,46	0
85	MG	5	3537	1/1	0.27	-0.39	34,34,34,34	0
85	MG	5	3484	1/1	0.25	-0.39	30,30,30,30	0
86	OHX	1	4191	7/7	0.23	-0.39	159,159,159,159	0
85	MG	5	3754	1/1	0.22	-0.39	50,50,50,50	0
85	MG	3	210	1/1	0.21	-0.39	64,64,64,64	0
85	MG	5	3682	1/1	0.21	-0.40	46,46,46,46	0
86	OHX	8	217	7/7	0.23	-0.40	62,62,62,62	0
85	MG	1	3416	1/1	0.22	-0.40	54,54,54,54	0
85	MG	6	2032	1/1	0.29	-0.40	51,51,51,51	0
86	OHX	6	2182	7/7	0.19	-0.41	147,147,147,147	0
85	MG	5	3463	1/1	0.26	-0.41	30,30,30,30	0
85	MG	1	3816	1/1	0.31	-0.41	56,56,56,56	0
86	OHX	6	2183	7/7	0.19	-0.42	142,142,142,142	0
85	MG	1	3638	1/1	0.32	-0.42	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	3484	1/1	0.24	-0.42	55,55,55,55	0
85	MG	6	1956	1/1	0.38	-0.42	57,57,57,57	0
85	MG	1	3842	1/1	0.20	-0.43	46,46,46,46	0
86	OHX	5	4153	7/7	0.23	-0.44	142,142,142,142	0
86	OHX	2	2179	7/7	0.31	-0.45	168,168,168,168	0
85	MG	1	3478	1/1	0.20	-0.45	51,51,51,51	0
86	OHX	1	4087	7/7	0.23	-0.45	136,136,136,136	0
86	OHX	5	4241	7/7	0.21	-0.45	142,142,142,142	0
85	MG	6	2002	1/1	0.16	-0.45	97,97,97,97	0
86	OHX	5	4132	7/7	0.22	-0.45	127,127,127,127	0
86	OHX	m5	304	7/7	0.20	-0.46	67,67,67,67	0
86	OHX	5	3911	7/7	0.20	-0.46	64,64,64,64	0
85	MG	1	3812	1/1	0.21	-0.46	60,60,60,60	0
86	OHX	7	217	7/7	0.23	-0.46	89,89,89,89	0
86	OHX	2	2115	7/7	0.19	-0.46	153,153,153,153	0
86	OHX	1	3945	7/7	0.20	-0.47	108,108,108,108	0
86	OHX	5	3991	7/7	0.26	-0.47	102,102,102,102	0
85	MG	5	3529	1/1	0.31	-0.47	58,58,58,58	0
86	OHX	5	3905	7/7	0.21	-0.47	64,64,64,64	0
85	MG	1	3708	1/1	0.21	-0.47	56,56,56,56	0
86	OHX	5	4102	7/7	0.30	-0.48	110,110,110,110	0
86	OHX	6	2104	7/7	0.20	-0.48	127,127,127,127	0
85	MG	5	3582	1/1	0.28	-0.48	33,33,33,33	0
86	OHX	1	4206	7/7	0.21	-0.48	134,134,134,134	0
86	OHX	6	2095	7/7	0.17	-0.49	129,129,129,129	0
86	OHX	5	4100	7/7	0.20	-0.49	162,162,162,162	0
85	MG	2	1950	1/1	0.24	-0.49	99,99,99,99	0
85	MG	1	3583	1/1	0.27	-0.50	36,36,36,36	0
87	ZN	d9	101	1/1	0.18	-0.51	81,81,81,81	0
85	MG	1	3642	1/1	0.21	-0.52	40,40,40,40	0
85	MG	5	3579	1/1	0.29	-0.52	48,48,48,48	0
86	OHX	5	4185	7/7	0.20	-0.52	168,168,168,168	0
85	MG	5	3643	1/1	0.20	-0.53	52,52,52,52	0
85	MG	5	3847	1/1	0.22	-0.53	56,56,56,56	0
85	MG	1	3502	1/1	0.25	-0.53	22,22,22,22	0
86	OHX	5	3972	7/7	0.18	-0.53	109,109,109,109	0
86	OHX	Q2	503	7/7	0.24	-0.53	95,95,95,95	0
86	OHX	2	2143	7/7	0.24	-0.53	177,177,177,177	0
86	OHX	2	2149	7/7	0.26	-0.53	176,176,176,176	0
85	MG	1	3421	1/1	0.37	-0.54	76,76,76,76	0
86	OHX	6	2049	7/7	0.23	-0.54	74,74,74,74	0
85	MG	1	3682	1/1	0.21	-0.54	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3555	1/1	0.25	-0.55	37,37,37,37	0
86	OHX	6	2186	7/7	0.17	-0.55	181,181,181,181	0
86	OHX	1	4189	7/7	0.18	-0.55	153,153,153,153	0
85	MG	M7	202	1/1	0.25	-0.55	37,37,37,37	0
86	OHX	1	4033	7/7	0.20	-0.55	126,126,126,126	0
85	MG	1	3468	1/1	0.19	-0.55	53,53,53,53	0
85	MG	1	3771	1/1	0.17	-0.55	56,56,56,56	0
85	MG	1	3598	1/1	0.28	-0.55	43,43,43,43	0
86	OHX	2	2046	7/7	0.14	-0.55	129,129,129,129	0
85	MG	5	3638	1/1	0.28	-0.55	46,46,46,46	0
86	OHX	5	4239	7/7	0.21	-0.56	110,110,110,110	0
85	MG	1	3637	1/1	0.36	-0.56	74,74,74,74	0
85	MG	1	3586	1/1	0.24	-0.57	51,51,51,51	0
86	OHX	5	3902	7/7	0.24	-0.57	56,56,56,56	0
85	MG	5	3460	1/1	0.23	-0.57	33,33,33,33	0
86	OHX	2	2151	7/7	0.18	-0.58	152,152,152,152	0
85	MG	5	3584	1/1	0.23	-0.58	45,45,45,45	0
86	OHX	m8	201	7/7	0.23	-0.58	145,145,145,145	0
85	MG	1	3672	1/1	0.21	-0.59	54,54,54,54	0
85	MG	5	3894	1/1	0.27	-0.59	57,57,57,57	0
86	OHX	5	4180	7/7	0.18	-0.59	138,138,138,138	0
85	MG	5	3668	1/1	0.23	-0.60	45,45,45,45	0
85	MG	6	2035	1/1	0.26	-0.60	62,62,62,62	0
85	MG	5	3776	1/1	0.23	-0.60	41,41,41,41	0
85	MG	5	3665	1/1	0.20	-0.60	56,56,56,56	0
86	OHX	1	4071	7/7	0.20	-0.60	120,120,120,120	0
85	MG	1	3803	1/1	0.27	-0.60	31,31,31,31	0
85	MG	2	1939	1/1	0.17	-0.60	71,71,71,71	0
85	MG	1	3488	1/1	0.24	-0.60	44,44,44,44	0
87	ZN	Q0	500	1/1	0.20	-0.60	52,52,52,52	0
85	MG	M0	302	1/1	0.23	-0.61	55,55,55,55	0
86	OHX	6	2173	7/7	0.18	-0.61	153,153,153,153	0
85	MG	1	3535	1/1	0.28	-0.61	32,32,32,32	0
85	MG	5	3614	1/1	0.29	-0.61	35,35,35,35	0
85	MG	8	206	1/1	0.22	-0.61	50,50,50,50	0
86	OHX	1	4188	7/7	0.19	-0.62	143,143,143,143	0
85	MG	1	3440	1/1	0.26	-0.62	38,38,38,38	0
86	OHX	5	4159	7/7	0.20	-0.62	121,121,121,121	0
85	MG	S6	301	1/1	0.24	-0.62	93,93,93,93	0
86	OHX	1	3882	7/7	0.21	-0.62	67,67,67,67	0
86	OHX	5	4215	7/7	0.19	-0.62	154,154,154,154	0
86	OHX	1	4200	7/7	0.28	-0.62	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	6	2174	7/7	0.19	-0.63	135,135,135,135	0
86	OHX	6	2046	7/7	0.22	-0.63	61,61,61,61	0
86	OHX	1	4082	7/7	0.23	-0.63	129,129,129,129	0
86	OHX	5	4181	7/7	0.20	-0.63	126,126,126,126	0
85	MG	5	3831	1/1	0.17	-0.64	56,56,56,56	0
85	MG	5	3726	1/1	0.20	-0.64	43,43,43,43	0
85	MG	5	3415	1/1	0.20	-0.64	59,59,59,59	0
85	MG	4	214	1/1	0.21	-0.64	43,43,43,43	0
86	OHX	m0	301	7/7	0.17	-0.65	125,125,125,125	0
86	OHX	6	2116	7/7	0.23	-0.65	144,144,144,144	0
86	OHX	1	4069	7/7	0.28	-0.65	111,111,111,111	0
86	OHX	5	4225	7/7	0.19	-0.65	167,167,167,167	0
86	OHX	l3	405	7/7	0.20	-0.65	123,123,123,123	0
85	MG	1	3667	1/1	0.24	-0.66	46,46,46,46	0
85	MG	5	3594	1/1	0.20	-0.66	32,32,32,32	0
86	OHX	5	4027	7/7	0.14	-0.66	140,140,140,140	0
85	MG	1	3595	1/1	0.23	-0.66	24,24,24,24	0
85	MG	6	1994	1/1	0.20	-0.66	71,71,71,71	0
85	MG	2	1966	1/1	0.24	-0.66	61,61,61,61	0
85	MG	M3	201	1/1	0.21	-0.67	44,44,44,44	0
86	OHX	5	3973	7/7	0.19	-0.67	95,95,95,95	0
86	OHX	2	2099	7/7	0.22	-0.67	156,156,156,156	0
85	MG	5	3674	1/1	0.21	-0.67	54,54,54,54	0
85	MG	1	3657	1/1	0.26	-0.67	50,50,50,50	0
85	MG	1	3427	1/1	0.32	-0.67	63,63,63,63	0
85	MG	6	1940	1/1	0.22	-0.68	54,54,54,54	0
86	OHX	2	2129	7/7	0.20	-0.68	127,127,127,127	0
85	MG	6	2016	1/1	0.24	-0.68	43,43,43,43	0
86	OHX	2	2176	7/7	0.20	-0.69	187,187,187,187	0
85	MG	6	1934	1/1	0.19	-0.69	61,61,61,61	0
85	MG	5	3494	1/1	0.18	-0.69	45,45,45,45	0
85	MG	6	1968	1/1	0.18	-0.69	60,60,60,60	0
86	OHX	l4	402	7/7	0.25	-0.70	168,168,168,168	0
86	OHX	1	4209	7/7	0.18	-0.70	139,139,139,139	0
85	MG	1	3526	1/1	0.22	-0.70	31,31,31,31	0
85	MG	6	1980	1/1	0.20	-0.70	52,52,52,52	0
86	OHX	1	3911	7/7	0.20	-0.70	88,88,88,88	0
85	MG	c1	201	1/1	0.21	-0.71	49,49,49,49	0
85	MG	5	3461	1/1	0.27	-0.72	34,34,34,34	0
86	OHX	1	3877	7/7	0.21	-0.72	55,55,55,55	0
85	MG	5	3628	1/1	0.19	-0.73	62,62,62,62	0
85	MG	5	3438	1/1	0.21	-0.73	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2001	1/1	0.21	-0.73	75,75,75,75	0
86	OHX	5	4191	7/7	0.20	-0.73	176,176,176,176	0
85	MG	1	3483	1/1	0.18	-0.74	34,34,34,34	0
86	OHX	5	4106	7/7	0.21	-0.75	131,131,131,131	0
87	ZN	q0	201	1/1	0.20	-0.75	34,34,34,34	0
85	MG	2	1953	1/1	0.20	-0.75	105,105,105,105	0
85	MG	1	3426	1/1	0.25	-0.75	29,29,29,29	0
86	OHX	5	4057	7/7	0.21	-0.75	120,120,120,120	0
85	MG	6	1982	1/1	0.17	-0.75	82,82,82,82	0
86	OHX	2	2034	7/7	0.18	-0.75	104,104,104,104	0
85	MG	2	2012	1/1	0.26	-0.76	69,69,69,69	0
87	ZN	Q2	501	1/1	0.16	-0.76	95,95,95,95	0
86	OHX	3	221	7/7	0.20	-0.76	130,130,130,130	0
86	OHX	6	2146	7/7	0.12	-0.76	136,136,136,136	0
85	MG	1	3564	1/1	0.21	-0.77	51,51,51,51	0
86	OHX	1	4160	7/7	0.22	-0.77	138,138,138,138	0
86	OHX	5	4206	7/7	0.20	-0.77	131,131,131,131	0
85	MG	m7	204	1/1	0.26	-0.77	39,39,39,39	0
85	MG	5	3730	1/1	0.20	-0.78	33,33,33,33	0
86	OHX	1	3883	7/7	0.21	-0.78	60,60,60,60	0
86	OHX	s8	303	7/7	0.22	-0.78	172,172,172,172	0
85	MG	1	3587	1/1	0.26	-0.78	38,38,38,38	0
85	MG	l7	302	1/1	0.23	-0.79	43,43,43,43	0
85	MG	S2	301	1/1	0.36	-0.79	48,48,48,48	0
86	OHX	5	4143	7/7	0.25	-0.79	125,125,125,125	0
86	OHX	1	3932	7/7	0.15	-0.80	109,109,109,109	0
86	OHX	5	3945	7/7	0.17	-0.80	90,90,90,90	0
85	MG	6	2003	1/1	0.27	-0.81	72,72,72,72	0
86	OHX	1	4106	7/7	0.17	-0.82	141,141,141,141	0
86	OHX	6	2070	7/7	0.16	-0.82	112,112,112,112	0
86	OHX	5	4186	7/7	0.21	-0.82	131,131,131,131	0
85	MG	4	218	1/1	0.15	-0.82	60,60,60,60	0
86	OHX	1	4006	7/7	0.20	-0.83	122,122,122,122	0
85	MG	O7	102	1/1	0.21	-0.83	42,42,42,42	0
85	MG	1	3412	1/1	0.27	-0.83	44,44,44,44	0
85	MG	2	1954	1/1	0.19	-0.83	68,68,68,68	0
86	OHX	2	2160	7/7	0.21	-0.83	163,163,163,163	0
86	OHX	5	3904	7/7	0.20	-0.83	62,62,62,62	0
86	OHX	5	3924	7/7	0.22	-0.84	76,76,76,76	0
85	MG	1	3438	1/1	0.22	-0.84	33,33,33,33	0
86	OHX	5	3954	7/7	0.18	-0.84	93,93,93,93	0
85	MG	5	3760	1/1	0.21	-0.84	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2135	7/7	0.19	-0.85	144,144,144,144	0
85	MG	5	3490	1/1	0.18	-0.85	33,33,33,33	0
86	OHX	6	2124	7/7	0.10	-0.85	138,138,138,138	0
85	MG	1	3740	1/1	0.34	-0.85	63,63,63,63	0
86	OHX	d9	102	7/7	0.19	-0.85	169,169,169,169	0
85	MG	6	1963	1/1	0.18	-0.86	57,57,57,57	0
85	MG	5	3430	1/1	0.24	-0.87	32,32,32,32	0
86	OHX	2	2052	7/7	0.18	-0.87	135,135,135,135	0
