



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:42 am GMT

PDB ID : 5TGA  
Title : Crystal structure of the *S.cerevisiae* 80S ribosome in complex with the A-site bound aminoacyl-tRNA analog ACCA-Pro  
Authors : Melnikov, S.; Mailliot, J.  
Deposited on : 2016-09-27  
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

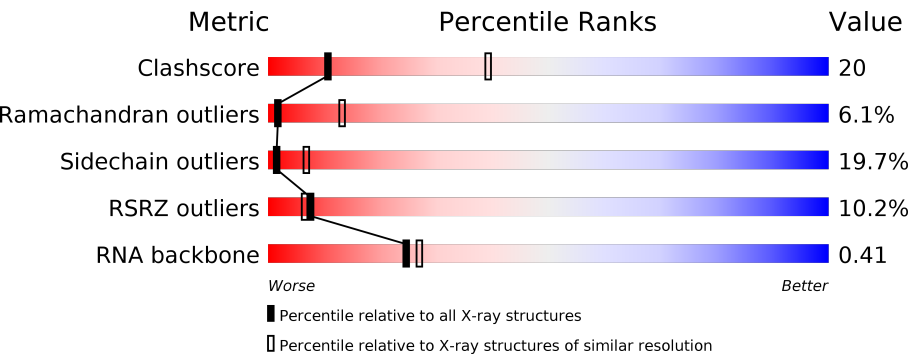
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28972

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)
RNA backbone	2435	1111 (3.80-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1829	<div><div>5%</div><div>25%45%23% . .</div></div>
2	S0	206	<div><div>48%</div><div>23%60%16% .</div></div>
2	s0	206	<div><div>17%</div><div>73%25% .</div></div>
3	S1	216	<div><div>23%</div><div>19%59%19% . .</div></div>
3	s1	216	<div><div>18%</div><div>76%20% .</div></div>
4	S2	217	<div><div>5%</div><div>28%57%14% .</div></div>

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Mol	Chain	Length	Quality of chain
4	s2	217	
5	S3	223	
5	s3	223	
6	S4	260	
6	s4	260	
7	S5	206	
7	s5	206	
8	S6	226	
8	s6	226	
9	S7	186	
9	s7	186	
10	S8	199	
10	s8	199	
11	S9	185	
11	s9	185	
12	C0	96	
13	C1	155	
13	c1	155	
14	C2	124	
14	c2	124	
15	C3	150	
15	c3	150	
16	C4	128	
16	c4	128	
17	C5	135	

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Mol	Chain	Length	Quality of chain
17	c5	135	
18	C6	142	
18	c6	142	
19	C7	125	
19	c7	125	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	110	
22	d0	110	
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	70	
27	d5	70	
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	

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Mol	Chain	Length	Quality of chain
30	D8	63	
30	d8	63	
31	D9	53	
31	d9	53	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	159	
36	1	3394	
36	5	3394	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	252	
39	l2	252	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	

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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	223	
44	l7	223	
45	L8	233	
45	l8	233	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	169	
48	m1	169	
49	M3	194	
49	m3	194	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	197	
52	m6	197	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	

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Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	100	
58	n2	100	
59	N3	136	
59	n3	136	
60	N4	135	
60	n4	135	
61	N5	121	
61	n5	121	
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	100	
66	o0	100	
67	O1	109	
67	o1	109	

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Mol	Chain	Length	Quality of chain
68	O2	127	
68	o2	127	
69	O3	106	
69	o3	106	
70	O4	112	
70	o4	112	
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	6	1800	

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Mol	Chain	Length	Quality of chain
81	c0	96	
82	sM	104	
83	m2	150	
84	p0	219	
85	p1	47	
85	p2	47	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	3407	-	-	-	X
86	OHX	1	3415	-	-	-	X
86	OHX	1	3418	-	-	-	X
86	OHX	1	3422	-	-	-	X
86	OHX	1	3436	-	-	-	X
86	OHX	1	3437	-	-	X	-
86	OHX	1	3439	-	-	-	X
86	OHX	1	3443	-	-	-	X
86	OHX	1	3451	-	-	-	X
86	OHX	1	3452	-	-	-	X
86	OHX	1	3455	-	-	-	X
86	OHX	1	3459	-	-	-	X
86	OHX	1	3464	-	-	-	X
86	OHX	1	3466	-	-	-	X
86	OHX	1	3470	-	-	-	X
86	OHX	1	3471	-	-	-	X
86	OHX	1	3474	-	-	-	X
86	OHX	1	3476	-	-	X	-
86	OHX	1	3479	-	-	X	X
86	OHX	1	3480	-	-	X	-
86	OHX	1	3483	-	-	-	X
86	OHX	1	3485	-	-	-	X
86	OHX	1	3486	-	-	-	X
86	OHX	1	3487	-	-	-	X
86	OHX	1	3494	-	-	X	-
86	OHX	1	3495	-	-	-	X
86	OHX	1	3500	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	3502	-	-	-	X
86	OHX	1	3505	-	-	-	X
86	OHX	1	3507	-	-	-	X
86	OHX	1	3511	-	-	X	-
86	OHX	1	3514	-	-	-	X
86	OHX	1	3518	-	-	X	-
86	OHX	1	3521	-	-	-	X
86	OHX	1	3530	-	-	-	X
86	OHX	1	3531	-	-	-	X
86	OHX	1	3532	-	-	-	X
86	OHX	1	3534	-	-	-	X
86	OHX	1	3536	-	-	-	X
86	OHX	1	3541	-	-	-	X
86	OHX	1	3542	-	-	-	X
86	OHX	1	3544	-	-	-	X
86	OHX	1	3545	-	-	-	X
86	OHX	1	3546	-	-	-	X
86	OHX	1	3547	-	-	-	X
86	OHX	1	3550	-	-	-	X
86	OHX	1	3561	-	-	-	X
86	OHX	1	3570	-	-	-	X
86	OHX	1	3575	-	-	-	X
86	OHX	1	3583	-	-	-	X
86	OHX	1	3585	-	-	-	X
86	OHX	1	3587	-	-	-	X
86	OHX	1	3592	-	-	-	X
86	OHX	1	3593	-	-	-	X
86	OHX	1	3598	-	-	-	X
86	OHX	1	3599	-	-	-	X
86	OHX	1	3603	-	-	-	X
86	OHX	1	3609	-	-	-	X
86	OHX	1	3613	-	-	-	X
86	OHX	1	3627	-	-	-	X
86	OHX	1	3631	-	-	-	X
86	OHX	1	3633	-	-	-	X
86	OHX	1	3635	-	-	-	X
86	OHX	1	3643	-	-	-	X
86	OHX	1	3647	-	-	X	-
86	OHX	1	3652	-	-	-	X
86	OHX	1	3656	-	-	-	X
86	OHX	1	3659	-	-	-	X
86	OHX	1	3661	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	3667	-	-	-	X
86	OHX	1	3669	-	-	-	X
86	OHX	1	3671	-	-	-	X
86	OHX	1	3675	-	-	-	X
86	OHX	1	3684	-	-	-	X
86	OHX	1	3688	-	-	-	X
86	OHX	1	3689	-	-	X	-
86	OHX	1	3691	-	-	X	-
86	OHX	1	3695	-	-	X	X
86	OHX	1	3702	-	-	-	X
86	OHX	1	3703	-	-	-	X
86	OHX	1	3708	-	-	-	X
86	OHX	1	3716	-	-	-	X
86	OHX	1	3725	-	-	-	X
86	OHX	1	3728	-	-	-	X
86	OHX	1	3729	-	-	-	X
86	OHX	1	3730	-	-	-	X
86	OHX	1	3733	-	-	-	X
86	OHX	1	3734	-	-	X	X
86	OHX	1	3737	-	-	X	X
86	OHX	1	3738	-	-	-	X
86	OHX	1	3739	-	-	-	X
86	OHX	1	3745	-	-	-	X
86	OHX	1	3746	-	-	X	-
86	OHX	1	3747	-	-	-	X
86	OHX	1	3748	-	-	-	X
86	OHX	1	3751	-	-	X	-
86	OHX	1	3753	-	-	X	-
86	OHX	1	3759	-	-	-	X
86	OHX	1	3760	-	-	-	X
86	OHX	1	3771	-	-	-	X
86	OHX	1	3774	-	-	-	X
86	OHX	1	3776	-	-	X	-
86	OHX	1	3777	-	-	X	-
86	OHX	1	3779	-	-	X	X
86	OHX	1	3783	-	-	-	X
86	OHX	1	3790	-	-	-	X
86	OHX	1	3791	-	-	X	-
86	OHX	1	3793	-	-	-	X
86	OHX	1	3795	-	-	-	X
86	OHX	1	3797	-	-	X	X
86	OHX	1	3798	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	3799	-	-	X	-
86	OHX	1	3800	-	-	X	-
86	OHX	1	3801	-	-	-	X
86	OHX	1	3802	-	-	-	X
86	OHX	1	3803	-	-	-	X
86	OHX	1	3804	-	-	X	-
86	OHX	1	3805	-	-	X	-
86	OHX	1	3809	-	-	X	-
86	OHX	1	3810	-	-	X	-
86	OHX	2	1905	-	-	-	X
86	OHX	2	1909	-	-	X	-
86	OHX	2	1913	-	-	-	X
86	OHX	2	1918	-	-	X	X
86	OHX	2	1933	-	-	-	X
86	OHX	2	1936	-	-	-	X
86	OHX	2	1938	-	-	-	X
86	OHX	2	1951	-	-	-	X
86	OHX	2	1962	-	-	X	-
86	OHX	2	1964	-	-	X	-
86	OHX	2	1969	-	-	X	-
86	OHX	2	1985	-	-	-	X
86	OHX	2	1989	-	-	-	X
86	OHX	2	2002	-	-	-	X
86	OHX	2	2005	-	-	-	X
86	OHX	2	2009	-	-	-	X
86	OHX	2	2021	-	-	-	X
86	OHX	2	2023	-	-	-	X
86	OHX	2	2029	-	-	-	X
86	OHX	2	2030	-	-	-	X
86	OHX	2	2032	-	-	-	X
86	OHX	2	2035	-	-	X	-
86	OHX	2	2041	-	-	-	X
86	OHX	2	2055	-	-	-	X
86	OHX	2	2060	-	-	-	X
86	OHX	2	2063	-	-	-	X
86	OHX	2	2069	-	-	-	X
86	OHX	2	2070	-	-	-	X
86	OHX	2	2077	-	-	-	X
86	OHX	2	2079	-	-	-	X
86	OHX	2	2080	-	-	-	X
86	OHX	2	2081	-	-	-	X
86	OHX	2	2085	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	2	2088	-	-	-	X
86	OHX	2	2089	-	-	-	X
86	OHX	3	202	-	-	-	X
86	OHX	3	203	-	-	-	X
86	OHX	4	201	-	-	-	X
86	OHX	4	208	-	-	-	X
86	OHX	4	209	-	-	-	X
86	OHX	4	212	-	-	-	X
86	OHX	4	213	-	-	-	X
86	OHX	4	214	-	-	-	X
86	OHX	4	216	-	-	-	X
86	OHX	4	218	-	-	-	X
86	OHX	5	3407	-	-	-	X
86	OHX	5	3417	-	-	-	X
86	OHX	5	3418	-	-	-	X
86	OHX	5	3428	-	-	-	X
86	OHX	5	3433	-	-	-	X
86	OHX	5	3434	-	-	-	X
86	OHX	5	3439	-	-	-	X
86	OHX	5	3440	-	-	-	X
86	OHX	5	3442	-	-	-	X
86	OHX	5	3444	-	-	-	X
86	OHX	5	3445	-	-	-	X
86	OHX	5	3448	-	-	-	X
86	OHX	5	3449	-	-	X	-
86	OHX	5	3452	-	-	-	X
86	OHX	5	3453	-	-	X	X
86	OHX	5	3454	-	-	-	X
86	OHX	5	3457	-	-	X	-
86	OHX	5	3458	-	-	-	X
86	OHX	5	3463	-	-	-	X
86	OHX	5	3465	-	-	X	X
86	OHX	5	3467	-	-	-	X
86	OHX	5	3474	-	-	-	X
86	OHX	5	3475	-	-	-	X
86	OHX	5	3477	-	-	-	X
86	OHX	5	3478	-	-	-	X
86	OHX	5	3482	-	-	X	-
86	OHX	5	3483	-	-	-	X
86	OHX	5	3484	-	-	-	X
86	OHX	5	3487	-	-	-	X
86	OHX	5	3488	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	3489	-	-	-	X
86	OHX	5	3490	-	-	-	X
86	OHX	5	3491	-	-	-	X
86	OHX	5	3492	-	-	-	X
86	OHX	5	3493	-	-	-	X
86	OHX	5	3496	-	-	-	X
86	OHX	5	3502	-	-	-	X
86	OHX	5	3503	-	-	-	X
86	OHX	5	3504	-	-	-	X
86	OHX	5	3506	-	-	-	X
86	OHX	5	3507	-	-	-	X
86	OHX	5	3509	-	-	-	X
86	OHX	5	3515	-	-	-	X
86	OHX	5	3520	-	-	-	X
86	OHX	5	3523	-	-	X	-
86	OHX	5	3524	-	-	X	-
86	OHX	5	3527	-	-	-	X
86	OHX	5	3528	-	-	-	X
86	OHX	5	3529	-	-	-	X
86	OHX	5	3531	-	-	-	X
86	OHX	5	3534	-	-	-	X
86	OHX	5	3539	-	-	-	X
86	OHX	5	3541	-	-	X	-
86	OHX	5	3542	-	-	-	X
86	OHX	5	3543	-	-	-	X
86	OHX	5	3549	-	-	-	X
86	OHX	5	3555	-	-	-	X
86	OHX	5	3557	-	-	-	X
86	OHX	5	3559	-	-	-	X
86	OHX	5	3561	-	-	-	X
86	OHX	5	3568	-	-	-	X
86	OHX	5	3569	-	-	-	X
86	OHX	5	3571	-	-	-	X
86	OHX	5	3572	-	-	-	X
86	OHX	5	3573	-	-	X	-
86	OHX	5	3579	-	-	-	X
86	OHX	5	3580	-	-	X	-
86	OHX	5	3587	-	-	-	X
86	OHX	5	3589	-	-	-	X
86	OHX	5	3590	-	-	X	-
86	OHX	5	3593	-	-	-	X
86	OHX	5	3594	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	3596	-	-	-	X
86	OHX	5	3597	-	-	X	X
86	OHX	5	3600	-	-	-	X
86	OHX	5	3602	-	-	X	X
86	OHX	5	3608	-	-	-	X
86	OHX	5	3610	-	-	-	X
86	OHX	5	3612	-	-	-	X
86	OHX	5	3616	-	-	-	X
86	OHX	5	3618	-	-	-	X
86	OHX	5	3619	-	-	-	X
86	OHX	5	3620	-	-	-	X
86	OHX	5	3623	-	-	-	X
86	OHX	5	3626	-	-	-	X
86	OHX	5	3628	-	-	-	X
86	OHX	5	3633	-	-	-	X
86	OHX	5	3636	-	-	-	X
86	OHX	5	3638	-	-	-	X
86	OHX	5	3647	-	-	-	X
86	OHX	5	3649	-	-	-	X
86	OHX	5	3651	-	-	-	X
86	OHX	5	3653	-	-	-	X
86	OHX	5	3655	-	-	-	X
86	OHX	5	3656	-	-	-	X
86	OHX	5	3657	-	-	-	X
86	OHX	5	3658	-	-	-	X
86	OHX	5	3659	-	-	X	-
86	OHX	5	3661	-	-	-	X
86	OHX	5	3672	-	-	-	X
86	OHX	5	3674	-	-	-	X
86	OHX	5	3676	-	-	-	X
86	OHX	5	3678	-	-	-	X
86	OHX	5	3680	-	-	-	X
86	OHX	5	3681	-	-	-	X
86	OHX	5	3685	-	-	-	X
86	OHX	5	3687	-	-	-	X
86	OHX	5	3688	-	-	X	X
86	OHX	5	3691	-	-	X	X
86	OHX	5	3692	-	-	-	X
86	OHX	5	3694	-	-	-	X
86	OHX	5	3702	-	-	-	X
86	OHX	5	3703	-	-	-	X
86	OHX	5	3705	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	3709	-	-	-	X
86	OHX	5	3716	-	-	X	X
86	OHX	5	3722	-	-	X	X
86	OHX	5	3724	-	-	-	X
86	OHX	5	3725	-	-	-	X
86	OHX	5	3727	-	-	X	-
86	OHX	5	3728	-	-	-	X
86	OHX	5	3729	-	-	X	-
86	OHX	5	3730	-	-	-	X
86	OHX	5	3735	-	-	-	X
86	OHX	5	3741	-	-	-	X
86	OHX	5	3742	-	-	-	X
86	OHX	5	3745	-	-	-	X
86	OHX	5	3749	-	-	-	X
86	OHX	5	3753	-	-	X	X
86	OHX	5	3756	-	-	-	X
86	OHX	5	3757	-	-	X	-
86	OHX	5	3767	-	-	-	X
86	OHX	5	3770	-	-	-	X
86	OHX	5	3772	-	-	-	X
86	OHX	5	3773	-	-	-	X
86	OHX	5	3779	-	-	X	X
86	OHX	5	3782	-	-	-	X
86	OHX	5	3785	-	-	-	X
86	OHX	5	3786	-	-	-	X
86	OHX	5	3789	-	-	-	X
86	OHX	5	3790	-	-	-	X
86	OHX	5	3792	-	-	-	X
86	OHX	5	3796	-	-	X	-
86	OHX	5	3797	-	-	-	X
86	OHX	5	3798	-	-	-	X
86	OHX	5	3802	-	-	-	X
86	OHX	5	3806	-	-	X	-
86	OHX	5	3808	-	-	X	X
86	OHX	5	3810	-	-	X	-
86	OHX	6	1903	-	-	-	X
86	OHX	6	1906	-	-	-	X
86	OHX	6	1909	-	-	X	-
86	OHX	6	1914	-	-	-	X
86	OHX	6	1918	-	-	-	X
86	OHX	6	1920	-	-	X	-
86	OHX	6	1929	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	6	1931	-	-	X	-
86	OHX	6	1939	-	-	-	X
86	OHX	6	1944	-	-	-	X
86	OHX	6	1945	-	-	-	X
86	OHX	6	1946	-	-	-	X
86	OHX	6	1947	-	-	-	X
86	OHX	6	1953	-	-	-	X
86	OHX	6	1959	-	-	-	X
86	OHX	6	1961	-	-	-	X
86	OHX	6	1966	-	-	-	X
86	OHX	6	1969	-	-	-	X
86	OHX	6	1977	-	-	-	X
86	OHX	6	1981	-	-	-	X
86	OHX	6	1985	-	-	-	X
86	OHX	6	1988	-	-	-	X
86	OHX	6	1989	-	-	-	X
86	OHX	6	1993	-	-	-	X
86	OHX	6	1995	-	-	-	X
86	OHX	6	2002	-	-	-	X
86	OHX	6	2003	-	-	-	X
86	OHX	6	2004	-	-	-	X
86	OHX	6	2006	-	-	-	X
86	OHX	6	2007	-	-	-	X
86	OHX	6	2008	-	-	-	X
86	OHX	6	2014	-	-	-	X
86	OHX	6	2015	-	-	-	X
86	OHX	6	2018	-	-	-	X
86	OHX	6	2019	-	-	-	X
86	OHX	6	2023	-	-	-	X
86	OHX	6	2028	-	-	-	X
86	OHX	6	2029	-	-	-	X
86	OHX	6	2036	-	-	-	X
86	OHX	6	2044	-	-	-	X
86	OHX	6	2052	-	-	-	X
86	OHX	6	2054	-	-	-	X
86	OHX	6	2060	-	-	-	X
86	OHX	6	2061	-	-	-	X
86	OHX	6	2068	-	-	-	X
86	OHX	6	2072	-	-	-	X
86	OHX	6	2077	-	-	-	X
86	OHX	6	2082	-	-	X	X
86	OHX	6	2083	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	6	2084	-	-	X	X
86	OHX	6	2085	-	-	-	X
86	OHX	6	2088	-	-	-	X
86	OHX	6	2090	-	-	X	-
86	OHX	6	2093	-	-	-	X
86	OHX	6	2095	-	-	-	X
86	OHX	6	2096	-	-	-	X
86	OHX	6	2098	-	-	X	-
86	OHX	7	203	-	-	-	X
86	OHX	7	205	-	-	-	X
86	OHX	7	209	-	-	-	X
86	OHX	7	211	-	-	-	X
86	OHX	7	213	-	-	-	X
86	OHX	8	206	-	-	-	X
86	OHX	8	207	-	-	X	-
86	OHX	8	208	-	-	-	X
86	OHX	8	209	-	-	-	X
86	OHX	8	210	-	-	-	X
86	OHX	8	212	-	-	X	-
86	OHX	8	213	-	-	-	X
86	OHX	8	216	-	-	-	X
86	OHX	8	221	-	-	X	-
86	OHX	C5	201	-	-	X	-
86	OHX	L4	401	-	-	X	-
86	OHX	M0	301	-	-	-	X
86	OHX	M0	302	-	-	-	X
86	OHX	M0	303	-	-	X	-
86	OHX	M0	304	-	-	X	-
86	OHX	O3	201	-	-	-	X
86	OHX	O7	102	-	-	X	-
86	OHX	Q2	502	-	-	X	-
86	OHX	S2	301	-	-	-	X
86	OHX	m0	302	-	-	-	X
86	OHX	m0	304	-	-	-	X
86	OHX	n3	202	-	-	-	X
86	OHX	o3	201	-	-	-	X
86	OHX	o9	101	-	-	-	X
87	MG	1	3815	-	-	-	X
87	MG	1	3820	-	-	-	X
87	MG	1	3822	-	-	-	X
87	MG	1	3824	-	-	-	X
87	MG	1	3828	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	1	3830	-	-	-	X
87	MG	1	3831	-	-	-	X
87	MG	1	3840	-	-	-	X
87	MG	1	3850	-	-	-	X
87	MG	1	3854	-	-	-	X
87	MG	1	3867	-	-	-	X
87	MG	1	3874	-	-	-	X
87	MG	1	3884	-	-	-	X
87	MG	1	3886	-	-	-	X
87	MG	1	3887	-	-	-	X
87	MG	1	3889	-	-	-	X
87	MG	1	3891	-	-	-	X
87	MG	1	3904	-	-	-	X
87	MG	1	3908	-	-	-	X
87	MG	1	3909	-	-	-	X
87	MG	1	3911	-	-	-	X
87	MG	1	3914	-	-	-	X
87	MG	1	3921	-	-	-	X
87	MG	1	3924	-	-	-	X
87	MG	1	3925	-	-	-	X
87	MG	1	3929	-	-	-	X
87	MG	1	3931	-	-	-	X
87	MG	1	3932	-	-	-	X
87	MG	1	3934	-	-	-	X
87	MG	1	3936	-	-	-	X
87	MG	1	3940	-	-	-	X
87	MG	1	3941	-	-	-	X
87	MG	1	3942	-	-	-	X
87	MG	1	3946	-	-	-	X
87	MG	1	3950	-	-	-	X
87	MG	1	3951	-	-	-	X
87	MG	1	3952	-	-	-	X
87	MG	1	3959	-	-	-	X
87	MG	1	3963	-	-	-	X
87	MG	1	3965	-	-	-	X
87	MG	1	3966	-	-	-	X
87	MG	1	3967	-	-	-	X
87	MG	1	3975	-	-	-	X
87	MG	1	3976	-	-	-	X
87	MG	1	3977	-	-	-	X
87	MG	1	3982	-	-	-	X
87	MG	1	3983	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	1	3989	-	-	-	X
87	MG	1	3992	-	-	-	X
87	MG	1	3993	-	-	-	X
87	MG	1	3994	-	-	-	X
87	MG	1	3997	-	-	-	X
87	MG	1	3998	-	-	-	X
87	MG	1	3999	-	-	-	X
87	MG	1	4007	-	-	-	X
87	MG	1	4009	-	-	-	X
87	MG	1	4010	-	-	-	X
87	MG	1	4012	-	-	-	X
87	MG	1	4013	-	-	-	X
87	MG	1	4017	-	-	-	X
87	MG	1	4019	-	-	-	X
87	MG	1	4020	-	-	-	X
87	MG	1	4022	-	-	-	X
87	MG	1	4024	-	-	-	X
87	MG	1	4025	-	-	-	X
87	MG	1	4034	-	-	-	X
87	MG	1	4040	-	-	-	X
87	MG	1	4041	-	-	-	X
87	MG	1	4050	-	-	-	X
87	MG	1	4059	-	-	-	X
87	MG	1	4060	-	-	-	X
87	MG	1	4061	-	-	-	X
87	MG	1	4082	-	-	-	X
87	MG	1	4091	-	-	-	X
87	MG	1	4093	-	-	-	X
87	MG	1	4094	-	-	-	X
87	MG	1	4111	-	-	-	X
87	MG	1	4116	-	-	-	X
87	MG	1	4134	-	-	-	X
87	MG	1	4135	-	-	-	X
87	MG	1	4137	-	-	-	X
87	MG	1	4139	-	-	-	X
87	MG	1	4140	-	-	-	X
87	MG	1	4143	-	-	-	X
87	MG	1	4151	-	-	-	X
87	MG	1	4157	-	-	-	X
87	MG	1	4159	-	-	-	X
87	MG	1	4160	-	-	-	X
87	MG	1	4170	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	1	4173	-	-	-	X
87	MG	1	4174	-	-	-	X
87	MG	1	4193	-	-	-	X
87	MG	1	4198	-	-	-	X
87	MG	1	4200	-	-	-	X
87	MG	1	4201	-	-	-	X
87	MG	1	4202	-	-	-	X
87	MG	1	4203	-	-	-	X
87	MG	1	4206	-	-	-	X
87	MG	1	4208	-	-	-	X
87	MG	1	4210	-	-	-	X
87	MG	1	4211	-	-	-	X
87	MG	1	4212	-	-	-	X
87	MG	1	4215	-	-	-	X
87	MG	1	4220	-	-	-	X
87	MG	1	4225	-	-	-	X
87	MG	1	4242	-	-	-	X
87	MG	1	4243	-	-	-	X
87	MG	1	4250	-	-	-	X
87	MG	1	4257	-	-	-	X
87	MG	1	4266	-	-	-	X
87	MG	1	4268	-	-	-	X
87	MG	1	4273	-	-	-	X
87	MG	1	4284	-	-	-	X
87	MG	1	4291	-	-	-	X
87	MG	1	4307	-	-	-	X
87	MG	1	4313	-	-	-	X
87	MG	1	4315	-	-	-	X
87	MG	1	4317	-	-	-	X
87	MG	1	4323	-	-	-	X
87	MG	1	4328	-	-	-	X
87	MG	1	4339	-	-	-	X
87	MG	1	4340	-	-	-	X
87	MG	1	4341	-	-	-	X
87	MG	1	4346	-	-	-	X
87	MG	1	4350	-	-	-	X
87	MG	1	4362	-	-	-	X
87	MG	1	4366	-	-	-	X
87	MG	1	4376	-	-	-	X
87	MG	1	4377	-	-	-	X
87	MG	1	4378	-	-	-	X
87	MG	1	4379	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	1	4383	-	-	-	X
87	MG	1	4385	-	-	-	X
87	MG	1	4387	-	-	-	X
87	MG	1	4391	-	-	-	X
87	MG	1	4392	-	-	-	X
87	MG	1	4393	-	-	-	X
87	MG	1	4395	-	-	-	X
87	MG	1	4396	-	-	-	X
87	MG	1	4397	-	-	-	X
87	MG	1	4408	-	-	-	X
87	MG	1	4410	-	-	-	X
87	MG	1	4411	-	-	-	X
87	MG	1	4412	-	-	-	X
87	MG	1	4424	-	-	-	X
87	MG	1	4431	-	-	-	X
87	MG	1	4432	-	-	-	X
87	MG	1	4433	-	-	-	X
87	MG	1	4437	-	-	-	X
87	MG	1	4444	-	-	-	X
87	MG	1	4447	-	-	-	X
87	MG	1	4451	-	-	-	X
87	MG	1	4461	-	-	-	X
87	MG	1	4469	-	-	-	X
87	MG	1	4471	-	-	-	X
87	MG	1	4478	-	-	-	X
87	MG	1	4480	-	-	-	X
87	MG	1	4485	-	-	-	X
87	MG	1	4496	-	-	-	X
87	MG	1	4505	-	-	-	X
87	MG	1	4507	-	-	-	X
87	MG	1	4508	-	-	-	X
87	MG	1	4511	-	-	-	X
87	MG	2	2099	-	-	-	X
87	MG	2	2100	-	-	-	X
87	MG	2	2103	-	-	-	X
87	MG	2	2109	-	-	-	X
87	MG	2	2112	-	-	-	X
87	MG	2	2117	-	-	-	X
87	MG	2	2127	-	-	-	X
87	MG	2	2128	-	-	-	X
87	MG	2	2130	-	-	-	X
87	MG	2	2133	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	2	2135	-	-	-	X
87	MG	2	2139	-	-	-	X
87	MG	2	2141	-	-	-	X
87	MG	2	2144	-	-	-	X
87	MG	2	2149	-	-	-	X
87	MG	2	2151	-	-	-	X
87	MG	2	2157	-	-	-	X
87	MG	2	2158	-	-	-	X
87	MG	2	2168	-	-	-	X
87	MG	2	2186	-	-	-	X
87	MG	2	2194	-	-	-	X
87	MG	2	2197	-	-	-	X
87	MG	2	2199	-	-	-	X
87	MG	2	2206	-	-	-	X
87	MG	2	2210	-	-	-	X
87	MG	2	2250	-	-	-	X
87	MG	2	2258	-	-	-	X
87	MG	2	2259	-	-	-	X
87	MG	4	222	-	-	-	X
87	MG	4	223	-	-	-	X
87	MG	4	224	-	-	-	X
87	MG	4	226	-	-	-	X
87	MG	4	230	-	-	-	X
87	MG	4	232	-	-	-	X
87	MG	4	238	-	-	-	X
87	MG	4	239	-	-	-	X
87	MG	4	244	-	-	-	X
87	MG	5	3820	-	-	-	X
87	MG	5	3822	-	-	-	X
87	MG	5	3823	-	-	-	X
87	MG	5	3824	-	-	-	X
87	MG	5	3825	-	-	-	X
87	MG	5	3829	-	-	-	X
87	MG	5	3830	-	-	-	X
87	MG	5	3833	-	-	-	X
87	MG	5	3834	-	-	-	X
87	MG	5	3835	-	-	-	X
87	MG	5	3836	-	-	-	X
87	MG	5	3837	-	-	-	X
87	MG	5	3841	-	-	-	X
87	MG	5	3844	-	-	-	X
87	MG	5	3846	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	5	3848	-	-	-	X
87	MG	5	3849	-	-	-	X
87	MG	5	3859	-	-	-	X
87	MG	5	3861	-	-	-	X
87	MG	5	3863	-	-	-	X
87	MG	5	3876	-	-	-	X
87	MG	5	3881	-	-	-	X
87	MG	5	3882	-	-	-	X
87	MG	5	3891	-	-	-	X
87	MG	5	3898	-	-	-	X
87	MG	5	3899	-	-	-	X
87	MG	5	3911	-	-	-	X
87	MG	5	3919	-	-	-	X
87	MG	5	3922	-	-	-	X
87	MG	5	3925	-	-	-	X
87	MG	5	3926	-	-	-	X
87	MG	5	3928	-	-	-	X
87	MG	5	3930	-	-	-	X
87	MG	5	3934	-	-	-	X
87	MG	5	3938	-	-	-	X
87	MG	5	3940	-	-	-	X
87	MG	5	3941	-	-	-	X
87	MG	5	3945	-	-	-	X
87	MG	5	3946	-	-	-	X
87	MG	5	3950	-	-	-	X
87	MG	5	3952	-	-	-	X
87	MG	5	3954	-	-	-	X
87	MG	5	3955	-	-	-	X
87	MG	5	3956	-	-	-	X
87	MG	5	3961	-	-	-	X
87	MG	5	3972	-	-	-	X
87	MG	5	3977	-	-	-	X
87	MG	5	3980	-	-	-	X
87	MG	5	3981	-	-	-	X
87	MG	5	3982	-	-	-	X
87	MG	5	3986	-	-	-	X
87	MG	5	3989	-	-	-	X
87	MG	5	3991	-	-	-	X
87	MG	5	3992	-	-	-	X
87	MG	5	3996	-	-	-	X
87	MG	5	3997	-	-	-	X
87	MG	5	3999	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	5	4000	-	-	-	X
87	MG	5	4001	-	-	-	X
87	MG	5	4002	-	-	-	X
87	MG	5	4005	-	-	-	X
87	MG	5	4006	-	-	-	X
87	MG	5	4013	-	-	-	X
87	MG	5	4017	-	-	-	X
87	MG	5	4019	-	-	-	X
87	MG	5	4021	-	-	-	X
87	MG	5	4022	-	-	-	X
87	MG	5	4023	-	-	-	X
87	MG	5	4025	-	-	-	X
87	MG	5	4026	-	-	-	X
87	MG	5	4027	-	-	-	X
87	MG	5	4029	-	-	-	X
87	MG	5	4030	-	-	-	X
87	MG	5	4031	-	-	-	X
87	MG	5	4037	-	-	-	X
87	MG	5	4040	-	-	-	X
87	MG	5	4041	-	-	-	X
87	MG	5	4045	-	-	-	X
87	MG	5	4047	-	-	-	X
87	MG	5	4048	-	-	-	X
87	MG	5	4053	-	-	-	X
87	MG	5	4075	-	-	-	X
87	MG	5	4089	-	-	-	X
87	MG	5	4096	-	-	-	X
87	MG	5	4097	-	-	-	X
87	MG	5	4105	-	-	-	X
87	MG	5	4111	-	-	-	X
87	MG	5	4115	-	-	-	X
87	MG	5	4118	-	-	-	X
87	MG	5	4127	-	-	-	X
87	MG	5	4131	-	-	-	X
87	MG	5	4133	-	-	-	X
87	MG	5	4142	-	-	-	X
87	MG	5	4150	-	-	-	X
87	MG	5	4154	-	-	-	X
87	MG	5	4156	-	-	-	X
87	MG	5	4159	-	-	-	X
87	MG	5	4167	-	-	-	X
87	MG	5	4170	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	5	4176	-	-	-	X
87	MG	5	4189	-	-	-	X
87	MG	5	4191	-	-	-	X
87	MG	5	4200	-	-	-	X
87	MG	5	4208	-	-	-	X
87	MG	5	4210	-	-	-	X
87	MG	5	4218	-	-	-	X
87	MG	5	4231	-	-	-	X
87	MG	5	4232	-	-	-	X
87	MG	5	4235	-	-	-	X
87	MG	5	4236	-	-	-	X
87	MG	5	4237	-	-	-	X
87	MG	5	4241	-	-	-	X
87	MG	5	4245	-	-	-	X
87	MG	5	4247	-	-	-	X
87	MG	5	4250	-	-	-	X
87	MG	5	4263	-	-	-	X
87	MG	5	4266	-	-	-	X
87	MG	5	4275	-	-	-	X
87	MG	5	4276	-	-	-	X
87	MG	5	4277	-	-	-	X
87	MG	5	4278	-	-	-	X
87	MG	5	4279	-	-	-	X
87	MG	5	4284	-	-	-	X
87	MG	5	4286	-	-	-	X
87	MG	5	4289	-	-	-	X
87	MG	5	4290	-	-	-	X
87	MG	5	4294	-	-	-	X
87	MG	5	4297	-	-	-	X
87	MG	5	4305	-	-	-	X
87	MG	5	4306	-	-	-	X
87	MG	5	4316	-	-	-	X
87	MG	5	4326	-	-	-	X
87	MG	5	4333	-	-	-	X
87	MG	5	4341	-	-	-	X
87	MG	5	4342	-	-	-	X
87	MG	5	4343	-	-	-	X
87	MG	5	4344	-	-	-	X
87	MG	5	4347	-	-	-	X
87	MG	5	4348	-	-	-	X
87	MG	5	4357	-	-	-	X
87	MG	5	4360	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	5	4361	-	-	-	X
87	MG	5	4362	-	-	-	X
87	MG	5	4363	-	-	-	X
87	MG	5	4365	-	-	-	X
87	MG	5	4370	-	-	-	X
87	MG	5	4372	-	-	-	X
87	MG	5	4384	-	-	-	X
87	MG	5	4390	-	-	-	X
87	MG	5	4396	-	-	-	X
87	MG	5	4401	-	-	-	X
87	MG	5	4403	-	-	-	X
87	MG	5	4404	-	-	-	X
87	MG	5	4405	-	-	-	X
87	MG	5	4409	-	-	-	X
87	MG	5	4415	-	-	-	X
87	MG	5	4427	-	-	-	X
87	MG	5	4429	-	-	-	X
87	MG	5	4436	-	-	-	X
87	MG	5	4438	-	-	-	X
87	MG	5	4439	-	-	-	X
87	MG	5	4442	-	-	-	X
87	MG	5	4443	-	-	-	X
87	MG	5	4447	-	-	-	X
87	MG	5	4448	-	-	-	X
87	MG	5	4452	-	-	-	X
87	MG	5	4453	-	-	-	X
87	MG	5	4459	-	-	-	X
87	MG	5	4461	-	-	-	X
87	MG	5	4463	-	-	-	X
87	MG	5	4467	-	-	-	X
87	MG	5	4477	-	-	-	X
87	MG	5	4478	-	-	-	X
87	MG	5	4480	-	-	-	X
87	MG	5	4482	-	-	-	X
87	MG	5	4483	-	-	-	X
87	MG	5	4487	-	-	-	X
87	MG	5	4491	-	-	-	X
87	MG	5	4498	-	-	-	X
87	MG	5	4501	-	-	-	X
87	MG	5	4502	-	-	-	X
87	MG	5	4504	-	-	-	X
87	MG	5	4512	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	5	4514	-	-	-	X
87	MG	5	4515	-	-	-	X
87	MG	5	4519	-	-	-	X
87	MG	5	4520	-	-	-	X
87	MG	5	4533	-	-	-	X
87	MG	5	4538	-	-	-	X
87	MG	5	4547	-	-	-	X
87	MG	5	4550	-	-	-	X
87	MG	5	4566	-	-	-	X
87	MG	5	4571	-	-	-	X
87	MG	5	4575	-	-	-	X
87	MG	5	4576	-	-	-	X
87	MG	6	2099	-	-	-	X
87	MG	6	2104	-	-	-	X
87	MG	6	2110	-	-	-	X
87	MG	6	2115	-	-	-	X
87	MG	6	2118	-	-	-	X
87	MG	6	2125	-	-	-	X
87	MG	6	2126	-	-	-	X
87	MG	6	2127	-	-	-	X
87	MG	6	2131	-	-	-	X
87	MG	6	2138	-	-	-	X
87	MG	6	2144	-	-	-	X
87	MG	6	2150	-	-	-	X
87	MG	6	2159	-	-	-	X
87	MG	6	2164	-	-	-	X
87	MG	6	2167	-	-	-	X
87	MG	6	2173	-	-	-	X
87	MG	6	2180	-	-	-	X
87	MG	6	2185	-	-	-	X
87	MG	6	2209	-	-	-	X
87	MG	6	2211	-	-	-	X
87	MG	6	2212	-	-	-	X
87	MG	6	2221	-	-	-	X
87	MG	6	2229	-	-	-	X
87	MG	6	2232	-	-	-	X
87	MG	6	2239	-	-	-	X
87	MG	6	2242	-	-	-	X
87	MG	6	2246	-	-	-	X
87	MG	6	2248	-	-	-	X
87	MG	6	2251	-	-	-	X
87	MG	6	2282	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	6	2285	-	-	-	X
87	MG	6	2296	-	-	-	X
87	MG	6	2303	-	-	-	X
87	MG	6	2308	-	-	-	X
87	MG	6	2309	-	-	-	X
87	MG	6	2310	-	-	-	X
87	MG	6	2311	-	-	-	X
87	MG	6	2313	-	-	-	X
87	MG	6	2316	-	-	-	X
87	MG	6	2318	-	-	-	X
87	MG	6	2328	-	-	-	X
87	MG	6	2329	-	-	-	X
87	MG	7	227	-	-	-	X
87	MG	7	229	-	-	-	X
87	MG	7	239	-	-	-	X
87	MG	8	222	-	-	-	X
87	MG	8	231	-	-	-	X
87	MG	C1	201	-	-	-	X
87	MG	C1	202	-	-	-	X
87	MG	C5	202	-	-	-	X
87	MG	D9	105	-	-	-	X
87	MG	L2	302	-	-	-	X
87	MG	L2	303	-	-	-	X
87	MG	L3	406	-	-	-	X
87	MG	L4	405	-	-	-	X
87	MG	L4	406	-	-	-	X
87	MG	L4	407	-	-	-	X
87	MG	L4	408	-	-	-	X
87	MG	L7	302	-	-	-	X
87	MG	M0	308	-	-	-	X
87	MG	M3	202	-	-	-	X
87	MG	M3	203	-	-	-	X
87	MG	M5	302	-	-	-	X
87	MG	M5	303	-	-	-	X
87	MG	M5	305	-	-	-	X
87	MG	M6	201	-	-	-	X
87	MG	M6	202	-	-	-	X
87	MG	M6	203	-	-	-	X
87	MG	M6	204	-	-	-	X
87	MG	M7	204	-	-	-	X
87	MG	M7	209	-	-	-	X
87	MG	M8	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	M8	203	-	-	-	X
87	MG	M8	204	-	-	-	X
87	MG	N0	201	-	-	-	X
87	MG	N0	202	-	-	-	X
87	MG	N1	201	-	-	-	X
87	MG	N3	201	-	-	-	X
87	MG	N3	203	-	-	-	X
87	MG	N6	202	-	-	-	X
87	MG	N8	202	-	-	-	X
87	MG	N8	203	-	-	-	X
87	MG	N8	205	-	-	-	X
87	MG	N8	207	-	-	-	X
87	MG	N9	102	-	-	-	X
87	MG	O1	202	-	-	-	X
87	MG	O1	203	-	-	-	X
87	MG	O1	204	-	-	-	X
87	MG	O1	206	-	-	-	X
87	MG	O2	202	-	-	-	X
87	MG	O2	203	-	-	-	X
87	MG	O3	202	-	-	-	X
87	MG	O3	203	-	-	-	X
87	MG	O5	202	-	-	-	X
87	MG	O7	107	-	-	-	X
87	MG	O7	109	-	-	-	X
87	MG	Q0	202	-	-	-	X
87	MG	S8	302	-	-	-	X
87	MG	c7	201	-	-	-	X
87	MG	c9	203	-	-	-	X
87	MG	d3	202	-	-	-	X
87	MG	d9	103	-	-	-	X
87	MG	l2	302	-	-	-	X
87	MG	l2	304	-	-	-	X
87	MG	l2	307	-	-	-	X
87	MG	l3	404	-	-	-	X
87	MG	l3	406	-	-	-	X
87	MG	l3	407	-	-	-	X
87	MG	l3	408	-	-	-	X
87	MG	l3	410	-	-	-	X
87	MG	l3	411	-	-	-	X
87	MG	l3	412	-	-	-	X
87	MG	l3	413	-	-	-	X
87	MG	l3	414	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	l5	307	-	-	-	X
87	MG	l5	308	-	-	-	X
87	MG	l5	309	-	-	-	X
87	MG	l7	301	-	-	-	X
87	MG	l7	302	-	-	-	X
87	MG	l7	303	-	-	-	X
87	MG	l7	305	-	-	-	X
87	MG	l7	306	-	-	-	X
87	MG	m5	505	-	-	-	X
87	MG	m6	201	-	-	-	X
87	MG	m6	202	-	-	-	X
87	MG	m7	202	-	-	-	X
87	MG	m7	204	-	-	-	X
87	MG	m7	206	-	-	-	X
87	MG	m7	207	-	-	-	X
87	MG	m7	208	-	-	-	X
87	MG	m7	209	-	-	-	X
87	MG	m8	1501	-	-	-	X
87	MG	m8	1503	-	-	-	X
87	MG	m8	1504	-	-	-	X
87	MG	m9	202	-	-	-	X
87	MG	n0	201	-	-	-	X
87	MG	n0	202	-	-	-	X
87	MG	n0	205	-	-	-	X
87	MG	n1	202	-	-	-	X
87	MG	n1	203	-	-	-	X
87	MG	n1	204	-	-	-	X
87	MG	n3	203	-	-	-	X
87	MG	n8	201	-	-	-	X
87	MG	n8	204	-	-	-	X
87	MG	n8	206	-	-	-	X
87	MG	n8	207	-	-	-	X
87	MG	n9	103	-	-	-	X
87	MG	o2	203	-	-	-	X
87	MG	o4	201	-	-	-	X
87	MG	o7	504	-	-	-	X
87	MG	q1	103	-	-	-	X
87	MG	q2	503	-	-	-	X
87	MG	q3	502	-	-	-	X
87	MG	s8	303	-	-	-	X
87	MG	s8	304	-	-	-	X
87	MG	sM	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
88	ZN	Q2	501	-	-	X	-
89	C	1	3401	-	-	-	X
90	8AN	1	3403	-	-	X	X
90	8AN	5	3403	-	-	X	X
91	PRO	5	3404	-	-	-	X



## 2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 414270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	1	0
			37970	16975	6720	12493	1782			

- 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			

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

- 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
			772	499	126	145	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- 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-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

- 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	S	0	0	0
			1105	708	203	194				
18	c6	142	Total	C	N	O	S	0	0	0
			1111	711	204	196				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	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
			2437	1541	418	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,Suppressor protein STM1,Ribosome-bound protein Stm1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	654	221	229				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	134	LEU	ASP	conflict	UNP P39015

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

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 5S ribosomal RNA.

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 5.8S ribosomal RNA.

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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O	0	0	0
			796	516	131	149			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	6	1795	Total	C	N	O	P	0	1	0
			38260	17105	6763	12596	1796			

- Molecule 81 is a protein called 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S Ribosomal Protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

- Molecule 82 is a protein called Suppressor protein STM1,Suppressor protein STM1,Ribosome-bound protein Stm1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
82	sM	104	Total	C	N	O	0	0	0
			681	404	140	137			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
sM	59	ALA	GLY	conflict	UNP P39015

- Molecule 83 is a protein called 60S Ribosomal Protein L12.

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

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

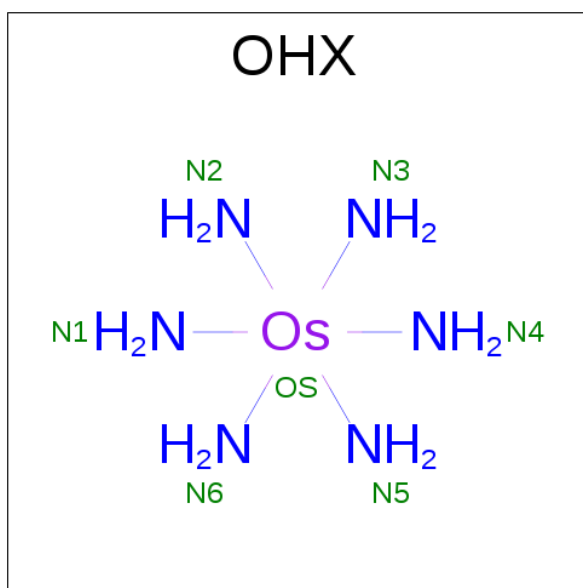
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
84	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 85 is a protein called 60S Ribosomal Protein P1/2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
85	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			
85	p2	46	Total	C	N	O	0	0	0
			230	138	46	46			



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



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

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

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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
			7	6	1		
86	2	1	Total	N	Os	0	0
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			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
			7	6	1		
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
			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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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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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 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
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
86	2	1	Total 7	N 6	Os 1	0	0
86	S2	1	Total 7	N 6	Os 1	0	0
86	S8	1	Total 7	N 6	Os 1	0	0
86	C3	1	Total 7	N 6	Os 1	0	0
86	C5	1	Total 7	N 6	Os 1	0	0
86	C8	1	Total 7	N 6	Os 1	0	0
86	C8	1	Total 7	N 6	Os 1	0	0
86	D9	1	Total 7	N 6	Os 1	0	0
86	SR	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L4	1	Total 7	N 6	Os 1	0	0
86	L5	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	M0	1	Total	N	Os	0	0
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86	M0	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	M8	1	Total	N	Os	0	0
			7	6	1		
86	M9	1	Total	N	Os	0	0
			7	6	1		
86	M9	1	Total	N	Os	0	0
			7	6	1		
86	M9	1	Total	N	Os	0	0
			7	6	1		
86	N8	1	Total	N	Os	0	0
			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	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
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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

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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
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	s1	1	Total 7	N 6	Os 1	0	0
86	s1	1	Total 7	N 6	Os 1	0	0
86	s4	1	Total 7	N 6	Os 1	0	0
86	s8	1	Total 7	N 6	Os 1	0	0
86	c1	1	Total 7	N 6	Os 1	0	0
86	c3	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0
86	c8	1	Total 7	N 6	Os 1	0	0
86	d9	1	Total 7	N 6	Os 1	0	0
86	sR	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	2	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	1	0
86	5	1	Total 7	N 6	Os 1	0	0

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

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

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

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

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

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

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

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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		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	1	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
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 7	N 6	Os 1	0	0
86	l2	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l4	1	Total 7	N 6	Os 1	0	0
86	l4	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	0	0
86	l9	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m1	1	Total 7	N 6	Os 1	0	0
86	m4	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m7	1	Total 7	N 6	Os 1	0	0
86	m9	1	Total 7	N 6	Os 1	0	0
86	n1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	n3	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	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	o9	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	n8	7	Total	Mg	0	0
			7	7		
87	c6	2	Total	Mg	0	0
			2	2		
87	Q0	2	Total	Mg	0	0
			2	2		
87	sM	2	Total	Mg	0	0
			2	2		
87	O3	2	Total	Mg	0	0
			2	2		
87	M9	2	Total	Mg	0	0
			2	2		
87	q0	1	Total	Mg	0	0
			1	1		
87	O2	4	Total	Mg	0	0
			4	4		
87	D9	3	Total	Mg	0	0
			3	3		
87	m9	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	M3	3	Total 3	Mg 3	0	0
87	D4	1	Total 1	Mg 1	0	0
87	S4	2	Total 2	Mg 2	0	0
87	l5	6	Total 6	Mg 6	0	0
87	m6	4	Total 4	Mg 4	0	0
87	o2	3	Total 3	Mg 3	0	0
87	d5	1	Total 1	Mg 1	0	0
87	d9	2	Total 2	Mg 2	0	0
87	m3	1	Total 1	Mg 1	0	0
87	d4	2	Total 2	Mg 2	0	0
87	s4	1	Total 1	Mg 1	0	0
87	M6	4	Total 4	Mg 4	0	0
87	N9	1	Total 1	Mg 1	0	0
87	p0	1	Total 1	Mg 1	0	0
87	n0	5	Total 5	Mg 5	0	0
87	C8	1	Total 1	Mg 1	0	0
87	n9	2	Total 2	Mg 2	0	0
87	M5	4	Total 4	Mg 4	0	0
87	S2	1	Total 1	Mg 1	0	0
87	N6	2	Total 2	Mg 2	0	0
87	D0	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	O5	2	Total 2	Mg 2	0	0
87	m5	3	Total 3	Mg 3	0	0
87	n6	1	Total 1	Mg 1	0	0
87	S8	1	Total 1	Mg 1	0	0
87	M8	3	Total 3	Mg 3	0	0
87	q3	1	Total 1	Mg 1	0	0
87	N3	3	Total 3	Mg 3	0	0
87	4	28	Total 28	Mg 28	0	0
87	L2	3	Total 3	Mg 3	0	0
87	o3	4	Total 4	Mg 4	0	0
87	O1	5	Total 5	Mg 5	0	0
87	s8	4	Total 4	Mg 4	0	0
87	m8	4	Total 4	Mg 4	0	0
87	n3	3	Total 3	Mg 3	0	0
87	l2	6	Total 6	Mg 6	0	0
87	N0	2	Total 2	Mg 2	0	0
87	L7	3	Total 3	Mg 3	0	0
87	6	235	Total 235	Mg 235	0	0
87	O4	1	Total 1	Mg 1	0	0
87	C1	2	Total 2	Mg 2	0	0
87	M1	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	D6	1	Total 1	Mg 1	0	0
87	S6	1	Total 1	Mg 1	0	0
87	c9	3	Total 3	Mg 3	0	0
87	l7	7	Total 7	Mg 7	0	0
87	L8	1	Total 1	Mg 1	0	0
87	SM	1	Total 1	Mg 1	0	0
87	o4	1	Total 1	Mg 1	0	0
87	O7	6	Total 6	Mg 6	0	0
87	s6	2	Total 2	Mg 2	0	0
87	M4	1	Total 1	Mg 1	0	0
87	1	698	Total 698	Mg 698	0	0
87	S1	1	Total 1	Mg 1	0	0
87	l8	1	Total 1	Mg 1	0	0
87	Q2	3	Total 3	Mg 3	0	0
87	o7	1	Total 1	Mg 1	0	0
87	m4	1	Total 1	Mg 1	0	0
87	s1	1	Total 1	Mg 1	0	0
87	q2	1	Total 1	Mg 1	0	0
87	c7	1	Total 1	Mg 1	0	0
87	L3	5	Total 5	Mg 5	0	0
87	8	19	Total 19	Mg 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	3	18	Total 18	Mg 18	0	0
87	C5	1	Total 1	Mg 1	0	0
87	q1	2	Total 2	Mg 2	0	0
87	l3	13	Total 13	Mg 13	0	0
87	N1	1	Total 1	Mg 1	0	0
87	2	170	Total 170	Mg 170	0	0
87	L4	7	Total 7	Mg 7	0	0
87	M0	5	Total 5	Mg 5	0	0
87	5	759	Total 759	Mg 759	0	0
87	n1	3	Total 3	Mg 3	0	0
87	c8	4	Total 4	Mg 4	0	0
87	l4	1	Total 1	Mg 1	0	0
87	d2	1	Total 1	Mg 1	0	0
87	d3	2	Total 2	Mg 2	0	0
87	E1	1	Total 1	Mg 1	0	0
87	m0	1	Total 1	Mg 1	0	0
87	M7	10	Total 10	Mg 10	0	0
87	N8	7	Total 7	Mg 7	0	0
87	l9	3	Total 3	Mg 3	0	0
87	7	28	Total 28	Mg 28	0	0
87	o6	1	Total 1	Mg 1	0	0

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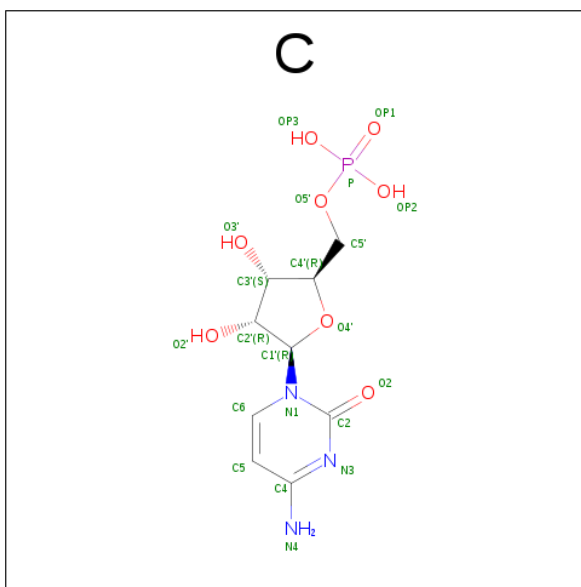
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	m7	8	Total	Mg	0	0
			8	8		

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

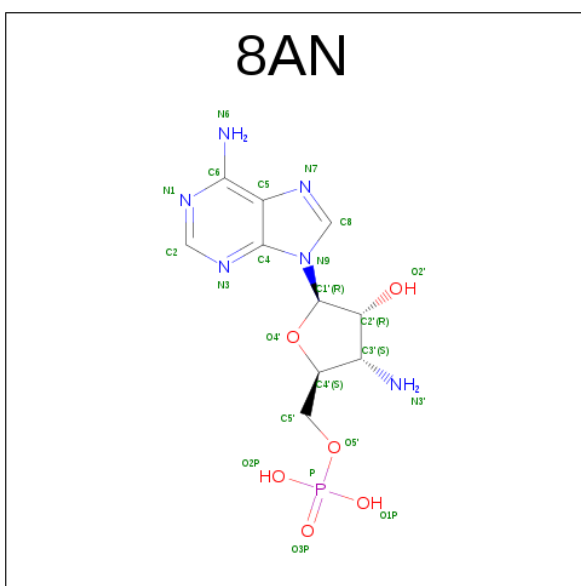
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total	Zn	0	0
			1	1		
88	D6	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		
88	Q3	1	Total	Zn	0	0
			1	1		
88	D9	1	Total	Zn	0	0
			1	1		
88	E1	1	Total	Zn	0	0
			1	1		
88	Q0	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0	0
			1	1		
88	q3	1	Total	Zn	0	0
			1	1		
88	d9	1	Total	Zn	0	0
			1	1		
88	D7	1	Total	Zn	0	0
			1	1		
88	d6	1	Total	Zn	0	0
			1	1		
88	o7	1	Total	Zn	0	0
			1	1		
88	O7	1	Total	Zn	0	0
			1	1		
88	q2	1	Total	Zn	0	0
			1	1		

- Molecule 89 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>3</sub>O<sub>8</sub>P).



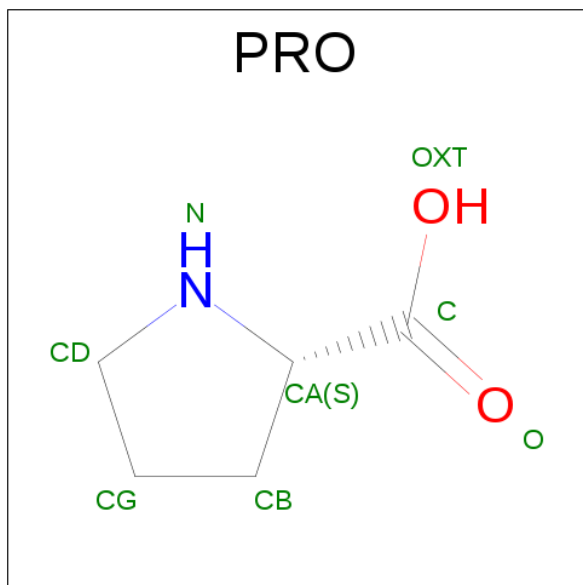
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
89	1	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
89	1	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
89	5	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
89	5	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

- Molecule 90 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (three-letter code: 8AN) (formula:  $C_{10}H_{15}N_6O_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
90	1	1	Total	C	N	O	P	0	0
			22	10	6	5	1		
90	5	1	Total	C	N	O	P	0	0
			22	10	6	5	1		

- Molecule 91 is PROLINE (three-letter code: PRO) (formula:  $C_5H_9NO_2$ ).



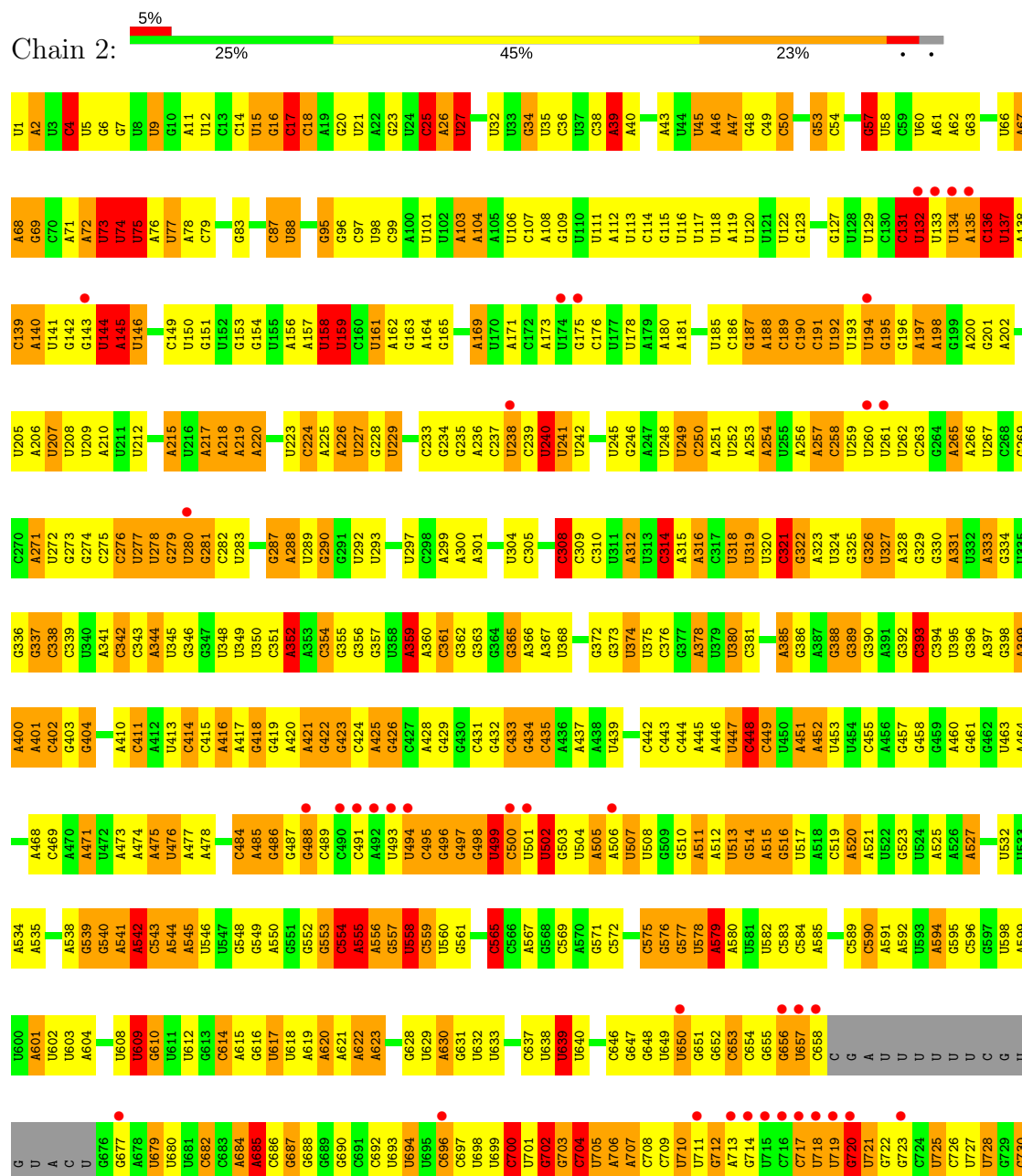
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
91	1	1	Total	C	N	O	0	0
			7	5	1	1		
91	5	1	Total	C	N	O	0	0
			7	5	1	1		



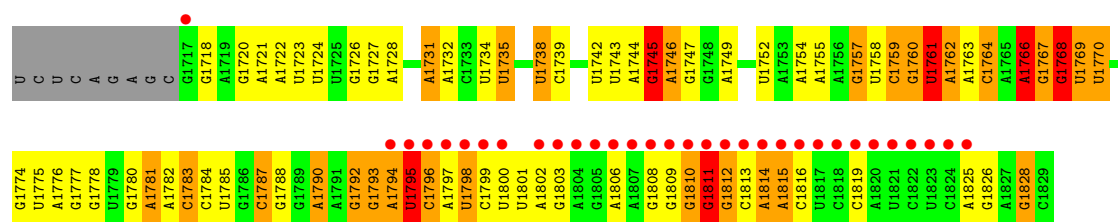
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

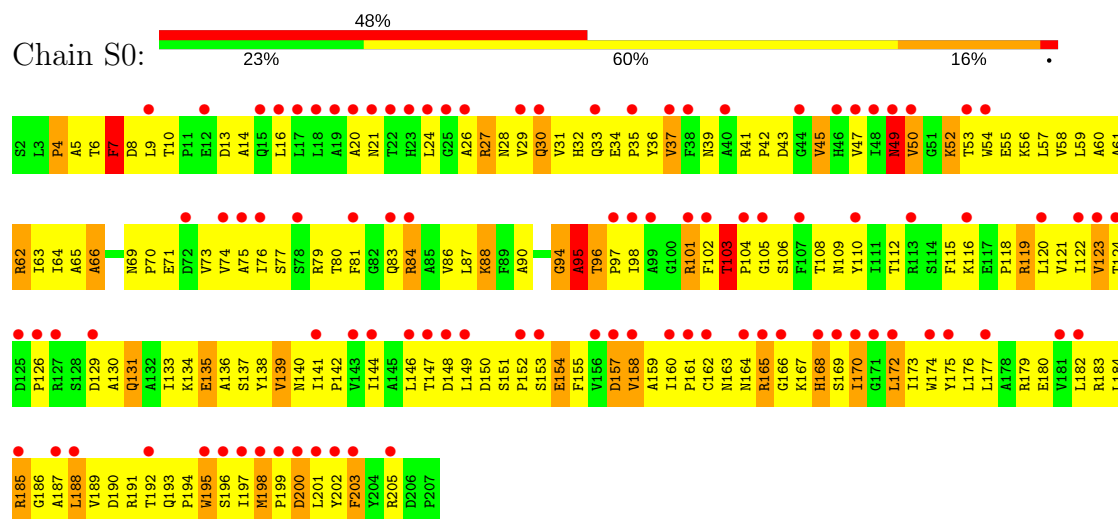
- Molecule 1: 18S ribosomal RNA



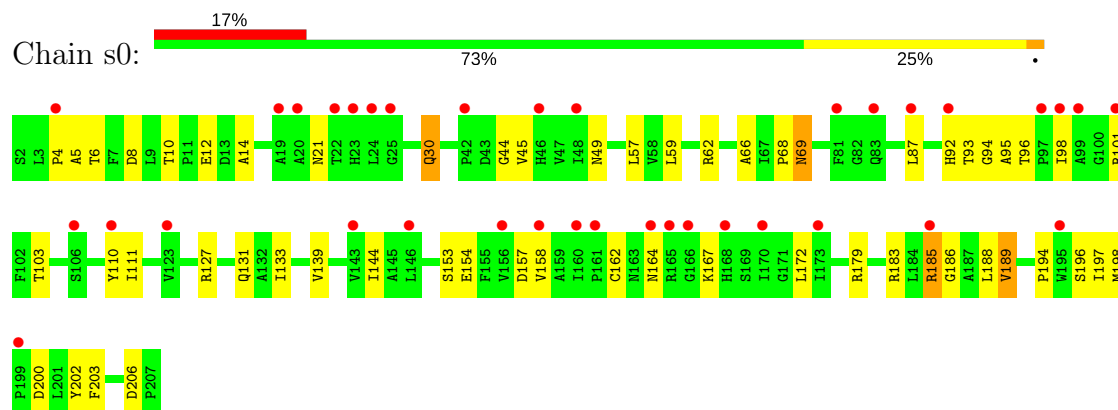
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U1582	A1583	G1584	U1585	A1586	A1587	C1588	C1589	G1590	C1591	A1592	G1593	A1594	U1595	C1596	A1597	U1598	C1599	A1600	G1601	C1602	U1603	G1604	G1605	A1606	G1607	U1608	U1609	A1610	A1611	U1612	U1613	A1614	C1615	U1616	A1617	U1618	C1619	C1620	U1621	G1622	C1623	G1624	C1625	U1626	G1629	U1630	A1631	C1634	A1635	C1636	A1637	C1638	A1639	C1640	C1641	C1642	C1643	A																																																								
U1520	G1521	U1522	G1523	A1524	A1525	A1526	C1527	U1528	C1529	C1530	G1531	U1532	C1533	G1534	U1535	C1536	G1537	U1538	C1539	G1540	G1541	G1542	G1543	U1544	A1545	G1546	A1547	U1550	U1551	U1552	G1553	U1554	A1555	U1556	U1557	U1558	A1559	U1560	U1561	G1562	U1563	U1564	C1565	U1566	U1567	C1568	A1569	A1570	C1571	G1572	A1573	C1574	G1575	A1576	A1577	U1578	U1579	U1643																																																								
G1458	C1459	A1460	G1461	G1462	G1466	U1467	U1468	C1469	A1470	C1470	A1471	C1472	U1473	G1474	A1475	C1476	G1477	G1478	A1479	G1480	G1481	C1482	A1483	G1484	C1485	U1486	A1487	U1488	G1489	C1490	A1491	U1492	U1493	A1494	C1495	G1496	U1497	G1498	G1499	C1500	C1501	G1502	A1503	G1504	A1505	G1506	U1507	U1508	C1509	U1510	U1511	G1512	C1513	A1514	U1515	A1516	U1517	U1518	G1519																																																							
G1385	G1386	G1387	A1388	C1389	U1390	U1398	C1399	A1400	A1401	G1402	C1403	U1407	G1408	A1409	G1410	A1411	G1412	U1413	U1414	C1415	G1416	A1417	G1418	C1419	G1420	A1421	A1422	U1423	A1424	A1427	G1428	G1429	U1430	C1431	U1432	G1433	U1434	G1435	A1436	C1439	A1444	G1445	A1446	C1447	G1448	U1449	A1450	C1451	U1452	G1453	A1454	U1455	G1456	C1457																																																												
A1321	A1322	G1323	G1324	A1325	A1331	C1332	C1333	U1334	U1335	A1336	A1337	C1338	C1339	U1340	A1341	U1342	U1343	A1344	A1345	A1346	U1347	A1348	A1349	U1350	G1351	G1352	U1353	G1354	C1355	U1356	A1357	G1358	C1359	A1360	U1361	U1362	C1363	G1364	C1365	U1366	G1367	C1368	U1369	U1370	A1371	U1372	C1373	C1374	A1375	U1376	U1377	A1378	C1379	U1380	U1381	A1382	G1383	A1384																																																								
U1259	U1260	G1261	U1262	G1263	U1266	G1267	C1268	U1269	G1270	C1271	U1272	G1273	C1274	A1275	U1276	G1277	G1278	C1279	C1280	G1281	U1282	U1283	C1284	U1285	U1286	A1287	G1288	U1289	U1290	G1291	G1292	U1293	G1294	U1294	C1295	U1296	U1297	G1298	G1299	A1300	U1301	U1302	U1303	C1304	U1305	C1306	U1307	G1308	C1309	U1310	U1311	A1312	U1313	C1314	U1315	U1316	C1317	U1318	U1319	U1320																																																						
A1189	C1190	U1191	C1192	A1193	A1194	C1195	A1196	G1197	U1198	G1199	G1200	A1201	A1202	A1203	A1204	C1207	A1208	G1212	G1213	U1214	C1215	G1216	A1217	G1218	A1226	A1227	U1228	G1229	U1230	U1231	U1234	C1235	U1236	G1237	A1238	U1239	U1240	G1241	A1242	G1243	A1244	G1245	C1246	U1247	C1248	U1249	U1250	U1251	C1252	U1253	U1254	G1255	A1256	U1257	U1258																																																											
A1125	G1126	G1130	A1131	A1132	A1133	C1134	U1135	U1136	U1137	A1138	A1139	G1140	G1141	A1142	A1143	U1144	U1145	G1146	A1147	C1148	G1149	C1150	A1151	A1152	G1153	G1154	C1155	A1156	A1157	C1158	C1159	U1160	C1161	G1162	A1163	G1164	G1165	A1166	U1167	U1168	G1169	G1170	A1171	C1172	C1173	C1174	U1175	G1176	C1180	U1181	U1182	A1183	A1184	U1185	U1186	U1187	G1188																																																									
A1062	U1063	A1064	U1065	C1066	U1067	A1068	C1069	U1070	U1071	G1074	C1077	C1078	U1079	U1080	A1081	C1082	C1083	A1084	C1085	A1086	A1087	U1088	A1089	U1090	C1091	A1092	C1093	U1094	C1095	U1096	A1097	U1098	C1099	G1099	G1100	G1101	U1102	U1103	U1104	C1105	U1106	G1107	C1108	U1109	G1110	G1111	G1112	A1113	G1114	U1115	A1116	U1117	U1118	U1119	U1120	C1121	G1122																																																									
U956	G957	A958	U959	C960	U961	C962	U963	U964	A965	C966	U967	U968	C969	G972	A973	U974	G975	U976	C977	U978	A979	G980	U981	C982	U983	A984	C985	U986	A987	U988	C989	A990	G991	C992	U993	A994	C995	U996	A997	U998	C999	A999	U999	C1000	U1001	A1002	U1003	C1004	U1005	C1006	U1007	A1008	U1009	C1010	G1011	U1012	A1013	U1014	U1015	C1016	U1017	U1018	A1019	C1020	U1021	G1022	C1023	U1024	A1025	C1026	U1027	A1028	C1029	U1030	A1031	C1032	U1033	C1034	G1035	A1036	C1037	U1038	A1039	C1040	U1041	A1042	C1043	U1044	C1045	G1046	U1052	C1053	U1054	U1055	C1056	U1057	C1058	U1059	A1060															
U861	A862	A863	U864	A865	G866	C867	G868	A869	C870	G871	A872	G876	C877	G878	G879	C880	A881	U882	C883	A884	U885	G886	A887	U888	C889	C890	U894	A895	U896	C897	A898	C899	A900	G901	C902	U903	G904	U909	C910	U911	U912	G913	A914	U915	U916	U917	U918	A919	U920	U921	A924	C925	A926	U927	A928	U929	U930	C931	U932	A933	U934	C935	U936	A937	U938	C939	A940	U941	C942	U943	A944	U945	C949	C950	U951	G952	C953	G954	A955	U959	U960	U961	C962	U963	A964	C965	U966	A967	U968	C969	G972	A973	U974	G975	U976	C977	U978	A979	G980	U981	C982	U983	A984	C985	U986	A987	U988	C989	A990	G991	C992	U993	A994	A995
U800	G801	A802	U803	A804	U805	C806	A807	U808	A809	C810	A811	A812	U813	G814	C815	A816	A817	A818	C819	U820	A821	U822	G823	G824	U825	U826	U827	U828	A829	U830	U831	U832	U833	G834	G837	G838	U839	U840	U841	C842	U843	A844	G845	U846	A847	U848	C849	U850	U851	C852	U853	U854	A855	U856	U857	U858	A859	U860																																																								
C731	G732	A733	C736	C737	A737	G738	G739	A740	C741	U742	U748	U749	U750	G751	A752	A753	A754	A755	U756	A757	U758	U759	A760	G761	A762	G763	U764	G765	U766	U767	U768	A769	G772	C773	A774	G775	G776	C777	G778	U779	A780	U781	U782	G783	C784	U785	C786	A789	U792	A793	U794	U795	U796	U797	U798	U799	U800																																																									



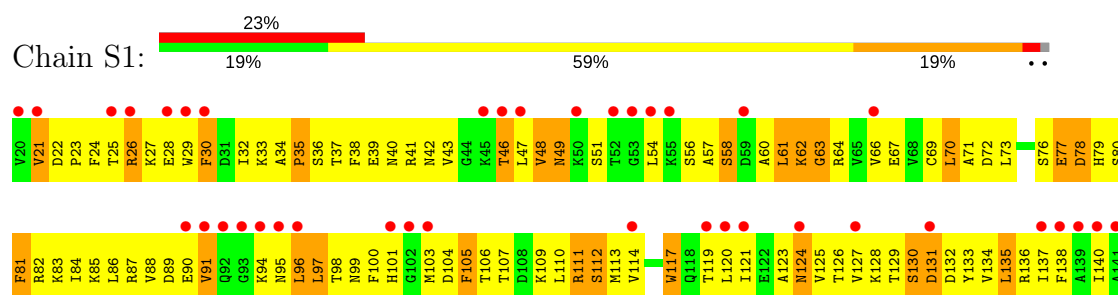
• Molecule 2: 40S ribosomal protein S0-A