86	OHX	5	3918	7/7	0.20	-0.87	68,68,68,68	0
85	MG	1	3614	1/1	0.23	-0.87	34,34,34,34	0
86	OHX	5	3966	7/7	0.20	-0.87	93,93,93,93	0
86	OHX	1	3908	7/7	0.18	-0.88	85,85,85,85	0
85	MG	1	3493	1/1	0.29	-0.88	72,72,72,72	0
86	OHX	1	4153	7/7	0.19	-0.88	149,149,149,149	0
85	MG	5	3419	1/1	0.27	-0.88	38,38,38,38	0
86	OHX	5	3914	7/7	0.19	-0.88	73,73,73,73	0
86	OHX	1	3971	7/7	0.15	-0.88	121,121,121,121	0
85	MG	1	3777	1/1	0.17	-0.89	49,49,49,49	0
86	OHX	1	4059	7/7	0.21	-0.90	115,115,115,115	0
86	OHX	1	4193	7/7	0.20	-0.90	148,148,148,148	0
86	OHX	5	3977	7/7	0.15	-0.90	96,96,96,96	0
85	MG	5	3507	1/1	0.27	-0.90	36,36,36,36	0
85	MG	1	3415	1/1	0.23	-0.90	38,38,38,38	0
85	MG	12	302	1/1	0.25	-0.90	45,45,45,45	0
86	OHX	5	4155	7/7	0.23	-0.91	141,141,141,141	0
85	MG	6	2017	1/1	0.23	-0.91	46,46,46,46	0
86	OHX	6	2072	7/7	0.14	-0.92	133,133,133,133	0
85	MG	6	2041	1/1	0.21	-0.92	69,69,69,69	0
85	MG	6	1905	1/1	0.20	-0.92	54,54,54,54	0
85	MG	1	3505	1/1	0.27	-0.92	43,43,43,43	0
85	MG	1	3556	1/1	0.26	-0.92	34,34,34,34	0
85	MG	1	3555	1/1	0.20	-0.92	37,37,37,37	0
86	OHX	1	3935	7/7	0.14	-0.92	107,107,107,107	0
86	OHX	m1	202	7/7	0.15	-0.93	160,160,160,160	0
85	MG	5	3575	1/1	0.25	-0.93	33,33,33,33	0
86	OHX	5	4105	7/7	0.22	-0.94	135,135,135,135	0
86	OHX	5	3953	7/7	0.18	-0.94	99,99,99,99	0
85	MG	5	3721	1/1	0.22	-0.95	59,59,59,59	0
85	MG	6	1914	1/1	0.25	-0.95	76,76,76,76	0
85	MG	5	3422	1/1	0.23	-0.95	39,39,39,39	0
85	MG	1	3582	1/1	0.26	-0.96	47,47,47,47	0
85	MG	5	3746	1/1	0.16	-0.96	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3990	7/7	0.22	-0.96	109,109,109,109	0
87	ZN	Q3	501	1/1	0.14	-0.96	65,65,65,65	0
85	MG	1	3608	1/1	0.22	-0.96	70,70,70,70	0
85	MG	5	3851	1/1	0.23	-0.97	49,49,49,49	0
85	MG	1	3429	1/1	0.16	-0.97	56,56,56,56	0
86	OHX	2	2088	7/7	0.19	-0.97	120,120,120,120	0
86	OHX	5	3931	7/7	0.20	-0.98	76,76,76,76	0
86	OHX	1	4171	7/7	0.11	-0.98	215,215,215,215	0
85	MG	1	3669	1/1	0.21	-0.98	54,54,54,54	0
86	OHX	m0	302	7/7	0.17	-0.98	136,136,136,136	0
86	OHX	1	4041	7/7	0.21	-0.98	133,133,133,133	0
86	OHX	2	2023	7/7	0.21	-0.98	87,87,87,87	0
86	OHX	N9	101	7/7	0.20	-0.99	68,68,68,68	0
85	MG	1	3605	1/1	0.20	-0.99	45,45,45,45	0
85	MG	2	1909	1/1	0.24	-0.99	72,72,72,72	0
86	OHX	4	234	7/7	0.13	-0.99	147,147,147,147	0
86	OHX	1	4118	7/7	0.13	-0.99	186,186,186,186	0
85	MG	n8	201	1/1	0.18	-1.00	40,40,40,40	0
85	MG	1	3721	1/1	0.16	-1.00	79,79,79,79	0
85	MG	5	3613	1/1	0.21	-1.01	51,51,51,51	0
85	MG	1	3789	1/1	0.21	-1.01	46,46,46,46	0
85	MG	5	3604	1/1	0.21	-1.01	37,37,37,37	0
86	OHX	1	3987	7/7	0.10	-1.01	117,117,117,117	0
86	OHX	5	4204	7/7	0.18	-1.01	154,154,154,154	0
85	MG	n8	204	1/1	0.21	-1.02	42,42,42,42	0
86	OHX	1	3891	7/7	0.18	-1.02	74,74,74,74	0
85	MG	5	3749	1/1	0.23	-1.02	39,39,39,39	0
86	OHX	2	2076	7/7	0.14	-1.02	127,127,127,127	0
85	MG	1	3806	1/1	0.16	-1.02	55,55,55,55	0
85	MG	S4	301	1/1	0.25	-1.03	71,71,71,71	0
85	MG	1	3444	1/1	0.15	-1.03	82,82,82,82	0
86	OHX	6	2088	7/7	0.14	-1.03	132,132,132,132	0
86	OHX	8	226	7/7	0.14	-1.03	132,132,132,132	0
85	MG	5	3482	1/1	0.21	-1.03	39,39,39,39	0
85	MG	1	3581	1/1	0.21	-1.04	43,43,43,43	0
86	OHX	1	3988	7/7	0.14	-1.04	112,112,112,112	0
85	MG	l2	301	1/1	0.26	-1.05	46,46,46,46	0
85	MG	1	3519	1/1	0.25	-1.05	31,31,31,31	0
86	OHX	O3	202	7/7	0.18	-1.05	124,124,124,124	0
86	OHX	5	4231	7/7	0.19	-1.05	114,114,114,114	0
85	MG	5	3801	1/1	0.20	-1.05	33,33,33,33	0
86	OHX	q1	102	7/7	0.22	-1.06	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3740	1/1	0.19	-1.06	43,43,43,43	0
86	OHX	1	4141	7/7	0.18	-1.06	114,114,114,114	0
86	OHX	6	2162	7/7	0.11	-1.06	125,125,125,125	0
86	OHX	5	4197	7/7	0.20	-1.06	129,129,129,129	0
85	MG	6	1973	1/1	0.18	-1.06	59,59,59,59	0
85	MG	5	3825	1/1	0.17	-1.06	42,42,42,42	0
86	OHX	2	2084	7/7	0.10	-1.06	145,145,145,145	0
86	OHX	2	2022	7/7	0.21	-1.07	78,78,78,78	0
85	MG	5	3820	1/1	0.20	-1.07	59,59,59,59	0
87	ZN	D9	101	1/1	0.13	-1.07	81,81,81,81	0
86	OHX	O2	201	7/7	0.17	-1.07	101,101,101,101	0
86	OHX	1	4085	7/7	0.19	-1.08	125,125,125,125	0
86	OHX	2	2144	7/7	0.23	-1.08	153,153,153,153	0
85	MG	q3	503	1/1	0.23	-1.08	74,74,74,74	0
85	MG	4	217	1/1	0.15	-1.09	61,61,61,61	0
86	OHX	5	3909	7/7	0.21	-1.09	64,64,64,64	0
86	OHX	1	3913	7/7	0.18	-1.09	83,83,83,83	0
86	OHX	6	2132	7/7	0.19	-1.10	132,132,132,132	0
86	OHX	1	3928	7/7	0.14	-1.10	95,95,95,95	0
86	OHX	2	2092	7/7	0.14	-1.11	155,155,155,155	0
86	OHX	5	3971	7/7	0.16	-1.11	86,86,86,86	0
85	MG	N6	201	1/1	0.21	-1.11	48,48,48,48	0
86	OHX	2	2130	7/7	0.19	-1.11	140,140,140,140	0
85	MG	1	3793	1/1	0.18	-1.12	57,57,57,57	0
85	MG	L2	301	1/1	0.25	-1.12	31,31,31,31	0
86	OHX	1	4007	7/7	0.20	-1.12	104,104,104,104	0
86	OHX	8	230	7/7	0.19	-1.12	139,139,139,139	0
86	OHX	5	4040	7/7	0.22	-1.12	105,105,105,105	0
85	MG	m7	201	1/1	0.22	-1.12	37,37,37,37	0
86	OHX	6	2057	7/7	0.17	-1.13	92,92,92,92	0
85	MG	5	3819	1/1	0.20	-1.13	65,65,65,65	0
86	OHX	6	2053	7/7	0.20	-1.13	82,82,82,82	0
86	OHX	5	3929	7/7	0.20	-1.13	76,76,76,76	0
86	OHX	6	2176	7/7	0.18	-1.14	112,112,112,112	0
86	OHX	6	2141	7/7	0.13	-1.14	164,164,164,164	0
86	OHX	1	4196	7/7	0.17	-1.14	149,149,149,149	0
86	OHX	5	4117	7/7	0.16	-1.14	133,133,133,133	0
86	OHX	1	3952	7/7	0.15	-1.14	117,117,117,117	0
86	OHX	2	2109	7/7	0.09	-1.14	145,145,145,145	0
86	OHX	M5	302	7/7	0.22	-1.14	120,120,120,120	0
86	OHX	6	2194	7/7	0.17	-1.15	192,192,192,192	0
86	OHX	1	3967	7/7	0.16	-1.15	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2068	7/7	0.13	-1.15	104,104,104,104	0
86	OHX	5	4166	7/7	0.18	-1.16	136,136,136,136	0
86	OHX	5	4173	7/7	0.20	-1.16	141,141,141,141	0
85	MG	M9	202	1/1	0.20	-1.16	71,71,71,71	0
86	OHX	L4	403	7/7	0.20	-1.16	143,143,143,143	0
86	OHX	1	4068	7/7	0.19	-1.16	131,131,131,131	0
86	OHX	2	2138	7/7	0.14	-1.16	177,177,177,177	0
86	OHX	8	218	7/7	0.10	-1.16	114,114,114,114	0
86	OHX	5	4020	7/7	0.12	-1.17	116,116,116,116	0
86	OHX	5	3960	7/7	0.15	-1.17	93,93,93,93	0
85	MG	1	3643	1/1	0.20	-1.17	43,43,43,43	0
85	MG	6	1960	1/1	0.17	-1.17	79,79,79,79	0
85	MG	5	3524	1/1	0.25	-1.18	43,43,43,43	0
85	MG	5	3466	1/1	0.19	-1.18	63,63,63,63	0
85	MG	5	3763	1/1	0.23	-1.18	73,73,73,73	0
86	OHX	2	2161	7/7	0.16	-1.19	171,171,171,171	0
86	OHX	c3	201	7/7	0.12	-1.19	159,159,159,159	0
86	OHX	2	2106	7/7	0.09	-1.20	122,122,122,122	0
87	ZN	e1	501	1/1	0.11	-1.20	167,167,167,167	0
85	MG	6	2025	1/1	0.14	-1.20	92,92,92,92	0
85	MG	6	1985	1/1	0.18	-1.20	71,71,71,71	0
85	MG	14	401	1/1	0.21	-1.20	43,43,43,43	0
86	OHX	l3	406	7/7	0.18	-1.21	142,142,142,142	0
86	OHX	4	224	7/7	0.21	-1.21	61,61,61,61	0
85	MG	1	3703	1/1	0.20	-1.21	43,43,43,43	0
85	MG	5	3848	1/1	0.23	-1.22	50,50,50,50	0
85	MG	1	3755	1/1	0.21	-1.22	65,65,65,65	0
86	OHX	O7	104	7/7	0.11	-1.22	101,101,101,101	0
86	OHX	1	4037	7/7	0.12	-1.22	133,133,133,133	0
86	OHX	n9	101	7/7	0.18	-1.22	70,70,70,70	0
85	MG	5	3826	1/1	0.20	-1.23	43,43,43,43	0
85	MG	6	1935	1/1	0.14	-1.23	78,78,78,78	0
87	ZN	E1	501	1/1	0.08	-1.23	122,122,122,122	0
86	OHX	8	221	7/7	0.12	-1.24	128,128,128,128	0
86	OHX	1	3922	7/7	0.16	-1.24	90,90,90,90	0
85	MG	2	1947	1/1	0.23	-1.24	92,92,92,92	0
85	MG	1	3568	1/1	0.16	-1.24	29,29,29,29	0
85	MG	6	2023	1/1	0.18	-1.24	47,47,47,47	0
86	OHX	1	4167	7/7	0.14	-1.24	147,147,147,147	0
85	MG	2	1975	1/1	0.19	-1.24	62,62,62,62	0
86	OHX	1	4002	7/7	0.14	-1.25	167,167,167,167	0
86	OHX	1	4040	7/7	0.08	-1.25	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	1	3897	7/7	0.17	-1.25	75,75,75,75	0
85	MG	5	3429	1/1	0.23	-1.25	29,29,29,29	0
85	MG	2	1990	1/1	0.11	-1.25	102,102,102,102	0
86	OHX	5	4112	7/7	0.17	-1.26	126,126,126,126	0
86	OHX	2	2131	7/7	0.12	-1.26	165,165,165,165	0
85	MG	2	1971	1/1	0.21	-1.26	85,85,85,85	0
86	OHX	5	4064	7/7	0.18	-1.27	116,116,116,116	0
86	OHX	7	226	7/7	0.19	-1.27	119,119,119,119	0
85	MG	1	3533	1/1	0.24	-1.27	41,41,41,41	0
85	MG	5	3627	1/1	0.18	-1.27	33,33,33,33	0
86	OHX	6	2189	7/7	0.19	-1.27	153,153,153,153	0
85	MG	5	3457	1/1	0.21	-1.28	31,31,31,31	0
85	MG	5	3427	1/1	0.15	-1.28	42,42,42,42	0
85	MG	1	3446	1/1	0.18	-1.28	52,52,52,52	0
86	OHX	1	4103	7/7	0.19	-1.29	119,119,119,119	0
85	MG	2	2020	1/1	0.15	-1.29	86,86,86,86	0
85	MG	8	201	1/1	0.12	-1.29	36,36,36,36	0
85	MG	5	3773	1/1	0.16	-1.29	70,70,70,70	0
87	ZN	d6	101	1/1	0.15	-1.29	64,64,64,64	0
86	OHX	1	4012	7/7	0.13	-1.29	116,116,116,116	0
85	MG	5	3839	1/1	0.15	-1.30	58,58,58,58	0
85	MG	5	3459	1/1	0.21	-1.30	72,72,72,72	0
87	ZN	D6	500	1/1	0.12	-1.30	86,86,86,86	0
86	OHX	5	4015	7/7	0.10	-1.30	124,124,124,124	0
86	OHX	O1	201	7/7	0.15	-1.30	118,118,118,118	0
85	MG	5	3878	1/1	0.19	-1.31	24,24,24,24	0
86	OHX	2	2048	7/7	0.14	-1.31	125,125,125,125	0
85	MG	5	3503	1/1	0.18	-1.31	53,53,53,53	0
85	MG	n6	201	1/1	0.23	-1.31	53,53,53,53	0
85	MG	m7	202	1/1	0.23	-1.31	36,36,36,36	0