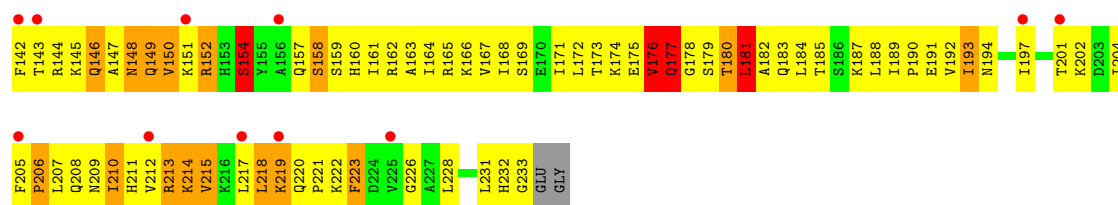


• Molecule 2: 40S ribosomal protein S0-A

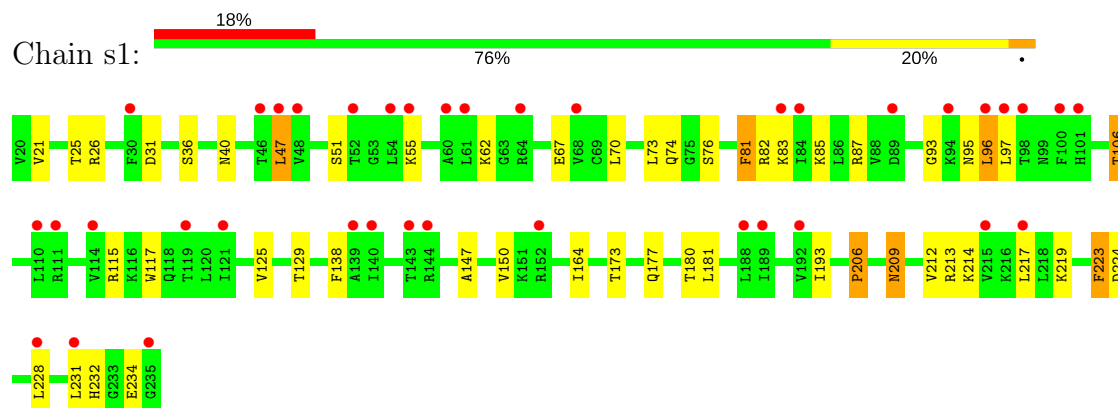


• Molecule 3: 40S ribosomal protein S1-A

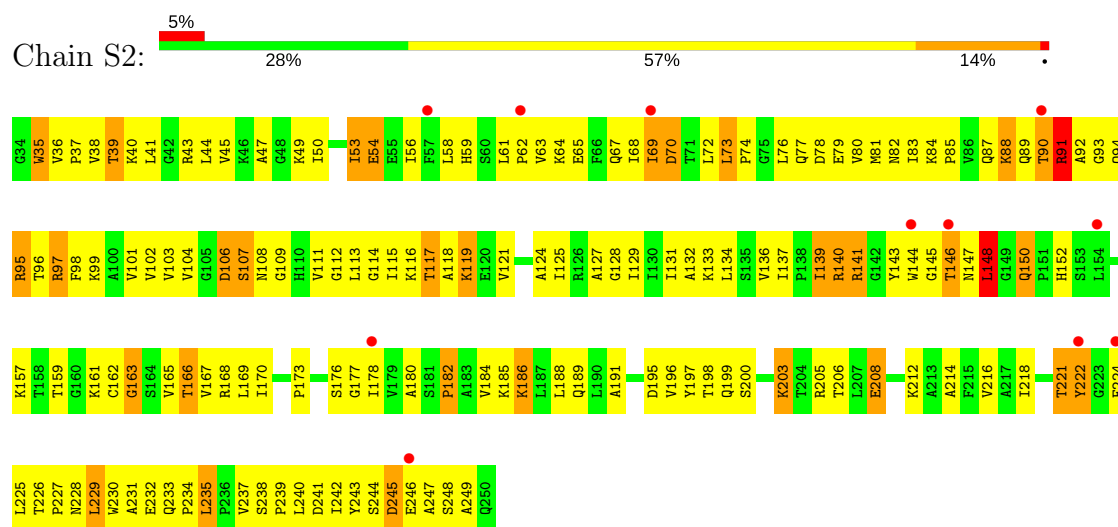




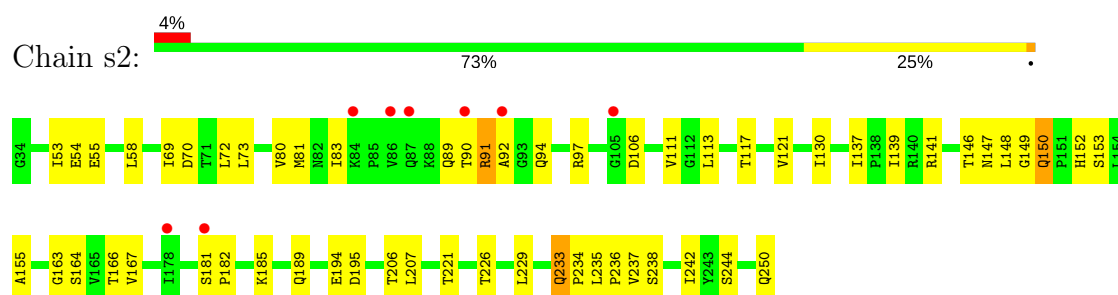
• Molecule 3: 40S ribosomal protein S1-A



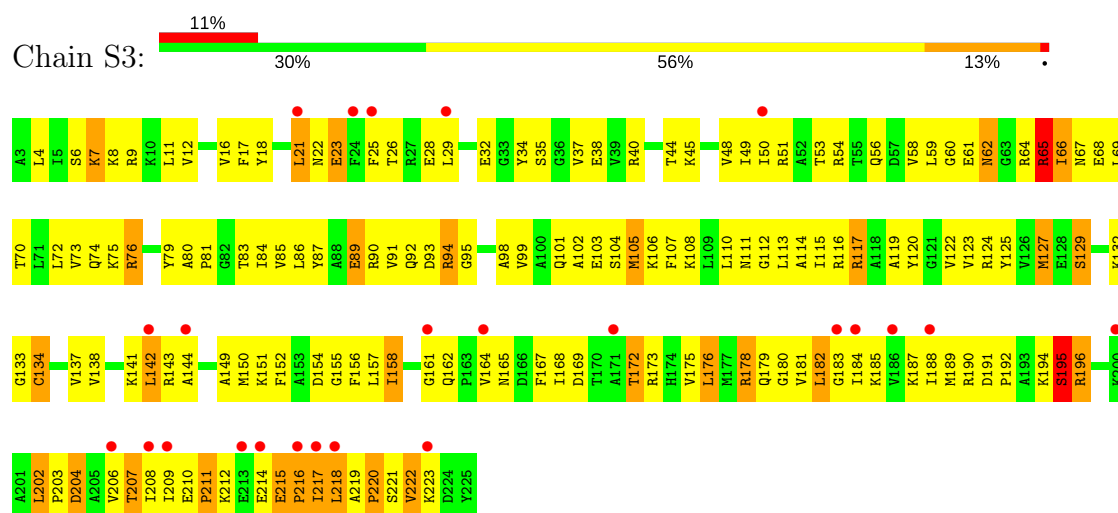
• Molecule 4: 40S ribosomal protein S2



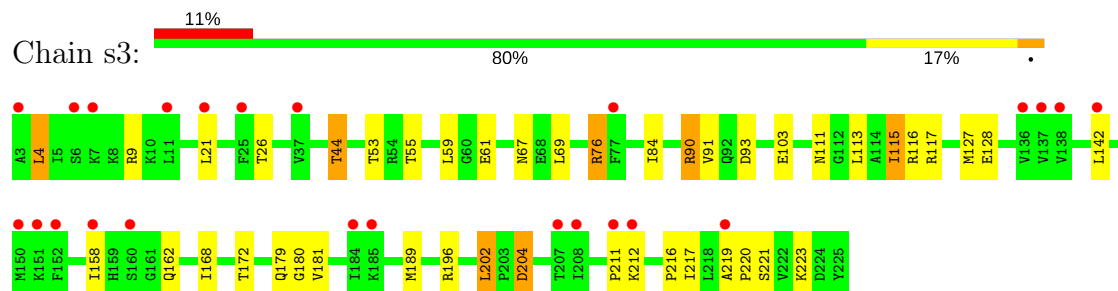
• Molecule 4: 40S ribosomal protein S2



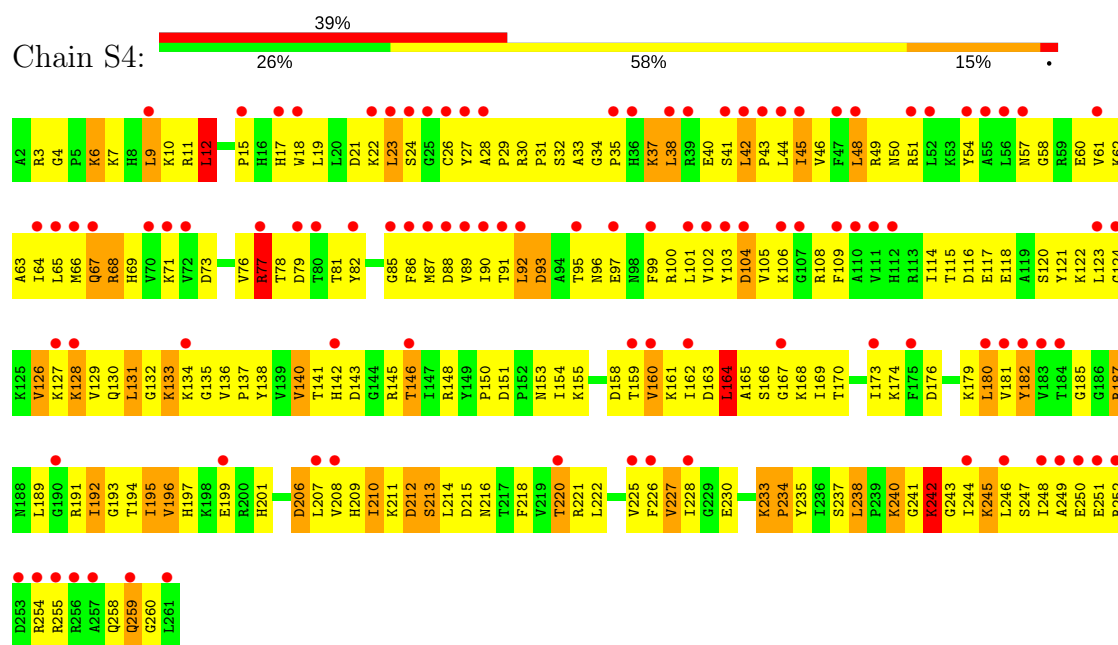
• Molecule 5: 40S ribosomal protein S3



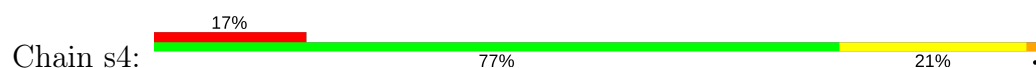
• Molecule 5: 40S ribosomal protein S3

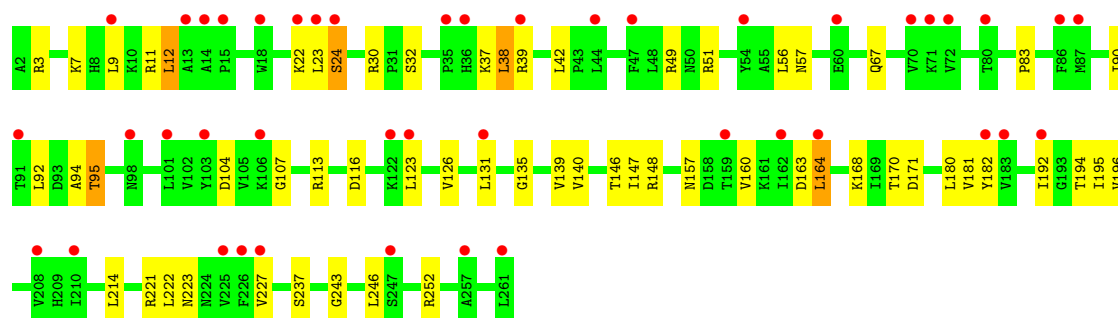


• Molecule 6: 40S ribosomal protein S4-A

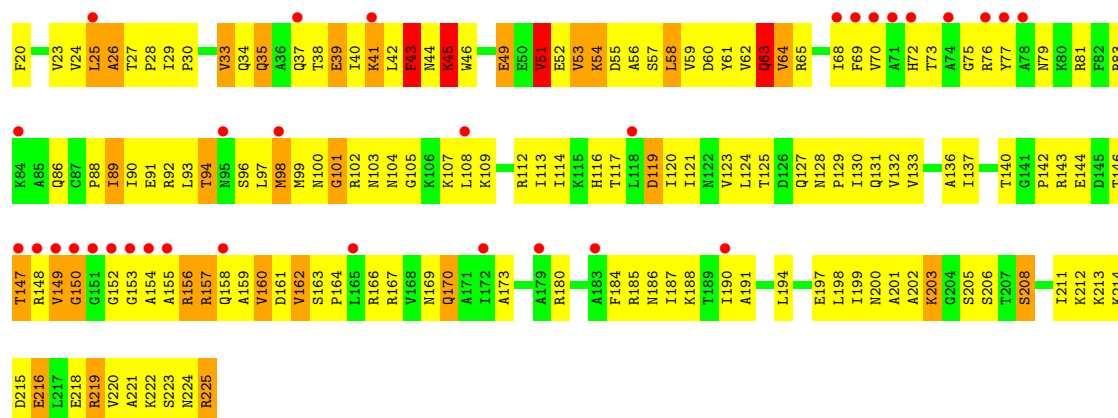


• Molecule 6: 40S ribosomal protein S4-A

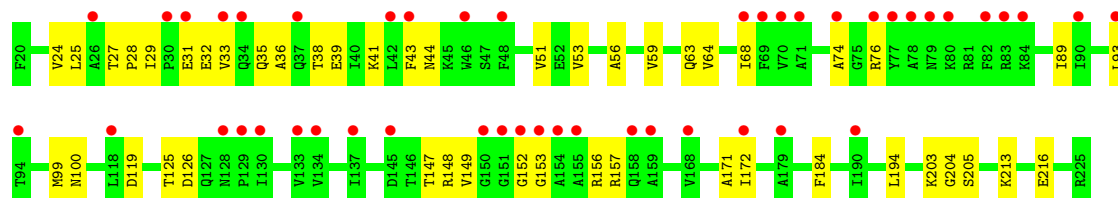
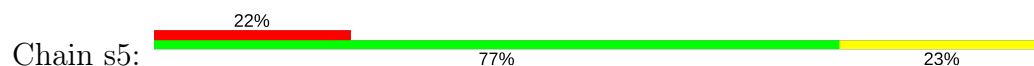




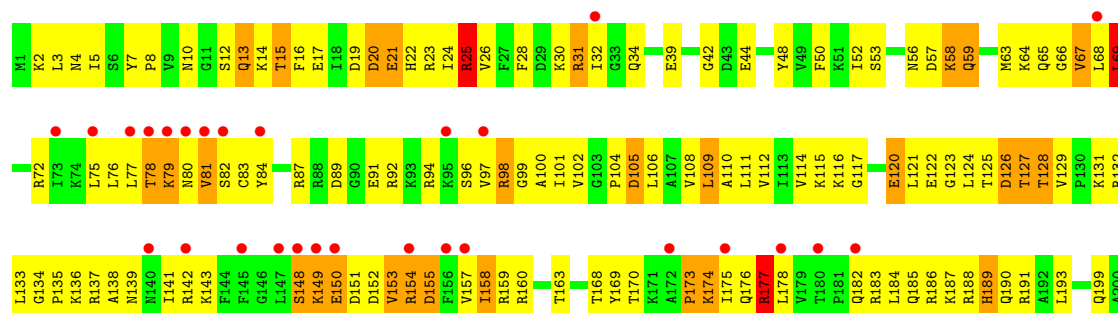
• Molecule 7: 40S ribosomal protein S5



• Molecule 7: 40S ribosomal protein S5

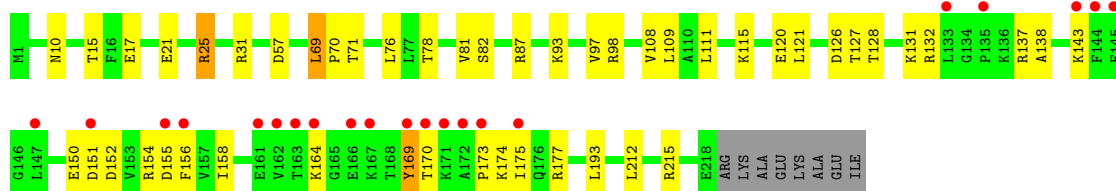
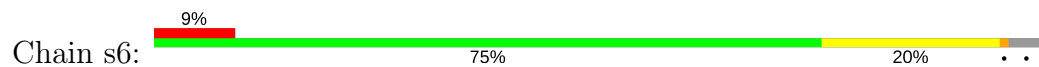


• Molecule 8: 40S ribosomal protein S6-A

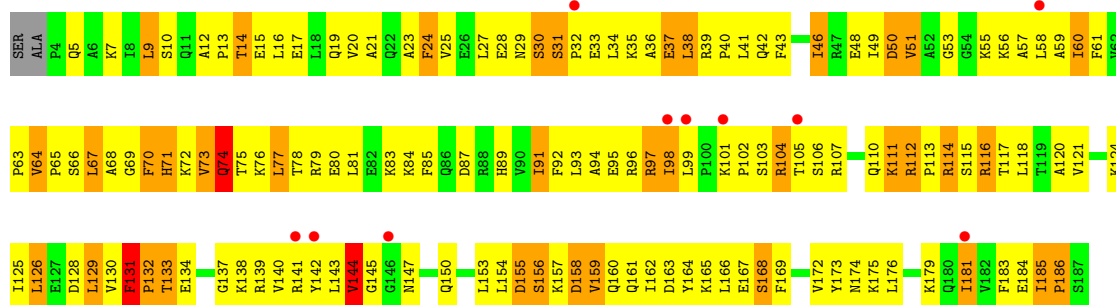




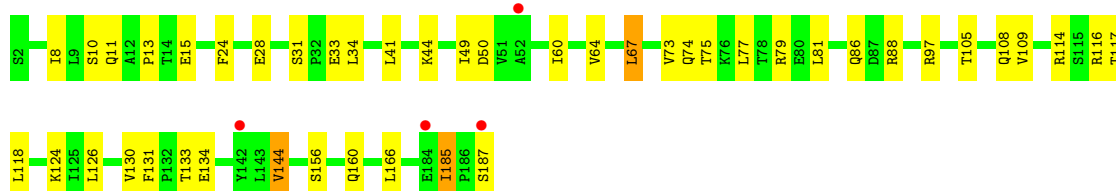
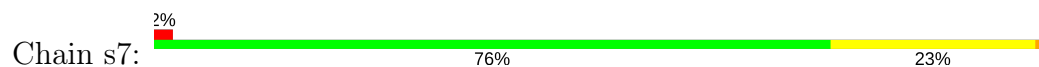
• Molecule 8: 40S ribosomal protein S6-A



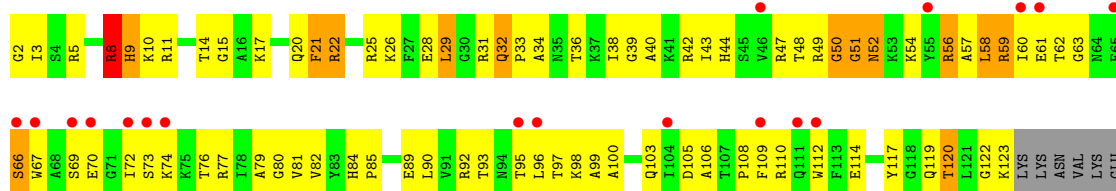
• Molecule 9: 40S ribosomal protein S7-A

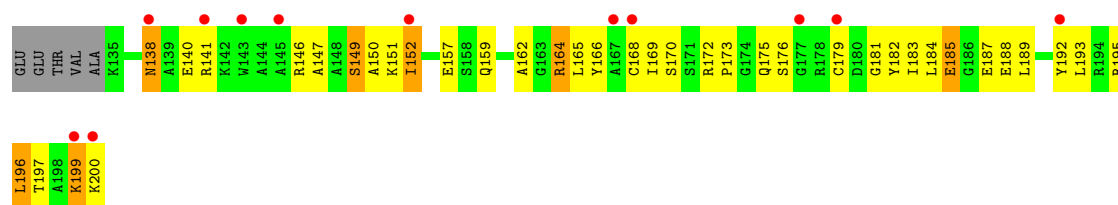


• Molecule 9: 40S ribosomal protein S7-A

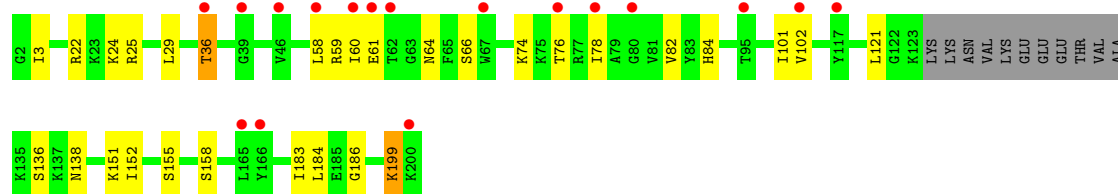
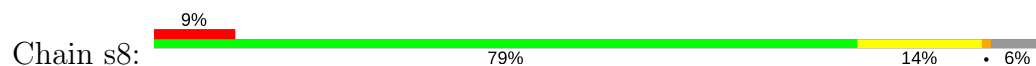


• Molecule 10: 40S ribosomal protein S8-A

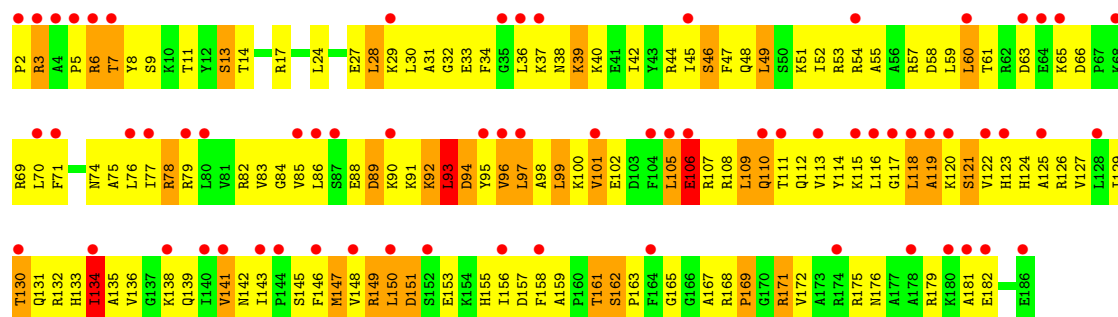




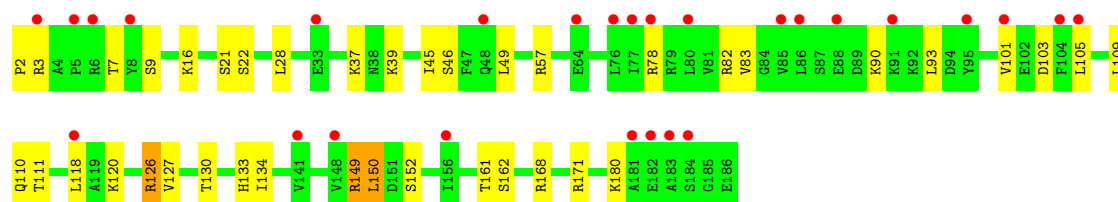
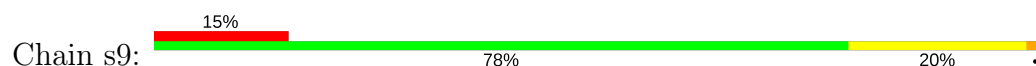
• Molecule 10: 40S ribosomal protein S8-A



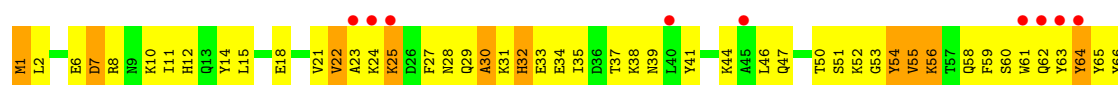
• Molecule 11: 40S ribosomal protein S9-A



• Molecule 11: 40S ribosomal protein S9-A



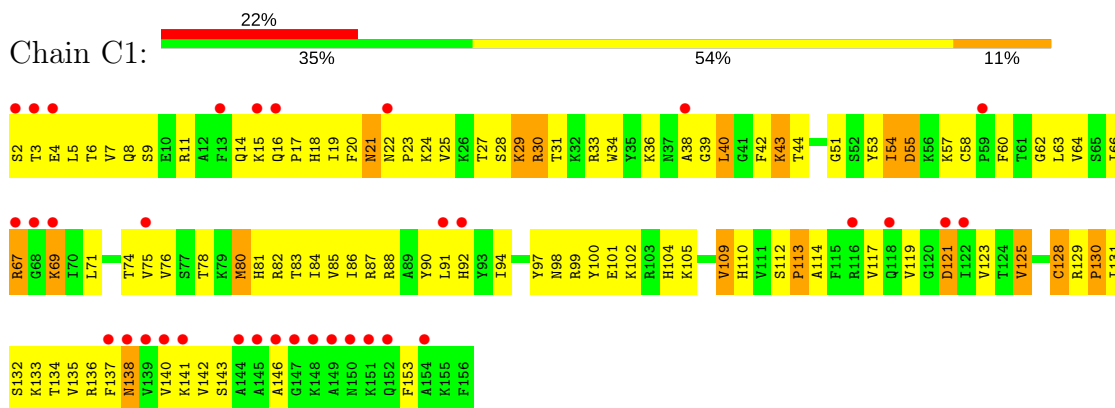
• Molecule 12: 40S ribosomal protein S10-A



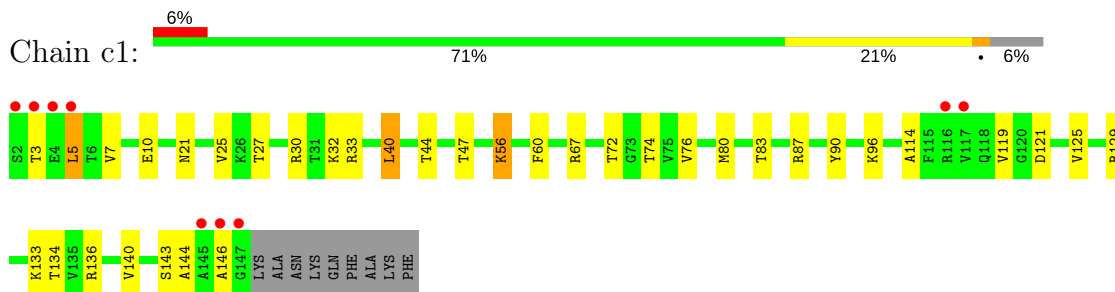




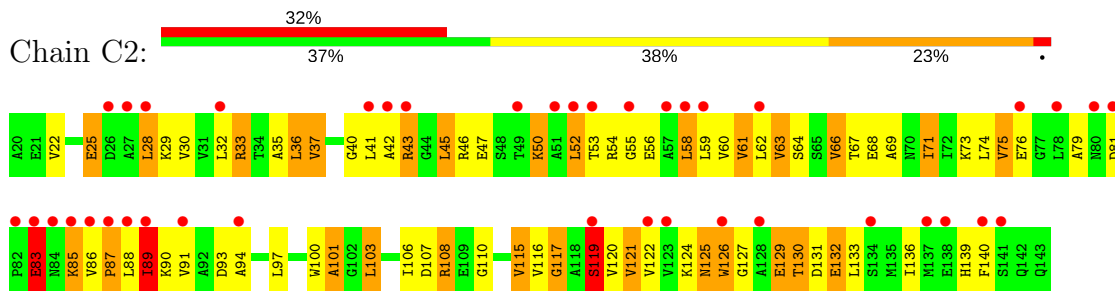
• Molecule 13: 40S ribosomal protein S11-A



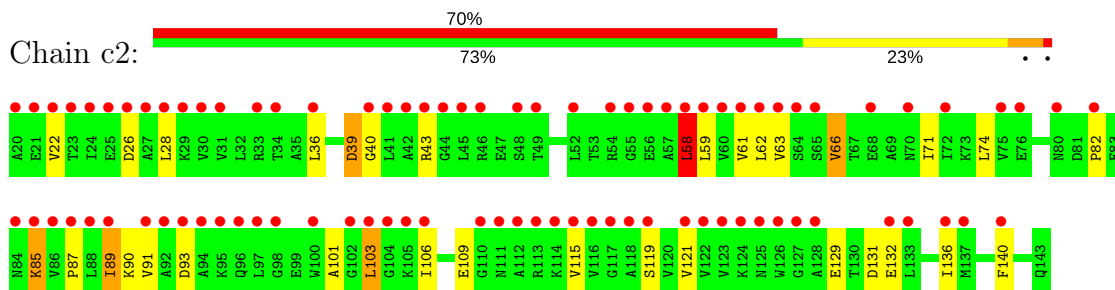
• Molecule 13: 40S ribosomal protein S11-A



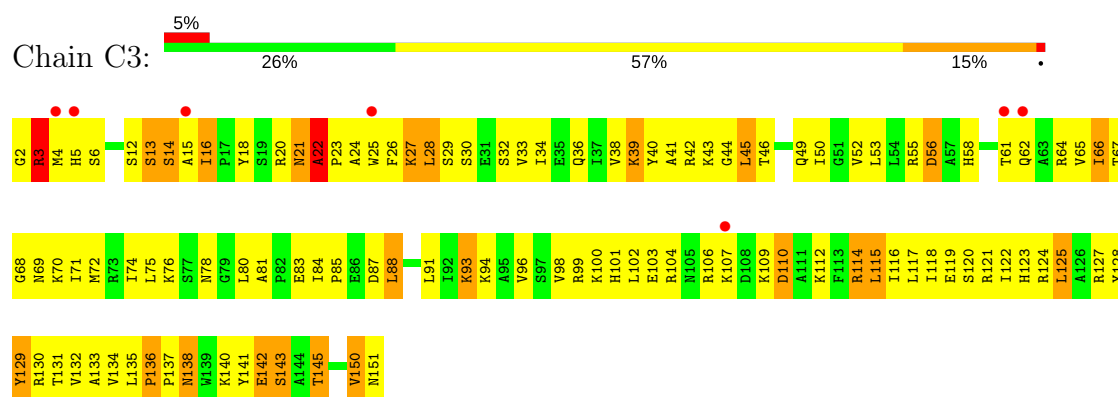
• Molecule 14: 40S ribosomal protein S12



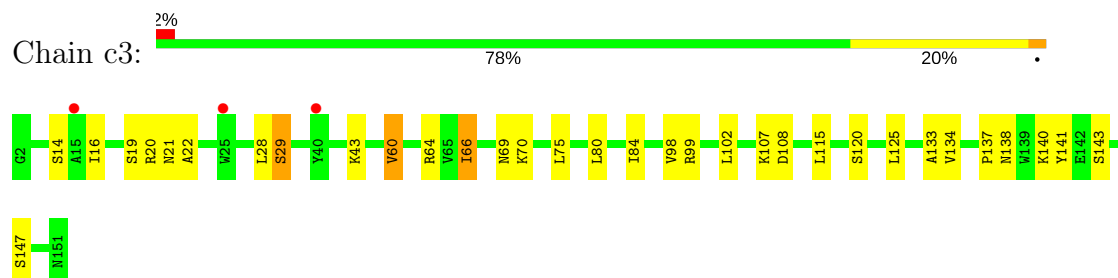
• Molecule 14: 40S ribosomal protein S12



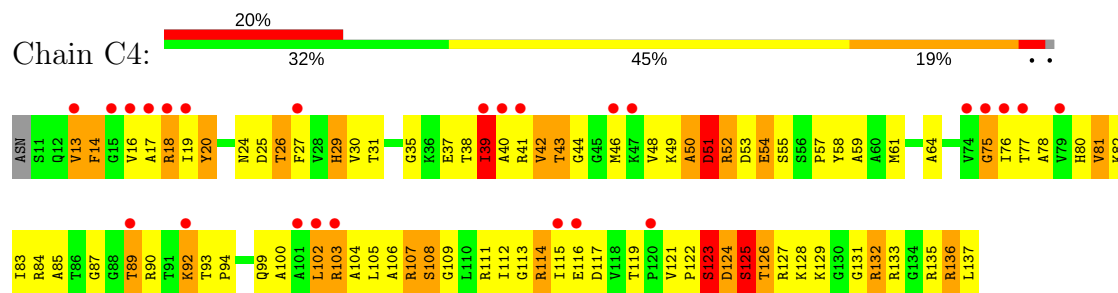
• Molecule 15: 40S ribosomal protein S13



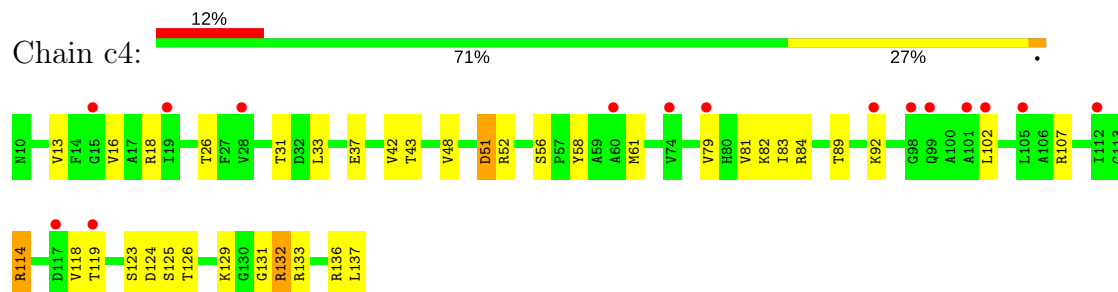
• Molecule 15: 40S ribosomal protein S13



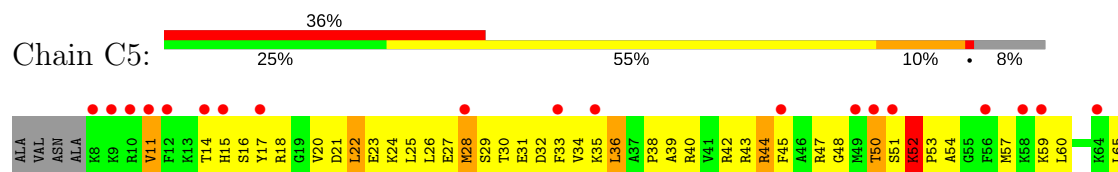
• Molecule 16: 40S ribosomal protein S14-B



• Molecule 16: 40S ribosomal protein S14-B



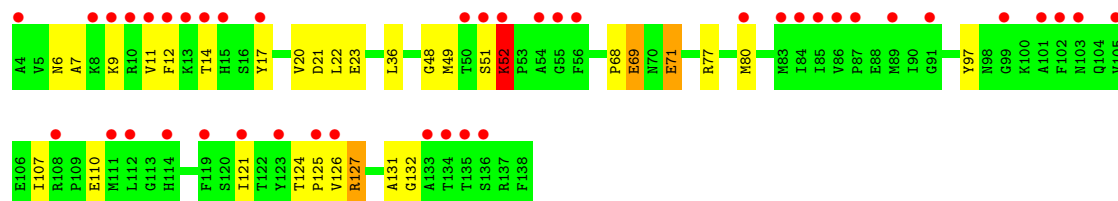
• Molecule 17: 40S ribosomal protein S15





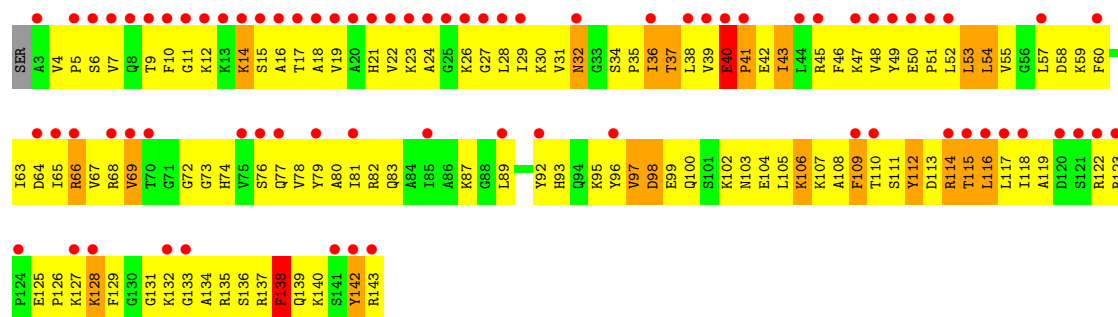
• Molecule 17: 40S ribosomal protein S15

Chain c5: 31% 77% 20% ..



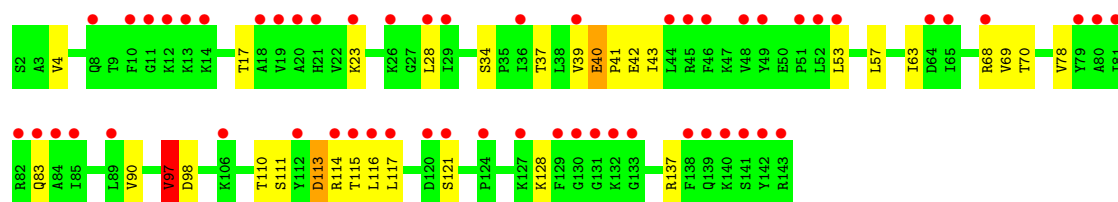
• Molecule 18: 40S ribosomal protein S16-A

Chain C6: 54% 18% 65% 14% ..



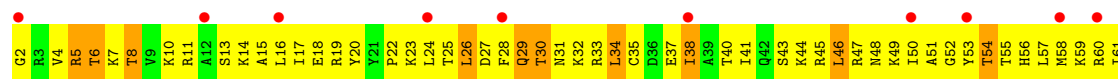
• Molecule 18: 40S ribosomal protein S16-A

Chain c6: 39% 77% 20% ..



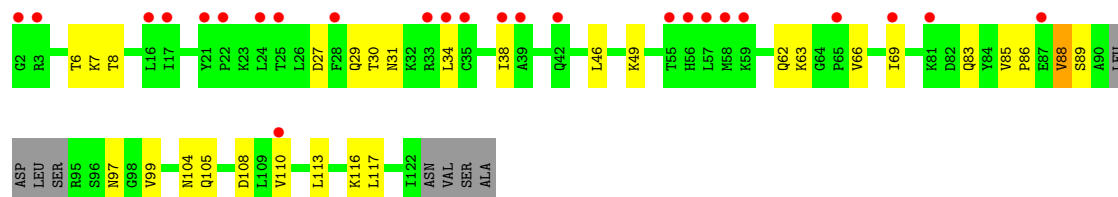
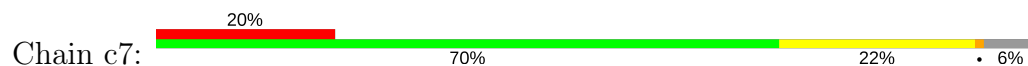
• Molecule 19: 40S ribosomal protein S17-B

Chain C7: 30% 26% 54% 14% ..

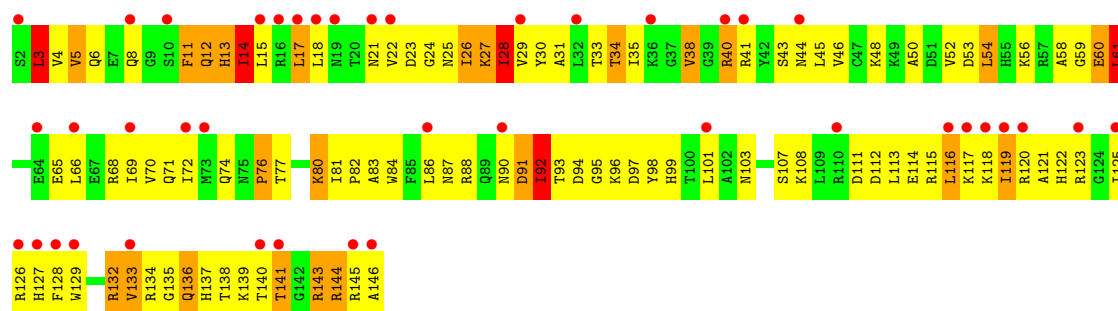




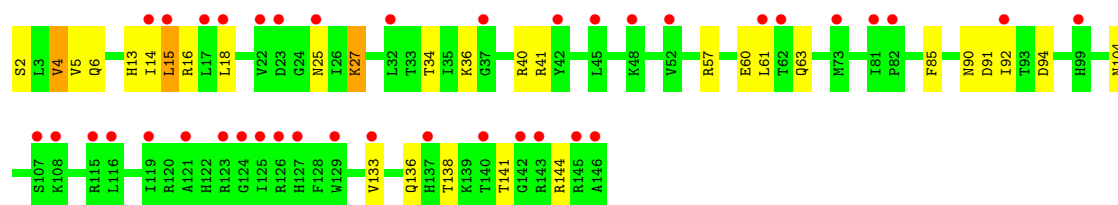
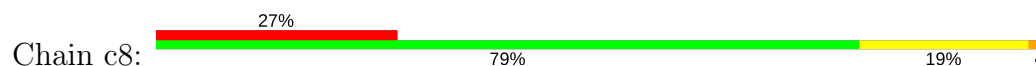
• Molecule 19: 40S ribosomal protein S17-B



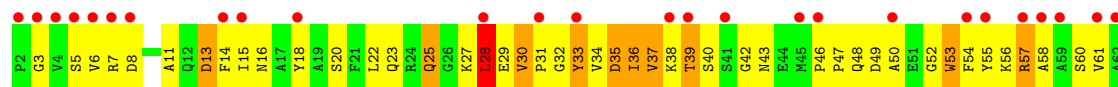
• Molecule 20: 40S ribosomal protein S18-A

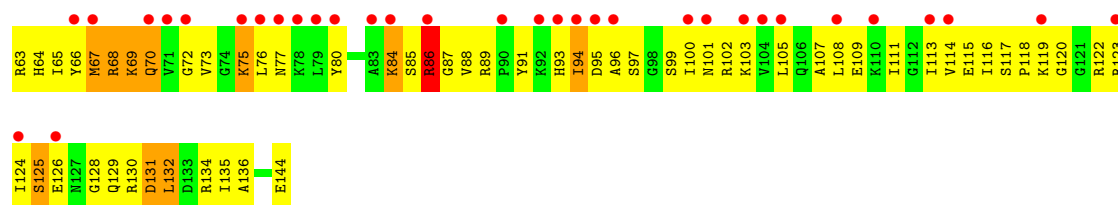


• Molecule 20: 40S ribosomal protein S18-A

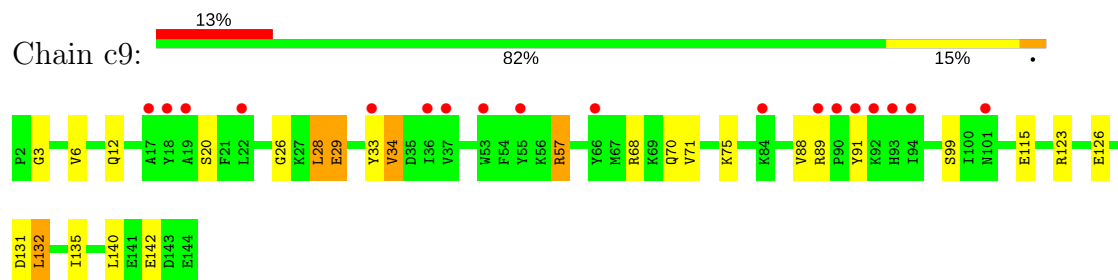


• Molecule 21: 40S ribosomal protein S19-A

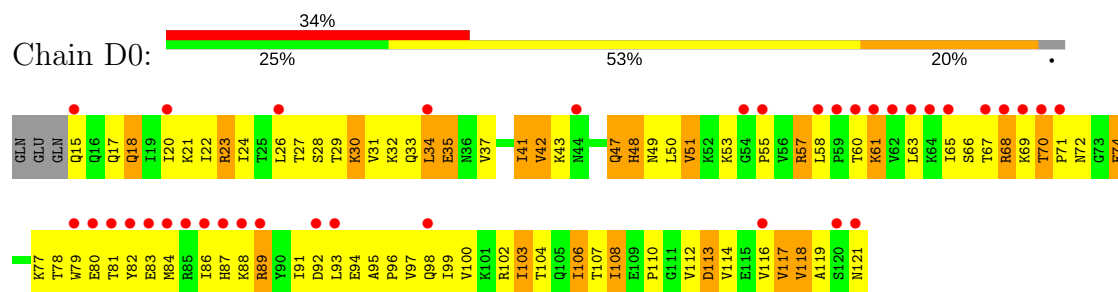




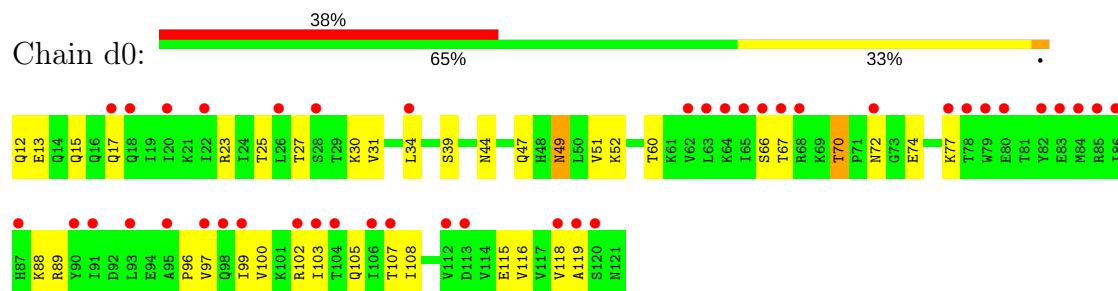
- Molecule 21: 40S ribosomal protein S19-A



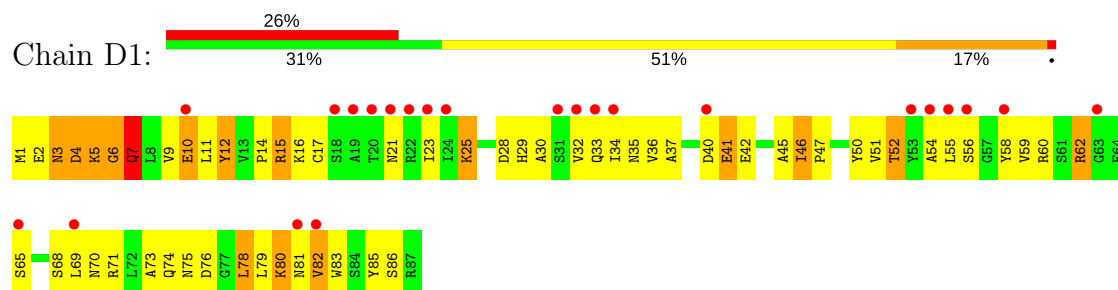
- Molecule 22: 40S ribosomal protein S20



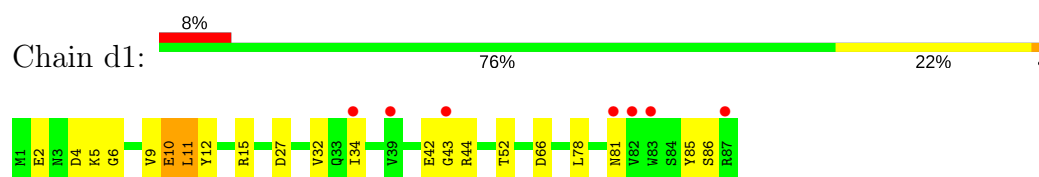
- Molecule 22: 40S ribosomal protein S20



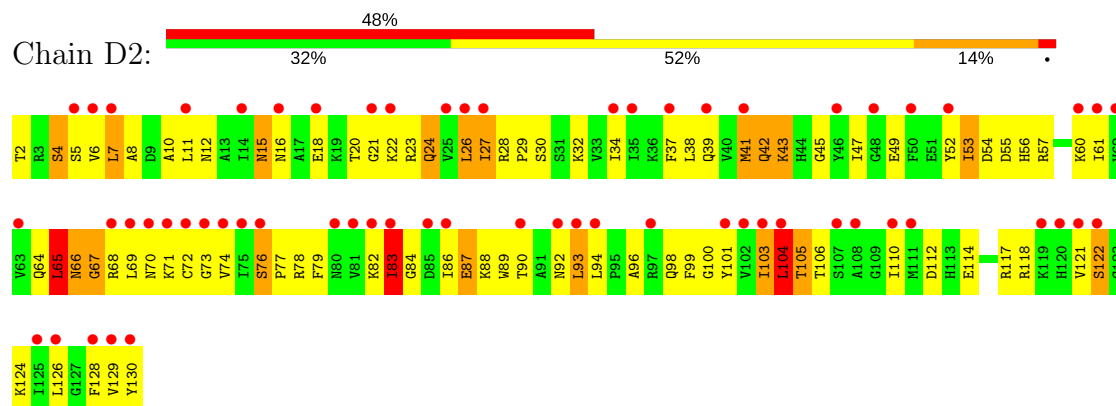
- Molecule 23: 40S ribosomal protein S21-A



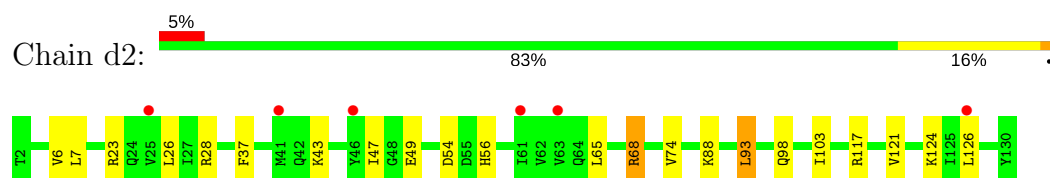
- Molecule 23: 40S ribosomal protein S21-A



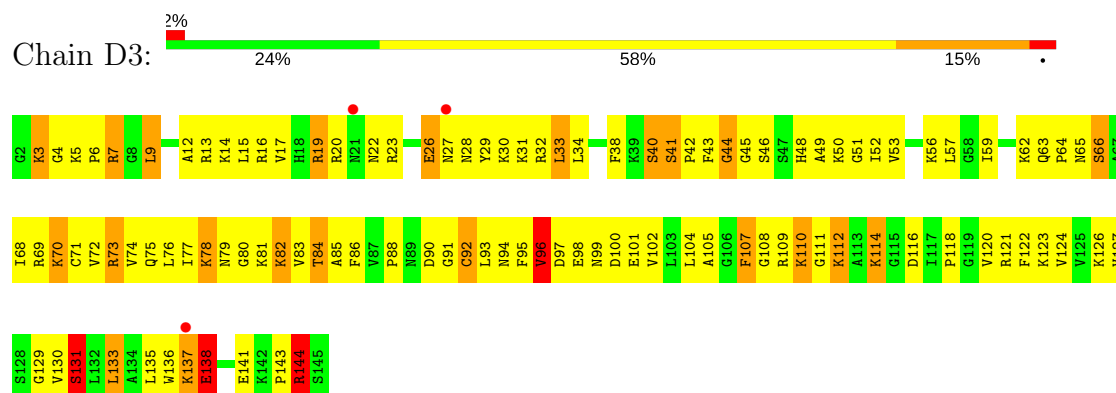
- Molecule 24: 40S ribosomal protein S22-A



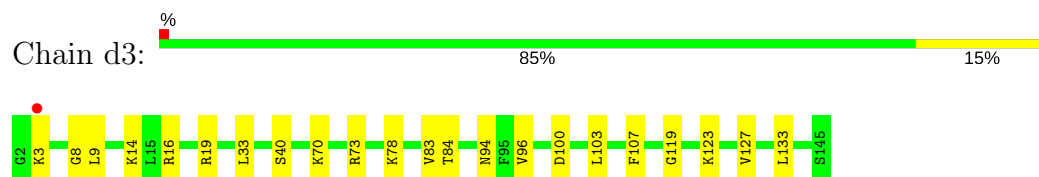
- Molecule 24: 40S ribosomal protein S22-A



- Molecule 25: 40S ribosomal protein S23-A

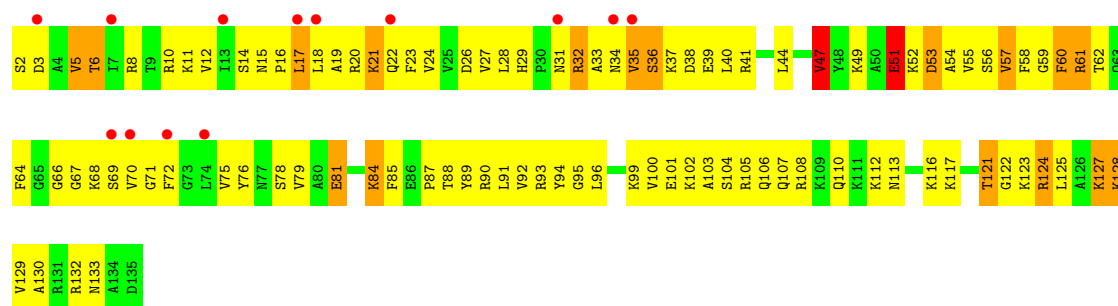


- Molecule 25: 40S ribosomal protein S23-A

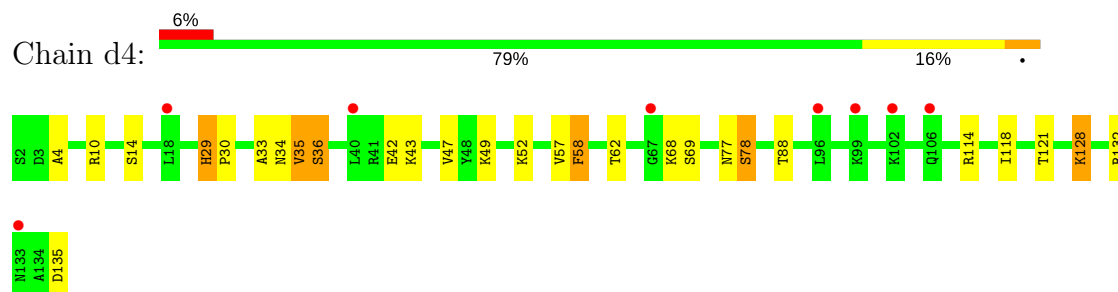


- Molecule 26: 40S ribosomal protein S24-A

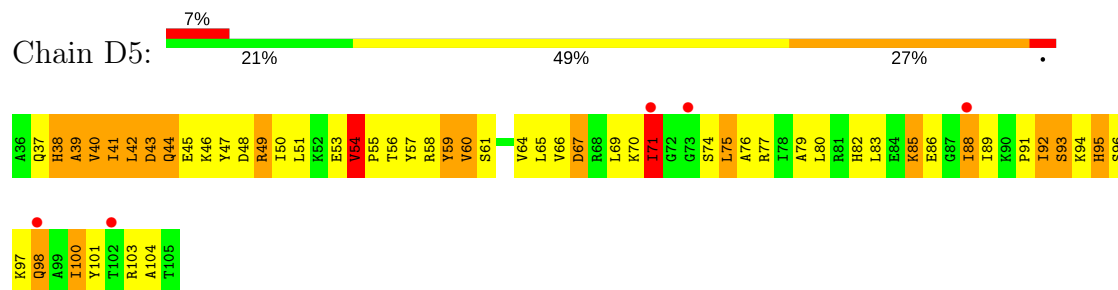




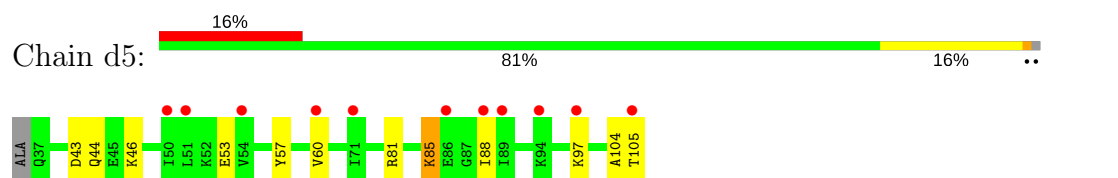
- Molecule 26: 40S ribosomal protein S24-A



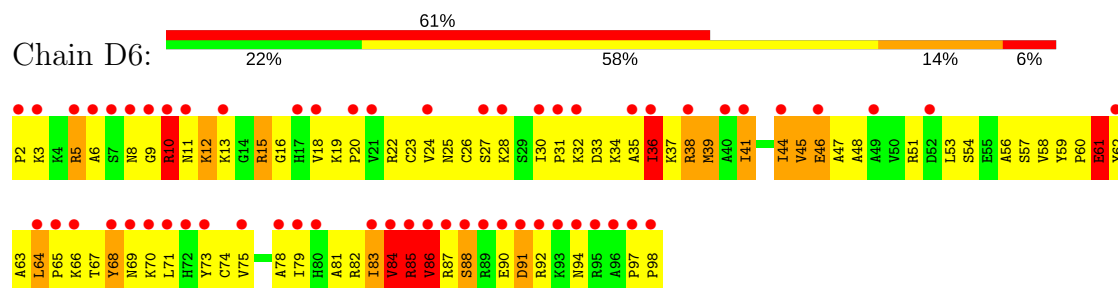
- Molecule 27: 40S ribosomal protein S25-A



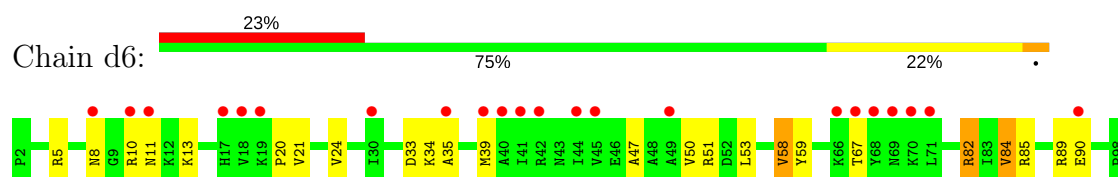
- Molecule 27: 40S ribosomal protein S25-A



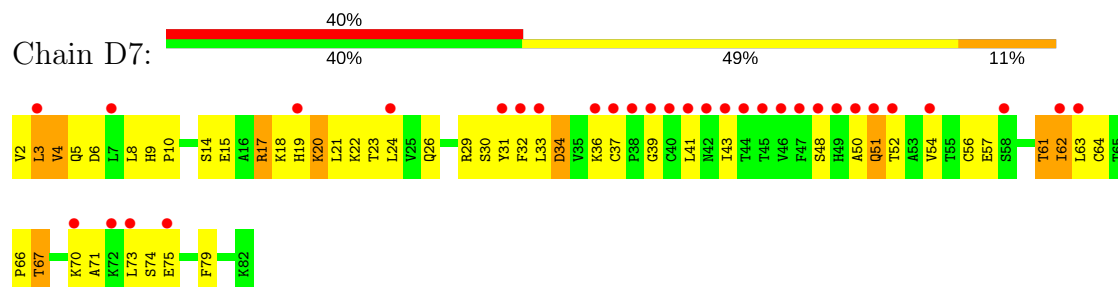
- Molecule 28: 40S ribosomal protein S26-B



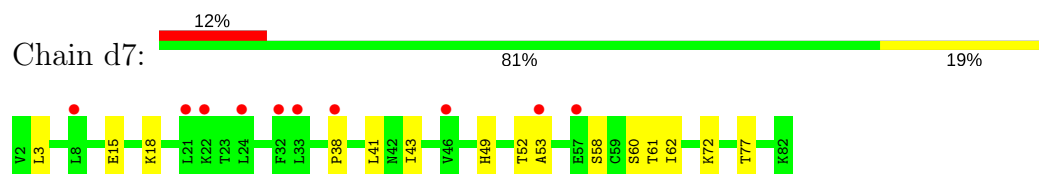
- Molecule 28: 40S ribosomal protein S26-B



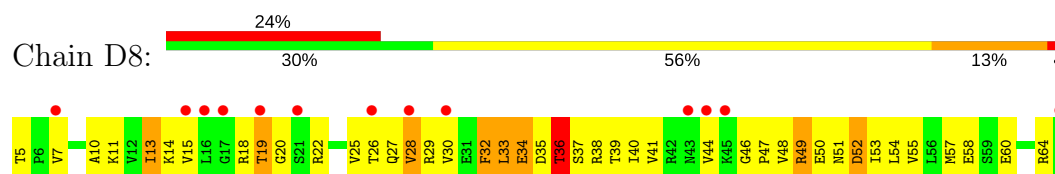
- Molecule 29: 40S ribosomal protein S27-A



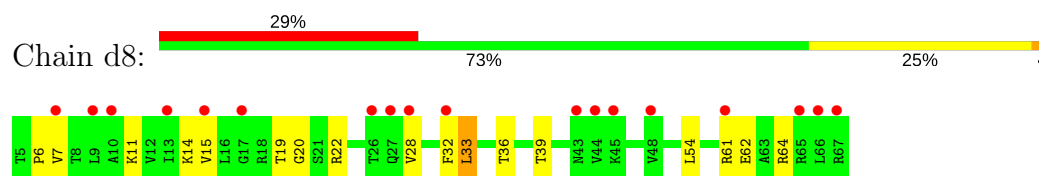
- Molecule 29: 40S ribosomal protein S27-A



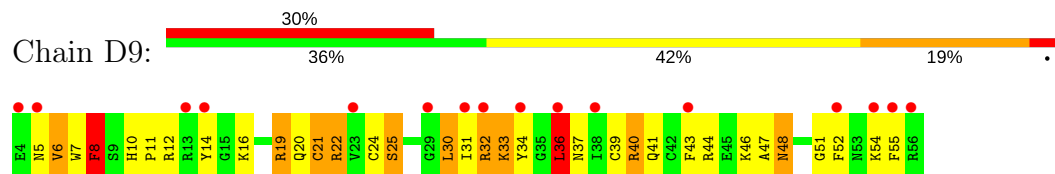
- Molecule 30: 40S ribosomal protein S28-A



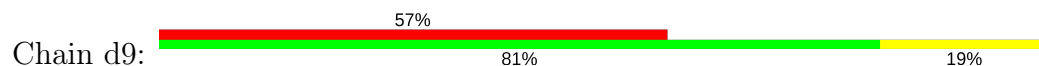
- Molecule 30: 40S ribosomal protein S28-A



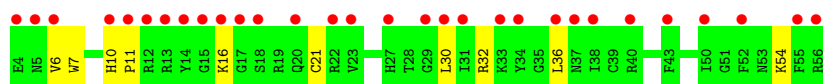
- Molecule 31: 40S ribosomal protein S29-A



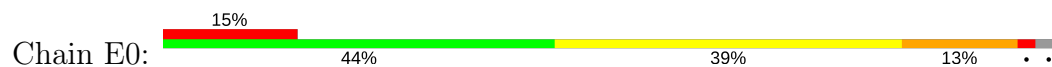
- Molecule 31: 40S ribosomal protein S29-A







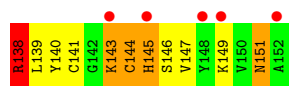
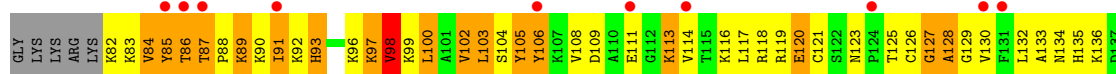
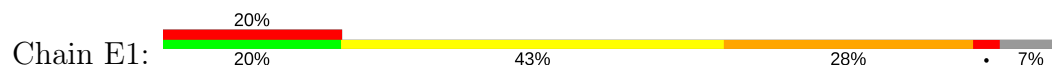
- Molecule 32: 40S ribosomal protein S30-A



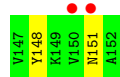
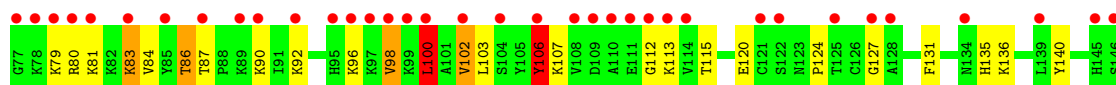
- Molecule 32: 40S ribosomal protein S30-A



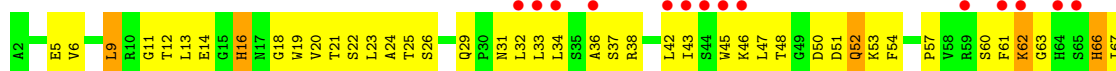
- Molecule 33: Ubiquitin-40S ribosomal protein S31

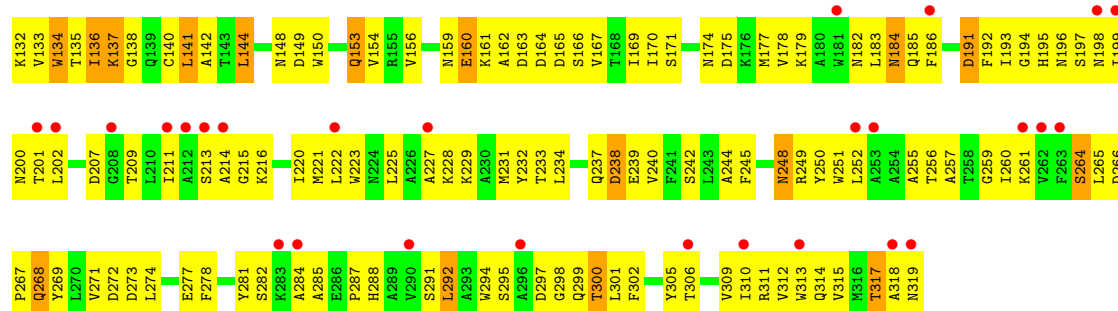


- Molecule 33: Ubiquitin-40S ribosomal protein S31

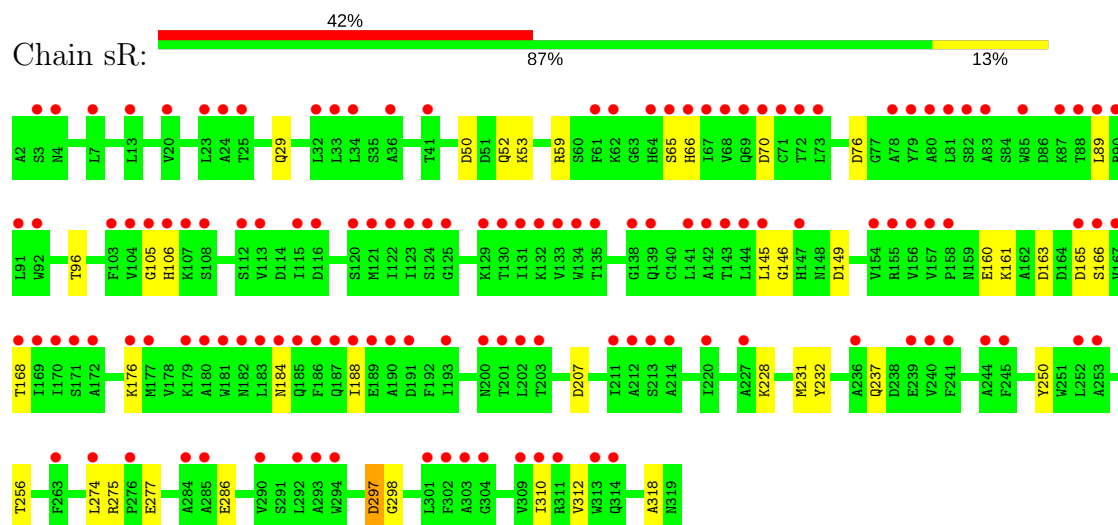


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

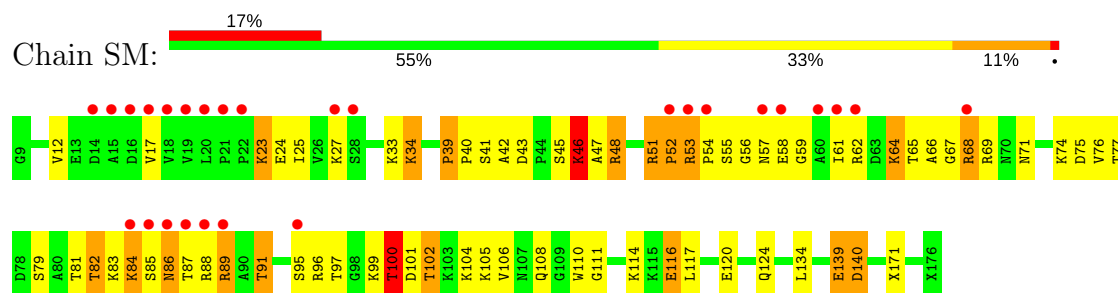




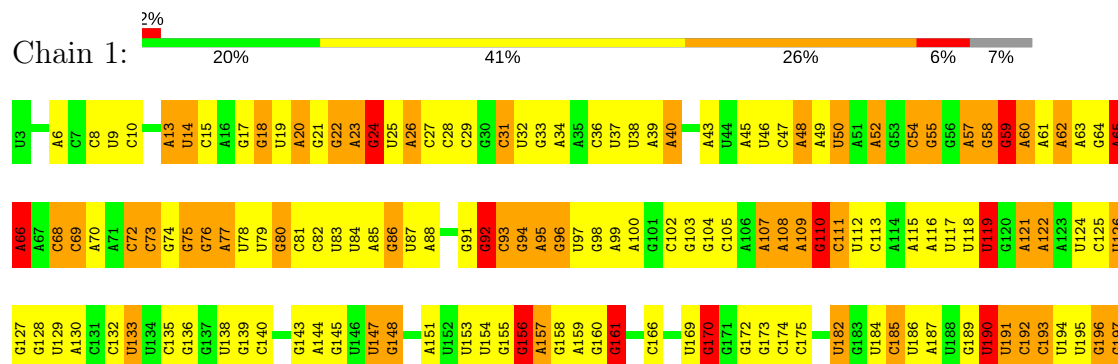
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 35: Suppressor protein STM1, Suppressor protein STM1, Ribosome-bound protein Stm1



- Molecule 36: 25S ribosomal RNA



A1153	C1092	A1025	A962	G901	C839	A646	A585	G517	C	U393	G333	G267	A198
A1154	A1093	A1026	G963	G902	C840	A647	C586	G518	C	G394	A334	A268	A199
C1155	U1094	A1027	G964	U903	A841	C648	U587	A519	C	A395	G335	G269	C200
G1157	U1095	A1028	A965	A904	G779	A649	G588	U520	C	A396	A336	U270	A201
A1158	G1097	G1029	U966	U905	A843	C650	A589	A521	U	A397	G337	G271	G202
A1159	U1098	A1030	A967	A906	G844	G651	G590	A522	G	A398	A338	G272	G203
C1160	C1032	C1081	G968	G907	G845	C652	G591	A523	C	A399	A339	A273	A204
G1161	A1099	U1033	C969	G908	A846	A653	A592	U524	U	G400	C340	G274	C205
U1162	U1100	U1034	A970	G909	C654	C654	G595	U525	C	U401	G341	G275	G206
A1163	G1101	G1035	G785	U911	G717	C655	C596	G530	C	A402	A342	U276	U207
A1164	A1102	A786	A656	G912	G718	A656	G597	G531	U	C403	U343	U277	C208
A1165	A1103	G1036	G787	G913	G719	A657	A598	A532	U	G404	A344	U278	A209
G1166	G1104	C1037	C788	G914	A720	C658	G599	A533	G	U405	G345	U279	U210
U1167	C1038	C789	A789	A914	G721	G659	C599	U534	U	G406	C346	U280	A211
U1168	U1041	U976	U790	A915	G722	A660	G600	G535	G	A407	G347	G281	G212
U1169	U1108	C977	A791	G916	G725	A661	U601	U540	G	A408	A348	G282	A213
G1170	G978	G917	G792	G917	G726	U662	A602	U541	G	A409	A349	G283	G214
U1171	C1045	A918	G793	C793	G727	C663	A603	U542	U	U410	C350	A284	U215
U1172	A1046	U919	U794	U794	G727	U664	G604	G543	A	U411	A351	A285	G216
U1173	A1047	U920	G795	G795	G728	A665	U605	C543	G	G412	A352	U286	U217
G1174	A1048	A921	G796	U796	G729	A666	C606	C544	G	U413	G353	G287	G218
C1175	A1049	U922	G797	G797	C730	C667	A607	U545	G	U414	U354	C288	A219
C1176	U1050	G923	U862	U798	G731	G668	A608	C546	G	G415	A355	A289	G220
G1177	G1115	C924	C863	G799	G732	U669	G609	C547	A	A416	C356	G290	A221
G1178	U985	G924	C864	G800	G733	C670	G610	G548	A	A417	A357	C291	A222
G1179	U986	A925	G864	G801	G734	U671	A611	U549	U	A418	G358	U292	U223
A1180	U987	A926	G867	C802	A735	A672	U612	A550	C	G419	U359	C293	C224
U1181	U988	C927	C868	C803	A736	U673	G613	A551	U	G420	G360	U294	C225
A1182	A1056	G928	G869	G804	C674	C674	C614	G552	C	G421	A361	G295	C226
U1183	A1057	A929	G870	G805	G742	C675	U615	U553	G	A422	U362	A296	G227
U1184	U930	U930	G871	G806	G743	C676	G616	A554	C	A423	G363	U298	U228
U1185	G933	C931	U871	A807	A744	A677	G617	U555	A	G424	G364	C299	G229
G1186	G934	U932	C873	A808	G778	C678	C618	U556	U	A425	A365	G300	U230
C1187	A997	A933	U874	G809	A747	U679	A619	A557	U	G426	A366	G301	G231
A1190	A998	G934	G875	A810	U748	G680	U620	U558	U	C427	A367	U302	G232
U1191	G999	U935	A876	U811	C749	U681	A621	A559	C	A428	G368	G303	G233
C1192	A1085	A936	A877	U811	G750	U682	A622	G560	A	H499	A369	G304	
A1193	U1066	G937	C877	U811	A751		U623	C561	C	U430	U370	U305	
G1194	U1067	G1001	G878	G815	G752	G685	G624	C562	U	G371	A371	A306	A238
A1195	C1068	U939	U879	A816	C753	G686	G625	U563	G	A372	A372	A307	G239
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A1217	U1021	U959	U898	A836	G774	A705	U644	G583	U	U	A391	G331	A265
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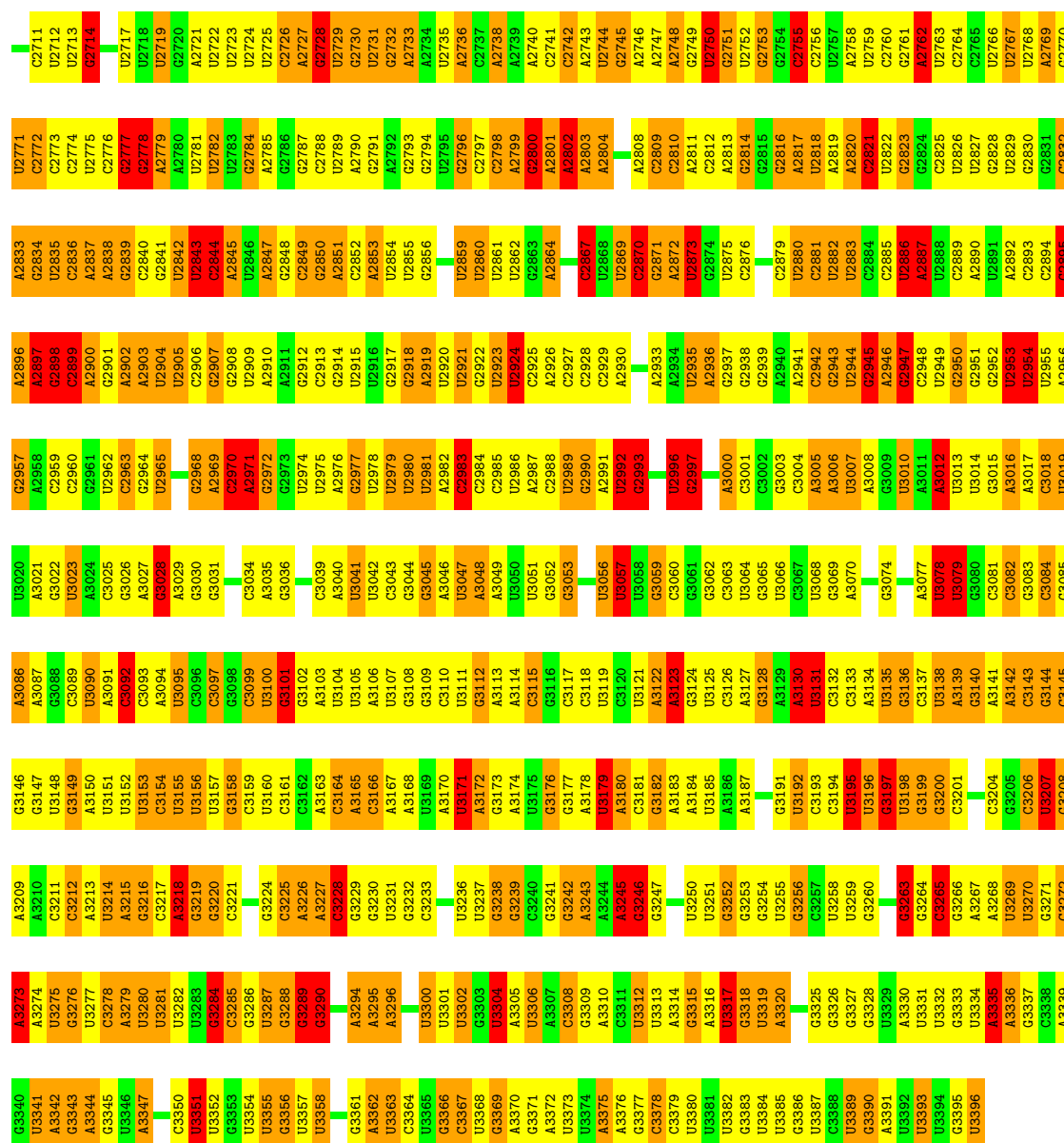




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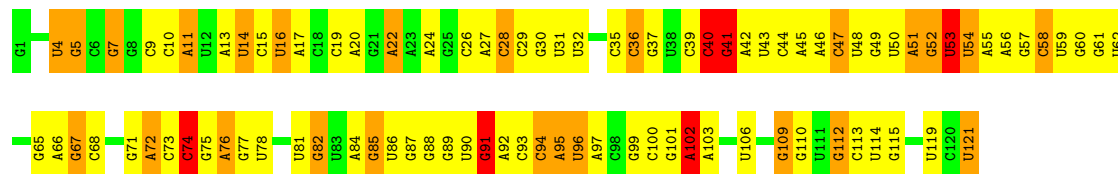
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• Molecule 37: 5S ribosomal RNA

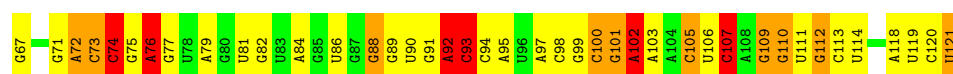
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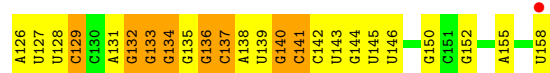
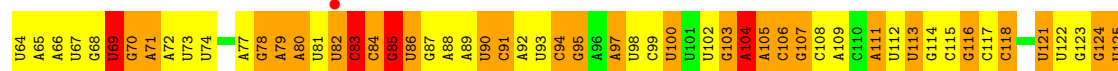
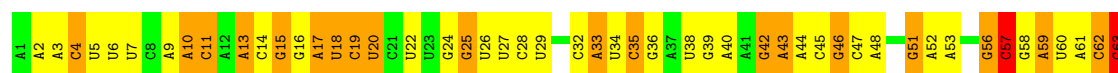
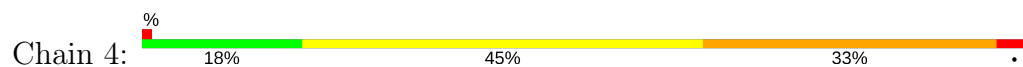
• Molecule 37: 5S ribosomal RNA

Chain 7: 28% 45% 19% 7%

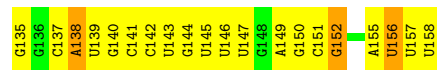
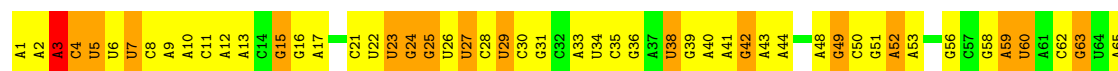




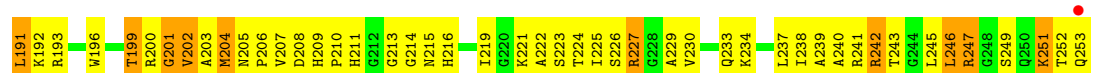
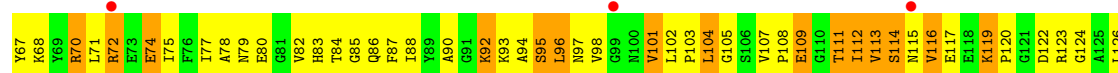
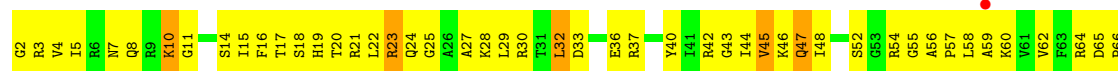
• Molecule 38: 5.8S ribosomal RNA



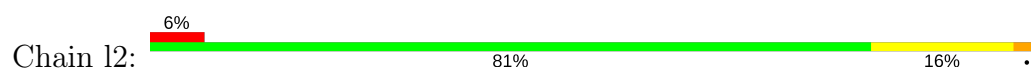
• Molecule 38: 5.8S ribosomal RNA

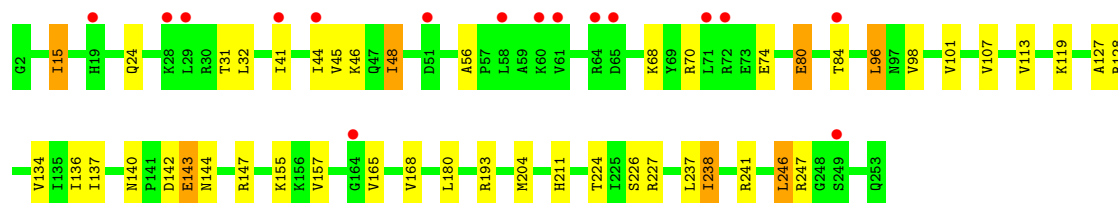


• Molecule 39: 60S ribosomal protein L2-A



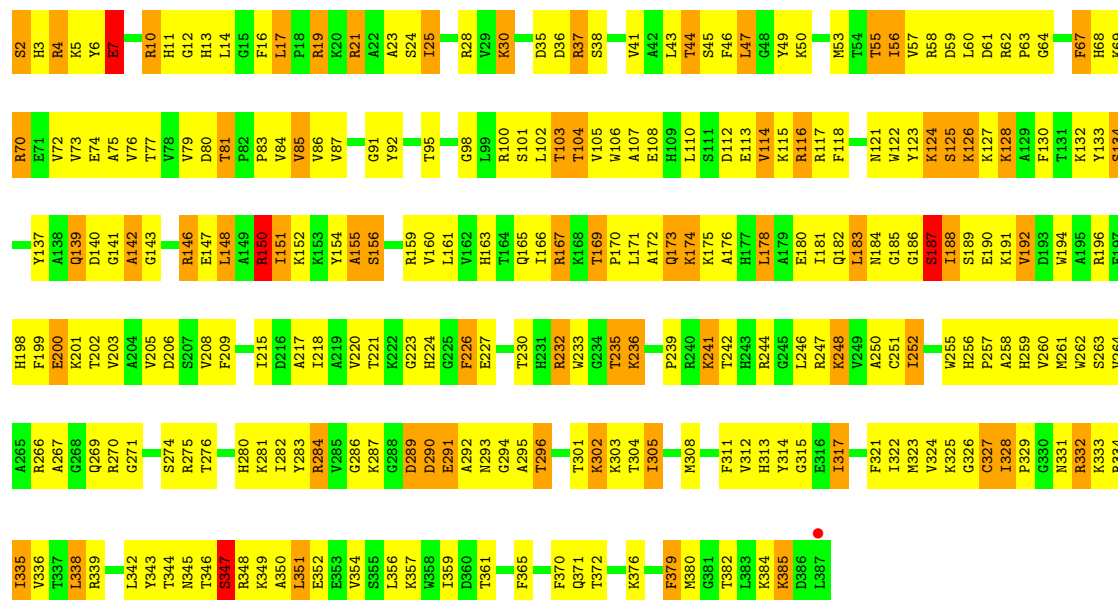
• Molecule 39: 60S ribosomal protein L2-A





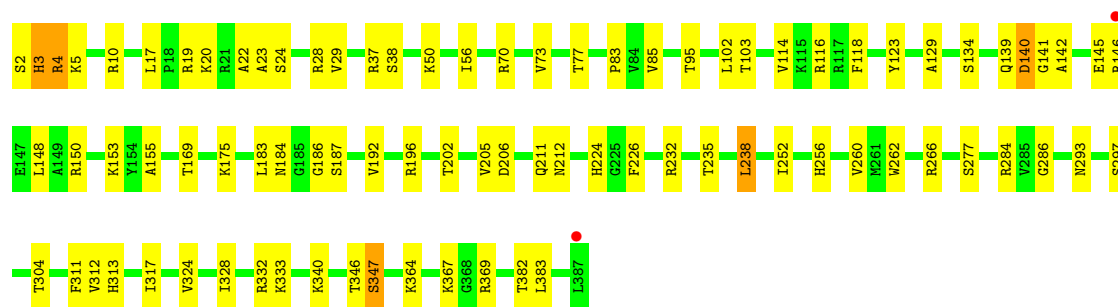
• Molecule 40: 60S ribosomal protein L3

Chain L3: 32% 50% 17%



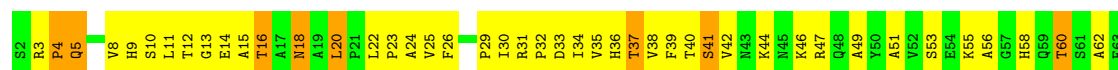
• Molecule 40: 60S ribosomal protein L3

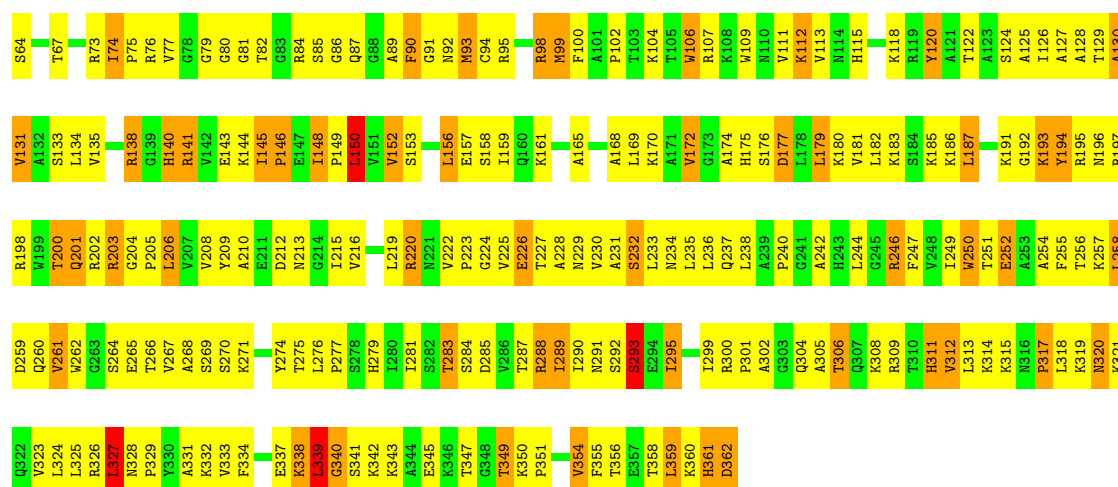
Chain l3: 78% 21%



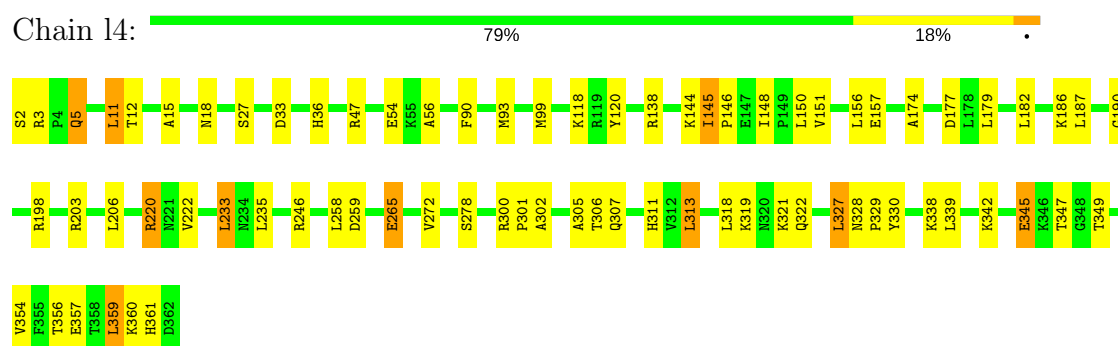
• Molecule 41: 60S ribosomal protein L4-A

Chain L4: 28% 54% 17%

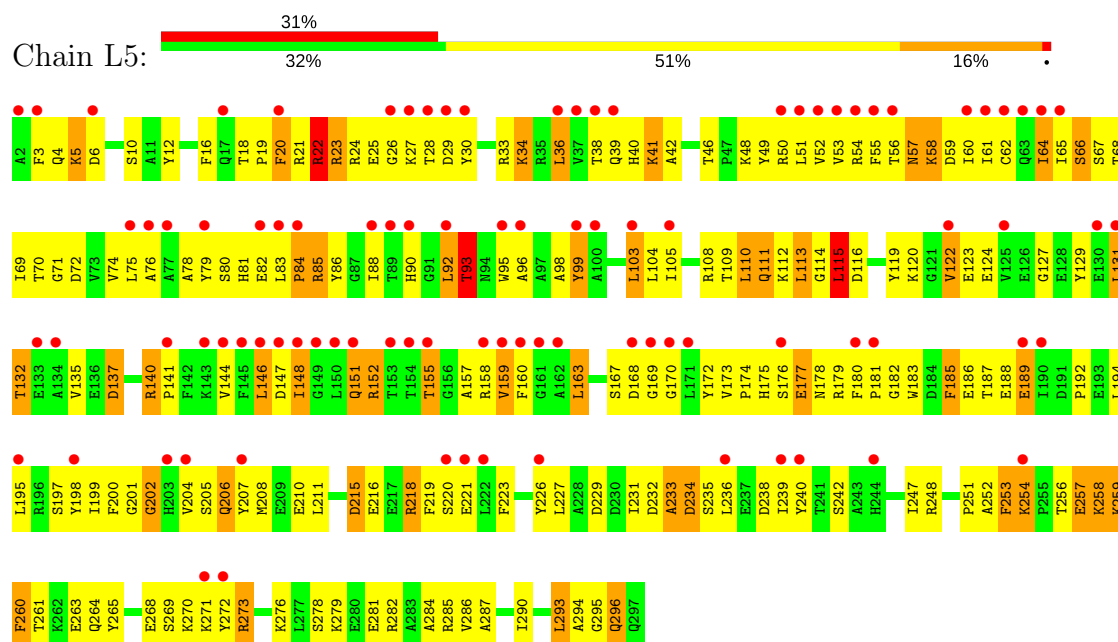




• Molecule 41: 60S ribosomal protein L4-A



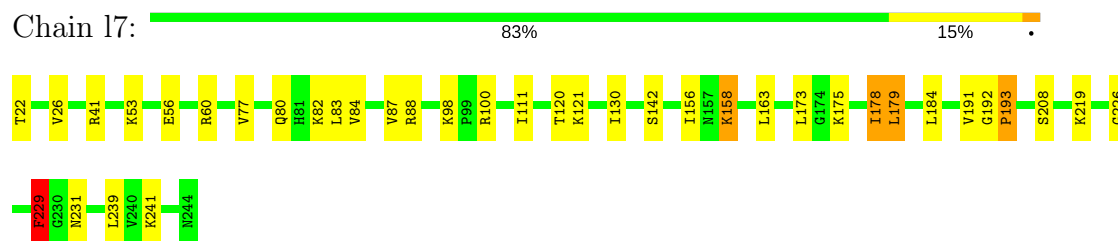
• Molecule 42: 60S ribosomal protein L5



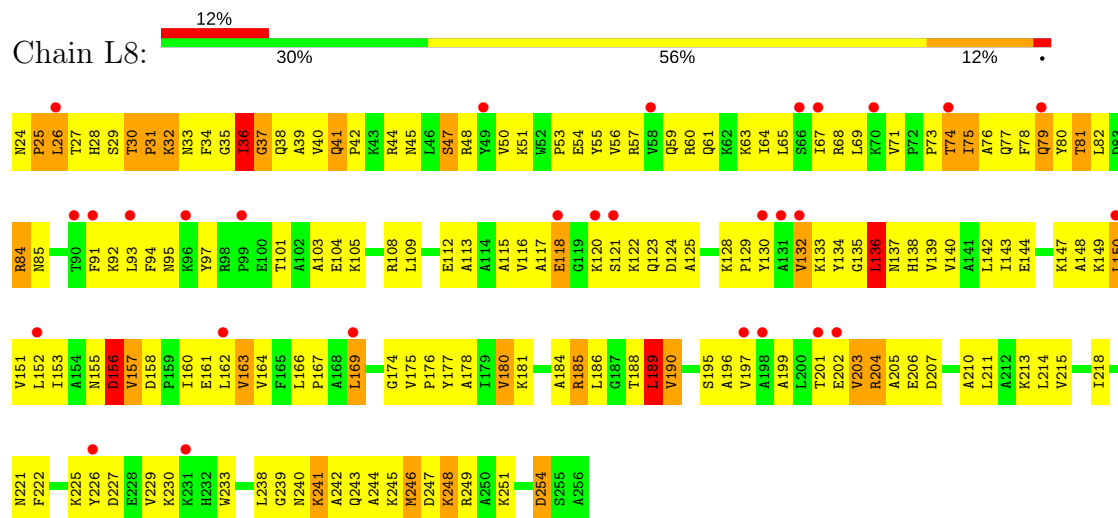
• Molecule 42: 60S ribosomal protein L5



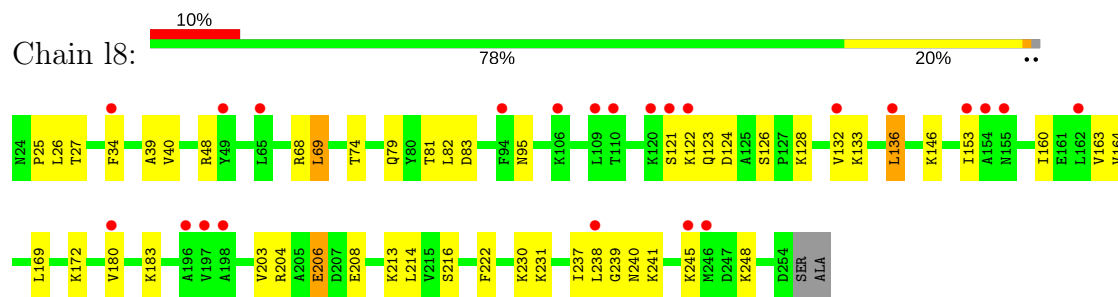
- Molecule 44: 60S ribosomal protein L7-A



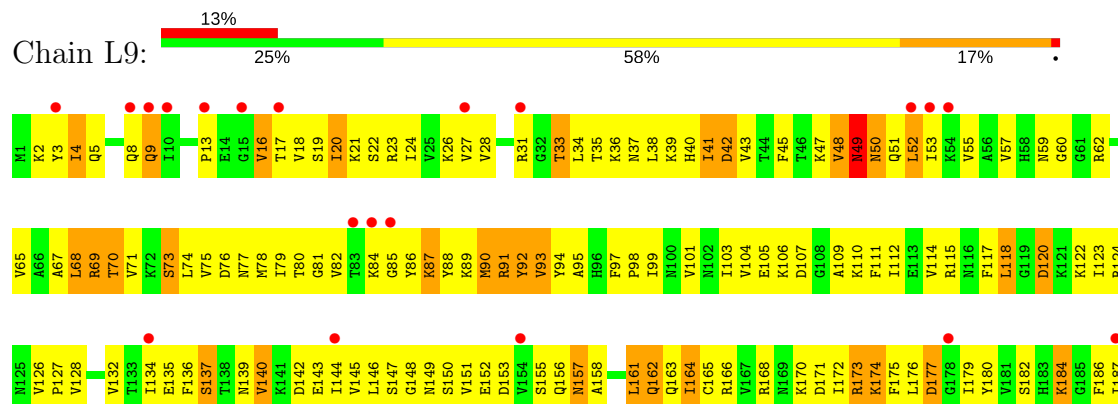
- Molecule 45: 60S ribosomal protein L8-A



- Molecule 45: 60S ribosomal protein L8-A

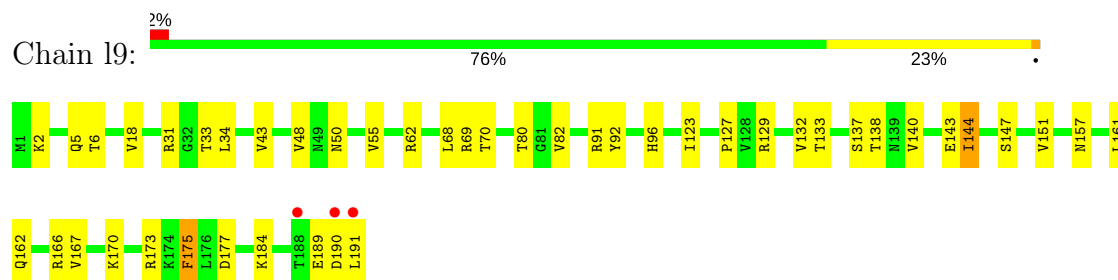


- Molecule 46: 60S ribosomal protein L9-A

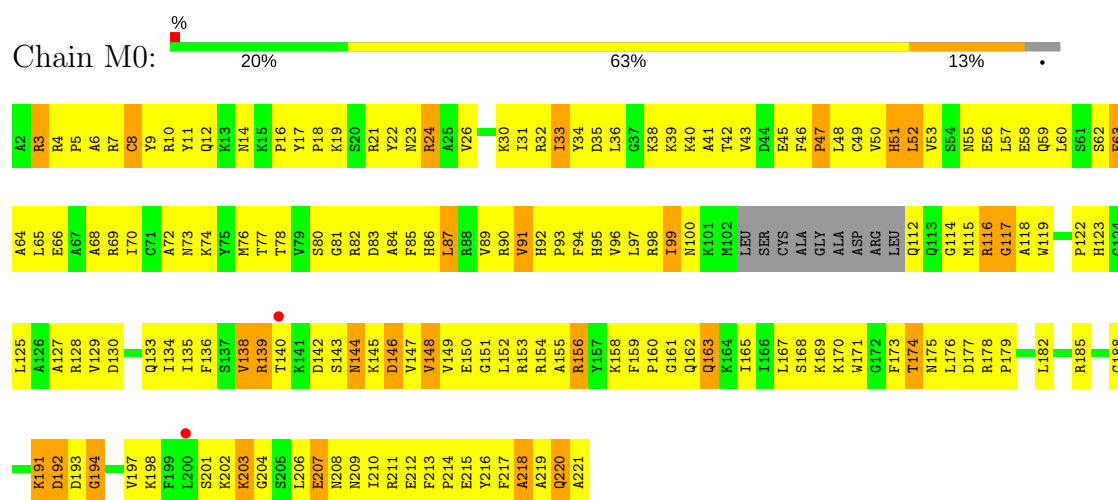




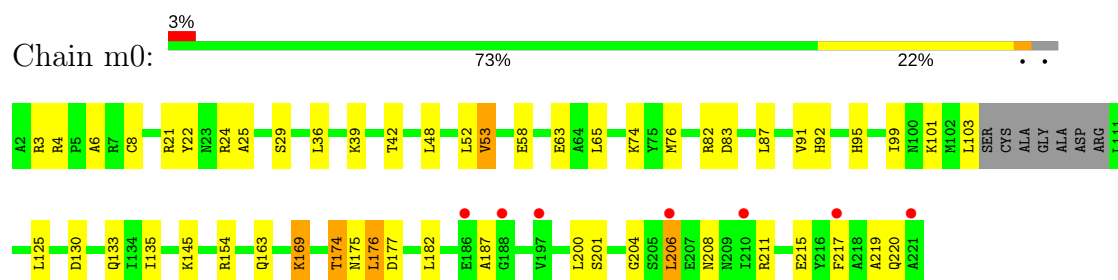
- Molecule 46: 60S ribosomal protein L9-A



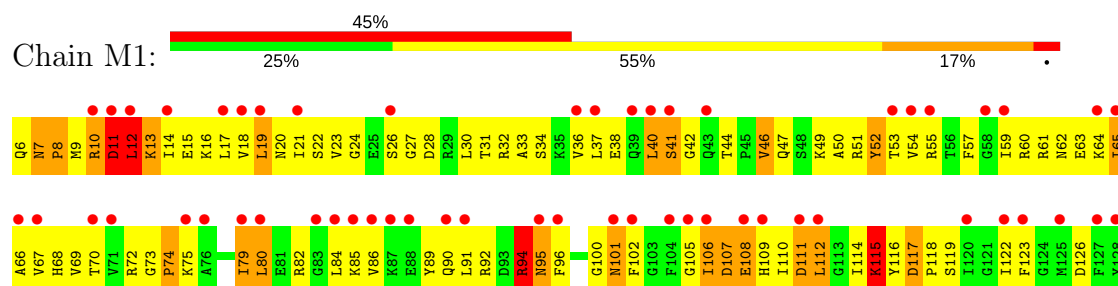
- Molecule 47: 60S ribosomal protein L10

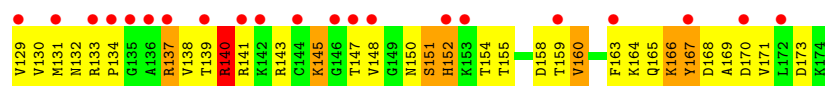


- Molecule 47: 60S ribosomal protein L10

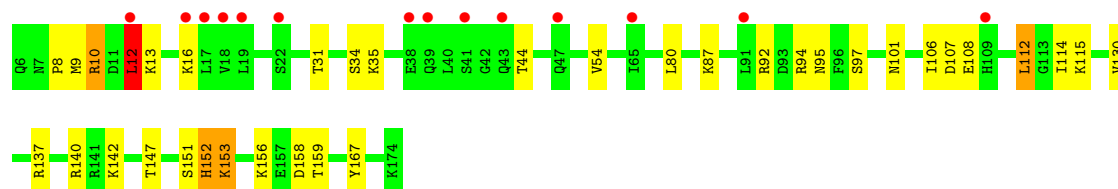
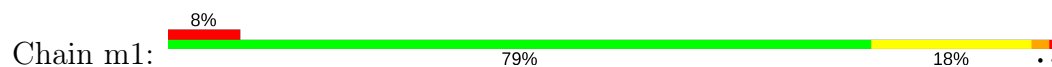


- Molecule 48: 60S ribosomal protein L11-B

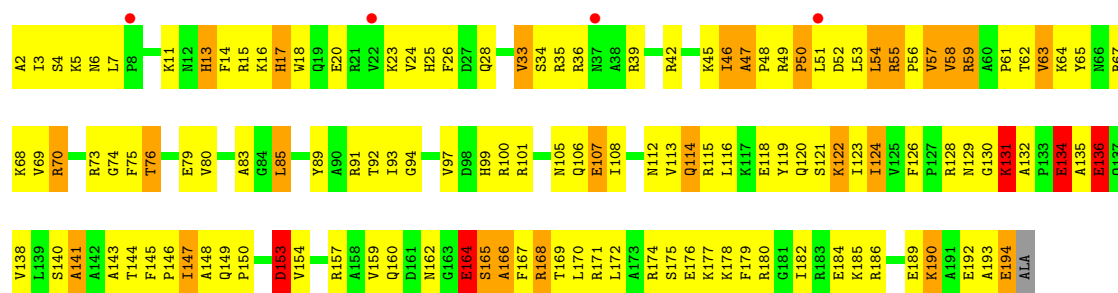




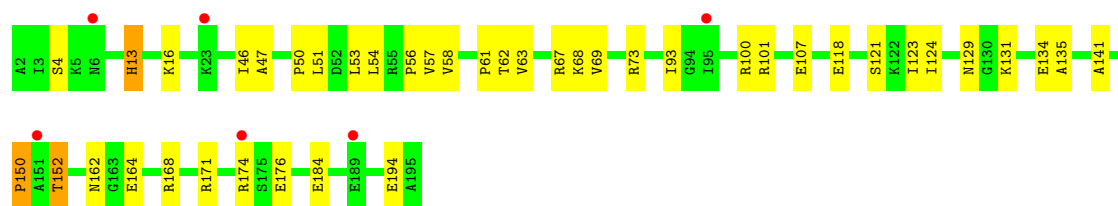
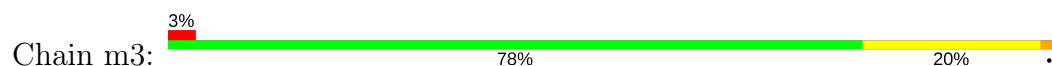
• Molecule 48: 60S ribosomal protein L11-B



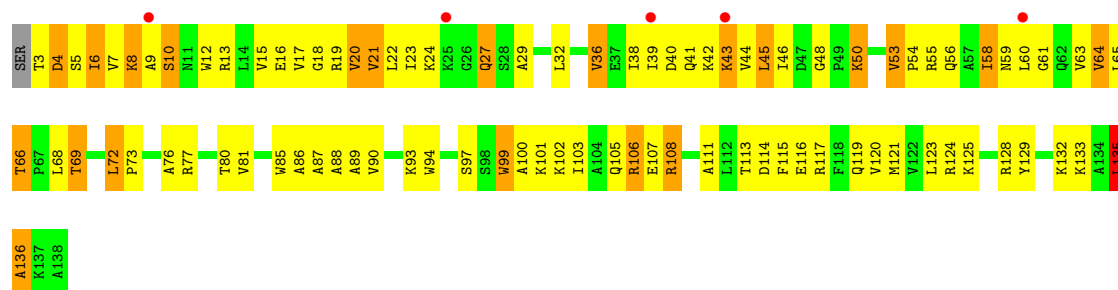
• Molecule 49: 60S ribosomal protein L13-A



• Molecule 49: 60S ribosomal protein L13-A

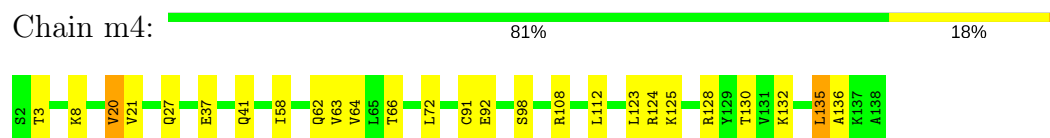


• Molecule 50: 60S ribosomal protein L14-A

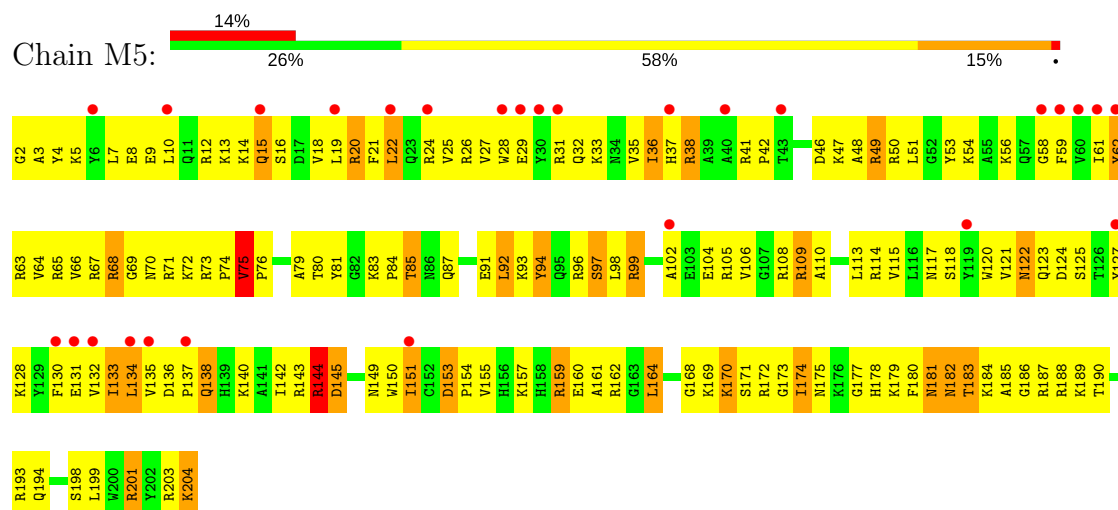




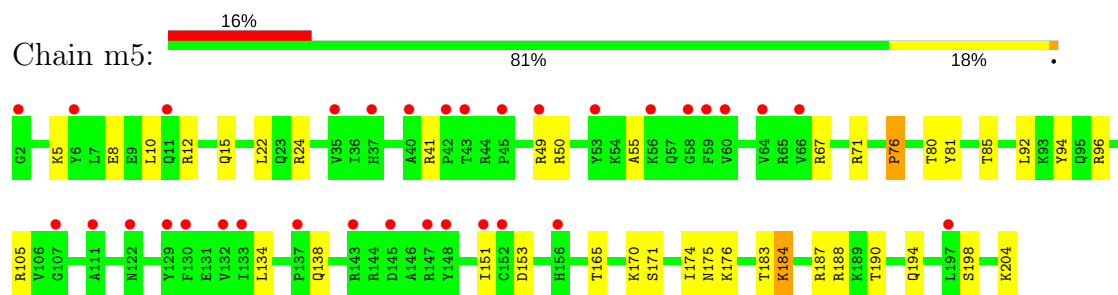
- Molecule 50: 60S ribosomal protein L14-A



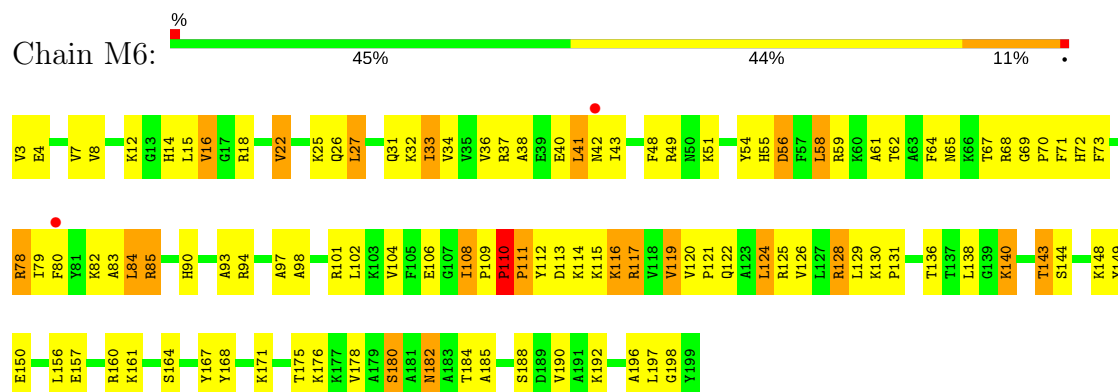
- Molecule 51: 60S ribosomal protein L15-A



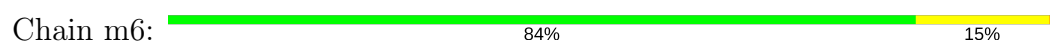
- Molecule 51: 60S ribosomal protein L15-A

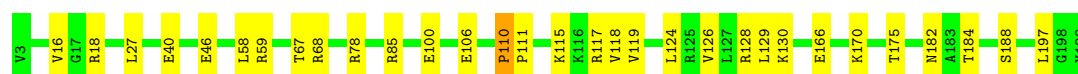


- Molecule 52: 60S ribosomal protein L16-A

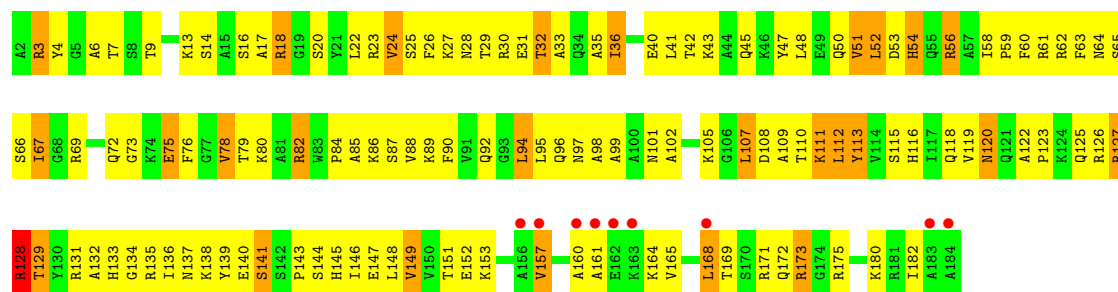


- Molecule 52: 60S ribosomal protein L16-A

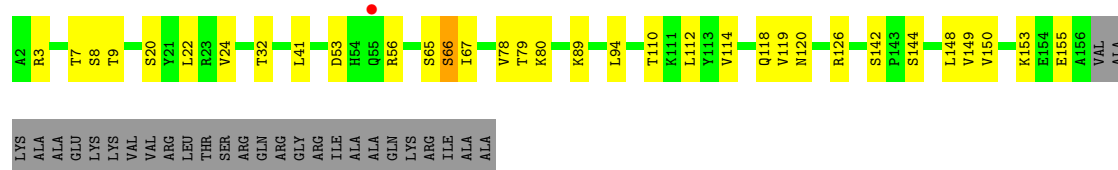




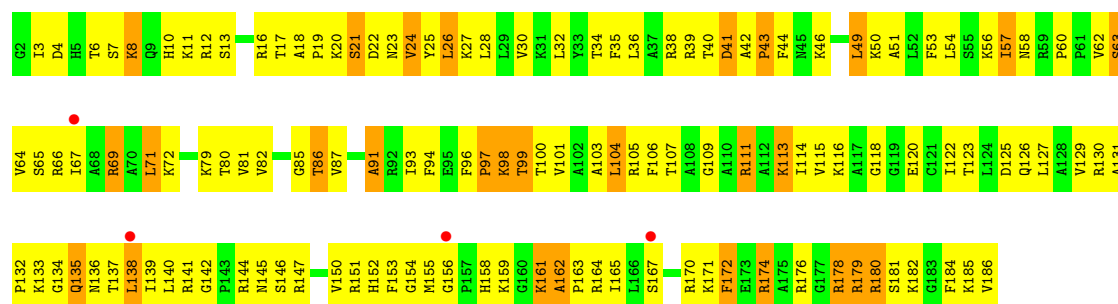
• Molecule 53: 60S ribosomal protein L17-A



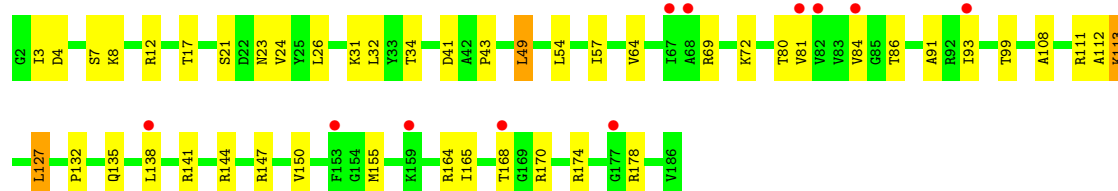
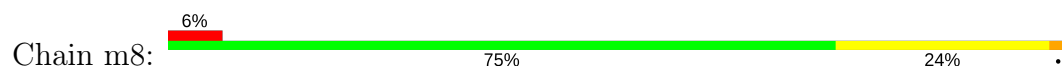
• Molecule 53: 60S ribosomal protein L17-A



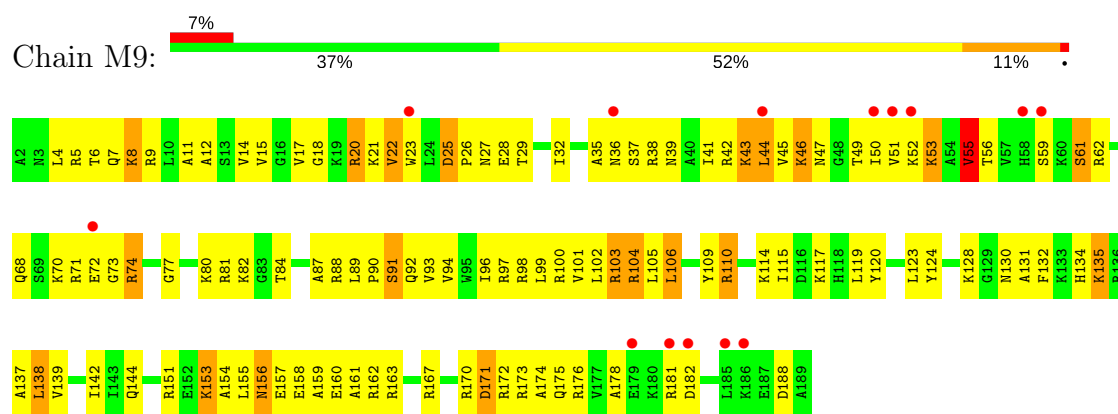
• Molecule 54: 60S ribosomal protein L18-A



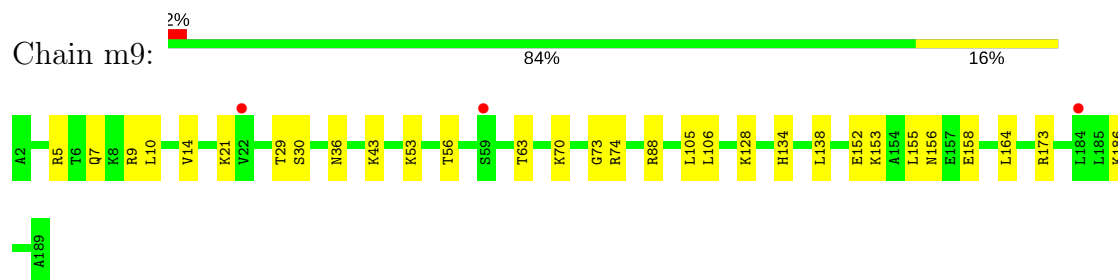
• Molecule 54: 60S ribosomal protein L18-A



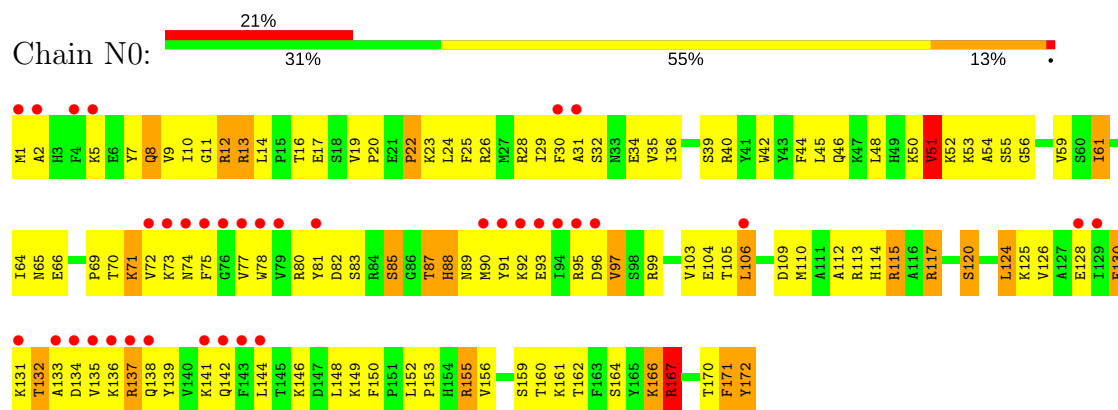
• Molecule 55: 60S ribosomal protein L19-A



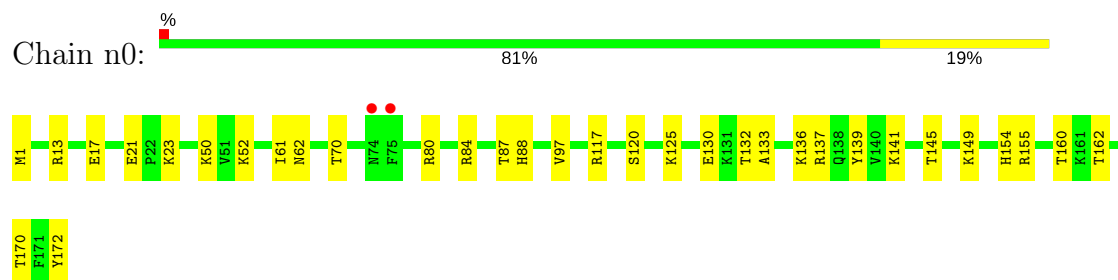
• Molecule 55: 60S ribosomal protein L19-A



• Molecule 56: 60S ribosomal protein L20-A

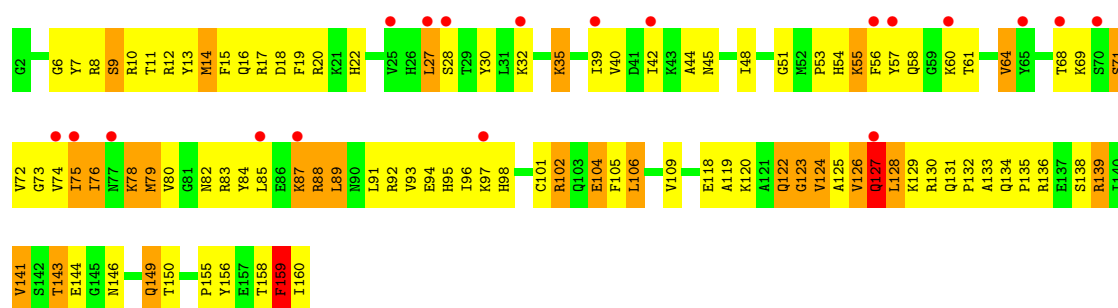


• Molecule 56: 60S ribosomal protein L20-A

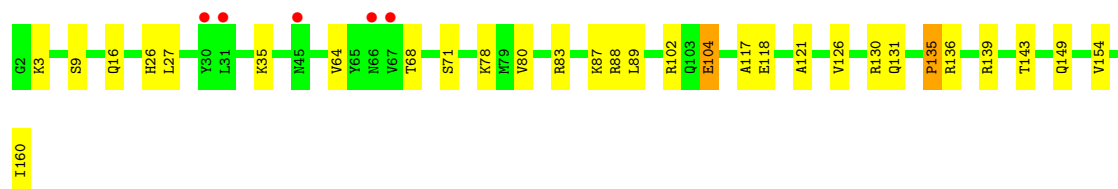
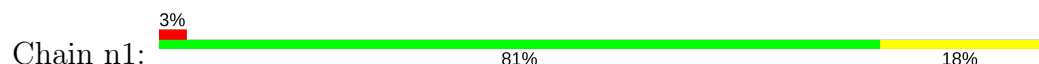


• Molecule 57: 60S ribosomal protein L21-A

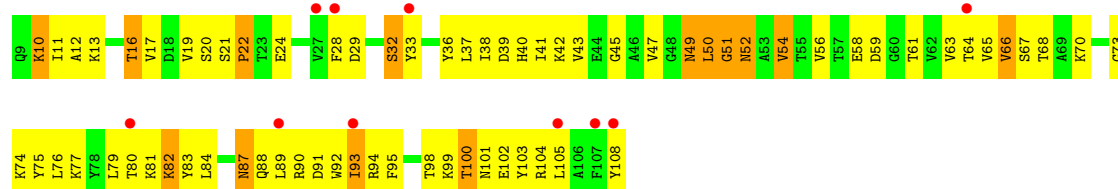




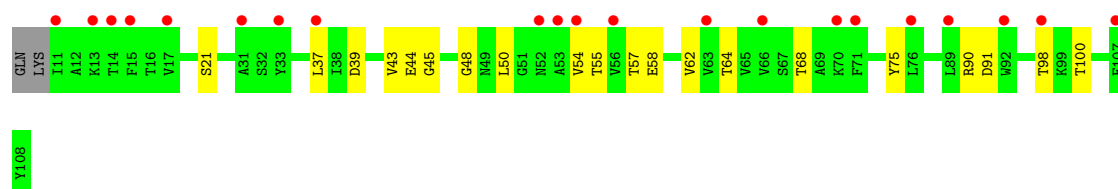
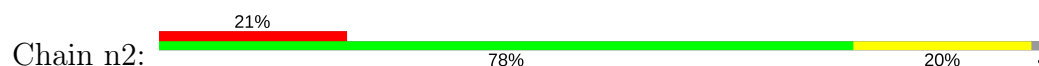
• Molecule 57: 60S ribosomal protein L21-A



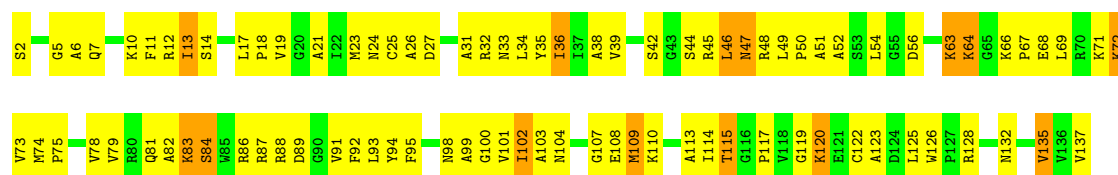
• Molecule 58: 60S ribosomal protein L22-A



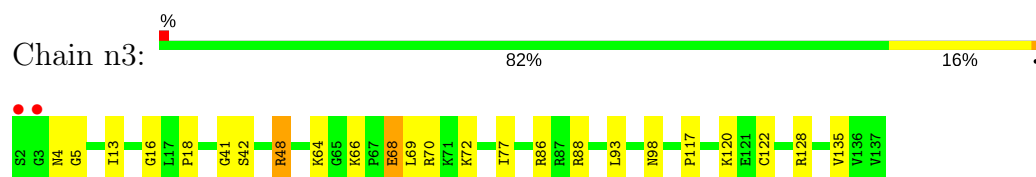
• Molecule 58: 60S ribosomal protein L22-A



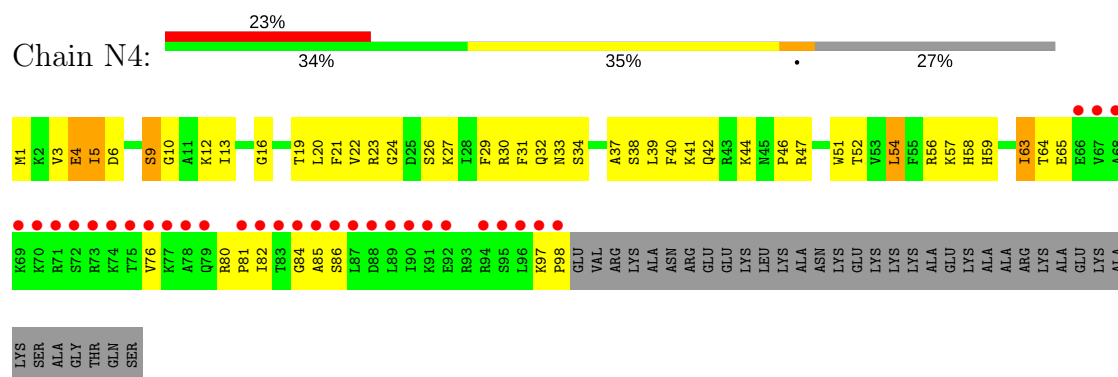
• Molecule 59: 60S ribosomal protein L23-A



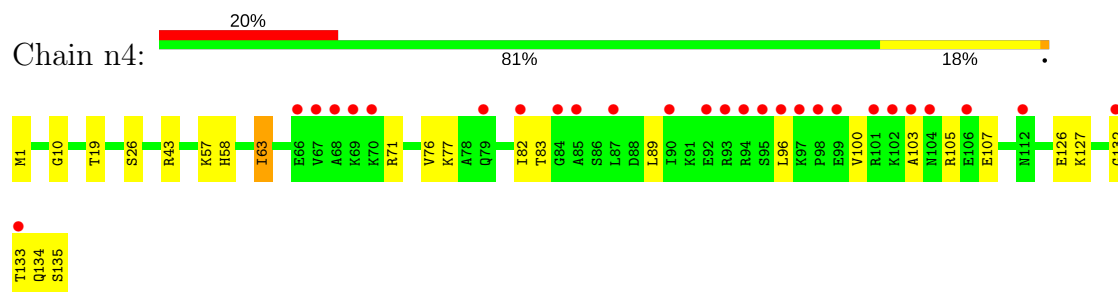
- Molecule 59: 60S ribosomal protein L23-A



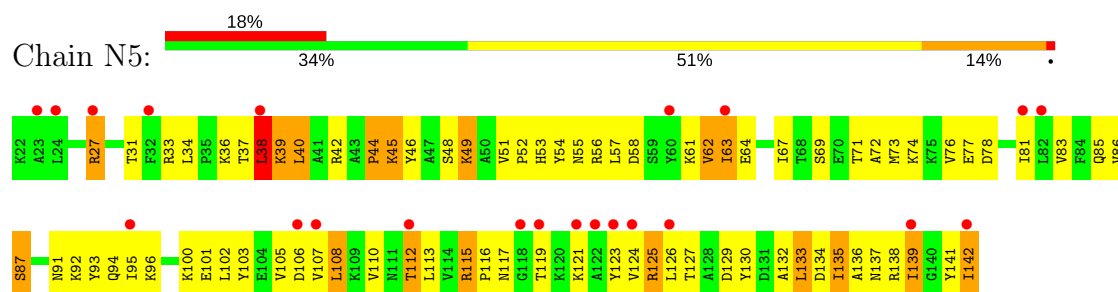
- Molecule 60: 60S ribosomal protein L24-A



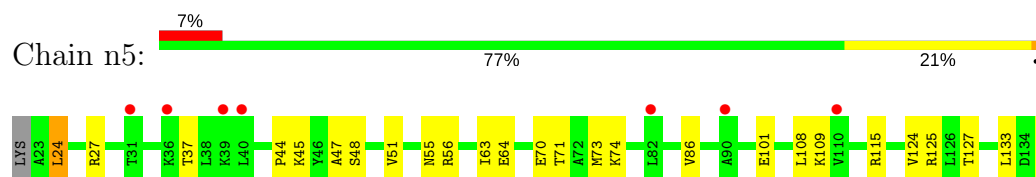
- Molecule 60: 60S ribosomal protein L24-A



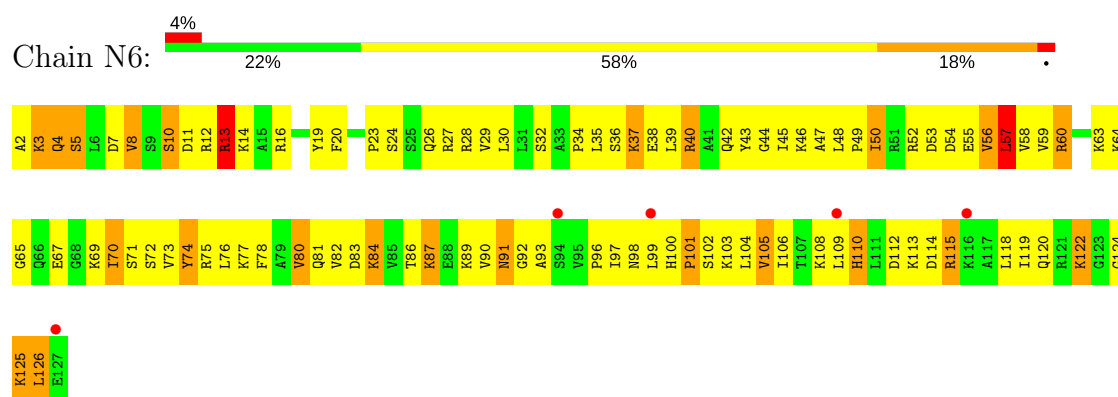
- Molecule 61: 60S ribosomal protein L25



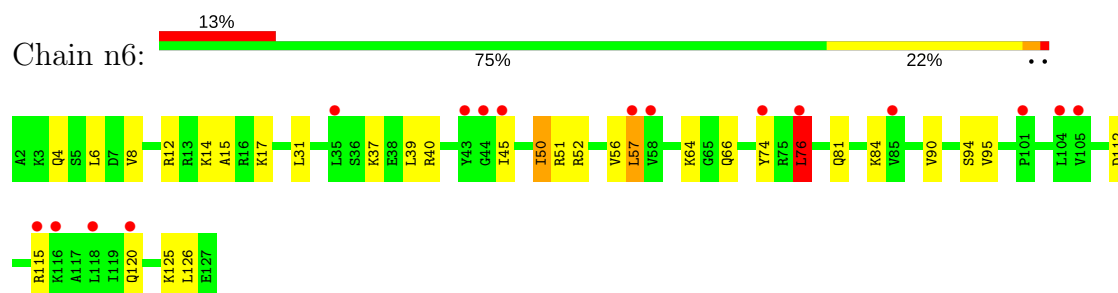
- Molecule 61: 60S ribosomal protein L25



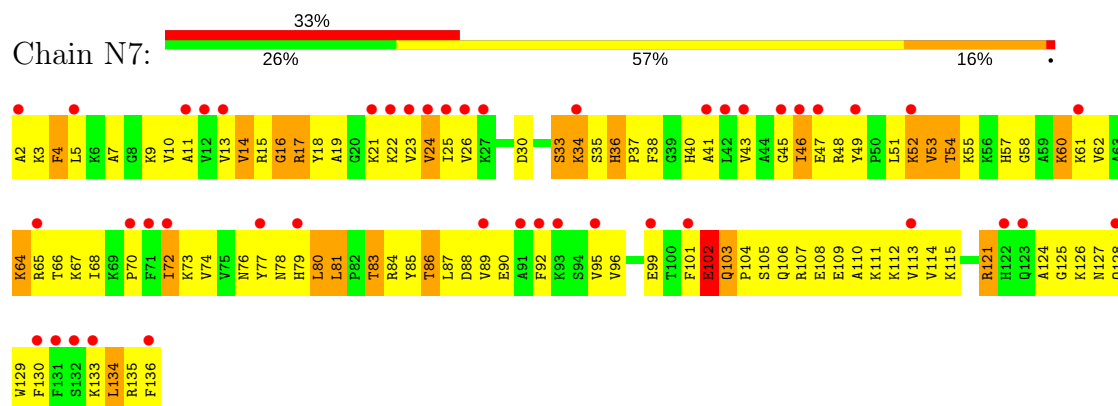
- Molecule 62: 60S ribosomal protein L26-A



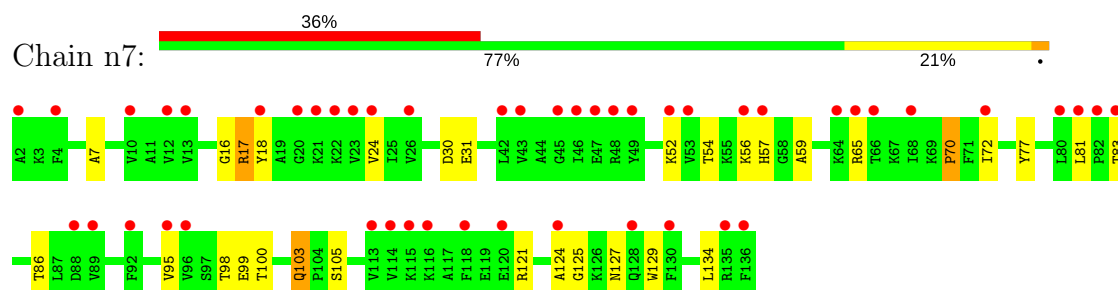
• Molecule 62: 60S ribosomal protein L26-A



• Molecule 63: 60S ribosomal protein L27-A

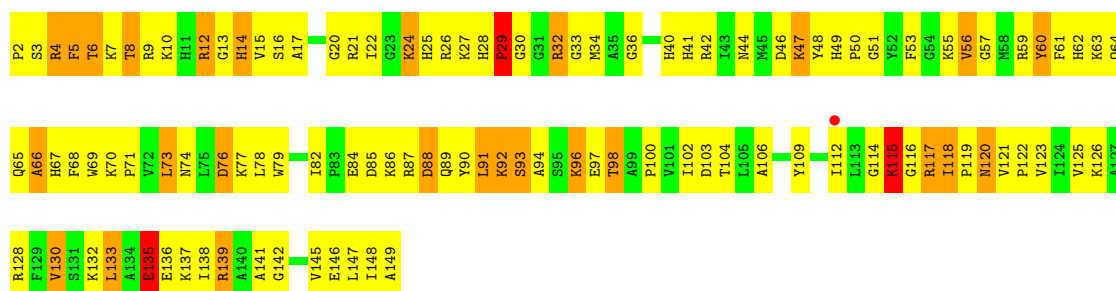


• Molecule 63: 60S ribosomal protein L27-A

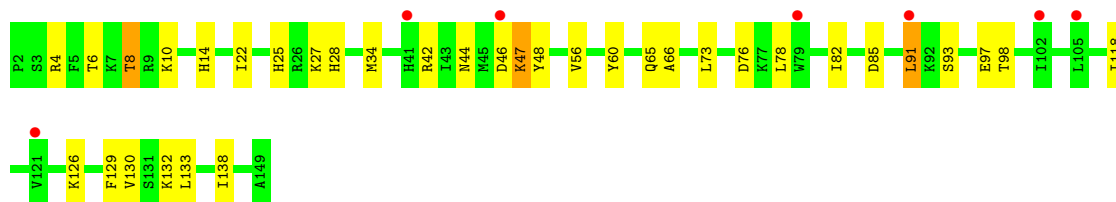
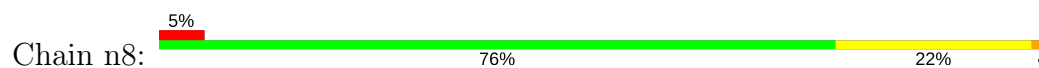


• Molecule 64: 60S ribosomal protein L28

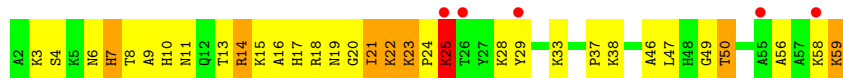
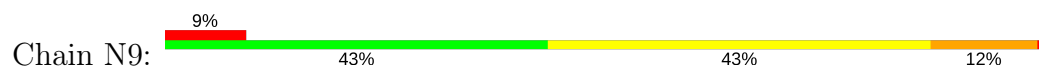




- Molecule 64: 60S ribosomal protein L28



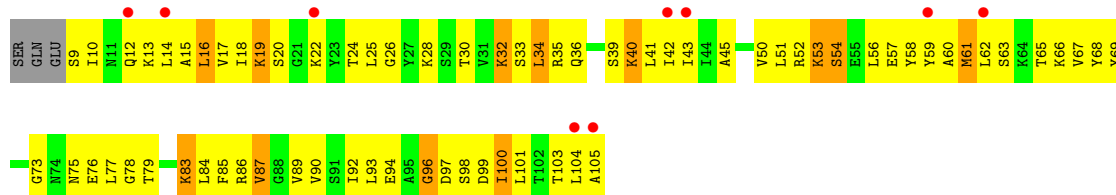
- Molecule 65: 60S ribosomal protein L29



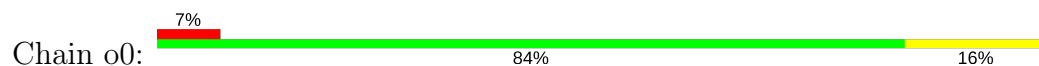
- Molecule 65: 60S ribosomal protein L29



- Molecule 66: 60S ribosomal protein L30

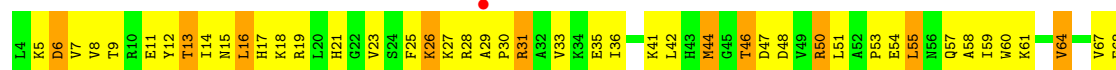


- Molecule 66: 60S ribosomal protein L30

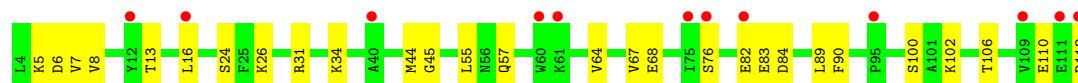
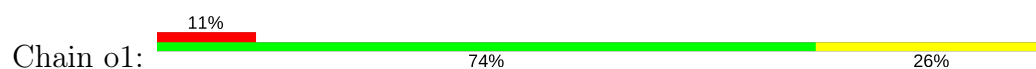




• Molecule 67: 60S ribosomal protein L31-A



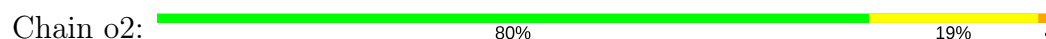
• Molecule 67: 60S ribosomal protein L31-A



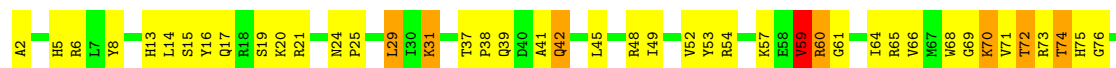
• Molecule 68: 60S ribosomal protein L32



• Molecule 68: 60S ribosomal protein L32




• Molecule 69: 60S ribosomal protein L33-A



• Molecule 69: 60S ribosomal protein L33-A

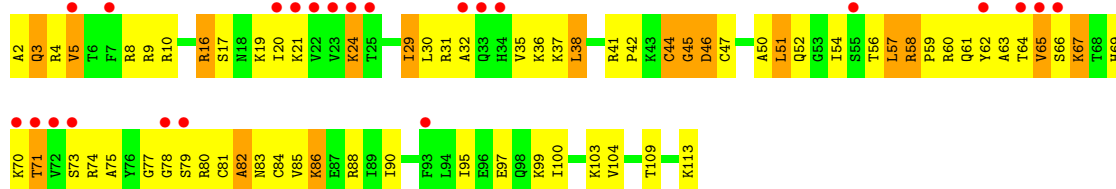


Chain o3:  85% 13% .




- Molecule 70: 60S ribosomal protein L34-A

Chain O4:  21% 38% 46% 15%



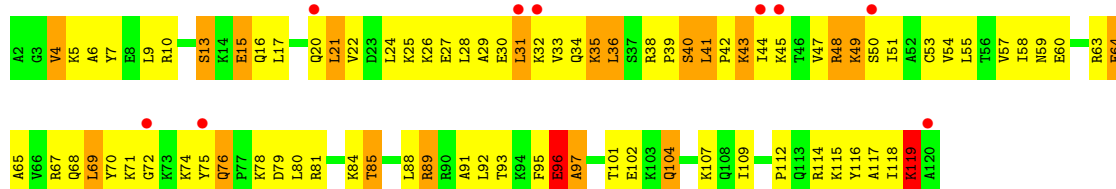
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:  9% 86% 13% .




- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  8% 29% 53% 16% .



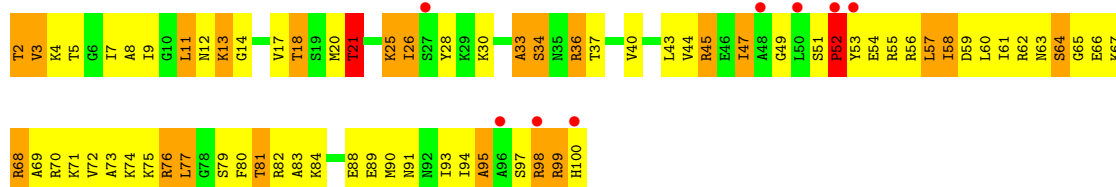
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:  2% 82% 14% .

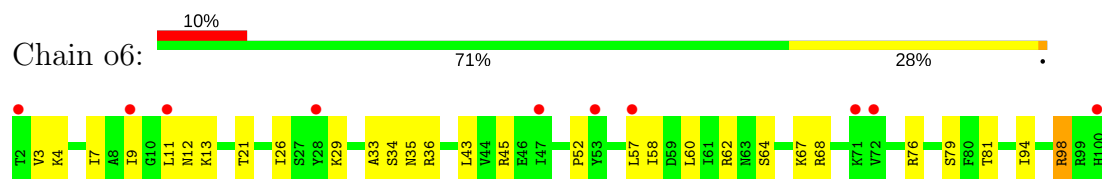


- Molecule 72: 60S ribosomal protein L36-A

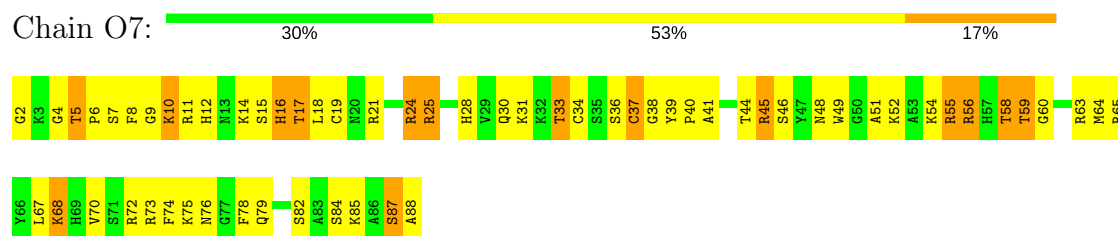
Chain O6:  8% 26% 49% 22% .



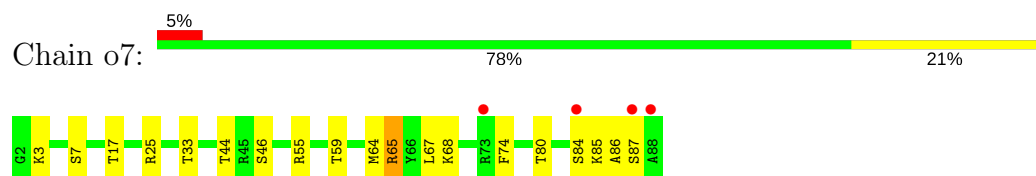
- Molecule 72: 60S ribosomal protein L36-A



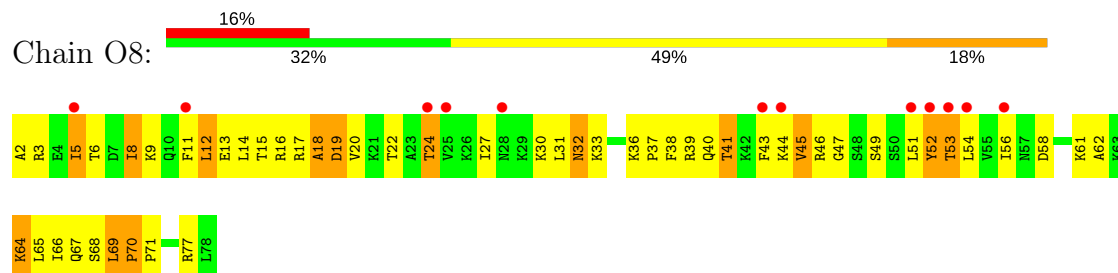
- Molecule 73: 60S ribosomal protein L37-A



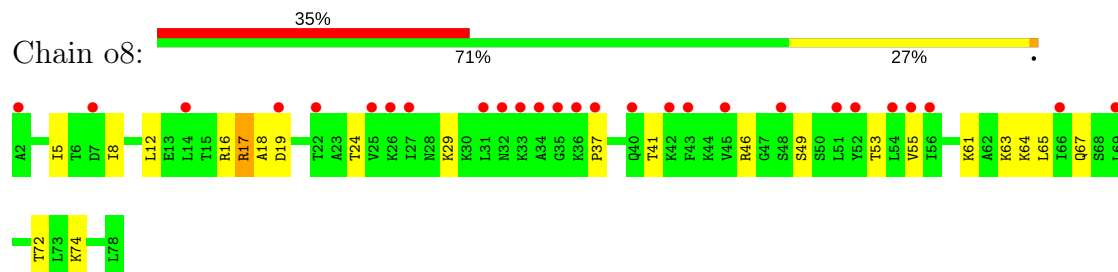
- Molecule 73: 60S ribosomal protein L37-A



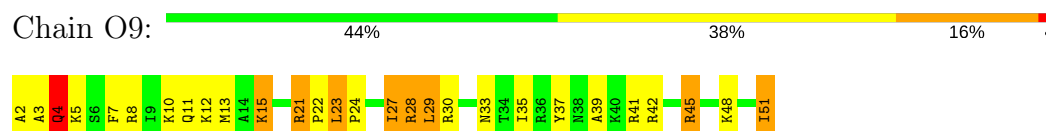
- Molecule 74: 60S ribosomal protein L38

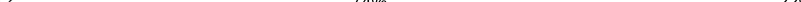


- Molecule 74: 60S ribosomal protein L38



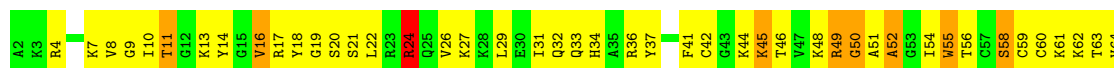
- Molecule 75: 60S ribosomal protein L39



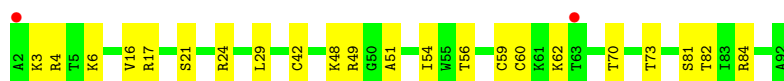
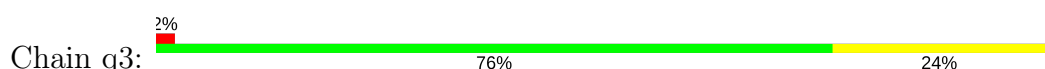
- Chain q2: 



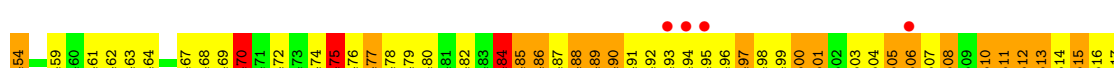
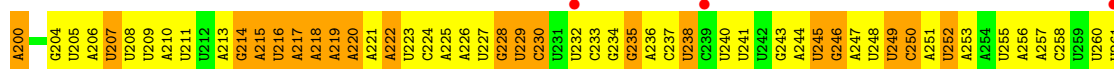
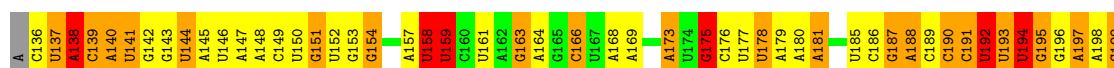
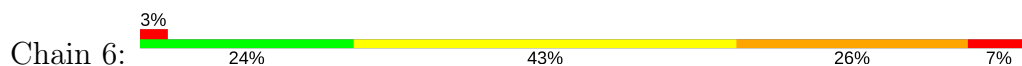
- Molecule 79: 60S ribosomal protein L43-A



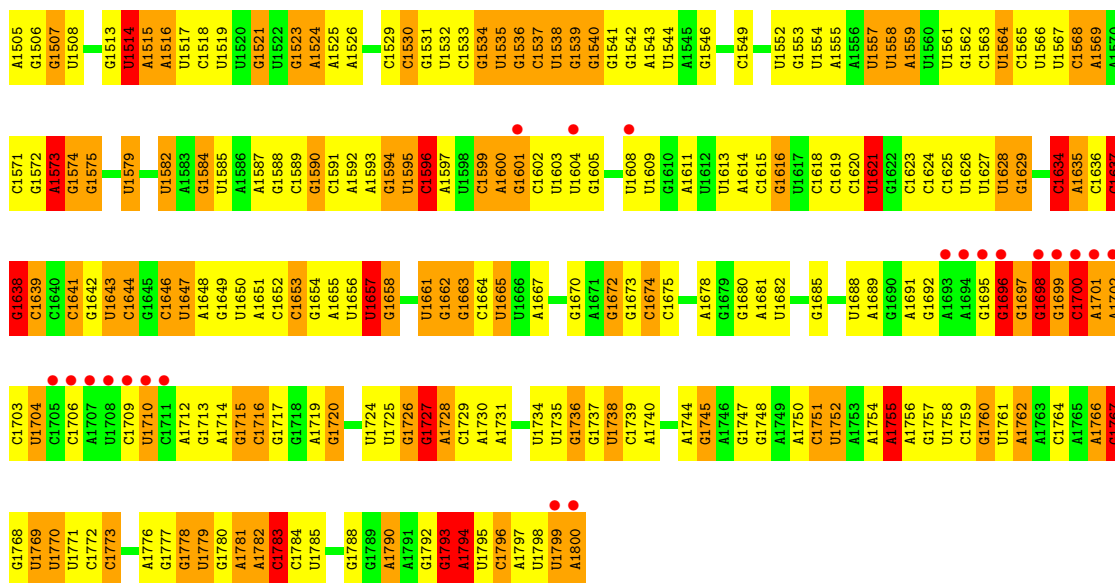
- Molecule 79: 60S ribosomal protein L43-A



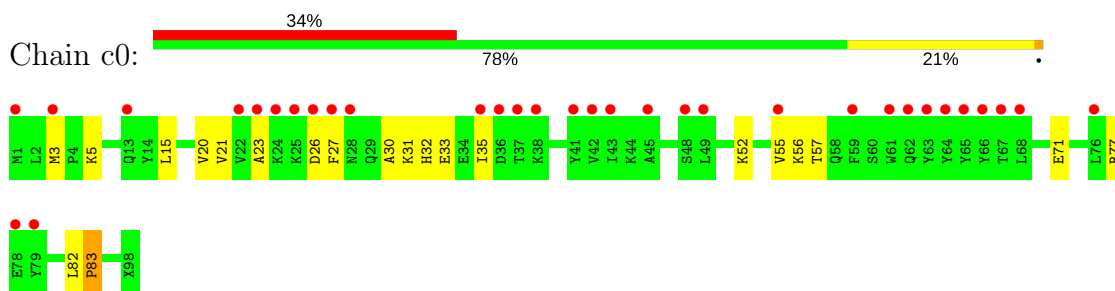
- Molecule 80: 18S ribosomal RNA



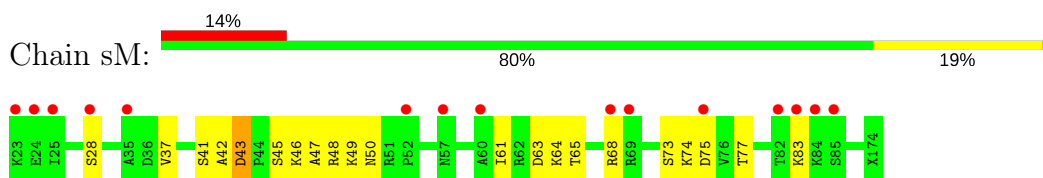




- Molecule 81: 40S ribosomal protein S10-A, 40S ribosomal protein S10-A, 40S Ribosomal Protein S10-A



- Molecule 82: Suppressor protein STM1, Suppressor protein STM1, Ribosome-bound protein Stm1

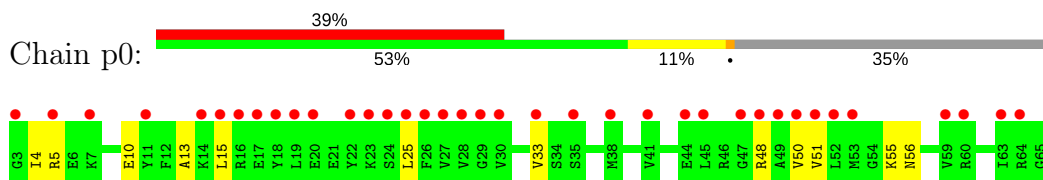


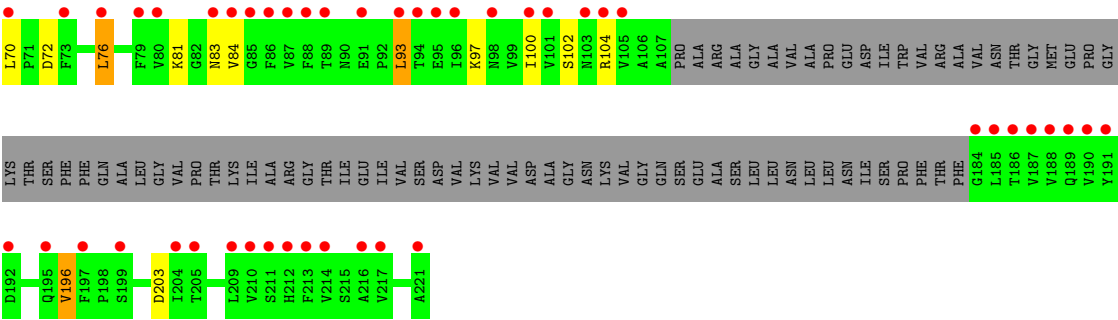
- Molecule 83: 60S Ribosomal Protein L12



There are no outlier residues recorded for this chain.