86	OHX	1	3912	7/7	0.19	-1.32	96,96,96,96	0
85	MG	M3	202	1/1	0.28	-1.32	86,86,86,86	0
85	MG	5	3751	1/1	0.11	-1.33	56,56,56,56	0
86	OHX	1	3918	7/7	0.15	-1.33	88,88,88,88	0
86	OHX	5	4034	7/7	0.12	-1.33	136,136,136,136	0
85	MG	5	3553	1/1	0.22	-1.33	41,41,41,41	0
85	MG	6	1975	1/1	0.19	-1.33	48,48,48,48	0
85	MG	5	3561	1/1	0.27	-1.33	38,38,38,38	0
86	OHX	5	4179	7/7	0.15	-1.34	153,153,153,153	0
85	MG	5	3620	1/1	0.11	-1.34	47,47,47,47	0
85	MG	1	3663	1/1	0.25	-1.34	35,35,35,35	0
86	OHX	6	2062	7/7	0.15	-1.34	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3676	1/1	0.16	-1.34	29,29,29,29	0
85	MG	1	3826	1/1	0.19	-1.34	54,54,54,54	0
85	MG	5	3818	1/1	0.12	-1.35	72,72,72,72	0
86	OHX	2	2031	7/7	0.14	-1.35	105,105,105,105	0
86	OHX	2	2066	7/7	0.11	-1.35	147,147,147,147	0
85	MG	2	1924	1/1	0.24	-1.36	87,87,87,87	0
86	OHX	2	2030	7/7	0.14	-1.36	114,114,114,114	0
86	OHX	2	2025	7/7	0.18	-1.36	91,91,91,91	0
86	OHX	5	4237	7/7	0.21	-1.36	191,191,191,191	0
86	OHX	4	226	7/7	0.14	-1.36	82,82,82,82	0
85	MG	5	3545	1/1	0.15	-1.37	71,71,71,71	0
86	OHX	2	2047	7/7	0.12	-1.37	117,117,117,117	0
85	MG	1	3837	1/1	0.25	-1.37	38,38,38,38	0
85	MG	1	3566	1/1	0.24	-1.37	37,37,37,37	0
85	MG	1	3764	1/1	0.18	-1.37	46,46,46,46	0
85	MG	7	212	1/1	0.21	-1.37	66,66,66,66	0
86	OHX	1	3957	7/7	0.18	-1.38	115,115,115,115	0
85	MG	5	3779	1/1	0.15	-1.38	57,57,57,57	0
86	OHX	5	3985	7/7	0.15	-1.38	102,102,102,102	0
86	OHX	1	4111	7/7	0.14	-1.38	123,123,123,123	0
86	OHX	2	2165	7/7	0.12	-1.38	171,171,171,171	0
86	OHX	6	2135	7/7	0.14	-1.38	149,149,149,149	0
86	OHX	4	236	7/7	0.18	-1.38	123,123,123,123	0
86	OHX	1	3917	7/7	0.16	-1.39	97,97,97,97	0
86	OHX	2	2146	7/7	0.17	-1.39	189,189,189,189	0
85	MG	5	3625	1/1	0.20	-1.39	44,44,44,44	0
85	MG	O4	201	1/1	0.15	-1.40	63,63,63,63	0
85	MG	1	3692	1/1	0.22	-1.40	51,51,51,51	0
85	MG	8	210	1/1	0.20	-1.40	44,44,44,44	0
85	MG	5	3411	1/1	0.21	-1.41	41,41,41,41	0
86	OHX	2	2079	7/7	0.10	-1.41	167,167,167,167	0
86	OHX	5	4238	7/7	0.14	-1.41	238,238,238,238	0
85	MG	2	2018	1/1	0.19	-1.42	67,67,67,67	0
86	OHX	5	4142	7/7	0.14	-1.42	139,139,139,139	0
86	OHX	1	4020	7/7	0.20	-1.43	127,127,127,127	0
86	OHX	6	2119	7/7	0.13	-1.44	120,120,120,120	0
85	MG	L4	402	1/1	0.20	-1.44	32,32,32,32	0
85	MG	1	3439	1/1	0.15	-1.44	52,52,52,52	0
86	OHX	5	4099	7/7	0.19	-1.44	110,110,110,110	0
86	OHX	2	2035	7/7	0.13	-1.45	95,95,95,95	0
86	OHX	m4	202	7/7	0.17	-1.45	223,223,223,223	0
85	MG	5	3462	1/1	0.21	-1.45	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4092	7/7	0.20	-1.45	132,132,132,132	0
86	OHX	2	2120	7/7	0.12	-1.45	155,155,155,155	0
85	MG	1	3459	1/1	0.21	-1.45	43,43,43,43	0
85	MG	1	3851	1/1	0.29	-1.45	36,36,36,36	0
86	OHX	5	4005	7/7	0.13	-1.46	78,78,78,78	0
87	ZN	O7	101	1/1	0.15	-1.46	41,41,41,41	0
86	OHX	2	2056	7/7	0.10	-1.46	141,141,141,141	0
86	OHX	1	3975	7/7	0.12	-1.47	110,110,110,110	0
85	MG	sM	301	1/1	0.17	-1.48	46,46,46,46	0
86	OHX	1	3961	7/7	0.17	-1.48	106,106,106,106	0
86	OHX	2	2091	7/7	0.16	-1.48	120,120,120,120	0
86	OHX	1	4218	7/7	0.10	-1.49	175,175,175,175	0
86	OHX	1	4154	7/7	0.13	-1.49	145,145,145,145	0
86	OHX	5	3974	7/7	0.15	-1.49	104,104,104,104	0
85	MG	Q2	502	1/1	0.17	-1.49	69,69,69,69	0
85	MG	5	3626	1/1	0.20	-1.49	46,46,46,46	0
86	OHX	5	3920	7/7	0.17	-1.49	71,71,71,71	0
87	ZN	q2	501	1/1	0.16	-1.49	93,93,93,93	0
85	MG	5	3442	1/1	0.22	-1.50	45,45,45,45	0
85	MG	5	3806	1/1	0.19	-1.50	45,45,45,45	0
85	MG	1	3570	1/1	0.21	-1.51	33,33,33,33	0
86	OHX	1	4105	7/7	0.12	-1.51	170,170,170,170	0
85	MG	6	2026	1/1	0.20	-1.51	86,86,86,86	0
86	OHX	1	4119	7/7	0.21	-1.51	127,127,127,127	0
86	OHX	1	4084	7/7	0.17	-1.52	131,131,131,131	0
86	OHX	2	2067	7/7	0.12	-1.52	159,159,159,159	0
86	OHX	2	2055	7/7	0.16	-1.52	135,135,135,135	0
85	MG	5	3486	1/1	0.21	-1.52	48,48,48,48	0
86	OHX	5	4126	7/7	0.10	-1.52	155,155,155,155	0
86	OHX	5	3934	7/7	0.14	-1.52	75,75,75,75	0
85	MG	5	3719	1/1	0.11	-1.52	48,48,48,48	0
86	OHX	2	2170	7/7	0.13	-1.52	153,153,153,153	0
87	ZN	q3	501	1/1	0.11	-1.53	73,73,73,73	0
86	OHX	1	4139	7/7	0.18	-1.53	122,122,122,122	0
86	OHX	2	2167	7/7	0.18	-1.53	132,132,132,132	0
86	OHX	2	2140	7/7	0.09	-1.53	172,172,172,172	0
86	OHX	6	2099	7/7	0.13	-1.53	162,162,162,162	0
85	MG	2	1922	1/1	0.21	-1.53	66,66,66,66	0
86	OHX	o2	201	7/7	0.09	-1.54	103,103,103,103	0
85	MG	D0	201	1/1	0.20	-1.54	77,77,77,77	0
85	MG	6	1929	1/1	0.17	-1.54	60,60,60,60	0
86	OHX	6	2108	7/7	0.11	-1.55	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3702	1/1	0.18	-1.55	66,66,66,66	0
85	MG	5	3790	1/1	0.13	-1.55	40,40,40,40	0
85	MG	6	1937	1/1	0.17	-1.55	43,43,43,43	0
85	MG	1	3569	1/1	0.18	-1.55	33,33,33,33	0
85	MG	5	3496	1/1	0.21	-1.56	28,28,28,28	0
86	OHX	1	4129	7/7	0.08	-1.56	152,152,152,152	0
86	OHX	5	3967	7/7	0.13	-1.56	102,102,102,102	0
86	OHX	6	2137	7/7	0.11	-1.56	130,130,130,130	0
86	OHX	1	3892	7/7	0.19	-1.56	74,74,74,74	0
85	MG	5	3699	1/1	0.21	-1.57	56,56,56,56	0
86	OHX	15	303	7/7	0.09	-1.57	146,146,146,146	0
86	OHX	6	2175	7/7	0.12	-1.57	165,165,165,165	0
86	OHX	5	4104	7/7	0.14	-1.57	123,123,123,123	0
85	MG	L3	402	1/1	0.19	-1.57	42,42,42,42	0
85	MG	6	1992	1/1	0.13	-1.57	66,66,66,66	0
86	OHX	1	4212	7/7	0.13	-1.58	141,141,141,141	0
85	MG	5	3475	1/1	0.15	-1.58	51,51,51,51	0
85	MG	5	3669	1/1	0.18	-1.59	49,49,49,49	0
86	OHX	6	2081	7/7	0.12	-1.59	110,110,110,110	0
85	MG	5	3729	1/1	0.19	-1.59	100,100,100,100	0
86	OHX	5	4025	7/7	0.16	-1.59	101,101,101,101	0
85	MG	5	3511	1/1	0.21	-1.59	32,32,32,32	0
86	OHX	1	4110	7/7	0.13	-1.59	143,143,143,143	0
86	OHX	1	4138	7/7	0.18	-1.59	141,141,141,141	0
85	MG	5	3632	1/1	0.19	-1.59	45,45,45,45	0
86	OHX	6	2128	7/7	0.17	-1.60	152,152,152,152	0
86	OHX	6	2083	7/7	0.11	-1.60	116,116,116,116	0
85	MG	m5	302	1/1	0.18	-1.61	56,56,56,56	0
86	OHX	1	3979	7/7	0.13	-1.61	127,127,127,127	0
86	OHX	D9	102	7/7	0.17	-1.61	149,149,149,149	0
86	OHX	2	2114	7/7	0.14	-1.62	126,126,126,126	0
86	OHX	6	2121	7/7	0.10	-1.62	146,146,146,146	0
86	OHX	L3	404	7/7	0.20	-1.62	121,121,121,121	0
86	OHX	5	3959	7/7	0.14	-1.62	94,94,94,94	0
86	OHX	6	2055	7/7	0.20	-1.62	78,78,78,78	0
85	MG	1	3458	1/1	0.19	-1.62	23,23,23,23	0
85	MG	5	3485	1/1	0.14	-1.63	67,67,67,67	0
86	OHX	5	4008	7/7	0.18	-1.63	112,112,112,112	0
86	OHX	2	2024	7/7	0.22	-1.63	90,90,90,90	0
86	OHX	1	4150	7/7	0.13	-1.63	161,161,161,161	0
85	MG	6	2021	1/1	0.15	-1.63	64,64,64,64	0
85	MG	1	3753	1/1	0.19	-1.64	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	s4	302	7/7	0.14	-1.65	155,155,155,155	0
86	OHX	o7	503	7/7	0.11	-1.65	108,108,108,108	0
85	MG	M5	301	1/1	0.14	-1.65	38,38,38,38	0
86	OHX	1	4143	7/7	0.16	-1.65	151,151,151,151	0
86	OHX	2	2128	7/7	0.11	-1.65	201,201,201,201	0
86	OHX	5	4031	7/7	0.14	-1.65	126,126,126,126	0
86	OHX	2	2040	7/7	0.15	-1.65	103,103,103,103	0
86	OHX	1	3969	7/7	0.18	-1.65	78,78,78,78	0
86	OHX	2	2075	7/7	0.16	-1.66	135,135,135,135	0
85	MG	5	3558	1/1	0.21	-1.66	28,28,28,28	0
86	OHX	6	2082	7/7	0.16	-1.66	116,116,116,116	0
86	OHX	6	2170	7/7	0.17	-1.66	163,163,163,163	0
85	MG	M0	301	1/1	0.19	-1.67	44,44,44,44	0
86	OHX	5	4002	7/7	0.13	-1.67	108,108,108,108	0
86	OHX	2	2095	7/7	0.09	-1.67	138,138,138,138	0
85	MG	1	3645	1/1	0.18	-1.67	45,45,45,45	0
85	MG	4	209	1/1	0.11	-1.67	31,31,31,31	0
86	OHX	2	2169	7/7	0.13	-1.68	145,145,145,145	0
85	MG	1	3602	1/1	0.18	-1.68	33,33,33,33	0
85	MG	1	3499	1/1	0.20	-1.68	34,34,34,34	0
85	MG	1	3809	1/1	0.11	-1.69	59,59,59,59	0
85	MG	2	1996	1/1	0.12	-1.69	85,85,85,85	0
85	MG	n8	202	1/1	0.17	-1.69	32,32,32,32	0
85	MG	1	3511	1/1	0.23	-1.69	34,34,34,34	0
86	OHX	5	4070	7/7	0.11	-1.69	121,121,121,121	0
86	OHX	2	2177	7/7	0.18	-1.69	188,188,188,188	0
85	MG	1	3739	1/1	0.14	-1.69	39,39,39,39	0
85	MG	5	3715	1/1	0.16	-1.69	47,47,47,47	0
86	OHX	6	2120	7/7	0.17	-1.70	119,119,119,119	0
85	MG	6	2010	1/1	0.14	-1.70	49,49,49,49	0
86	OHX	1	4204	7/7	0.15	-1.70	142,142,142,142	0
86	OHX	sR	401	7/7	0.09	-1.70	167,167,167,167	0
86	OHX	5	4189	7/7	0.19	-1.70	133,133,133,133	0
86	OHX	1	3934	7/7	0.19	-1.70	107,107,107,107	0
86	OHX	2	2096	7/7	0.11	-1.71	175,175,175,175	0
85	MG	5	3502	1/1	0.21	-1.71	29,29,29,29	0
86	OHX	7	222	7/7	0.16	-1.71	106,106,106,106	0
86	OHX	7	224	7/7	0.16	-1.71	140,140,140,140	0
86	OHX	1	3983	7/7	0.20	-1.72	98,98,98,98	0
86	OHX	5	4161	7/7	0.13	-1.72	148,148,148,148	0
85	MG	1	3621	1/1	0.18	-1.73	70,70,70,70	0
85	MG	1	3834	1/1	0.18	-1.74	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3462	1/1	0.19	-1.74	24,24,24,24	0
86	OHX	5	4202	7/7	0.19	-1.75	141,141,141,141	0
86	OHX	6	2093	7/7	0.13	-1.75	132,132,132,132	0
85	MG	1	3457	1/1	0.26	-1.75	53,53,53,53	0
85	MG	1	3593	1/1	0.25	-1.75	63,63,63,63	0
86	OHX	5	4074	7/7	0.20	-1.76	102,102,102,102	0
86	OHX	1	4035	7/7	0.07	-1.76	138,138,138,138	0
86	OHX	5	3952	7/7	0.14	-1.77	94,94,94,94	0