- Molecule 84: 60S acidic ribosomal protein P0





● Molecule 85: 60S Ribosomal Protein P1/2



There are no outlier residues recorded for this chain.

● Molecule 85: 60S Ribosomal Protein P1/2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	435.45Å 288.14Å 304.16Å 90.00° 99.11° 90.00°	Depositor
Resolution (Å)	149.31 – 3.30 149.31 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.3 (149.31-3.30) 92.3 (149.31-3.30)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.211 , 0.265 0.212 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	82.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 69.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	414270	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OHX, MG, 8AN

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	0.75	7/42467 (0.0%)	1.40	452/66169 (0.7%)
2	S0	0.54	1/1617 (0.1%)	0.63	0/2215
2	s0	0.51	0/1623	0.70	0/2222
3	S1	0.37	0/1735	0.62	1/2335 (0.0%)
3	s1	0.48	0/1748	0.67	3/2352 (0.1%)
4	S2	0.46	0/1665	0.69	0/2263
4	s2	0.61	0/1665	0.78	2/2263 (0.1%)
5	S3	0.46	0/1759	0.63	1/2368 (0.0%)
5	s3	0.48	0/1759	0.64	1/2368 (0.0%)
6	S4	0.45	0/2109	0.71	0/2839
6	s4	0.55	0/2109	0.78	3/2839 (0.1%)
7	S5	0.39	0/1629	0.59	0/2202
7	s5	0.46	0/1629	0.63	0/2202
8	S6	0.47	0/1823	0.64	0/2439
8	s6	0.56	0/1779	0.77	2/2379 (0.1%)
9	S7	0.44	0/1506	0.66	0/2028
9	s7	0.51	0/1516	0.69	1/2043 (0.0%)
10	S8	0.50	0/1514	0.67	0/2021
10	s8	0.59	0/1514	0.74	0/2021
11	S9	0.48	0/1519	0.65	0/2035
11	s9	0.55	0/1519	0.74	1/2035 (0.0%)
12	C0	0.41	0/789	0.69	1/1067 (0.1%)
13	C1	0.52	0/1239	0.65	0/1673
13	c1	0.60	0/1194	0.78	1/1610 (0.1%)
14	C2	0.40	0/898	0.67	0/1220
14	c2	0.33	0/898	0.61	1/1220 (0.1%)
15	C3	0.48	0/1215	0.66	1/1638 (0.1%)
15	c3	0.53	0/1215	0.70	0/1638
16	C4	0.37	0/901	0.62	0/1217
16	c4	0.50	0/960	0.66	0/1290
17	C5	0.48	0/998	0.65	0/1341
17	c5	0.51	0/1060	0.68	0/1426

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	C6	0.43	0/1125	0.68	2/1510 (0.1%)
18	c6	0.55	1/1131 (0.1%)	0.69	1/1518 (0.1%)
19	C7	0.43	0/935	0.67	0/1254
19	c7	0.48	0/914	0.66	0/1224
20	C8	0.48	0/1211	0.69	2/1628 (0.1%)
20	c8	0.46	0/1211	0.67	1/1628 (0.1%)
21	C9	0.45	0/1130	0.64	0/1517
21	c9	0.50	0/1130	0.66	3/1517 (0.2%)
22	D0	0.47	0/865	0.68	0/1169
22	d0	0.45	0/892	0.65	0/1205
23	D1	0.44	0/693	0.65	0/935
23	d1	0.64	0/693	0.75	1/935 (0.1%)
24	D2	0.49	0/1038	0.74	3/1395 (0.2%)
24	d2	0.59	0/1038	0.77	1/1395 (0.1%)
25	D3	0.57	0/1139	0.72	1/1518 (0.1%)
25	d3	0.63	0/1139	0.83	0/1518
26	D4	0.46	0/1087	0.63	0/1449
26	d4	0.55	0/1087	0.74	0/1449
27	D5	0.42	0/571	0.68	0/768
27	d5	0.45	0/566	0.60	0/761
28	D6	0.43	0/782	0.70	1/1047 (0.1%)
28	d6	0.58	0/782	0.68	0/1047
29	D7	0.44	0/620	0.64	0/838
29	d7	0.48	0/620	0.70	0/838
30	D8	0.40	0/499	0.60	0/670
30	d8	0.43	0/499	0.63	0/670
31	D9	0.59	0/452	0.71	1/600 (0.2%)
31	d9	0.52	0/452	0.64	0/600
32	E0	0.45	0/483	0.61	0/643
32	e0	0.55	0/499	0.72	0/665
33	E1	0.43	0/577	0.73	0/770
33	e1	0.40	0/619	0.72	2/822 (0.2%)
34	SR	0.40	0/2490	0.61	1/3389 (0.0%)
34	sR	0.41	0/2495	0.61	0/3395
35	SM	0.49	0/984	0.67	0/1323
36	1	1.08	150/75394 (0.2%)	1.76	2353/117545 (2.0%)
36	5	1.16	238/75414 (0.3%)	1.85	2720/117575 (2.3%)
37	3	0.96	4/2883 (0.1%)	1.60	55/4491 (1.2%)
37	7	1.09	5/2883 (0.2%)	1.77	83/4491 (1.8%)
38	4	1.01	3/3746 (0.1%)	1.72	114/5832 (2.0%)
38	8	0.95	2/3746 (0.1%)	1.62	75/5832 (1.3%)
39	L2	0.58	0/1948	0.77	0/2617
39	l2	0.61	0/1946	0.82	2/2614 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
40	L3	0.65	2/3146 (0.1%)	0.81	3/4228 (0.1%)
40	l3	0.73	0/3146	0.84	4/4228 (0.1%)
41	L4	0.67	1/2800 (0.0%)	0.84	4/3790 (0.1%)
41	l4	0.68	1/2800 (0.0%)	0.81	2/3790 (0.1%)
42	L5	0.59	0/2425	0.71	2/3271 (0.1%)
42	l5	0.73	2/2408 (0.1%)	0.77	1/3248 (0.0%)
43	L6	0.65	1/1260 (0.1%)	0.77	0/1694
43	l6	0.68	0/1269	0.79	0/1705
44	L7	0.66	0/1821	0.80	4/2451 (0.2%)
44	l7	0.71	0/1828	0.86	3/2461 (0.1%)
45	L8	0.49	0/1836	0.64	1/2481 (0.0%)
45	l8	0.48	0/1795	0.65	1/2429 (0.0%)
46	L9	0.58	0/1539	0.74	0/2073
46	l9	0.70	0/1539	0.77	0/2073
47	M0	0.72	1/1741 (0.1%)	0.77	0/2335
47	m0	0.85	2/1758 (0.1%)	0.83	0/2358
48	M1	0.52	0/1374	0.70	0/1842
48	m1	0.66	0/1374	0.80	2/1842 (0.1%)
49	M3	0.63	0/1568	0.78	0/2106
49	m3	0.59	0/1573	0.76	0/2113
50	M4	0.61	0/1068	0.72	0/1438
50	m4	0.66	0/1074	0.79	2/1446 (0.1%)
51	M5	0.63	0/1757	0.77	0/2354
51	m5	0.57	0/1757	0.73	0/2354
52	M6	0.74	0/1585	0.83	4/2128 (0.2%)
52	m6	0.83	1/1585 (0.1%)	0.84	2/2128 (0.1%)
53	M7	0.69	0/1443	0.82	2/1944 (0.1%)
53	m7	0.77	0/1250	0.84	0/1683
54	M8	0.66	1/1465 (0.1%)	0.84	2/1965 (0.1%)
54	m8	0.64	0/1465	0.84	2/1965 (0.1%)
55	M9	0.49	0/1538	0.66	0/2050
55	m9	0.58	0/1538	0.67	0/2050
56	N0	0.65	0/1481	0.78	1/1990 (0.1%)
56	n0	0.68	0/1481	0.78	0/1990
57	N1	0.66	0/1300	0.78	1/1743 (0.1%)
57	n1	0.69	1/1300 (0.1%)	0.74	0/1743
58	N2	0.44	0/812	0.62	0/1099
58	n2	0.54	0/794	0.67	0/1076
59	N3	0.66	0/1018	0.82	0/1369
59	n3	0.78	2/1018 (0.2%)	0.90	2/1369 (0.1%)
60	N4	0.54	0/712	0.68	0/958
60	n4	0.61	0/1052	0.71	0/1398
61	N5	0.57	0/979	0.75	3/1321 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	n5	0.56	0/974	0.74	0/1314
62	N6	0.62	0/1004	0.84	3/1341 (0.2%)
62	n6	0.62	0/1004	0.80	2/1341 (0.1%)
63	N7	0.48	0/1118	0.61	0/1497
63	n7	0.49	0/1118	0.61	0/1497
64	N8	0.68	1/1204 (0.1%)	0.84	2/1612 (0.1%)
64	n8	0.72	1/1204 (0.1%)	0.90	3/1612 (0.2%)
65	N9	0.64	0/473	0.78	0/629
65	n9	0.68	0/473	0.89	0/629
66	O0	0.42	0/751	0.59	0/1008
66	o0	0.50	0/775	0.72	0/1040
67	O1	0.60	0/890	0.74	0/1196
67	o1	0.74	0/897	0.76	0/1205
68	O2	0.68	0/1041	0.81	0/1394
68	o2	0.70	0/1041	0.82	1/1394 (0.1%)
69	O3	0.81	0/868	0.85	1/1168 (0.1%)
69	o3	0.77	0/868	0.82	0/1168
70	O4	0.54	0/890	0.70	2/1189 (0.2%)
70	o4	0.55	0/890	0.69	0/1189
71	O5	0.60	1/978 (0.1%)	0.70	0/1301
71	o5	0.58	0/974	0.69	1/1297 (0.1%)
72	O6	0.57	0/778	0.72	0/1034
72	o6	0.51	0/777	0.76	0/1033
73	O7	0.58	0/696	0.77	1/923 (0.1%)
73	o7	0.62	0/696	0.89	1/923 (0.1%)
74	O8	0.48	0/618	0.62	0/826
74	o8	0.47	0/614	0.63	0/822
75	O9	0.70	0/443	0.88	2/588 (0.3%)
75	o9	0.69	0/443	0.86	0/588
76	Q0	0.70	0/423	0.85	2/562 (0.4%)
76	q0	0.86	1/423 (0.2%)	1.00	3/562 (0.5%)
77	Q1	0.61	0/234	0.76	0/300
77	q1	0.68	0/234	0.84	0/300
78	Q2	0.91	1/860 (0.1%)	0.85	1/1136 (0.1%)
78	q2	0.81	1/860 (0.1%)	0.83	1/1136 (0.1%)
79	Q3	0.64	1/701 (0.1%)	0.77	0/934
79	q3	0.69	0/701	0.81	2/934 (0.2%)
80	6	0.97	84/42790 (0.2%)	1.64	980/66673 (1.5%)
81	c0	0.40	0/718	0.60	1/968 (0.1%)
82	sM	0.51	0/481	0.62	0/644
84	p0	0.42	0/1092	0.62	1/1474 (0.1%)
All	All	0.87	517/430468 (0.1%)	1.41	6951/632045 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	S1	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	1
17	c5	0	1
18	c6	0	2
19	C7	0	2
19	c7	0	1
22	d0	0	1
24	d2	0	1
25	D3	0	1
27	D5	0	2
27	d5	0	1
28	D6	0	3
33	E1	0	3
33	e1	0	1
39	L2	0	1
39	l2	0	3
40	L3	0	1
40	l3	0	1
41	l4	0	1
42	L5	0	2
42	l5	0	2
43	L6	0	1
44	l7	0	2
45	L8	0	1
47	M0	0	1
48	m1	0	1
49	m3	0	1
50	m4	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
53	m7	0	1
55	m9	0	1
56	N0	0	2
56	n0	0	2
59	n3	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
62	N6	0	1
64	N8	0	1
64	n8	0	1
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
68	o2	0	2
70	o4	0	1
78	Q2	0	1
78	q2	0	1
All	All	0	67

The worst 5 of 517 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2707	C	C4-N4	22.02	1.53	1.33
78	Q2	17	CYS	CB-SG	16.14	2.09	1.82
47	m0	92	HIS	C-N	-13.33	1.08	1.34
80	6	89	G	C6-O6	13.07	1.35	1.24
36	5	2606	G	N7-C5	12.96	1.47	1.39

The worst 5 of 6951 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3144	G	O5'-P-OP1	-41.01	61.49	110.70
36	5	2707	C	N3-C4-C5	-37.89	106.74	121.90
36	5	2707	C	C6-N1-C2	-27.23	109.41	120.30
36	5	1779	C	C2-N3-C4	-24.43	107.69	119.90
36	5	1134	G	C5-N7-C8	-21.53	93.53	104.30

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
19	C7	22	PRO	Peptide
3	S1	131	ASP	Peptide
9	S7	131	PHE	Peptide
10	S8	8	ARG	Peptide

## 5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37970	0	19103	1241	0
2	S0	1577	0	1567	205	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	213	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	181	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	161	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	232	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	154	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	158	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	155	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	133	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	180	0
11	s9	1494	0	1573	0	0
12	C0	772	0	727	69	0
13	C1	1213	0	1257	122	0
13	c1	1168	0	1233	0	0
14	C2	890	0	887	75	0
14	c2	890	0	887	0	0
15	C3	1192	0	1255	109	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	105	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	125	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	153	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	101	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	127	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	107	0
22	d0	882	0	939	0	0
23	D1	684	0	672	98	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	111	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	116	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	110	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	75	0
27	d5	558	0	598	0	0
28	D6	769	0	814	104	0
28	d6	769	0	814	0	0
29	D7	610	0	631	53	0
29	d7	610	0	632	0	0
30	D8	497	0	535	45	0
30	d8	497	0	535	0	0
31	D9	442	0	428	41	0
31	d9	442	0	427	0	0
32	E0	475	0	525	45	0
32	e0	491	0	542	0	0
33	E1	566	0	601	68	0
33	e1	608	0	657	0	0
34	SR	2437	0	2386	199	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	977	82	0
36	1	67355	0	33836	2006	0
36	5	67376	0	33839	1949	0
37	3	2579	0	1304	79	0
37	7	2579	0	1303	77	0
38	4	3353	0	1695	112	0
38	8	3353	0	1695	115	0
39	L2	1914	0	1981	224	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	322	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2858	309	0
41	l4	2748	0	2859	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	L5	2375	0	2325	244	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	118	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	174	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	167	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	169	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	202	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	133	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	174	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	102	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	189	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1658	130	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	143	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1542	154	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	136	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	144	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	129	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	65	0
58	n2	778	0	791	0	0
59	N3	1003	0	1047	96	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	38	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	89	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	101	0
62	n6	993	0	1081	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	N7	1092	0	1155	110	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	154	0
64	n8	1173	0	1214	0	0
65	N9	462	0	491	46	0
65	n9	462	0	491	0	0
66	O0	743	0	797	73	0
66	o0	767	0	816	0	0
67	O1	876	0	911	75	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	123	0
68	o2	1020	0	1089	0	0
69	O3	850	0	880	76	0
69	o3	850	0	880	0	0
70	O4	880	0	945	105	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	110	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	94	0
72	o6	770	0	846	0	0
73	O7	681	0	683	85	0
73	o7	681	0	682	0	0
74	O8	612	0	682	51	0
74	o8	608	0	671	0	0
75	O9	436	0	475	40	0
75	o9	436	0	475	0	0
76	Q0	417	0	456	45	0
76	q0	417	0	456	0	0
77	Q1	233	0	284	16	0
77	q1	233	0	284	0	0
78	Q2	847	0	915	86	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	76	0
79	q3	694	0	734	0	0
80	6	38260	0	19242	1254	0
81	c0	762	0	691	0	0
82	sM	681	0	544	0	0
83	m2	750	0	178	0	0
84	p0	1077	0	1041	0	0
85	p1	235	0	52	0	0
85	p2	230	0	49	0	0
86	1	2870	0	0	343	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	2	1323	0	0	134	0
86	3	84	0	0	5	0
86	4	126	0	0	10	0
86	5	2898	0	0	310	0
86	6	1386	0	0	142	0
86	7	91	0	0	2	0
86	8	147	0	0	22	0
86	C3	7	0	0	2	0
86	C5	7	0	0	5	0
86	C8	14	0	0	3	0
86	D9	7	0	0	1	0
86	L3	21	0	0	6	0
86	L4	7	0	0	5	0
86	L5	7	0	0	0	0
86	M0	28	0	0	14	0
86	M5	7	0	0	1	0
86	M7	7	0	0	0	0
86	M8	7	0	0	0	0
86	M9	21	0	0	2	0
86	N8	7	0	0	0	0
86	N9	7	0	0	2	0
86	O1	7	0	0	2	0
86	O3	7	0	0	0	0
86	O7	14	0	0	8	0
86	Q2	7	0	0	5	0
86	S2	7	0	0	2	0
86	S8	7	0	0	3	0
86	SR	7	0	0	0	0
86	c1	7	0	0	0	0
86	c3	7	0	0	0	0
86	c5	14	0	0	0	0
86	c8	7	0	0	0	0
86	d9	7	0	0	0	0
86	l2	7	0	0	0	0
86	l3	14	0	0	0	0
86	l4	14	0	0	0	0
86	l5	21	0	0	0	0
86	l9	7	0	0	0	0
86	m0	28	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	m7	7	0	0	0	0
86	m9	7	0	0	0	0
86	n1	7	0	0	0	0
86	n3	14	0	0	0	0
86	n9	7	0	0	0	0
86	o3	7	0	0	0	0
86	o7	14	0	0	0	0
86	o9	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	1	698	0	0	0	0
87	2	170	0	0	0	0
87	3	18	0	0	0	0
87	4	28	0	0	0	0
87	5	759	0	0	0	0
87	6	235	0	0	0	0
87	7	28	0	0	0	0
87	8	19	0	0	0	0
87	C1	2	0	0	0	0
87	C5	1	0	0	0	0
87	C8	1	0	0	0	0
87	D0	1	0	0	0	0
87	D4	1	0	0	0	0
87	D6	1	0	0	0	0
87	D9	3	0	0	0	0
87	E1	1	0	0	0	0
87	L2	3	0	0	0	0
87	L3	5	0	0	0	0
87	L4	7	0	0	0	0
87	L7	3	0	0	0	0
87	L8	1	0	0	0	0
87	M0	5	0	0	0	0
87	M1	2	0	0	0	0
87	M3	3	0	0	0	0
87	M4	1	0	0	0	0
87	M5	4	0	0	0	0
87	M6	4	0	0	0	0
87	M7	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	M8	3	0	0	0	0
87	M9	2	0	0	0	0
87	N0	2	0	0	0	0
87	N1	1	0	0	0	0
87	N3	3	0	0	0	0
87	N6	2	0	0	0	0
87	N8	7	0	0	0	0
87	N9	1	0	0	0	0
87	O1	5	0	0	0	0
87	O2	4	0	0	0	0
87	O3	2	0	0	0	0
87	O4	1	0	0	0	0
87	O5	2	0	0	0	0
87	O7	6	0	0	0	0
87	Q0	2	0	0	0	0
87	Q2	3	0	0	0	0
87	S1	1	0	0	0	0
87	S2	1	0	0	0	0
87	S4	2	0	0	0	0
87	S6	1	0	0	0	0
87	S8	1	0	0	0	0
87	SM	1	0	0	0	0
87	c6	2	0	0	0	0
87	c7	1	0	0	0	0
87	c8	4	0	0	0	0
87	c9	3	0	0	0	0
87	d2	1	0	0	0	0
87	d3	2	0	0	0	0
87	d4	2	0	0	0	0
87	d5	1	0	0	0	0
87	d9	2	0	0	0	0
87	l2	6	0	0	0	0
87	l3	13	0	0	0	0
87	l4	1	0	0	0	0
87	l5	6	0	0	0	0
87	l7	7	0	0	0	0
87	l8	1	0	0	0	0
87	l9	3	0	0	0	0
87	m0	1	0	0	0	0
87	m3	1	0	0	0	0
87	m4	1	0	0	0	0
87	m5	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	m6	4	0	0	0	0
87	m7	8	0	0	0	0
87	m8	4	0	0	0	0
87	m9	1	0	0	0	0
87	n0	5	0	0	0	0
87	n1	3	0	0	0	0
87	n3	3	0	0	0	0
87	n6	1	0	0	0	0
87	n8	7	0	0	0	0
87	n9	2	0	0	0	0
87	o2	3	0	0	0	0
87	o3	4	0	0	0	0
87	o4	1	0	0	0	0
87	o6	1	0	0	0	0
87	o7	1	0	0	0	0
87	p0	1	0	0	0	0
87	q0	1	0	0	0	0
87	q1	2	0	0	0	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
87	s1	1	0	0	0	0
87	s4	1	0	0	0	0
87	s6	2	0	0	0	0
87	s8	4	0	0	0	0
87	sM	2	0	0	0	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	1	0
88	Q2	1	0	0	2	0
88	Q3	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
89	1	40	0	22	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	5	40	0	22	6	0
90	1	22	0	11	14	0
90	5	22	0	10	9	0
91	1	7	0	7	0	0
91	5	7	0	7	2	0
All	All	414270	0	297568	14106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 14106 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	2.09	1.47
73:O7:87:SER:O	86:O7:102:OHX:N3	1.78	1.16
78:Q2:17:CYS:SG	88:Q2:501:ZN:ZN	1.39	1.11
78:Q2:17:CYS:CB	88:Q2:501:ZN:ZN	1.30	1.10
86:2:2062:OHX:N5	11:S9:8:TYR:O	1.87	1.08

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	204/206 (99%)	150 (74%)	34 (17%)	20 (10%)	1	4
2	s0	204/206 (99%)	151 (74%)	30 (15%)	23 (11%)	0	3
3	S1	212/216 (98%)	149 (70%)	42 (20%)	21 (10%)	1	4
3	s1	214/216 (99%)	174 (81%)	29 (14%)	11 (5%)	2	17
4	S2	215/217 (99%)	176 (82%)	22 (10%)	17 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	s2	215/217 (99%)	177 (82%)	23 (11%)	15 (7%)	1	10
5	S3	221/223 (99%)	177 (80%)	34 (15%)	10 (4%)	3	20
5	s3	221/223 (99%)	172 (78%)	31 (14%)	18 (8%)	1	7
6	S4	258/260 (99%)	204 (79%)	40 (16%)	14 (5%)	2	15
6	s4	258/260 (99%)	207 (80%)	30 (12%)	21 (8%)	1	7
7	S5	204/206 (99%)	168 (82%)	21 (10%)	15 (7%)	1	9
7	s5	204/206 (99%)	156 (76%)	30 (15%)	18 (9%)	1	6
8	S6	224/226 (99%)	194 (87%)	18 (8%)	12 (5%)	2	15
8	s6	216/226 (96%)	186 (86%)	18 (8%)	12 (6%)	2	14
9	S7	182/186 (98%)	133 (73%)	25 (14%)	24 (13%)	0	2
9	s7	184/186 (99%)	147 (80%)	23 (12%)	14 (8%)	1	9
10	S8	184/199 (92%)	146 (79%)	29 (16%)	9 (5%)	2	18
10	s8	184/199 (92%)	150 (82%)	27 (15%)	7 (4%)	4	24
11	S9	183/185 (99%)	143 (78%)	28 (15%)	12 (7%)	1	11
11	s9	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	4	28
12	C0	94/96 (98%)	67 (71%)	16 (17%)	11 (12%)	0	3
13	C1	153/155 (99%)	128 (84%)	18 (12%)	7 (5%)	3	19
13	c1	144/155 (93%)	114 (79%)	19 (13%)	11 (8%)	1	9
14	C2	122/124 (98%)	73 (60%)	27 (22%)	22 (18%)	0	1
14	c2	122/124 (98%)	70 (57%)	31 (25%)	21 (17%)	0	1
15	C3	148/150 (99%)	120 (81%)	23 (16%)	5 (3%)	4	27
15	c3	148/150 (99%)	115 (78%)	20 (14%)	13 (9%)	1	6
16	C4	125/128 (98%)	97 (78%)	16 (13%)	12 (10%)	1	5
16	c4	126/128 (98%)	98 (78%)	20 (16%)	8 (6%)	1	12
17	C5	122/135 (90%)	90 (74%)	18 (15%)	14 (12%)	0	3
17	c5	133/135 (98%)	100 (75%)	13 (10%)	20 (15%)	0	1
18	C6	139/142 (98%)	115 (83%)	18 (13%)	6 (4%)	3	21
18	c6	140/142 (99%)	120 (86%)	12 (9%)	8 (6%)	2	14
19	C7	116/125 (93%)	90 (78%)	18 (16%)	8 (7%)	1	10
19	c7	113/125 (90%)	92 (81%)	11 (10%)	10 (9%)	1	6
20	C8	143/145 (99%)	109 (76%)	25 (18%)	9 (6%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	c8	143/145 (99%)	120 (84%)	15 (10%)	8 (6%)	2	14
21	C9	141/143 (99%)	114 (81%)	19 (14%)	8 (6%)	2	14
21	c9	141/143 (99%)	120 (85%)	15 (11%)	6 (4%)	3	21
22	D0	105/110 (96%)	86 (82%)	14 (13%)	5 (5%)	2	18
22	d0	108/110 (98%)	82 (76%)	14 (13%)	12 (11%)	0	3
23	D1	85/87 (98%)	65 (76%)	11 (13%)	9 (11%)	0	4
23	d1	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	1	10
24	D2	127/129 (98%)	102 (80%)	21 (16%)	4 (3%)	5	30
24	d2	127/129 (98%)	100 (79%)	25 (20%)	2 (2%)	11	43
25	D3	142/144 (99%)	109 (77%)	22 (16%)	11 (8%)	1	8
25	d3	142/144 (99%)	119 (84%)	20 (14%)	3 (2%)	8	38
26	D4	132/134 (98%)	108 (82%)	16 (12%)	8 (6%)	2	13
26	d4	132/134 (98%)	100 (76%)	19 (14%)	13 (10%)	1	4
27	D5	68/70 (97%)	49 (72%)	11 (16%)	8 (12%)	0	2
27	d5	67/70 (96%)	51 (76%)	13 (19%)	3 (4%)	3	20
28	D6	95/97 (98%)	62 (65%)	18 (19%)	15 (16%)	0	1
28	d6	95/97 (98%)	71 (75%)	13 (14%)	11 (12%)	0	3
29	D7	79/81 (98%)	62 (78%)	13 (16%)	4 (5%)	2	17
29	d7	79/81 (98%)	58 (73%)	15 (19%)	6 (8%)	1	9
30	D8	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	4	28
30	d8	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	7
31	D9	51/53 (96%)	36 (71%)	8 (16%)	7 (14%)	0	2
31	d9	51/53 (96%)	42 (82%)	6 (12%)	3 (6%)	2	14
32	E0	58/62 (94%)	47 (81%)	7 (12%)	4 (7%)	1	10
32	e0	60/62 (97%)	43 (72%)	10 (17%)	7 (12%)	0	3
33	E1	69/76 (91%)	39 (56%)	15 (22%)	15 (22%)	0	0
33	e1	74/76 (97%)	38 (51%)	19 (26%)	17 (23%)	0	0
34	SR	316/318 (99%)	275 (87%)	31 (10%)	10 (3%)	5	29
34	sR	316/318 (99%)	259 (82%)	44 (14%)	13 (4%)	3	22
35	SM	131/159 (82%)	95 (72%)	18 (14%)	18 (14%)	0	2
39	L2	250/252 (99%)	222 (89%)	17 (7%)	11 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	l2	250/252 (99%)	201 (80%)	39 (16%)	10 (4%)	3	23
40	L3	384/386 (100%)	323 (84%)	44 (12%)	17 (4%)	3	20
40	l3	384/386 (100%)	331 (86%)	35 (9%)	18 (5%)	3	19
41	L4	359/361 (99%)	284 (79%)	50 (14%)	25 (7%)	1	10
41	l4	359/361 (99%)	275 (77%)	57 (16%)	27 (8%)	1	9
42	L5	294/296 (99%)	225 (76%)	43 (15%)	26 (9%)	1	6
42	l5	292/296 (99%)	243 (83%)	42 (14%)	7 (2%)	7	35
43	L6	152/175 (87%)	131 (86%)	18 (12%)	3 (2%)	9	39
43	l6	153/175 (87%)	123 (80%)	25 (16%)	5 (3%)	4	28
44	L7	220/223 (99%)	185 (84%)	26 (12%)	9 (4%)	3	22
44	l7	221/223 (99%)	195 (88%)	18 (8%)	8 (4%)	4	26
45	L8	231/233 (99%)	180 (78%)	35 (15%)	16 (7%)	1	10
45	l8	229/233 (98%)	179 (78%)	33 (14%)	17 (7%)	1	9
46	L9	189/191 (99%)	159 (84%)	22 (12%)	8 (4%)	3	22
46	l9	189/191 (99%)	156 (82%)	25 (13%)	8 (4%)	3	22
47	M0	207/220 (94%)	166 (80%)	30 (14%)	11 (5%)	2	16
47	m0	209/220 (95%)	164 (78%)	30 (14%)	15 (7%)	1	10
48	M1	167/169 (99%)	132 (79%)	16 (10%)	19 (11%)	0	3
48	m1	167/169 (99%)	137 (82%)	18 (11%)	12 (7%)	1	10
49	M3	191/194 (98%)	148 (78%)	28 (15%)	15 (8%)	1	8
49	m3	192/194 (99%)	153 (80%)	26 (14%)	13 (7%)	1	10
50	M4	134/137 (98%)	109 (81%)	14 (10%)	11 (8%)	1	7
50	m4	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	12	44
51	M5	201/203 (99%)	171 (85%)	21 (10%)	9 (4%)	3	20
51	m5	201/203 (99%)	169 (84%)	26 (13%)	6 (3%)	5	30
52	M6	195/197 (99%)	180 (92%)	13 (7%)	2 (1%)	18	53
52	m6	195/197 (99%)	179 (92%)	13 (7%)	3 (2%)	12	44
53	M7	181/183 (99%)	144 (80%)	26 (14%)	11 (6%)	2	13
53	m7	153/183 (84%)	127 (83%)	24 (16%)	2 (1%)	14	48
54	M8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	4	28
54	m8	183/185 (99%)	151 (82%)	18 (10%)	14 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	M9	186/188 (99%)	159 (86%)	23 (12%)	4 (2%)	8	37
55	m9	186/188 (99%)	165 (89%)	20 (11%)	1 (0%)	32	66
56	N0	170/172 (99%)	149 (88%)	16 (9%)	5 (3%)	5	31
56	n0	170/172 (99%)	150 (88%)	17 (10%)	3 (2%)	10	42
57	N1	157/159 (99%)	133 (85%)	16 (10%)	8 (5%)	2	17
57	n1	157/159 (99%)	132 (84%)	21 (13%)	4 (2%)	6	34
58	N2	98/100 (98%)	70 (71%)	23 (24%)	5 (5%)	2	17
58	n2	96/100 (96%)	82 (85%)	10 (10%)	4 (4%)	3	22
59	N3	134/136 (98%)	118 (88%)	14 (10%)	2 (2%)	12	44
59	n3	134/136 (98%)	120 (90%)	9 (7%)	5 (4%)	4	25
60	N4	96/135 (71%)	73 (76%)	17 (18%)	6 (6%)	1	12
60	n4	133/135 (98%)	103 (77%)	19 (14%)	11 (8%)	1	7
61	N5	119/121 (98%)	99 (83%)	14 (12%)	6 (5%)	2	17
61	n5	118/121 (98%)	103 (87%)	9 (8%)	6 (5%)	2	17
62	N6	124/126 (98%)	100 (81%)	19 (15%)	5 (4%)	3	23
62	n6	124/126 (98%)	108 (87%)	7 (6%)	9 (7%)	1	9
63	N7	133/135 (98%)	109 (82%)	16 (12%)	8 (6%)	2	13
63	n7	133/135 (98%)	105 (79%)	16 (12%)	12 (9%)	1	6
64	N8	146/148 (99%)	109 (75%)	28 (19%)	9 (6%)	2	13
64	n8	146/148 (99%)	114 (78%)	22 (15%)	10 (7%)	1	10
65	N9	56/58 (97%)	44 (79%)	10 (18%)	2 (4%)	4	26
65	n9	56/58 (97%)	37 (66%)	11 (20%)	8 (14%)	0	1
66	O0	95/100 (95%)	85 (90%)	8 (8%)	2 (2%)	8	38
66	o0	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	9	39
67	O1	107/109 (98%)	93 (87%)	9 (8%)	5 (5%)	3	19
67	o1	107/109 (98%)	91 (85%)	11 (10%)	5 (5%)	3	19
68	O2	125/127 (98%)	94 (75%)	22 (18%)	9 (7%)	1	10
68	o2	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	2	18
69	O3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	5	31
69	o3	104/106 (98%)	92 (88%)	6 (6%)	6 (6%)	2	14
70	O4	110/112 (98%)	94 (86%)	12 (11%)	4 (4%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	o4	110/112 (98%)	91 (83%)	16 (14%)	3 (3%)	6	32
71	O5	117/119 (98%)	98 (84%)	11 (9%)	8 (7%)	1	10
71	o5	117/119 (98%)	100 (86%)	13 (11%)	4 (3%)	4	27
72	O6	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	0	4
72	o6	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	7
73	O7	85/87 (98%)	67 (79%)	17 (20%)	1 (1%)	15	50
73	o7	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	4	26
74	O8	75/77 (97%)	61 (81%)	12 (16%)	2 (3%)	6	32
74	o8	75/77 (97%)	60 (80%)	9 (12%)	6 (8%)	1	8
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	8	38
75	o9	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
76	Q0	50/52 (96%)	40 (80%)	8 (16%)	2 (4%)	3	23
76	q0	50/52 (96%)	41 (82%)	8 (16%)	1 (2%)	9	39
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	3 (13%)	1 (4%)	3	21
78	Q2	103/105 (98%)	79 (77%)	19 (18%)	5 (5%)	2	18
78	q2	103/105 (98%)	90 (87%)	8 (8%)	5 (5%)	2	18
79	Q3	89/91 (98%)	76 (85%)	7 (8%)	6 (7%)	1	11
79	q3	89/91 (98%)	78 (88%)	8 (9%)	3 (3%)	4	27
81	c0	82/96 (85%)	63 (77%)	11 (13%)	8 (10%)	1	4
82	sM	61/104 (59%)	38 (62%)	15 (25%)	8 (13%)	0	2
84	p0	139/219 (64%)	115 (83%)	17 (12%)	7 (5%)	2	17
All	All	22262/22948 (97%)	17987 (81%)	2915 (13%)	1360 (6%)	2	13

5 of 1360 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	5	ALA
2	S0	30	GLN
2	S0	36	TYR
2	S0	95	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/173 (95%)	133 (81%)	31 (19%)	2	8
2	s0	165/173 (95%)	128 (78%)	37 (22%)	1	4
3	S1	191/192 (100%)	152 (80%)	39 (20%)	1	6
3	s1	192/192 (100%)	148 (77%)	44 (23%)	1	4
4	S2	176/176 (100%)	139 (79%)	37 (21%)	1	5
4	s2	176/176 (100%)	132 (75%)	44 (25%)	1	2
5	S3	182/182 (100%)	149 (82%)	33 (18%)	2	9
5	s3	182/182 (100%)	150 (82%)	32 (18%)	2	10
6	S4	221/221 (100%)	176 (80%)	45 (20%)	1	6
6	s4	221/221 (100%)	179 (81%)	42 (19%)	2	8
7	S5	173/173 (100%)	143 (83%)	30 (17%)	2	11
7	s5	173/173 (100%)	146 (84%)	27 (16%)	3	15
8	S6	188/193 (97%)	147 (78%)	41 (22%)	1	5
8	s6	187/193 (97%)	149 (80%)	38 (20%)	1	6
9	S7	165/166 (99%)	132 (80%)	33 (20%)	1	6
9	s7	165/166 (99%)	132 (80%)	33 (20%)	1	6
10	S8	150/160 (94%)	126 (84%)	24 (16%)	3	14
10	s8	150/160 (94%)	125 (83%)	25 (17%)	2	12
11	S9	158/158 (100%)	124 (78%)	34 (22%)	1	5
11	s9	158/158 (100%)	122 (77%)	36 (23%)	1	4
12	C0	77/89 (86%)	63 (82%)	14 (18%)	2	9
13	C1	129/136 (95%)	110 (85%)	19 (15%)	3	17
13	c1	129/136 (95%)	102 (79%)	27 (21%)	1	5
14	C2	88/100 (88%)	65 (74%)	23 (26%)	0	2
14	c2	88/100 (88%)	69 (78%)	19 (22%)	1	5
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	c3	127/127 (100%)	104 (82%)	23 (18%)	2	9
16	C4	81/97 (84%)	58 (72%)	23 (28%)	0	2
16	c4	97/97 (100%)	65 (67%)	32 (33%)	0	1
17	C5	101/111 (91%)	85 (84%)	16 (16%)	3	14
17	c5	103/111 (93%)	88 (85%)	15 (15%)	3	18
18	C6	117/118 (99%)	93 (80%)	24 (20%)	1	6
18	c6	118/118 (100%)	94 (80%)	24 (20%)	1	6
19	C7	94/113 (83%)	73 (78%)	21 (22%)	1	4
19	c7	92/113 (81%)	73 (79%)	19 (21%)	1	6
20	C8	128/128 (100%)	96 (75%)	32 (25%)	1	2
20	c8	128/128 (100%)	104 (81%)	24 (19%)	2	8
21	C9	115/115 (100%)	88 (76%)	27 (24%)	1	3
21	c9	115/115 (100%)	92 (80%)	23 (20%)	1	6
22	D0	100/103 (97%)	76 (76%)	24 (24%)	1	3
22	d0	103/103 (100%)	76 (74%)	27 (26%)	0	2
23	D1	74/74 (100%)	63 (85%)	11 (15%)	3	17
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	5
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	6
24	d2	110/110 (100%)	90 (82%)	20 (18%)	2	9
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	10
25	d3	119/119 (100%)	100 (84%)	19 (16%)	3	14
26	D4	112/112 (100%)	91 (81%)	21 (19%)	2	8
26	d4	112/112 (100%)	91 (81%)	21 (19%)	2	8
27	D5	61/61 (100%)	44 (72%)	17 (28%)	0	2
27	d5	61/61 (100%)	52 (85%)	9 (15%)	3	17
28	D6	83/83 (100%)	63 (76%)	20 (24%)	1	3
28	d6	83/83 (100%)	67 (81%)	16 (19%)	1	7
29	D7	70/70 (100%)	61 (87%)	9 (13%)	5	22
29	d7	70/70 (100%)	61 (87%)	9 (13%)	5	22
30	D8	56/56 (100%)	44 (79%)	12 (21%)	1	5
30	d8	56/56 (100%)	43 (77%)	13 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	D9	47/47 (100%)	35 (74%)	12 (26%)	0	2
31	d9	47/47 (100%)	40 (85%)	7 (15%)	3	17
32	E0	51/53 (96%)	45 (88%)	6 (12%)	6	26
32	e0	53/53 (100%)	37 (70%)	16 (30%)	0	1
33	E1	62/66 (94%)	50 (81%)	12 (19%)	1	7
33	e1	66/66 (100%)	50 (76%)	16 (24%)	1	3
34	SR	259/261 (99%)	226 (87%)	33 (13%)	5	23
34	sR	260/261 (100%)	231 (89%)	29 (11%)	7	29
35	SM	97/107 (91%)	76 (78%)	21 (22%)	1	5
39	L2	193/194 (100%)	155 (80%)	38 (20%)	1	7
39	l2	192/194 (99%)	153 (80%)	39 (20%)	1	6
40	L3	319/322 (99%)	249 (78%)	70 (22%)	1	5
40	l3	321/322 (100%)	252 (78%)	69 (22%)	1	5
41	L4	288/288 (100%)	232 (81%)	56 (19%)	1	7
41	l4	288/288 (100%)	234 (81%)	54 (19%)	2	8
42	L5	244/244 (100%)	198 (81%)	46 (19%)	2	8
42	l5	243/244 (100%)	189 (78%)	54 (22%)	1	4
43	L6	134/152 (88%)	114 (85%)	20 (15%)	3	17
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	10
44	L7	186/187 (100%)	160 (86%)	26 (14%)	4	19
44	l7	187/187 (100%)	155 (83%)	32 (17%)	2	11
45	L8	187/191 (98%)	157 (84%)	30 (16%)	3	14
45	l8	177/191 (93%)	142 (80%)	35 (20%)	1	6
46	L9	171/171 (100%)	130 (76%)	41 (24%)	1	3
46	l9	171/171 (100%)	132 (77%)	39 (23%)	1	4
47	M0	177/186 (95%)	151 (85%)	26 (15%)	3	17
47	m0	179/186 (96%)	138 (77%)	41 (23%)	1	4
48	M1	147/147 (100%)	119 (81%)	28 (19%)	2	8
48	m1	147/147 (100%)	120 (82%)	27 (18%)	2	9
49	M3	154/154 (100%)	124 (80%)	30 (20%)	1	7
49	m3	154/154 (100%)	123 (80%)	31 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	M4	107/108 (99%)	87 (81%)	20 (19%)	2	8
50	m4	108/108 (100%)	85 (79%)	23 (21%)	1	5
51	M5	175/175 (100%)	140 (80%)	35 (20%)	1	6
51	m5	175/175 (100%)	140 (80%)	35 (20%)	1	6
52	M6	160/160 (100%)	139 (87%)	21 (13%)	5	22
52	m6	160/160 (100%)	135 (84%)	25 (16%)	3	15
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	4
53	m7	125/145 (86%)	94 (75%)	31 (25%)	1	2
54	M8	150/150 (100%)	124 (83%)	26 (17%)	2	11
54	m8	150/150 (100%)	116 (77%)	34 (23%)	1	4
55	M9	153/153 (100%)	129 (84%)	24 (16%)	3	15
55	m9	153/153 (100%)	125 (82%)	28 (18%)	2	9
56	N0	156/156 (100%)	127 (81%)	29 (19%)	2	8
56	n0	156/156 (100%)	128 (82%)	28 (18%)	2	10
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	4
57	n1	136/136 (100%)	109 (80%)	27 (20%)	1	6
58	N2	87/87 (100%)	70 (80%)	17 (20%)	1	7
58	n2	85/87 (98%)	69 (81%)	16 (19%)	2	8
59	N3	104/104 (100%)	89 (86%)	15 (14%)	4	18
59	n3	104/104 (100%)	89 (86%)	15 (14%)	4	18
60	N4	57/114 (50%)	50 (88%)	7 (12%)	5	25
60	n4	100/114 (88%)	85 (85%)	15 (15%)	3	16
61	N5	104/105 (99%)	82 (79%)	22 (21%)	1	5
61	n5	104/105 (99%)	82 (79%)	22 (21%)	1	5
62	N6	109/109 (100%)	85 (78%)	24 (22%)	1	4
62	n6	109/109 (100%)	85 (78%)	24 (22%)	1	4
63	N7	115/115 (100%)	93 (81%)	22 (19%)	2	7
63	n7	115/115 (100%)	93 (81%)	22 (19%)	2	7
64	N8	118/118 (100%)	93 (79%)	25 (21%)	1	5
64	n8	118/118 (100%)	94 (80%)	24 (20%)	1	6
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0	1
66	O0	81/84 (96%)	68 (84%)	13 (16%)	3	14
66	o0	84/84 (100%)	70 (83%)	14 (17%)	2	12
67	O1	92/96 (96%)	68 (74%)	24 (26%)	0	2
67	o1	94/96 (98%)	72 (77%)	22 (23%)	1	3
68	O2	109/109 (100%)	89 (82%)	20 (18%)	2	9
68	o2	109/109 (100%)	90 (83%)	19 (17%)	2	10
69	O3	90/90 (100%)	75 (83%)	15 (17%)	2	12
69	o3	90/90 (100%)	78 (87%)	12 (13%)	4	21
70	O4	95/95 (100%)	80 (84%)	15 (16%)	3	14
70	o4	95/95 (100%)	82 (86%)	13 (14%)	4	20
71	O5	104/104 (100%)	79 (76%)	25 (24%)	1	3
71	o5	103/104 (99%)	83 (81%)	20 (19%)	1	7
72	O6	81/81 (100%)	59 (73%)	22 (27%)	0	2
72	o6	80/81 (99%)	58 (72%)	22 (28%)	0	2
73	O7	70/70 (100%)	54 (77%)	16 (23%)	1	4
73	o7	70/70 (100%)	54 (77%)	16 (23%)	1	4
74	O8	68/68 (100%)	51 (75%)	17 (25%)	1	2
74	o8	67/68 (98%)	50 (75%)	17 (25%)	0	2
75	O9	45/45 (100%)	37 (82%)	8 (18%)	2	10
75	o9	45/45 (100%)	39 (87%)	6 (13%)	4	21
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1	5
76	q0	47/47 (100%)	34 (72%)	13 (28%)	0	2
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
78	Q2	90/90 (100%)	65 (72%)	25 (28%)	0	2
78	q2	90/90 (100%)	66 (73%)	24 (27%)	0	2
79	Q3	71/71 (100%)	63 (89%)	8 (11%)	7	28
79	q3	71/71 (100%)	54 (76%)	17 (24%)	1	3
81	c0	73/78 (94%)	60 (82%)	13 (18%)	2	10
82	sM	54/54 (100%)	40 (74%)	14 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
84	p0	105/186 (56%)	82 (78%)	23 (22%)	<b>1</b> <b>5</b>
All	All	18727/19202 (98%)	15037 (80%)	3690 (20%)	<b>1</b> <b>7</b>

5 of 3690 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
71	O5	4	VAL
8	s6	169	TYR
64	n8	14	HIS
73	O7	16	HIS
3	s1	177	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
47	M0	59	GLN
64	N8	67	HIS
62	n6	120	GLN
47	M0	144	ASN
54	M8	145	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1829 (97%)	519 (29%)	0
36	1	3145/3394 (92%)	765 (24%)	0
36	5	3145/3394 (92%)	772 (24%)	0
37	3	120/121 (99%)	22 (18%)	0
37	7	120/121 (99%)	23 (19%)	0
38	4	157/158 (99%)	42 (26%)	0
38	8	157/158 (99%)	40 (25%)	0
80	6	1791/1800 (99%)	489 (27%)	0
All	All	10411/10975 (94%)	2672 (25%)	0

5 of 2672 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C

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Mol	Chain	Res	Type
1	2	17	C
1	2	25	C
1	2	26	A

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3561 ligands modelled in this entry, 2208 are monoatomic - leaving 1353 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	$\# Z  > 2$
89	C	1	3401	-	15,21,22	1.02	0	16,30,33	1.24	2 (12%)
89	C	1	3402	90	15,21,22	0.83	0	16,30,33	1.03	1 (6%)
90	8AN	1	3403	89	17,24,25	1.14	1 (5%)	14,35,38	2.25	5 (35%)
91	PRO	1	3404	-	6,7,8	0.95	1 (16%)	7,8,10	1.49	1 (14%)
86	OHX	1	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3409	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3410	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3411	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3412	-	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	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3422	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3431	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3437	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3438	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3441	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3450	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3455	86	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3456	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3461	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3464	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3465	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3469	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3472	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3476	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3477	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3478	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3479	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3480	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3488	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3489	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3493	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3494	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3495	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3498	-	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	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3502	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3504	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3505	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3506	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3508	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3510	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3511	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3513	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3517	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3518	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3519	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3530	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3535	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3536	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3538	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3539	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3540	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3541	-	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	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3546	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3547	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3553	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3559	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3560	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3562	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3571	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3575	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3579	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3581	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3582	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3584	36	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	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3587	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3588	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3590	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3595	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3596	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3598	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3599	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3600	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3601	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3602	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3605	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3606	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3612	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3615	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3616	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3617	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3619	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3624	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3625	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3627	-	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	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3629	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3639	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3647	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3651	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3656	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3661	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3663	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3667	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3669	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3670	-	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	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3675	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3678	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3681	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3685	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3687	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3688	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3689	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3691	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3695	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3696	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3697	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3699	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3700	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3703	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3705	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3709	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3711	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3713	-	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	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3715	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3716	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3717	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3718	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3719	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3721	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3722	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3723	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3724	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3725	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3726	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3727	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3728	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3729	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3730	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3731	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3732	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3733	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3734	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3735	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3736	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3737	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3738	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3739	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3740	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3741	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3742	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3743	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3744	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3745	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3746	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3747	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3748	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3749	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3750	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3751	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3752	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3753	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3754	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3755	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3756	86,36	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	3757	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3758	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3759	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3760	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3761	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3762	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3763	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3764	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3765	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3766	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3767	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3768	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3769	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3770	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3771	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3772	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3773	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3774	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3775	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3776	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3777	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3778	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3779	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3780	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3781	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3782	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3783	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3784	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3785	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3786	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3787	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3788	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3789	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3790	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3791	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3792	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3793	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3794	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3795	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3796	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3797	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3798	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3799	86	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3800	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3801	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3802	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3803	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3804	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3805	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3806	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3807	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3808	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3809	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3810	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3811	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3812	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3813	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3814	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1906	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1907	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1909	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1910	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1914	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1915	1,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1916	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1918	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1919	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1921	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1922	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1928	-	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	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1933	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1940	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1942	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1943	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1945	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1948	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1952	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1954	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1961	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1965	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1969	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1970	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1971	-	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	1972	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1973	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1975	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1976	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1977	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1979	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1980	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1984	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1988	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1989	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1990	1,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1991	1,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1993	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1998	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2003	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2008	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2013	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2014	-	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	2015	1,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2018	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2022	86	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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2027	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2028	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2029	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2030	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2031	86	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	86	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	86	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	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	86	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	1	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	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2053	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2054	86	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	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2059	86	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	1	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	86	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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2069	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2070	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2071	86	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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2074	86	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	1,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2077	1,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2078	86	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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2081	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2082	1,86	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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2085	86	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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2088	1,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2089	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	205	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	207	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	209	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	211	86	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	3	212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	208	38	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	212	38	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	214	38	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	215	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	216	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	218	86	0,6,6	0.00	-	0,15,15	0.00	-
89	C	5	3401	86	15,21,22	1.02	1 (6%)	16,30,33	1.24	2 (12%)
89	C	5	3402	90	15,21,22	0.83	0	16,30,33	1.04	1 (6%)
90	8AN	5	3403	89	17,24,25	8.70	3 (17%)	14,35,38	2.21	4 (28%)
91	PRO	5	3404	-	6,7,8	0.96	1 (16%)	7,8,10	1.49	1 (14%)
86	OHX	5	3405	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3406	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3407	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3409	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3410	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3411	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3413	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3420	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3421	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3423	36	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	3424	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3429	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3430	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3433	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3434	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3437	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3438	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3444	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3447	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3448	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3449	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3451	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3454	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3455	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3457	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3459	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3460	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3462	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3464	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3465	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3466	36	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	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3468	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3471	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3474	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3475	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3477	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3478	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3480	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3482	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3483	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3486	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3488	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3489	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3492	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3493	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3501	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3502	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3503	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3505	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3506	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3507	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3508	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3509	86	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3511	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3512	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3513	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3514	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3517	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3518	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3519	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3522	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3523	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3524	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3527	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3531	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3533	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3534	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3536	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3537	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3539	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3540	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3541	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3542	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3543	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3547	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3551	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3552	-	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	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3557	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3558	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3560	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3561	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3564	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3569	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3570	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3571	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3572	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3573	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3577	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3579	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3581	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3582	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3583	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3586	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3587	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3590	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3593	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3594	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3595	-	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	3596	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3598	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3599	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3602	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3603	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3605	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3606	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3607	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3608	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3609	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3612	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3615	89,86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3620	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3624	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3625	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3629	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3632	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3633	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3634	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3635	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3636	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3637	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3638	-	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	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3642	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3644	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3645	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3647	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3649	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3650	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3651	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3652	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3654	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3655	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3657	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3658	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3659	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3660	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3661	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3664	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3670	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3673	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3674	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3675	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3676	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3681	-	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	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3683	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3688	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3689	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3691	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3693	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3696	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3697	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3699	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3700	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3701	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3702	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3703	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3704	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3708	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3709	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3710	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3713	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3715	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3716	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3719	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3720	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3721	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3722	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3723	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3724	-	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	3725	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3726	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3727	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3728	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3729	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3730	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3731	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3732	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3733	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3734	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3735	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3736	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3737	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3738	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3739	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3740	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3741	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3742	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3743	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3744	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3745	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3746	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3747	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3748	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3749	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3750	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3751	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3752	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3753	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3754	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3755	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3756	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3757	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3758	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3759	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3760	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3761	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3762	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3763	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3764	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3765	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3766	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3767	86,36	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	3768	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3769	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3770	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3771	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3772	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3773	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3774	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3775	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3776	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3777	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3778	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3779	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3780	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3781	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3782	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3783	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3784	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3785	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3786	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3787	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3788	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3789	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3790	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3791	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3792	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3793	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3794	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3795	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3796	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3797	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3798	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3799	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3800	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3801	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3802	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3803	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3804	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3805	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3806	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3807	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3808	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3809	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3810	86	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3811	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3812	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3813	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3814	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3815	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3816	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3817	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3818	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1901	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1904	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1907	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1909	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1911	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1913	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1914	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1917	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1918	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1919	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1920	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1923	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1925	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1927	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1928	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1930	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1931	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1935	80	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	1936	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1938	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1939	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1941	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1942	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1944	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1945	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1948	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1949	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1950	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1952	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1954	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1955	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1957	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1958	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1959	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1962	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1963	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1964	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1965	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1971	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1973	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1974	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1975	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1976	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1978	80	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	1979	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1980	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1982	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1983	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1984	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1989	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1990	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1991	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1993	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1998	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2002	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2003	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2005	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2007	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2009	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2010	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2012	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2015	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2016	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2017	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2018	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2020	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2021	-	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	2022	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2024	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2026	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2028	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2032	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2034	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2036	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2037	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2041	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2042	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2043	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2045	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2046	86	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	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2050	80	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	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2053	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2054	80,86	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	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2057	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2058	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2059	86	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	86	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	80	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	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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2068	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2069	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2070	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2071	86	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	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2075	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2076	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2077	86	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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2083	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2084	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2085	80	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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2089	80	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2090	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2091	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2092	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2093	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2094	80,86	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	80,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2097	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2098	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	201	37	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	203	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	209	86,37	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	7	210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	211	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	202	38	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	203	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	207	38,86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	211	38	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	212	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	216	38	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	38	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	219	38	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	221	86	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	17	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	201	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	202	86,36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	D9	102	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	301	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	302	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	303	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	304	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	201	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	M9	202	86	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	N8	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	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	102	73	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	Q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S2	301	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	301	-	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	c1	201	86	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	c5	202	17	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d9	102	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l2	301	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	401	-	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	l5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	301	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	303	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	304	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	501	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m7	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	502	-	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	o7	503	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q1	101	86	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	301	-	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	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	301	-	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
89	C	1	3401	-	-	0/3/25/26	0/2/2/2
89	C	1	3402	90	-	0/3/25/26	0/2/2/2
90	8AN	1	3403	89	-	0/3/25/26	0/3/3/3
91	PRO	1	3404	-	-	0/0/9/11	0/1/1/1
86	OHX	1	3405	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3406	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3407	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3408	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3409	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3410	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3411	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3412	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3413	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3414	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3415	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3416	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3417	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3418	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3419	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3420	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3421	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3422	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3423	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3424	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3425	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3426	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3427	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3428	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3429	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3430	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3431	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3432	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3433	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3434	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3435	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3436	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3437	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3438	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3439	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3440	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3441	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3442	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3443	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3444	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3445	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3446	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3447	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3448	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3449	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3450	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3451	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3452	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3453	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3454	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3455	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3456	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3457	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3458	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3459	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3460	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3461	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3462	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3463	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3464	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3465	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3466	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3467	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3468	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3469	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3470	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3471	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3472	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3473	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3474	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3475	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3476	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3477	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3478	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3479	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3480	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3481	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3482	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3483	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3484	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3485	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3486	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3487	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3488	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3489	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3490	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3491	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3492	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3493	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3494	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3495	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3496	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3497	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3498	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3499	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3500	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3501	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3502	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3503	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3504	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3505	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3506	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3507	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3508	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3509	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3510	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3511	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3512	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3513	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3514	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3515	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3516	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3517	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3518	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3519	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3520	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3521	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3522	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3523	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3524	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3525	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3526	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3527	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3528	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3529	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3530	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3531	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3532	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3533	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3534	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3535	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3536	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3537	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3538	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3539	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3540	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3541	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3542	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3543	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3544	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3545	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3546	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3547	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3548	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3549	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3550	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3551	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3552	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3553	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3554	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3555	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3556	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3557	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3558	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3559	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3560	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3561	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3562	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3563	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3564	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3565	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3566	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3567	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3568	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3569	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3570	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3571	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3572	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3573	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3574	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3575	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3576	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3577	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3578	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3579	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3580	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3581	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3582	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3583	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3584	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3585	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3586	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3587	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3588	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3589	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3590	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3591	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3592	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3593	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3594	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3595	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3596	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3597	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3598	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3599	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3600	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3601	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3602	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3603	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3604	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3605	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3606	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3607	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3608	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3609	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3610	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3611	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3612	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3613	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3614	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3615	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3616	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3617	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3618	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3619	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3620	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3621	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3622	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3623	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3624	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3625	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3626	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3627	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3628	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3629	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3630	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3631	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3632	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3633	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3634	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3635	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3636	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3637	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3638	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3639	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3640	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3641	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3642	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3643	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3644	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3645	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3646	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3647	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3648	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3649	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3650	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3651	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3652	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3653	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3654	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3655	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3656	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3657	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3658	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3659	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3660	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3661	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3662	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3663	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3664	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3665	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3666	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3667	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3668	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3669	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3670	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3671	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3672	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3673	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3674	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3675	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3676	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3677	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3678	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3679	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3680	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3681	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3682	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3683	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3684	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3685	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3686	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3687	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3688	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3689	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3690	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3691	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3692	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3693	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3694	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3695	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3696	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3697	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3698	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3699	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3700	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3701	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3702	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3703	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3704	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3705	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3706	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3707	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3708	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3709	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3710	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3711	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3712	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3713	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3714	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3715	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3716	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3717	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3718	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3719	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3720	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3721	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3722	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3723	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3724	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3725	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3726	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3727	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3728	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3729	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3730	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3731	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3732	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3733	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3734	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3735	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3736	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3737	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3738	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3739	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3740	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3741	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3742	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3743	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3744	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3745	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3746	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3747	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3748	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3749	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3750	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3751	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3752	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3753	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3754	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3755	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3756	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3757	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3758	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3759	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3760	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3761	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3762	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3763	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3764	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3765	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3766	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3767	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3768	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3769	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3770	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3771	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3772	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3773	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3774	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3775	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3776	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3777	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3778	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3779	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3780	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3781	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3782	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3783	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3784	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3785	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3786	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3787	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3788	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3789	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3790	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3791	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3792	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3793	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3794	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3795	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3796	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3797	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3798	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3799	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3800	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3801	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3802	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3803	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3804	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3805	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3806	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3807	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3808	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3809	86,36	-	0/0/0/0	0/0/0/0
86	OHX	1	3810	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3811	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3812	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3813	86	-	0/0/0/0	0/0/0/0
86	OHX	1	3814	86,36	-	0/0/0/0	0/0/0/0
86	OHX	2	1901	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1902	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1903	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1904	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1905	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1906	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1907	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1908	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1909	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1910	1	-	0/0/0/0	0/0/0/0
86	OHX	2	1911	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1912	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1913	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1914	1	-	0/0/0/0	0/0/0/0
86	OHX	2	1915	1,86	-	0/0/0/0	0/0/0/0
86	OHX	2	1916	1	-	0/0/0/0	0/0/0/0
86	OHX	2	1917	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1918	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1919	1	-	0/0/0/0	0/0/0/0
86	OHX	2	1920	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1921	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1922	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1923	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1924	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1925	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1926	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1927	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1928	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1929	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1930	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1931	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1932	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1933	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	1934	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1935	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1936	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1937	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1938	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1939	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1940	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1941	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1942	1	-	0/0/0/0	0/0/0/0
86	OHX	2	1943	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1944	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1945	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1946	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1947	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1948	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1949	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1950	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1951	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1952	1	-	0/0/0/0	0/0/0/0
86	OHX	2	1953	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1954	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1955	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1956	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1957	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1958	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1959	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1960	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1961	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1962	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1963	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1964	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1965	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1966	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1967	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1968	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1969	1	-	0/0/0/0	0/0/0/0
86	OHX	2	1970	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1971	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1972	1	-	0/0/0/0	0/0/0/0
86	OHX	2	1973	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1974	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1975	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	1976	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1977	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1978	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1979	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1980	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1981	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1982	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1983	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1984	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1985	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1986	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1987	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1988	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1989	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1990	1,86	-	0/0/0/0	0/0/0/0
86	OHX	2	1991	1,86	-	0/0/0/0	0/0/0/0
86	OHX	2	1992	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1993	1	-	0/0/0/0	0/0/0/0
86	OHX	2	1994	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1995	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1996	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1997	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1998	86	-	0/0/0/0	0/0/0/0
86	OHX	2	1999	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2000	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2001	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2002	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2003	1	-	0/0/0/0	0/0/0/0
86	OHX	2	2004	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2005	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2006	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2007	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2008	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2009	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2010	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2011	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2012	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2013	1	-	0/0/0/0	0/0/0/0
86	OHX	2	2014	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2015	1,86	-	0/0/0/0	0/0/0/0
86	OHX	2	2016	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2017	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2018	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2019	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2020	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2021	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2022	86	-	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	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2027	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2028	1	-	0/0/0/0	0/0/0/0
86	OHX	2	2029	1	-	0/0/0/0	0/0/0/0
86	OHX	2	2030	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2031	86	-	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	86	-	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	86	-	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	1	-	0/0/0/0	0/0/0/0
86	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2048	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2050	1	-	0/0/0/0	0/0/0/0
86	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2052	1	-	0/0/0/0	0/0/0/0
86	OHX	2	2053	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2054	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2059	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1	-	0/0/0/0	0/0/0/0
86	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2064	86	-	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	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2069	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2070	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2071	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2073	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2074	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2076	1,86	-	0/0/0/0	0/0/0/0
86	OHX	2	2077	1,86	-	0/0/0/0	0/0/0/0
86	OHX	2	2078	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2080	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2081	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2082	1,86	-	0/0/0/0	0/0/0/0
86	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2084	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2085	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2087	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2088	1,86	-	0/0/0/0	0/0/0/0
86	OHX	2	2089	86	-	0/0/0/0	0/0/0/0
86	OHX	3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	3	204	-	-	0/0/0/0	0/0/0/0
86	OHX	3	205	86	-	0/0/0/0	0/0/0/0
86	OHX	3	206	-	-	0/0/0/0	0/0/0/0
86	OHX	3	207	86	-	0/0/0/0	0/0/0/0
86	OHX	3	208	-	-	0/0/0/0	0/0/0/0
86	OHX	3	209	86	-	0/0/0/0	0/0/0/0
86	OHX	3	210	-	-	0/0/0/0	0/0/0/0
86	OHX	3	211	86	-	0/0/0/0	0/0/0/0
86	OHX	3	212	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	4	202	-	-	0/0/0/0	0/0/0/0
86	OHX	4	203	-	-	0/0/0/0	0/0/0/0
86	OHX	4	204	-	-	0/0/0/0	0/0/0/0
86	OHX	4	205	-	-	0/0/0/0	0/0/0/0
86	OHX	4	206	-	-	0/0/0/0	0/0/0/0
86	OHX	4	207	-	-	0/0/0/0	0/0/0/0
86	OHX	4	208	38	-	0/0/0/0	0/0/0/0
86	OHX	4	209	-	-	0/0/0/0	0/0/0/0
86	OHX	4	210	-	-	0/0/0/0	0/0/0/0
86	OHX	4	211	-	-	0/0/0/0	0/0/0/0
86	OHX	4	212	38	-	0/0/0/0	0/0/0/0
86	OHX	4	213	-	-	0/0/0/0	0/0/0/0
86	OHX	4	214	38	-	0/0/0/0	0/0/0/0
86	OHX	4	215	86	-	0/0/0/0	0/0/0/0
86	OHX	4	216	86	-	0/0/0/0	0/0/0/0
86	OHX	4	217	-	-	0/0/0/0	0/0/0/0
86	OHX	4	218	86	-	0/0/0/0	0/0/0/0
89	C	5	3401	86	-	0/3/25/26	0/2/2/2
89	C	5	3402	90	-	0/3/25/26	0/2/2/2
90	8AN	5	3403	89	-	0/3/25/26	0/3/3/3
91	PRO	5	3404	-	-	0/0/9/11	0/1/1/1
86	OHX	5	3405	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3406	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3407	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3408	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3409	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3410	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3411	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3412	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3413	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3414	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3415	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3416	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3417	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3418	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3419	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3420	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3421	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3422	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3423	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3424	36	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3425	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3426	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3427	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3428	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3429	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3430	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3431	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3432	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3433	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3434	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3435	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3436	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3437	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3438	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3439	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3440	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3441	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3442	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3443	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3444	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3445	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3446	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3447	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3448	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3449	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3450	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3451	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3452	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3453	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3454	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3455	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3456	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3457	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3458	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3459	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3460	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3461	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3462	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3463	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3464	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3465	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3466	36	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3467	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3468	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3469	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3470	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3471	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3472	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3473	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3474	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3475	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3476	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3477	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3478	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3479	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3480	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3481	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3482	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3483	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3484	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3485	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3486	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3487	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3488	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3489	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3490	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3491	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3492	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3493	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3494	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3495	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3496	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3497	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3498	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3499	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3500	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3501	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3502	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3503	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3504	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3505	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3506	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3507	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3508	36	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3509	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3510	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3511	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3512	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3513	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3514	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3515	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3516	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3517	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3518	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3519	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3520	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3521	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3522	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3523	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3524	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3525	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3526	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3527	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3528	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3529	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3530	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3531	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3532	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3533	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3534	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3535	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3536	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3537	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3538	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3539	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3540	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3541	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3542	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3543	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3544	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3545	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3546	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3547	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3548	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3549	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3550	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3551	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3552	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3553	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3554	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3555	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3556	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3557	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3558	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3559	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3560	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3561	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3562	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3563	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3564	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3565	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3566	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3567	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3568	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3569	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3570	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3571	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3572	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3573	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3574	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3575	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3576	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3577	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3578	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3579	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3580	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3581	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3582	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3583	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3584	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3585	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3586	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3587	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3588	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3589	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3590	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3591	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3592	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3593	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3594	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3595	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3596	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3597	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3598	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3599	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3600	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3601	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3602	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3603	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3604	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3605	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3606	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3607	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3608	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3609	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3610	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3611	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3612	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3613	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3614	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3615	89,86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3616	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3617	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3618	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3619	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3620	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3621	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3622	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3623	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3624	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3625	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3626	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3627	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3628	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3629	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3630	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3631	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3632	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3633	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3634	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3635	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3636	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3637	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3638	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3639	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3640	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3641	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3642	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3643	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3644	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3645	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3646	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3647	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3648	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3649	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3650	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3651	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3652	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3653	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3654	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3655	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3656	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3657	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3658	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3659	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3660	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3661	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3662	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3663	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3664	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3665	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3666	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3667	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3668	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3669	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3670	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3671	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3672	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3673	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3674	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3675	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3676	36	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3677	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3678	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3679	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3680	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3681	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3682	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3683	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3684	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3685	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3686	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3687	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3688	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3689	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3690	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3691	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3692	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3693	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3694	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3695	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3696	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3697	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3698	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3699	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3700	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3701	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3702	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3703	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3704	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3705	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3706	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3707	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3708	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3709	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3710	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3711	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3712	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3713	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3714	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3715	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3716	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3717	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3718	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3719	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3720	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3721	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3722	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3723	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3724	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3725	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3726	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3727	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3728	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3729	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3730	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3731	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3732	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3733	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3734	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3735	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3736	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3737	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3738	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3739	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3740	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3741	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3742	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3743	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3744	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3745	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3746	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3747	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3748	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3749	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3750	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3751	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3752	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3753	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3754	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3755	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3756	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3757	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3758	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3759	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3760	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3761	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3762	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3763	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3764	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3765	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3766	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3767	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3768	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3769	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3770	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3771	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3772	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3773	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3774	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3775	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3776	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3777	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3778	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3779	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3780	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3781	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3782	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3783	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3784	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3785	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3786	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3787	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3788	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3789	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3790	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3791	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3792	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3793	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3794	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3795	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3796	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3797	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3798	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3799	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3800	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3801	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3802	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3803	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3804	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3805	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3806	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3807	86,36	-	0/0/0/0	0/0/0/0
86	OHX	5	3808	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3809	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3810	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3811	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3812	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3813	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3814	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3815	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3816	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3817	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3818	86,36	-	0/0/0/0	0/0/0/0
86	OHX	6	1901	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1902	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1903	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1904	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1905	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1906	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1907	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1908	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1909	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	1910	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1911	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1912	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1913	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1914	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	1915	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1916	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1917	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1918	86	-	0/0/0/0	0/0/0/0
86	OHX	6	1919	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	1920	86	-	0/0/0/0	0/0/0/0
86	OHX	6	1921	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1922	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1923	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1924	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1925	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1926	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	1927	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1928	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1929	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1930	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1931	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	1932	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1933	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1934	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1935	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1936	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1937	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1938	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	1939	86	-	0/0/0/0	0/0/0/0
86	OHX	6	1940	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1941	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1942	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1943	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1944	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1945	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1946	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1947	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1948	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	1949	86	-	0/0/0/0	0/0/0/0
86	OHX	6	1950	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1951	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1952	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	1953	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1954	86	-	0/0/0/0	0/0/0/0
86	OHX	6	1955	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1956	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1957	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1958	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1959	86	-	0/0/0/0	0/0/0/0
86	OHX	6	1960	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1961	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1962	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1963	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1964	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1965	86	-	0/0/0/0	0/0/0/0
86	OHX	6	1966	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1967	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1968	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	1969	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1970	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1971	86	-	0/0/0/0	0/0/0/0
86	OHX	6	1972	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1973	86	-	0/0/0/0	0/0/0/0
86	OHX	6	1974	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1975	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	1976	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1977	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1978	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1979	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1980	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1981	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1982	86	-	0/0/0/0	0/0/0/0
86	OHX	6	1983	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1984	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1985	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1986	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1987	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1988	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1989	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1990	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1991	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1992	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1993	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1994	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1995	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1996	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1997	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1998	80	-	0/0/0/0	0/0/0/0
86	OHX	6	1999	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2000	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2001	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2002	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2003	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2004	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2005	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2006	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2007	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2008	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2009	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2010	80,86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2011	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2012	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2013	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2014	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2015	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2016	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2017	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2018	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2019	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2020	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2021	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2022	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2023	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2024	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2025	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2026	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2027	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2028	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2029	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2030	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2031	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2032	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2033	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2034	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2035	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2036	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2037	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2038	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2039	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2040	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2041	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2042	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2043	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2045	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2046	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2050	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2052	80	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2053	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2054	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2056	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2057	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2058	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2059	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2061	86	-	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	80	-	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	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2068	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2069	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2070	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2071	86	-	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	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	86	-	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	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2083	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2085	80	-	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	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2089	80	-	0/0/0/0	0/0/0/0
86	OHX	6	2090	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2091	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2092	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2093	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2094	80,86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2096	80,86	-	0/0/0/0	0/0/0/0
86	OHX	6	2097	86	-	0/0/0/0	0/0/0/0
86	OHX	6	2098	86	-	0/0/0/0	0/0/0/0
86	OHX	7	201	37	-	0/0/0/0	0/0/0/0
86	OHX	7	202	-	-	0/0/0/0	0/0/0/0
86	OHX	7	203	86	-	0/0/0/0	0/0/0/0
86	OHX	7	204	-	-	0/0/0/0	0/0/0/0
86	OHX	7	205	-	-	0/0/0/0	0/0/0/0
86	OHX	7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	7	208	-	-	0/0/0/0	0/0/0/0
86	OHX	7	209	86,37	-	0/0/0/0	0/0/0/0
86	OHX	7	210	-	-	0/0/0/0	0/0/0/0
86	OHX	7	211	86	-	0/0/0/0	0/0/0/0
86	OHX	7	212	-	-	0/0/0/0	0/0/0/0
86	OHX	7	213	-	-	0/0/0/0	0/0/0/0
86	OHX	8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	8	202	38	-	0/0/0/0	0/0/0/0
86	OHX	8	203	86	-	0/0/0/0	0/0/0/0
86	OHX	8	204	-	-	0/0/0/0	0/0/0/0
86	OHX	8	205	-	-	0/0/0/0	0/0/0/0
86	OHX	8	206	-	-	0/0/0/0	0/0/0/0
86	OHX	8	207	38,86	-	0/0/0/0	0/0/0/0
86	OHX	8	208	-	-	0/0/0/0	0/0/0/0
86	OHX	8	209	-	-	0/0/0/0	0/0/0/0
86	OHX	8	210	-	-	0/0/0/0	0/0/0/0
86	OHX	8	211	38	-	0/0/0/0	0/0/0/0
86	OHX	8	212	86	-	0/0/0/0	0/0/0/0
86	OHX	8	213	-	-	0/0/0/0	0/0/0/0
86	OHX	8	214	-	-	0/0/0/0	0/0/0/0
86	OHX	8	215	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	38	-	0/0/0/0	0/0/0/0
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	38	-	0/0/0/0	0/0/0/0
86	OHX	8	219	38	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	86	-	0/0/0/0	0/0/0/0
86	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	17	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	86	-	0/0/0/0	0/0/0/0
86	OHX	C8	202	86,36	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	D9	102	86	-	0/0/0/0	0/0/0/0
86	OHX	L3	401	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	402	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	401	-	-	0/0/0/0	0/0/0/0
86	OHX	L5	301	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	301	86	-	0/0/0/0	0/0/0/0
86	OHX	M0	302	86	-	0/0/0/0	0/0/0/0
86	OHX	M0	303	86	-	0/0/0/0	0/0/0/0
86	OHX	M0	304	86	-	0/0/0/0	0/0/0/0
86	OHX	M5	301	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	201	-	-	0/0/0/0	0/0/0/0
86	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	202	86	-	0/0/0/0	0/0/0/0
86	OHX	M9	203	-	-	0/0/0/0	0/0/0/0
86	OHX	N8	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	86	-	0/0/0/0	0/0/0/0
86	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	102	73	-	0/0/0/0	0/0/0/0
86	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	S2	301	86	-	0/0/0/0	0/0/0/0
86	OHX	S8	301	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c1	201	86	-	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	c5	202	17	-	0/0/0/0	0/0/0/0
86	OHX	c8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	86	-	0/0/0/0	0/0/0/0
86	OHX	l2	301	86	-	0/0/0/0	0/0/0/0
86	OHX	l3	401	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	401	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	301	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	302	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	301	86	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	m0	302	86	-	0/0/0/0	0/0/0/0
86	OHX	m0	303	86	-	0/0/0/0	0/0/0/0
86	OHX	m0	304	86	-	0/0/0/0	0/0/0/0
86	OHX	m1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	501	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	502	-	-	0/0/0/0	0/0/0/0
86	OHX	m7	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	503	86	-	0/0/0/0	0/0/0/0
86	OHX	o9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	q1	101	86	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	301	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	5	3403	8AN	C3'-N3'	-35.11	0.93	1.47
90	5	3403	8AN	C5-C4	-2.45	1.35	1.40
89	5	3401	C	C4-N3	-2.01	1.31	1.35
91	1	3404	PRO	CA-C	2.04	1.52	1.50
91	5	3404	PRO	CA-C	2.09	1.53	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	5	3403	8AN	N3-C2-N1	-5.92	123.70	128.86
90	1	3403	8AN	N3-C2-N1	-5.90	123.72	128.86
89	5	3402	C	C6-N1-C2	-3.18	116.13	121.28
89	1	3402	C	C6-N1-C2	-3.16	116.16	121.28
90	1	3403	8AN	C4-C5-N7	-2.93	106.58	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