86	OHX	1	4066	7/7	0.15	-1.77	156,156,156,156	0
85	MG	1	3784	1/1	0.21	-1.77	35,35,35,35	0
85	MG	1	3509	1/1	0.22	-1.77	23,23,23,23	0
85	MG	1	3763	1/1	0.15	-1.77	52,52,52,52	0
86	OHX	6	2094	7/7	0.13	-1.77	133,133,133,133	0
86	OHX	5	4073	7/7	0.11	-1.78	163,163,163,163	0
85	MG	5	3742	1/1	0.15	-1.78	39,39,39,39	0
85	MG	1	3571	1/1	0.14	-1.78	26,26,26,26	0
86	OHX	6	2177	7/7	0.18	-1.79	129,129,129,129	0
86	OHX	2	2137	7/7	0.18	-1.79	146,146,146,146	0
86	OHX	5	4089	7/7	0.18	-1.79	124,124,124,124	0
86	OHX	5	4107	7/7	0.15	-1.80	98,98,98,98	0
86	OHX	6	2148	7/7	0.24	-1.80	149,149,149,149	0
86	OHX	1	4018	7/7	0.12	-1.80	145,145,145,145	0
85	MG	5	3645	1/1	0.15	-1.80	43,43,43,43	0
86	OHX	1	4162	7/7	0.13	-1.80	118,118,118,118	0
85	MG	5	3884	1/1	0.18	-1.80	63,63,63,63	0
86	OHX	1	4149	7/7	0.15	-1.81	126,126,126,126	0
86	OHX	SR	401	7/7	0.14	-1.81	171,171,171,171	0
86	OHX	1	4086	7/7	0.15	-1.81	150,150,150,150	0
86	OHX	1	4074	7/7	0.27	-1.81	126,126,126,126	0
85	MG	6	1951	1/1	0.18	-1.81	63,63,63,63	0
86	OHX	4	227	7/7	0.17	-1.82	96,96,96,96	0
85	MG	1	3460	1/1	0.19	-1.82	57,57,57,57	0
85	MG	5	3869	1/1	0.17	-1.82	53,53,53,53	0
86	OHX	5	4056	7/7	0.09	-1.83	150,150,150,150	0
85	MG	o7	502	1/1	0.17	-1.83	38,38,38,38	0
86	OHX	1	3884	7/7	0.18	-1.83	64,64,64,64	0
85	MG	2	1942	1/1	0.16	-1.84	74,74,74,74	0
85	MG	m5	301	1/1	0.12	-1.84	39,39,39,39	0
85	MG	5	3816	1/1	0.09	-1.85	47,47,47,47	0
85	MG	5	3497	1/1	0.17	-1.85	39,39,39,39	0
86	OHX	2	2121	7/7	0.15	-1.85	149,149,149,149	0
85	MG	1	3635	1/1	0.18	-1.85	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	4046	7/7	0.10	-1.86	134,134,134,134	0
86	OHX	5	3999	7/7	0.14	-1.86	80,80,80,80	0
86	OHX	5	4042	7/7	0.16	-1.86	111,111,111,111	0
86	OHX	6	2096	7/7	0.12	-1.86	157,157,157,157	0
86	OHX	8	232	7/7	0.17	-1.86	142,142,142,142	0
86	OHX	1	4135	7/7	0.14	-1.86	159,159,159,159	0
86	OHX	c8	203	7/7	0.15	-1.87	157,157,157,157	0
85	MG	1	3579	1/1	0.17	-1.87	28,28,28,28	0
86	OHX	1	4187	7/7	0.15	-1.87	113,113,113,113	0
85	MG	1	3819	1/1	0.18	-1.87	56,56,56,56	0
86	OHX	1	4061	7/7	0.16	-1.87	105,105,105,105	0
86	OHX	5	4233	7/7	0.16	-1.87	138,138,138,138	0
86	OHX	1	4003	7/7	0.09	-1.87	151,151,151,151	0
86	OHX	S8	302	7/7	0.17	-1.88	175,175,175,175	0
86	OHX	5	4036	7/7	0.14	-1.88	132,132,132,132	0
86	OHX	2	2073	7/7	0.18	-1.88	122,122,122,122	0
86	OHX	2	2123	7/7	0.09	-1.88	154,154,154,154	0
86	OHX	1	4093	7/7	0.19	-1.89	98,98,98,98	0
86	OHX	1	3907	7/7	0.17	-1.89	72,72,72,72	0
85	MG	5	3593	1/1	0.20	-1.89	29,29,29,29	0
86	OHX	1	3919	7/7	0.15	-1.89	88,88,88,88	0
85	MG	1	3532	1/1	0.19	-1.90	29,29,29,29	0
85	MG	5	3402	1/1	0.16	-1.90	33,33,33,33	0
86	OHX	5	4060	7/7	0.11	-1.90	156,156,156,156	0
85	MG	1	3625	1/1	0.11	-1.91	47,47,47,47	0
85	MG	N8	202	1/1	0.14	-1.91	52,52,52,52	0
85	MG	5	3600	1/1	0.22	-1.91	43,43,43,43	0
86	OHX	2	2098	7/7	0.14	-1.91	126,126,126,126	0
85	MG	1	3689	1/1	0.20	-1.91	86,86,86,86	0
85	MG	5	3591	1/1	0.20	-1.91	35,35,35,35	0
86	OHX	5	4098	7/7	0.12	-1.92	149,149,149,149	0
85	MG	1	3660	1/1	0.19	-1.92	48,48,48,48	0
86	OHX	1	4163	7/7	0.20	-1.92	155,155,155,155	0
86	OHX	5	3951	7/7	0.14	-1.92	79,79,79,79	0
86	OHX	2	2068	7/7	0.12	-1.93	118,118,118,118	0
85	MG	M7	201	1/1	0.24	-1.93	36,36,36,36	0
86	OHX	6	2164	7/7	0.13	-1.93	192,192,192,192	0
85	MG	1	3573	1/1	0.23	-1.94	34,34,34,34	0
85	MG	1	3552	1/1	0.25	-1.94	36,36,36,36	0
86	OHX	5	4088	7/7	0.20	-1.95	121,121,121,121	0
85	MG	1	3528	1/1	0.26	-1.95	36,36,36,36	0
85	MG	5	3817	1/1	0.18	-1.96	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	1992	1/1	0.12	-1.96	68,68,68,68	0
85	MG	2	2021	1/1	0.17	-1.96	116,116,116,116	0
86	OHX	1	4008	7/7	0.12	-1.96	128,128,128,128	0
85	MG	1	3835	1/1	0.18	-1.97	30,30,30,30	0
85	MG	s4	301	1/1	0.13	-1.97	55,55,55,55	0
85	MG	1	3577	1/1	0.19	-1.97	28,28,28,28	0
86	OHX	1	3889	7/7	0.19	-1.97	71,71,71,71	0
86	OHX	1	3962	7/7	0.16	-1.97	99,99,99,99	0
86	OHX	5	3990	7/7	0.16	-1.98	108,108,108,108	0
85	MG	1	3441	1/1	0.18	-1.99	45,45,45,45	0
85	MG	5	3768	1/1	0.24	-2.00	43,43,43,43	0
85	MG	5	3852	1/1	0.21	-2.00	59,59,59,59	0
86	OHX	6	2144	7/7	0.16	-2.00	145,145,145,145	0
86	OHX	2	2166	7/7	0.07	-2.01	168,168,168,168	0
86	OHX	1	4136	7/7	0.10	-2.01	166,166,166,166	0
86	OHX	6	2200	7/7	0.18	-2.01	152,152,152,152	0
86	OHX	6	2058	7/7	0.17	-2.02	97,97,97,97	0
86	OHX	6	2048	7/7	0.20	-2.02	68,68,68,68	0
86	OHX	2	2150	7/7	0.14	-2.02	197,197,197,197	0
86	OHX	2	2153	7/7	0.12	-2.03	158,158,158,158	0
86	OHX	2	2085	7/7	0.15	-2.03	121,121,121,121	0
86	OHX	2	2173	7/7	0.18	-2.03	170,170,170,170	0
86	OHX	1	3938	7/7	0.15	-2.03	101,101,101,101	0
86	OHX	1	3974	7/7	0.10	-2.03	107,107,107,107	0
86	OHX	5	4168	7/7	0.14	-2.04	173,173,173,173	0
85	MG	1	3434	1/1	0.18	-2.04	35,35,35,35	0
85	MG	1	3559	1/1	0.17	-2.04	52,52,52,52	0
86	OHX	2	2097	7/7	0.10	-2.04	161,161,161,161	0
85	MG	5	3670	1/1	0.17	-2.05	32,32,32,32	0
86	OHX	5	4120	7/7	0.10	-2.05	138,138,138,138	0
86	OHX	6	2172	7/7	0.19	-2.05	153,153,153,153	0
86	OHX	1	3976	7/7	0.10	-2.05	116,116,116,116	0
86	OHX	5	4072	7/7	0.11	-2.05	131,131,131,131	0
85	MG	6	1977	1/1	0.15	-2.05	78,78,78,78	0
86	OHX	1	3920	7/7	0.17	-2.06	93,93,93,93	0
86	OHX	5	4158	7/7	0.13	-2.07	132,132,132,132	0
86	OHX	6	2085	7/7	0.16	-2.07	110,110,110,110	0
86	OHX	5	3998	7/7	0.13	-2.07	118,118,118,118	0
86	OHX	o3	203	7/7	0.11	-2.07	113,113,113,113	0
85	MG	1	3839	1/1	0.21	-2.08	25,25,25,25	0
85	MG	5	3513	1/1	0.14	-2.08	34,34,34,34	0
85	MG	5	3745	1/1	0.17	-2.08	46,46,46,46	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	0.17	-2.09	27,27,27,27	0
86	OHX	1	3999	7/7	0.10	-2.09	109,109,109,109	0
85	MG	1	3531	1/1	0.16	-2.10	63,63,63,63	0
85	MG	q1	101	1/1	0.20	-2.10	44,44,44,44	0
85	MG	N3	203	1/1	0.11	-2.11	54,54,54,54	0
86	OHX	L3	405	7/7	0.10	-2.11	119,119,119,119	0
85	MG	1	3596	1/1	0.24	-2.11	27,27,27,27	0
86	OHX	5	4145	7/7	0.17	-2.11	134,134,134,134	0
85	MG	6	2015	1/1	0.17	-2.11	71,71,71,71	0
85	MG	1	3677	1/1	0.17	-2.11	72,72,72,72	0
85	MG	5	3662	1/1	0.19	-2.11	33,33,33,33	0
85	MG	6	1989	1/1	0.21	-2.12	78,78,78,78	0
86	OHX	5	3923	7/7	0.17	-2.12	65,65,65,65	0
86	OHX	6	2077	7/7	0.13	-2.12	100,100,100,100	0
85	MG	5	3552	1/1	0.26	-2.12	37,37,37,37	0
86	OHX	2	2132	7/7	0.14	-2.12	162,162,162,162	0
86	OHX	1	4155	7/7	0.15	-2.13	157,157,157,157	0
86	OHX	1	3950	7/7	0.15	-2.13	105,105,105,105	0
86	OHX	6	2123	7/7	0.14	-2.13	111,111,111,111	0
85	MG	5	3523	1/1	0.17	-2.13	36,36,36,36	0
86	OHX	5	4021	7/7	0.12	-2.14	116,116,116,116	0
86	OHX	N1	201	7/7	0.17	-2.14	70,70,70,70	0
86	OHX	5	3907	7/7	0.20	-2.14	54,54,54,54	0
85	MG	1	3575	1/1	0.21	-2.15	43,43,43,43	0
86	OHX	4	232	7/7	0.11	-2.15	122,122,122,122	0
86	OHX	1	4094	7/7	0.09	-2.15	140,140,140,140	0
86	OHX	6	2167	7/7	0.07	-2.15	180,180,180,180	0
86	OHX	5	4114	7/7	0.20	-2.15	112,112,112,112	0
86	OHX	5	4188	7/7	0.12	-2.15	132,132,132,132	0
85	MG	1	3847	1/1	0.22	-2.15	30,30,30,30	0
85	MG	5	3504	1/1	0.17	-2.16	45,45,45,45	0
85	MG	O7	103	1/1	0.23	-2.16	44,44,44,44	0
86	OHX	6	2163	7/7	0.16	-2.16	139,139,139,139	0
86	OHX	1	3929	7/7	0.16	-2.17	84,84,84,84	0
85	MG	5	3456	1/1	0.15	-2.17	51,51,51,51	0
85	MG	5	3832	1/1	0.09	-2.17	70,70,70,70	0
85	MG	1	3515	1/1	0.16	-2.17	41,41,41,41	0
86	OHX	1	3953	7/7	0.09	-2.18	114,114,114,114	0
86	OHX	1	3904	7/7	0.18	-2.18	80,80,80,80	0
85	MG	5	3704	1/1	0.15	-2.18	61,61,61,61	0
86	OHX	2	2044	7/7	0.13	-2.18	106,106,106,106	0
85	MG	2	2003	1/1	0.20	-2.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3598	1/1	0.19	-2.19	35,35,35,35	0
86	OHX	5	3915	7/7	0.16	-2.19	68,68,68,68	0
86	OHX	6	2159	7/7	0.07	-2.19	123,123,123,123	0
86	OHX	2	2028	7/7	0.18	-2.19	106,106,106,106	0
86	OHX	1	4168	7/7	0.21	-2.19	152,152,152,152	0
86	OHX	5	3982	7/7	0.17	-2.19	98,98,98,98	0
86	OHX	6	2153	7/7	0.14	-2.19	156,156,156,156	0
86	OHX	1	3893	7/7	0.18	-2.20	75,75,75,75	0
86	OHX	m5	305	7/7	0.14	-2.20	128,128,128,128	0
86	OHX	2	2072	7/7	0.10	-2.20	151,151,151,151	0
85	MG	6	2033	1/1	0.16	-2.21	60,60,60,60	0
86	OHX	5	3927	7/7	0.14	-2.21	86,86,86,86	0
86	OHX	1	3890	7/7	0.16	-2.21	65,65,65,65	0
85	MG	5	3828	1/1	0.17	-2.21	29,29,29,29	0
86	OHX	2	2155	7/7	0.13	-2.22	244,244,244,244	0
86	OHX	2	2069	7/7	0.11	-2.22	132,132,132,132	0
85	MG	5	3833	1/1	0.20	-2.23	40,40,40,40	0
86	OHX	m6	203	7/7	0.14	-2.23	101,101,101,101	0
86	OHX	1	3925	7/7	0.16	-2.23	89,89,89,89	0
85	MG	5	3439	1/1	0.14	-2.24	59,59,59,59	0
85	MG	5	3661	1/1	0.17	-2.24	59,59,59,59	0
86	OHX	1	4184	7/7	0.08	-2.24	245,245,245,245	0
86	OHX	1	3906	7/7	0.17	-2.25	91,91,91,91	0
86	OHX	6	2122	7/7	0.11	-2.25	138,138,138,138	0
85	MG	c8	202	1/1	0.23	-2.25	63,63,63,63	0
86	OHX	8	227	7/7	0.14	-2.25	150,150,150,150	0
86	OHX	1	3991	7/7	0.10	-2.25	122,122,122,122	0
86	OHX	6	2073	7/7	0.14	-2.26	131,131,131,131	0
85	MG	5	3535	1/1	0.13	-2.26	53,53,53,53	0
86	OHX	8	219	7/7	0.09	-2.26	114,114,114,114	0
86	OHX	5	3950	7/7	0.18	-2.26	105,105,105,105	0
85	MG	1	3841	1/1	0.16	-2.26	33,33,33,33	0
86	OHX	l3	404	7/7	0.10	-2.27	105,105,105,105	0
85	MG	1	3734	1/1	0.22	-2.27	40,40,40,40	0
85	MG	1	3506	1/1	0.18	-2.28	42,42,42,42	0
85	MG	1	3747	1/1	0.16	-2.28	40,40,40,40	0
85	MG	2	1984	1/1	0.17	-2.28	69,69,69,69	0
86	OHX	5	4213	7/7	0.14	-2.28	149,149,149,149	0
86	OHX	n3	203	7/7	0.11	-2.28	91,91,91,91	0
86	OHX	5	4187	7/7	0.11	-2.28	144,144,144,144	0
87	ZN	o7	501	1/1	0.13	-2.29	47,47,47,47	0
86	OHX	1	3982	7/7	0.17	-2.29	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	1	3888	7/7	0.17	-2.29	70,70,70,70	0
86	OHX	1	4053	7/7	0.07	-2.29	137,137,137,137	0
86	OHX	1	3997	7/7	0.15	-2.30	137,137,137,137	0
85	MG	5	3703	1/1	0.20	-2.30	40,40,40,40	0
85	MG	1	3558	1/1	0.09	-2.30	57,57,57,57	0
85	MG	5	3855	1/1	0.17	-2.30	65,65,65,65	0
86	OHX	5	4129	7/7	0.10	-2.30	184,184,184,184	0
86	OHX	5	3928	7/7	0.17	-2.31	69,69,69,69	0
86	OHX	5	3926	7/7	0.17	-2.31	78,78,78,78	0
86	OHX	2	2054	7/7	0.13	-2.31	121,121,121,121	0
86	OHX	1	4026	7/7	0.16	-2.31	128,128,128,128	0
86	OHX	5	3968	7/7	0.13	-2.32	100,100,100,100	0
86	OHX	6	2133	7/7	0.12	-2.32	166,166,166,166	0
85	MG	1	3798	1/1	0.15	-2.32	82,82,82,82	0
85	MG	5	3616	1/1	0.10	-2.32	51,51,51,51	0
86	OHX	q2	502	7/7	0.13	-2.32	98,98,98,98	0
86	OHX	5	4046	7/7	0.09	-2.33	129,129,129,129	0
86	OHX	6	2145	7/7	0.12	-2.33	136,136,136,136	0
86	OHX	1	4058	7/7	0.12	-2.33	142,142,142,142	0
86	OHX	5	4039	7/7	0.13	-2.33	123,123,123,123	0
86	OHX	5	3958	7/7	0.16	-2.33	78,78,78,78	0
86	OHX	6	2149	7/7	0.10	-2.33	113,113,113,113	0
86	OHX	6	2066	7/7	0.10	-2.33	96,96,96,96	0
86	OHX	6	2101	7/7	0.12	-2.33	118,118,118,118	0
86	OHX	6	2117	7/7	0.08	-2.34	117,117,117,117	0
86	OHX	5	3935	7/7	0.17	-2.34	80,80,80,80	0
86	OHX	6	2076	7/7	0.18	-2.34	117,117,117,117	0
86	OHX	5	3948	7/7	0.19	-2.34	86,86,86,86	0
86	OHX	5	3910	7/7	0.18	-2.35	61,61,61,61	0
86	OHX	1	3972	7/7	0.10	-2.35	104,104,104,104	0
85	MG	1	3783	1/1	0.21	-2.36	57,57,57,57	0
86	OHX	6	2050	7/7	0.21	-2.36	75,75,75,75	0
86	OHX	1	4039	7/7	0.16	-2.36	117,117,117,117	0
85	MG	5	3755	1/1	0.13	-2.36	48,48,48,48	0
85	MG	1	3433	1/1	0.18	-2.37	44,44,44,44	0
86	OHX	1	4122	7/7	0.11	-2.37	136,136,136,136	0
86	OHX	5	4075	7/7	0.17	-2.37	135,135,135,135	0
86	OHX	6	2086	7/7	0.11	-2.38	115,115,115,115	0
85	MG	6	1961	1/1	0.17	-2.38	47,47,47,47	0
86	OHX	6	2059	7/7	0.15	-2.38	86,86,86,86	0
85	MG	5	3424	1/1	0.17	-2.39	62,62,62,62	0
85	MG	1	3664	1/1	0.15	-2.39	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2203	7/7	0.11	-2.39	197,197,197,197	0
86	OHX	1	4199	7/7	0.15	-2.39	176,176,176,176	0
86	OHX	5	4195	7/7	0.20	-2.40	91,91,91,91	0
86	OHX	2	2070	7/7	0.10	-2.43	133,133,133,133	0
86	OHX	5	4033	7/7	0.12	-2.43	125,125,125,125	0
86	OHX	1	3977	7/7	0.15	-2.43	108,108,108,108	0
86	OHX	5	3994	7/7	0.19	-2.44	100,100,100,100	0
86	OHX	5	3919	7/7	0.17	-2.44	67,67,67,67	0
85	MG	1	3684	1/1	0.11	-2.44	45,45,45,45	0
86	OHX	5	4156	7/7	0.16	-2.45	120,120,120,120	0
86	OHX	5	3975	7/7	0.15	-2.46	102,102,102,102	0
85	MG	1	3710	1/1	0.16	-2.47	44,44,44,44	0
85	MG	1	3788	1/1	0.15	-2.47	52,52,52,52	0
86	OHX	1	4031	7/7	0.10	-2.47	134,134,134,134	0
85	MG	1	3578	1/1	0.10	-2.47	32,32,32,32	0
85	MG	5	3890	1/1	0.15	-2.48	29,29,29,29	0
86	OHX	6	2097	7/7	0.10	-2.49	127,127,127,127	0
86	OHX	6	2166	7/7	0.12	-2.49	152,152,152,152	0
86	OHX	5	4003	7/7	0.15	-2.50	116,116,116,116	0
86	OHX	3	214	7/7	0.14	-2.50	101,101,101,101	0
86	OHX	6	2060	7/7	0.15	-2.50	86,86,86,86	0
85	MG	1	3861	1/1	0.20	-2.51	26,26,26,26	0
85	MG	1	3425	1/1	0.16	-2.51	50,50,50,50	0
85	MG	5	3858	1/1	0.22	-2.51	49,49,49,49	0
85	MG	1	3417	1/1	0.15	-2.51	36,36,36,36	0
86	OHX	5	4000	7/7	0.16	-2.51	120,120,120,120	0
86	OHX	5	4149	7/7	0.15	-2.52	152,152,152,152	0
85	MG	1	3561	1/1	0.18	-2.52	42,42,42,42	0
86	OHX	5	3939	7/7	0.14	-2.52	84,84,84,84	0
86	OHX	5	3922	7/7	0.16	-2.53	69,69,69,69	0
86	OHX	5	4119	7/7	0.12	-2.53	144,144,144,144	0
86	OHX	2	2086	7/7	0.09	-2.53	130,130,130,130	0
85	MG	5	3465	1/1	0.21	-2.54	38,38,38,38	0
86	OHX	5	4004	7/7	0.13	-2.54	128,128,128,128	0
86	OHX	1	3958	7/7	0.17	-2.54	105,105,105,105	0
86	OHX	1	3984	7/7	0.14	-2.54	112,112,112,112	0
86	OHX	1	3985	7/7	0.16	-2.55	115,115,115,115	0
85	MG	1	3757	1/1	0.17	-2.55	62,62,62,62	0
86	OHX	2	2119	7/7	0.14	-2.55	144,144,144,144	0
86	OHX	O7	105	7/7	0.12	-2.56	103,103,103,103	0
86	OHX	2	2107	7/7	0.14	-2.56	141,141,141,141	0
86	OHX	5	4035	7/7	0.15	-2.56	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4116	7/7	0.14	-2.56	124,124,124,124	0
86	OHX	2	2037	7/7	0.15	-2.56	107,107,107,107	0
86	OHX	2	2082	7/7	0.10	-2.56	139,139,139,139	0
86	OHX	2	2152	7/7	0.10	-2.57	182,182,182,182	0
86	OHX	1	3901	7/7	0.16	-2.57	85,85,85,85	0
86	OHX	1	4043	7/7	0.09	-2.57	115,115,115,115	0
86	OHX	1	4038	7/7	0.10	-2.58	105,105,105,105	0
85	MG	5	3741	1/1	0.18	-2.58	56,56,56,56	0
86	OHX	1	4030	7/7	0.14	-2.59	117,117,117,117	0
86	OHX	1	3964	7/7	0.10	-2.59	115,115,115,115	0
85	MG	5	3866	1/1	0.23	-2.60	49,49,49,49	0
86	OHX	6	2064	7/7	0.15	-2.60	103,103,103,103	0
86	OHX	1	3947	7/7	0.16	-2.60	102,102,102,102	0
86	OHX	5	4103	7/7	0.15	-2.60	119,119,119,119	0
86	OHX	5	3993	7/7	0.15	-2.61	113,113,113,113	0
85	MG	5	3516	1/1	0.15	-2.61	40,40,40,40	0
86	OHX	2	2113	7/7	0.09	-2.62	167,167,167,167	0
86	OHX	2	2154	7/7	0.18	-2.62	152,152,152,152	0
85	MG	5	3588	1/1	0.14	-2.63	29,29,29,29	0
86	OHX	5	3957	7/7	0.15	-2.63	77,77,77,77	0
86	OHX	1	3951	7/7	0.13	-2.63	95,95,95,95	0
86	OHX	1	4052	7/7	0.08	-2.63	128,128,128,128	0
85	MG	1	3810	1/1	0.16	-2.64	62,62,62,62	0
86	OHX	c5	201	7/7	0.09	-2.64	172,172,172,172	0
86	OHX	2	2141	7/7	0.12	-2.65	143,143,143,143	0
86	OHX	6	2142	7/7	0.14	-2.66	132,132,132,132	0
85	MG	5	3871	1/1	0.20	-2.66	39,39,39,39	0
85	MG	L3	401	1/1	0.10	-2.66	75,75,75,75	0
85	MG	5	3592	1/1	0.19	-2.67	44,44,44,44	0
86	OHX	1	3916	7/7	0.20	-2.67	87,87,87,87	0
86	OHX	5	3943	7/7	0.14	-2.67	78,78,78,78	0
86	OHX	1	4075	7/7	0.10	-2.67	137,137,137,137	0
85	MG	1	3542	1/1	0.17	-2.68	31,31,31,31	0
85	MG	5	3445	1/1	0.17	-2.68	30,30,30,30	0
86	OHX	7	219	7/7	0.16	-2.68	105,105,105,105	0
86	OHX	6	2157	7/7	0.14	-2.68	152,152,152,152	0
86	OHX	5	4167	7/7	0.13	-2.70	197,197,197,197	0
85	MG	5	3602	1/1	0.12	-2.70	47,47,47,47	0
86	OHX	5	3933	7/7	0.15	-2.70	79,79,79,79	0
86	OHX	6	2069	7/7	0.13	-2.71	92,92,92,92	0
86	OHX	1	3949	7/7	0.12	-2.71	98,98,98,98	0
86	OHX	5	4182	7/7	0.13	-2.72	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	7	223	7/7	0.10	-2.72	111,111,111,111	0
86	OHX	5	4122	7/7	0.10	-2.72	154,154,154,154	0
86	OHX	2	2043	7/7	0.10	-2.73	107,107,107,107	0
86	OHX	6	2151	7/7	0.14	-2.74	121,121,121,121	0
85	MG	4	215	1/1	0.15	-2.74	59,59,59,59	0
86	OHX	1	4081	7/7	0.11	-2.75	140,140,140,140	0
86	OHX	8	225	7/7	0.12	-2.75	144,144,144,144	0
86	OHX	6	2091	7/7	0.11	-2.75	116,116,116,116	0
86	OHX	6	2115	7/7	0.12	-2.75	133,133,133,133	0
85	MG	2	1930	1/1	0.14	-2.76	67,67,67,67	0
86	OHX	6	2136	7/7	0.15	-2.77	137,137,137,137	0
86	OHX	5	4092	7/7	0.12	-2.78	134,134,134,134	0
86	OHX	5	3961	7/7	0.15	-2.78	99,99,99,99	0
86	OHX	6	2197	7/7	0.09	-2.78	180,180,180,180	0
85	MG	7	211	1/1	0.19	-2.78	37,37,37,37	0
85	MG	7	213	1/1	0.15	-2.79	73,73,73,73	0
86	OHX	1	4102	7/7	0.14	-2.80	152,152,152,152	0
86	OHX	6	2195	7/7	0.12	-2.80	193,193,193,193	0
86	OHX	6	2107	7/7	0.10	-2.80	119,119,119,119	0
86	OHX	2	2125	7/7	0.10	-2.80	143,143,143,143	0
86	OHX	5	3978	7/7	0.13	-2.81	109,109,109,109	0
85	MG	1	3481	1/1	0.20	-2.81	78,78,78,78	0
86	OHX	2	2103	7/7	0.09	-2.81	202,202,202,202	0
86	OHX	6	2098	7/7	0.11	-2.82	156,156,156,156	0
86	OHX	1	3915	7/7	0.16	-2.82	79,79,79,79	0
86	OHX	1	3900	7/7	0.14	-2.82	75,75,75,75	0
86	OHX	6	2138	7/7	0.12	-2.83	125,125,125,125	0
86	OHX	5	4067	7/7	0.17	-2.83	134,134,134,134	0
86	OHX	3	223	7/7	0.14	-2.84	136,136,136,136	0
86	OHX	5	4242	7/7	0.17	-2.84	165,165,165,165	0
85	MG	1	3473	1/1	0.14	-2.85	39,39,39,39	0
86	OHX	5	3980	7/7	0.12	-2.85	89,89,89,89	0
85	MG	7	214	1/1	0.15	-2.85	53,53,53,53	0
86	OHX	6	2191	7/7	0.15	-2.86	150,150,150,150	0
86	OHX	6	2087	7/7	0.12	-2.86	125,125,125,125	0
86	OHX	2	2175	7/7	0.14	-2.87	145,145,145,145	0
86	OHX	L3	406	7/7	0.09	-2.87	164,164,164,164	0
85	MG	1	3496	1/1	0.15	-2.87	53,53,53,53	0
86	OHX	5	4028	7/7	0.15	-2.88	118,118,118,118	0
86	OHX	3	219	7/7	0.10	-2.88	135,135,135,135	0
86	OHX	2	2117	7/7	0.12	-2.89	166,166,166,166	0
85	MG	1	3698	1/1	0.17	-2.90	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	4042	7/7	0.12	-2.90	149,149,149,149	0
86	OHX	1	3921	7/7	0.14	-2.90	105,105,105,105	0
85	MG	1	3630	1/1	0.16	-2.92	67,67,67,67	0
85	MG	1	3411	1/1	0.16	-2.92	50,50,50,50	0