665 monomers are involved in 1055 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	1	3401	C	4	0
89	1	3402	C	4	0
90	1	3403	8AN	14	0
86	1	3407	OHX	2	0
86	1	3410	OHX	1	0
86	1	3411	OHX	3	0
86	1	3413	OHX	1	0
86	1	3414	OHX	1	0
86	1	3415	OHX	1	0
86	1	3417	OHX	1	0
86	1	3418	OHX	1	0
86	1	3419	OHX	1	0
86	1	3420	OHX	1	0
86	1	3421	OHX	1	0
86	1	3423	OHX	1	0
86	1	3424	OHX	2	0
86	1	3430	OHX	1	0
86	1	3431	OHX	1	0
86	1	3432	OHX	1	0
86	1	3433	OHX	1	0
86	1	3434	OHX	1	0
86	1	3437	OHX	5	0
86	1	3438	OHX	3	0
86	1	3440	OHX	1	0
86	1	3441	OHX	2	0
86	1	3442	OHX	1	0
86	1	3446	OHX	1	0
86	1	3447	OHX	1	0
86	1	3448	OHX	1	0
86	1	3450	OHX	3	0
86	1	3453	OHX	3	0
86	1	3455	OHX	3	0
86	1	3456	OHX	1	0
86	1	3457	OHX	1	0
86	1	3460	OHX	1	0
86	1	3461	OHX	1	0
86	1	3463	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3465	OHX	1	0
86	1	3467	OHX	1	0
86	1	3468	OHX	1	0
86	1	3469	OHX	1	0
86	1	3474	OHX	2	0
86	1	3475	OHX	3	0
86	1	3476	OHX	4	0
86	1	3478	OHX	2	0
86	1	3479	OHX	5	0
86	1	3480	OHX	5	0
86	1	3482	OHX	1	0
86	1	3483	OHX	1	0
86	1	3484	OHX	2	0
86	1	3488	OHX	1	0
86	1	3494	OHX	7	0
86	1	3495	OHX	1	0
86	1	3496	OHX	1	0
86	1	3499	OHX	1	0
86	1	3500	OHX	5	0
86	1	3504	OHX	1	0
86	1	3505	OHX	3	0
86	1	3507	OHX	1	0
86	1	3508	OHX	2	0
86	1	3509	OHX	1	0
86	1	3511	OHX	4	0
86	1	3513	OHX	1	0
86	1	3516	OHX	2	0
86	1	3517	OHX	2	0
86	1	3518	OHX	5	0
86	1	3519	OHX	1	0
86	1	3522	OHX	1	0
86	1	3523	OHX	1	0
86	1	3524	OHX	2	0
86	1	3528	OHX	1	0
86	1	3530	OHX	1	0
86	1	3533	OHX	1	0
86	1	3535	OHX	3	0
86	1	3536	OHX	3	0
86	1	3538	OHX	3	0
86	1	3539	OHX	2	0
86	1	3541	OHX	3	0
86	1	3542	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3543	OHX	2	0
86	1	3544	OHX	2	0
86	1	3545	OHX	2	0
86	1	3546	OHX	3	0
86	1	3548	OHX	1	0
86	1	3550	OHX	2	0
86	1	3551	OHX	1	0
86	1	3553	OHX	3	0
86	1	3556	OHX	1	0
86	1	3562	OHX	2	0
86	1	3566	OHX	2	0
86	1	3570	OHX	2	0
86	1	3571	OHX	1	0
86	1	3574	OHX	1	0
86	1	3575	OHX	1	0
86	1	3576	OHX	1	0
86	1	3577	OHX	1	0
86	1	3578	OHX	1	0
86	1	3583	OHX	2	0
86	1	3584	OHX	2	0
86	1	3586	OHX	2	0
86	1	3587	OHX	2	0
86	1	3588	OHX	1	0
86	1	3590	OHX	2	0
86	1	3595	OHX	1	0
86	1	3596	OHX	3	0
86	1	3598	OHX	1	0
86	1	3599	OHX	1	0
86	1	3602	OHX	2	0
86	1	3605	OHX	1	0
86	1	3606	OHX	2	0
86	1	3607	OHX	1	0
86	1	3611	OHX	1	0
86	1	3614	OHX	1	0
86	1	3620	OHX	1	0
86	1	3625	OHX	1	0
86	1	3627	OHX	1	0
86	1	3631	OHX	1	0
86	1	3632	OHX	1	0
86	1	3634	OHX	1	0
86	1	3636	OHX	1	0
86	1	3639	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3640	OHX	2	0
86	1	3642	OHX	1	0
86	1	3647	OHX	6	0
86	1	3649	OHX	1	0
86	1	3651	OHX	1	0
86	1	3652	OHX	1	0
86	1	3653	OHX	1	0
86	1	3654	OHX	1	0
86	1	3656	OHX	1	0
86	1	3660	OHX	1	0
86	1	3662	OHX	1	0
86	1	3663	OHX	2	0
86	1	3665	OHX	1	0
86	1	3666	OHX	2	0
86	1	3667	OHX	2	0
86	1	3670	OHX	1	0
86	1	3672	OHX	1	0
86	1	3675	OHX	1	0
86	1	3676	OHX	1	0
86	1	3678	OHX	1	0
86	1	3684	OHX	1	0
86	1	3685	OHX	3	0
86	1	3686	OHX	1	0
86	1	3687	OHX	1	0
86	1	3688	OHX	2	0
86	1	3689	OHX	4	0
86	1	3690	OHX	1	0
86	1	3691	OHX	5	0
86	1	3695	OHX	4	0
86	1	3698	OHX	1	0
86	1	3699	OHX	2	0
86	1	3702	OHX	1	0
86	1	3703	OHX	1	0
86	1	3704	OHX	1	0
86	1	3705	OHX	2	0
86	1	3707	OHX	1	0
86	1	3710	OHX	2	0
86	1	3711	OHX	2	0
86	1	3715	OHX	1	0
86	1	3716	OHX	2	0
86	1	3718	OHX	1	0
86	1	3721	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3722	OHX	1	0
86	1	3728	OHX	2	0
86	1	3729	OHX	2	0
86	1	3730	OHX	3	0
86	1	3731	OHX	1	0
86	1	3734	OHX	5	0
86	1	3736	OHX	1	0
86	1	3737	OHX	11	0
86	1	3740	OHX	1	0
86	1	3741	OHX	3	0
86	1	3742	OHX	2	0
86	1	3744	OHX	3	0
86	1	3746	OHX	4	0
86	1	3750	OHX	2	0
86	1	3751	OHX	9	0
86	1	3753	OHX	4	0
86	1	3754	OHX	1	0
86	1	3755	OHX	1	0
86	1	3757	OHX	3	0
86	1	3758	OHX	2	0
86	1	3762	OHX	3	0
86	1	3767	OHX	1	0
86	1	3768	OHX	2	0
86	1	3774	OHX	1	0
86	1	3775	OHX	2	0
86	1	3776	OHX	4	0
86	1	3777	OHX	4	0
86	1	3778	OHX	1	0
86	1	3779	OHX	4	0
86	1	3780	OHX	2	0
86	1	3781	OHX	2	0
86	1	3786	OHX	1	0
86	1	3787	OHX	2	0
86	1	3788	OHX	1	0
86	1	3790	OHX	1	0
86	1	3791	OHX	4	0
86	1	3792	OHX	1	0
86	1	3794	OHX	3	0
86	1	3797	OHX	4	0
86	1	3799	OHX	5	0
86	1	3800	OHX	6	0
86	1	3801	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3802	OHX	1	0
86	1	3804	OHX	4	0
86	1	3805	OHX	4	0
86	1	3808	OHX	3	0
86	1	3809	OHX	7	0
86	1	3810	OHX	5	0
86	1	3813	OHX	1	0
86	1	3814	OHX	3	0
86	2	1901	OHX	1	0
86	2	1904	OHX	1	0
86	2	1906	OHX	1	0
86	2	1909	OHX	5	0
86	2	1912	OHX	1	0
86	2	1913	OHX	1	0
86	2	1914	OHX	2	0
86	2	1915	OHX	1	0
86	2	1917	OHX	1	0
86	2	1918	OHX	5	0
86	2	1921	OHX	2	0
86	2	1923	OHX	1	0
86	2	1924	OHX	1	0
86	2	1925	OHX	1	0
86	2	1926	OHX	1	0
86	2	1927	OHX	1	0
86	2	1928	OHX	1	0
86	2	1932	OHX	1	0
86	2	1935	OHX	1	0
86	2	1936	OHX	1	0
86	2	1937	OHX	1	0
86	2	1938	OHX	1	0
86	2	1941	OHX	1	0
86	2	1943	OHX	2	0
86	2	1944	OHX	1	0
86	2	1945	OHX	1	0
86	2	1946	OHX	1	0
86	2	1949	OHX	2	0
86	2	1950	OHX	1	0
86	2	1952	OHX	1	0
86	2	1953	OHX	2	0
86	2	1954	OHX	3	0
86	2	1955	OHX	1	0
86	2	1956	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	1961	OHX	1	0
86	2	1962	OHX	4	0
86	2	1963	OHX	2	0
86	2	1964	OHX	4	0
86	2	1965	OHX	1	0
86	2	1966	OHX	1	0
86	2	1969	OHX	4	0
86	2	1970	OHX	2	0
86	2	1971	OHX	1	0
86	2	1973	OHX	1	0
86	2	1974	OHX	1	0
86	2	1975	OHX	2	0
86	2	1976	OHX	1	0
86	2	1977	OHX	3	0
86	2	1981	OHX	1	0
86	2	1984	OHX	2	0
86	2	1988	OHX	1	0
86	2	1990	OHX	3	0
86	2	1992	OHX	1	0
86	2	1993	OHX	1	0
86	2	1995	OHX	1	0
86	2	1997	OHX	2	0
86	2	2003	OHX	3	0
86	2	2004	OHX	1	0
86	2	2006	OHX	1	0
86	2	2008	OHX	1	0
86	2	2009	OHX	2	0
86	2	2010	OHX	1	0
86	2	2011	OHX	1	0
86	2	2013	OHX	1	0
86	2	2016	OHX	1	0
86	2	2017	OHX	1	0
86	2	2018	OHX	1	0
86	2	2021	OHX	1	0
86	2	2022	OHX	1	0
86	2	2023	OHX	1	0
86	2	2030	OHX	2	0
86	2	2033	OHX	1	0
86	2	2034	OHX	1	0
86	2	2035	OHX	4	0
86	2	2037	OHX	2	0
86	2	2042	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2043	OHX	1	0
86	2	2044	OHX	2	0
86	2	2047	OHX	1	0
86	2	2048	OHX	1	0
86	2	2050	OHX	1	0
86	2	2051	OHX	1	0
86	2	2053	OHX	3	0
86	2	2054	OHX	2	0
86	2	2057	OHX	1	0
86	2	2061	OHX	1	0
86	2	2062	OHX	1	0
86	2	2063	OHX	1	0
86	2	2064	OHX	3	0
86	2	2067	OHX	1	0
86	2	2068	OHX	1	0
86	2	2069	OHX	2	0
86	2	2071	OHX	2	0
86	2	2073	OHX	2	0
86	2	2076	OHX	3	0
86	2	2078	OHX	2	0
86	2	2081	OHX	1	0
86	2	2084	OHX	1	0
86	2	2085	OHX	3	0
86	2	2087	OHX	2	0
86	2	2088	OHX	1	0
86	3	201	OHX	1	0
86	3	202	OHX	1	0
86	3	205	OHX	1	0
86	3	206	OHX	1	0
86	3	212	OHX	1	0
86	4	205	OHX	1	0
86	4	206	OHX	2	0
86	4	209	OHX	1	0
86	4	210	OHX	1	0
86	4	213	OHX	3	0
86	4	218	OHX	2	0
89	5	3401	C	3	0
89	5	3402	C	4	0
90	5	3403	8AN	9	0
91	5	3404	PRO	2	0
86	5	3405	OHX	1	0
86	5	3407	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3412	OHX	1	0
86	5	3413	OHX	2	0
86	5	3415	OHX	1	0
86	5	3417	OHX	1	0
86	5	3421	OHX	2	0
86	5	3423	OHX	1	0
86	5	3426	OHX	1	0
86	5	3429	OHX	2	0
86	5	3430	OHX	1	0
86	5	3436	OHX	1	0
86	5	3438	OHX	1	0
86	5	3439	OHX	1	0
86	5	3443	OHX	1	0
86	5	3447	OHX	3	0
86	5	3448	OHX	3	0
86	5	3449	OHX	4	0
86	5	3450	OHX	1	0
86	5	3451	OHX	3	0
86	5	3453	OHX	4	0
86	5	3455	OHX	3	0
86	5	3457	OHX	4	0
86	5	3458	OHX	1	0
86	5	3459	OHX	1	0
86	5	3460	OHX	2	0
86	5	3461	OHX	2	0
86	5	3464	OHX	2	0
86	5	3465	OHX	4	0
86	5	3467	OHX	3	0
86	5	3468	OHX	2	0
86	5	3470	OHX	1	0
86	5	3471	OHX	3	0
86	5	3477	OHX	2	0
86	5	3482	OHX	4	0
86	5	3484	OHX	1	0
86	5	3486	OHX	2	0
86	5	3489	OHX	2	0
86	5	3490	OHX	1	0
86	5	3491	OHX	1	0
86	5	3495	OHX	1	0
86	5	3496	OHX	1	0
86	5	3497	OHX	2	0
86	5	3498	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3501	OHX	2	0
86	5	3502	OHX	1	0
86	5	3504	OHX	1	0
86	5	3505	OHX	3	0
86	5	3506	OHX	1	0
86	5	3507	OHX	3	0
86	5	3508	OHX	3	0
86	5	3509	OHX	3	0
86	5	3511	OHX	1	0
86	5	3512	OHX	2	0
86	5	3514	OHX	3	0
86	5	3515	OHX	1	0
86	5	3517	OHX	1	0
86	5	3521	OHX	2	0
86	5	3523	OHX	7	0
86	5	3524	OHX	4	0
86	5	3525	OHX	1	0
86	5	3527	OHX	2	0
86	5	3529	OHX	3	0
86	5	3531	OHX	1	0
86	5	3532	OHX	1	0
86	5	3533	OHX	1	0
86	5	3535	OHX	1	0
86	5	3537	OHX	1	0
86	5	3538	OHX	2	0
86	5	3539	OHX	3	0
86	5	3541	OHX	4	0
86	5	3543	OHX	2	0
86	5	3545	OHX	1	0
86	5	3547	OHX	2	0
86	5	3555	OHX	1	0
86	5	3556	OHX	1	0
86	5	3557	OHX	1	0
86	5	3558	OHX	1	0
86	5	3559	OHX	2	0
86	5	3560	OHX	1	0
86	5	3562	OHX	1	0
86	5	3565	OHX	2	0
86	5	3567	OHX	1	0
86	5	3569	OHX	3	0
86	5	3571	OHX	3	0
86	5	3572	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3573	OHX	4	0
86	5	3574	OHX	1	0
86	5	3578	OHX	1	0
86	5	3580	OHX	5	0
86	5	3585	OHX	1	0
86	5	3586	OHX	1	0
86	5	3587	OHX	2	0
86	5	3590	OHX	4	0
86	5	3592	OHX	1	0
86	5	3596	OHX	1	0
86	5	3597	OHX	4	0
86	5	3598	OHX	1	0
86	5	3599	OHX	3	0
86	5	3601	OHX	1	0
86	5	3602	OHX	5	0
86	5	3608	OHX	1	0
86	5	3609	OHX	2	0
86	5	3611	OHX	1	0
86	5	3612	OHX	2	0
86	5	3613	OHX	2	0
86	5	3615	OHX	1	0
86	5	3617	OHX	1	0
86	5	3619	OHX	1	0
86	5	3623	OHX	1	0
86	5	3625	OHX	1	0
86	5	3626	OHX	1	0
86	5	3631	OHX	1	0
86	5	3632	OHX	1	0
86	5	3633	OHX	1	0
86	5	3636	OHX	3	0
86	5	3638	OHX	1	0
86	5	3639	OHX	2	0
86	5	3642	OHX	2	0
86	5	3645	OHX	1	0
86	5	3648	OHX	2	0
86	5	3653	OHX	2	0
86	5	3654	OHX	1	0
86	5	3655	OHX	1	0
86	5	3659	OHX	5	0
86	5	3660	OHX	1	0
86	5	3662	OHX	1	0
86	5	3667	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3669	OHX	1	0
86	5	3671	OHX	1	0
86	5	3674	OHX	2	0
86	5	3676	OHX	1	0
86	5	3679	OHX	1	0
86	5	3680	OHX	1	0
86	5	3685	OHX	1	0
86	5	3688	OHX	4	0
86	5	3691	OHX	5	0
86	5	3692	OHX	1	0
86	5	3693	OHX	2	0
86	5	3700	OHX	1	0
86	5	3701	OHX	1	0
86	5	3704	OHX	1	0
86	5	3705	OHX	2	0
86	5	3706	OHX	1	0
86	5	3708	OHX	2	0
86	5	3709	OHX	3	0
86	5	3711	OHX	1	0
86	5	3713	OHX	2	0
86	5	3716	OHX	5	0
86	5	3717	OHX	2	0
86	5	3718	OHX	1	0
86	5	3720	OHX	1	0
86	5	3722	OHX	4	0
86	5	3724	OHX	3	0
86	5	3727	OHX	4	0
86	5	3729	OHX	5	0
86	5	3730	OHX	1	0
86	5	3735	OHX	2	0
86	5	3736	OHX	2	0
86	5	3741	OHX	1	0
86	5	3745	OHX	1	0
86	5	3749	OHX	2	0
86	5	3753	OHX	4	0
86	5	3757	OHX	4	0
86	5	3758	OHX	1	0
86	5	3759	OHX	1	0
86	5	3761	OHX	3	0
86	5	3762	OHX	1	0
86	5	3765	OHX	2	0
86	5	3767	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3769	OHX	2	0
86	5	3770	OHX	1	0
86	5	3771	OHX	1	0
86	5	3772	OHX	3	0
86	5	3773	OHX	1	0
86	5	3775	OHX	1	0
86	5	3776	OHX	1	0
86	5	3777	OHX	1	0
86	5	3779	OHX	4	0
86	5	3781	OHX	1	0
86	5	3783	OHX	1	0
86	5	3786	OHX	1	0
86	5	3788	OHX	2	0
86	5	3789	OHX	1	0
86	5	3793	OHX	1	0
86	5	3794	OHX	3	0
86	5	3796	OHX	4	0
86	5	3799	OHX	1	0
86	5	3801	OHX	3	0
86	5	3802	OHX	3	0
86	5	3803	OHX	3	0
86	5	3804	OHX	2	0
86	5	3805	OHX	3	0
86	5	3806	OHX	5	0
86	5	3807	OHX	1	0
86	5	3808	OHX	6	0
86	5	3809	OHX	3	0
86	5	3810	OHX	6	0
86	5	3811	OHX	2	0
86	5	3814	OHX	3	0
86	5	3815	OHX	3	0
86	5	3816	OHX	3	0
86	5	3817	OHX	2	0
86	5	3818	OHX	2	0
86	6	1901	OHX	1	0
86	6	1903	OHX	1	0
86	6	1909	OHX	4	0
86	6	1910	OHX	2	0
86	6	1911	OHX	3	0
86	6	1912	OHX	2	0
86	6	1914	OHX	2	0
86	6	1915	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	1916	OHX	2	0
86	6	1918	OHX	3	0
86	6	1919	OHX	2	0
86	6	1920	OHX	4	0
86	6	1921	OHX	3	0
86	6	1922	OHX	1	0
86	6	1925	OHX	1	0
86	6	1926	OHX	1	0
86	6	1928	OHX	1	0
86	6	1929	OHX	1	0
86	6	1931	OHX	4	0
86	6	1934	OHX	1	0
86	6	1938	OHX	3	0
86	6	1939	OHX	3	0
86	6	1949	OHX	2	0
86	6	1951	OHX	3	0
86	6	1952	OHX	1	0
86	6	1955	OHX	1	0
86	6	1956	OHX	1	0
86	6	1957	OHX	1	0
86	6	1959	OHX	2	0
86	6	1961	OHX	1	0
86	6	1963	OHX	1	0
86	6	1965	OHX	3	0
86	6	1966	OHX	2	0
86	6	1967	OHX	1	0
86	6	1968	OHX	1	0
86	6	1969	OHX	1	0
86	6	1974	OHX	1	0
86	6	1975	OHX	2	0
86	6	1978	OHX	2	0
86	6	1980	OHX	1	0
86	6	1983	OHX	1	0
86	6	1984	OHX	1	0
86	6	1985	OHX	1	0
86	6	1991	OHX	2	0
86	6	1992	OHX	1	0
86	6	1997	OHX	2	0
86	6	2000	OHX	1	0
86	6	2002	OHX	3	0
86	6	2004	OHX	1	0
86	6	2005	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2006	OHX	1	0
86	6	2008	OHX	1	0
86	6	2009	OHX	3	0
86	6	2015	OHX	2	0
86	6	2016	OHX	3	0
86	6	2018	OHX	1	0
86	6	2019	OHX	1	0
86	6	2021	OHX	1	0
86	6	2023	OHX	1	0
86	6	2028	OHX	1	0
86	6	2032	OHX	2	0
86	6	2034	OHX	1	0
86	6	2035	OHX	2	0
86	6	2038	OHX	1	0
86	6	2041	OHX	1	0
86	6	2042	OHX	1	0
86	6	2043	OHX	2	0
86	6	2045	OHX	1	0
86	6	2051	OHX	2	0
86	6	2053	OHX	1	0
86	6	2054	OHX	1	0
86	6	2056	OHX	3	0
86	6	2057	OHX	1	0
86	6	2058	OHX	2	0
86	6	2061	OHX	2	0
86	6	2065	OHX	1	0
86	6	2066	OHX	1	0
86	6	2067	OHX	3	0
86	6	2068	OHX	1	0
86	6	2069	OHX	3	0
86	6	2070	OHX	1	0
86	6	2071	OHX	1	0
86	6	2074	OHX	2	0
86	6	2075	OHX	2	0
86	6	2077	OHX	1	0
86	6	2079	OHX	1	0
86	6	2082	OHX	4	0
86	6	2083	OHX	4	0
86	6	2084	OHX	4	0
86	6	2088	OHX	2	0
86	6	2090	OHX	4	0
86	6	2091	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2092	OHX	1	0
86	6	2094	OHX	1	0
86	6	2097	OHX	2	0
86	6	2098	OHX	5	0
86	7	203	OHX	1	0
86	7	211	OHX	2	0
86	8	201	OHX	2	0
86	8	202	OHX	1	0
86	8	203	OHX	3	0
86	8	204	OHX	1	0
86	8	206	OHX	1	0
86	8	207	OHX	4	0
86	8	211	OHX	1	0
86	8	212	OHX	4	0
86	8	213	OHX	2	0
86	8	215	OHX	1	0
86	8	216	OHX	1	0
86	8	219	OHX	2	0
86	8	221	OHX	4	0
86	C3	201	OHX	2	0
86	C5	201	OHX	5	0
86	C8	201	OHX	2	0
86	C8	202	OHX	3	0
86	D9	102	OHX	1	0
86	L3	401	OHX	3	0
86	L3	402	OHX	3	0
86	L4	401	OHX	5	0
86	M0	301	OHX	2	0
86	M0	302	OHX	3	0
86	M0	303	OHX	4	0
86	M0	304	OHX	6	0
86	M5	301	OHX	1	0
86	M9	203	OHX	2	0
86	N9	101	OHX	2	0
86	O1	201	OHX	2	0
86	O7	102	OHX	7	0
86	O7	103	OHX	1	0
86	Q2	502	OHX	5	0
86	S2	301	OHX	2	0
86	S8	301	OHX	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
83	m2	2
82	sM	2
2	S0	1
35	SM	1
81	c0	1
47	m0	1
1	2	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1798:U	O3'	1799:C	P	144.70
1	sM	85:SER	C	119:UNK	N	44.14
1	sM	139:UNK	C	155:UNK	N	37.81
1	SM	141:ALA	C	151:UNK	N	26.32
1	c0	84:GLU	C	87:UNK	N	7.55

## 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	1781/1829 (97%)	0.32	93 (5%) 28 26	53, 90, 174, 223	0
2	S0	206/206 (100%)	1.99	98 (47%) 0 0	91, 107, 116, 121	0
2	s0	206/206 (100%)	1.06	36 (17%) 2 1	68, 84, 96, 105	0
3	S1	214/216 (99%)	1.09	50 (23%) 1 1	104, 134, 158, 165	0
3	s1	216/216 (100%)	1.06	38 (17%) 2 1	72, 84, 102, 115	0
4	S2	217/217 (100%)	0.31	11 (5%) 29 26	75, 86, 98, 108	0
4	s2	217/217 (100%)	0.45	8 (3%) 42 38	55, 68, 78, 87	0
5	S3	223/223 (100%)	0.65	24 (10%) 6 5	82, 93, 112, 124	0
5	s3	223/223 (100%)	0.70	24 (10%) 6 5	74, 99, 116, 124	0
6	S4	260/260 (100%)	1.81	101 (38%) 0 0	69, 91, 98, 119	0
6	s4	260/260 (100%)	0.96	43 (16%) 2 2	47, 69, 82, 106	0
7	S5	206/206 (100%)	0.77	32 (15%) 2 2	96, 112, 124, 132	0
7	s5	206/206 (100%)	1.01	46 (22%) 1 1	79, 97, 113, 121	0
8	S6	226/226 (100%)	0.65	28 (12%) 4 4	72, 106, 120, 125	0
8	s6	218/226 (96%)	0.50	21 (9%) 9 8	49, 77, 94, 110	0
9	S7	184/186 (98%)	0.40	10 (5%) 26 25	90, 114, 139, 144	0
9	s7	186/186 (100%)	0.12	4 (2%) 62 60	65, 96, 124, 132	0
10	S8	188/199 (94%)	1.00	30 (15%) 2 2	63, 79, 113, 125	0
10	s8	188/199 (94%)	0.58	17 (9%) 10 10	46, 66, 107, 124	0
11	S9	185/185 (100%)	1.74	67 (36%) 0 1	81, 95, 126, 141	0
11	s9	185/185 (100%)	0.84	27 (14%) 3 2	57, 74, 104, 122	0
12	C0	96/96 (100%)	0.59	9 (9%) 9 9	84, 105, 126, 135	0
13	C1	155/155 (100%)	1.26	34 (21%) 1 1	64, 76, 112, 121	0
13	c1	146/155 (94%)	0.48	9 (6%) 21 21	48, 61, 89, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
14	C2	124/124 (100%)	1.57	40 (32%)	0	1	133, 139, 151, 157	0
14	c2	124/124 (100%)	3.26	87 (70%)	0	0	167, 183, 195, 200	0
15	C3	150/150 (100%)	0.43	7 (4%)	32	30	75, 88, 104, 108	0
15	c3	150/150 (100%)	0.01	3 (2%)	65	63	57, 70, 86, 88	0
16	C4	127/128 (99%)	0.88	25 (19%)	1	1	75, 129, 142, 144	0
16	c4	128/128 (100%)	0.98	15 (11%)	5	4	54, 86, 94, 104	0
17	C5	124/135 (91%)	1.87	49 (39%)	0	0	79, 94, 110, 126	0
17	c5	135/135 (100%)	1.62	42 (31%)	0	1	67, 97, 112, 115	0
18	C6	141/142 (99%)	2.45	76 (53%)	0	0	82, 102, 107, 110	0
18	c6	142/142 (100%)	1.89	56 (39%)	0	0	73, 91, 104, 121	0
19	C7	120/125 (96%)	1.61	38 (31%)	0	1	91, 105, 124, 126	0
19	c7	117/125 (93%)	0.98	25 (21%)	1	1	78, 91, 105, 112	0
20	C8	145/145 (100%)	1.38	41 (28%)	1	1	77, 97, 120, 127	0
20	c8	145/145 (100%)	1.34	39 (26%)	1	1	73, 89, 109, 114	0
21	C9	143/143 (100%)	1.80	59 (41%)	0	0	85, 99, 111, 120	0
21	c9	143/143 (100%)	0.77	18 (12%)	4	4	76, 85, 99, 107	0
22	D0	107/110 (97%)	1.57	37 (34%)	0	1	77, 105, 124, 127	0
22	d0	110/110 (100%)	1.85	42 (38%)	0	0	74, 102, 127, 134	0
23	D1	87/87 (100%)	1.43	23 (26%)	1	1	87, 95, 109, 115	0
23	d1	87/87 (100%)	0.52	7 (8%)	13	12	65, 73, 93, 100	0
24	D2	129/129 (100%)	2.07	62 (48%)	0	0	73, 84, 90, 100	0
24	d2	129/129 (100%)	0.71	6 (4%)	32	30	53, 61, 68, 76	0
25	D3	144/144 (100%)	0.28	3 (2%)	64	61	64, 71, 83, 97	0
25	d3	144/144 (100%)	0.03	1 (0%)	87	87	45, 52, 62, 77	0
26	D4	134/134 (100%)	0.76	13 (9%)	8	8	81, 102, 113, 118	0
26	d4	134/134 (100%)	0.43	8 (5%)	23	21	56, 76, 87, 91	0
27	D5	70/70 (100%)	0.62	5 (7%)	17	17	108, 118, 124, 125	0
27	d5	69/70 (98%)	1.11	11 (15%)	2	2	89, 104, 111, 113	0
28	D6	97/97 (100%)	2.36	59 (60%)	0	0	79, 94, 142, 143	0
28	d6	97/97 (100%)	1.18	22 (22%)	1	1	58, 72, 97, 100	0
29	D7	81/81 (100%)	1.69	32 (39%)	0	0	90, 106, 133, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	d7	81/81 (100%)	0.88	10 (12%) 5 4	66, 83, 117, 120	0
30	D8	63/63 (100%)	1.13	15 (23%) 1 1	106, 122, 129, 131	0
30	d8	63/63 (100%)	1.40	18 (28%) 1 1	96, 110, 117, 119	0
31	D9	53/53 (100%)	1.39	16 (30%) 1 1	75, 80, 100, 104	0
31	d9	53/53 (100%)	2.42	30 (56%) 0 0	71, 83, 117, 130	0
32	E0	60/62 (96%)	0.83	9 (15%) 3 2	70, 100, 125, 128	0
32	e0	62/62 (100%)	0.03	3 (4%) 31 29	55, 79, 104, 105	0
33	E1	71/76 (93%)	1.28	15 (21%) 1 1	96, 129, 140, 142	0
33	e1	76/76 (100%)	2.21	38 (50%) 0 0	100, 155, 176, 179	0
34	SR	318/318 (100%)	1.04	60 (18%) 1 1	100, 111, 126, 148	0
34	sR	318/318 (100%)	1.80	134 (42%) 0 0	96, 110, 122, 137	0
35	SM	133/159 (83%)	1.20	27 (20%) 1 1	54, 86, 117, 122	0
36	1	3149/3394 (92%)	0.13	52 (1%) 70 67	30, 54, 125, 221	0
36	5	3150/3394 (92%)	0.12	30 (0%) 82 81	31, 50, 117, 193	0
37	3	121/121 (100%)	0.03	0 100 100	40, 70, 86, 94	0
37	7	121/121 (100%)	-0.13	0 100 100	35, 53, 64, 71	0
38	4	158/158 (100%)	0.00	2 (1%) 77 75	40, 60, 96, 129	0
38	8	158/158 (100%)	-0.02	1 (0%) 89 88	42, 64, 97, 126	0
39	L2	252/252 (100%)	0.45	6 (2%) 59 56	40, 57, 74, 83	0
39	l2	252/252 (100%)	0.57	16 (6%) 21 20	38, 56, 74, 87	0
40	L3	386/386 (100%)	0.04	1 (0%) 93 93	38, 57, 69, 83	0
40	l3	386/386 (100%)	-0.12	2 (0%) 90 90	30, 42, 56, 76	0
41	L4	361/361 (100%)	-0.16	0 100 100	34, 48, 63, 70	0
41	l4	361/361 (100%)	-0.10	0 100 100	37, 52, 70, 76	0
42	L5	296/296 (100%)	1.36	93 (31%) 0 1	51, 76, 94, 108	0
42	l5	294/296 (99%)	0.72	17 (5%) 24 23	42, 54, 75, 94	0
43	L6	156/175 (89%)	0.22	1 (0%) 89 88	44, 53, 66, 77	0
43	l6	157/175 (89%)	-0.01	1 (0%) 89 88	44, 54, 71, 83	0
44	L7	222/223 (99%)	0.11	1 (0%) 90 90	35, 45, 70, 99	0
44	l7	223/223 (100%)	-0.03	0 100 100	35, 43, 74, 102	0
45	L8	233/233 (100%)	0.83	29 (12%) 4 4	65, 83, 108, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	l8	231/233 (99%)	0.75	23 (9%) 8 7	72, 87, 109, 112	0
46	L9	191/191 (100%)	0.66	24 (12%) 4 4	57, 65, 74, 85	0
46	l9	191/191 (100%)	0.16	3 (1%) 72 69	39, 48, 63, 72	0
47	M0	211/220 (95%)	0.05	2 (0%) 84 83	41, 54, 88, 102	0
47	m0	213/220 (96%)	0.17	7 (3%) 47 44	36, 50, 74, 87	0
48	M1	169/169 (100%)	1.89	76 (44%) 0 0	62, 77, 87, 93	0
48	m1	169/169 (100%)	0.75	14 (8%) 12 11	45, 61, 68, 72	0
49	M3	193/194 (99%)	0.35	4 (2%) 64 61	35, 58, 94, 119	0
49	m3	194/194 (100%)	0.48	6 (3%) 49 48	38, 67, 100, 109	0
50	M4	136/137 (99%)	0.06	5 (3%) 42 38	50, 59, 70, 74	0
50	m4	137/137 (100%)	-0.23	0 100 100	44, 50, 66, 72	0
51	M5	203/203 (100%)	0.86	28 (13%) 3 3	38, 55, 66, 68	0
51	m5	203/203 (100%)	0.99	33 (16%) 2 2	42, 61, 73, 76	0
52	M6	197/197 (100%)	-0.02	2 (1%) 82 81	38, 45, 63, 65	0
52	m6	197/197 (100%)	-0.04	0 100 100	31, 37, 63, 68	0
53	M7	183/183 (100%)	0.26	9 (4%) 30 28	41, 47, 96, 121	0
53	m7	155/183 (84%)	-0.02	1 (0%) 89 88	37, 42, 52, 70	0
54	M8	185/185 (100%)	0.36	4 (2%) 62 60	37, 48, 61, 75	0
54	m8	185/185 (100%)	0.60	11 (5%) 23 22	37, 52, 62, 69	0
55	M9	188/188 (100%)	0.40	14 (7%) 15 15	61, 73, 137, 144	0
55	m9	188/188 (100%)	0.13	3 (1%) 72 69	49, 63, 121, 132	0
56	N0	172/172 (100%)	1.02	36 (20%) 1 1	46, 54, 65, 73	0
56	n0	172/172 (100%)	0.10	2 (1%) 79 77	38, 45, 55, 63	0
57	N1	159/159 (100%)	0.79	19 (11%) 5 4	37, 51, 92, 98	0
57	n1	159/159 (100%)	0.34	5 (3%) 49 48	36, 44, 78, 83	0
58	N2	100/100 (100%)	0.60	10 (10%) 8 7	92, 102, 107, 115	0
58	n2	98/100 (98%)	1.07	21 (21%) 1 1	74, 85, 91, 93	0
59	N3	136/136 (100%)	0.41	0 100 100	44, 54, 64, 69	0
59	n3	136/136 (100%)	0.25	2 (1%) 74 70	31, 38, 47, 50	0
60	N4	98/135 (72%)	2.14	31 (31%) 0 1	55, 67, 134, 136	0
60	n4	135/135 (100%)	1.03	27 (20%) 1 1	39, 83, 109, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
61	N5	121/121 (100%)	1.07	22 (18%) 1 1	57, 69, 85, 107	0
61	n5	120/121 (99%)	0.58	8 (6%) 19 18	56, 69, 87, 93	0
62	N6	126/126 (100%)	0.53	5 (3%) 39 36	44, 61, 70, 79	0
62	n6	126/126 (100%)	1.06	16 (12%) 4 4	50, 66, 80, 83	0
63	N7	135/135 (100%)	1.56	44 (32%) 0 1	83, 96, 107, 111	0
63	n7	135/135 (100%)	1.52	48 (35%) 0 1	82, 96, 113, 117	0
64	N8	148/148 (100%)	0.45	1 (0%) 87 87	31, 49, 67, 75	0
64	n8	148/148 (100%)	0.67	7 (4%) 32 30	33, 54, 68, 71	0
65	N9	58/58 (100%)	0.78	5 (8%) 11 11	34, 54, 89, 101	0
65	n9	58/58 (100%)	0.18	2 (3%) 46 42	35, 52, 73, 77	0
66	O0	97/100 (97%)	0.56	9 (9%) 9 9	80, 88, 103, 106	0
66	o0	100/100 (100%)	0.34	7 (7%) 17 17	72, 83, 100, 103	0
67	O1	109/109 (100%)	0.49	4 (3%) 42 38	55, 65, 88, 92	0
67	o1	109/109 (100%)	0.97	12 (11%) 6 5	43, 53, 80, 96	0
68	O2	127/127 (100%)	-0.06	2 (1%) 72 69	33, 44, 55, 67	0
68	o2	127/127 (100%)	-0.12	0 100 100	34, 49, 59, 64	0
69	O3	106/106 (100%)	0.19	0 100 100	37, 45, 66, 74	0
69	o3	106/106 (100%)	0.26	0 100 100	36, 42, 65, 74	0
70	O4	112/112 (100%)	1.19	23 (20%) 1 1	54, 74, 103, 109	0
70	o4	112/112 (100%)	0.79	10 (8%) 10 10	51, 73, 105, 111	0
71	O5	119/119 (100%)	0.70	9 (7%) 15 14	55, 70, 77, 80	0
71	o5	119/119 (100%)	0.30	2 (1%) 70 67	63, 71, 86, 95	0
72	O6	99/99 (100%)	0.64	8 (8%) 13 12	55, 67, 92, 100	0
72	o6	99/99 (100%)	0.71	10 (10%) 8 7	61, 72, 86, 99	0
73	O7	87/87 (100%)	0.30	0 100 100	41, 46, 67, 75	0
73	o7	87/87 (100%)	0.42	4 (4%) 33 31	37, 49, 77, 91	0
74	O8	77/77 (100%)	0.92	12 (15%) 2 2	82, 92, 103, 106	0
74	o8	77/77 (100%)	1.76	27 (35%) 0 1	81, 89, 97, 99	0
75	O9	50/50 (100%)	0.42	0 100 100	47, 55, 57, 57	0
75	o9	50/50 (100%)	0.47	2 (4%) 39 36	48, 55, 60, 62	0
76	Q0	52/52 (100%)	0.50	4 (7%) 14 13	49, 53, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
76	q0	52/52 (100%)	-0.01	1 (1%) 67 65	36, 40, 49, 54	0
77	Q1	25/25 (100%)	0.30	0 100 100	57, 62, 66, 66	0
77	q1	25/25 (100%)	0.04	0 100 100	45, 47, 48, 50	0
78	Q2	105/105 (100%)	0.51	8 (7%) 15 14	41, 51, 72, 93	0
78	q2	105/105 (100%)	0.40	4 (3%) 41 37	42, 50, 64, 85	0
79	Q3	91/91 (100%)	0.20	2 (2%) 62 60	46, 59, 74, 81	0
79	q3	91/91 (100%)	0.28	2 (2%) 62 60	42, 55, 67, 73	0
80	6	1795/1800 (99%)	0.17	60 (3%) 47 44	38, 75, 157, 227	0
81	c0	84/96 (87%)	1.66	33 (39%) 0 0	94, 126, 139, 141	0
82	sM	63/104 (60%)	1.32	15 (23%) 1 1	47, 97, 105, 110	0
83	m2	0/150	-	-	-	-
84	p0	143/219 (65%)	2.45	86 (60%) 0 0	88, 109, 177, 181	0
85	p1	0/47	-	-	-	-
85	p2	0/47	-	-	-	-
All	All	33015/34167 (96%)	0.57	3374 (10%) 7 6	30, 69, 125, 227	0

The worst 5 of 3374 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	86	SER	15.3
60	N4	75	THR	13.0
60	N4	84	GLY	12.8
1	2	1807	A	12.6
1	2	1806	A	11.8