86	OHX	6	2134	7/7	0.15	-2.93	135,135,135,135	0
86	OHX	5	4177	7/7	0.10	-2.93	159,159,159,159	0
85	MG	5	3566	1/1	0.19	-2.93	30,30,30,30	0
85	MG	1	3666	1/1	0.13	-2.93	54,54,54,54	0
86	OHX	5	4053	7/7	0.10	-2.94	131,131,131,131	0
86	OHX	5	3925	7/7	0.16	-2.94	81,81,81,81	0
86	OHX	1	3879	7/7	0.20	-2.94	58,58,58,58	0
85	MG	5	3531	1/1	0.21	-2.95	33,33,33,33	0
86	OHX	2	2087	7/7	0.09	-2.95	140,140,140,140	0
86	OHX	2	2089	7/7	0.11	-2.95	129,129,129,129	0
85	MG	5	3748	1/1	0.13	-2.95	66,66,66,66	0
86	OHX	6	2113	7/7	0.14	-2.96	133,133,133,133	0
86	OHX	5	4059	7/7	0.14	-2.96	130,130,130,130	0
85	MG	1	3504	1/1	0.20	-2.96	29,29,29,29	0
86	OHX	1	4000	7/7	0.10	-2.97	139,139,139,139	0
86	OHX	2	2104	7/7	0.18	-2.97	128,128,128,128	0
85	MG	5	3701	1/1	0.17	-2.97	40,40,40,40	0
86	OHX	2	2093	7/7	0.06	-2.98	158,158,158,158	0
86	OHX	6	2196	7/7	0.12	-2.98	171,171,171,171	0
86	OHX	5	4044	7/7	0.12	-2.98	122,122,122,122	0
86	OHX	4	230	7/7	0.08	-2.98	125,125,125,125	0
85	MG	1	3467	1/1	0.13	-2.99	62,62,62,62	0
86	OHX	5	3989	7/7	0.14	-2.99	97,97,97,97	0
85	MG	1	3487	1/1	0.17	-2.99	49,49,49,49	0
86	OHX	6	2105	7/7	0.11	-2.99	119,119,119,119	0
85	MG	1	3529	1/1	0.22	-2.99	46,46,46,46	0
86	OHX	5	4080	7/7	0.11	-2.99	143,143,143,143	0
86	OHX	5	4078	7/7	0.17	-2.99	108,108,108,108	0
86	OHX	5	4125	7/7	0.20	-2.99	133,133,133,133	0
86	OHX	l5	304	7/7	0.08	-3.00	144,144,144,144	0
85	MG	5	3707	1/1	0.18	-3.00	60,60,60,60	0
86	OHX	C3	201	7/7	0.08	-3.00	167,167,167,167	0
85	MG	1	3704	1/1	0.20	-3.00	47,47,47,47	0
86	OHX	1	4036	7/7	0.15	-3.00	112,112,112,112	0
86	OHX	5	4050	7/7	0.12	-3.01	116,116,116,116	0
86	OHX	5	4097	7/7	0.10	-3.01	130,130,130,130	0
86	OHX	2	2058	7/7	0.12	-3.02	125,125,125,125	0
85	MG	5	3448	1/1	0.16	-3.03	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	2	2053	7/7	0.13	-3.03	136,136,136,136	0
86	OHX	1	4090	7/7	0.08	-3.03	191,191,191,191	0
86	OHX	5	4049	7/7	0.13	-3.04	106,106,106,106	0
85	MG	1	3818	1/1	0.12	-3.05	41,41,41,41	0
86	OHX	2	2157	7/7	0.12	-3.05	260,260,260,260	0
86	OHX	5	3996	7/7	0.13	-3.06	108,108,108,108	0
86	OHX	5	3970	7/7	0.13	-3.06	84,84,84,84	0
85	MG	1	3475	1/1	0.18	-3.07	27,27,27,27	0
85	MG	1	3521	1/1	0.12	-3.07	39,39,39,39	0
85	MG	6	1922	1/1	0.14	-3.08	70,70,70,70	0
85	MG	1	3423	1/1	0.10	-3.08	36,36,36,36	0
86	OHX	6	2198	7/7	0.13	-3.09	149,149,149,149	0
86	OHX	2	2045	7/7	0.12	-3.09	121,121,121,121	0
86	OHX	M0	304	7/7	0.12	-3.09	120,120,120,120	0
85	MG	5	3835	1/1	0.15	-3.09	48,48,48,48	0
86	OHX	D3	202	7/7	0.09	-3.11	148,148,148,148	0
85	MG	1	3520	1/1	0.13	-3.13	42,42,42,42	0
86	OHX	6	2106	7/7	0.11	-3.15	134,134,134,134	0
86	OHX	5	4196	7/7	0.16	-3.15	125,125,125,125	0
86	OHX	3	217	7/7	0.11	-3.15	125,125,125,125	0
86	OHX	5	4023	7/7	0.14	-3.16	109,109,109,109	0
86	OHX	1	4089	7/7	0.08	-3.16	136,136,136,136	0
85	MG	5	3404	1/1	0.17	-3.16	48,48,48,48	0
85	MG	5	3408	1/1	0.09	-3.16	32,32,32,32	0
86	OHX	5	3992	7/7	0.09	-3.16	129,129,129,129	0
85	MG	2	1962	1/1	0.20	-3.17	143,143,143,143	0
86	OHX	1	3994	7/7	0.10	-3.17	111,111,111,111	0
86	OHX	5	4163	7/7	0.17	-3.17	145,145,145,145	0
86	OHX	1	4004	7/7	0.14	-3.17	118,118,118,118	0
86	OHX	7	218	7/7	0.15	-3.17	96,96,96,96	0
85	MG	5	3679	1/1	0.16	-3.18	40,40,40,40	0
85	MG	5	3423	1/1	0.15	-3.19	46,46,46,46	0
86	OHX	5	4115	7/7	0.09	-3.20	130,130,130,130	0
86	OHX	6	2131	7/7	0.08	-3.20	148,148,148,148	0
86	OHX	1	4044	7/7	0.06	-3.20	129,129,129,129	0
85	MG	5	3559	1/1	0.18	-3.23	52,52,52,52	0
86	OHX	8	223	7/7	0.09	-3.24	120,120,120,120	0
85	MG	1	3758	1/1	0.19	-3.24	43,43,43,43	0
85	MG	5	3590	1/1	0.21	-3.24	31,31,31,31	0
85	MG	5	3441	1/1	0.17	-3.24	32,32,32,32	0
85	MG	1	3659	1/1	0.11	-3.25	40,40,40,40	0
85	MG	1	3868	1/1	0.13	-3.26	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3955	7/7	0.12	-3.26	86,86,86,86	0
86	OHX	5	4054	7/7	0.09	-3.26	138,138,138,138	0
86	OHX	1	3965	7/7	0.12	-3.26	110,110,110,110	0
85	MG	6	2007	1/1	0.18	-3.28	48,48,48,48	0
86	OHX	2	2101	7/7	0.08	-3.28	145,145,145,145	0
86	OHX	1	4100	7/7	0.12	-3.30	156,156,156,156	0
85	MG	5	3518	1/1	0.17	-3.30	40,40,40,40	0
86	OHX	6	2061	7/7	0.16	-3.31	90,90,90,90	0
86	OHX	1	4156	7/7	0.10	-3.31	118,118,118,118	0
86	OHX	1	3944	7/7	0.14	-3.31	99,99,99,99	0
86	OHX	5	4160	7/7	0.17	-3.32	118,118,118,118	0
85	MG	5	3639	1/1	0.13	-3.32	53,53,53,53	0
86	OHX	5	4127	7/7	0.10	-3.32	142,142,142,142	0
86	OHX	1	4057	7/7	0.08	-3.32	158,158,158,158	0
86	OHX	1	4133	7/7	0.12	-3.32	131,131,131,131	0
86	OHX	6	2143	7/7	0.09	-3.33	148,148,148,148	0
86	OHX	5	4118	7/7	0.08	-3.35	151,151,151,151	0
85	MG	1	3838	1/1	0.18	-3.36	37,37,37,37	0
86	OHX	1	4079	7/7	0.12	-3.37	127,127,127,127	0
85	MG	1	3463	1/1	0.19	-3.37	28,28,28,28	0
86	OHX	1	4027	7/7	0.09	-3.37	120,120,120,120	0
86	OHX	1	4045	7/7	0.17	-3.37	118,118,118,118	0
86	OHX	1	3946	7/7	0.16	-3.39	99,99,99,99	0
85	MG	1	3869	1/1	0.13	-3.39	54,54,54,54	0
86	OHX	5	4051	7/7	0.10	-3.40	108,108,108,108	0
86	OHX	5	4220	7/7	0.11	-3.41	151,151,151,151	0
86	OHX	6	2188	7/7	0.17	-3.41	171,171,171,171	0
85	MG	6	1999	1/1	0.14	-3.41	54,54,54,54	0
85	MG	1	3461	1/1	0.17	-3.42	33,33,33,33	0
86	OHX	1	3989	7/7	0.15	-3.43	101,101,101,101	0
86	OHX	2	2071	7/7	0.08	-3.43	128,128,128,128	0
86	OHX	2	2168	7/7	0.10	-3.43	163,163,163,163	0
86	OHX	2	2060	7/7	0.10	-3.44	134,134,134,134	0
86	OHX	1	4142	7/7	0.16	-3.44	135,135,135,135	0
86	OHX	5	4032	7/7	0.14	-3.46	136,136,136,136	0
86	OHX	5	4076	7/7	0.11	-3.48	120,120,120,120	0
85	MG	5	3560	1/1	0.19	-3.49	34,34,34,34	0
86	OHX	5	3976	7/7	0.15	-3.49	85,85,85,85	0
85	MG	1	3513	1/1	0.18	-3.50	28,28,28,28	0
85	MG	5	3691	1/1	0.12	-3.50	54,54,54,54	0
86	OHX	8	222	7/7	0.12	-3.51	123,123,123,123	0
86	OHX	5	4209	7/7	0.15	-3.51	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3943	7/7	0.16	-3.51	101,101,101,101	0
86	OHX	2	2112	7/7	0.15	-3.52	140,140,140,140	0
85	MG	5	3546	1/1	0.12	-3.52	37,37,37,37	0
86	OHX	6	2102	7/7	0.16	-3.52	123,123,123,123	0
86	OHX	6	2154	7/7	0.14	-3.54	143,143,143,143	0
86	OHX	6	2080	7/7	0.14	-3.54	104,104,104,104	0
86	OHX	2	2077	7/7	0.06	-3.54	139,139,139,139	0
86	OHX	5	4082	7/7	0.17	-3.54	132,132,132,132	0
85	MG	5	3454	1/1	0.09	-3.55	42,42,42,42	0
86	OHX	5	4207	7/7	0.15	-3.56	142,142,142,142	0
86	OHX	1	4024	7/7	0.12	-3.57	141,141,141,141	0
85	MG	1	3766	1/1	0.13	-3.57	41,41,41,41	0
86	OHX	d4	201	7/7	0.10	-3.57	157,157,157,157	0
85	MG	1	3419	1/1	0.18	-3.58	55,55,55,55	0
86	OHX	5	4111	7/7	0.10	-3.58	119,119,119,119	0
85	MG	2	1979	1/1	0.19	-3.60	72,72,72,72	0
86	OHX	5	4058	7/7	0.12	-3.60	128,128,128,128	0
86	OHX	1	3895	7/7	0.15	-3.60	75,75,75,75	0
86	OHX	5	4022	7/7	0.16	-3.60	112,112,112,112	0
86	OHX	1	4073	7/7	0.13	-3.60	131,131,131,131	0
85	MG	5	3698	1/1	0.15	-3.60	46,46,46,46	0
86	OHX	6	2103	7/7	0.10	-3.60	130,130,130,130	0
86	OHX	1	3966	7/7	0.11	-3.61	98,98,98,98	0
85	MG	5	3540	1/1	0.18	-3.61	46,46,46,46	0
86	OHX	5	3940	7/7	0.12	-3.62	94,94,94,94	0
86	OHX	1	3887	7/7	0.16	-3.63	70,70,70,70	0
85	MG	2	1908	1/1	0.12	-3.63	74,74,74,74	0
86	OHX	2	2059	7/7	0.08	-3.64	113,113,113,113	0
86	OHX	6	2109	7/7	0.10	-3.65	120,120,120,120	0
86	OHX	6	2114	7/7	0.10	-3.65	132,132,132,132	0
86	OHX	2	2036	7/7	0.17	-3.65	124,124,124,124	0
85	MG	1	3546	1/1	0.12	-3.65	47,47,47,47	0
86	OHX	5	4055	7/7	0.14	-3.66	119,119,119,119	0
85	MG	1	3436	1/1	0.16	-3.66	50,50,50,50	0
86	OHX	1	3981	7/7	0.10	-3.67	112,112,112,112	0
86	OHX	5	4026	7/7	0.15	-3.69	122,122,122,122	0
86	OHX	3	215	7/7	0.09	-3.69	115,115,115,115	0
85	MG	1	3776	1/1	0.18	-3.69	72,72,72,72	0
86	OHX	5	4236	7/7	0.16	-3.70	158,158,158,158	0
86	OHX	5	3984	7/7	0.13	-3.70	91,91,91,91	0
86	OHX	1	4113	7/7	0.10	-3.73	128,128,128,128	0
86	OHX	1	4056	7/7	0.09	-3.73	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	4001	7/7	0.12	-3.73	106,106,106,106	0
86	OHX	5	4084	7/7	0.11	-3.74	122,122,122,122	0
85	MG	5	3836	1/1	0.14	-3.75	68,68,68,68	0
85	MG	5	3478	1/1	0.15	-3.75	33,33,33,33	0
86	OHX	5	4101	7/7	0.10	-3.80	134,134,134,134	0
86	OHX	6	2074	7/7	0.12	-3.81	93,93,93,93	0
86	OHX	1	4095	7/7	0.10	-3.81	159,159,159,159	0
86	OHX	5	4024	7/7	0.13	-3.81	93,93,93,93	0
86	OHX	1	4021	7/7	0.13	-3.81	119,119,119,119	0
86	OHX	1	4114	7/7	0.13	-3.81	147,147,147,147	0
86	OHX	6	2078	7/7	0.10	-3.82	109,109,109,109	0
85	MG	6	1925	1/1	0.20	-3.82	51,51,51,51	0
86	OHX	1	4063	7/7	0.06	-3.83	182,182,182,182	0
86	OHX	5	3965	7/7	0.13	-3.85	100,100,100,100	0
86	OHX	5	4095	7/7	0.10	-3.85	138,138,138,138	0
86	OHX	5	3942	7/7	0.19	-3.86	88,88,88,88	0
86	OHX	5	4009	7/7	0.12	-3.86	116,116,116,116	0
86	OHX	1	4088	7/7	0.12	-3.87	145,145,145,145	0
85	MG	1	3751	1/1	0.11	-3.88	43,43,43,43	0
85	MG	1	3775	1/1	0.10	-3.89	41,41,41,41	0
85	MG	1	3735	1/1	0.09	-3.89	48,48,48,48	0
86	OHX	1	3998	7/7	0.09	-3.90	133,133,133,133	0