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
87	MG	4	222	1/1	0.88	0.55	93.73	46,46,46,46	0
87	MG	1	4013	1/1	0.95	0.61	71.59	47,47,47,47	0
87	MG	2	2258	1/1	0.97	0.50	65.88	74,74,74,74	1
87	MG	5	4480	1/1	0.96	0.72	59.48	50,50,50,50	1
87	MG	5	3930	1/1	0.99	0.54	57.37	34,34,34,34	0
87	MG	1	3936	1/1	0.86	0.75	56.04	31,31,31,31	0
87	MG	5	4404	1/1	0.96	0.93	55.72	38,38,38,38	1
87	MG	5	3955	1/1	0.98	0.48	54.85	32,32,32,32	0
87	MG	5	4019	1/1	0.97	0.56	53.34	30,30,30,30	0
87	MG	2	2259	1/1	0.71	1.52	51.82	74,74,74,74	1
86	OHX	5	3792	7/7	0.86	0.51	51.13	51,51,51,51	7
87	MG	1	4093	1/1	0.91	0.87	50.10	43,43,43,43	0
87	MG	5	4131	1/1	0.76	0.78	47.47	35,35,35,35	1
87	MG	5	3941	1/1	0.98	0.55	47.14	30,30,30,30	0
87	MG	5	3911	1/1	0.02	1.38	44.38	53,53,53,53	1
87	MG	5	4519	1/1	0.90	0.83	44.22	42,42,42,42	1
87	MG	5	3961	1/1	0.96	0.64	42.81	29,29,29,29	0
87	MG	5	4031	1/1	0.92	0.66	42.49	30,30,30,30	0
87	MG	5	4278	1/1	0.96	0.51	42.25	35,35,35,35	1
87	MG	5	4023	1/1	0.97	0.69	42.12	32,32,32,32	0
87	MG	1	4408	1/1	0.67	1.03	41.56	56,56,56,56	1
87	MG	5	4231	1/1	0.84	0.67	40.33	35,35,35,35	1
87	MG	2	2117	1/1	0.54	0.33	39.17	74,74,74,74	0
87	MG	5	4463	1/1	0.97	0.73	38.70	36,36,36,36	1
86	OHX	1	3521	7/7	0.97	0.48	37.54	59,59,59,59	7
87	MG	5	4438	1/1	0.83	0.51	36.73	40,40,40,40	0
87	MG	1	3925	1/1	0.85	0.75	36.33	49,49,49,49	0
87	MG	1	3820	1/1	0.81	0.51	34.75	44,44,44,44	0
87	MG	1	4444	1/1	0.70	0.73	34.72	41,41,41,41	1
87	MG	6	2099	1/1	0.97	0.54	33.74	43,43,43,43	0
87	MG	N8	203	1/1	0.96	0.62	33.27	33,33,33,33	0
87	MG	5	4277	1/1	0.97	0.52	32.72	35,35,35,35	1
87	MG	6	2150	1/1	0.81	0.50	32.49	59,59,59,59	0
87	MG	1	4496	1/1	0.94	0.79	32.04	56,56,56,56	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4307	1/1	0.90	0.74	31.75	58,58,58,58	1
87	MG	1	3965	1/1	0.94	0.48	31.53	31,31,31,31	0
87	MG	6	2311	1/1	0.83	0.91	31.49	60,60,60,60	1
86	OHX	5	3676	7/7	0.90	0.41	31.11	42,42,42,42	7
87	MG	5	4286	1/1	0.92	0.62	30.97	34,34,34,34	1
86	OHX	5	3782	7/7	0.83	0.58	30.65	45,45,45,45	7
87	MG	1	3887	1/1	0.94	0.62	30.51	31,31,31,31	0
87	MG	5	4448	1/1	0.76	0.61	30.22	42,42,42,42	1
87	MG	5	3934	1/1	0.94	0.62	30.16	35,35,35,35	0
87	MG	5	3938	1/1	0.97	0.69	30.09	28,28,28,28	0
87	MG	17	306	1/1	0.84	1.64	29.92	37,37,37,37	1
87	MG	5	3999	1/1	0.91	0.78	29.87	32,32,32,32	0
87	MG	M6	201	1/1	0.89	0.79	29.40	40,40,40,40	1
87	MG	5	3925	1/1	0.68	0.48	29.15	43,43,43,43	1
87	MG	1	4094	1/1	0.92	0.52	28.32	48,48,48,48	0
87	MG	5	4241	1/1	0.96	0.40	28.24	38,38,38,38	1
87	MG	5	4477	1/1	0.97	1.27	28.06	38,38,38,38	1
87	MG	5	3950	1/1	0.97	0.60	27.78	36,36,36,36	0
87	MG	1	3975	1/1	0.93	0.54	27.74	41,41,41,41	0
87	MG	5	4167	1/1	0.91	0.76	27.69	39,39,39,39	0
87	MG	5	3940	1/1	0.98	0.70	27.67	34,34,34,34	0
87	MG	1	4379	1/1	0.98	0.49	27.66	33,33,33,33	0
87	MG	1	4022	1/1	0.96	0.77	27.58	22,22,22,22	0
87	MG	1	3874	1/1	0.95	0.68	27.29	31,31,31,31	0
87	MG	1	3951	1/1	0.84	0.76	27.16	35,35,35,35	0
87	MG	5	3945	1/1	0.95	0.43	27.13	41,41,41,41	0
87	MG	5	3919	1/1	0.96	0.65	27.07	44,44,44,44	0
87	MG	1	3946	1/1	0.93	0.61	26.96	39,39,39,39	0
87	MG	5	3989	1/1	0.91	0.51	26.93	32,32,32,32	0
87	MG	6	2180	1/1	0.96	0.41	26.85	52,52,52,52	0
87	MG	5	4306	1/1	0.96	0.73	26.66	35,35,35,35	1
87	MG	5	4482	1/1	0.85	0.41	26.55	45,45,45,45	1
87	MG	1	4010	1/1	0.89	0.56	26.50	41,41,41,41	0
87	MG	1	3914	1/1	0.96	0.44	26.34	34,34,34,34	0
87	MG	6	2296	1/1	0.95	0.71	25.89	54,54,54,54	1
87	MG	5	3830	1/1	0.89	0.33	25.67	31,31,31,31	0
87	MG	1	4511	1/1	0.90	0.53	25.53	52,52,52,52	0
87	MG	1	3950	1/1	0.98	0.48	25.26	31,31,31,31	0
87	MG	5	3837	1/1	0.99	0.66	25.12	33,33,33,33	0
87	MG	5	4013	1/1	0.95	0.53	25.06	39,39,39,39	0
87	MG	1	4139	1/1	0.91	0.60	24.51	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3688	7/7	0.95	0.53	24.36	37,37,37,37	7
87	MG	n3	203	1/1	0.98	0.46	24.25	29,29,29,29	0
87	MG	1	4019	1/1	0.99	0.72	24.25	27,27,27,27	0
87	MG	5	3992	1/1	0.96	0.62	24.03	33,33,33,33	0
87	MG	1	3989	1/1	0.93	0.65	24.02	37,37,37,37	0
87	MG	5	4342	1/1	0.87	0.64	23.50	34,34,34,34	0
87	MG	1	4412	1/1	0.95	0.49	23.37	32,32,32,32	1
87	MG	O3	202	1/1	0.93	0.87	23.29	38,38,38,38	1
87	MG	1	4082	1/1	0.90	0.49	23.24	52,52,52,52	1
87	MG	5	4343	1/1	0.96	0.96	23.23	53,53,53,53	1
87	MG	6	2308	1/1	0.90	0.68	23.13	51,51,51,51	1
87	MG	1	3941	1/1	0.98	0.50	23.10	36,36,36,36	0
87	MG	1	4266	1/1	0.94	0.62	23.07	33,33,33,33	0
87	MG	5	4017	1/1	0.96	0.65	22.92	33,33,33,33	0
87	MG	5	4210	1/1	0.97	0.56	22.91	35,35,35,35	1
87	MG	2	2109	1/1	0.93	0.68	22.73	73,73,73,73	0
87	MG	5	4478	1/1	0.95	0.45	22.47	33,33,33,33	0
87	MG	5	4415	1/1	0.84	0.50	22.46	33,33,33,33	1
87	MG	2	2128	1/1	0.94	0.47	22.43	60,60,60,60	0
87	MG	5	4279	1/1	0.94	0.57	22.40	36,36,36,36	1
87	MG	l3	414	1/1	0.83	0.58	21.94	32,32,32,32	1
87	MG	1	3940	1/1	0.96	0.65	21.80	38,38,38,38	0
87	MG	5	4360	1/1	0.68	0.43	21.43	50,50,50,50	0
87	MG	1	4041	1/1	0.93	0.43	21.42	33,33,33,33	0
87	MG	5	4396	1/1	0.94	0.46	21.41	52,52,52,52	1
87	MG	1	3921	1/1	0.96	0.48	21.33	37,37,37,37	0
87	MG	2	2194	1/1	0.69	0.60	21.17	72,72,72,72	0
87	MG	6	2126	1/1	0.96	0.46	21.12	43,43,43,43	0
87	MG	5	3946	1/1	0.97	0.57	21.03	33,33,33,33	0
87	MG	5	4156	1/1	0.77	0.63	20.83	41,41,41,41	0
87	MG	1	4395	1/1	0.87	0.66	20.72	34,34,34,34	1
87	MG	1	4350	1/1	0.73	0.45	20.71	40,40,40,40	1
87	MG	5	3972	1/1	0.96	0.62	20.71	31,31,31,31	0
87	MG	1	3997	1/1	0.90	0.57	20.67	43,43,43,43	0
87	MG	1	4198	1/1	0.93	0.52	20.61	47,47,47,47	0
87	MG	1	4469	1/1	0.71	0.36	20.57	55,55,55,55	0
87	MG	1	4220	1/1	0.87	0.55	20.40	39,39,39,39	0
87	MG	1	3942	1/1	0.98	0.60	20.30	32,32,32,32	0
87	MG	m6	201	1/1	0.89	1.03	20.08	38,38,38,38	1
87	MG	5	4533	1/1	0.98	0.60	19.93	36,36,36,36	1
87	MG	5	4006	1/1	0.96	0.60	19.85	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	2	2099	1/1	0.90	0.48	19.85	63,63,63,63	0
87	MG	5	4037	1/1	0.93	0.49	19.67	35,35,35,35	0
86	OHX	1	3771	7/7	0.96	0.52	19.52	52,52,52,52	7
87	MG	1	4346	1/1	0.75	0.72	19.51	48,48,48,48	1
87	MG	5	3991	1/1	0.98	0.50	19.48	34,34,34,34	0
87	MG	5	4029	1/1	0.98	0.55	19.07	26,26,26,26	0
87	MG	5	4208	1/1	0.90	0.49	18.90	32,32,32,32	0
87	MG	1	3994	1/1	0.93	0.41	18.87	56,56,56,56	0
87	MG	M5	305	1/1	0.68	2.52	18.69	69,69,69,69	0
87	MG	1	3998	1/1	0.97	0.55	18.66	27,27,27,27	0
87	MG	m7	209	1/1	0.94	0.80	18.65	42,42,42,42	1
87	MG	5	3952	1/1	0.92	0.53	18.49	34,34,34,34	0
87	MG	5	4467	1/1	0.92	0.38	18.47	37,37,37,37	0
87	MG	1	3867	1/1	0.87	0.55	18.40	42,42,42,42	0
87	MG	5	4235	1/1	0.90	0.50	18.30	38,38,38,38	0
87	MG	1	4447	1/1	0.96	0.35	18.19	44,44,44,44	0
87	MG	1	4478	1/1	0.98	1.01	18.06	47,47,47,47	1
87	MG	6	2125	1/1	0.94	0.50	18.03	40,40,40,40	0
86	OHX	5	3767	7/7	0.84	0.53	18.01	39,39,39,39	7
87	MG	1	4203	1/1	0.92	0.93	17.84	42,42,42,42	1
87	MG	1	4396	1/1	0.98	0.58	17.77	45,45,45,45	1
86	OHX	5	3730	7/7	0.87	0.40	17.67	42,42,42,42	7
86	OHX	5	3785	7/7	0.82	0.37	17.65	53,53,53,53	7
87	MG	5	4515	1/1	0.95	0.55	17.63	34,34,34,34	0
87	MG	2	2112	1/1	0.96	0.59	17.62	69,69,69,69	0
87	MG	6	2118	1/1	0.94	0.37	17.46	38,38,38,38	0
87	MG	5	4005	1/1	0.95	0.48	17.43	30,30,30,30	0
86	OHX	1	3695	7/7	0.92	0.48	17.29	56,56,56,56	7
86	OHX	5	3515	7/7	0.98	0.34	17.26	40,40,40,40	7
87	MG	1	3952	1/1	0.94	0.51	17.11	48,48,48,48	0
87	MG	1	3963	1/1	0.94	0.44	17.09	31,31,31,31	0
87	MG	5	3986	1/1	0.94	0.40	17.04	35,35,35,35	0
86	OHX	5	3797	7/7	0.86	0.49	16.80	42,42,42,42	7
86	OHX	6	2052	7/7	0.80	0.47	16.59	127,127,127,127	7
87	MG	1	4151	1/1	0.90	0.40	16.36	50,50,50,50	0
87	MG	5	4001	1/1	0.95	0.59	16.30	36,36,36,36	0
87	MG	2	2158	1/1	0.89	0.40	16.26	68,68,68,68	0
87	MG	m7	207	1/1	0.98	0.52	16.18	41,41,41,41	1
87	MG	5	4096	1/1	0.95	0.40	16.17	34,34,34,34	0
87	MG	1	3967	1/1	0.94	0.49	16.17	40,40,40,40	0
86	OHX	5	3741	7/7	0.90	0.52	16.15	53,53,53,53	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4048	1/1	0.78	0.37	16.00	34,34,34,34	0
87	MG	5	4571	1/1	0.94	0.64	15.98	34,34,34,34	1
87	MG	5	4021	1/1	0.89	0.63	15.90	36,36,36,36	0
87	MG	5	4111	1/1	0.96	0.57	15.88	36,36,36,36	0
87	MG	n0	202	1/1	0.95	0.93	15.77	38,38,38,38	1
87	MG	5	3825	1/1	0.81	0.32	15.71	48,48,48,48	0
87	MG	5	3824	1/1	0.91	0.44	15.56	39,39,39,39	0
87	MG	1	4392	1/1	0.94	1.03	15.53	37,37,37,37	1
87	MG	d3	202	1/1	0.93	1.91	15.50	49,49,49,49	1
87	MG	N8	205	1/1	0.94	0.57	15.47	31,31,31,31	1
87	MG	O2	203	1/1	0.68	0.86	15.43	44,44,44,44	1
87	MG	5	4297	1/1	0.95	0.66	15.22	33,33,33,33	1
87	MG	4	223	1/1	0.90	0.50	15.19	32,32,32,32	0
87	MG	5	4022	1/1	0.98	0.52	15.15	31,31,31,31	0
87	MG	5	3823	1/1	0.98	0.36	15.08	33,33,33,33	0
87	MG	5	3829	1/1	0.96	0.47	14.78	39,39,39,39	0
87	MG	5	3841	1/1	0.95	0.39	14.78	43,43,43,43	0
87	MG	1	4173	1/1	0.84	0.46	14.76	52,52,52,52	0
87	MG	1	4431	1/1	0.99	0.45	14.71	42,42,42,42	1
87	MG	1	4211	1/1	0.68	0.48	14.70	58,58,58,58	0
87	MG	5	4176	1/1	0.81	0.42	14.67	45,45,45,45	0
87	MG	1	3992	1/1	0.97	0.50	14.66	27,27,27,27	0
86	OHX	5	3612	7/7	0.93	0.42	14.64	39,39,39,39	7
87	MG	5	4502	1/1	0.97	0.42	14.60	42,42,42,42	1
87	MG	5	3954	1/1	0.95	0.41	14.50	40,40,40,40	0
87	MG	5	4538	1/1	0.98	0.80	14.43	48,48,48,48	1
87	MG	1	4313	1/1	0.95	0.44	14.39	41,41,41,41	1
87	MG	1	3884	1/1	0.69	0.44	14.32	50,50,50,50	0
86	OHX	1	3729	7/7	0.91	0.39	14.27	57,57,57,57	7
87	MG	5	4189	1/1	0.96	0.41	14.24	35,35,35,35	1
87	MG	L4	408	1/1	0.94	0.66	14.23	34,34,34,34	1
87	MG	n1	202	1/1	0.98	0.98	14.19	40,40,40,40	1
87	MG	1	4461	1/1	0.87	1.07	14.19	54,54,54,54	1
87	MG	5	3848	1/1	0.95	0.44	14.13	33,33,33,33	0
87	MG	6	2328	1/1	0.95	1.14	14.12	54,54,54,54	1
86	OHX	6	1981	7/7	0.97	0.42	14.06	45,45,45,45	7
87	MG	5	4150	1/1	0.77	0.39	13.99	41,41,41,41	1
87	MG	5	3849	1/1	0.99	0.44	13.97	34,34,34,34	0
87	MG	N3	201	1/1	0.98	0.59	13.97	39,39,39,39	0
87	MG	5	4461	1/1	0.96	0.87	13.91	45,45,45,45	1
87	MG	1	4383	1/1	0.96	0.53	13.85	33,33,33,33	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4432	1/1	0.79	1.19	13.79	47,47,47,47	1
86	OHX	6	1959	7/7	0.95	0.35	13.79	57,57,57,57	7
87	MG	5	3996	1/1	0.95	0.54	13.70	31,31,31,31	0
87	MG	O2	202	1/1	0.84	0.41	13.70	32,32,32,32	0
87	MG	5	4002	1/1	0.98	0.44	13.69	37,37,37,37	0
87	MG	5	4276	1/1	0.93	0.45	13.65	33,33,33,33	1
86	OHX	5	3549	7/7	0.95	0.50	13.60	55,55,55,55	7
87	MG	M6	203	1/1	0.95	0.87	13.42	40,40,40,40	1
86	OHX	4	214	7/7	0.94	0.41	13.40	46,46,46,46	7
87	MG	n0	205	1/1	0.98	0.85	13.37	41,41,41,41	1
87	MG	6	2318	1/1	0.97	0.38	13.36	54,54,54,54	0
87	MG	6	2232	1/1	0.79	0.54	13.32	53,53,53,53	0
86	OHX	2	1985	7/7	0.98	0.35	13.29	59,59,59,59	7
87	MG	1	4315	1/1	0.98	0.46	13.26	35,35,35,35	1
86	OHX	1	3802	7/7	0.89	0.42	13.18	63,63,63,63	7
87	MG	1	4242	1/1	0.97	0.38	13.12	37,37,37,37	0
87	MG	5	4498	1/1	0.97	0.53	13.04	45,45,45,45	1
87	MG	1	4135	1/1	0.91	0.38	12.97	41,41,41,41	0
87	MG	5	4289	1/1	0.82	0.43	12.96	57,57,57,57	1
87	MG	1	4376	1/1	0.98	0.64	12.95	34,34,34,34	1
87	MG	L2	303	1/1	0.90	0.69	12.93	53,53,53,53	0
87	MG	5	4347	1/1	0.74	0.73	12.92	60,60,60,60	0
86	OHX	5	3542	7/7	0.92	0.35	12.91	84,84,84,84	7
86	OHX	5	3722	7/7	0.94	0.28	12.84	76,76,76,76	7
87	MG	M8	202	1/1	0.95	1.44	12.76	39,39,39,39	1
87	MG	7	227	1/1	0.92	1.31	12.70	50,50,50,50	1
86	OHX	5	3685	7/7	0.93	0.26	12.68	88,88,88,88	7
87	MG	5	4263	1/1	0.92	0.79	12.66	32,32,32,32	1
87	MG	5	4439	1/1	0.82	0.33	12.53	40,40,40,40	0
87	MG	1	3977	1/1	0.99	0.44	12.51	41,41,41,41	0
87	MG	5	4097	1/1	0.95	0.43	12.42	40,40,40,40	0
86	OHX	5	3674	7/7	0.94	0.40	12.37	39,39,39,39	7
87	MG	1	3932	1/1	0.96	0.49	12.27	28,28,28,28	0
87	MG	5	4284	1/1	0.97	0.30	12.23	44,44,44,44	1
87	MG	5	3891	1/1	0.97	0.53	12.22	39,39,39,39	0
87	MG	5	4200	1/1	0.94	0.52	12.20	43,43,43,43	1
87	MG	1	4160	1/1	0.94	0.44	12.20	46,46,46,46	0
86	OHX	1	3730	7/7	0.91	0.29	12.19	59,59,59,59	7
86	OHX	1	3774	7/7	0.79	0.39	12.18	53,53,53,53	7
86	OHX	6	2060	7/7	0.82	0.42	12.15	58,58,58,58	7
86	OHX	6	1993	7/7	0.80	0.34	12.14	78,78,78,78	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3977	1/1	0.92	0.56	12.14	55,55,55,55	0
87	MG	1	4007	1/1	0.95	0.49	12.08	46,46,46,46	0
86	OHX	5	3465	7/7	0.98	0.38	12.08	40,40,40,40	7
86	OHX	5	3756	7/7	0.79	0.36	12.07	42,42,42,42	7
87	MG	15	307	1/1	0.92	0.78	12.05	46,46,46,46	1
86	OHX	2	2029	7/7	0.89	0.33	12.01	95,95,95,95	7
86	OHX	1	3702	7/7	0.95	0.38	11.99	42,42,42,42	7
86	OHX	5	3681	7/7	0.93	0.45	11.94	80,80,80,80	7
87	MG	1	3886	1/1	0.92	0.34	11.93	39,39,39,39	0
87	MG	2	2151	1/1	0.93	0.52	11.88	58,58,58,58	0
87	MG	5	4491	1/1	0.98	0.61	11.86	35,35,35,35	1
87	MG	5	3835	1/1	0.83	0.46	11.84	37,37,37,37	0
87	MG	N0	201	1/1	0.97	1.23	11.80	49,49,49,49	1
87	MG	1	4020	1/1	0.96	0.49	11.79	32,32,32,32	0
87	MG	5	4030	1/1	0.94	0.48	11.78	34,34,34,34	0
86	OHX	5	3594	7/7	0.96	0.35	11.74	42,42,42,42	7
87	MG	6	2159	1/1	0.92	0.53	11.73	45,45,45,45	0
87	MG	1	3976	1/1	0.92	0.45	11.72	44,44,44,44	0
86	OHX	6	2068	7/7	0.86	0.37	11.65	83,83,83,83	7
87	MG	1	4134	1/1	0.40	1.23	11.63	49,49,49,49	1
87	MG	5	3980	1/1	0.90	0.45	11.61	58,58,58,58	0
86	OHX	6	2003	7/7	0.93	0.35	11.55	61,61,61,61	7
87	MG	1	4025	1/1	0.97	0.45	11.46	39,39,39,39	0
87	MG	1	3929	1/1	0.94	0.56	11.41	40,40,40,40	0
86	OHX	6	2036	7/7	0.75	0.40	11.40	48,48,48,48	7
87	MG	1	4210	1/1	0.98	0.54	11.37	47,47,47,47	0
87	MG	6	2221	1/1	0.91	0.31	11.35	53,53,53,53	1
86	OHX	5	3753	7/7	0.95	0.28	11.25	49,49,49,49	7
87	MG	M6	202	1/1	0.99	0.78	11.23	41,41,41,41	1
86	OHX	1	3737	7/7	0.80	0.38	11.22	42,42,42,42	7
87	MG	1	4250	1/1	0.96	0.44	11.16	53,53,53,53	1
86	OHX	6	1985	7/7	0.95	0.24	11.09	90,90,90,90	7
87	MG	o4	201	1/1	0.94	1.40	11.04	70,70,70,70	1
86	OHX	5	3633	7/7	0.93	0.40	11.01	43,43,43,43	7
86	OHX	1	3656	7/7	0.95	0.36	10.98	69,69,69,69	7
87	MG	M6	204	1/1	0.67	0.51	10.89	39,39,39,39	1
87	MG	5	4370	1/1	0.96	1.03	10.81	47,47,47,47	1
87	MG	n9	103	1/1	0.98	0.83	10.81	40,40,40,40	1
87	MG	5	4026	1/1	0.97	0.50	10.79	37,37,37,37	0
87	MG	1	4174	1/1	0.96	0.35	10.78	35,35,35,35	0
87	MG	1	4393	1/1	0.87	0.24	10.75	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4403	1/1	0.98	0.35	10.73	40,40,40,40	1
86	OHX	6	2018	7/7	0.95	0.40	10.67	54,54,54,54	7
86	OHX	5	3745	7/7	0.90	0.47	10.65	37,37,37,37	7
87	MG	O3	203	1/1	0.87	0.60	10.63	47,47,47,47	1
87	MG	l5	308	1/1	0.96	1.26	10.62	49,49,49,49	1
87	MG	M0	308	1/1	0.98	0.80	10.60	44,44,44,44	1
87	MG	1	3822	1/1	0.90	0.38	10.60	34,34,34,34	0
87	MG	1	3924	1/1	0.95	0.51	10.57	36,36,36,36	0
87	MG	2	2206	1/1	0.93	0.27	10.51	58,58,58,58	0
87	MG	5	4247	1/1	0.95	0.48	10.50	37,37,37,37	0
86	OHX	5	3509	7/7	0.95	0.23	10.48	66,66,66,66	7
87	MG	5	4452	1/1	0.88	1.04	10.48	38,38,38,38	1
87	MG	m7	206	1/1	0.77	0.48	10.47	35,35,35,35	0
87	MG	5	4348	1/1	0.86	1.51	10.47	46,46,46,46	1
87	MG	1	4208	1/1	0.93	0.79	10.37	47,47,47,47	1
86	OHX	o9	101	7/7	0.87	0.45	10.36	52,52,52,52	7
87	MG	5	4384	1/1	0.97	0.38	10.32	34,34,34,34	1
87	MG	5	4362	1/1	0.92	0.50	10.28	49,49,49,49	1
87	MG	1	4200	1/1	0.78	0.39	10.23	51,51,51,51	0
87	MG	l3	411	1/1	0.93	0.51	10.21	33,33,33,33	1
87	MG	5	4344	1/1	0.90	0.46	10.17	35,35,35,35	1
87	MG	1	4507	1/1	0.95	0.68	10.14	36,36,36,36	1
87	MG	6	2127	1/1	0.95	0.33	10.13	45,45,45,45	0
87	MG	l2	304	1/1	0.97	0.72	10.11	44,44,44,44	1
87	MG	2	2157	1/1	0.91	0.37	10.10	103,103,103,103	0
87	MG	1	4437	1/1	0.94	0.47	10.04	39,39,39,39	1
87	MG	5	3822	1/1	0.87	0.32	10.04	48,48,48,48	0
87	MG	5	4142	1/1	0.80	0.33	10.03	40,40,40,40	0
87	MG	O5	202	1/1	0.97	0.76	10.01	54,54,54,54	1
87	MG	1	3889	1/1	0.99	0.35	10.00	37,37,37,37	0
87	MG	6	2251	1/1	0.85	0.42	9.93	74,74,74,74	0
87	MG	1	4385	1/1	0.96	0.37	9.92	32,32,32,32	1
86	OHX	5	3658	7/7	0.82	0.48	9.85	51,51,51,51	7
87	MG	1	3824	1/1	0.95	0.32	9.84	55,55,55,55	0
87	MG	1	3908	1/1	0.97	0.41	9.82	43,43,43,43	0
86	OHX	2	2088	7/7	0.98	0.26	9.80	94,94,94,94	7
87	MG	5	3899	1/1	0.97	0.38	9.80	32,32,32,32	0
87	MG	1	4268	1/1	0.96	0.42	9.78	32,32,32,32	0
86	OHX	5	3529	7/7	0.98	0.26	9.73	51,51,51,51	7
87	MG	1	4317	1/1	0.94	0.84	9.70	38,38,38,38	1
87	MG	1	3966	1/1	0.95	0.40	9.70	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	l3	406	1/1	0.96	0.55	9.69	31,31,31,31	1
86	OHX	4	212	7/7	0.91	0.34	9.69	42,42,42,42	7
87	MG	7	239	1/1	0.96	0.80	9.69	50,50,50,50	1
86	OHX	5	3703	7/7	0.76	0.31	9.64	86,86,86,86	7
87	MG	Q0	202	1/1	0.79	0.90	9.63	54,54,54,54	0
87	MG	o7	504	1/1	0.96	0.48	9.55	37,37,37,37	1
86	OHX	5	3602	7/7	0.97	0.30	9.47	86,86,86,86	7
86	OHX	5	3716	7/7	0.98	0.31	9.45	60,60,60,60	7
87	MG	l7	303	1/1	0.94	0.26	9.44	34,34,34,34	1
87	MG	N1	201	1/1	0.96	0.52	9.43	42,42,42,42	1
87	MG	1	4411	1/1	0.95	0.38	9.43	42,42,42,42	1
87	MG	5	4501	1/1	0.94	0.41	9.42	33,33,33,33	1
87	MG	1	4091	1/1	0.97	0.38	9.41	39,39,39,39	0
86	OHX	1	3598	7/7	0.97	0.31	9.41	100,100,100,100	7
87	MG	6	2229	1/1	0.81	0.38	9.41	45,45,45,45	0
87	MG	1	4341	1/1	0.94	0.70	9.38	38,38,38,38	1
87	MG	5	3859	1/1	0.94	0.42	9.36	32,32,32,32	0
86	OHX	1	3739	7/7	0.83	0.44	9.35	52,52,52,52	7
87	MG	N8	207	1/1	0.97	1.16	9.32	39,39,39,39	1
87	MG	5	4361	1/1	0.89	0.70	9.29	37,37,37,37	1
87	MG	6	2211	1/1	0.91	0.38	9.27	50,50,50,50	0
87	MG	m7	204	1/1	0.89	0.58	9.24	40,40,40,40	1
86	OHX	2	2069	7/7	0.96	0.25	9.19	78,78,78,78	7
87	MG	q2	503	1/1	0.95	0.74	9.17	42,42,42,42	1
87	MG	5	4550	1/1	0.84	0.98	9.17	49,49,49,49	1
87	MG	5	3997	1/1	0.99	0.32	9.16	31,31,31,31	0
87	MG	M3	203	1/1	0.97	0.69	9.14	46,46,46,46	1
87	MG	6	2239	1/1	0.89	0.29	9.14	56,56,56,56	1
86	OHX	1	3443	7/7	0.99	0.26	9.09	61,61,61,61	7
87	MG	m6	202	1/1	0.88	0.65	9.03	36,36,36,36	1
87	MG	1	3982	1/1	0.99	0.36	9.01	31,31,31,31	0
87	MG	l7	301	1/1	0.23	0.74	9.01	36,36,36,36	1
87	MG	1	4505	1/1	0.86	0.48	8.95	51,51,51,51	0
87	MG	5	3882	1/1	0.92	0.41	8.91	37,37,37,37	0
86	OHX	5	3808	7/7	0.92	0.34	8.90	83,83,83,83	7
87	MG	l3	413	1/1	0.95	0.72	8.83	32,32,32,32	1
87	MG	O1	203	1/1	0.83	1.06	8.78	57,57,57,57	0
87	MG	m7	202	1/1	0.84	0.53	8.78	36,36,36,36	0
87	MG	5	4027	1/1	0.88	0.42	8.77	41,41,41,41	0
86	OHX	1	3635	7/7	0.95	0.33	8.77	45,45,45,45	7
86	OHX	5	3610	7/7	0.96	0.50	8.71	60,60,60,60	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3583	7/7	0.96	0.34	8.69	54,54,54,54	7
86	OHX	6	2015	7/7	0.96	0.32	8.67	65,65,65,65	7
87	MG	1	4215	1/1	0.80	0.34	8.67	37,37,37,37	0
87	MG	5	4127	1/1	0.93	0.52	8.64	44,44,44,44	1
87	MG	5	4429	1/1	0.97	0.30	8.64	37,37,37,37	1
87	MG	N0	202	1/1	0.66	0.74	8.64	51,51,51,51	1
86	OHX	6	2082	7/7	0.97	0.27	8.63	54,54,54,54	7
87	MG	5	4504	1/1	0.97	0.67	8.60	39,39,39,39	1
87	MG	5	4290	1/1	0.86	0.42	8.60	72,72,72,72	0
87	MG	C1	201	1/1	0.99	1.02	8.59	69,69,69,69	0
86	OHX	5	3491	7/7	0.98	0.32	8.58	51,51,51,51	7
87	MG	8	222	1/1	0.94	0.37	8.58	41,41,41,41	0
87	MG	N8	202	1/1	0.90	1.02	8.55	37,37,37,37	0
87	MG	M3	202	1/1	1.00	0.53	8.53	49,49,49,49	1
86	OHX	6	2028	7/7	0.82	0.38	8.50	58,58,58,58	7
87	MG	5	3928	1/1	0.99	0.29	8.41	38,38,38,38	0
86	OHX	1	3790	7/7	0.89	0.32	8.41	69,69,69,69	7
86	OHX	2	2080	7/7	0.86	0.32	8.41	66,66,66,66	7
86	OHX	5	3749	7/7	0.95	0.37	8.38	39,39,39,39	7
87	MG	S8	302	1/1	0.86	1.01	8.37	69,69,69,69	1
87	MG	5	4453	1/1	0.99	0.44	8.36	33,33,33,33	1
87	MG	O7	107	1/1	0.94	0.60	8.35	42,42,42,42	1
87	MG	5	3876	1/1	0.96	0.36	8.32	33,33,33,33	0
86	OHX	2	1933	7/7	0.96	0.28	8.32	71,71,71,71	7
87	MG	5	4040	1/1	0.92	0.32	8.29	35,35,35,35	0
86	OHX	5	3543	7/7	0.97	0.37	8.23	60,60,60,60	7
87	MG	1	3934	1/1	0.96	0.36	8.22	40,40,40,40	0
87	MG	1	4116	1/1	0.92	0.37	8.20	36,36,36,36	0
87	MG	1	4012	1/1	0.93	0.41	8.14	35,35,35,35	0
87	MG	l7	302	1/1	0.96	0.61	8.12	35,35,35,35	1
87	MG	2	2144	1/1	0.90	0.31	8.09	66,66,66,66	0
87	MG	5	4159	1/1	0.94	0.36	8.09	37,37,37,37	0
87	MG	N9	102	1/1	0.89	0.32	8.08	38,38,38,38	0
86	OHX	1	3748	7/7	0.96	0.24	8.06	89,89,89,89	7
87	MG	5	3956	1/1	0.85	0.35	8.02	47,47,47,47	0
86	OHX	5	3487	7/7	0.98	0.34	7.99	48,48,48,48	7
86	OHX	1	3661	7/7	0.95	0.34	7.99	45,45,45,45	7
87	MG	1	4060	1/1	0.86	0.32	7.99	44,44,44,44	0
87	MG	1	3999	1/1	0.97	0.50	7.98	32,32,32,32	0
87	MG	5	4409	1/1	0.97	0.33	7.95	39,39,39,39	0
87	MG	5	4459	1/1	0.91	0.34	7.94	36,36,36,36	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3680	7/7	0.97	0.34	7.92	38,38,38,38	7
87	MG	5	3898	1/1	0.96	0.37	7.92	39,39,39,39	0
87	MG	1	3983	1/1	0.98	0.36	7.90	40,40,40,40	0
86	OHX	6	2054	7/7	0.91	0.28	7.90	65,65,65,65	7
87	MG	6	2185	1/1	0.98	0.31	7.86	44,44,44,44	0
87	MG	M8	204	1/1	0.98	0.73	7.84	46,46,46,46	1
87	MG	M7	204	1/1	0.86	0.51	7.79	40,40,40,40	0
86	OHX	2	2030	7/7	0.78	0.43	7.78	112,112,112,112	7
86	OHX	5	3608	7/7	0.96	0.35	7.78	44,44,44,44	7
86	OHX	2	2055	7/7	0.88	0.35	7.75	72,72,72,72	7
86	OHX	5	3653	7/7	0.97	0.28	7.74	64,64,64,64	7
87	MG	5	4275	1/1	0.88	0.46	7.69	36,36,36,36	1
87	MG	2	2199	1/1	0.96	0.36	7.69	81,81,81,81	0
86	OHX	1	3505	7/7	0.96	0.29	7.69	50,50,50,50	7
86	OHX	1	3669	7/7	0.96	0.40	7.68	54,54,54,54	7
86	OHX	2	2002	7/7	0.94	0.29	7.67	86,86,86,86	7
87	MG	5	4443	1/1	0.99	0.36	7.67	32,32,32,32	0
86	OHX	5	3568	7/7	0.96	0.32	7.67	53,53,53,53	7
86	OHX	5	3655	7/7	0.90	0.31	7.66	47,47,47,47	7
86	OHX	6	2085	7/7	0.85	0.41	7.61	128,128,128,128	7
86	OHX	5	3579	7/7	0.94	0.26	7.61	55,55,55,55	7
87	MG	5	4487	1/1	0.85	0.35	7.54	37,37,37,37	0
87	MG	1	4397	1/1	0.96	0.40	7.54	38,38,38,38	1
87	MG	m9	202	1/1	0.96	0.69	7.51	54,54,54,54	1
86	OHX	5	3434	7/7	0.98	0.31	7.45	38,38,38,38	7
86	OHX	1	3436	7/7	0.98	0.34	7.42	46,46,46,46	7
87	MG	6	2246	1/1	0.94	0.33	7.40	50,50,50,50	1
86	OHX	5	3649	7/7	0.86	0.37	7.36	41,41,41,41	7
86	OHX	5	3620	7/7	0.95	0.34	7.35	42,42,42,42	7
87	MG	5	4170	1/1	0.86	0.57	7.33	36,36,36,36	1
86	OHX	m0	304	7/7	0.96	0.34	7.33	43,43,43,43	7
87	MG	5	4566	1/1	0.81	0.32	7.31	40,40,40,40	0
87	MG	4	238	1/1	0.72	0.31	7.30	59,59,59,59	0
87	MG	C1	202	1/1	0.94	1.17	7.29	72,72,72,72	1
86	OHX	1	3798	7/7	0.95	0.27	7.28	93,93,93,93	7
87	MG	5	4401	1/1	0.84	0.34	7.27	48,48,48,48	0
87	MG	5	3861	1/1	0.96	0.35	7.27	36,36,36,36	0
87	MG	1	4291	1/1	0.95	0.53	7.27	41,41,41,41	0
86	OHX	1	3546	7/7	0.95	0.27	7.23	52,52,52,52	7
86	OHX	5	3569	7/7	0.97	0.27	7.20	78,78,78,78	7
86	OHX	1	3418	7/7	0.99	0.28	7.20	49,49,49,49	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3545	7/7	0.94	0.25	7.20	91,91,91,91	7
86	OHX	1	3570	7/7	0.97	0.28	7.17	41,41,41,41	7
87	MG	5	4390	1/1	0.94	0.42	7.16	39,39,39,39	1
86	OHX	1	3627	7/7	0.95	0.38	7.16	45,45,45,45	7
87	MG	5	4237	1/1	0.96	0.46	7.12	36,36,36,36	1
86	OHX	1	3745	7/7	0.89	0.25	7.09	72,72,72,72	7
86	OHX	1	3544	7/7	0.98	0.29	7.08	52,52,52,52	7
86	OHX	3	203	7/7	0.98	0.26	7.06	56,56,56,56	7
86	OHX	6	1995	7/7	0.97	0.24	7.03	113,113,113,113	7
87	MG	2	2135	1/1	0.48	0.40	7.01	72,72,72,72	0
87	MG	1	3904	1/1	0.96	0.28	6.97	42,42,42,42	0
86	OHX	6	1989	7/7	0.90	0.30	6.91	84,84,84,84	7
86	OHX	2	2009	7/7	0.97	0.33	6.90	70,70,70,70	7
87	MG	1	4391	1/1	0.86	0.54	6.89	37,37,37,37	1
87	MG	1	4009	1/1	0.94	0.61	6.88	48,48,48,48	0
87	MG	n8	207	1/1	0.98	0.76	6.77	39,39,39,39	1
87	MG	2	2210	1/1	0.85	0.34	6.75	69,69,69,69	0
87	MG	8	231	1/1	0.83	0.54	6.74	50,50,50,50	0
87	MG	M8	203	1/1	0.98	0.76	6.73	41,41,41,41	0
87	MG	2	2139	1/1	0.80	0.44	6.73	70,70,70,70	0
87	MG	4	239	1/1	0.99	0.60	6.72	40,40,40,40	1
87	MG	1	4243	1/1	0.92	0.28	6.70	45,45,45,45	0
87	MG	1	4059	1/1	0.99	0.27	6.70	38,38,38,38	0
87	MG	5	4341	1/1	0.99	0.67	6.68	46,46,46,46	0
87	MG	6	2310	1/1	0.97	0.79	6.68	48,48,48,48	1
87	MG	5	4053	1/1	0.90	0.47	6.67	44,44,44,44	0
86	OHX	5	3600	7/7	0.97	0.28	6.67	57,57,57,57	7
87	MG	L4	406	1/1	0.96	0.67	6.66	38,38,38,38	1
87	MG	5	4245	1/1	0.79	0.29	6.64	65,65,65,65	0
87	MG	6	2209	1/1	0.93	0.29	6.62	46,46,46,46	0
87	MG	5	4191	1/1	0.93	0.38	6.59	44,44,44,44	1
87	MG	l3	410	1/1	0.99	0.58	6.58	31,31,31,31	1
87	MG	5	4427	1/1	0.91	0.52	6.56	39,39,39,39	1
87	MG	l2	307	1/1	0.96	0.92	6.52	46,46,46,46	1
86	OHX	1	3759	7/7	0.88	0.27	6.52	45,45,45,45	7
86	OHX	1	3474	7/7	0.98	0.36	6.49	90,90,90,90	7
87	MG	M5	302	1/1	0.99	0.58	6.47	42,42,42,42	1
87	MG	O1	206	1/1	0.99	0.61	6.45	59,59,59,59	1
86	OHX	1	3728	7/7	0.89	0.32	6.44	37,37,37,37	7
87	MG	1	4366	1/1	0.99	0.41	6.41	42,42,42,42	1
86	OHX	1	3734	7/7	0.97	0.24	6.40	52,52,52,52	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4024	1/1	0.99	0.33	6.38	37,37,37,37	0
87	MG	5	4363	1/1	0.94	0.34	6.35	42,42,42,42	0
87	MG	2	2127	1/1	0.95	0.33	6.31	60,60,60,60	0
87	MG	1	4508	1/1	0.82	0.32	6.25	37,37,37,37	1
87	MG	1	4323	1/1	0.95	0.40	6.23	42,42,42,42	1
86	OHX	6	2006	7/7	0.98	0.27	6.23	54,54,54,54	7
87	MG	l3	404	1/1	0.87	0.39	6.19	33,33,33,33	0
86	OHX	1	3530	7/7	0.94	0.24	6.18	67,67,67,67	7
86	OHX	5	3638	7/7	0.95	0.34	6.17	73,73,73,73	7
87	MG	6	2131	1/1	0.94	0.35	6.16	53,53,53,53	0
86	OHX	6	1966	7/7	0.96	0.31	6.16	56,56,56,56	7
86	OHX	1	3671	7/7	0.93	0.32	6.14	85,85,85,85	7
87	MG	5	4520	1/1	0.86	0.39	6.11	43,43,43,43	0
87	MG	M5	303	1/1	0.98	0.73	6.05	41,41,41,41	1
91	PRO	5	3404	7/8	0.82	0.31	6.03	71,71,71,71	0
86	OHX	5	3527	7/7	0.96	0.25	6.02	49,49,49,49	7
87	MG	1	4480	1/1	0.86	0.65	6.00	48,48,48,48	0
87	MG	o2	203	1/1	0.96	0.36	5.99	34,34,34,34	1
86	OHX	5	3453	7/7	0.98	0.30	5.98	79,79,79,79	7
86	OHX	1	3738	7/7	0.93	0.27	5.98	68,68,68,68	7
86	OHX	5	3692	7/7	0.96	0.30	5.96	38,38,38,38	7
86	OHX	1	3733	7/7	0.83	0.40	5.95	46,46,46,46	7
86	OHX	5	3507	7/7	0.99	0.32	5.92	62,62,62,62	7
86	OHX	1	3652	7/7	0.98	0.32	5.92	58,58,58,58	7
86	OHX	8	208	7/7	0.96	0.23	5.91	63,63,63,63	7
87	MG	1	4212	1/1	0.98	0.31	5.89	41,41,41,41	1
86	OHX	1	3716	7/7	0.95	0.35	5.89	61,61,61,61	7
87	MG	n0	201	1/1	0.69	0.31	5.87	49,49,49,49	1
87	MG	5	4075	1/1	0.97	0.29	5.87	36,36,36,36	0
87	MG	5	4316	1/1	0.65	0.36	5.85	74,74,74,74	0
86	OHX	5	3709	7/7	0.83	0.27	5.85	41,41,41,41	7
86	OHX	5	3728	7/7	0.87	0.37	5.83	57,57,57,57	7
86	OHX	6	2019	7/7	0.97	0.28	5.83	55,55,55,55	7
87	MG	5	4154	1/1	0.88	0.28	5.82	44,44,44,44	0
87	MG	5	4372	1/1	0.95	0.39	5.82	38,38,38,38	1
87	MG	m8	1504	1/1	0.96	0.94	5.82	42,42,42,42	1
86	OHX	5	3561	7/7	0.97	0.31	5.78	51,51,51,51	7
86	OHX	5	3587	7/7	0.92	0.30	5.78	53,53,53,53	7
87	MG	6	2248	1/1	0.86	0.36	5.76	53,53,53,53	0
86	OHX	7	205	7/7	0.99	0.22	5.76	68,68,68,68	7
87	MG	1	4140	1/1	0.89	0.35	5.72	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4362	1/1	0.99	0.27	5.70	42,42,42,42	0
87	MG	5	3844	1/1	0.94	0.25	5.70	36,36,36,36	0
87	MG	5	4115	1/1	0.85	0.36	5.66	35,35,35,35	0
86	OHX	6	2095	7/7	0.85	0.38	5.66	73,73,73,73	7
87	MG	5	3982	1/1	0.83	0.32	5.63	57,57,57,57	0
86	OHX	5	3786	7/7	0.94	0.33	5.63	42,42,42,42	7
86	OHX	2	2089	7/7	0.85	0.28	5.61	121,121,121,121	7
87	MG	5	4405	1/1	0.93	0.79	5.60	70,70,70,70	1
86	OHX	1	3593	7/7	0.97	0.27	5.60	56,56,56,56	7
87	MG	1	3931	1/1	0.95	0.42	5.58	41,41,41,41	0
86	OHX	2	2021	7/7	0.92	0.30	5.57	72,72,72,72	7
86	OHX	5	3735	7/7	0.94	0.26	5.53	62,62,62,62	7
86	OHX	5	3790	7/7	0.84	0.38	5.52	40,40,40,40	7
86	OHX	1	3495	7/7	0.98	0.26	5.52	44,44,44,44	7
86	OHX	5	3724	7/7	0.95	0.28	5.51	58,58,58,58	7
86	OHX	5	3742	7/7	0.86	0.33	5.45	49,49,49,49	7
87	MG	2	2186	1/1	0.94	0.29	5.45	65,65,65,65	0
87	MG	1	4157	1/1	0.84	0.34	5.44	42,42,42,42	0
87	MG	5	3863	1/1	0.94	0.34	5.43	35,35,35,35	0
87	MG	L4	405	1/1	0.98	0.36	5.43	38,38,38,38	1
87	MG	O7	109	1/1	0.97	0.59	5.42	46,46,46,46	1
87	MG	6	2329	1/1	0.69	0.43	5.42	48,48,48,48	0
87	MG	1	3909	1/1	0.99	0.32	5.41	43,43,43,43	0
87	MG	1	3959	1/1	0.86	0.36	5.40	55,55,55,55	0
87	MG	L4	407	1/1	0.97	0.46	5.39	55,55,55,55	1
86	OHX	2	1936	7/7	0.98	0.27	5.33	72,72,72,72	7
86	OHX	6	1929	7/7	0.99	0.29	5.32	53,53,53,53	7
86	OHX	8	210	7/7	0.98	0.31	5.31	49,49,49,49	7
87	MG	6	2316	1/1	0.95	0.31	5.29	60,60,60,60	1
86	OHX	5	3626	7/7	0.96	0.27	5.28	69,69,69,69	7
86	OHX	6	1961	7/7	0.96	0.33	5.26	65,65,65,65	7
87	MG	4	232	1/1	0.73	0.35	5.22	42,42,42,42	0
86	OHX	8	213	7/7	0.87	0.27	5.22	77,77,77,77	7
87	MG	5	4232	1/1	0.96	0.67	5.20	35,35,35,35	1
87	MG	5	4436	1/1	0.89	0.33	5.18	39,39,39,39	0
87	MG	s8	304	1/1	0.62	0.50	5.17	56,56,56,56	0
86	OHX	1	3422	7/7	0.98	0.30	5.16	56,56,56,56	7
86	OHX	2	2063	7/7	0.86	0.33	5.16	81,81,81,81	7
86	OHX	4	218	7/7	0.93	0.27	5.15	51,51,51,51	7
87	MG	1	4451	1/1	0.96	0.55	5.15	58,58,58,58	1
87	MG	L2	302	1/1	0.99	0.62	5.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	m7	208	1/1	0.98	0.57	5.14	40,40,40,40	1
87	MG	1	3828	1/1	0.97	0.44	5.14	40,40,40,40	0
86	OHX	2	2005	7/7	0.95	0.34	5.12	86,86,86,86	7
86	OHX	1	3466	7/7	0.98	0.25	5.11	45,45,45,45	7
86	OHX	6	2088	7/7	0.97	0.27	5.09	71,71,71,71	7
86	OHX	5	3504	7/7	0.98	0.23	5.08	75,75,75,75	7
90	8AN	5	3403	22/23	0.84	0.29	5.07	42,97,101,102	0
86	OHX	1	3502	7/7	0.97	0.26	5.07	63,63,63,63	7
87	MG	1	3830	1/1	0.93	0.41	5.06	40,40,40,40	0
87	MG	1	4378	1/1	0.80	0.39	5.04	41,41,41,41	1
87	MG	6	2110	1/1	0.93	0.26	5.00	82,82,82,82	0
87	MG	n1	203	1/1	0.98	0.45	5.00	37,37,37,37	1
87	MG	6	2313	1/1	0.85	0.27	4.98	71,71,71,71	0
87	MG	5	4365	1/1	0.88	0.33	4.97	45,45,45,45	0
86	OHX	1	3803	7/7	0.93	0.30	4.96	48,48,48,48	7
87	MG	5	4236	1/1	0.93	0.30	4.96	42,42,42,42	0
86	OHX	1	3609	7/7	0.98	0.29	4.94	49,49,49,49	7
87	MG	s8	303	1/1	0.79	0.39	4.93	46,46,46,46	0
87	MG	2	2100	1/1	0.97	0.34	4.93	66,66,66,66	0
86	OHX	1	3760	7/7	0.94	0.34	4.93	52,52,52,52	7
86	OHX	1	3451	7/7	0.96	0.31	4.92	77,77,77,77	7
86	OHX	1	3793	7/7	0.94	0.30	4.91	46,46,46,46	7
87	MG	1	3993	1/1	0.89	0.29	4.89	28,28,28,28	0
87	MG	O1	202	1/1	0.94	0.80	4.88	60,60,60,60	1
86	OHX	2	2085	7/7	0.90	0.32	4.86	93,93,93,93	7
86	OHX	5	3458	7/7	0.99	0.30	4.84	42,42,42,42	7
86	OHX	5	3616	7/7	0.98	0.34	4.84	46,46,46,46	7
86	OHX	5	3672	7/7	0.95	0.27	4.83	71,71,71,71	7
87	MG	1	4340	1/1	0.92	0.35	4.78	49,49,49,49	1
86	OHX	1	3779	7/7	0.97	0.25	4.78	50,50,50,50	7
86	OHX	1	3452	7/7	0.98	0.26	4.77	70,70,70,70	7
87	MG	1	3891	1/1	0.90	0.30	4.75	45,45,45,45	0
86	OHX	5	3452	7/7	0.98	0.30	4.74	70,70,70,70	7
86	OHX	6	1945	7/7	0.98	0.28	4.74	58,58,58,58	7
87	MG	L7	302	1/1	0.89	0.62	4.72	44,44,44,44	0
86	OHX	8	216	7/7	0.88	0.26	4.71	67,67,67,67	7
86	OHX	6	2044	7/7	0.91	0.28	4.71	78,78,78,78	7
86	OHX	3	202	7/7	0.98	0.27	4.70	48,48,48,48	7
86	OHX	4	209	7/7	0.98	0.27	4.67	45,45,45,45	7
87	MG	5	4357	1/1	0.99	0.33	4.66	36,36,36,36	1
86	OHX	5	3798	7/7	0.89	0.30	4.66	73,73,73,73	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3474	7/7	0.97	0.20	4.66	78,78,78,78	7
86	OHX	7	211	7/7	0.97	0.26	4.64	52,52,52,52	7
87	MG	5	4105	1/1	0.99	0.28	4.61	38,38,38,38	0
87	MG	1	4387	1/1	0.99	0.35	4.59	51,51,51,51	1
87	MG	5	4025	1/1	0.96	0.44	4.58	32,32,32,32	0
87	MG	1	3854	1/1	0.94	0.28	4.54	48,48,48,48	0
86	OHX	5	3694	7/7	0.95	0.27	4.54	55,55,55,55	7
86	OHX	1	3547	7/7	0.97	0.34	4.53	56,56,56,56	7
87	MG	7	229	1/1	0.81	0.31	4.50	38,38,38,38	0
87	MG	5	4326	1/1	0.95	0.32	4.48	53,53,53,53	0
86	OHX	5	3555	7/7	0.96	0.27	4.48	60,60,60,60	7
87	MG	L3	406	1/1	0.98	0.40	4.48	39,39,39,39	1
86	OHX	5	3490	7/7	0.98	0.29	4.47	50,50,50,50	7
86	OHX	5	3539	7/7	0.96	0.28	4.47	54,54,54,54	7
87	MG	n8	204	1/1	0.97	0.54	4.46	55,55,55,55	1
86	OHX	2	2032	7/7	0.91	0.26	4.44	82,82,82,82	7
87	MG	1	3911	1/1	0.96	0.33	4.44	40,40,40,40	0
87	MG	5	4483	1/1	0.95	0.26	4.42	34,34,34,34	1
87	MG	1	4050	1/1	0.90	0.40	4.42	35,35,35,35	0
86	OHX	5	3772	7/7	0.82	0.39	4.39	115,115,115,115	7
86	OHX	1	3659	7/7	0.93	0.28	4.37	48,48,48,48	7
87	MG	5	3981	1/1	0.90	0.47	4.36	50,50,50,50	0
87	MG	5	4041	1/1	0.72	0.34	4.36	51,51,51,51	0
86	OHX	5	3557	7/7	0.96	0.24	4.36	49,49,49,49	7
86	OHX	1	3643	7/7	0.98	0.24	4.33	52,52,52,52	7
86	OHX	5	3444	7/7	0.99	0.27	4.32	70,70,70,70	7
87	MG	q1	103	1/1	0.96	0.43	4.32	46,46,46,46	1
86	OHX	7	213	7/7	0.84	0.28	4.31	56,56,56,56	7
86	OHX	1	3633	7/7	0.97	0.26	4.27	79,79,79,79	7
87	MG	1	4061	1/1	0.91	0.31	4.27	32,32,32,32	0
87	MG	5	4000	1/1	0.99	0.32	4.26	34,34,34,34	0
86	OHX	5	3618	7/7	0.98	0.29	4.25	52,52,52,52	7
86	OHX	5	3789	7/7	0.86	0.37	4.24	90,90,90,90	7
87	MG	1	4201	1/1	0.98	0.28	4.23	38,38,38,38	0
86	OHX	1	3486	7/7	0.98	0.24	4.21	65,65,65,65	7
86	OHX	5	3520	7/7	0.98	0.28	4.20	42,42,42,42	7
87	MG	l7	305	1/1	0.97	0.45	4.19	40,40,40,40	0
87	MG	n8	201	1/1	0.96	0.37	4.18	33,33,33,33	0
87	MG	1	4017	1/1	0.97	0.40	4.18	35,35,35,35	0
86	OHX	5	3687	7/7	0.96	0.28	4.15	46,46,46,46	7
87	MG	6	2173	1/1	0.93	0.42	4.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2061	7/7	0.97	0.22	4.13	102,102,102,102	7
87	MG	1	4206	1/1	0.85	0.20	4.13	48,48,48,48	0
87	MG	5	3926	1/1	0.94	0.26	4.12	65,65,65,65	0
86	OHX	6	1953	7/7	0.96	0.20	4.09	137,137,137,137	7
86	OHX	5	3531	7/7	0.95	0.24	4.09	57,57,57,57	7
86	OHX	6	2008	7/7	0.93	0.27	4.08	82,82,82,82	7
86	OHX	5	3417	7/7	0.99	0.20	4.07	63,63,63,63	0
87	MG	5	4118	1/1	0.97	0.40	4.05	32,32,32,32	1
87	MG	5	4047	1/1	0.88	0.47	4.04	40,40,40,40	1
87	MG	4	244	1/1	0.80	0.43	4.04	41,41,41,41	1
86	OHX	6	2096	7/7	0.80	0.29	4.03	78,78,78,78	7
86	OHX	6	2084	7/7	0.98	0.20	4.02	79,79,79,79	7
87	MG	5	4514	1/1	0.98	0.37	4.01	30,30,30,30	1
86	OHX	6	2023	7/7	0.88	0.23	3.99	80,80,80,80	7
87	MG	1	4225	1/1	0.90	0.43	3.99	37,37,37,37	1
87	MG	M7	209	1/1	0.99	0.35	3.98	42,42,42,42	0
87	MG	5	4089	1/1	0.97	0.25	3.96	37,37,37,37	0
87	MG	5	4266	1/1	0.99	0.24	3.96	42,42,42,42	1
86	OHX	1	3531	7/7	0.98	0.24	3.94	49,49,49,49	7
87	MG	l3	407	1/1	0.92	0.40	3.92	38,38,38,38	1
86	OHX	n3	202	7/7	0.89	0.45	3.90	44,44,44,44	7
87	MG	5	3833	1/1	0.98	0.34	3.90	59,59,59,59	0
86	OHX	1	3532	7/7	0.97	0.26	3.89	59,59,59,59	7
87	MG	2	2130	1/1	0.91	0.36	3.89	75,75,75,75	0
86	OHX	1	3747	7/7	0.85	0.33	3.87	46,46,46,46	7
86	OHX	6	1939	7/7	0.98	0.22	3.82	103,103,103,103	7
86	OHX	6	2072	7/7	0.87	0.32	3.81	66,66,66,66	7
87	MG	l3	412	1/1	0.92	0.42	3.81	34,34,34,34	0
86	OHX	6	2093	7/7	0.87	0.30	3.81	83,83,83,83	7
87	MG	2	2103	1/1	0.82	0.24	3.80	65,65,65,65	0
87	MG	c7	201	1/1	0.97	0.52	3.80	81,81,81,81	1
87	MG	1	4040	1/1	0.96	0.31	3.79	47,47,47,47	0
87	MG	5	4447	1/1	0.99	0.31	3.79	34,34,34,34	1
86	OHX	5	3657	7/7	0.97	0.26	3.79	41,41,41,41	7
86	OHX	4	213	7/7	0.93	0.22	3.77	64,64,64,64	7
87	MG	1	4485	1/1	0.88	0.45	3.72	63,63,63,63	0
87	MG	2	2197	1/1	0.84	0.40	3.71	76,76,76,76	0
87	MG	1	4273	1/1	0.98	0.42	3.68	45,45,45,45	1
87	MG	1	4257	1/1	0.98	0.41	3.68	44,44,44,44	1
86	OHX	5	3445	7/7	0.99	0.23	3.67	63,63,63,63	7
87	MG	5	3922	1/1	1.00	0.44	3.67	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4202	1/1	0.93	0.29	3.67	59,59,59,59	1
86	OHX	6	2029	7/7	0.95	0.23	3.64	82,82,82,82	7
86	OHX	5	3702	7/7	0.86	0.27	3.64	86,86,86,86	7
86	OHX	2	2079	7/7	0.85	0.32	3.62	103,103,103,103	7
87	MG	5	4133	1/1	0.77	0.23	3.60	57,57,57,57	0
86	OHX	1	3550	7/7	0.98	0.20	3.60	55,55,55,55	7
86	OHX	m0	302	7/7	0.98	0.47	3.59	45,45,45,45	7
86	OHX	2	2077	7/7	0.84	0.27	3.58	139,139,139,139	7
86	OHX	1	3708	7/7	0.88	0.28	3.57	103,103,103,103	7
86	OHX	5	3492	7/7	0.97	0.27	3.55	42,42,42,42	7
86	OHX	5	3597	7/7	0.98	0.27	3.55	46,46,46,46	7
86	OHX	1	3684	7/7	0.88	0.30	3.54	81,81,81,81	7
87	MG	5	4218	1/1	0.83	0.24	3.50	41,41,41,41	0
86	OHX	5	3448	7/7	0.99	0.26	3.48	46,46,46,46	7
86	OHX	1	3534	7/7	0.96	0.29	3.47	65,65,65,65	7
87	MG	2	2250	1/1	0.96	0.22	3.47	79,79,79,79	0
86	OHX	6	2077	7/7	0.80	0.28	3.47	85,85,85,85	7
86	OHX	1	3464	7/7	0.99	0.33	3.46	50,50,50,50	7
86	OHX	5	3705	7/7	0.95	0.27	3.45	46,46,46,46	7
87	MG	5	4250	1/1	0.86	0.23	3.45	58,58,58,58	0
87	MG	2	2149	1/1	0.77	0.25	3.45	92,92,92,92	0
87	MG	12	302	1/1	0.88	0.45	3.44	36,36,36,36	0
86	OHX	4	216	7/7	0.91	0.25	3.44	73,73,73,73	7
86	OHX	5	3503	7/7	0.99	0.20	3.44	104,104,104,104	7
87	MG	5	4294	1/1	0.93	0.27	3.42	39,39,39,39	0
86	OHX	5	3572	7/7	0.98	0.21	3.41	66,66,66,66	7
87	MG	5	3846	1/1	0.96	0.31	3.40	43,43,43,43	0
86	OHX	2	1938	7/7	0.97	0.28	3.38	70,70,70,70	7
87	MG	1	4339	1/1	0.71	0.86	3.38	73,73,73,73	1
86	OHX	6	1969	7/7	0.96	0.24	3.37	68,68,68,68	7
86	OHX	1	3471	7/7	0.99	0.27	3.37	43,43,43,43	7
86	OHX	5	3725	7/7	0.97	0.20	3.37	75,75,75,75	7
86	OHX	6	1906	7/7	0.99	0.25	3.35	55,55,55,55	7
86	OHX	8	206	7/7	0.95	0.23	3.34	94,94,94,94	7
86	OHX	7	203	7/7	0.98	0.22	3.33	54,54,54,54	7
87	MG	n1	204	1/1	0.86	0.34	3.31	56,56,56,56	0
86	OHX	5	3656	7/7	0.96	0.32	3.30	58,58,58,58	7
87	MG	d9	103	1/1	0.93	0.93	3.29	83,83,83,83	1
87	MG	5	4576	1/1	0.66	0.37	3.29	53,53,53,53	0
86	OHX	1	3675	7/7	0.89	0.31	3.28	49,49,49,49	7
87	MG	1	4328	1/1	0.74	0.35	3.28	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3603	7/7	0.96	0.29	3.27	128,128,128,128	7
86	OHX	6	1947	7/7	0.98	0.24	3.25	59,59,59,59	7
86	OHX	1	3487	7/7	0.98	0.26	3.24	74,74,74,74	7
86	OHX	5	3506	7/7	0.96	0.25	3.24	41,41,41,41	7
87	MG	q3	502	1/1	0.97	0.41	3.23	43,43,43,43	1
87	MG	1	4111	1/1	0.92	0.36	3.22	40,40,40,40	1
86	OHX	6	1977	7/7	0.98	0.23	3.20	86,86,86,86	7
87	MG	O1	204	1/1	0.91	0.35	3.20	63,63,63,63	0
86	OHX	1	3575	7/7	0.99	0.24	3.18	47,47,47,47	7
86	OHX	6	2002	7/7	0.97	0.23	3.16	52,52,52,52	7
86	OHX	5	3439	7/7	0.99	0.22	3.16	57,57,57,57	7
87	MG	2	2141	1/1	0.96	0.29	3.15	67,67,67,67	0
86	OHX	1	3587	7/7	0.97	0.25	3.15	77,77,77,77	7
87	MG	4	226	1/1	0.95	0.36	3.14	61,61,61,61	0
86	OHX	1	3507	7/7	0.98	0.29	3.14	60,60,60,60	7
86	OHX	6	2007	7/7	0.88	0.37	3.14	62,62,62,62	7
86	OHX	5	3463	7/7	0.98	0.24	3.13	58,58,58,58	7
86	OHX	2	2041	7/7	0.82	0.39	3.12	83,83,83,83	7
86	OHX	5	3433	7/7	0.99	0.22	3.10	47,47,47,47	7
87	MG	5	4575	1/1	0.99	0.39	3.10	48,48,48,48	1
86	OHX	4	208	7/7	0.91	0.22	3.09	85,85,85,85	7
87	MG	6	2115	1/1	0.79	0.25	3.08	75,75,75,75	0
86	OHX	5	3773	7/7	0.93	0.22	3.08	145,145,145,145	7
86	OHX	1	3483	7/7	0.99	0.26	3.07	55,55,55,55	7
86	OHX	5	3571	7/7	0.94	0.24	3.05	62,62,62,62	7
87	MG	1	4034	1/1	0.84	0.20	3.04	54,54,54,54	0
87	MG	m5	505	1/1	0.96	0.49	3.04	58,58,58,58	0
87	MG	1	4410	1/1	0.96	0.41	3.04	56,56,56,56	0
86	OHX	5	3418	7/7	0.99	0.24	3.02	58,58,58,58	7
87	MG	1	4137	1/1	0.91	0.25	3.02	38,38,38,38	0
86	OHX	2	2070	7/7	0.94	0.24	3.02	78,78,78,78	7
87	MG	5	4442	1/1	0.84	0.29	3.00	34,34,34,34	1
86	OHX	5	3483	7/7	0.99	0.31	3.00	49,49,49,49	7
86	OHX	1	3613	7/7	0.97	0.25	3.00	62,62,62,62	7
87	MG	l3	408	1/1	0.96	0.41	2.99	31,31,31,31	0
86	OHX	5	3636	7/7	0.98	0.39	2.97	44,44,44,44	7
86	OHX	M0	302	7/7	0.97	0.34	2.94	48,48,48,48	7
90	8AN	1	3403	22/23	0.78	0.34	2.94	48,103,107,107	0
86	OHX	2	1913	7/7	0.99	0.27	2.92	87,87,87,87	7
86	OHX	6	1944	7/7	0.94	0.19	2.92	60,60,60,60	7
87	MG	6	2212	1/1	0.78	0.28	2.91	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3795	7/7	0.86	0.29	2.89	79,79,79,79	7
87	MG	5	4045	1/1	0.92	0.26	2.88	40,40,40,40	0
86	OHX	5	3478	7/7	0.99	0.30	2.86	45,45,45,45	7
87	MG	6	2144	1/1	0.98	0.26	2.86	55,55,55,55	0
86	OHX	1	3688	7/7	0.91	0.27	2.86	54,54,54,54	7
86	OHX	5	3477	7/7	0.98	0.26	2.85	44,44,44,44	7
87	MG	6	2167	1/1	0.94	0.22	2.84	55,55,55,55	0
86	OHX	1	3585	7/7	0.97	0.24	2.84	54,54,54,54	7
86	OHX	5	3488	7/7	0.97	0.27	2.84	48,48,48,48	7
87	MG	m8	1501	1/1	0.98	0.64	2.83	42,42,42,42	1
87	MG	m8	1503	1/1	0.96	0.56	2.81	52,52,52,52	0
86	OHX	5	3489	7/7	0.98	0.22	2.81	51,51,51,51	7
86	OHX	1	3561	7/7	0.94	0.28	2.81	76,76,76,76	7
87	MG	5	4333	1/1	0.94	0.29	2.80	43,43,43,43	0
86	OHX	2	2081	7/7	0.78	0.23	2.79	120,120,120,120	7
86	OHX	5	3593	7/7	0.98	0.27	2.77	44,44,44,44	7
86	OHX	6	1918	7/7	0.98	0.24	2.76	56,56,56,56	7
86	OHX	1	3415	7/7	0.99	0.24	2.75	53,53,53,53	7
86	OHX	1	3459	7/7	0.98	0.21	2.74	81,81,81,81	7
86	OHX	1	3592	7/7	0.98	0.27	2.74	52,52,52,52	7
86	OHX	1	3631	7/7	0.95	0.37	2.73	51,51,51,51	7
87	MG	1	4284	1/1	0.95	0.23	2.70	50,50,50,50	0
86	OHX	5	3496	7/7	0.98	0.25	2.70	48,48,48,48	7
86	OHX	1	3801	7/7	0.98	0.25	2.70	57,57,57,57	7
87	MG	2	2168	1/1	0.94	0.41	2.69	68,68,68,68	0
86	OHX	1	3470	7/7	0.97	0.30	2.68	88,88,88,88	7
86	OHX	2	1951	7/7	0.99	0.22	2.67	87,87,87,87	7
86	OHX	1	3455	7/7	0.99	0.24	2.65	70,70,70,70	7
87	MG	l5	309	1/1	0.95	0.52	2.65	54,54,54,54	1
87	MG	1	3815	1/1	0.91	0.28	2.63	44,44,44,44	0
87	MG	2	2133	1/1	0.83	0.29	2.63	76,76,76,76	0
87	MG	6	2164	1/1	0.78	0.37	2.63	87,87,87,87	0
86	OHX	5	3628	7/7	0.98	0.28	2.62	66,66,66,66	7
87	MG	5	4547	1/1	0.91	0.24	2.62	46,46,46,46	0
86	OHX	5	3428	7/7	0.99	0.24	2.62	64,64,64,64	0
86	OHX	1	3703	7/7	0.93	0.31	2.61	101,101,101,101	7
87	MG	1	3831	1/1	0.94	0.23	2.61	44,44,44,44	0
86	OHX	5	3647	7/7	0.87	0.28	2.61	35,35,35,35	7
86	OHX	5	3442	7/7	0.99	0.23	2.58	56,56,56,56	7
87	MG	4	224	1/1	0.82	0.35	2.57	37,37,37,37	0
86	OHX	2	1918	7/7	0.99	0.19	2.56	80,80,80,80	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4193	1/1	0.66	0.54	2.54	40,40,40,40	1
87	MG	5	4305	1/1	0.96	0.28	2.53	34,34,34,34	1
87	MG	N3	203	1/1	0.87	0.53	2.52	51,51,51,51	0
86	OHX	5	3619	7/7	0.98	0.26	2.51	38,38,38,38	7
86	OHX	1	3514	7/7	0.99	0.21	2.51	50,50,50,50	7
86	OHX	6	1914	7/7	0.98	0.25	2.46	52,52,52,52	7
86	OHX	5	3484	7/7	0.97	0.27	2.45	57,57,57,57	7
86	OHX	5	3779	7/7	0.87	0.26	2.45	122,122,122,122	7
87	MG	1	3850	1/1	0.95	0.27	2.45	37,37,37,37	0
87	MG	6	2242	1/1	0.93	0.24	2.44	55,55,55,55	1
87	MG	4	230	1/1	0.84	0.29	2.44	47,47,47,47	0
86	OHX	5	3802	7/7	0.97	0.22	2.44	55,55,55,55	7
87	MG	5	4512	1/1	0.96	0.46	2.43	53,53,53,53	1
86	OHX	7	209	7/7	0.95	0.27	2.42	40,40,40,40	7
86	OHX	S2	301	7/7	0.98	0.27	2.40	81,81,81,81	7
87	MG	1	4170	1/1	0.87	0.24	2.40	45,45,45,45	0
86	OHX	5	3691	7/7	0.97	0.23	2.39	54,54,54,54	7
86	OHX	5	3596	7/7	0.96	0.26	2.38	43,43,43,43	7
86	OHX	5	3528	7/7	0.98	0.25	2.37	62,62,62,62	7
87	MG	5	3820	1/1	0.92	0.27	2.34	32,32,32,32	0
86	OHX	5	3651	7/7	0.94	0.24	2.33	63,63,63,63	7
86	OHX	1	3485	7/7	0.98	0.24	2.33	87,87,87,87	7
86	OHX	O3	201	7/7	0.95	0.30	2.33	49,49,49,49	7
86	OHX	6	1903	7/7	0.99	0.23	2.33	63,63,63,63	3
86	OHX	M0	301	7/7	0.99	0.39	2.30	49,49,49,49	7
86	OHX	1	3479	7/7	0.99	0.26	2.30	55,55,55,55	7
86	OHX	1	3667	7/7	0.97	0.28	2.30	49,49,49,49	7
87	MG	D9	105	1/1	0.96	0.50	2.30	76,76,76,76	0
87	MG	1	3840	1/1	0.82	0.20	2.29	43,43,43,43	0
87	MG	5	3881	1/1	0.96	0.25	2.29	41,41,41,41	0
87	MG	6	2285	1/1	0.66	0.21	2.29	68,68,68,68	1
86	OHX	6	1988	7/7	0.97	0.22	2.29	57,57,57,57	7
87	MG	1	4433	1/1	0.98	0.32	2.27	43,43,43,43	0
86	OHX	5	3407	7/7	0.99	0.25	2.26	44,44,44,44	2
86	OHX	1	3407	7/7	0.99	0.24	2.25	48,48,48,48	2
86	OHX	5	3770	7/7	0.90	0.31	2.25	96,96,96,96	7
87	MG	1	4471	1/1	0.97	0.26	2.25	33,33,33,33	1
86	OHX	5	3467	7/7	0.99	0.22	2.24	66,66,66,66	7
86	OHX	5	3559	7/7	0.97	0.23	2.22	53,53,53,53	7
86	OHX	2	1989	7/7	0.90	0.24	2.21	104,104,104,104	7
86	OHX	1	3439	7/7	0.99	0.24	2.20	69,69,69,69	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3836	1/1	0.99	0.23	2.20	34,34,34,34	0
86	OHX	4	201	7/7	0.99	0.26	2.20	52,52,52,52	2
86	OHX	1	3541	7/7	0.98	0.26	2.19	54,54,54,54	7
86	OHX	5	3475	7/7	0.98	0.21	2.19	81,81,81,81	7
86	OHX	5	3589	7/7	0.98	0.24	2.17	46,46,46,46	7
86	OHX	1	3536	7/7	0.98	0.25	2.17	54,54,54,54	7
87	MG	C5	202	1/1	0.86	0.61	2.16	76,76,76,76	0
87	MG	5	3834	1/1	0.84	0.33	2.16	46,46,46,46	0
86	OHX	8	209	7/7	0.97	0.20	2.15	88,88,88,88	7
87	MG	1	4159	1/1	0.96	0.23	2.15	45,45,45,45	0
87	MG	6	2104	1/1	0.96	0.33	2.14	52,52,52,52	0
89	C	1	3401	20/21	0.86	0.26	2.14	54,111,113,113	0
86	OHX	1	3725	7/7	0.90	0.31	2.14	68,68,68,68	7
86	OHX	5	3623	7/7	0.97	0.26	2.13	46,46,46,46	7
87	MG	6	2282	1/1	0.90	0.34	2.12	55,55,55,55	0
86	OHX	6	2014	7/7	0.97	0.28	2.12	74,74,74,74	7
86	OHX	1	3599	7/7	0.97	0.23	2.11	42,42,42,42	7
86	OHX	5	3661	7/7	0.91	0.29	2.10	50,50,50,50	7
86	OHX	6	1946	7/7	0.98	0.22	2.10	71,71,71,71	7
86	OHX	5	3493	7/7	0.96	0.23	2.10	67,67,67,67	7
87	MG	6	2309	1/1	0.79	0.25	2.10	65,65,65,65	0
86	OHX	5	3454	7/7	0.99	0.18	2.10	77,77,77,77	7
86	OHX	1	3542	7/7	0.99	0.26	2.08	49,49,49,49	7
86	OHX	o3	201	7/7	0.99	0.31	2.07	51,51,51,51	7
86	OHX	5	3534	7/7	0.97	0.23	2.06	42,42,42,42	7
86	OHX	2	1905	7/7	0.99	0.26	2.05	71,71,71,71	7
86	OHX	6	2004	7/7	0.98	0.26	2.04	54,54,54,54	7
86	OHX	5	3502	7/7	0.98	0.24	2.04	46,46,46,46	7
86	OHX	2	2023	7/7	0.96	0.24	2.04	71,71,71,71	7
86	OHX	1	3783	7/7	0.86	0.33	2.04	48,48,48,48	7
86	OHX	5	3678	7/7	0.88	0.29	2.03	51,51,51,51	7
86	OHX	5	3440	7/7	0.99	0.25	2.01	51,51,51,51	7
86	OHX	1	3797	7/7	0.99	0.18	2.00	85,85,85,85	7
86	OHX	5	3431	7/7	0.98	0.23	2.00	61,61,61,61	7
86	OHX	1	3672	7/7	0.95	0.28	1.99	46,46,46,46	7
86	OHX	5	3432	7/7	0.99	0.25	1.99	59,59,59,59	7
87	MG	1	4377	1/1	0.97	0.44	1.99	35,35,35,35	1
86	OHX	1	3522	7/7	0.99	0.27	1.98	40,40,40,40	7
87	MG	8	226	1/1	0.96	0.28	1.98	63,63,63,63	0
86	OHX	5	3731	7/7	0.98	0.28	1.97	48,48,48,48	7
86	OHX	2	1959	7/7	0.97	0.17	1.97	127,127,127,127	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	1974	7/7	0.97	0.21	1.96	137,137,137,137	7
86	OHX	5	3419	7/7	0.99	0.25	1.95	55,55,55,55	7
86	OHX	5	3588	7/7	0.98	0.21	1.94	43,43,43,43	7
87	MG	N6	202	1/1	0.96	0.48	1.94	58,58,58,58	1
86	OHX	5	3677	7/7	0.96	0.24	1.94	48,48,48,48	7
86	OHX	1	3686	7/7	0.92	0.23	1.93	117,117,117,117	7
87	MG	5	4246	1/1	0.98	0.23	1.93	45,45,45,45	0
86	OHX	8	201	7/7	0.99	0.22	1.92	55,55,55,55	7
86	OHX	1	3776	7/7	0.98	0.23	1.92	59,59,59,59	7
86	OHX	1	3518	7/7	0.99	0.23	1.91	41,41,41,41	7
87	MG	1	3918	1/1	0.97	0.23	1.91	57,57,57,57	0
86	OHX	5	3617	7/7	0.97	0.15	1.90	74,74,74,74	7
86	OHX	6	2040	7/7	0.93	0.27	1.90	58,58,58,58	7
86	OHX	1	3611	7/7	0.96	0.25	1.90	42,42,42,42	7
86	OHX	1	3642	7/7	0.96	0.26	1.86	52,52,52,52	7
86	OHX	1	3618	7/7	0.97	0.21	1.86	78,78,78,78	7
86	OHX	1	3490	7/7	0.98	0.34	1.84	54,54,54,54	7
86	OHX	5	3642	7/7	0.95	0.32	1.84	39,39,39,39	7
86	OHX	1	3655	7/7	0.96	0.21	1.84	64,64,64,64	7
86	OHX	M7	201	7/7	0.92	0.26	1.84	42,42,42,42	7
87	MG	2	2101	1/1	0.85	0.26	1.83	73,73,73,73	0
87	MG	1	3980	1/1	0.88	0.34	1.83	54,54,54,54	0
86	OHX	1	3492	7/7	0.97	0.18	1.82	113,113,113,113	7
86	OHX	1	3520	7/7	0.98	0.24	1.82	52,52,52,52	7
87	MG	1	3907	1/1	0.86	0.20	1.81	59,59,59,59	0
86	OHX	3	212	7/7	0.89	0.28	1.80	79,79,79,79	7
86	OHX	5	3495	7/7	0.99	0.20	1.80	47,47,47,47	7
86	OHX	6	2045	7/7	0.87	0.29	1.78	61,61,61,61	7
86	OHX	5	3663	7/7	0.93	0.26	1.78	57,57,57,57	7
87	MG	5	3838	1/1	0.91	0.26	1.76	40,40,40,40	0
86	OHX	1	3632	7/7	0.98	0.25	1.76	43,43,43,43	7
87	MG	2	2121	1/1	0.99	0.28	1.76	73,73,73,73	0
87	MG	n8	206	1/1	0.95	0.47	1.76	37,37,37,37	1
86	OHX	5	3560	7/7	0.97	0.27	1.76	50,50,50,50	7
86	OHX	1	3445	7/7	0.99	0.26	1.75	51,51,51,51	7
86	OHX	5	3455	7/7	0.99	0.25	1.75	54,54,54,54	7
86	OHX	1	3662	7/7	0.89	0.23	1.74	60,60,60,60	7
86	OHX	6	1909	7/7	0.98	0.17	1.74	79,79,79,79	7
86	OHX	6	1931	7/7	0.94	0.22	1.72	71,71,71,71	7
87	MG	5	4379	1/1	0.95	0.34	1.72	37,37,37,37	1
86	OHX	6	1921	7/7	0.98	0.31	1.72	51,51,51,51	7
87	MG	5	4123	1/1	0.86	0.28	1.71	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3746	7/7	0.96	0.20	1.71	71,71,71,71	7
86	OHX	1	3438	7/7	0.99	0.23	1.70	59,59,59,59	7
86	OHX	1	3647	7/7	0.97	0.26	1.70	64,64,64,64	7
86	OHX	1	3447	7/7	0.99	0.23	1.68	69,69,69,69	7
86	OHX	5	3607	7/7	0.92	0.24	1.67	112,112,112,112	7
86	OHX	1	3620	7/7	0.97	0.26	1.67	60,60,60,60	7
86	OHX	6	1955	7/7	0.98	0.17	1.67	145,145,145,145	7
87	MG	1	4000	1/1	0.93	0.24	1.65	39,39,39,39	0
87	MG	5	4510	1/1	0.91	0.25	1.64	33,33,33,33	0
86	OHX	1	3690	7/7	0.97	0.23	1.63	66,66,66,66	7
86	OHX	5	3514	7/7	0.99	0.24	1.62	39,39,39,39	7
86	OHX	6	1962	7/7	0.98	0.23	1.61	62,62,62,62	7
86	OHX	1	3419	7/7	0.99	0.19	1.60	66,66,66,66	7
87	MG	5	4574	1/1	0.86	0.33	1.60	49,49,49,49	0
87	MG	5	4288	1/1	0.99	0.23	1.60	39,39,39,39	1
86	OHX	2	2018	7/7	0.91	0.20	1.58	102,102,102,102	7
86	OHX	6	1972	7/7	0.98	0.25	1.58	59,59,59,59	7
87	MG	1	4329	1/1	0.87	0.35	1.57	60,60,60,60	0
87	MG	1	3829	1/1	0.91	0.32	1.57	58,58,58,58	0
87	MG	5	4411	1/1	0.92	0.38	1.57	55,55,55,55	0
86	OHX	2	1969	7/7	0.94	0.26	1.56	62,62,62,62	7
87	MG	sM	202	1/1	0.96	0.47	1.56	44,44,44,44	0
86	OHX	2	1919	7/7	0.99	0.20	1.55	78,78,78,78	7
86	OHX	8	205	7/7	0.97	0.23	1.55	64,64,64,64	7
86	OHX	5	3650	7/7	0.90	0.28	1.55	46,46,46,46	7
86	OHX	6	1980	7/7	0.95	0.23	1.53	61,61,61,61	7
86	OHX	1	3709	7/7	0.97	0.17	1.53	59,59,59,59	7
87	MG	1	4026	1/1	0.99	0.23	1.52	40,40,40,40	0
86	OHX	1	3535	7/7	0.95	0.30	1.52	47,47,47,47	7
86	OHX	1	3497	7/7	0.99	0.23	1.51	50,50,50,50	7
86	OHX	2	2051	7/7	0.95	0.27	1.51	86,86,86,86	7
86	OHX	1	3473	7/7	0.97	0.25	1.50	60,60,60,60	7
86	OHX	1	3499	7/7	0.98	0.26	1.49	54,54,54,54	7
86	OHX	1	3799	7/7	0.98	0.26	1.48	54,54,54,54	7
86	OHX	1	3751	7/7	0.95	0.13	1.48	146,146,146,146	7
87	MG	1	4390	1/1	0.88	0.24	1.48	36,36,36,36	1
86	OHX	2	2071	7/7	0.85	0.34	1.48	94,94,94,94	7
86	OHX	5	3532	7/7	0.96	0.24	1.47	38,38,38,38	7
86	OHX	1	3434	7/7	0.99	0.19	1.47	68,68,68,68	7
87	MG	6	2138	1/1	0.81	0.68	1.46	73,73,73,73	0
86	OHX	6	2098	7/7	0.99	0.20	1.46	113,113,113,113	7
86	OHX	1	3506	7/7	0.99	0.25	1.46	38,38,38,38	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	2	2105	1/1	0.90	0.33	1.46	72,72,72,72	0
86	OHX	2	1963	7/7	0.98	0.18	1.46	83,83,83,83	7
86	OHX	7	207	7/7	0.97	0.20	1.45	78,78,78,78	7
86	OHX	5	3746	7/7	0.84	0.21	1.45	149,149,149,149	7
86	OHX	6	1904	7/7	0.99	0.18	1.45	71,71,71,71	7
87	MG	1	4424	1/1	0.79	0.46	1.44	54,54,54,54	0
86	OHX	5	3429	7/7	0.99	0.21	1.44	49,49,49,49	7
86	OHX	5	3533	7/7	0.96	0.22	1.42	47,47,47,47	7
86	OHX	5	3511	7/7	0.94	0.26	1.41	61,61,61,61	7
86	OHX	19	201	7/7	0.92	0.31	1.41	62,62,62,62	7
86	OHX	8	202	7/7	0.99	0.24	1.41	49,49,49,49	2
86	OHX	1	3743	7/7	0.97	0.21	1.41	76,76,76,76	7
86	OHX	N9	101	7/7	0.99	0.21	1.41	58,58,58,58	7
87	MG	1	4314	1/1	0.97	0.28	1.41	40,40,40,40	1
86	OHX	2	1988	7/7	0.96	0.20	1.39	80,80,80,80	7
86	OHX	5	3727	7/7	0.99	0.24	1.39	53,53,53,53	7
86	OHX	5	3659	7/7	0.96	0.19	1.38	58,58,58,58	7
86	OHX	1	3682	7/7	0.95	0.17	1.38	75,75,75,75	7
87	MG	5	4525	1/1	0.95	0.26	1.37	41,41,41,41	0
87	MG	1	3902	1/1	0.93	0.24	1.37	43,43,43,43	0
86	OHX	1	3526	7/7	0.97	0.22	1.36	47,47,47,47	7
87	MG	1	4404	1/1	0.68	0.25	1.34	57,57,57,57	0
87	MG	1	3899	1/1	0.74	0.23	1.34	40,40,40,40	0
87	MG	1	4076	1/1	0.87	0.21	1.33	76,76,76,76	0
86	OHX	1	3650	7/7	0.98	0.17	1.32	96,96,96,96	7
86	OHX	1	3778	7/7	0.94	0.32	1.32	56,56,56,56	7
86	OHX	5	3437	7/7	0.98	0.18	1.30	100,100,100,100	0
86	OHX	5	3580	7/7	0.97	0.23	1.30	63,63,63,63	7
87	MG	5	4313	1/1	0.91	0.21	1.30	57,57,57,57	0
86	OHX	2	2074	7/7	0.90	0.37	1.30	92,92,92,92	7
86	OHX	5	3624	7/7	0.91	0.26	1.29	51,51,51,51	7
87	MG	1	4177	1/1	0.99	0.28	1.29	49,49,49,49	1
86	OHX	2	1922	7/7	0.98	0.20	1.28	75,75,75,75	7
87	MG	6	2108	1/1	0.96	0.23	1.28	98,98,98,98	0
86	OHX	2	2060	7/7	0.68	0.45	1.28	98,98,98,98	7
86	OHX	1	3456	7/7	0.99	0.18	1.27	85,85,85,85	7
86	OHX	5	3519	7/7	0.97	0.14	1.26	132,132,132,132	7
87	MG	5	4028	1/1	0.96	0.29	1.25	38,38,38,38	0
86	OHX	1	3717	7/7	0.98	0.24	1.24	50,50,50,50	7
86	OHX	1	3763	7/7	0.91	0.26	1.24	64,64,64,64	7
86	OHX	1	3812	7/7	0.93	0.32	1.24	88,88,88,88	7
86	OHX	1	3424	7/7	0.99	0.22	1.23	49,49,49,49	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	l4	401	7/7	0.93	0.31	1.23	69,69,69,69	7
86	OHX	5	3693	7/7	0.97	0.24	1.22	45,45,45,45	7
87	MG	1	4421	1/1	0.95	0.21	1.21	41,41,41,41	1
86	OHX	1	3800	7/7	0.99	0.23	1.21	41,41,41,41	7
86	OHX	o7	503	7/7	0.94	0.26	1.20	53,53,53,53	7
86	OHX	5	3558	7/7	0.97	0.20	1.20	45,45,45,45	7
86	OHX	6	1932	7/7	0.99	0.23	1.19	47,47,47,47	7
87	MG	6	2303	1/1	0.98	0.44	1.19	78,78,78,78	0
87	MG	s8	302	1/1	0.97	0.28	1.19	45,45,45,45	0
86	OHX	1	3517	7/7	0.96	0.26	1.18	61,61,61,61	7
86	OHX	1	3423	7/7	0.99	0.23	1.18	62,62,62,62	7
86	OHX	1	3722	7/7	0.92	0.29	1.18	69,69,69,69	7
87	MG	5	4148	1/1	0.99	0.28	1.16	32,32,32,32	1
87	MG	5	4268	1/1	0.98	0.18	1.15	46,46,46,46	0
87	MG	o3	202	1/1	0.86	0.38	1.15	53,53,53,53	0
86	OHX	1	3576	7/7	0.97	0.22	1.15	53,53,53,53	7
87	MG	5	4495	1/1	0.89	0.23	1.14	53,53,53,53	0
86	OHX	1	3663	7/7	0.96	0.33	1.13	48,48,48,48	7
86	OHX	1	3405	7/7	1.00	0.21	1.13	48,48,48,48	0
86	OHX	5	3408	7/7	0.99	0.22	1.12	42,42,42,42	2
86	OHX	1	3431	7/7	0.99	0.17	1.11	86,86,86,86	7
87	MG	5	4220	1/1	0.93	0.21	1.09	49,49,49,49	1
86	OHX	1	3509	7/7	0.98	0.29	1.08	42,42,42,42	7
86	OHX	1	3442	7/7	0.99	0.21	1.08	55,55,55,55	7
87	MG	1	4445	1/1	0.95	0.25	1.08	41,41,41,41	0
86	OHX	O1	201	7/7	0.89	0.32	1.06	77,77,77,77	7
86	OHX	1	3757	7/7	0.83	0.26	1.06	49,49,49,49	7
87	MG	1	3991	1/1	0.95	0.28	1.06	36,36,36,36	0
89	C	5	3401	20/21	0.83	0.25	1.05	48,105,107,107	0
86	OHX	1	3721	7/7	0.92	0.21	1.05	96,96,96,96	7
86	OHX	1	3657	7/7	0.96	0.24	1.03	40,40,40,40	7
86	OHX	1	3687	7/7	0.92	0.23	1.02	61,61,61,61	7
87	MG	6	2268	1/1	0.91	0.31	1.01	84,84,84,84	0
86	OHX	6	2039	7/7	0.99	0.22	1.01	46,46,46,46	7
86	OHX	1	3579	7/7	0.96	0.23	1.00	53,53,53,53	7
86	OHX	5	3751	7/7	0.93	0.23	1.00	61,61,61,61	7
86	OHX	5	3801	7/7	0.97	0.23	0.99	66,66,66,66	7
86	OHX	1	3533	7/7	0.96	0.18	0.99	129,129,129,129	7
86	OHX	5	3595	7/7	0.99	0.26	0.99	46,46,46,46	7
87	MG	l2	303	1/1	0.75	0.29	0.99	55,55,55,55	1
86	OHX	4	202	7/7	0.99	0.21	0.98	55,55,55,55	7
86	OHX	6	1928	7/7	0.98	0.17	0.98	118,118,118,118	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3535	7/7	0.97	0.28	0.97	42,42,42,42	7
87	MG	5	4446	1/1	0.94	0.32	0.97	45,45,45,45	0
87	MG	1	4143	1/1	0.81	0.44	0.97	54,54,54,54	0
86	OHX	1	3513	7/7	0.99	0.23	0.96	49,49,49,49	7
86	OHX	1	3421	7/7	0.99	0.24	0.95	48,48,48,48	7
86	OHX	5	3613	7/7	0.96	0.22	0.95	70,70,70,70	7
86	OHX	5	3562	7/7	0.98	0.22	0.94	51,51,51,51	7
86	OHX	5	3760	7/7	0.94	0.17	0.94	89,89,89,89	7
86	OHX	1	3435	7/7	0.99	0.24	0.93	45,45,45,45	7
86	OHX	1	3484	7/7	0.98	0.20	0.93	62,62,62,62	7
87	MG	c8	205	1/1	0.74	0.31	0.92	93,93,93,93	0
86	OHX	2	1914	7/7	0.99	0.25	0.91	69,69,69,69	7
86	OHX	5	3686	7/7	0.91	0.27	0.91	56,56,56,56	7
86	OHX	6	1990	7/7	0.90	0.28	0.91	65,65,65,65	7
87	MG	5	3939	1/1	0.98	0.26	0.90	39,39,39,39	0
86	OHX	3	206	7/7	0.98	0.20	0.89	81,81,81,81	7
87	MG	d2	201	1/1	0.92	0.29	0.89	46,46,46,46	0
87	MG	o6	201	1/1	0.99	0.39	0.88	69,69,69,69	1
87	MG	2	2193	1/1	0.89	0.21	0.88	71,71,71,71	0
87	MG	6	2188	1/1	0.95	0.19	0.88	52,52,52,52	0
86	OHX	5	3699	7/7	0.95	0.23	0.87	39,39,39,39	7
86	OHX	5	3734	7/7	0.97	0.23	0.87	70,70,70,70	7
87	MG	1	4256	1/1	0.91	0.21	0.85	58,58,58,58	0
86	OHX	4	207	7/7	0.97	0.19	0.84	61,61,61,61	7
86	OHX	7	202	7/7	0.98	0.18	0.84	60,60,60,60	7
86	OHX	1	3425	7/7	0.99	0.22	0.84	71,71,71,71	7
86	OHX	5	3523	7/7	0.91	0.20	0.84	120,120,120,120	7
87	MG	1	3917	1/1	0.97	0.19	0.83	49,49,49,49	0
86	OHX	1	3448	7/7	0.99	0.19	0.81	59,59,59,59	7
86	OHX	6	1978	7/7	0.98	0.20	0.81	52,52,52,52	7
87	MG	5	3933	1/1	0.98	0.22	0.81	46,46,46,46	0
87	MG	2	2240	1/1	0.91	0.31	0.81	66,66,66,66	0
86	OHX	5	3430	7/7	0.99	0.22	0.81	40,40,40,40	7
86	OHX	5	3411	7/7	0.99	0.22	0.80	50,50,50,50	7
86	OHX	3	207	7/7	0.95	0.17	0.79	85,85,85,85	7
87	MG	5	4528	1/1	0.86	0.36	0.79	83,83,83,83	1
86	OHX	l5	303	7/7	0.92	0.25	0.78	69,69,69,69	7
86	OHX	1	3469	7/7	0.99	0.20	0.77	75,75,75,75	7
86	OHX	5	3476	7/7	0.99	0.24	0.76	46,46,46,46	7
86	OHX	5	3409	7/7	1.00	0.23	0.76	57,57,57,57	1
87	MG	1	3858	1/1	0.99	0.21	0.75	51,51,51,51	0
87	MG	1	4129	1/1	0.94	0.26	0.74	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	c1	201	7/7	0.97	0.20	0.73	79,79,79,79	7
86	OHX	1	3420	7/7	0.99	0.18	0.73	59,59,59,59	7
87	MG	1	4033	1/1	0.96	0.34	0.73	73,73,73,73	0
87	MG	5	4035	1/1	0.98	0.19	0.73	46,46,46,46	0
86	OHX	1	3586	7/7	0.98	0.20	0.72	50,50,50,50	7
87	MG	1	4312	1/1	0.96	0.23	0.72	41,41,41,41	0
86	OHX	2	1904	7/7	0.99	0.18	0.71	89,89,89,89	7
86	OHX	6	1926	7/7	0.99	0.20	0.70	55,55,55,55	7
86	OHX	5	3422	7/7	0.99	0.20	0.70	55,55,55,55	7
86	OHX	1	3805	7/7	0.97	0.26	0.69	73,73,73,73	7
86	OHX	1	3493	7/7	0.99	0.19	0.69	56,56,56,56	7
86	OHX	1	3595	7/7	0.97	0.20	0.69	95,95,95,95	7
87	MG	c9	203	1/1	0.62	0.40	0.68	87,87,87,87	0
87	MG	6	2195	1/1	0.82	0.24	0.68	46,46,46,46	0
87	MG	1	4418	1/1	0.98	0.40	0.68	60,60,60,60	1
87	MG	2	2098	1/1	0.78	0.23	0.67	80,80,80,80	0
86	OHX	4	203	7/7	0.97	0.22	0.67	61,61,61,61	7
86	OHX	5	3485	7/7	0.98	0.27	0.67	46,46,46,46	7
87	MG	5	4562	1/1	0.75	0.38	0.67	68,68,68,68	0
86	OHX	5	3420	7/7	0.99	0.22	0.66	56,56,56,56	7
87	MG	1	4004	1/1	0.95	0.26	0.66	44,44,44,44	0
86	OHX	L3	401	7/7	0.97	0.22	0.65	56,56,56,56	7
86	OHX	6	2037	7/7	0.87	0.25	0.65	75,75,75,75	7
86	OHX	5	3581	7/7	0.97	0.26	0.65	46,46,46,46	7
87	MG	2	2235	1/1	0.86	0.27	0.64	102,102,102,102	1
86	OHX	l3	401	7/7	0.98	0.25	0.64	52,52,52,52	7
86	OHX	5	3625	7/7	0.94	0.24	0.63	52,52,52,52	7
87	MG	6	2154	1/1	0.91	0.26	0.63	76,76,76,76	0
87	MG	5	4469	1/1	1.00	0.25	0.63	38,38,38,38	0
86	OHX	2	2031	7/7	0.94	0.25	0.62	90,90,90,90	7
86	OHX	6	1954	7/7	0.97	0.18	0.62	149,149,149,149	7
87	MG	1	3971	1/1	0.97	0.23	0.62	43,43,43,43	0
86	OHX	6	1987	7/7	0.97	0.21	0.62	70,70,70,70	7
86	OHX	5	3584	7/7	0.98	0.23	0.62	52,52,52,52	7
87	MG	6	2181	1/1	0.98	0.32	0.62	55,55,55,55	0
86	OHX	o7	502	7/7	0.99	0.24	0.61	64,64,64,64	7
87	MG	8	234	1/1	0.92	0.23	0.61	41,41,41,41	1
86	OHX	2	2062	7/7	0.89	0.30	0.61	85,85,85,85	7
86	OHX	1	3488	7/7	0.99	0.25	0.61	49,49,49,49	7
87	MG	5	4375	1/1	0.86	0.26	0.60	61,61,61,61	0
86	OHX	2	2048	7/7	0.88	0.30	0.60	83,83,83,83	7
86	OHX	3	204	7/7	0.98	0.21	0.60	85,85,85,85	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2067	7/7	0.96	0.30	0.60	70,70,70,70	7
86	OHX	5	3787	7/7	0.89	0.22	0.60	111,111,111,111	7
88	ZN	d7	101	1/1	0.86	0.27	0.59	135,135,135,135	0
86	OHX	5	3710	7/7	0.92	0.32	0.59	79,79,79,79	7
86	OHX	7	201	7/7	0.99	0.23	0.59	70,70,70,70	7
86	OHX	5	3637	7/7	0.90	0.20	0.59	109,109,109,109	7
86	OHX	1	3762	7/7	0.91	0.16	0.59	63,63,63,63	7
87	MG	2	2172	1/1	0.94	0.25	0.58	65,65,65,65	0
87	MG	2	2104	1/1	0.95	0.22	0.57	70,70,70,70	0
86	OHX	Q2	502	7/7	0.99	0.22	0.57	45,45,45,45	7
86	OHX	1	3504	7/7	0.98	0.17	0.56	90,90,90,90	7
86	OHX	2	2020	7/7	0.87	0.25	0.53	84,84,84,84	7
86	OHX	2	1923	7/7	0.99	0.21	0.52	80,80,80,80	7
86	OHX	1	3810	7/7	0.98	0.24	0.52	62,62,62,62	7
87	MG	5	4567	1/1	0.97	0.31	0.52	48,48,48,48	1
87	MG	2	2114	1/1	0.92	0.32	0.52	79,79,79,79	0
86	OHX	2	2015	7/7	0.94	0.21	0.51	87,87,87,87	7
87	MG	2	2170	1/1	0.89	0.21	0.51	78,78,78,78	0
86	OHX	5	3564	7/7	0.96	0.25	0.50	89,89,89,89	7
86	OHX	1	3511	7/7	0.96	0.23	0.49	66,66,66,66	7
86	OHX	6	2011	7/7	0.98	0.21	0.49	57,57,57,57	7
86	OHX	1	3411	7/7	0.99	0.18	0.48	64,64,64,64	0
86	OHX	5	3416	7/7	0.99	0.25	0.47	46,46,46,46	7
87	MG	s6	302	1/1	0.91	0.35	0.47	75,75,75,75	0
86	OHX	1	3406	7/7	0.99	0.20	0.46	58,58,58,58	2
86	OHX	1	3553	7/7	0.97	0.22	0.46	60,60,60,60	7
87	MG	5	4033	1/1	0.90	0.19	0.46	43,43,43,43	0
87	MG	6	2266	1/1	0.94	0.20	0.45	71,71,71,71	0
86	OHX	5	3410	7/7	0.99	0.21	0.44	58,58,58,58	2
87	MG	2	2256	1/1	0.87	0.26	0.43	66,66,66,66	0
87	MG	L2	301	1/1	0.93	0.28	0.42	39,39,39,39	0
86	OHX	L4	401	7/7	0.97	0.26	0.41	59,59,59,59	7
86	OHX	5	3552	7/7	0.97	0.22	0.41	47,47,47,47	7
87	MG	6	2149	1/1	0.96	0.29	0.40	65,65,65,65	0
86	OHX	5	3501	7/7	0.98	0.20	0.38	57,57,57,57	7
87	MG	1	4402	1/1	0.91	0.19	0.38	48,48,48,48	0
87	MG	1	4065	1/1	0.78	0.27	0.38	50,50,50,50	0
86	OHX	1	3477	7/7	0.99	0.23	0.38	62,62,62,62	7
86	OHX	5	3757	7/7	0.99	0.17	0.38	75,75,75,75	7
86	OHX	6	1908	7/7	0.99	0.21	0.38	71,71,71,71	7
86	OHX	1	3794	7/7	0.98	0.22	0.37	68,68,68,68	7
86	OHX	6	2070	7/7	0.95	0.20	0.37	71,71,71,71	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	d4	202	1/1	0.87	0.27	0.37	55,55,55,55	0
86	OHX	6	2027	7/7	0.85	0.34	0.37	83,83,83,83	7
86	OHX	5	3715	7/7	0.94	0.22	0.36	69,69,69,69	7
86	OHX	6	2000	7/7	0.95	0.32	0.36	63,63,63,63	7
87	MG	5	4174	1/1	0.92	0.22	0.35	41,41,41,41	0
86	OHX	1	3437	7/7	0.99	0.20	0.35	61,61,61,61	7
87	MG	m5	503	1/1	0.99	0.22	0.34	48,48,48,48	0
86	OHX	5	3574	7/7	0.97	0.22	0.34	53,53,53,53	7
87	MG	M9	204	1/1	0.55	0.21	0.34	70,70,70,70	0
86	OHX	1	3617	7/7	0.94	0.24	0.34	36,36,36,36	7
86	OHX	1	3476	7/7	0.98	0.22	0.33	70,70,70,70	7
86	OHX	2	1947	7/7	0.96	0.17	0.33	130,130,130,130	7
86	OHX	1	3549	7/7	0.98	0.22	0.33	54,54,54,54	7
86	OHX	1	3813	7/7	0.96	0.25	0.33	60,60,60,60	7
88	ZN	D7	101	1/1	0.57	0.39	0.32	147,147,147,147	0
86	OHX	6	1911	7/7	0.98	0.19	0.32	59,59,59,59	7
86	OHX	2	1992	7/7	0.97	0.23	0.32	75,75,75,75	7
86	OHX	6	2078	7/7	0.94	0.20	0.32	93,93,93,93	7
86	OHX	5	3546	7/7	0.97	0.23	0.31	52,52,52,52	7
86	OHX	6	2041	7/7	0.88	0.27	0.31	62,62,62,62	7
86	OHX	5	3471	7/7	0.99	0.15	0.29	76,76,76,76	7
86	OHX	5	3468	7/7	0.99	0.22	0.28	63,63,63,63	7
86	OHX	6	2026	7/7	0.94	0.24	0.27	151,151,151,151	7
86	OHX	5	3517	7/7	0.97	0.23	0.27	56,56,56,56	7
86	OHX	4	217	7/7	0.94	0.23	0.27	70,70,70,70	7
86	OHX	1	3596	7/7	0.97	0.21	0.27	70,70,70,70	7
86	OHX	5	3447	7/7	0.99	0.21	0.27	60,60,60,60	7
87	MG	5	3958	1/1	0.94	0.32	0.27	61,61,61,61	0
87	MG	1	4436	1/1	0.96	0.20	0.27	41,41,41,41	0
86	OHX	5	3667	7/7	0.98	0.23	0.26	41,41,41,41	7
86	OHX	1	3519	7/7	0.98	0.21	0.25	50,50,50,50	7
86	OHX	5	3541	7/7	0.98	0.20	0.25	55,55,55,55	7
86	OHX	6	1937	7/7	0.97	0.18	0.25	88,88,88,88	7
86	OHX	6	1960	7/7	0.97	0.23	0.24	72,72,72,72	7
86	OHX	6	1949	7/7	0.98	0.22	0.24	73,73,73,73	7
87	MG	5	3843	1/1	0.96	0.23	0.23	62,62,62,62	0
86	OHX	2	1973	7/7	0.96	0.19	0.23	103,103,103,103	7
86	OHX	1	3457	7/7	0.98	0.27	0.21	50,50,50,50	7
86	OHX	1	3548	7/7	0.98	0.19	0.21	59,59,59,59	7
86	OHX	q1	101	7/7	0.99	0.24	0.20	46,46,46,46	7
86	OHX	1	3685	7/7	0.96	0.17	0.20	95,95,95,95	7
86	OHX	n9	101	7/7	0.99	0.22	0.20	59,59,59,59	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	m5	502	7/7	0.89	0.28	0.20	78,78,78,78	7
86	OHX	1	3417	7/7	0.99	0.20	0.19	56,56,56,56	7
87	MG	6	2106	1/1	0.91	0.26	0.19	68,68,68,68	0
86	OHX	5	3803	7/7	0.98	0.21	0.18	69,69,69,69	7
86	OHX	7	206	7/7	0.99	0.21	0.17	67,67,67,67	7
86	OHX	5	3611	7/7	0.97	0.21	0.17	52,52,52,52	7
86	OHX	6	1997	7/7	0.94	0.20	0.17	94,94,94,94	7
86	OHX	1	3429	7/7	1.00	0.22	0.14	62,62,62,62	7
87	MG	5	4140	1/1	0.83	0.20	0.13	82,82,82,82	0
86	OHX	5	3424	7/7	0.99	0.19	0.13	70,70,70,70	0
87	MG	5	3915	1/1	0.95	0.21	0.13	39,39,39,39	0
86	OHX	1	3601	7/7	0.98	0.19	0.12	49,49,49,49	7
86	OHX	2	2067	7/7	0.87	0.29	0.12	92,92,92,92	7
86	OHX	2	1941	7/7	0.97	0.19	0.11	92,92,92,92	7
86	OHX	6	2043	7/7	0.90	0.24	0.11	86,86,86,86	7
86	OHX	1	3573	7/7	0.97	0.24	0.11	58,58,58,58	7
86	OHX	2	1956	7/7	0.97	0.17	0.10	91,91,91,91	7
86	OHX	2	1987	7/7	0.97	0.22	0.08	75,75,75,75	7
86	OHX	5	3668	7/7	0.96	0.22	0.08	39,39,39,39	7
86	OHX	6	1916	7/7	0.99	0.18	0.08	65,65,65,65	7
86	OHX	1	3758	7/7	0.95	0.20	0.07	55,55,55,55	7
86	OHX	2	2076	7/7	0.97	0.15	0.07	122,122,122,122	7
86	OHX	6	2013	7/7	0.88	0.31	0.06	82,82,82,82	7
86	OHX	5	3606	7/7	0.96	0.16	0.06	74,74,74,74	7
86	OHX	5	3673	7/7	0.98	0.23	0.06	44,44,44,44	7
86	OHX	5	3518	7/7	0.97	0.18	0.06	60,60,60,60	7
86	OHX	5	3462	7/7	0.97	0.20	0.05	56,56,56,56	7
86	OHX	1	3480	7/7	0.97	0.23	0.05	75,75,75,75	7
86	OHX	6	2035	7/7	0.94	0.33	0.05	82,82,82,82	7
86	OHX	6	1983	7/7	0.97	0.19	0.04	95,95,95,95	7
86	OHX	N8	201	7/7	0.90	0.27	0.04	94,94,94,94	7
87	MG	5	4081	1/1	0.93	0.18	0.04	48,48,48,48	0
86	OHX	1	3524	7/7	0.98	0.19	0.03	55,55,55,55	7
86	OHX	3	211	7/7	0.94	0.23	0.03	81,81,81,81	7
87	MG	1	3986	1/1	0.97	0.21	0.02	54,54,54,54	0
86	OHX	1	3786	7/7	0.98	0.25	0.02	73,73,73,73	7
86	OHX	5	3788	7/7	0.98	0.24	0.02	58,58,58,58	7
86	OHX	2	2078	7/7	0.91	0.17	0.02	102,102,102,102	7
86	OHX	1	3707	7/7	0.91	0.15	0.01	106,106,106,106	7
86	OHX	6	1919	7/7	0.98	0.17	0.01	68,68,68,68	7
86	OHX	1	3465	7/7	0.99	0.22	-0.00	62,62,62,62	7
86	OHX	1	3416	7/7	0.99	0.20	-0.01	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3645	7/7	0.94	0.25	-0.01	68,68,68,68	7
86	OHX	1	3475	7/7	0.99	0.20	-0.01	49,49,49,49	7
86	OHX	6	1920	7/7	0.99	0.16	-0.02	114,114,114,114	7
86	OHX	1	3673	7/7	0.94	0.23	-0.03	47,47,47,47	7
86	OHX	1	3428	7/7	0.99	0.16	-0.03	79,79,79,79	0
86	OHX	5	3795	7/7	0.92	0.26	-0.03	54,54,54,54	7
87	MG	1	4079	1/1	0.92	0.27	-0.04	43,43,43,43	0
86	OHX	1	3750	7/7	0.98	0.22	-0.04	46,46,46,46	7
86	OHX	1	3744	7/7	0.97	0.26	-0.05	60,60,60,60	7
86	OHX	5	3446	7/7	0.99	0.22	-0.06	56,56,56,56	7
87	MG	3	225	1/1	0.93	0.30	-0.06	68,68,68,68	0
87	MG	1	4318	1/1	0.41	0.17	-0.06	115,115,115,115	0
86	OHX	5	3499	7/7	0.98	0.20	-0.06	46,46,46,46	7
86	OHX	1	3641	7/7	0.98	0.15	-0.08	89,89,89,89	7
86	OHX	1	3700	7/7	0.95	0.24	-0.08	47,47,47,47	7
87	MG	6	2203	1/1	0.87	0.21	-0.09	68,68,68,68	0
87	MG	5	4381	1/1	0.76	0.19	-0.09	79,79,79,79	0
86	OHX	1	3582	7/7	0.97	0.18	-0.10	67,67,67,67	7
86	OHX	1	3538	7/7	0.96	0.22	-0.10	62,62,62,62	7
86	OHX	5	3421	7/7	0.99	0.21	-0.10	45,45,45,45	7
87	MG	5	4230	1/1	0.93	0.15	-0.10	55,55,55,55	0
86	OHX	5	3660	7/7	0.84	0.21	-0.10	42,42,42,42	7
86	OHX	5	3582	7/7	0.97	0.19	-0.12	67,67,67,67	7
87	MG	1	4133	1/1	0.94	0.13	-0.12	83,83,83,83	0
86	OHX	8	204	7/7	0.97	0.22	-0.13	66,66,66,66	7
87	MG	1	3910	1/1	0.94	0.27	-0.13	44,44,44,44	0
86	OHX	6	2032	7/7	0.97	0.21	-0.13	61,61,61,61	7
87	MG	1	3821	1/1	0.86	0.19	-0.13	55,55,55,55	0
86	OHX	6	2047	7/7	0.94	0.23	-0.14	67,67,67,67	7
87	MG	7	223	1/1	0.83	0.21	-0.14	52,52,52,52	0
86	OHX	5	3805	7/7	0.98	0.21	-0.14	88,88,88,88	7
87	MG	5	4199	1/1	0.86	0.19	-0.14	41,41,41,41	0
87	MG	5	4321	1/1	0.99	0.22	-0.14	66,66,66,66	1
87	MG	6	2170	1/1	0.93	0.21	-0.14	49,49,49,49	0
86	OHX	2	2052	7/7	0.83	0.20	-0.14	189,189,189,189	7
86	OHX	6	1958	7/7	0.97	0.17	-0.15	77,77,77,77	7
86	OHX	2	2010	7/7	0.86	0.22	-0.15	101,101,101,101	7
87	MG	5	4410	1/1	0.95	0.22	-0.17	47,47,47,47	1
86	OHX	5	3500	7/7	0.97	0.18	-0.17	75,75,75,75	7
86	OHX	6	2053	7/7	0.85	0.22	-0.17	85,85,85,85	7
86	OHX	5	3752	7/7	0.94	0.23	-0.17	49,49,49,49	7
86	OHX	1	3770	7/7	0.86	0.25	-0.17	141,141,141,141	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	8	219	7/7	0.86	0.26	-0.17	92,92,92,92	7
87	MG	1	4248	1/1	0.82	0.17	-0.17	55,55,55,55	0
86	OHX	4	204	7/7	0.99	0.20	-0.17	57,57,57,57	7
86	OHX	5	3497	7/7	0.98	0.20	-0.18	62,62,62,62	7
86	OHX	n3	201	7/7	0.99	0.23	-0.18	55,55,55,55	7
86	OHX	2	2054	7/7	0.97	0.21	-0.18	87,87,87,87	7
86	OHX	1	3558	7/7	0.97	0.20	-0.20	62,62,62,62	7
87	MG	5	3984	1/1	0.83	0.30	-0.21	50,50,50,50	0
87	MG	1	4289	1/1	0.94	0.19	-0.21	57,57,57,57	0
86	OHX	1	3461	7/7	0.99	0.14	-0.21	96,96,96,96	7
87	MG	2	2146	1/1	0.82	0.24	-0.21	86,86,86,86	0
87	MG	N8	204	1/1	0.89	0.28	-0.21	48,48,48,48	0
86	OHX	2	1901	7/7	0.99	0.22	-0.21	81,81,81,81	0
87	MG	1	4077	1/1	0.95	0.20	-0.22	54,54,54,54	0
86	OHX	7	204	7/7	0.99	0.18	-0.23	43,43,43,43	7
86	OHX	1	3624	7/7	0.88	0.26	-0.24	63,63,63,63	7
86	OHX	5	3508	7/7	0.98	0.21	-0.24	38,38,38,38	7
86	OHX	2	1948	7/7	0.98	0.20	-0.24	67,67,67,67	7
86	OHX	5	3443	7/7	0.99	0.15	-0.24	82,82,82,82	7
87	MG	5	4171	1/1	0.91	0.22	-0.25	115,115,115,115	0
86	OHX	2	1916	7/7	0.97	0.17	-0.25	89,89,89,89	7
86	OHX	5	3721	7/7	0.93	0.20	-0.25	50,50,50,50	7
86	OHX	2	2046	7/7	0.88	0.16	-0.25	114,114,114,114	7
86	OHX	6	1901	7/7	1.00	0.21	-0.25	62,62,62,62	0
86	OHX	2	1927	7/7	0.98	0.18	-0.26	94,94,94,94	7
86	OHX	1	3644	7/7	0.97	0.15	-0.26	91,91,91,91	7
87	MG	6	2210	1/1	0.83	0.24	-0.27	79,79,79,79	0
87	MG	c8	202	1/1	0.76	0.28	-0.27	81,81,81,81	0
86	OHX	1	3578	7/7	0.99	0.21	-0.28	40,40,40,40	7
86	OHX	1	3508	7/7	0.98	0.15	-0.28	71,71,71,71	7
86	OHX	2	1967	7/7	0.97	0.20	-0.28	92,92,92,92	7
86	OHX	1	3731	7/7	0.91	0.18	-0.30	100,100,100,100	7
86	OHX	2	1965	7/7	0.95	0.20	-0.30	91,91,91,91	7
86	OHX	1	3426	7/7	0.99	0.19	-0.30	71,71,71,71	7
86	OHX	2	2027	7/7	0.94	0.14	-0.32	111,111,111,111	7
86	OHX	6	1924	7/7	0.99	0.20	-0.33	54,54,54,54	7
86	OHX	O7	103	7/7	0.96	0.24	-0.34	60,60,60,60	7
86	OHX	1	3755	7/7	0.86	0.25	-0.34	79,79,79,79	7
86	OHX	6	1956	7/7	0.97	0.16	-0.35	90,90,90,90	7
86	OHX	5	3412	7/7	0.99	0.19	-0.36	64,64,64,64	7
86	OHX	5	3486	7/7	0.98	0.19	-0.37	64,64,64,64	7
87	MG	S6	301	1/1	0.98	0.23	-0.37	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	1999	7/7	0.93	0.19	-0.37	94,94,94,94	7
86	OHX	1	3784	7/7	0.93	0.20	-0.38	66,66,66,66	7
86	OHX	2	1915	7/7	0.97	0.14	-0.40	122,122,122,122	7
86	OHX	2	1976	7/7	0.97	0.18	-0.40	92,92,92,92	7
86	OHX	1	3430	7/7	0.99	0.21	-0.40	55,55,55,55	7
86	OHX	2	1917	7/7	0.98	0.18	-0.41	85,85,85,85	7
86	OHX	m7	201	7/7	0.92	0.22	-0.41	49,49,49,49	7
86	OHX	2	2028	7/7	0.94	0.17	-0.41	134,134,134,134	7
87	MG	2	2183	1/1	0.95	0.21	-0.42	66,66,66,66	0
86	OHX	1	3489	7/7	1.00	0.16	-0.42	89,89,89,89	7
86	OHX	1	3408	7/7	0.99	0.19	-0.43	59,59,59,59	2
86	OHX	1	3691	7/7	0.96	0.21	-0.44	67,67,67,67	7
87	MG	p0	301	1/1	0.64	0.31	-0.44	93,93,93,93	0
86	OHX	5	3435	7/7	0.99	0.21	-0.44	50,50,50,50	7
86	OHX	1	3554	7/7	0.98	0.20	-0.44	78,78,78,78	7
86	OHX	2	1949	7/7	0.95	0.15	-0.45	108,108,108,108	7
86	OHX	6	2090	7/7	0.97	0.19	-0.45	68,68,68,68	7
87	MG	2	2234	1/1	0.98	0.24	-0.45	76,76,76,76	0
87	MG	5	4121	1/1	0.84	0.20	-0.46	52,52,52,52	0
86	OHX	O7	102	7/7	0.97	0.20	-0.46	73,73,73,73	7
87	MG	1	3885	1/1	0.92	0.23	-0.47	41,41,41,41	0
86	OHX	2	1909	7/7	0.99	0.17	-0.47	94,94,94,94	7
86	OHX	6	1979	7/7	0.96	0.23	-0.47	79,79,79,79	7
87	MG	2	2159	1/1	0.74	0.22	-0.48	75,75,75,75	0
86	OHX	6	1923	7/7	0.99	0.16	-0.48	71,71,71,71	7
86	OHX	6	1952	7/7	0.98	0.16	-0.48	84,84,84,84	7
86	OHX	2	1902	7/7	1.00	0.18	-0.48	86,86,86,86	0
86	OHX	6	2069	7/7	0.96	0.16	-0.49	78,78,78,78	7
86	OHX	2	2068	7/7	0.93	0.20	-0.49	66,66,66,66	7
86	OHX	8	212	7/7	0.95	0.18	-0.49	85,85,85,85	7
86	OHX	5	3413	7/7	0.99	0.17	-0.49	51,51,51,51	7
86	OHX	s1	302	7/7	0.90	0.25	-0.49	93,93,93,93	7
86	OHX	d9	102	7/7	0.95	0.27	-0.50	97,97,97,97	7
87	MG	1	4428	1/1	0.80	0.14	-0.50	67,67,67,67	0
86	OHX	5	3406	7/7	1.00	0.19	-0.50	48,48,48,48	0
86	OHX	5	3670	7/7	0.96	0.18	-0.51	51,51,51,51	7
86	OHX	q2	502	7/7	0.99	0.20	-0.51	51,51,51,51	7
86	OHX	2	2007	7/7	0.94	0.18	-0.52	101,101,101,101	7
86	OHX	2	1958	7/7	0.98	0.19	-0.52	75,75,75,75	7
87	MG	5	4542	1/1	0.90	0.24	-0.52	45,45,45,45	0
86	OHX	5	3441	7/7	0.99	0.18	-0.52	54,54,54,54	7
86	OHX	c5	202	7/7	0.88	0.26	-0.53	98,98,98,98	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3426	7/7	0.99	0.20	-0.54	59,59,59,59	7
86	OHX	L5	301	7/7	0.95	0.18	-0.55	78,78,78,78	7
86	OHX	5	3764	7/7	0.95	0.19	-0.55	71,71,71,71	7
86	OHX	6	1973	7/7	0.97	0.19	-0.55	86,86,86,86	7
86	OHX	12	301	7/7	0.98	0.22	-0.55	63,63,63,63	7
86	OHX	1	3581	7/7	0.98	0.17	-0.56	54,54,54,54	7
86	OHX	L3	403	7/7	0.91	0.23	-0.58	85,85,85,85	7
86	OHX	5	3470	7/7	0.98	0.18	-0.58	90,90,90,90	7
87	MG	1	3838	1/1	0.98	0.23	-0.59	59,59,59,59	0
86	OHX	2	1964	7/7	0.97	0.15	-0.59	101,101,101,101	7
86	OHX	2	1925	7/7	0.98	0.12	-0.60	112,112,112,112	7
86	OHX	2	2065	7/7	0.88	0.15	-0.60	110,110,110,110	7
87	MG	5	3975	1/1	0.90	0.16	-0.61	74,74,74,74	0
86	OHX	6	1917	7/7	0.99	0.20	-0.61	55,55,55,55	7
87	MG	2	2131	1/1	0.97	0.15	-0.62	73,73,73,73	0
86	OHX	2	2057	7/7	0.93	0.23	-0.62	67,67,67,67	7
86	OHX	1	3679	7/7	0.96	0.20	-0.63	42,42,42,42	7
87	MG	c6	202	1/1	0.82	0.25	-0.63	87,87,87,87	0
86	OHX	6	1912	7/7	0.99	0.18	-0.64	72,72,72,72	7
86	OHX	6	2057	7/7	0.94	0.17	-0.64	78,78,78,78	7
86	OHX	5	3754	7/7	0.88	0.16	-0.65	161,161,161,161	7
86	OHX	1	3668	7/7	0.99	0.21	-0.65	50,50,50,50	7
87	MG	2	2179	1/1	0.97	0.18	-0.66	85,85,85,85	0
86	OHX	1	3625	7/7	0.98	0.15	-0.66	61,61,61,61	7
86	OHX	1	3432	7/7	0.99	0.17	-0.66	64,64,64,64	7
86	OHX	5	3545	7/7	0.99	0.20	-0.66	46,46,46,46	7
86	OHX	2	2025	7/7	0.93	0.19	-0.66	94,94,94,94	7
86	OHX	8	203	7/7	0.97	0.17	-0.67	86,86,86,86	7
86	OHX	2	1908	7/7	0.98	0.15	-0.67	104,104,104,104	0
86	OHX	5	3480	7/7	0.98	0.20	-0.70	63,63,63,63	7
87	MG	5	4300	1/1	0.97	0.21	-0.71	32,32,32,32	0
86	OHX	1	3500	7/7	0.99	0.19	-0.71	41,41,41,41	7
86	OHX	5	3521	7/7	0.98	0.18	-0.71	56,56,56,56	7
86	OHX	6	1999	7/7	0.95	0.18	-0.72	85,85,85,85	7
87	MG	Q0	203	1/1	0.94	0.15	-0.72	52,52,52,52	0
86	OHX	1	3715	7/7	0.94	0.18	-0.72	77,77,77,77	7
86	OHX	5	3598	7/7	0.98	0.17	-0.73	73,73,73,73	7
86	OHX	l3	402	7/7	0.94	0.23	-0.73	73,73,73,73	7
86	OHX	M9	201	7/7	0.98	0.19	-0.74	68,68,68,68	7
86	OHX	4	206	7/7	0.99	0.16	-0.74	88,88,88,88	7
86	OHX	2	2042	7/7	0.92	0.16	-0.74	113,113,113,113	7
86	OHX	2	2043	7/7	0.91	0.14	-0.75	119,119,119,119	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	1982	7/7	0.95	0.17	-0.76	98,98,98,98	7
86	OHX	s8	301	7/7	0.94	0.18	-0.77	104,104,104,104	7
87	MG	O1	205	1/1	0.97	0.22	-0.78	65,65,65,65	0
86	OHX	2	1939	7/7	0.98	0.16	-0.78	98,98,98,98	7
88	ZN	q3	501	1/1	0.99	0.15	-0.78	64,64,64,64	0
86	OHX	5	3460	7/7	0.99	0.19	-0.79	68,68,68,68	7
86	OHX	1	3653	7/7	0.98	0.14	-0.79	59,59,59,59	7
86	OHX	6	1910	7/7	1.00	0.19	-0.79	60,60,60,60	7
86	OHX	6	2074	7/7	0.79	0.19	-0.80	108,108,108,108	7
87	MG	5	3908	1/1	0.97	0.15	-0.80	76,76,76,76	0
86	OHX	5	3464	7/7	0.99	0.19	-0.80	45,45,45,45	7
86	OHX	1	3523	7/7	0.98	0.17	-0.81	95,95,95,95	7
86	OHX	6	1971	7/7	0.95	0.16	-0.81	85,85,85,85	7
86	OHX	sR	401	7/7	0.92	0.20	-0.81	122,122,122,122	7
86	OHX	n1	201	7/7	0.99	0.19	-0.81	48,48,48,48	7
86	OHX	2	1903	7/7	0.99	0.18	-0.82	90,90,90,90	0
86	OHX	3	205	7/7	0.97	0.15	-0.82	80,80,80,80	7
86	OHX	D9	102	7/7	0.96	0.19	-0.83	83,83,83,83	7
87	MG	6	2155	1/1	0.97	0.20	-0.84	72,72,72,72	0
86	OHX	1	3467	7/7	0.99	0.12	-0.84	113,113,113,113	7
86	OHX	2	1907	7/7	0.99	0.15	-0.84	93,93,93,93	7
86	OHX	5	3537	7/7	0.97	0.13	-0.85	114,114,114,114	7
87	MG	n0	203	1/1	0.95	0.20	-0.85	41,41,41,41	0
87	MG	1	3868	1/1	0.80	0.23	-0.85	70,70,70,70	0
86	OHX	6	2030	7/7	0.93	0.19	-0.86	105,105,105,105	7
86	OHX	2	2038	7/7	0.94	0.21	-0.87	85,85,85,85	7
86	OHX	5	3547	7/7	0.97	0.12	-0.88	136,136,136,136	7
86	OHX	5	3586	7/7	0.97	0.14	-0.88	83,83,83,83	7
86	OHX	5	3706	7/7	0.97	0.16	-0.88	74,74,74,74	7
86	OHX	6	1927	7/7	0.98	0.13	-0.89	109,109,109,109	7
86	OHX	5	3563	7/7	0.97	0.13	-0.89	93,93,93,93	7
86	OHX	6	2034	7/7	0.81	0.23	-0.89	134,134,134,134	7
86	OHX	l5	301	7/7	0.92	0.17	-0.90	90,90,90,90	7
86	OHX	6	1902	7/7	0.99	0.17	-0.90	77,77,77,77	2
87	MG	L7	301	1/1	0.94	0.18	-0.91	39,39,39,39	0
87	MG	1	4008	1/1	0.99	0.16	-0.91	52,52,52,52	0
86	OHX	2	1921	7/7	0.98	0.15	-0.91	88,88,88,88	7
86	OHX	1	3409	7/7	0.99	0.15	-0.92	58,58,58,58	1
86	OHX	1	3768	7/7	0.92	0.18	-0.92	50,50,50,50	7
86	OHX	2	2035	7/7	0.99	0.16	-0.92	95,95,95,95	7
87	MG	1	4275	1/1	0.98	0.15	-0.92	46,46,46,46	0
86	OHX	L3	402	7/7	0.98	0.18	-0.93	67,67,67,67	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3410	7/7	1.00	0.18	-0.93	53,53,53,53	3
86	OHX	2	1935	7/7	0.97	0.15	-0.93	98,98,98,98	7
86	OHX	1	3597	7/7	0.98	0.19	-0.94	37,37,37,37	7
86	OHX	5	3713	7/7	0.94	0.17	-0.94	70,70,70,70	7
86	OHX	M8	201	7/7	0.95	0.20	-0.94	53,53,53,53	7
86	OHX	2	1980	7/7	0.92	0.25	-0.95	93,93,93,93	7
86	OHX	1	3615	7/7	0.96	0.18	-0.96	68,68,68,68	7
86	OHX	6	1943	7/7	0.98	0.14	-0.97	108,108,108,108	7
87	MG	s4	302	1/1	0.86	0.19	-0.97	55,55,55,55	0
86	OHX	2	1977	7/7	0.98	0.12	-0.97	138,138,138,138	7
86	OHX	5	3717	7/7	0.96	0.18	-1.00	56,56,56,56	7
86	OHX	5	3415	7/7	0.99	0.18	-1.00	74,74,74,74	1
86	OHX	6	1933	7/7	0.97	0.16	-1.01	82,82,82,82	7
86	OHX	1	3698	7/7	0.97	0.20	-1.01	51,51,51,51	7
86	OHX	5	3459	7/7	0.98	0.17	-1.02	80,80,80,80	7
86	OHX	1	3564	7/7	0.98	0.20	-1.02	54,54,54,54	7
87	MG	1	3836	1/1	0.95	0.17	-1.03	38,38,38,38	1
87	MG	6	2102	1/1	0.94	0.12	-1.04	81,81,81,81	0
86	OHX	6	1992	7/7	0.96	0.18	-1.04	71,71,71,71	7
86	OHX	2	1910	7/7	0.98	0.17	-1.05	94,94,94,94	7
86	OHX	1	3412	7/7	1.00	0.20	-1.06	47,47,47,47	7
86	OHX	1	3433	7/7	0.99	0.20	-1.06	53,53,53,53	7
87	MG	6	2198	1/1	0.77	0.19	-1.06	90,90,90,90	0
86	OHX	2	1911	7/7	0.97	0.14	-1.08	109,109,109,109	0
86	OHX	1	3712	7/7	0.98	0.19	-1.09	62,62,62,62	7
87	MG	5	4468	1/1	0.92	0.20	-1.09	43,43,43,43	0
86	OHX	m0	303	7/7	0.93	0.21	-1.10	86,86,86,86	7
87	MG	1	4458	1/1	0.98	0.17	-1.10	47,47,47,47	0
86	OHX	M9	202	7/7	0.97	0.16	-1.10	78,78,78,78	7
86	OHX	2	2047	7/7	0.93	0.17	-1.10	106,106,106,106	7
86	OHX	M0	303	7/7	0.88	0.16	-1.10	96,96,96,96	7
86	OHX	6	2038	7/7	0.94	0.14	-1.11	88,88,88,88	7
88	ZN	Q3	501	1/1	0.99	0.10	-1.11	73,73,73,73	0
86	OHX	2	1991	7/7	0.95	0.13	-1.11	104,104,104,104	7
86	OHX	1	3584	7/7	0.92	0.14	-1.12	106,106,106,106	7
86	OHX	2	2026	7/7	0.95	0.20	-1.12	93,93,93,93	7
86	OHX	C5	201	7/7	0.93	0.19	-1.13	112,112,112,112	7
86	OHX	1	3543	7/7	0.96	0.17	-1.14	64,64,64,64	7
86	OHX	5	3405	7/7	0.99	0.17	-1.15	48,48,48,48	3
86	OHX	1	3719	7/7	0.97	0.17	-1.16	86,86,86,86	7
87	MG	5	4195	1/1	0.94	0.21	-1.16	35,35,35,35	1
86	OHX	2	1946	7/7	0.96	0.12	-1.16	110,110,110,110	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	l5	302	7/7	0.95	0.16	-1.16	88,88,88,88	7
87	MG	5	3965	1/1	0.95	0.16	-1.16	55,55,55,55	0
88	ZN	E1	501	1/1	0.91	0.08	-1.17	132,132,132,132	0
86	OHX	6	2022	7/7	0.76	0.22	-1.17	139,139,139,139	7
87	MG	5	4248	1/1	0.95	0.21	-1.18	39,39,39,39	1
86	OHX	s1	301	7/7	0.99	0.15	-1.18	80,80,80,80	0
87	MG	5	4537	1/1	0.95	0.20	-1.18	38,38,38,38	0
87	MG	6	2240	1/1	0.70	0.15	-1.19	74,74,74,74	0
86	OHX	1	3628	7/7	0.98	0.14	-1.19	74,74,74,74	7
86	OHX	5	3807	7/7	0.98	0.13	-1.19	147,147,147,147	7
86	OHX	6	1951	7/7	0.98	0.13	-1.20	133,133,133,133	7
86	OHX	2	1924	7/7	0.98	0.15	-1.20	89,89,89,89	7
86	OHX	5	3556	7/7	0.97	0.12	-1.20	107,107,107,107	7
86	OHX	2	1943	7/7	0.96	0.15	-1.21	95,95,95,95	7
87	MG	5	4302	1/1	1.00	0.19	-1.22	40,40,40,40	0
86	OHX	1	3572	7/7	0.96	0.15	-1.23	95,95,95,95	7
86	OHX	1	3478	7/7	0.99	0.19	-1.23	58,58,58,58	7
86	OHX	2	1997	7/7	0.98	0.14	-1.23	88,88,88,88	7
86	OHX	2	1993	7/7	0.96	0.18	-1.23	80,80,80,80	7
86	OHX	6	1986	7/7	0.97	0.17	-1.24	73,73,73,73	7
86	OHX	1	3638	7/7	0.97	0.17	-1.29	82,82,82,82	7
86	OHX	C8	202	7/7	0.98	0.14	-1.29	94,94,94,94	7
86	OHX	2	1972	7/7	0.98	0.16	-1.30	81,81,81,81	7
86	OHX	2	1940	7/7	0.98	0.15	-1.30	85,85,85,85	7
87	MG	5	3842	1/1	0.94	0.15	-1.31	45,45,45,45	0
87	MG	c8	203	1/1	0.89	0.12	-1.31	86,86,86,86	0
87	MG	6	2176	1/1	0.94	0.16	-1.32	73,73,73,73	0
86	OHX	6	1922	7/7	0.99	0.16	-1.32	58,58,58,58	7
86	OHX	5	3718	7/7	0.93	0.10	-1.33	136,136,136,136	7
86	OHX	M5	301	7/7	0.98	0.18	-1.34	75,75,75,75	7
87	MG	6	2142	1/1	0.97	0.21	-1.34	73,73,73,73	0
86	OHX	2	1978	7/7	0.97	0.12	-1.34	121,121,121,121	7
87	MG	5	4063	1/1	0.91	0.19	-1.35	37,37,37,37	0
86	OHX	m5	501	7/7	0.98	0.18	-1.35	81,81,81,81	7
87	MG	S4	301	1/1	0.93	0.21	-1.35	76,76,76,76	0
86	OHX	2	1945	7/7	0.97	0.13	-1.36	110,110,110,110	7
86	OHX	2	2003	7/7	0.94	0.16	-1.38	103,103,103,103	7
86	OHX	5	3436	7/7	0.99	0.20	-1.38	54,54,54,54	7
88	ZN	q2	501	1/1	0.97	0.09	-1.41	69,69,69,69	0
87	MG	l9	203	1/1	0.99	0.15	-1.41	46,46,46,46	1
86	OHX	1	3414	7/7	0.99	0.15	-1.41	67,67,67,67	0
88	ZN	o7	501	1/1	1.00	0.14	-1.41	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3530	7/7	0.99	0.14	-1.41	94,94,94,94	7
87	MG	1	4101	1/1	0.93	0.16	-1.41	57,57,57,57	0
87	MG	6	2122	1/1	0.93	0.17	-1.42	49,49,49,49	0
87	MG	5	3909	1/1	0.94	0.18	-1.42	49,49,49,49	0
86	OHX	2	1966	7/7	0.97	0.19	-1.43	61,61,61,61	7
86	OHX	2	2014	7/7	0.97	0.16	-1.43	80,80,80,80	7
86	OHX	SR	401	7/7	0.96	0.12	-1.43	130,130,130,130	7
86	OHX	6	1913	7/7	0.98	0.15	-1.44	85,85,85,85	7
87	MG	6	2205	1/1	0.87	0.14	-1.45	84,84,84,84	0
86	OHX	S8	301	7/7	0.91	0.16	-1.47	108,108,108,108	7
88	ZN	Q0	201	1/1	1.00	0.13	-1.47	53,53,53,53	0
87	MG	1	4029	1/1	0.89	0.16	-1.47	62,62,62,62	0
88	ZN	d9	101	1/1	1.00	0.10	-1.48	81,81,81,81	0
86	OHX	1	3807	7/7	0.94	0.11	-1.50	112,112,112,112	7
86	OHX	2	1950	7/7	0.97	0.17	-1.50	97,97,97,97	7
87	MG	5	4456	1/1	0.93	0.10	-1.51	100,100,100,100	0
88	ZN	O7	101	1/1	0.99	0.14	-1.56	47,47,47,47	0
86	OHX	2	2040	7/7	0.96	0.16	-1.57	88,88,88,88	7
86	OHX	2	1932	7/7	0.97	0.16	-1.57	92,92,92,92	7
86	OHX	M0	304	7/7	0.91	0.15	-1.57	96,96,96,96	7
86	OHX	1	3580	7/7	0.97	0.16	-1.57	89,89,89,89	7
88	ZN	D9	101	1/1	0.99	0.09	-1.58	79,79,79,79	0
87	MG	C8	203	1/1	0.89	0.06	-1.58	96,96,96,96	0
86	OHX	1	3453	7/7	0.99	0.15	-1.59	74,74,74,74	7
88	ZN	q0	201	1/1	0.99	0.15	-1.59	40,40,40,40	0
87	MG	O4	201	1/1	0.93	0.14	-1.60	77,77,77,77	0
87	MG	1	4068	1/1	0.94	0.13	-1.62	62,62,62,62	0
87	MG	O2	204	1/1	0.97	0.18	-1.63	33,33,33,33	0
87	MG	6	2204	1/1	0.96	0.17	-1.65	47,47,47,47	0
87	MG	M0	307	1/1	0.87	0.16	-1.67	45,45,45,45	0
87	MG	5	4076	1/1	0.89	0.19	-1.67	56,56,56,56	0
87	MG	6	2137	1/1	0.92	0.12	-1.68	83,83,83,83	0
88	ZN	d6	500	1/1	0.98	0.08	-1.68	67,67,67,67	0
86	OHX	2	1984	7/7	0.85	0.14	-1.70	177,177,177,177	7
86	OHX	6	1991	7/7	0.96	0.15	-1.71	83,83,83,83	7
86	OHX	5	3689	7/7	0.90	0.12	-1.72	116,116,116,116	7
86	OHX	1	3591	7/7	0.98	0.12	-1.73	90,90,90,90	7
86	OHX	5	3630	7/7	0.98	0.16	-1.73	75,75,75,75	7
88	ZN	D6	101	1/1	0.99	0.07	-1.74	88,88,88,88	0
87	MG	6	2302	1/1	0.92	0.11	-1.76	106,106,106,106	0
86	OHX	5	3427	7/7	1.00	0.17	-1.77	66,66,66,66	7
87	MG	2	2188	1/1	0.92	0.18	-1.77	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
88	ZN	Q2	501	1/1	0.93	0.04	-1.78	73,73,73,73	0
86	OHX	2	1986	7/7	0.98	0.16	-1.79	80,80,80,80	7
86	OHX	2	2037	7/7	0.97	0.16	-1.79	60,60,60,60	7
87	MG	c9	201	1/1	0.83	0.10	-1.80	78,78,78,78	0
87	MG	5	4143	1/1	0.98	0.19	-1.81	34,34,34,34	1
86	OHX	6	2092	7/7	0.89	0.13	-1.81	104,104,104,104	7
86	OHX	1	3814	7/7	0.94	0.17	-1.82	149,149,149,149	7
87	MG	5	3867	1/1	0.94	0.14	-1.83	41,41,41,41	0
86	OHX	1	3494	7/7	0.99	0.17	-1.83	66,66,66,66	7
86	OHX	2	2008	7/7	0.97	0.15	-1.87	83,83,83,83	7
86	OHX	6	1941	7/7	0.98	0.14	-1.99	79,79,79,79	7
87	MG	2	2138	1/1	0.75	0.14	-2.01	76,76,76,76	0
86	OHX	m0	301	7/7	0.98	0.13	-2.04	86,86,86,86	7
86	OHX	5	3707	7/7	0.96	0.16	-2.06	46,46,46,46	7
87	MG	n8	202	1/1	0.82	0.17	-2.06	51,51,51,51	0
87	MG	n3	204	1/1	0.94	0.14	-2.06	42,42,42,42	0
87	MG	2	2143	1/1	0.91	0.08	-2.07	91,91,91,91	0
86	OHX	5	3708	7/7	0.94	0.20	-2.10	43,43,43,43	7
86	OHX	6	2091	7/7	0.96	0.15	-2.13	96,96,96,96	7
87	MG	O7	105	1/1	0.95	0.10	-2.13	51,51,51,51	0
86	OHX	6	1994	7/7	0.97	0.13	-2.14	76,76,76,76	7
86	OHX	5	3640	7/7	0.97	0.14	-2.16	73,73,73,73	7
86	OHX	2	2082	7/7	0.94	0.08	-2.24	137,137,137,137	7
87	MG	5	4205	1/1	0.94	0.11	-2.26	60,60,60,60	0
86	OHX	1	3491	7/7	0.98	0.12	-2.29	118,118,118,118	7
87	MG	2	2165	1/1	0.82	0.18	-2.30	98,98,98,98	0
86	OHX	5	3592	7/7	0.99	0.12	-2.31	63,63,63,63	7
86	OHX	c5	201	7/7	0.92	0.20	-2.34	118,118,118,118	7
86	OHX	6	1907	7/7	0.98	0.14	-2.34	76,76,76,76	0
86	OHX	5	3671	7/7	0.94	0.19	-2.47	56,56,56,56	7
86	OHX	1	3450	7/7	0.99	0.17	-2.48	46,46,46,46	7
88	ZN	e1	501	1/1	0.91	0.04	-2.50	163,163,163,163	0
87	MG	6	2298	1/1	0.98	0.12	-2.51	86,86,86,86	0
86	OHX	1	3590	7/7	0.98	0.12	-2.52	91,91,91,91	7
86	OHX	1	3540	7/7	0.98	0.10	-2.52	128,128,128,128	7
87	MG	6	2190	1/1	0.99	0.16	-2.68	44,44,44,44	0
86	OHX	2	1990	7/7	0.97	0.13	-2.70	111,111,111,111	7
86	OHX	5	3456	7/7	0.98	0.14	-2.70	115,115,115,115	0
86	OHX	1	3537	7/7	0.97	0.12	-2.71	112,112,112,112	7
87	MG	1	4311	1/1	0.97	0.12	-2.76	57,57,57,57	1
87	MG	1	3847	1/1	0.98	0.10	-2.88	49,49,49,49	0
86	OHX	1	3562	7/7	0.99	0.15	-2.91	71,71,71,71	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2064	7/7	0.93	0.08	-2.98	130,130,130,130	7
87	MG	6	2289	1/1	0.91	0.14	-3.03	57,57,57,57	0
87	MG	6	2201	1/1	0.83	0.09	-3.06	83,83,83,83	0
86	OHX	2	1982	7/7	0.98	0.11	-3.12	100,100,100,100	7
86	OHX	6	1970	7/7	0.97	0.13	-3.13	88,88,88,88	7
86	OHX	1	3600	7/7	0.98	0.14	-3.16	68,68,68,68	7
87	MG	5	3826	1/1	0.95	0.14	-3.16	35,35,35,35	0
86	OHX	6	1996	7/7	0.96	0.13	-3.18	90,90,90,90	7
86	OHX	2	1937	7/7	0.97	0.15	-3.40	94,94,94,94	7
87	MG	5	4192	1/1	0.94	0.13	-3.51	36,36,36,36	0
87	MG	1	4326	1/1	0.96	0.14	-3.53	42,42,42,42	0
86	OHX	1	3602	7/7	0.95	0.09	-3.69	152,152,152,152	7
87	MG	1	3846	1/1	0.93	0.18	-3.89	35,35,35,35	0
87	MG	1	3930	1/1	0.96	0.13	-4.10	41,41,41,41	0
87	MG	5	3889	1/1	0.91	0.08	-4.19	111,111,111,111	0
87	MG	5	4441	1/1	0.99	0.14	-4.49	33,33,33,33	0
87	MG	M7	210	1/1	0.98	0.13	-4.99	45,45,45,45	1
87	MG	5	4034	1/1	0.96	0.09	-5.06	45,45,45,45	0
86	OHX	1	3651	7/7	0.93	0.07	-5.10	199,199,199,199	7
87	MG	1	4097	1/1	0.97	0.19	-5.11	42,42,42,42	0
86	OHX	2	1975	7/7	0.99	0.11	-5.12	112,112,112,112	7
87	MG	5	4032	1/1	0.95	0.12	-6.03	49,49,49,49	0
87	MG	1	4168	1/1	0.97	0.15	-6.21	35,35,35,35	1
87	MG	1	4423	1/1	0.92	0.16	-6.71	40,40,40,40	1
86	OHX	8	221	7/7	0.99	0.16	-	74,74,74,74	7
86	OHX	2	1983	7/7	0.97	0.27	-	70,70,70,70	7
87	MG	1	4290	1/1	0.96	0.28	-	40,40,40,40	1
86	OHX	5	3737	7/7	0.90	0.25	-	73,73,73,73	7
87	MG	1	4175	1/1	0.90	0.77	-	46,46,46,46	0
87	MG	1	4459	1/1	0.70	0.35	-	46,46,46,46	1
87	MG	5	3895	1/1	0.96	0.14	-	59,59,59,59	0
87	MG	1	4276	1/1	0.93	0.62	-	37,37,37,37	0
87	MG	6	2160	1/1	0.96	0.42	-	59,59,59,59	0
87	MG	1	4403	1/1	0.96	0.35	-	65,65,65,65	0
87	MG	1	4337	1/1	0.97	0.34	-	42,42,42,42	0
86	OHX	5	3816	7/7	0.97	0.29	-	43,43,43,43	7
87	MG	6	2274	1/1	0.59	0.60	-	42,42,42,42	1
87	MG	3	214	1/1	0.76	0.34	-	46,46,46,46	0
87	MG	1	4263	1/1	0.95	0.20	-	45,45,45,45	1
87	MG	5	4095	1/1	0.93	0.77	-	60,60,60,60	0
86	OHX	5	3775	7/7	0.95	0.24	-	59,59,59,59	7
86	OHX	1	3510	7/7	0.97	0.27	-	93,93,93,93	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	2	2096	1/1	0.87	0.44	-	61,61,61,61	0
87	MG	1	4227	1/1	0.68	0.88	-	45,45,45,45	0
87	MG	2	2201	1/1	0.60	0.51	-	61,61,61,61	0
87	MG	5	3962	1/1	0.90	0.55	-	44,44,44,44	0
87	MG	7	233	1/1	0.93	0.17	-	52,52,52,52	0
87	MG	5	3973	1/1	0.96	0.49	-	34,34,34,34	0
87	MG	1	4419	1/1	0.95	0.45	-	34,34,34,34	1
87	MG	1	4251	1/1	0.90	0.39	-	45,45,45,45	1
86	OHX	1	3714	7/7	0.96	0.29	-	45,45,45,45	7
87	MG	1	3833	1/1	0.97	0.21	-	84,84,84,84	0
87	MG	1	4136	1/1	0.90	0.63	-	58,58,58,58	0
87	MG	5	4064	1/1	0.95	0.22	-	64,64,64,64	0
87	MG	1	3956	1/1	0.94	0.55	-	40,40,40,40	0
87	MG	5	4544	1/1	0.84	0.76	-	37,37,37,37	0
86	OHX	5	3577	7/7	0.91	0.34	-	53,53,53,53	7
86	OHX	8	207	7/7	0.98	0.14	-	74,74,74,74	7
86	OHX	5	3704	7/7	0.94	0.30	-	67,67,67,67	7
86	OHX	5	3665	7/7	0.96	0.48	-	47,47,47,47	7
87	MG	S1	301	1/1	1.00	0.13	-	105,105,105,105	0
87	MG	5	4122	1/1	0.97	0.21	-	48,48,48,48	1
87	MG	2	2153	1/1	0.98	0.23	-	72,72,72,72	0
87	MG	1	3961	1/1	0.94	0.57	-	37,37,37,37	0
87	MG	1	4023	1/1	0.92	0.32	-	45,45,45,45	0
87	MG	8	228	1/1	0.92	0.31	-	46,46,46,46	1
87	MG	5	4307	1/1	0.99	0.23	-	41,41,41,41	1
86	OHX	1	3681	7/7	0.93	0.49	-	56,56,56,56	7
87	MG	19	204	1/1	0.87	0.33	-	41,41,41,41	1
86	OHX	5	3524	7/7	0.98	0.17	-	88,88,88,88	7
87	MG	5	4126	1/1	0.90	0.18	-	55,55,55,55	0
87	MG	6	2147	1/1	0.95	0.43	-	58,58,58,58	0
87	MG	6	2284	1/1	0.81	0.35	-	59,59,59,59	0
87	MG	6	2305	1/1	0.65	0.78	-	98,98,98,98	0
87	MG	1	3863	1/1	0.96	0.36	-	38,38,38,38	0
87	MG	5	4193	1/1	0.95	0.88	-	39,39,39,39	1
87	MG	1	4255	1/1	0.94	0.98	-	48,48,48,48	0
87	MG	1	3864	1/1	0.93	0.60	-	55,55,55,55	0
87	MG	5	4320	1/1	0.95	0.38	-	35,35,35,35	1
87	MG	5	4207	1/1	0.94	0.43	-	62,62,62,62	0
87	MG	1	4042	1/1	0.83	0.21	-	50,50,50,50	0
86	OHX	1	3726	7/7	0.95	0.22	-	54,54,54,54	7
87	MG	6	2177	1/1	0.96	0.29	-	80,80,80,80	0
86	OHX	2	1954	7/7	0.94	0.26	-	88,88,88,88	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4455	1/1	0.77	0.50	-	37,37,37,37	1
87	MG	5	4530	1/1	0.88	0.35	-	43,43,43,43	0
87	MG	6	2152	1/1	0.90	0.45	-	50,50,50,50	0
87	MG	5	4374	1/1	0.93	0.27	-	45,45,45,45	1
87	MG	7	236	1/1	0.89	0.12	-	44,44,44,44	0
87	MG	c9	202	1/1	0.59	0.34	-	80,80,80,80	0
87	MG	2	2249	1/1	0.73	0.63	-	97,97,97,97	0
87	MG	6	2271	1/1	0.80	0.36	-	42,42,42,42	0
86	OHX	1	3713	7/7	0.97	0.30	-	58,58,58,58	7
87	MG	6	2189	1/1	0.85	0.45	-	47,47,47,47	0
86	OHX	5	3498	7/7	0.98	0.17	-	66,66,66,66	7
87	MG	5	4325	1/1	0.96	0.17	-	74,74,74,74	0
86	OHX	5	3567	7/7	0.99	0.27	-	39,39,39,39	7
87	MG	1	3905	1/1	0.97	0.20	-	48,48,48,48	0
87	MG	1	4347	1/1	0.69	0.57	-	41,41,41,41	1
87	MG	1	4057	1/1	0.92	0.51	-	38,38,38,38	0
87	MG	1	4238	1/1	0.89	0.29	-	46,46,46,46	0
87	MG	1	4239	1/1	0.90	0.21	-	45,45,45,45	0
87	MG	1	4336	1/1	0.92	0.42	-	43,43,43,43	0
87	MG	2	2216	1/1	0.64	0.28	-	69,69,69,69	0
87	MG	5	4152	1/1	0.97	0.35	-	40,40,40,40	0
86	OHX	1	3560	7/7	0.92	0.46	-	72,72,72,72	7
87	MG	5	4296	1/1	0.98	0.28	-	48,48,48,48	1
87	MG	1	3883	1/1	0.88	0.41	-	48,48,48,48	0
87	MG	1	4096	1/1	0.92	0.59	-	76,76,76,76	0
89	C	1	3402	20/21	0.83	0.30	-	50,107,109,109	0
86	OHX	5	3646	7/7	0.97	0.35	-	52,52,52,52	7
86	OHX	5	3750	7/7	0.86	0.14	-	131,131,131,131	7
86	OHX	5	3585	7/7	0.97	0.53	-	44,44,44,44	7
86	OHX	1	3571	7/7	0.97	0.25	-	64,64,64,64	7
87	MG	5	4497	1/1	0.98	0.22	-	41,41,41,41	1
86	OHX	5	3769	7/7	0.83	0.54	-	78,78,78,78	7
87	MG	5	3944	1/1	0.99	0.47	-	32,32,32,32	0
86	OHX	1	3440	7/7	0.99	0.14	-	75,75,75,75	7
87	MG	7	217	1/1	0.88	0.64	-	43,43,43,43	0
87	MG	d9	104	1/1	0.81	0.19	-	109,109,109,109	0
86	OHX	5	3536	7/7	0.95	0.39	-	53,53,53,53	7
86	OHX	1	3658	7/7	0.97	0.24	-	49,49,49,49	7
87	MG	5	3873	1/1	0.92	0.52	-	45,45,45,45	0
87	MG	1	3844	1/1	0.90	0.71	-	39,39,39,39	0
87	MG	o3	205	1/1	0.93	0.72	-	35,35,35,35	1
87	MG	5	4125	1/1	0.93	0.36	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	1957	7/7	0.98	0.18	-	63,63,63,63	7
87	MG	1	4169	1/1	0.73	0.46	-	72,72,72,72	0
87	MG	5	4144	1/1	0.96	0.23	-	44,44,44,44	0
87	MG	5	4444	1/1	0.95	0.58	-	39,39,39,39	0
87	MG	m7	203	1/1	0.94	0.37	-	33,33,33,33	0
87	MG	5	4317	1/1	0.86	0.18	-	102,102,102,102	0
87	MG	5	4184	1/1	0.98	0.38	-	40,40,40,40	1
87	MG	5	4421	1/1	0.87	0.17	-	46,46,46,46	0
87	MG	5	4109	1/1	0.90	0.35	-	40,40,40,40	0
87	MG	1	3968	1/1	0.90	0.29	-	43,43,43,43	0
86	OHX	1	3606	7/7	0.95	0.26	-	68,68,68,68	7
86	OHX	5	3576	7/7	0.99	0.16	-	56,56,56,56	7
87	MG	6	2243	1/1	0.96	0.39	-	68,68,68,68	0
87	MG	5	4087	1/1	0.76	0.48	-	36,36,36,36	0
87	MG	5	4281	1/1	0.76	0.54	-	44,44,44,44	1
87	MG	3	215	1/1	0.97	0.40	-	51,51,51,51	0
87	MG	5	4496	1/1	0.97	0.13	-	57,57,57,57	0
87	MG	6	2237	1/1	0.87	0.25	-	55,55,55,55	0
86	OHX	5	3762	7/7	0.70	0.44	-	53,53,53,53	7
87	MG	M7	211	1/1	0.68	0.22	-	75,75,75,75	0
87	MG	1	4486	1/1	0.77	0.23	-	53,53,53,53	0
86	OHX	2	1929	7/7	0.98	0.28	-	66,66,66,66	7
87	MG	1	4491	1/1	0.95	0.14	-	36,36,36,36	0
87	MG	5	4433	1/1	0.96	0.66	-	45,45,45,45	1
87	MG	5	3827	1/1	0.90	0.71	-	46,46,46,46	0
87	MG	5	4460	1/1	1.00	0.30	-	62,62,62,62	0
87	MG	6	2276	1/1	0.94	0.52	-	40,40,40,40	0
87	MG	6	2105	1/1	0.97	0.38	-	49,49,49,49	0
86	OHX	2	1955	7/7	0.96	0.18	-	91,91,91,91	7
86	OHX	C3	201	7/7	0.93	0.33	-	99,99,99,99	7
87	MG	1	3988	1/1	0.86	0.26	-	42,42,42,42	0
87	MG	1	4466	1/1	0.82	0.51	-	43,43,43,43	0
87	MG	1	4327	1/1	0.93	0.45	-	51,51,51,51	0
87	MG	5	4223	1/1	0.78	0.26	-	53,53,53,53	0
87	MG	1	4247	1/1	0.92	0.90	-	44,44,44,44	1
87	MG	5	4274	1/1	0.95	0.33	-	46,46,46,46	0
87	MG	6	2186	1/1	0.97	0.32	-	53,53,53,53	0
87	MG	1	3875	1/1	0.96	0.62	-	35,35,35,35	0
87	MG	1	4052	1/1	0.82	0.41	-	49,49,49,49	0
87	MG	7	224	1/1	0.93	0.38	-	55,55,55,55	0
87	MG	1	4373	1/1	0.90	0.33	-	69,69,69,69	0
87	MG	5	3907	1/1	0.90	0.69	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4053	1/1	0.98	0.23	-	44,44,44,44	0
87	MG	7	216	1/1	0.99	0.33	-	53,53,53,53	0
87	MG	6	2214	1/1	0.85	0.57	-	79,79,79,79	0
87	MG	6	2132	1/1	0.88	0.35	-	69,69,69,69	0
87	MG	5	4082	1/1	0.76	0.19	-	62,62,62,62	0
87	MG	1	3960	1/1	0.91	0.61	-	43,43,43,43	0
87	MG	5	4431	1/1	0.98	0.39	-	44,44,44,44	1
86	OHX	6	2051	7/7	0.90	0.36	-	82,82,82,82	7
87	MG	5	4383	1/1	0.91	0.27	-	53,53,53,53	0
86	OHX	2	2039	7/7	0.93	0.18	-	103,103,103,103	7
87	MG	5	4366	1/1	0.93	0.49	-	41,41,41,41	0
87	MG	6	2113	1/1	0.79	0.18	-	75,75,75,75	0
87	MG	5	3976	1/1	0.95	0.40	-	41,41,41,41	0
86	OHX	5	3599	7/7	0.98	0.15	-	56,56,56,56	7
86	OHX	2	1906	7/7	0.99	0.17	-	82,82,82,82	7
87	MG	5	3897	1/1	0.99	0.28	-	52,52,52,52	0
86	OHX	1	3481	7/7	0.98	0.23	-	88,88,88,88	7
87	MG	d5	201	1/1	0.05	0.31	-	124,124,124,124	0
87	MG	17	304	1/1	0.92	0.14	-	49,49,49,49	1
86	OHX	2	1928	7/7	0.98	0.27	-	75,75,75,75	7
87	MG	1	3842	1/1	0.95	0.63	-	45,45,45,45	0
87	MG	5	3865	1/1	0.88	0.52	-	44,44,44,44	0
86	OHX	8	214	7/7	0.95	0.18	-	100,100,100,100	7
87	MG	6	2322	1/1	0.99	0.20	-	62,62,62,62	0
87	MG	5	4546	1/1	0.98	0.35	-	34,34,34,34	1
87	MG	6	2263	1/1	0.92	0.77	-	40,40,40,40	0
87	MG	2	2231	1/1	0.94	0.30	-	82,82,82,82	0
87	MG	5	3850	1/1	0.78	0.37	-	65,65,65,65	0
87	MG	L8	301	1/1	0.87	0.54	-	82,82,82,82	0
86	OHX	2	2017	7/7	0.97	0.13	-	108,108,108,108	7
87	MG	5	4378	1/1	0.91	0.20	-	55,55,55,55	0
86	OHX	1	3616	7/7	0.96	0.29	-	60,60,60,60	7
87	MG	5	4151	1/1	0.89	0.39	-	52,52,52,52	0
86	OHX	8	215	7/7	0.94	0.51	-	48,48,48,48	7
87	MG	6	2178	1/1	0.87	0.32	-	54,54,54,54	0
87	MG	5	4466	1/1	0.91	0.33	-	39,39,39,39	0
87	MG	1	3949	1/1	0.96	0.46	-	31,31,31,31	0
87	MG	1	4003	1/1	0.91	0.46	-	44,44,44,44	0
87	MG	5	4445	1/1	0.97	0.36	-	32,32,32,32	1
86	OHX	1	3777	7/7	0.90	0.31	-	68,68,68,68	7
87	MG	15	306	1/1	0.71	0.31	-	54,54,54,54	0
86	OHX	5	3553	7/7	0.98	0.14	-	84,84,84,84	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3854	1/1	0.70	0.50	-	72,72,72,72	0
89	C	5	3402	20/21	0.87	0.28	-	43,100,102,102	0
87	MG	5	4119	1/1	0.93	0.33	-	61,61,61,61	0
87	MG	5	3885	1/1	0.86	0.34	-	58,58,58,58	0
87	MG	1	4322	1/1	0.71	0.35	-	65,65,65,65	0
86	OHX	5	3601	7/7	0.96	0.18	-	89,89,89,89	7
86	OHX	5	3469	7/7	0.99	0.23	-	49,49,49,49	7
87	MG	5	3910	1/1	0.76	0.18	-	88,88,88,88	0
87	MG	5	4180	1/1	0.87	0.32	-	51,51,51,51	0
87	MG	5	3918	1/1	0.90	0.58	-	50,50,50,50	0
87	MG	5	3917	1/1	0.87	0.21	-	39,39,39,39	0
86	OHX	6	2065	7/7	0.89	0.17	-	129,129,129,129	7
87	MG	1	4320	1/1	0.89	0.68	-	36,36,36,36	1
87	MG	5	4219	1/1	0.88	0.54	-	39,39,39,39	0
87	MG	5	4090	1/1	0.79	0.13	-	52,52,52,52	0
87	MG	1	3903	1/1	0.91	0.49	-	51,51,51,51	0
87	MG	5	3995	1/1	0.98	0.64	-	34,34,34,34	0
87	MG	1	4069	1/1	0.92	0.16	-	56,56,56,56	0
87	MG	1	3843	1/1	0.98	0.51	-	43,43,43,43	0
87	MG	1	4456	1/1	0.95	0.64	-	56,56,56,56	1
86	OHX	3	210	7/7	0.94	0.26	-	53,53,53,53	7
87	MG	5	3904	1/1	0.90	0.34	-	44,44,44,44	0
87	MG	1	4099	1/1	0.92	0.20	-	59,59,59,59	0
86	OHX	2	2022	7/7	0.93	0.25	-	66,66,66,66	7
87	MG	1	4484	1/1	0.60	0.73	-	49,49,49,49	1
87	MG	L3	408	1/1	0.96	0.81	-	53,53,53,53	1
87	MG	1	4067	1/1	0.73	0.46	-	71,71,71,71	0
86	OHX	1	3607	7/7	0.95	0.19	-	55,55,55,55	7
87	MG	6	2253	1/1	0.92	0.46	-	47,47,47,47	0
87	MG	5	4523	1/1	0.91	0.26	-	43,43,43,43	1
87	MG	5	4043	1/1	0.86	0.38	-	37,37,37,37	0
86	OHX	5	3570	7/7	0.97	0.12	-	98,98,98,98	7
87	MG	1	3895	1/1	0.86	0.51	-	44,44,44,44	0
87	MG	1	4500	1/1	0.91	0.13	-	49,49,49,49	0
87	MG	8	230	1/1	0.90	0.19	-	72,72,72,72	0
86	OHX	1	3665	7/7	0.96	0.36	-	59,59,59,59	7
87	MG	5	4382	1/1	0.94	0.53	-	47,47,47,47	0
86	OHX	1	3634	7/7	0.96	0.08	-	121,121,121,121	7
86	OHX	5	3513	7/7	0.97	0.10	-	107,107,107,107	7
87	MG	1	3834	1/1	0.77	0.62	-	71,71,71,71	0
87	MG	5	4301	1/1	0.89	0.38	-	37,37,37,37	0
87	MG	5	4526	1/1	0.97	0.28	-	51,51,51,51	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	M1	201	1/1	0.49	0.28	-	73,73,73,73	0
87	MG	5	4398	1/1	0.98	0.25	-	38,38,38,38	1
87	MG	D6	102	1/1	0.93	0.79	-	77,77,77,77	0
87	MG	5	4020	1/1	0.93	0.50	-	30,30,30,30	0
87	MG	O2	201	1/1	0.94	0.44	-	30,30,30,30	0
86	OHX	1	3693	7/7	0.96	0.32	-	81,81,81,81	7
86	OHX	1	3699	7/7	0.92	0.24	-	44,44,44,44	7
86	OHX	1	3515	7/7	0.98	0.21	-	98,98,98,98	7
86	OHX	1	3563	7/7	0.98	0.30	-	50,50,50,50	7
87	MG	1	4188	1/1	0.91	0.31	-	47,47,47,47	0
87	MG	5	4340	1/1	0.96	0.56	-	34,34,34,34	0
87	MG	5	4364	1/1	0.99	0.17	-	35,35,35,35	1
87	MG	1	4237	1/1	0.93	0.41	-	54,54,54,54	0
87	MG	6	2109	1/1	0.94	0.35	-	47,47,47,47	0
87	MG	5	4267	1/1	0.88	0.37	-	38,38,38,38	0
86	OHX	2	2034	7/7	0.83	0.41	-	86,86,86,86	7
87	MG	5	4408	1/1	0.56	0.57	-	57,57,57,57	0
87	MG	2	2229	1/1	0.95	0.14	-	84,84,84,84	0
87	MG	1	3927	1/1	0.96	0.87	-	40,40,40,40	0
86	OHX	6	2076	7/7	0.79	0.40	-	74,74,74,74	7
86	OHX	6	2058	7/7	0.94	0.18	-	148,148,148,148	7
87	MG	6	2304	1/1	0.62	0.37	-	52,52,52,52	1
87	MG	5	3821	1/1	0.92	0.58	-	54,54,54,54	0
86	OHX	5	3461	7/7	0.97	0.32	-	72,72,72,72	7
87	MG	1	4051	1/1	0.97	0.30	-	41,41,41,41	0
87	MG	1	4448	1/1	0.96	0.29	-	37,37,37,37	1
87	MG	M0	309	1/1	0.65	0.48	-	46,46,46,46	1
91	PRO	1	3404	7/8	0.85	0.29	-	75,75,75,75	0
87	MG	1	4108	1/1	0.92	0.34	-	56,56,56,56	0
87	MG	5	3994	1/1	0.99	0.64	-	21,21,21,21	0
87	MG	2	2094	1/1	0.90	0.50	-	62,62,62,62	0
87	MG	1	4180	1/1	0.79	0.27	-	58,58,58,58	0
87	MG	1	4482	1/1	0.90	0.48	-	46,46,46,46	0
87	MG	l3	409	1/1	0.87	0.43	-	41,41,41,41	1
86	OHX	6	2025	7/7	0.91	0.17	-	113,113,113,113	7
87	MG	6	2168	1/1	0.76	0.33	-	59,59,59,59	0
87	MG	1	4141	1/1	0.82	0.27	-	51,51,51,51	0
87	MG	1	4264	1/1	0.85	0.53	-	53,53,53,53	0
86	OHX	6	2089	7/7	0.84	0.30	-	74,74,74,74	7
87	MG	1	4305	1/1	0.91	0.38	-	59,59,59,59	0
87	MG	2	2189	1/1	0.94	0.23	-	94,94,94,94	0
86	OHX	1	3636	7/7	0.96	0.26	-	75,75,75,75	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4463	1/1	0.99	0.26	-	51,51,51,51	0
87	MG	6	2290	1/1	0.84	0.29	-	52,52,52,52	0
87	MG	1	4455	1/1	0.94	0.40	-	43,43,43,43	0
87	MG	5	3875	1/1	0.98	0.49	-	31,31,31,31	0
87	MG	7	237	1/1	0.72	0.36	-	53,53,53,53	1
87	MG	1	4249	1/1	0.96	0.16	-	54,54,54,54	0
87	MG	1	4301	1/1	0.83	0.68	-	52,52,52,52	0
87	MG	5	4545	1/1	0.83	0.42	-	34,34,34,34	1
86	OHX	2	1934	7/7	0.98	0.19	-	103,103,103,103	7
86	OHX	1	3446	7/7	0.98	0.22	-	65,65,65,65	7
86	OHX	5	3800	7/7	0.92	0.21	-	87,87,87,87	7
86	OHX	5	3644	7/7	0.94	0.32	-	47,47,47,47	7
87	MG	1	3995	1/1	0.96	0.72	-	36,36,36,36	0
87	MG	1	4223	1/1	0.99	0.24	-	37,37,37,37	1
87	MG	5	3878	1/1	0.96	0.58	-	54,54,54,54	0
87	MG	1	4205	1/1	0.99	0.20	-	52,52,52,52	1
87	MG	5	4318	1/1	0.81	0.30	-	64,64,64,64	0
86	OHX	6	2048	7/7	0.94	0.29	-	51,51,51,51	7
87	MG	2	2171	1/1	0.89	0.37	-	90,90,90,90	0
87	MG	5	4521	1/1	0.88	0.57	-	59,59,59,59	0
87	MG	1	4293	1/1	0.55	0.22	-	127,127,127,127	0
87	MG	5	4430	1/1	0.95	0.32	-	45,45,45,45	0
87	MG	6	2233	1/1	0.90	0.47	-	83,83,83,83	0
87	MG	1	4214	1/1	0.54	0.41	-	36,36,36,36	0
86	OHX	1	3740	7/7	0.94	0.38	-	70,70,70,70	7
87	MG	5	4397	1/1	0.51	0.47	-	38,38,38,38	1
87	MG	1	3841	1/1	0.92	0.25	-	55,55,55,55	0
87	MG	5	4387	1/1	0.92	0.31	-	45,45,45,45	0
87	MG	1	4018	1/1	0.89	0.58	-	30,30,30,30	0
87	MG	s1	303	1/1	0.97	0.17	-	77,77,77,77	0
86	OHX	1	3735	7/7	0.85	0.49	-	71,71,71,71	7
87	MG	5	4464	1/1	0.76	0.38	-	66,66,66,66	0
86	OHX	6	1965	7/7	0.98	0.15	-	83,83,83,83	7
86	OHX	1	3482	7/7	0.99	0.20	-	59,59,59,59	7
87	MG	5	4262	1/1	0.75	0.48	-	39,39,39,39	0
86	OHX	5	3449	7/7	0.99	0.19	-	72,72,72,72	7
86	OHX	5	3551	7/7	0.96	0.20	-	66,66,66,66	7
87	MG	2	2203	1/1	0.77	0.14	-	85,85,85,85	0
86	OHX	2	1995	7/7	0.98	0.19	-	86,86,86,86	7
87	MG	1	4119	1/1	0.92	0.23	-	52,52,52,52	0
87	MG	5	3948	1/1	0.92	0.60	-	24,24,24,24	0
87	MG	1	3862	1/1	0.88	0.41	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3957	1/1	0.97	0.46	-	34,34,34,34	0
86	OHX	5	3451	7/7	0.99	0.28	-	43,43,43,43	7
86	OHX	5	3639	7/7	0.92	0.27	-	138,138,138,138	7
87	MG	1	4048	1/1	0.95	0.28	-	44,44,44,44	0
87	MG	5	3932	1/1	0.93	0.22	-	39,39,39,39	0
86	OHX	1	3766	7/7	0.90	0.23	-	59,59,59,59	7
87	MG	5	4391	1/1	0.85	0.42	-	52,52,52,52	0
87	MG	5	4003	1/1	0.98	0.62	-	27,27,27,27	0
87	MG	1	4443	1/1	0.79	0.52	-	41,41,41,41	1
87	MG	5	4056	1/1	0.94	0.40	-	40,40,40,40	0
87	MG	1	4221	1/1	0.90	0.35	-	43,43,43,43	0
87	MG	2	2212	1/1	0.90	0.75	-	86,86,86,86	0
86	OHX	1	3559	7/7	0.95	0.23	-	90,90,90,90	7
87	MG	1	4308	1/1	0.98	0.36	-	55,55,55,55	0
86	OHX	5	3479	7/7	0.97	0.22	-	79,79,79,79	7
87	MG	5	4412	1/1	0.83	0.40	-	39,39,39,39	0
86	OHX	8	220	7/7	0.87	0.28	-	77,77,77,77	7
87	MG	1	3888	1/1	0.98	0.22	-	66,66,66,66	0
86	OHX	1	3718	7/7	0.94	0.32	-	73,73,73,73	7
87	MG	5	4065	1/1	0.97	0.11	-	39,39,39,39	0
87	MG	6	2249	1/1	0.83	0.24	-	53,53,53,53	0
87	MG	5	4067	1/1	0.68	0.49	-	54,54,54,54	0
87	MG	6	2288	1/1	0.98	0.14	-	65,65,65,65	0
87	MG	2	2162	1/1	0.77	0.69	-	85,85,85,85	0
87	MG	5	4253	1/1	0.89	0.35	-	44,44,44,44	0
87	MG	6	2300	1/1	0.49	0.31	-	82,82,82,82	0
87	MG	5	4194	1/1	0.95	0.34	-	39,39,39,39	0
86	OHX	1	3676	7/7	0.93	0.22	-	71,71,71,71	7
86	OHX	5	3736	7/7	0.95	0.18	-	93,93,93,93	7
87	MG	8	233	1/1	0.83	0.13	-	88,88,88,88	0
87	MG	5	4450	1/1	0.99	0.21	-	44,44,44,44	0
86	OHX	5	3781	7/7	0.88	0.26	-	53,53,53,53	7
87	MG	6	2171	1/1	0.95	0.22	-	79,79,79,79	0
86	OHX	5	3548	7/7	0.97	0.30	-	48,48,48,48	7
87	MG	5	4084	1/1	0.96	0.23	-	41,41,41,41	0
87	MG	5	3845	1/1	0.89	0.30	-	46,46,46,46	0
87	MG	5	4484	1/1	0.88	0.28	-	39,39,39,39	1
87	MG	6	2254	1/1	0.98	0.21	-	53,53,53,53	0
87	MG	L3	407	1/1	0.91	0.32	-	51,51,51,51	1
87	MG	2	2106	1/1	0.97	0.24	-	60,60,60,60	0
87	MG	5	4004	1/1	0.97	0.59	-	42,42,42,42	0
87	MG	6	2269	1/1	0.97	0.12	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3640	7/7	0.98	0.32	-	83,83,83,83	7
86	OHX	6	2021	7/7	0.97	0.23	-	53,53,53,53	7
87	MG	1	3878	1/1	0.92	0.56	-	46,46,46,46	0
86	OHX	5	3759	7/7	0.88	0.13	-	110,110,110,110	7
87	MG	5	4304	1/1	0.86	0.14	-	70,70,70,70	0
87	MG	1	4407	1/1	1.00	0.11	-	47,47,47,47	1