85	MG	1	3424	1/1	0.17	-3.90	44,44,44,44	0
85	MG	1	3590	1/1	0.20	-3.91	42,42,42,42	0
86	OHX	1	4120	7/7	0.12	-3.93	133,133,133,133	0
86	OHX	5	4205	7/7	0.11	-3.94	153,153,153,153	0
86	OHX	1	4055	7/7	0.09	-3.96	121,121,121,121	0
85	MG	5	3688	1/1	0.12	-3.98	76,76,76,76	0
85	MG	5	3557	1/1	0.15	-3.98	46,46,46,46	0
85	MG	5	3696	1/1	0.16	-3.98	54,54,54,54	0
85	MG	5	3472	1/1	0.19	-3.99	57,57,57,57	0
86	OHX	1	4128	7/7	0.10	-3.99	147,147,147,147	0
85	MG	5	3401	1/1	0.12	-4.00	61,61,61,61	0
86	OHX	1	4032	7/7	0.11	-4.00	129,129,129,129	0
86	OHX	2	2081	7/7	0.08	-4.01	158,158,158,158	0
86	OHX	7	227	7/7	0.13	-4.01	150,150,150,150	0
86	OHX	5	4066	7/7	0.13	-4.02	140,140,140,140	0
86	OHX	5	4137	7/7	0.10	-4.04	147,147,147,147	0
85	MG	5	3677	1/1	0.22	-4.05	48,48,48,48	0
85	MG	5	3786	1/1	0.14	-4.05	31,31,31,31	0
85	MG	5	3692	1/1	0.14	-4.09	43,43,43,43	0
86	OHX	1	3937	7/7	0.14	-4.10	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	2	2074	7/7	0.12	-4.11	151,151,151,151	0
86	OHX	1	4211	7/7	0.15	-4.12	139,139,139,139	0
86	OHX	1	4049	7/7	0.08	-4.13	114,114,114,114	0
85	MG	1	3489	1/1	0.13	-4.13	39,39,39,39	0
86	OHX	8	224	7/7	0.09	-4.13	126,126,126,126	0
86	OHX	19	202	7/7	0.09	-4.14	132,132,132,132	0
86	OHX	5	3969	7/7	0.13	-4.17	94,94,94,94	0
86	OHX	1	4047	7/7	0.11	-4.18	115,115,115,115	0
86	OHX	6	2118	7/7	0.10	-4.19	144,144,144,144	0
86	OHX	1	3936	7/7	0.12	-4.19	91,91,91,91	0
86	OHX	1	4078	7/7	0.10	-4.19	129,129,129,129	0
85	MG	2	1940	1/1	0.08	-4.19	71,71,71,71	0
85	MG	5	3477	1/1	0.18	-4.20	39,39,39,39	0
85	MG	6	2014	1/1	0.16	-4.20	41,41,41,41	0
86	OHX	2	2062	7/7	0.08	-4.20	136,136,136,136	0
85	MG	1	3658	1/1	0.14	-4.21	36,36,36,36	0
86	OHX	5	4043	7/7	0.10	-4.21	127,127,127,127	0
86	OHX	2	2061	7/7	0.10	-4.22	131,131,131,131	0
86	OHX	5	3979	7/7	0.12	-4.23	91,91,91,91	0
86	OHX	5	4138	7/7	0.18	-4.23	134,134,134,134	0
86	OHX	1	3993	7/7	0.07	-4.24	127,127,127,127	0
86	OHX	C5	201	7/7	0.08	-4.25	176,176,176,176	0
85	MG	6	1995	1/1	0.13	-4.26	57,57,57,57	0
86	OHX	1	4028	7/7	0.07	-4.26	147,147,147,147	0
86	OHX	5	3988	7/7	0.10	-4.28	112,112,112,112	0
86	OHX	1	3996	7/7	0.11	-4.29	111,111,111,111	0
86	OHX	1	3927	7/7	0.14	-4.30	96,96,96,96	0
86	OHX	2	2049	7/7	0.09	-4.30	123,123,123,123	0
86	OHX	5	4165	7/7	0.08	-4.32	158,158,158,158	0
86	OHX	2	2164	7/7	0.07	-4.32	181,181,181,181	0
85	MG	1	3600	1/1	0.10	-4.34	41,41,41,41	0
85	MG	5	3587	1/1	0.22	-4.34	28,28,28,28	0
86	OHX	5	4194	7/7	0.13	-4.34	129,129,129,129	0
86	OHX	1	3992	7/7	0.12	-4.34	117,117,117,117	0
85	MG	5	3793	1/1	0.17	-4.35	46,46,46,46	0
85	MG	5	3512	1/1	0.16	-4.36	29,29,29,29	0
86	OHX	6	2075	7/7	0.11	-4.36	111,111,111,111	0
85	MG	4	210	1/1	0.17	-4.37	44,44,44,44	0
86	OHX	4	231	7/7	0.11	-4.37	114,114,114,114	0
85	MG	1	3601	1/1	0.08	-4.37	29,29,29,29	0
86	OHX	5	4212	7/7	0.09	-4.39	207,207,207,207	0
86	OHX	1	4121	7/7	0.11	-4.39	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4174	7/7	0.13	-4.40	139,139,139,139	0
86	OHX	4	228	7/7	0.11	-4.40	104,104,104,104	0
85	MG	1	3469	1/1	0.18	-4.40	46,46,46,46	0
85	MG	1	3477	1/1	0.14	-4.42	36,36,36,36	0
86	OHX	1	3954	7/7	0.15	-4.43	128,128,128,128	0
86	OHX	1	4048	7/7	0.09	-4.44	110,110,110,110	0
86	OHX	8	229	7/7	0.11	-4.44	144,144,144,144	0
86	OHX	5	4140	7/7	0.10	-4.45	138,138,138,138	0
85	MG	1	3492	1/1	0.18	-4.45	35,35,35,35	0
86	OHX	1	3970	7/7	0.13	-4.46	108,108,108,108	0
85	MG	1	3699	1/1	0.14	-4.47	47,47,47,47	0
85	MG	5	3447	1/1	0.16	-4.48	49,49,49,49	0
85	MG	5	3767	1/1	0.15	-4.48	65,65,65,65	0
86	OHX	5	4109	7/7	0.13	-4.48	128,128,128,128	0
86	OHX	1	3940	7/7	0.09	-4.51	100,100,100,100	0
85	MG	5	3536	1/1	0.11	-4.51	41,41,41,41	0
85	MG	1	3407	1/1	0.15	-4.52	44,44,44,44	0
86	OHX	5	3981	7/7	0.14	-4.52	101,101,101,101	0
85	MG	1	3442	1/1	0.10	-4.53	47,47,47,47	0
85	MG	5	3789	1/1	0.12	-4.53	54,54,54,54	0
86	OHX	1	4011	7/7	0.10	-4.54	123,123,123,123	0
86	OHX	6	2112	7/7	0.10	-4.55	111,111,111,111	0
86	OHX	1	3995	7/7	0.13	-4.55	113,113,113,113	0
86	OHX	5	4193	7/7	0.13	-4.55	156,156,156,156	0
86	OHX	6	2158	7/7	0.09	-4.57	146,146,146,146	0
85	MG	1	3857	1/1	0.17	-4.57	64,64,64,64	0
86	OHX	6	2130	7/7	0.10	-4.59	127,127,127,127	0
86	OHX	5	4201	7/7	0.15	-4.60	146,146,146,146	0
85	MG	5	3629	1/1	0.16	-4.60	57,57,57,57	0
86	OHX	1	4180	7/7	0.12	-4.60	155,155,155,155	0
86	OHX	4	229	7/7	0.11	-4.61	120,120,120,120	0
86	OHX	1	4158	7/7	0.15	-4.61	154,154,154,154	0
85	MG	5	3863	1/1	0.17	-4.63	41,41,41,41	0
86	OHX	1	4104	7/7	0.11	-4.63	128,128,128,128	0
86	OHX	1	4005	7/7	0.11	-4.63	95,95,95,95	0
85	MG	5	3897	1/1	0.16	-4.64	46,46,46,46	0
85	MG	1	3754	1/1	0.13	-4.65	50,50,50,50	0
86	OHX	1	4157	7/7	0.07	-4.66	140,140,140,140	0
85	MG	1	3437	1/1	0.11	-4.66	45,45,45,45	0
85	MG	1	3584	1/1	0.13	-4.67	45,45,45,45	0
85	MG	1	3836	1/1	0.16	-4.68	56,56,56,56	0
86	OHX	6	2161	7/7	0.10	-4.68	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4006	7/7	0.12	-4.69	100,100,100,100	0
86	OHX	5	4077	7/7	0.11	-4.75	111,111,111,111	0
85	MG	1	3495	1/1	0.13	-4.75	45,45,45,45	0
86	OHX	1	4017	7/7	0.12	-4.75	136,136,136,136	0
86	OHX	7	221	7/7	0.10	-4.75	101,101,101,101	0
85	MG	1	3543	1/1	0.14	-4.76	36,36,36,36	0
86	OHX	2	2064	7/7	0.12	-4.76	118,118,118,118	0
85	MG	1	3451	1/1	0.12	-4.77	46,46,46,46	0
86	OHX	5	4048	7/7	0.09	-4.78	111,111,111,111	0
85	MG	5	3406	1/1	0.14	-4.78	42,42,42,42	0
86	OHX	2	2065	7/7	0.12	-4.79	142,142,142,142	0
85	MG	1	3512	1/1	0.17	-4.80	43,43,43,43	0
85	MG	6	1910	1/1	0.21	-4.80	51,51,51,51	0
86	OHX	1	3968	7/7	0.16	-4.81	104,104,104,104	0
86	OHX	6	2071	7/7	0.12	-4.81	95,95,95,95	0
86	OHX	1	4072	7/7	0.14	-4.82	136,136,136,136	0
85	MG	5	3493	1/1	0.17	-4.84	62,62,62,62	0
86	OHX	5	4018	7/7	0.11	-4.85	122,122,122,122	0
86	OHX	1	4060	7/7	0.08	-4.85	152,152,152,152	0
86	OHX	1	3931	7/7	0.13	-4.86	83,83,83,83	0
86	OHX	5	4131	7/7	0.13	-4.86	135,135,135,135	0
86	OHX	5	4230	7/7	0.08	-4.87	171,171,171,171	0
86	OHX	1	4098	7/7	0.10	-4.88	145,145,145,145	0
86	OHX	2	2080	7/7	0.10	-4.89	143,143,143,143	0
86	OHX	1	4108	7/7	0.07	-4.90	129,129,129,129	0
85	MG	6	1990	1/1	0.11	-4.91	53,53,53,53	0
85	MG	5	3605	1/1	0.17	-4.92	42,42,42,42	0
86	OHX	2	2108	7/7	0.10	-4.93	163,163,163,163	0
86	OHX	1	4112	7/7	0.10	-4.93	143,143,143,143	0
86	OHX	2	2057	7/7	0.09	-4.93	111,111,111,111	0
86	OHX	5	4013	7/7	0.12	-4.94	111,111,111,111	0
85	MG	6	2029	1/1	0.15	-4.94	105,105,105,105	0
86	OHX	1	3963	7/7	0.09	-4.95	82,82,82,82	0
85	MG	1	3550	1/1	0.13	-5.00	39,39,39,39	0
86	OHX	1	4080	7/7	0.09	-5.01	133,133,133,133	0
86	OHX	5	4091	7/7	0.09	-5.01	135,135,135,135	0
85	MG	1	3662	1/1	0.14	-5.03	43,43,43,43	0
85	MG	5	3845	1/1	0.19	-5.05	42,42,42,42	0
85	MG	5	3879	1/1	0.17	-5.05	37,37,37,37	0
85	MG	5	3642	1/1	0.13	-5.06	41,41,41,41	0
85	MG	1	3623	1/1	0.15	-5.07	45,45,45,45	0
85	MG	1	3820	1/1	0.18	-5.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2125	7/7	0.07	-5.12	138,138,138,138	0
86	OHX	5	4121	7/7	0.07	-5.13	157,157,157,157	0
86	OHX	5	4210	7/7	0.12	-5.13	148,148,148,148	0
86	OHX	1	4050	7/7	0.12	-5.14	116,116,116,116	0
86	OHX	5	4198	7/7	0.13	-5.14	128,128,128,128	0
86	OHX	6	2111	7/7	0.14	-5.14	129,129,129,129	0
86	OHX	6	2110	7/7	0.14	-5.15	134,134,134,134	0
86	OHX	1	3910	7/7	0.12	-5.19	80,80,80,80	0
86	OHX	1	4169	7/7	0.11	-5.20	169,169,169,169	0
86	OHX	3	220	7/7	0.11	-5.20	148,148,148,148	0
85	MG	5	3678	1/1	0.12	-5.21	45,45,45,45	0
86	OHX	5	3987	7/7	0.10	-5.22	103,103,103,103	0
86	OHX	6	2180	7/7	0.09	-5.23	164,164,164,164	0
86	OHX	5	4128	7/7	0.14	-5.24	122,122,122,122	0
86	OHX	2	2127	7/7	0.07	-5.26	154,154,154,154	0
86	OHX	2	2122	7/7	0.11	-5.27	148,148,148,148	0
85	MG	5	3854	1/1	0.26	-5.27	84,84,84,84	0
86	OHX	7	220	7/7	0.10	-5.27	104,104,104,104	0
86	OHX	5	4029	7/7	0.09	-5.27	109,109,109,109	0
85	MG	1	3560	1/1	0.14	-5.30	31,31,31,31	0
86	OHX	1	4107	7/7	0.12	-5.33	144,144,144,144	0
86	OHX	1	3980	7/7	0.11	-5.35	108,108,108,108	0
86	OHX	1	3986	7/7	0.10	-5.35	82,82,82,82	0
86	OHX	6	2127	7/7	0.18	-5.40	129,129,129,129	0
86	OHX	1	4151	7/7	0.10	-5.40	159,159,159,159	0
86	OHX	5	4083	7/7	0.06	-5.42	134,134,134,134	0
86	OHX	1	4091	7/7	0.15	-5.45	132,132,132,132	0
86	OHX	3	216	7/7	0.12	-5.46	109,109,109,109	0
86	OHX	6	2129	7/7	0.09	-5.47	141,141,141,141	0
86	OHX	1	4181	7/7	0.13	-5.48	163,163,163,163	0
85	MG	5	3436	1/1	0.18	-5.51	32,32,32,32	0
86	OHX	5	3944	7/7	0.18	-5.54	79,79,79,79	0
86	OHX	5	4224	7/7	0.09	-5.57	139,139,139,139	0
86	OHX	5	4247	7/7	0.11	-5.59	145,145,145,145	0
85	MG	5	3530	1/1	0.11	-5.62	32,32,32,32	0
85	MG	1	3743	1/1	0.10	-5.63	57,57,57,57	0
85	MG	5	3702	1/1	0.10	-5.70	62,62,62,62	0
86	OHX	3	218	7/7	0.10	-5.75	129,129,129,129	0
85	MG	5	3452	1/1	0.14	-5.79	32,32,32,32	0
86	OHX	5	4007	7/7	0.12	-5.80	112,112,112,112	0
86	OHX	1	4025	7/7	0.09	-5.81	116,116,116,116	0
85	MG	5	3785	1/1	0.12	-5.84	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
86	OHX	5	4065	7/7	0.07	-5.86	148,148,148,148	0
86	OHX	1	3898	7/7	0.16	-5.92	74,74,74,74	0
85	MG	5	3655	1/1	0.08	-5.94	30,30,30,30	0
86	OHX	6	2089	7/7	0.08	-5.94	116,116,116,116	0
86	OHX	1	4019	7/7	0.07	-5.96	125,125,125,125	0
86	OHX	1	4096	7/7	0.15	-5.97	125,125,125,125	0
86	OHX	5	4124	7/7	0.15	-5.98	134,134,134,134	0
86	OHX	6	2090	7/7	0.12	-6.00	122,122,122,122	0
86	OHX	2	2105	7/7	0.06	-6.04	143,143,143,143	0
86	OHX	5	4061	7/7	0.09	-6.06	122,122,122,122	0
86	OHX	5	4154	7/7	0.11	-6.07	146,146,146,146	0
86	OHX	1	4014	7/7	0.11	-6.13	129,129,129,129	0
85	MG	1	3750	1/1	0.10	-6.14	31,31,31,31	0
85	MG	8	211	1/1	0.14	-6.15	63,63,63,63	0
86	OHX	1	3959	7/7	0.14	-6.19	100,100,100,100	0
86	OHX	1	4131	7/7	0.09	-6.21	153,153,153,153	0
86	OHX	1	4101	7/7	0.07	-6.24	151,151,151,151	0
86	OHX	5	4047	7/7	0.07	-6.28	114,114,114,114	0
85	MG	1	3449	1/1	0.13	-6.29	36,36,36,36	0
85	MG	1	3634	1/1	0.17	-6.29	72,72,72,72	0
86	OHX	1	4064	7/7	0.09	-6.33	129,129,129,129	0
86	OHX	5	4062	7/7	0.08	-6.37	119,119,119,119	0
86	OHX	5	3962	7/7	0.12	-6.38	85,85,85,85	0
86	OHX	6	2155	7/7	0.09	-6.42	117,117,117,117	0
86	OHX	1	4076	7/7	0.12	-6.45	152,152,152,152	0
86	OHX	2	2078	7/7	0.09	-6.46	131,131,131,131	0
86	OHX	5	4052	7/7	0.11	-6.46	115,115,115,115	0
86	OHX	3	222	7/7	0.08	-6.47	172,172,172,172	0
86	OHX	2	2094	7/7	0.08	-6.53	159,159,159,159	0
86	OHX	5	4164	7/7	0.08	-6.57	132,132,132,132	0
86	OHX	1	4126	7/7	0.13	-6.57	152,152,152,152	0
85	MG	1	3712	1/1	0.10	-6.60	54,54,54,54	0
86	OHX	1	3933	7/7	0.13	-6.64	90,90,90,90	0
86	OHX	5	4147	7/7	0.17	-6.66	151,151,151,151	0
86	OHX	6	2152	7/7	0.07	-6.71	161,161,161,161	0
86	OHX	5	4030	7/7	0.13	-6.72	116,116,116,116	0
85	MG	5	3637	1/1	0.11	-6.73	56,56,56,56	0
86	OHX	5	4135	7/7	0.10	-6.76	137,137,137,137	0
86	OHX	2	2126	7/7	0.12	-6.78	141,141,141,141	0
86	OHX	1	4134	7/7	0.09	-6.78	174,174,174,174	0
85	MG	1	3474	1/1	0.12	-6.81	31,31,31,31	0
86	OHX	1	4125	7/7	0.12	-6.84	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3732	1/1	0.07	-6.86	75,75,75,75	0
85	MG	1	3862	1/1	0.11	-6.86	81,81,81,81	0
86	OHX	1	3942	7/7	0.14	-6.88	105,105,105,105	0
86	OHX	1	4016	7/7	0.10	-6.95	129,129,129,129	0
86	OHX	5	4041	7/7	0.08	-7.03	128,128,128,128	0
86	OHX	6	2169	7/7	0.11	-7.07	167,167,167,167	0
86	OHX	1	4097	7/7	0.10	-7.15	156,156,156,156	0
85	MG	1	3453	1/1	0.09	-7.16	39,39,39,39	0
86	OHX	5	4152	7/7	0.11	-7.20	123,123,123,123	0
85	MG	1	3799	1/1	0.14	-7.26	60,60,60,60	0
86	OHX	5	4016	7/7	0.11	-7.31	110,110,110,110	0
86	OHX	1	4034	7/7	0.07	-7.31	134,134,134,134	0
86	OHX	5	4017	7/7	0.09	-7.38	106,106,106,106	0
86	OHX	5	4214	7/7	0.08	-7.39	110,110,110,110	0
85	MG	1	3627	1/1	0.10	-7.41	41,41,41,41	0
86	OHX	1	4173	7/7	0.10	-7.41	129,129,129,129	0
86	OHX	5	4090	7/7	0.08	-7.45	121,121,121,121	0
86	OHX	3	224	7/7	0.08	-7.47	145,145,145,145	0
85	MG	6	2012	1/1	0.19	-7.49	68,68,68,68	0
85	MG	6	1998	1/1	0.12	-7.50	96,96,96,96	0
85	MG	6	2018	1/1	0.14	-7.62	49,49,49,49	0
85	MG	1	3817	1/1	0.10	-7.67	41,41,41,41	0
86	OHX	2	2124	7/7	0.07	-7.77	136,136,136,136	0
86	OHX	2	2051	7/7	0.10	-7.86	121,121,121,121	0
86	OHX	1	3956	7/7	0.11	-7.87	109,109,109,109	0
85	MG	1	3759	1/1	0.13	-7.90	31,31,31,31	0
86	OHX	1	4161	7/7	0.10	-7.91	112,112,112,112	0
86	OHX	8	220	7/7	0.07	-7.92	118,118,118,118	0
86	OHX	5	4019	7/7	0.08	-7.94	113,113,113,113	0
85	MG	5	3883	1/1	0.14	-7.98	36,36,36,36	0
85	MG	1	3617	1/1	0.12	-8.18	67,67,67,67	0
85	MG	6	1928	1/1	0.17	-8.19	62,62,62,62	0
86	OHX	5	4171	7/7	0.10	-8.21	129,129,129,129	0
85	MG	1	3604	1/1	0.12	-8.25	43,43,43,43	0
86	OHX	1	3960	7/7	0.13	-8.31	101,101,101,101	0
86	OHX	1	4023	7/7	0.10	-8.34	125,125,125,125	0
86	OHX	6	2140	7/7	0.08	-8.41	138,138,138,138	0
86	OHX	6	2067	7/7	0.14	-8.46	96,96,96,96	0
86	OHX	6	2092	7/7	0.10	-8.51	109,109,109,109	0
85	MG	5	3434	1/1	0.12	-8.59	53,53,53,53	0
85	MG	6	2031	1/1	0.11	-8.61	60,60,60,60	0
86	OHX	5	4038	7/7	0.10	-8.64	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4109	7/7	0.09	-8.67	130,130,130,130	0
86	OHX	2	2100	7/7	0.07	-8.84	150,150,150,150	0
86	OHX	5	4123	7/7	0.08	-8.84	144,144,144,144	0
86	OHX	6	2079	7/7	0.12	-8.96	104,104,104,104	0
86	OHX	5	4012	7/7	0.09	-8.98	111,111,111,111	0
85	MG	5	3861	1/1	0.20	-9.00	67,67,67,67	0
86	OHX	6	2139	7/7	0.06	-9.03	143,143,143,143	0
86	OHX	5	4141	7/7	0.09	-9.10	126,126,126,126	0
86	OHX	2	2063	7/7	0.07	-9.23	117,117,117,117	0
85	MG	6	1972	1/1	0.14	-9.27	54,54,54,54	0
86	OHX	2	2111	7/7	0.07	-9.47	170,170,170,170	0
85	MG	8	203	1/1	0.14	-9.62	52,52,52,52	0
85	MG	1	3741	1/1	0.12	-9.63	35,35,35,35	0
85	MG	5	3808	1/1	0.19	-9.67	51,51,51,51	0
85	MG	1	3648	1/1	0.14	-9.73	43,43,43,43	0
86	OHX	4	235	7/7	0.06	-9.87	139,139,139,139	0
86	OHX	1	4207	7/7	0.11	-9.99	147,147,147,147	0
85	MG	5	3431	1/1	0.14	-10.04	69,69,69,69	0
86	OHX	1	4065	7/7	0.09	-10.17	156,156,156,156	0
86	OHX	1	4029	7/7	0.10	-10.22	144,144,144,144	0
85	MG	6	1986	1/1	0.11	-10.31	48,48,48,48	0
86	OHX	1	3978	7/7	0.08	-10.36	111,111,111,111	0
85	MG	1	3641	1/1	0.11	-10.43	70,70,70,70	0
86	OHX	5	4011	7/7	0.09	-10.72	98,98,98,98	0
86	OHX	1	4054	7/7	0.10	-10.80	125,125,125,125	0
86	OHX	5	4069	7/7	0.10	-10.81	121,121,121,121	0
86	OHX	5	4045	7/7	0.06	-10.96	112,112,112,112	0
86	OHX	1	4178	7/7	0.08	-11.10	113,113,113,113	0
86	OHX	1	4013	7/7	0.07	-11.14	117,117,117,117	0
86	OHX	5	4063	7/7	0.07	-11.30	134,134,134,134	0
86	OHX	5	3983	7/7	0.11	-11.44	96,96,96,96	0
86	OHX	7	225	7/7	0.14	-11.55	154,154,154,154	0
86	OHX	1	4159	7/7	0.08	-11.61	138,138,138,138	0
85	MG	2	2010	1/1	0.19	-11.88	72,72,72,72	0
86	OHX	5	4087	7/7	0.08	-12.05	116,116,116,116	0
86	OHX	1	4010	7/7	0.12	-12.16	128,128,128,128	0
86	OHX	1	4197	7/7	0.09	-12.27	151,151,151,151	0
86	OHX	5	4001	7/7	0.13	-12.41	99,99,99,99	0
85	MG	1	3647	1/1	0.15	-12.67	38,38,38,38	0
86	OHX	2	2118	7/7	0.07	-12.69	154,154,154,154	0
86	OHX	5	4094	7/7	0.09	-12.70	128,128,128,128	0
86	OHX	5	4133	7/7	0.08	-12.72	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	5	3891	1/1	0.13	-12.82	92,92,92,92	0
85	MG	1	3792	1/1	0.11	-13.13	49,49,49,49	0
86	OHX	1	4009	7/7	0.10	-13.21	114,114,114,114	0
85	MG	5	3458	1/1	0.15	-13.58	43,43,43,43	0
86	OHX	5	3917	7/7	0.19	-13.67	72,72,72,72	0
85	MG	1	3774	1/1	0.20	-14.00	92,92,92,92	0
86	OHX	5	4176	7/7	0.13	-14.79	157,157,157,157	0
86	OHX	2	2110	7/7	0.08	-15.25	128,128,128,128	0
85	MG	1	3640	1/1	0.09	-15.44	64,64,64,64	0
86	OHX	2	2050	7/7	0.10	-15.67	109,109,109,109	0
86	OHX	6	2150	7/7	0.11	-15.83	145,145,145,145	0
86	OHX	5	4081	7/7	0.07	-16.05	120,120,120,120	0
85	MG	1	3744	1/1	0.18	-17.85	55,55,55,55	0
85	MG	1	3454	1/1	0.18	-19.00	52,52,52,52	0
85	MG	5	3843	1/1	0.14	-20.22	50,50,50,50	0
85	MG	1	3749	1/1	0.15	-20.27	60,60,60,60	0
86	OHX	1	4015	7/7	0.09	-21.29	131,131,131,131	0
86	OHX	5	4068	7/7	0.11	-21.37	122,122,122,122	0
86	OHX	5	4113	7/7	0.10	-21.81	153,153,153,153	0
86	OHX	5	4093	7/7	0.13	-26.27	156,156,156,156	0
85	MG	1	3405	1/1	0.15	-26.60	66,66,66,66	0
85	MG	1	3711	1/1	0.10	-32.93	61,61,61,61	0
85	MG	5	3658	1/1	0.10	-37.83	58,58,58,58	0
85	MG	2	1997	1/1	0.11	-38.50	111,111,111,111	0
85	MG	5	3714	1/1	0.10	-58.69	72,72,72,72	0
85	MG	5	3810	1/1	0.12	-79.67	83,83,83,83	0
85	MG	5	3859	1/1	0.45	-	93,93,93,93	0
85	MG	1	3845	1/1	0.36	-	39,39,39,39	0
85	MG	1	3846	1/1	0.27	-	42,42,42,42	0
85	MG	1	3760	1/1	0.15	-	100,100,100,100	0
85	MG	o1	201	1/1	0.92	-	99,99,99,99	0
85	MG	1	3808	1/1	0.13	-	89,89,89,89	0
85	MG	5	3886	1/1	0.45	-	93,93,93,93	0
85	MG	7	210	1/1	0.15	-	81,81,81,81	0
85	MG	1	3501	1/1	0.32	-	72,72,72,72	0
85	MG	4	219	1/1	0.27	-	48,48,48,48	0
85	MG	3	208	1/1	0.19	-	82,82,82,82	0
85	MG	6	2044	1/1	0.53	-	76,76,76,76	0
85	MG	5	3877	1/1	0.31	-	51,51,51,51	0
85	MG	5	3874	1/1	0.41	-	56,56,56,56	0
85	MG	1	3797	1/1	0.29	-	73,73,73,73	0
85	MG	1	3491	1/1	0.33	-	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	3681	1/1	0.35	-	43,43,43,43	0
85	MG	6	1978	1/1	0.15	-	69,69,69,69	0
85	MG	6	1923	1/1	0.51	-	103,103,103,103	0
85	MG	1	3856	1/1	0.15	-	50,50,50,50	0
85	MG	5	3800	1/1	0.19	-	41,41,41,41	0
85	MG	1	3549	1/1	0.22	-	51,51,51,51	0
85	MG	1	3852	1/1	0.30	-	63,63,63,63	0
85	MG	6	2040	1/1	0.52	-	77,77,77,77	0
85	MG	2	2019	1/1	0.39	-	71,71,71,71	0
85	MG	1	3613	1/1	0.16	-	45,45,45,45	0
85	MG	5	3653	1/1	0.35	-	120,120,120,120	0
85	MG	6	1997	1/1	0.35	-	97,97,97,97	0
85	MG	2	1952	1/1	0.62	-	99,99,99,99	0
85	MG	5	3733	1/1	0.31	-	60,60,60,60	0
85	MG	7	215	1/1	0.23	-	62,62,62,62	0
85	MG	1	3801	1/1	0.12	-	61,61,61,61	0
85	MG	5	3618	1/1	0.37	-	34,34,34,34	0
85	MG	5	3885	1/1	0.35	-	64,64,64,64	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.