87	MG	1	4274	1/1	0.86	0.86	-	43,43,43,43	1
87	MG	2	2113	1/1	0.70	0.62	-	68,68,68,68	0
86	OHX	6	2063	7/7	0.90	0.54	-	77,77,77,77	7
87	MG	5	3906	1/1	0.96	0.53	-	48,48,48,48	0
87	MG	5	4093	1/1	0.95	0.79	-	34,34,34,34	0
87	MG	1	4217	1/1	0.62	0.98	-	39,39,39,39	1
87	MG	5	4077	1/1	0.94	0.26	-	34,34,34,34	0
87	MG	1	4150	1/1	0.79	0.22	-	73,73,73,73	0
87	MG	5	4298	1/1	0.93	0.13	-	106,106,106,106	0
86	OHX	6	2005	7/7	0.95	0.21	-	80,80,80,80	7
87	MG	5	4155	1/1	0.66	0.29	-	80,80,80,80	0
86	OHX	4	215	7/7	0.92	0.23	-	74,74,74,74	7
87	MG	1	4254	1/1	0.98	0.30	-	51,51,51,51	0
87	MG	2	2223	1/1	0.88	0.40	-	69,69,69,69	0
87	MG	5	3870	1/1	0.97	0.49	-	34,34,34,34	0
87	MG	5	4500	1/1	0.89	0.22	-	54,54,54,54	0
87	MG	1	3852	1/1	0.95	0.70	-	30,30,30,30	0
86	OHX	1	3792	7/7	0.95	0.16	-	147,147,147,147	7
86	OHX	2	2024	7/7	0.90	0.28	-	91,91,91,91	7
87	MG	1	4429	1/1	0.96	0.42	-	49,49,49,49	1
87	MG	1	4493	1/1	0.86	0.25	-	46,46,46,46	0
86	OHX	6	2042	7/7	0.91	0.48	-	54,54,54,54	7
87	MG	1	4375	1/1	0.94	0.57	-	43,43,43,43	1
87	MG	5	4334	1/1	0.98	0.41	-	37,37,37,37	0
87	MG	5	4050	1/1	0.76	0.53	-	42,42,42,42	0
87	MG	5	4201	1/1	0.94	0.19	-	43,43,43,43	0
86	OHX	5	3604	7/7	0.94	0.27	-	70,70,70,70	7
87	MG	5	4356	1/1	0.98	0.69	-	45,45,45,45	0
87	MG	5	4185	1/1	0.89	0.22	-	50,50,50,50	0
87	MG	5	4240	1/1	0.92	0.38	-	37,37,37,37	1
87	MG	6	2234	1/1	0.83	0.22	-	79,79,79,79	0
87	MG	6	2187	1/1	0.92	0.29	-	77,77,77,77	0
87	MG	5	4222	1/1	0.72	0.42	-	49,49,49,49	0
86	OHX	5	3726	7/7	0.90	0.23	-	62,62,62,62	7
87	MG	5	4393	1/1	0.93	0.42	-	34,34,34,34	0
87	MG	5	3923	1/1	0.89	0.23	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3612	7/7	0.97	0.34	-	46,46,46,46	7
87	MG	m5	504	1/1	0.93	0.15	-	45,45,45,45	0
87	MG	2	2251	1/1	0.87	0.44	-	59,59,59,59	1
87	MG	1	4131	1/1	0.93	0.24	-	63,63,63,63	0
87	MG	5	4570	1/1	0.90	0.44	-	50,50,50,50	0
87	MG	5	4190	1/1	0.90	0.40	-	44,44,44,44	1
86	OHX	5	3696	7/7	0.94	0.27	-	49,49,49,49	7
87	MG	1	4344	1/1	0.95	0.22	-	40,40,40,40	0
87	MG	5	4062	1/1	0.91	0.45	-	39,39,39,39	0
87	MG	1	3880	1/1	0.93	0.24	-	49,49,49,49	0
86	OHX	1	3767	7/7	0.90	0.28	-	45,45,45,45	7
86	OHX	1	3765	7/7	0.96	0.20	-	93,93,93,93	7
87	MG	2	2160	1/1	0.93	0.29	-	67,67,67,67	0
87	MG	2	2225	1/1	0.62	0.52	-	58,58,58,58	1
86	OHX	5	3629	7/7	0.81	0.49	-	67,67,67,67	7
87	MG	1	3825	1/1	0.91	0.50	-	38,38,38,38	0
87	MG	L3	405	1/1	0.96	0.25	-	42,42,42,42	0
87	MG	6	2117	1/1	0.93	0.38	-	61,61,61,61	0
87	MG	5	4386	1/1	0.84	0.42	-	37,37,37,37	1
87	MG	1	3855	1/1	0.97	0.39	-	32,32,32,32	0
87	MG	5	4147	1/1	0.98	0.51	-	36,36,36,36	0
86	OHX	6	2079	7/7	0.89	0.31	-	60,60,60,60	7
87	MG	1	4240	1/1	0.88	0.27	-	46,46,46,46	0
87	MG	1	3948	1/1	0.96	0.18	-	34,34,34,34	0
87	MG	6	2291	1/1	0.96	0.32	-	65,65,65,65	0
87	MG	5	4518	1/1	0.90	0.80	-	41,41,41,41	0
86	OHX	6	1938	7/7	0.96	0.19	-	69,69,69,69	7
87	MG	1	4300	1/1	0.75	0.37	-	46,46,46,46	0
87	MG	6	2286	1/1	0.88	0.12	-	65,65,65,65	0
87	MG	1	4125	1/1	0.90	0.43	-	35,35,35,35	0
87	MG	5	4251	1/1	0.88	0.27	-	51,51,51,51	0
87	MG	1	4506	1/1	0.71	0.23	-	94,94,94,94	0
87	MG	1	3964	1/1	0.79	0.60	-	51,51,51,51	0
87	MG	5	4440	1/1	0.86	0.40	-	33,33,33,33	0
87	MG	Q2	505	1/1	0.91	0.20	-	45,45,45,45	1
87	MG	3	229	1/1	0.76	0.52	-	52,52,52,52	1
87	MG	5	4216	1/1	0.99	0.17	-	44,44,44,44	0
87	MG	1	4144	1/1	0.84	0.43	-	41,41,41,41	0
87	MG	5	4145	1/1	0.88	0.33	-	49,49,49,49	0
87	MG	N6	201	1/1	0.78	0.29	-	63,63,63,63	0
87	MG	1	3969	1/1	0.91	0.32	-	41,41,41,41	0
87	MG	1	3926	1/1	0.98	0.49	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	7	220	1/1	0.87	0.21	-	58,58,58,58	0
87	MG	6	2244	1/1	0.75	0.29	-	53,53,53,53	0
86	OHX	1	3460	7/7	0.98	0.27	-	60,60,60,60	7
87	MG	6	2162	1/1	0.79	0.46	-	53,53,53,53	0
87	MG	6	2332	1/1	0.30	0.25	-	213,213,213,213	0
87	MG	5	4565	1/1	0.95	0.24	-	37,37,37,37	0
87	MG	1	4104	1/1	0.87	0.51	-	52,52,52,52	0
87	MG	L3	404	1/1	0.95	0.42	-	42,42,42,42	1
87	MG	5	4449	1/1	0.82	0.33	-	48,48,48,48	0
87	MG	2	2124	1/1	0.85	0.51	-	77,77,77,77	0
87	MG	6	2139	1/1	0.87	0.64	-	63,63,63,63	0
87	MG	6	2213	1/1	0.97	0.79	-	68,68,68,68	1
87	MG	1	4285	1/1	0.92	0.63	-	52,52,52,52	0
87	MG	6	2333	1/1	0.37	0.49	-	59,59,59,59	1
86	OHX	1	3772	7/7	0.82	0.41	-	61,61,61,61	7
86	OHX	1	3775	7/7	0.90	0.23	-	84,84,84,84	7
87	MG	M9	205	1/1	0.95	0.51	-	68,68,68,68	1
87	MG	L4	404	1/1	0.95	0.62	-	42,42,42,42	1
87	MG	5	3839	1/1	0.98	0.48	-	55,55,55,55	0
87	MG	6	2236	1/1	1.00	0.18	-	54,54,54,54	0
87	MG	1	4502	1/1	0.90	0.24	-	46,46,46,46	0
87	MG	5	4388	1/1	0.86	0.27	-	40,40,40,40	0
87	MG	D0	201	1/1	0.82	0.47	-	71,71,71,71	0
87	MG	5	4516	1/1	0.70	0.48	-	62,62,62,62	1
86	OHX	1	3706	7/7	0.96	0.69	-	60,60,60,60	7
87	MG	5	4149	1/1	0.84	0.43	-	50,50,50,50	0
86	OHX	8	217	7/7	0.90	0.24	-	82,82,82,82	7
87	MG	1	4055	1/1	0.70	0.36	-	51,51,51,51	0
87	MG	5	4130	1/1	0.81	0.37	-	35,35,35,35	1
86	OHX	1	3664	7/7	0.95	0.40	-	65,65,65,65	7
87	MG	1	4233	1/1	0.91	0.15	-	63,63,63,63	0
87	MG	5	3831	1/1	0.96	0.19	-	43,43,43,43	0
87	MG	2	2118	1/1	0.83	0.95	-	46,46,46,46	0
87	MG	O7	104	1/1	0.92	0.22	-	81,81,81,81	0
86	OHX	1	3568	7/7	0.97	0.13	-	79,79,79,79	7
86	OHX	5	3643	7/7	0.96	0.32	-	53,53,53,53	7
86	OHX	1	3782	7/7	0.92	0.48	-	55,55,55,55	7
87	MG	1	4287	1/1	0.90	0.24	-	40,40,40,40	1
87	MG	5	4555	1/1	0.82	0.21	-	53,53,53,53	0
87	MG	5	4254	1/1	0.91	0.32	-	38,38,38,38	1
86	OHX	6	1905	7/7	0.99	0.18	-	74,74,74,74	0
87	MG	1	3892	1/1	0.87	0.43	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3569	7/7	0.97	0.16	-	79,79,79,79	7
87	MG	6	2146	1/1	0.98	0.49	-	37,37,37,37	0
87	MG	2	2238	1/1	0.94	0.32	-	89,89,89,89	0
87	MG	6	2217	1/1	0.92	0.63	-	66,66,66,66	0
86	OHX	2	1970	7/7	0.96	0.22	-	89,89,89,89	7
87	MG	M3	201	1/1	0.94	0.23	-	45,45,45,45	0
86	OHX	1	3565	7/7	0.98	0.32	-	84,84,84,84	7
87	MG	1	4267	1/1	0.95	0.28	-	36,36,36,36	0
86	OHX	5	3774	7/7	0.96	0.15	-	66,66,66,66	7
86	OHX	5	3755	7/7	0.79	0.65	-	49,49,49,49	7
87	MG	1	4338	1/1	0.93	0.63	-	37,37,37,37	1
87	MG	1	4102	1/1	0.92	0.57	-	44,44,44,44	0
87	MG	6	2216	1/1	0.94	0.18	-	86,86,86,86	0
87	MG	1	4190	1/1	0.90	0.32	-	65,65,65,65	0
87	MG	6	2175	1/1	0.88	0.22	-	56,56,56,56	0
86	OHX	5	3664	7/7	0.95	0.24	-	63,63,63,63	7
87	MG	5	4293	1/1	0.84	0.62	-	43,43,43,43	0
87	MG	5	4561	1/1	0.86	0.29	-	41,41,41,41	0
87	MG	5	4103	1/1	0.84	0.68	-	35,35,35,35	0
87	MG	4	240	1/1	0.91	0.19	-	57,57,57,57	0
87	MG	5	4012	1/1	0.94	0.47	-	33,33,33,33	0
87	MG	1	4252	1/1	0.85	0.28	-	58,58,58,58	0
86	OHX	1	3496	7/7	0.99	0.27	-	45,45,45,45	7
86	OHX	2	1961	7/7	0.94	0.15	-	112,112,112,112	7
86	OHX	5	3473	7/7	0.99	0.16	-	61,61,61,61	7
87	MG	5	3929	1/1	0.98	0.49	-	39,39,39,39	0
87	MG	6	2314	1/1	0.93	0.38	-	48,48,48,48	0
87	MG	1	4213	1/1	0.93	0.38	-	35,35,35,35	0
87	MG	1	4209	1/1	0.92	0.24	-	67,67,67,67	1
87	MG	5	4198	1/1	0.81	0.57	-	43,43,43,43	0
87	MG	1	4107	1/1	0.88	0.23	-	69,69,69,69	0
87	MG	5	4157	1/1	0.95	0.30	-	51,51,51,51	0
87	MG	1	4409	1/1	0.96	0.25	-	46,46,46,46	0
87	MG	1	4015	1/1	0.96	0.54	-	53,53,53,53	0
87	MG	5	4252	1/1	0.76	0.68	-	58,58,58,58	0
86	OHX	3	201	7/7	0.98	0.20	-	71,71,71,71	7
87	MG	2	2230	1/1	0.06	0.31	-	124,124,124,124	0
87	MG	1	3935	1/1	0.95	0.53	-	32,32,32,32	0
87	MG	2	2116	1/1	0.97	0.32	-	89,89,89,89	0
86	OHX	6	2056	7/7	0.81	0.18	-	97,97,97,97	7
87	MG	1	4245	1/1	0.95	0.79	-	47,47,47,47	1
87	MG	1	3861	1/1	0.94	0.35	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4315	1/1	0.81	0.43	-	31,31,31,31	1
86	OHX	2	1953	7/7	0.97	0.15	-	64,64,64,64	7
87	MG	3	213	1/1	0.95	0.15	-	78,78,78,78	0
87	MG	5	4138	1/1	0.95	0.29	-	100,100,100,100	0
87	MG	1	4283	1/1	0.98	0.34	-	38,38,38,38	1
87	MG	1	4372	1/1	0.71	0.41	-	76,76,76,76	0
87	MG	1	3981	1/1	0.93	0.62	-	51,51,51,51	0
87	MG	5	4114	1/1	0.86	0.41	-	43,43,43,43	0
86	OHX	1	3804	7/7	0.91	0.29	-	67,67,67,67	7
87	MG	1	4260	1/1	0.77	0.34	-	40,40,40,40	0
87	MG	5	4239	1/1	0.91	0.28	-	34,34,34,34	1
87	MG	5	4563	1/1	0.78	0.43	-	85,85,85,85	0
87	MG	5	4179	1/1	0.85	0.29	-	44,44,44,44	0
86	OHX	5	3683	7/7	0.95	0.29	-	60,60,60,60	7
87	MG	5	4072	1/1	0.91	0.44	-	55,55,55,55	0
87	MG	1	4194	1/1	0.98	0.41	-	47,47,47,47	1
87	MG	5	4472	1/1	0.97	0.17	-	42,42,42,42	0
87	MG	5	4328	1/1	0.94	0.25	-	53,53,53,53	0
87	MG	1	4113	1/1	0.96	0.26	-	49,49,49,49	0
87	MG	6	2241	1/1	0.94	0.16	-	70,70,70,70	0
87	MG	5	4269	1/1	0.98	0.26	-	39,39,39,39	1
87	MG	1	4226	1/1	0.84	0.12	-	72,72,72,72	0
86	OHX	3	209	7/7	0.92	0.22	-	82,82,82,82	7
87	MG	6	2275	1/1	0.98	0.20	-	67,67,67,67	1
87	MG	6	2140	1/1	0.94	0.33	-	44,44,44,44	0
87	MG	2	2120	1/1	0.83	0.21	-	70,70,70,70	0
87	MG	6	2133	1/1	0.94	0.26	-	39,39,39,39	0
87	MG	5	4124	1/1	0.79	0.49	-	57,57,57,57	0
86	OHX	6	1915	7/7	0.99	0.27	-	63,63,63,63	7
87	MG	6	2306	1/1	0.83	0.49	-	79,79,79,79	0
86	OHX	1	3501	7/7	0.97	0.28	-	83,83,83,83	7
87	MG	5	4402	1/1	0.91	0.26	-	42,42,42,42	1
87	MG	5	4310	1/1	0.89	0.17	-	50,50,50,50	0
87	MG	1	3871	1/1	0.94	0.35	-	46,46,46,46	0
87	MG	M5	304	1/1	0.98	0.58	-	40,40,40,40	1
86	OHX	6	2097	7/7	0.96	0.24	-	70,70,70,70	7
87	MG	6	2206	1/1	0.85	0.22	-	67,67,67,67	0
87	MG	5	3957	1/1	0.98	0.45	-	30,30,30,30	0
87	MG	7	235	1/1	0.81	0.30	-	60,60,60,60	0
86	OHX	2	2056	7/7	0.90	0.09	-	155,155,155,155	7
87	MG	1	4030	1/1	0.96	0.24	-	46,46,46,46	0
86	OHX	1	3683	7/7	0.94	0.34	-	61,61,61,61	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3819	1/1	0.94	0.39	-	106,106,106,106	0
87	MG	4	231	1/1	0.97	0.27	-	56,56,56,56	0
86	OHX	1	3614	7/7	0.93	0.39	-	53,53,53,53	7
87	MG	5	4422	1/1	0.93	0.23	-	35,35,35,35	0
87	MG	1	3953	1/1	0.97	0.63	-	38,38,38,38	0
87	MG	1	4386	1/1	0.92	0.33	-	53,53,53,53	0
87	MG	6	2319	1/1	0.98	0.26	-	57,57,57,57	0
87	MG	5	4137	1/1	0.72	0.55	-	63,63,63,63	0
87	MG	5	4042	1/1	0.98	0.50	-	35,35,35,35	0
87	MG	6	2101	1/1	0.92	0.62	-	39,39,39,39	0
86	OHX	5	3522	7/7	0.97	0.28	-	56,56,56,56	7
87	MG	1	4186	1/1	0.93	0.25	-	43,43,43,43	0
87	MG	5	4106	1/1	0.90	0.40	-	35,35,35,35	0
87	MG	4	242	1/1	0.88	0.45	-	45,45,45,45	0
87	MG	2	2092	1/1	0.96	0.61	-	40,40,40,40	0
87	MG	5	4371	1/1	0.90	0.36	-	38,38,38,38	1
86	OHX	5	3505	7/7	0.98	0.17	-	59,59,59,59	7
86	OHX	5	3714	7/7	0.93	0.22	-	82,82,82,82	7
87	MG	6	2270	1/1	0.91	0.55	-	61,61,61,61	0
87	MG	5	4261	1/1	0.88	0.30	-	44,44,44,44	0
87	MG	8	239	1/1	0.91	0.29	-	71,71,71,71	0
87	MG	5	4049	1/1	0.89	0.17	-	48,48,48,48	0
86	OHX	5	3482	7/7	0.99	0.24	-	54,54,54,54	7
86	OHX	2	1960	7/7	0.94	0.21	-	97,97,97,97	7
87	MG	5	4465	1/1	0.96	0.15	-	44,44,44,44	0
87	MG	2	2257	1/1	0.57	0.42	-	121,121,121,121	0
86	OHX	2	2059	7/7	0.90	0.25	-	66,66,66,66	7
87	MG	6	2192	1/1	0.77	0.20	-	75,75,75,75	0
87	MG	1	4359	1/1	0.76	0.45	-	51,51,51,51	1
87	MG	1	4196	1/1	0.92	0.23	-	55,55,55,55	0
87	MG	1	4001	1/1	0.98	0.56	-	28,28,28,28	0
86	OHX	1	3610	7/7	0.97	0.18	-	110,110,110,110	7
87	MG	5	4339	1/1	0.95	0.41	-	43,43,43,43	0
87	MG	5	4426	1/1	0.78	0.44	-	62,62,62,62	0
87	MG	8	232	1/1	0.80	0.44	-	64,64,64,64	0
87	MG	1	4464	1/1	0.80	1.89	-	60,60,60,60	0
86	OHX	1	3645	7/7	0.97	0.22	-	58,58,58,58	7
87	MG	6	2153	1/1	0.90	0.46	-	44,44,44,44	0
87	MG	6	2297	1/1	0.93	0.21	-	70,70,70,70	1
87	MG	5	4007	1/1	0.90	0.52	-	28,28,28,28	0
86	OHX	5	3796	7/7	0.92	0.29	-	63,63,63,63	7
87	MG	1	4046	1/1	0.94	0.27	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3985	1/1	0.99	0.63	-	28,28,28,28	0
87	MG	8	224	1/1	0.90	0.35	-	52,52,52,52	0
87	MG	5	3942	1/1	0.87	0.38	-	40,40,40,40	0
87	MG	5	4244	1/1	0.76	0.28	-	58,58,58,58	0
87	MG	1	4036	1/1	0.86	0.35	-	41,41,41,41	0
87	MG	1	4054	1/1	0.09	0.33	-	105,105,105,105	0
87	MG	5	4273	1/1	0.97	0.44	-	34,34,34,34	1
87	MG	1	3919	1/1	0.99	0.45	-	42,42,42,42	0
87	MG	7	219	1/1	0.90	0.28	-	39,39,39,39	0
86	OHX	6	1940	7/7	0.98	0.21	-	64,64,64,64	7
87	MG	1	4149	1/1	0.95	0.19	-	82,82,82,82	0
87	MG	O7	108	1/1	0.79	0.30	-	69,69,69,69	0
87	MG	1	4049	1/1	0.95	0.24	-	42,42,42,42	0
86	OHX	2	1942	7/7	0.97	0.17	-	74,74,74,74	7
86	OHX	6	1942	7/7	0.98	0.19	-	70,70,70,70	7
87	MG	5	4113	1/1	0.96	0.29	-	39,39,39,39	0
87	MG	1	3943	1/1	0.92	0.61	-	38,38,38,38	0
87	MG	5	4350	1/1	0.95	0.22	-	44,44,44,44	1
87	MG	1	4232	1/1	0.92	0.55	-	61,61,61,61	0
87	MG	6	2174	1/1	0.96	0.37	-	58,58,58,58	0
87	MG	2	2209	1/1	0.81	0.29	-	71,71,71,71	0
87	MG	5	3900	1/1	0.90	0.20	-	41,41,41,41	0
87	MG	5	4188	1/1	0.93	0.44	-	45,45,45,45	0
87	MG	1	4481	1/1	0.92	0.10	-	82,82,82,82	0
87	MG	1	4446	1/1	0.87	0.52	-	45,45,45,45	1
86	OHX	5	3666	7/7	0.97	0.31	-	65,65,65,65	7
87	MG	1	4235	1/1	0.91	0.31	-	49,49,49,49	1
87	MG	2	2195	1/1	0.88	0.55	-	65,65,65,65	0
86	OHX	1	3454	7/7	0.99	0.31	-	61,61,61,61	7
87	MG	5	3924	1/1	0.96	0.30	-	42,42,42,42	0
87	MG	1	4142	1/1	0.92	0.35	-	45,45,45,45	1
87	MG	5	4536	1/1	0.86	0.31	-	42,42,42,42	1
87	MG	5	4108	1/1	0.99	0.23	-	49,49,49,49	0
86	OHX	5	3811	7/7	0.96	0.61	-	44,44,44,44	7
87	MG	1	4509	1/1	0.95	0.16	-	90,90,90,90	0
87	MG	1	4355	1/1	0.74	0.64	-	67,67,67,67	0
87	MG	6	2315	1/1	0.86	0.30	-	54,54,54,54	0
87	MG	2	2192	1/1	0.84	0.43	-	64,64,64,64	0
87	MG	5	4066	1/1	0.92	0.33	-	53,53,53,53	0
86	OHX	2	2086	7/7	0.81	0.30	-	105,105,105,105	7
87	MG	5	4225	1/1	0.92	0.36	-	71,71,71,71	0
87	MG	5	4214	1/1	0.78	0.31	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4510	1/1	0.83	0.26	-	50,50,50,50	0
87	MG	5	4508	1/1	0.97	0.44	-	40,40,40,40	1
87	MG	M7	208	1/1	0.93	0.30	-	40,40,40,40	0
87	MG	3	227	1/1	0.69	0.37	-	78,78,78,78	0
87	MG	5	3993	1/1	0.94	0.46	-	29,29,29,29	0
87	MG	6	2228	1/1	0.90	0.88	-	59,59,59,59	1
87	MG	1	4462	1/1	0.69	0.35	-	53,53,53,53	0
87	MG	1	3901	1/1	0.97	0.27	-	66,66,66,66	0
87	MG	1	4345	1/1	0.77	0.29	-	44,44,44,44	1
87	MG	5	4474	1/1	0.78	0.31	-	62,62,62,62	0
87	MG	1	4335	1/1	0.81	0.67	-	45,45,45,45	1
87	MG	5	4486	1/1	0.97	0.34	-	46,46,46,46	0
87	MG	5	4392	1/1	0.82	0.51	-	134,134,134,134	0
87	MG	6	2197	1/1	0.77	0.24	-	60,60,60,60	0
87	MG	2	2148	1/1	0.84	0.48	-	130,130,130,130	0
86	OHX	5	3425	7/7	0.99	0.22	-	49,49,49,49	7
87	MG	3	223	1/1	0.92	0.11	-	62,62,62,62	0
87	MG	1	4146	1/1	0.83	0.22	-	50,50,50,50	0
86	OHX	7	208	7/7	0.97	0.21	-	54,54,54,54	7
87	MG	6	2107	1/1	0.80	0.23	-	47,47,47,47	0
86	OHX	2	1920	7/7	0.99	0.21	-	84,84,84,84	7
87	MG	5	4061	1/1	0.95	0.18	-	51,51,51,51	0
87	MG	1	3958	1/1	0.85	0.63	-	32,32,32,32	0
87	MG	1	4184	1/1	0.84	0.16	-	63,63,63,63	0
87	MG	5	4181	1/1	0.71	0.34	-	55,55,55,55	0
86	OHX	8	211	7/7	0.94	0.17	-	105,105,105,105	7
87	MG	5	3828	1/1	0.79	0.46	-	54,54,54,54	0
86	OHX	1	3789	7/7	0.94	0.36	-	56,56,56,56	7
87	MG	6	2141	1/1	0.91	0.39	-	40,40,40,40	0
87	MG	1	4164	1/1	0.94	0.20	-	62,62,62,62	0
87	MG	5	4086	1/1	0.87	0.43	-	48,48,48,48	0
87	MG	5	4039	1/1	0.87	0.45	-	57,57,57,57	0
86	OHX	1	3629	7/7	0.95	0.09	-	186,186,186,186	7
86	OHX	1	3720	7/7	0.96	0.15	-	104,104,104,104	7
86	OHX	M9	203	7/7	0.82	0.25	-	78,78,78,78	7
87	MG	6	2224	1/1	0.97	0.46	-	47,47,47,47	0
86	OHX	5	3815	7/7	0.96	0.34	-	66,66,66,66	7
86	OHX	6	2080	7/7	0.77	0.21	-	126,126,126,126	7
87	MG	1	4087	1/1	0.40	0.65	-	101,101,101,101	0
87	MG	c8	204	1/1	0.93	0.34	-	81,81,81,81	0
87	MG	1	4332	1/1	0.91	0.48	-	37,37,37,37	1
87	MG	5	4406	1/1	0.99	0.31	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3641	7/7	0.98	0.22	-	52,52,52,52	7
86	OHX	2	2045	7/7	0.92	0.38	-	73,73,73,73	7
87	MG	5	3832	1/1	0.92	0.53	-	35,35,35,35	0
87	MG	5	4044	1/1	0.93	0.50	-	35,35,35,35	0
86	OHX	2	2083	7/7	0.91	0.20	-	106,106,106,106	7
87	MG	1	4064	1/1	0.84	0.51	-	56,56,56,56	0
87	MG	4	236	1/1	0.94	0.12	-	98,98,98,98	0
87	MG	6	2182	1/1	0.98	0.22	-	51,51,51,51	0
87	MG	6	2327	1/1	0.96	0.39	-	78,78,78,78	0
87	MG	5	3819	1/1	0.98	0.46	-	36,36,36,36	0
87	MG	5	4454	1/1	0.94	0.27	-	47,47,47,47	0
87	MG	o3	203	1/1	0.89	0.38	-	40,40,40,40	1
87	MG	5	4107	1/1	0.50	0.33	-	59,59,59,59	0
87	MG	6	2136	1/1	0.99	0.28	-	54,54,54,54	0
87	MG	1	4258	1/1	0.85	0.55	-	77,77,77,77	0
87	MG	5	4187	1/1	0.88	0.58	-	53,53,53,53	0
87	MG	2	2237	1/1	0.98	0.16	-	80,80,80,80	0
87	MG	2	2248	1/1	0.94	0.12	-	78,78,78,78	0
86	OHX	2	1981	7/7	0.97	0.26	-	106,106,106,106	7
86	OHX	6	1936	7/7	0.99	0.22	-	57,57,57,57	7
87	MG	o2	202	1/1	0.90	0.26	-	49,49,49,49	0
86	OHX	5	3771	7/7	0.97	0.24	-	60,60,60,60	7
87	MG	5	4312	1/1	0.88	0.32	-	29,29,29,29	0
86	OHX	6	2033	7/7	0.95	0.20	-	67,67,67,67	7
86	OHX	6	2071	7/7	0.94	0.30	-	55,55,55,55	7
86	OHX	2	1998	7/7	0.96	0.14	-	94,94,94,94	7
87	MG	5	4183	1/1	0.72	0.40	-	54,54,54,54	0
87	MG	5	4270	1/1	0.98	0.08	-	45,45,45,45	0
87	MG	7	230	1/1	0.88	0.42	-	37,37,37,37	1
87	MG	6	2207	1/1	0.64	0.43	-	93,93,93,93	0
87	MG	1	4465	1/1	0.01	1.10	-	109,109,109,109	0
87	MG	5	4166	1/1	0.93	0.57	-	44,44,44,44	0
86	OHX	5	3481	7/7	0.98	0.26	-	69,69,69,69	7
87	MG	5	4139	1/1	0.99	0.18	-	38,38,38,38	0
87	MG	4	241	1/1	0.73	0.56	-	53,53,53,53	0
87	MG	5	4345	1/1	0.95	0.10	-	95,95,95,95	0
87	MG	6	2281	1/1	0.61	0.41	-	124,124,124,124	0
86	OHX	5	3765	7/7	0.97	0.25	-	42,42,42,42	7
87	MG	SM	201	1/1	0.68	0.31	-	55,55,55,55	0
87	MG	1	4181	1/1	0.93	0.25	-	75,75,75,75	0
87	MG	n9	102	1/1	0.64	0.32	-	37,37,37,37	0
86	OHX	6	2087	7/7	0.76	0.45	-	71,71,71,71	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4434	1/1	0.71	0.28	-	93,93,93,93	0
87	MG	5	4264	1/1	0.68	0.35	-	63,63,63,63	0
87	MG	5	4323	1/1	0.85	0.68	-	36,36,36,36	1
87	MG	6	2219	1/1	0.85	0.35	-	60,60,60,60	0
86	OHX	1	3723	7/7	0.93	0.50	-	57,57,57,57	7
87	MG	5	3847	1/1	0.92	0.65	-	38,38,38,38	0
87	MG	M7	205	1/1	0.96	0.42	-	42,42,42,42	0
87	MG	6	2235	1/1	0.91	0.20	-	76,76,76,76	0
87	MG	5	3964	1/1	0.95	0.44	-	33,33,33,33	0
87	MG	c6	201	1/1	0.81	0.41	-	97,97,97,97	0
86	OHX	5	3632	7/7	0.97	0.18	-	63,63,63,63	7
87	MG	2	2207	1/1	0.99	0.25	-	61,61,61,61	0
87	MG	6	2278	1/1	0.50	0.24	-	83,83,83,83	0
87	MG	1	4457	1/1	0.84	0.56	-	43,43,43,43	0
87	MG	2	2173	1/1	0.59	0.64	-	116,116,116,116	0
87	MG	O5	201	1/1	0.88	0.23	-	58,58,58,58	0
87	MG	1	4045	1/1	0.99	0.20	-	35,35,35,35	0
87	MG	1	4236	1/1	0.84	0.28	-	52,52,52,52	0
87	MG	1	4454	1/1	0.87	0.33	-	50,50,50,50	0
86	OHX	6	2066	7/7	0.87	0.28	-	70,70,70,70	7
87	MG	1	4187	1/1	0.94	0.21	-	47,47,47,47	1
86	OHX	5	3791	7/7	0.94	0.24	-	68,68,68,68	7
87	MG	1	3869	1/1	0.89	0.37	-	62,62,62,62	0
86	OHX	5	3472	7/7	0.99	0.25	-	53,53,53,53	7
87	MG	5	4432	1/1	0.81	0.34	-	36,36,36,36	1
86	OHX	5	3591	7/7	0.98	0.27	-	52,52,52,52	7
86	OHX	6	2016	7/7	0.94	0.16	-	91,91,91,91	7
86	OHX	5	3466	7/7	0.99	0.16	-	63,63,63,63	7
87	MG	2	2126	1/1	0.81	0.64	-	69,69,69,69	0
87	MG	5	3856	1/1	0.82	0.45	-	35,35,35,35	0
87	MG	6	2260	1/1	0.83	0.29	-	55,55,55,55	0
87	MG	5	4338	1/1	0.68	0.66	-	39,39,39,39	1
86	OHX	5	3729	7/7	0.97	0.33	-	58,58,58,58	7
87	MG	5	4135	1/1	0.57	0.67	-	69,69,69,69	0
87	MG	12	306	1/1	0.94	0.48	-	53,53,53,53	1
87	MG	5	4054	1/1	0.93	0.50	-	50,50,50,50	0
87	MG	6	2247	1/1	0.98	0.20	-	50,50,50,50	0
87	MG	5	4377	1/1	0.95	0.29	-	36,36,36,36	1
87	MG	6	2272	1/1	0.69	0.19	-	98,98,98,98	0
87	MG	2	2253	1/1	0.72	0.28	-	76,76,76,76	0
87	MG	1	3970	1/1	0.86	0.32	-	66,66,66,66	0
87	MG	1	4413	1/1	0.92	0.34	-	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4259	1/1	0.92	0.15	-	54,54,54,54	0
87	MG	1	4071	1/1	0.96	0.43	-	40,40,40,40	0
86	OHX	5	3615	7/7	0.93	0.31	-	51,51,51,51	7
87	MG	1	4430	1/1	0.95	0.32	-	49,49,49,49	0
87	MG	2	2164	1/1	0.83	0.28	-	122,122,122,122	0
87	MG	1	4292	1/1	0.94	0.19	-	39,39,39,39	0
86	OHX	1	3648	7/7	0.95	0.30	-	65,65,65,65	7
87	MG	1	3896	1/1	0.90	0.49	-	66,66,66,66	0
87	MG	1	4073	1/1	0.87	0.22	-	37,37,37,37	0
87	MG	1	4371	1/1	0.93	0.26	-	43,43,43,43	1
86	OHX	1	3680	7/7	0.98	0.36	-	60,60,60,60	7
87	MG	6	2172	1/1	0.98	0.33	-	76,76,76,76	0
87	MG	2	2247	1/1	0.50	0.38	-	115,115,115,115	0
86	OHX	1	3727	7/7	0.90	0.15	-	141,141,141,141	7
86	OHX	5	3723	7/7	0.95	0.30	-	62,62,62,62	7
86	OHX	1	3785	7/7	0.89	0.25	-	47,47,47,47	7
87	MG	5	4287	1/1	0.98	0.27	-	39,39,39,39	1
86	OHX	5	3690	7/7	0.92	0.28	-	90,90,90,90	7
86	OHX	6	2075	7/7	0.94	0.31	-	54,54,54,54	7
86	OHX	1	3710	7/7	0.91	0.26	-	55,55,55,55	7
87	MG	5	4257	1/1	0.97	0.52	-	29,29,29,29	0
87	MG	5	4258	1/1	0.91	0.23	-	57,57,57,57	0
86	OHX	5	3747	7/7	0.92	0.21	-	66,66,66,66	7
87	MG	1	3881	1/1	0.97	0.24	-	47,47,47,47	0
87	MG	1	4154	1/1	0.99	0.24	-	81,81,81,81	0
87	MG	1	4381	1/1	1.00	0.19	-	60,60,60,60	0
87	MG	7	214	1/1	0.94	0.22	-	46,46,46,46	0
86	OHX	6	2024	7/7	0.84	0.23	-	86,86,86,86	7
87	MG	5	4291	1/1	0.96	0.22	-	35,35,35,35	1
87	MG	5	4046	1/1	0.86	0.42	-	51,51,51,51	0
86	OHX	1	3749	7/7	0.92	0.41	-	62,62,62,62	7
86	OHX	14	402	7/7	0.97	0.19	-	55,55,55,55	7
87	MG	1	4120	1/1	0.94	0.40	-	51,51,51,51	0
87	MG	n8	203	1/1	0.94	0.21	-	41,41,41,41	0
86	OHX	2	2013	7/7	0.95	0.08	-	158,158,158,158	7
87	MG	5	4549	1/1	0.81	0.20	-	77,77,77,77	0
87	MG	L4	403	1/1	0.94	0.41	-	34,34,34,34	0
87	MG	2	2214	1/1	0.78	0.60	-	78,78,78,78	0
87	MG	5	4506	1/1	0.92	0.25	-	38,38,38,38	1
87	MG	5	3937	1/1	0.86	0.78	-	33,33,33,33	0
86	OHX	2	2033	7/7	0.96	0.12	-	113,113,113,113	7
86	OHX	m4	201	7/7	0.86	0.52	-	101,101,101,101	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4083	1/1	0.91	0.46	-	29,29,29,29	0
87	MG	1	4388	1/1	0.98	0.27	-	35,35,35,35	1
87	MG	5	4462	1/1	0.65	0.34	-	54,54,54,54	0
87	MG	1	4280	1/1	0.89	0.22	-	76,76,76,76	0
87	MG	1	3853	1/1	0.74	0.96	-	41,41,41,41	0
87	MG	1	4192	1/1	0.92	0.36	-	38,38,38,38	0
87	MG	6	2259	1/1	0.84	0.32	-	48,48,48,48	0
87	MG	5	4146	1/1	0.93	0.34	-	43,43,43,43	0
87	MG	2	2108	1/1	0.85	0.64	-	59,59,59,59	0
87	MG	2	2196	1/1	0.47	0.99	-	82,82,82,82	0
87	MG	N3	202	1/1	0.81	0.45	-	67,67,67,67	0
87	MG	4	219	1/1	0.94	0.58	-	54,54,54,54	0
87	MG	5	4376	1/1	0.60	0.28	-	72,72,72,72	0
87	MG	1	4158	1/1	0.89	0.40	-	42,42,42,42	1
86	OHX	5	3538	7/7	0.97	0.25	-	42,42,42,42	7
87	MG	1	3837	1/1	0.85	0.30	-	41,41,41,41	0
87	MG	1	4204	1/1	0.93	0.50	-	60,60,60,60	0
87	MG	1	4167	1/1	0.96	0.67	-	42,42,42,42	1
87	MG	6	2169	1/1	0.84	0.16	-	85,85,85,85	0
87	MG	1	3845	1/1	0.91	0.41	-	44,44,44,44	0
87	MG	1	4095	1/1	0.54	0.70	-	41,41,41,41	0
87	MG	1	4156	1/1	0.94	0.11	-	60,60,60,60	0
87	MG	5	4573	1/1	0.95	0.48	-	30,30,30,30	0
87	MG	6	2283	1/1	0.76	1.34	-	69,69,69,69	1
87	MG	5	3905	1/1	0.46	0.73	-	71,71,71,71	0
86	OHX	5	3414	7/7	0.99	0.23	-	43,43,43,43	7
87	MG	6	2215	1/1	0.86	0.15	-	52,52,52,52	0
86	OHX	1	3689	7/7	0.97	0.26	-	55,55,55,55	7
87	MG	1	3876	1/1	0.89	0.35	-	30,30,30,30	0
87	MG	n0	204	1/1	0.89	0.33	-	45,45,45,45	0
87	MG	5	3858	1/1	0.99	0.23	-	58,58,58,58	0
86	OHX	1	3670	7/7	0.95	0.28	-	50,50,50,50	7
87	MG	5	4136	1/1	0.89	0.33	-	48,48,48,48	0
87	MG	5	4425	1/1	0.98	0.30	-	48,48,48,48	1
86	OHX	1	3742	7/7	0.92	0.39	-	41,41,41,41	7
87	MG	3	226	1/1	0.49	0.23	-	65,65,65,65	0
87	MG	5	4551	1/1	0.96	0.60	-	41,41,41,41	1
86	OHX	2	1971	7/7	0.98	0.32	-	80,80,80,80	7
87	MG	2	2123	1/1	0.92	0.37	-	68,68,68,68	0
87	MG	5	4346	1/1	0.90	0.19	-	68,68,68,68	1
87	MG	3	220	1/1	0.98	0.17	-	55,55,55,55	0
86	OHX	2	2036	7/7	0.95	0.20	-	123,123,123,123	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4084	1/1	0.76	0.52	-	49,49,49,49	0
87	MG	1	4166	1/1	0.95	0.60	-	36,36,36,36	0
87	MG	5	3902	1/1	0.97	0.26	-	71,71,71,71	0
87	MG	5	3894	1/1	0.94	0.35	-	40,40,40,40	1
87	MG	13	403	1/1	0.97	0.54	-	26,26,26,26	0
86	OHX	2	1996	7/7	0.97	0.29	-	93,93,93,93	7
87	MG	2	2182	1/1	0.85	0.38	-	87,87,87,87	0
86	OHX	2	2075	7/7	0.90	0.37	-	87,87,87,87	7
87	MG	18	301	1/1	0.80	0.51	-	70,70,70,70	0
87	MG	5	3851	1/1	0.85	0.48	-	36,36,36,36	0
87	MG	6	2312	1/1	0.94	0.29	-	75,75,75,75	0
87	MG	1	4342	1/1	0.83	0.32	-	58,58,58,58	0
87	MG	2	2200	1/1	0.84	0.56	-	65,65,65,65	0
87	MG	5	4539	1/1	0.86	0.61	-	56,56,56,56	0
87	MG	7	215	1/1	0.93	0.51	-	27,27,27,27	0
87	MG	5	4036	1/1	0.96	0.54	-	34,34,34,34	0
86	OHX	2	2072	7/7	0.82	0.33	-	104,104,104,104	7
87	MG	5	4202	1/1	0.93	0.35	-	32,32,32,32	1
86	OHX	1	3756	7/7	0.86	0.34	-	59,59,59,59	7
86	OHX	6	1950	7/7	0.94	0.14	-	100,100,100,100	7
87	MG	5	3912	1/1	0.94	0.69	-	40,40,40,40	0
87	MG	5	4255	1/1	0.89	0.39	-	37,37,37,37	0
87	MG	5	4221	1/1	0.79	0.24	-	54,54,54,54	0
87	MG	6	2227	1/1	0.99	0.13	-	52,52,52,52	0
87	MG	5	4559	1/1	0.94	0.37	-	73,73,73,73	1
87	MG	5	4011	1/1	0.97	0.53	-	33,33,33,33	0
87	MG	8	223	1/1	0.89	0.14	-	60,60,60,60	0
87	MG	5	4265	1/1	0.65	0.67	-	61,61,61,61	0
87	MG	2	2154	1/1	0.50	0.99	-	68,68,68,68	0
87	MG	5	4299	1/1	0.82	0.51	-	47,47,47,47	0
87	MG	5	4314	1/1	0.96	0.18	-	33,33,33,33	0
86	OHX	6	1974	7/7	0.98	0.27	-	67,67,67,67	7
87	MG	m8	1502	1/1	0.98	0.16	-	47,47,47,47	0
87	MG	5	4080	1/1	0.92	0.43	-	37,37,37,37	0
87	MG	2	2198	1/1	0.47	0.55	-	120,120,120,120	0
87	MG	5	4437	1/1	0.84	0.40	-	37,37,37,37	1
87	MG	1	4114	1/1	0.81	0.26	-	67,67,67,67	0
87	MG	d3	201	1/1	0.87	0.53	-	47,47,47,47	0
87	MG	6	2145	1/1	0.95	0.51	-	33,33,33,33	0
87	MG	6	2320	1/1	0.81	0.31	-	62,62,62,62	0
87	MG	5	4209	1/1	0.94	0.12	-	50,50,50,50	0
87	MG	6	2238	1/1	0.70	0.26	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4138	1/1	0.82	0.34	-	46,46,46,46	0
87	MG	1	4115	1/1	0.89	0.49	-	49,49,49,49	0
86	OHX	5	3450	7/7	0.99	0.23	-	41,41,41,41	7
87	MG	5	4568	1/1	0.80	0.34	-	38,38,38,38	1
86	OHX	5	3423	7/7	0.99	0.16	-	56,56,56,56	7
87	MG	1	4468	1/1	0.80	0.20	-	70,70,70,70	1
87	MG	8	235	1/1	0.95	0.68	-	61,61,61,61	1
87	MG	1	4472	1/1	0.86	0.46	-	61,61,61,61	0
87	MG	1	3894	1/1	0.90	0.47	-	53,53,53,53	0
87	MG	5	4101	1/1	0.73	0.32	-	49,49,49,49	0
86	OHX	5	3810	7/7	0.98	0.26	-	63,63,63,63	7
87	MG	5	3884	1/1	0.86	0.44	-	40,40,40,40	0
86	OHX	5	3578	7/7	0.98	0.25	-	55,55,55,55	7
87	MG	1	4016	1/1	0.94	0.89	-	38,38,38,38	0
87	MG	6	2220	1/1	0.85	0.31	-	47,47,47,47	0
87	MG	1	4488	1/1	0.90	0.16	-	55,55,55,55	0
87	MG	5	4303	1/1	0.99	0.16	-	43,43,43,43	1
86	OHX	5	3758	7/7	0.85	0.32	-	42,42,42,42	7
87	MG	s8	305	1/1	0.90	0.17	-	56,56,56,56	0
87	MG	5	4507	1/1	0.89	0.48	-	46,46,46,46	1
87	MG	5	4524	1/1	0.82	0.30	-	47,47,47,47	0
87	MG	n3	205	1/1	0.98	0.28	-	34,34,34,34	1
87	MG	6	2135	1/1	0.90	0.60	-	50,50,50,50	0
87	MG	1	4352	1/1	0.86	0.27	-	52,52,52,52	0
87	MG	5	3974	1/1	0.90	0.33	-	36,36,36,36	0
87	MG	5	4485	1/1	0.91	0.25	-	95,95,95,95	0
87	MG	5	4529	1/1	0.75	0.47	-	37,37,37,37	1
86	OHX	2	2016	7/7	0.93	0.17	-	101,101,101,101	7
86	OHX	6	2012	7/7	0.86	0.30	-	64,64,64,64	7
87	MG	5	4572	1/1	0.57	0.39	-	69,69,69,69	0
86	OHX	2	2004	7/7	0.97	0.13	-	89,89,89,89	7
86	OHX	2	1952	7/7	0.97	0.10	-	131,131,131,131	7
87	MG	1	3933	1/1	0.90	0.52	-	49,49,49,49	0
86	OHX	5	3720	7/7	0.60	0.43	-	73,73,73,73	7
87	MG	1	3939	1/1	0.95	0.51	-	37,37,37,37	0
87	MG	2	2232	1/1	0.89	0.08	-	90,90,90,90	0
86	OHX	1	3808	7/7	0.90	0.29	-	60,60,60,60	7
87	MG	8	240	1/1	0.92	0.13	-	72,72,72,72	0
87	MG	M4	201	1/1	0.94	0.19	-	53,53,53,53	0
86	OHX	1	3791	7/7	0.97	0.24	-	68,68,68,68	7
87	MG	5	4394	1/1	0.93	0.73	-	62,62,62,62	0
87	MG	1	4222	1/1	0.90	0.26	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4336	1/1	0.76	0.43	-	69,69,69,69	0
87	MG	5	4380	1/1	0.87	0.27	-	45,45,45,45	0
87	MG	7	231	1/1	0.88	0.70	-	43,43,43,43	0
86	OHX	5	3778	7/7	0.91	0.19	-	109,109,109,109	7
87	MG	1	4195	1/1	0.88	0.44	-	52,52,52,52	0
87	MG	6	2112	1/1	0.94	0.51	-	42,42,42,42	0
87	MG	4	220	1/1	0.66	0.34	-	64,64,64,64	0
87	MG	5	4511	1/1	0.99	0.87	-	52,52,52,52	1
86	OHX	1	3752	7/7	0.92	0.11	-	180,180,180,180	7
87	MG	2	2177	1/1	0.78	0.40	-	69,69,69,69	0
87	MG	5	4424	1/1	0.95	0.21	-	63,63,63,63	0
87	MG	6	2103	1/1	0.94	0.22	-	66,66,66,66	0
87	MG	2	2093	1/1	0.71	0.45	-	74,74,74,74	0
86	OHX	m9	201	7/7	0.91	0.19	-	70,70,70,70	7
87	MG	3	218	1/1	0.95	0.46	-	35,35,35,35	0
87	MG	5	3901	1/1	0.55	0.36	-	67,67,67,67	0
87	MG	1	4224	1/1	0.60	0.28	-	74,74,74,74	0
86	OHX	5	3813	7/7	0.66	0.23	-	173,173,173,173	7
86	OHX	5	3733	7/7	0.98	0.21	-	57,57,57,57	7
87	MG	1	4145	1/1	0.89	0.27	-	47,47,47,47	0
86	OHX	6	2001	7/7	0.96	0.35	-	68,68,68,68	7
87	MG	1	3990	1/1	0.94	0.69	-	31,31,31,31	0
87	MG	1	4426	1/1	0.67	1.07	-	63,63,63,63	0
87	MG	19	202	1/1	0.92	0.30	-	38,38,38,38	0
86	OHX	6	2055	7/7	0.95	0.48	-	59,59,59,59	7
87	MG	1	4475	1/1	0.95	0.40	-	62,62,62,62	0
86	OHX	6	2050	7/7	0.88	0.12	-	132,132,132,132	7
87	MG	1	4155	1/1	0.76	0.18	-	54,54,54,54	0
87	MG	6	2279	1/1	0.98	0.43	-	80,80,80,80	0
87	MG	5	4458	1/1	0.94	0.25	-	38,38,38,38	1
86	OHX	2	2001	7/7	0.95	0.27	-	82,82,82,82	7
87	MG	1	4261	1/1	0.92	0.55	-	41,41,41,41	1
87	MG	1	4182	1/1	0.86	0.21	-	55,55,55,55	0
87	MG	5	4128	1/1	0.88	0.27	-	40,40,40,40	0
87	MG	5	4295	1/1	0.99	0.41	-	43,43,43,43	0
87	MG	5	3921	1/1	0.42	0.55	-	51,51,51,51	0
87	MG	1	4367	1/1	0.54	0.73	-	92,92,92,92	0
86	OHX	2	1994	7/7	0.96	0.12	-	111,111,111,111	7
87	MG	1	3947	1/1	0.96	0.50	-	37,37,37,37	0
87	MG	6	2120	1/1	0.95	0.32	-	43,43,43,43	0
87	MG	5	4351	1/1	0.92	0.31	-	59,59,59,59	0
87	MG	1	4489	1/1	0.96	0.64	-	56,56,56,56	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	4	228	1/1	0.93	0.13	-	58,58,58,58	0
87	MG	5	4018	1/1	0.87	0.36	-	34,34,34,34	0
86	OHX	1	3512	7/7	0.99	0.15	-	74,74,74,74	7
87	MG	1	4080	1/1	0.90	0.45	-	51,51,51,51	0
87	MG	1	4085	1/1	0.93	0.58	-	46,46,46,46	0
87	MG	1	4353	1/1	0.96	0.30	-	59,59,59,59	0
87	MG	2	2169	1/1	0.57	0.25	-	101,101,101,101	0
87	MG	1	4112	1/1	0.79	0.90	-	48,48,48,48	0
87	MG	1	4295	1/1	0.61	0.44	-	41,41,41,41	1
87	MG	1	4127	1/1	0.93	0.39	-	49,49,49,49	0
87	MG	2	2166	1/1	0.89	0.68	-	55,55,55,55	0
87	MG	1	3906	1/1	0.94	0.39	-	42,42,42,42	1
86	OHX	5	3748	7/7	0.94	0.42	-	54,54,54,54	7
87	MG	6	2292	1/1	0.93	0.19	-	50,50,50,50	1
87	MG	1	4474	1/1	0.97	0.67	-	55,55,55,55	0
87	MG	1	3818	1/1	0.93	0.51	-	58,58,58,58	0
87	MG	6	2262	1/1	0.80	0.63	-	114,114,114,114	0
87	MG	1	4304	1/1	0.93	0.49	-	44,44,44,44	1
87	MG	L7	303	1/1	0.97	0.17	-	42,42,42,42	0
86	OHX	5	3438	7/7	0.97	0.27	-	48,48,48,48	7
87	MG	7	240	1/1	0.98	0.56	-	53,53,53,53	1
86	OHX	6	2094	7/7	0.85	0.32	-	102,102,102,102	7
87	MG	o2	201	1/1	0.87	0.54	-	35,35,35,35	1
87	MG	M1	202	1/1	0.86	0.16	-	72,72,72,72	0
87	MG	3	221	1/1	0.76	0.16	-	70,70,70,70	0
86	OHX	6	2086	7/7	0.86	0.26	-	147,147,147,147	7
86	OHX	1	3441	7/7	0.99	0.21	-	52,52,52,52	7
86	OHX	6	2083	7/7	0.97	0.24	-	82,82,82,82	7
87	MG	1	4389	1/1	0.98	0.32	-	59,59,59,59	1
87	MG	1	3823	1/1	0.94	0.43	-	31,31,31,31	0
87	MG	7	225	1/1	0.89	0.17	-	39,39,39,39	0
86	OHX	5	3662	7/7	0.95	0.27	-	45,45,45,45	7
87	MG	5	4349	1/1	0.03	0.67	-	41,41,41,41	1
86	OHX	1	3697	7/7	0.92	0.10	-	169,169,169,169	7
87	MG	1	4441	1/1	0.99	0.14	-	43,43,43,43	1
87	MG	5	4088	1/1	0.84	0.30	-	42,42,42,42	1
86	OHX	5	3780	7/7	0.95	0.17	-	110,110,110,110	7
87	MG	1	4058	1/1	0.83	0.65	-	44,44,44,44	0
87	MG	5	3978	1/1	0.87	0.37	-	40,40,40,40	0
87	MG	5	4015	1/1	0.96	0.74	-	38,38,38,38	0
87	MG	1	4246	1/1	0.73	0.76	-	41,41,41,41	1
86	OHX	2	2044	7/7	0.87	0.17	-	134,134,134,134	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3886	1/1	0.71	0.17	-	97,97,97,97	0
86	OHX	1	3809	7/7	0.98	0.19	-	83,83,83,83	7
86	OHX	1	3660	7/7	0.77	0.34	-	127,127,127,127	7
87	MG	5	4311	1/1	0.97	0.36	-	37,37,37,37	1
87	MG	5	3970	1/1	0.97	0.68	-	38,38,38,38	0
87	MG	6	2280	1/1	0.97	0.18	-	46,46,46,46	0
87	MG	1	4089	1/1	0.90	0.25	-	44,44,44,44	0
87	MG	2	2136	1/1	0.66	0.29	-	71,71,71,71	0
87	MG	5	4083	1/1	0.92	0.23	-	36,36,36,36	1
87	MG	1	4416	1/1	0.99	0.26	-	60,60,60,60	0
86	OHX	2	1912	7/7	0.98	0.14	-	109,109,109,109	0
87	MG	1	4147	1/1	0.83	0.39	-	48,48,48,48	0
86	OHX	5	3566	7/7	0.98	0.22	-	96,96,96,96	7
86	OHX	1	3567	7/7	0.98	0.36	-	48,48,48,48	7
87	MG	1	4189	1/1	1.00	0.21	-	46,46,46,46	0
87	MG	6	2225	1/1	0.83	0.52	-	55,55,55,55	0
87	MG	5	4120	1/1	0.84	0.68	-	39,39,39,39	0
86	OHX	2	2012	7/7	0.97	0.13	-	102,102,102,102	7
87	MG	6	2323	1/1	0.52	0.34	-	70,70,70,70	0
87	MG	5	4319	1/1	0.84	0.34	-	59,59,59,59	0
87	MG	2	2213	1/1	0.90	0.38	-	55,55,55,55	0
86	OHX	5	3526	7/7	0.98	0.31	-	46,46,46,46	7
86	OHX	1	3806	7/7	0.89	0.29	-	54,54,54,54	7
87	MG	1	4309	1/1	0.90	0.36	-	44,44,44,44	1
87	MG	5	4182	1/1	0.96	0.28	-	66,66,66,66	0
87	MG	1	4361	1/1	0.74	0.30	-	67,67,67,67	0
87	MG	5	4476	1/1	0.86	0.55	-	46,46,46,46	0
87	MG	6	2331	1/1	0.95	0.53	-	76,76,76,76	0
87	MG	5	4327	1/1	0.77	0.66	-	82,82,82,82	0
87	MG	1	4153	1/1	0.80	0.64	-	101,101,101,101	0
87	MG	2	2218	1/1	0.93	0.19	-	82,82,82,82	0
86	OHX	6	2010	7/7	0.94	0.33	-	84,84,84,84	7
87	MG	5	3959	1/1	0.98	0.38	-	35,35,35,35	0
87	MG	1	4324	1/1	0.85	0.24	-	54,54,54,54	0
87	MG	5	3868	1/1	0.89	0.36	-	36,36,36,36	0
87	MG	1	4343	1/1	0.59	0.57	-	62,62,62,62	0
87	MG	5	4332	1/1	0.88	0.15	-	106,106,106,106	0
87	MG	1	3882	1/1	0.88	0.21	-	49,49,49,49	0
87	MG	6	2299	1/1	0.88	0.39	-	59,59,59,59	0
86	OHX	5	3621	7/7	0.97	0.29	-	43,43,43,43	7
86	OHX	1	3516	7/7	0.96	0.22	-	65,65,65,65	7
87	MG	1	4368	1/1	0.97	0.20	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4450	1/1	0.99	0.12	-	54,54,54,54	0
87	MG	1	4118	1/1	0.86	0.74	-	42,42,42,42	0
87	MG	5	4196	1/1	0.80	0.17	-	52,52,52,52	0
87	MG	5	4413	1/1	0.45	0.30	-	72,72,72,72	0
87	MG	1	4152	1/1	0.92	0.18	-	75,75,75,75	0
87	MG	2	2111	1/1	0.93	0.46	-	63,63,63,63	0
87	MG	2	2091	1/1	0.87	0.79	-	44,44,44,44	0
87	MG	1	4103	1/1	0.91	0.21	-	88,88,88,88	0
87	MG	m6	203	1/1	0.82	0.24	-	41,41,41,41	1
87	MG	1	3955	1/1	0.97	0.46	-	36,36,36,36	0
87	MG	5	4479	1/1	0.61	0.62	-	56,56,56,56	1
86	OHX	2	2050	7/7	0.97	0.10	-	96,96,96,96	7
87	MG	D9	104	1/1	0.84	0.10	-	85,85,85,85	0
86	OHX	1	3677	7/7	0.95	0.36	-	74,74,74,74	7
87	MG	2	2097	1/1	0.92	0.24	-	82,82,82,82	0
87	MG	5	4354	1/1	0.59	0.91	-	61,61,61,61	0
87	MG	6	2202	1/1	0.73	0.57	-	81,81,81,81	0
86	OHX	2	1930	7/7	0.98	0.31	-	77,77,77,77	7
87	MG	1	4234	1/1	0.88	0.45	-	51,51,51,51	0
86	OHX	5	3711	7/7	0.95	0.28	-	83,83,83,83	7
86	OHX	1	3529	7/7	0.98	0.24	-	66,66,66,66	7
86	OHX	5	3544	7/7	0.97	0.14	-	99,99,99,99	7
87	MG	o3	204	1/1	0.86	0.55	-	37,37,37,37	1
87	MG	2	2242	1/1	0.80	0.20	-	85,85,85,85	0
87	MG	7	226	1/1	0.93	0.19	-	64,64,64,64	0
86	OHX	1	3503	7/7	0.98	0.28	-	57,57,57,57	7
87	MG	1	4086	1/1	0.89	0.29	-	57,57,57,57	0
87	MG	7	218	1/1	0.97	0.49	-	30,30,30,30	0
87	MG	3	219	1/1	0.89	0.32	-	63,63,63,63	0
87	MG	1	4163	1/1	0.90	0.48	-	52,52,52,52	0
86	OHX	5	3648	7/7	0.88	0.40	-	69,69,69,69	7
87	MG	1	4044	1/1	0.96	0.22	-	69,69,69,69	0
87	MG	2	2156	1/1	0.30	0.47	-	86,86,86,86	0
87	MG	2	2221	1/1	0.72	0.39	-	61,61,61,61	0
87	MG	1	3928	1/1	0.98	0.39	-	43,43,43,43	0
86	OHX	1	3626	7/7	0.96	0.35	-	84,84,84,84	7
87	MG	2	2125	1/1	0.97	0.46	-	85,85,85,85	0
87	MG	1	3897	1/1	0.92	0.40	-	43,43,43,43	0
87	MG	2	2228	1/1	0.95	0.61	-	56,56,56,56	0
87	MG	5	4014	1/1	0.93	0.30	-	30,30,30,30	0
87	MG	1	4483	1/1	0.88	0.37	-	59,59,59,59	0
86	OHX	1	3566	7/7	0.96	0.20	-	92,92,92,92	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3987	1/1	0.97	0.49	-	45,45,45,45	0
86	OHX	5	3740	7/7	0.93	0.22	-	62,62,62,62	7
87	MG	q1	102	1/1	0.95	0.30	-	43,43,43,43	0
87	MG	l2	305	1/1	0.70	0.33	-	71,71,71,71	0
87	MG	1	4106	1/1	0.84	0.28	-	45,45,45,45	0
86	OHX	5	3793	7/7	0.92	0.32	-	58,58,58,58	7
86	OHX	2	2061	7/7	0.94	0.22	-	78,78,78,78	7
87	MG	5	4400	1/1	0.81	0.43	-	43,43,43,43	1
87	MG	1	3979	1/1	0.93	0.63	-	45,45,45,45	0
87	MG	5	4078	1/1	0.88	0.61	-	41,41,41,41	0
87	MG	5	4163	1/1	0.87	0.40	-	59,59,59,59	0
87	MG	1	4183	1/1	0.85	0.38	-	37,37,37,37	0
87	MG	5	3888	1/1	0.89	0.26	-	37,37,37,37	0
87	MG	5	4541	1/1	0.82	0.25	-	56,56,56,56	0
87	MG	1	4294	1/1	0.74	0.29	-	58,58,58,58	0
87	MG	N8	208	1/1	0.94	0.86	-	45,45,45,45	1
86	OHX	1	3589	7/7	0.94	0.25	-	50,50,50,50	7
87	MG	6	2273	1/1	0.79	0.25	-	80,80,80,80	0
86	OHX	1	3472	7/7	0.99	0.23	-	54,54,54,54	7
87	MG	5	4197	1/1	0.97	0.29	-	36,36,36,36	0
87	MG	1	4427	1/1	0.99	0.20	-	55,55,55,55	1
86	OHX	1	3527	7/7	0.97	0.31	-	81,81,81,81	7
87	MG	2	2155	1/1	0.95	0.56	-	60,60,60,60	0
87	MG	1	4179	1/1	0.71	1.32	-	53,53,53,53	1
87	MG	5	4070	1/1	0.91	0.22	-	49,49,49,49	0
87	MG	5	4060	1/1	0.92	0.32	-	45,45,45,45	0
87	MG	6	2255	1/1	0.87	0.37	-	54,54,54,54	0
87	MG	5	3935	1/1	0.85	0.37	-	54,54,54,54	0
86	OHX	1	3741	7/7	0.98	0.20	-	56,56,56,56	7
87	MG	sM	201	1/1	0.92	0.15	-	48,48,48,48	0
86	OHX	1	3736	7/7	0.90	0.16	-	113,113,113,113	7
87	MG	6	2200	1/1	0.81	1.15	-	74,74,74,74	0
87	MG	5	4505	1/1	0.82	0.22	-	49,49,49,49	0
87	MG	1	4005	1/1	0.89	0.42	-	29,29,29,29	0
87	MG	2	2175	1/1	0.66	0.27	-	87,87,87,87	0
87	MG	1	3945	1/1	0.86	0.40	-	43,43,43,43	0
87	MG	1	3916	1/1	0.63	0.20	-	86,86,86,86	0
87	MG	1	4434	1/1	0.74	0.43	-	38,38,38,38	1
86	OHX	5	3695	7/7	0.95	0.48	-	55,55,55,55	7
87	MG	5	3966	1/1	0.84	0.50	-	39,39,39,39	0
87	MG	5	4092	1/1	0.98	0.26	-	36,36,36,36	1
87	MG	6	2250	1/1	0.93	0.70	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	2	2241	1/1	0.95	0.56	-	60,60,60,60	0
87	MG	2	2090	1/1	0.86	0.36	-	83,83,83,83	0
87	MG	2	2190	1/1	0.85	0.24	-	78,78,78,78	0
87	MG	5	4117	1/1	0.95	0.71	-	46,46,46,46	0
87	MG	5	4554	1/1	0.94	0.26	-	43,43,43,43	0
87	MG	1	3860	1/1	0.88	0.36	-	49,49,49,49	0
87	MG	4	233	1/1	0.94	0.25	-	43,43,43,43	1
87	MG	1	4492	1/1	0.89	0.31	-	65,65,65,65	0
87	MG	5	4160	1/1	0.95	0.34	-	67,67,67,67	0
87	MG	6	2151	1/1	0.86	0.56	-	47,47,47,47	0
86	OHX	5	3684	7/7	0.96	0.59	-	43,43,43,43	7
87	MG	4	225	1/1	0.91	0.33	-	55,55,55,55	0
87	MG	2	2204	1/1	0.73	0.19	-	106,106,106,106	0
86	OHX	1	3753	7/7	0.98	0.25	-	51,51,51,51	7
87	MG	1	4399	1/1	0.90	0.30	-	54,54,54,54	0
87	MG	5	4211	1/1	0.76	0.25	-	46,46,46,46	0
87	MG	1	3912	1/1	0.91	0.24	-	52,52,52,52	0
87	MG	6	2252	1/1	0.93	0.39	-	47,47,47,47	0
87	MG	1	4197	1/1	0.12	0.43	-	56,56,56,56	0
86	OHX	6	1963	7/7	0.98	0.24	-	72,72,72,72	7
87	MG	15	305	1/1	0.82	0.14	-	62,62,62,62	0
87	MG	1	4105	1/1	0.83	0.56	-	47,47,47,47	0
87	MG	6	2301	1/1	0.77	0.49	-	57,57,57,57	0
86	OHX	6	1935	7/7	0.98	0.23	-	56,56,56,56	7
87	MG	M0	305	1/1	0.92	0.22	-	62,62,62,62	0
87	MG	5	4161	1/1	0.96	0.48	-	38,38,38,38	0
87	MG	6	2121	1/1	0.96	0.38	-	61,61,61,61	0
87	MG	2	2110	1/1	0.82	0.56	-	66,66,66,66	0
86	OHX	5	3744	7/7	0.93	0.30	-	56,56,56,56	7
86	OHX	5	3738	7/7	0.93	0.22	-	53,53,53,53	7
87	MG	5	3877	1/1	0.90	0.59	-	38,38,38,38	0
87	MG	6	2143	1/1	0.93	0.72	-	86,86,86,86	0
86	OHX	5	3635	7/7	0.85	0.23	-	81,81,81,81	7
87	MG	1	4126	1/1	0.37	0.42	-	66,66,66,66	0
86	OHX	7	210	7/7	0.94	0.26	-	63,63,63,63	7
87	MG	1	4037	1/1	0.98	0.46	-	45,45,45,45	0
87	MG	6	2191	1/1	0.78	0.41	-	86,86,86,86	0
86	OHX	1	3528	7/7	0.98	0.23	-	68,68,68,68	7
87	MG	1	4370	1/1	0.67	0.42	-	41,41,41,41	1
87	MG	s6	301	1/1	0.95	0.13	-	71,71,71,71	0
86	OHX	6	1968	7/7	0.97	0.30	-	74,74,74,74	7
87	MG	5	4509	1/1	0.93	0.23	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3458	7/7	0.98	0.22	-	79,79,79,79	7
87	MG	5	4543	1/1	0.57	0.70	-	41,41,41,41	1
87	MG	l3	405	1/1	0.93	0.31	-	35,35,35,35	0
86	OHX	1	3761	7/7	0.88	0.29	-	117,117,117,117	7
87	MG	1	4002	1/1	0.97	0.53	-	36,36,36,36	0
87	MG	6	2179	1/1	0.91	0.12	-	67,67,67,67	0
86	OHX	5	3743	7/7	0.95	0.17	-	105,105,105,105	7
87	MG	5	4058	1/1	0.94	0.42	-	37,37,37,37	0
87	MG	1	4299	1/1	0.99	0.22	-	44,44,44,44	1
87	MG	5	4395	1/1	0.93	0.26	-	41,41,41,41	0
86	OHX	5	3614	7/7	0.93	0.43	-	60,60,60,60	7
87	MG	5	4535	1/1	0.81	0.77	-	56,56,56,56	0
87	MG	5	4368	1/1	0.81	0.34	-	53,53,53,53	1
87	MG	Q2	504	1/1	0.91	0.30	-	50,50,50,50	0
86	OHX	1	3666	7/7	0.92	0.43	-	62,62,62,62	7
87	MG	1	4032	1/1	0.89	0.59	-	49,49,49,49	0
87	MG	S2	302	1/1	0.89	0.35	-	75,75,75,75	0
87	MG	6	2194	1/1	0.88	0.57	-	52,52,52,52	0
87	MG	5	4055	1/1	0.87	0.27	-	33,33,33,33	0
86	OHX	6	1925	7/7	0.96	0.20	-	87,87,87,87	7
87	MG	4	221	1/1	0.97	0.35	-	65,65,65,65	0
87	MG	1	4365	1/1	0.70	0.60	-	38,38,38,38	1
87	MG	5	4419	1/1	0.77	0.23	-	39,39,39,39	1
87	MG	5	4227	1/1	0.92	0.18	-	48,48,48,48	0
86	OHX	2	1968	7/7	0.96	0.38	-	77,77,77,77	7
87	MG	5	3947	1/1	0.91	0.35	-	43,43,43,43	0
87	MG	1	3893	1/1	0.97	0.37	-	51,51,51,51	0
87	MG	1	4473	1/1	0.82	0.34	-	51,51,51,51	0
86	OHX	5	3712	7/7	0.91	0.66	-	36,36,36,36	7
87	MG	5	3869	1/1	0.83	0.21	-	62,62,62,62	0
87	MG	1	4360	1/1	0.78	0.68	-	55,55,55,55	1
87	MG	5	4068	1/1	0.93	0.43	-	42,42,42,42	0
87	MG	1	4495	1/1	0.67	0.41	-	71,71,71,71	0
86	OHX	5	3701	7/7	0.88	0.14	-	120,120,120,120	7
86	OHX	5	3761	7/7	0.93	0.26	-	69,69,69,69	7
87	MG	2	2185	1/1	0.70	0.54	-	74,74,74,74	0
86	OHX	5	3768	7/7	0.73	0.63	-	47,47,47,47	7
87	MG	5	4330	1/1	0.86	0.19	-	79,79,79,79	0
87	MG	1	4028	1/1	0.95	0.16	-	48,48,48,48	0
87	MG	5	3864	1/1	0.77	0.32	-	35,35,35,35	0
87	MG	5	3969	1/1	0.97	0.42	-	41,41,41,41	0
87	MG	E1	502	1/1	0.86	0.25	-	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4322	1/1	0.56	0.45	-	62,62,62,62	0
87	MG	4	235	1/1	0.85	0.43	-	90,90,90,90	1
87	MG	5	4203	1/1	0.70	0.42	-	36,36,36,36	1
87	MG	6	2218	1/1	0.94	0.13	-	81,81,81,81	0
87	MG	1	4302	1/1	0.90	0.45	-	48,48,48,48	0
87	MG	5	4079	1/1	0.66	0.37	-	44,44,44,44	0
87	MG	5	4165	1/1	0.75	0.19	-	54,54,54,54	0
87	MG	7	232	1/1	0.88	0.25	-	50,50,50,50	0
87	MG	5	3866	1/1	0.87	0.33	-	34,34,34,34	0
87	MG	4	243	1/1	0.61	0.76	-	57,57,57,57	1
87	MG	5	4337	1/1	0.94	0.16	-	47,47,47,47	0
87	MG	5	4527	1/1	0.91	0.22	-	55,55,55,55	0
87	MG	1	4460	1/1	0.97	0.35	-	75,75,75,75	0
86	OHX	2	1957	7/7	0.97	0.18	-	79,79,79,79	7
87	MG	2	2254	1/1	0.81	0.26	-	97,97,97,97	0
87	MG	1	3920	1/1	0.95	0.29	-	52,52,52,52	0
86	OHX	1	3674	7/7	0.94	0.42	-	64,64,64,64	7
87	MG	1	4467	1/1	0.95	0.51	-	58,58,58,58	0
87	MG	1	3972	1/1	0.88	0.48	-	41,41,41,41	0
87	MG	1	4039	1/1	0.84	0.53	-	32,32,32,32	0
87	MG	1	3962	1/1	0.96	0.23	-	46,46,46,46	0
87	MG	1	4230	1/1	0.86	0.37	-	41,41,41,41	1
87	MG	5	4260	1/1	0.81	0.17	-	59,59,59,59	0
86	OHX	1	3608	7/7	0.93	0.27	-	51,51,51,51	7
87	MG	S4	302	1/1	0.79	1.59	-	87,87,87,87	0
87	MG	1	4279	1/1	0.93	0.22	-	58,58,58,58	0
87	MG	2	2219	1/1	0.88	0.38	-	62,62,62,62	0
87	MG	1	4306	1/1	0.69	0.11	-	126,126,126,126	0
87	MG	N8	206	1/1	0.62	0.39	-	39,39,39,39	0
86	OHX	5	3631	7/7	0.96	0.32	-	89,89,89,89	7
86	OHX	5	3766	7/7	0.94	0.29	-	66,66,66,66	7
87	MG	5	4569	1/1	0.84	0.36	-	117,117,117,117	0
86	OHX	2	2049	7/7	0.83	0.32	-	84,84,84,84	7
87	MG	1	3900	1/1	0.65	0.17	-	104,104,104,104	0
87	MG	6	2222	1/1	0.69	0.18	-	81,81,81,81	0
87	MG	4	246	1/1	0.94	0.39	-	51,51,51,51	0
87	MG	2	2119	1/1	0.86	0.45	-	92,92,92,92	0
86	OHX	5	3698	7/7	0.96	0.16	-	66,66,66,66	7
87	MG	2	2187	1/1	0.99	0.13	-	87,87,87,87	0
87	MG	l3	415	1/1	0.83	0.35	-	36,36,36,36	1
87	MG	8	225	1/1	0.92	0.25	-	55,55,55,55	0
87	MG	1	4066	1/1	0.72	0.35	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2157	1/1	0.97	0.47	-	46,46,46,46	0
86	OHX	1	3781	7/7	0.87	0.28	-	63,63,63,63	7
87	MG	5	4353	1/1	0.99	0.33	-	39,39,39,39	1
87	MG	5	4355	1/1	0.79	0.60	-	53,53,53,53	0
87	MG	1	4011	1/1	0.96	0.61	-	31,31,31,31	0
87	MG	8	236	1/1	0.91	0.30	-	57,57,57,57	0
87	MG	5	4517	1/1	0.91	0.19	-	54,54,54,54	0
87	MG	6	2231	1/1	0.53	0.28	-	86,86,86,86	0
86	OHX	4	211	7/7	0.97	0.13	-	99,99,99,99	7
87	MG	M7	202	1/1	0.83	0.63	-	52,52,52,52	0
87	MG	1	4072	1/1	0.90	0.46	-	40,40,40,40	0
87	MG	6	2295	1/1	0.86	0.35	-	58,58,58,58	1
87	MG	1	3898	1/1	0.96	0.38	-	48,48,48,48	0
86	OHX	1	3732	7/7	0.94	0.30	-	55,55,55,55	7
87	MG	5	4577	1/1	0.93	0.53	-	44,44,44,44	0
87	MG	1	4006	1/1	0.92	0.46	-	39,39,39,39	0
87	MG	1	4406	1/1	0.76	0.41	-	46,46,46,46	1
87	MG	5	4540	1/1	0.93	0.49	-	39,39,39,39	1
86	OHX	6	2059	7/7	0.94	0.25	-	104,104,104,104	7
87	MG	1	4269	1/1	0.90	0.27	-	68,68,68,68	0
87	MG	D9	103	1/1	0.64	0.15	-	94,94,94,94	0
87	MG	5	4249	1/1	0.86	0.33	-	60,60,60,60	0
87	MG	6	2230	1/1	0.96	0.40	-	59,59,59,59	0
86	OHX	5	3457	7/7	0.99	0.24	-	67,67,67,67	7
87	MG	1	4357	1/1	0.85	0.20	-	49,49,49,49	0
87	MG	5	4158	1/1	0.87	0.35	-	45,45,45,45	0
87	MG	1	4310	1/1	1.00	0.13	-	45,45,45,45	1
87	MG	3	230	1/1	0.94	0.13	-	58,58,58,58	0
86	OHX	6	2020	7/7	0.93	0.26	-	49,49,49,49	7
87	MG	1	3839	1/1	0.95	0.67	-	46,46,46,46	0
86	OHX	1	3463	7/7	0.99	0.24	-	74,74,74,74	7
87	MG	2	2176	1/1	0.94	0.40	-	84,84,84,84	0
86	OHX	1	3539	7/7	0.96	0.16	-	147,147,147,147	7
87	MG	5	4024	1/1	0.94	0.74	-	37,37,37,37	0
87	MG	5	3874	1/1	0.97	0.34	-	43,43,43,43	0
86	OHX	1	3594	7/7	0.97	0.15	-	74,74,74,74	7
86	OHX	5	3622	7/7	0.95	0.31	-	74,74,74,74	7
87	MG	1	4078	1/1	0.95	0.37	-	31,31,31,31	0
87	MG	5	4335	1/1	0.93	0.23	-	35,35,35,35	0
87	MG	5	4206	1/1	0.92	0.49	-	40,40,40,40	0
87	MG	2	2150	1/1	0.66	0.66	-	74,74,74,74	0
86	OHX	5	3776	7/7	0.91	0.32	-	80,80,80,80	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2166	1/1	0.85	0.30	-	88,88,88,88	0
87	MG	1	3873	1/1	0.97	0.73	-	39,39,39,39	0
87	MG	5	4215	1/1	0.96	0.36	-	38,38,38,38	0
86	OHX	5	3806	7/7	0.68	0.49	-	76,76,76,76	7
87	MG	1	3877	1/1	0.91	0.65	-	39,39,39,39	0
87	MG	1	3973	1/1	0.97	0.41	-	29,29,29,29	0
87	MG	M7	203	1/1	0.98	0.38	-	36,36,36,36	0
86	OHX	1	3773	7/7	0.91	0.28	-	71,71,71,71	7
87	MG	1	4316	1/1	0.99	0.54	-	51,51,51,51	0
87	MG	6	2123	1/1	0.94	0.23	-	67,67,67,67	0
87	MG	2	2236	1/1	0.99	0.25	-	64,64,64,64	0
87	MG	1	3827	1/1	0.91	0.20	-	67,67,67,67	0
86	OHX	2	2006	7/7	0.95	0.30	-	72,72,72,72	7
87	MG	5	4226	1/1	0.96	0.39	-	36,36,36,36	0
87	MG	2	2239	1/1	0.65	1.30	-	86,86,86,86	0
87	MG	3	222	1/1	0.96	0.31	-	45,45,45,45	0
87	MG	2	2215	1/1	0.92	0.27	-	78,78,78,78	0
87	MG	5	4373	1/1	0.66	0.23	-	38,38,38,38	1
87	MG	D4	201	1/1	0.78	0.28	-	83,83,83,83	0
87	MG	6	2193	1/1	0.89	0.31	-	57,57,57,57	0
87	MG	5	3951	1/1	0.86	0.98	-	39,39,39,39	0
86	OHX	3	208	7/7	0.97	0.21	-	85,85,85,85	7
87	MG	2	2202	1/1	0.85	0.22	-	69,69,69,69	0
87	MG	1	4172	1/1	0.87	0.14	-	53,53,53,53	0
87	MG	5	4352	1/1	0.95	0.62	-	54,54,54,54	1
87	MG	1	3870	1/1	0.93	0.46	-	34,34,34,34	0
86	OHX	5	3652	7/7	0.98	0.18	-	65,65,65,65	7
86	OHX	1	3649	7/7	0.96	0.23	-	52,52,52,52	7
86	OHX	1	3449	7/7	0.98	0.19	-	88,88,88,88	7
86	OHX	6	2073	7/7	0.84	0.35	-	64,64,64,64	7
87	MG	5	4489	1/1	0.91	0.17	-	57,57,57,57	0
87	MG	6	2128	1/1	0.67	0.28	-	68,68,68,68	0
87	MG	5	4238	1/1	0.84	0.30	-	33,33,33,33	1
87	MG	5	3880	1/1	0.85	0.48	-	34,34,34,34	0
87	MG	m6	204	1/1	0.99	0.31	-	40,40,40,40	0
87	MG	6	2184	1/1	0.72	0.18	-	69,69,69,69	0
87	MG	1	3859	1/1	0.95	0.25	-	89,89,89,89	0
87	MG	1	3816	1/1	0.96	0.67	-	49,49,49,49	0
87	MG	1	4348	1/1	0.78	0.15	-	191,191,191,191	0
87	MG	1	4487	1/1	0.75	0.54	-	62,62,62,62	0
87	MG	17	307	1/1	0.84	0.39	-	38,38,38,38	1
87	MG	5	3871	1/1	0.86	0.39	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4162	1/1	0.95	0.37	-	49,49,49,49	0
87	MG	6	2111	1/1	0.89	0.55	-	49,49,49,49	0
87	MG	5	4407	1/1	0.93	0.30	-	48,48,48,48	0
87	MG	1	3996	1/1	0.92	0.53	-	32,32,32,32	0
87	MG	1	4090	1/1	0.91	0.31	-	50,50,50,50	0
86	OHX	5	3700	7/7	0.88	0.48	-	43,43,43,43	7
87	MG	5	4272	1/1	0.97	0.33	-	48,48,48,48	0
87	MG	1	4265	1/1	0.98	0.32	-	56,56,56,56	0
87	MG	1	4470	1/1	0.81	0.44	-	35,35,35,35	1
87	MG	O7	106	1/1	0.89	1.38	-	59,59,59,59	0
87	MG	5	3879	1/1	0.94	0.41	-	33,33,33,33	0
87	MG	5	4389	1/1	0.81	0.41	-	63,63,63,63	0
87	MG	2	2244	1/1	0.80	0.15	-	78,78,78,78	0
86	OHX	m1	201	7/7	0.84	0.38	-	73,73,73,73	7
86	OHX	4	210	7/7	0.96	0.14	-	101,101,101,101	7
86	OHX	1	3588	7/7	0.99	0.22	-	47,47,47,47	7
87	MG	1	4178	1/1	0.76	0.38	-	93,93,93,93	0
87	MG	1	4262	1/1	0.94	0.17	-	74,74,74,74	0
87	MG	2	2226	1/1	0.98	0.21	-	76,76,76,76	0
86	OHX	5	3605	7/7	0.88	0.44	-	44,44,44,44	7
86	OHX	5	3554	7/7	0.97	0.23	-	57,57,57,57	7
86	OHX	5	3565	7/7	0.97	0.35	-	72,72,72,72	7
87	MG	5	4168	1/1	0.92	0.23	-	45,45,45,45	0
87	MG	1	4162	1/1	0.85	0.23	-	42,42,42,42	0
86	OHX	1	3764	7/7	0.94	0.42	-	49,49,49,49	7
87	MG	5	4057	1/1	0.90	0.23	-	45,45,45,45	0
87	MG	6	2208	1/1	0.84	0.15	-	67,67,67,67	0
87	MG	5	4009	1/1	0.93	0.41	-	38,38,38,38	0
87	MG	6	2261	1/1	0.95	0.36	-	60,60,60,60	0
87	MG	1	3974	1/1	0.95	0.31	-	54,54,54,54	0
87	MG	5	4177	1/1	0.98	0.31	-	42,42,42,42	0
86	OHX	1	3788	7/7	0.94	0.22	-	105,105,105,105	7
87	MG	6	2148	1/1	0.99	0.57	-	45,45,45,45	0
87	MG	1	4191	1/1	0.91	0.17	-	90,90,90,90	0
87	MG	1	3879	1/1	0.77	0.62	-	61,61,61,61	0
87	MG	5	4292	1/1	0.95	0.39	-	37,37,37,37	0
87	MG	1	4075	1/1	0.90	0.28	-	43,43,43,43	0
87	MG	5	4309	1/1	0.76	0.30	-	74,74,74,74	0
86	OHX	2	1944	7/7	0.97	0.23	-	72,72,72,72	7
87	MG	1	4281	1/1	0.83	0.30	-	40,40,40,40	0
87	MG	5	4071	1/1	0.82	0.71	-	89,89,89,89	0
86	OHX	1	3724	7/7	0.92	0.31	-	100,100,100,100	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3682	7/7	0.94	0.33	-	75,75,75,75	7
87	MG	5	4534	1/1	0.98	0.17	-	54,54,54,54	0
86	OHX	1	3557	7/7	0.97	0.18	-	87,87,87,87	7
87	MG	5	4473	1/1	0.81	0.30	-	49,49,49,49	0
86	OHX	1	3692	7/7	0.95	0.22	-	65,65,65,65	7
87	MG	5	4490	1/1	0.99	0.18	-	46,46,46,46	0
87	MG	1	4453	1/1	0.91	0.29	-	82,82,82,82	0
87	MG	1	4331	1/1	0.92	0.15	-	86,86,86,86	0
87	MG	1	4035	1/1	0.78	0.34	-	44,44,44,44	0
87	MG	5	4488	1/1	0.77	0.35	-	46,46,46,46	0
87	MG	5	3949	1/1	0.86	0.45	-	28,28,28,28	0
87	MG	5	3988	1/1	0.95	0.58	-	28,28,28,28	0
87	MG	5	3893	1/1	0.85	0.36	-	47,47,47,47	0
87	MG	1	4364	1/1	0.89	0.78	-	70,70,70,70	0
87	MG	1	3978	1/1	0.95	0.66	-	28,28,28,28	0
87	MG	1	4031	1/1	0.92	0.52	-	44,44,44,44	0
87	MG	5	4285	1/1	0.97	0.25	-	38,38,38,38	1
87	MG	2	2122	1/1	0.82	0.37	-	68,68,68,68	0
87	MG	1	4512	1/1	0.76	0.39	-	41,41,41,41	0
87	MG	1	4476	1/1	0.92	0.37	-	81,81,81,81	0
87	MG	5	3963	1/1	0.89	1.02	-	43,43,43,43	0
86	OHX	1	3551	7/7	0.95	0.29	-	65,65,65,65	7
86	OHX	6	2009	7/7	0.97	0.31	-	56,56,56,56	7
87	MG	1	4400	1/1	0.92	0.35	-	59,59,59,59	0
87	MG	1	4452	1/1	0.97	0.41	-	44,44,44,44	0
87	MG	5	4470	1/1	0.96	0.26	-	36,36,36,36	1
87	MG	1	4296	1/1	0.90	0.15	-	72,72,72,72	0
87	MG	1	4271	1/1	0.91	0.34	-	48,48,48,48	0
87	MG	1	4038	1/1	0.96	0.34	-	45,45,45,45	0
87	MG	1	3832	1/1	0.89	0.69	-	39,39,39,39	0
86	OHX	5	3609	7/7	0.98	0.20	-	96,96,96,96	7
87	MG	5	4385	1/1	0.89	0.34	-	34,34,34,34	1
86	OHX	6	2062	7/7	0.93	0.24	-	74,74,74,74	7
87	MG	6	2317	1/1	0.50	0.45	-	59,59,59,59	0
87	MG	1	4415	1/1	0.95	0.22	-	60,60,60,60	1
87	MG	6	2264	1/1	0.97	0.35	-	46,46,46,46	1
87	MG	7	222	1/1	0.83	0.19	-	61,61,61,61	0
87	MG	5	4224	1/1	0.97	0.36	-	38,38,38,38	0
87	MG	5	4234	1/1	1.00	0.22	-	44,44,44,44	0
86	OHX	1	3413	7/7	0.99	0.22	-	55,55,55,55	1
86	OHX	5	3814	7/7	0.98	0.21	-	70,70,70,70	7
87	MG	5	4367	1/1	0.91	0.19	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4475	1/1	0.98	0.30	-	39,39,39,39	0
86	OHX	5	3763	7/7	0.86	0.32	-	56,56,56,56	7
87	MG	1	3835	1/1	0.93	0.63	-	41,41,41,41	0
86	OHX	c3	201	7/7	0.92	0.32	-	79,79,79,79	7
87	MG	1	4356	1/1	0.96	0.26	-	88,88,88,88	0
86	OHX	2	1979	7/7	0.98	0.21	-	75,75,75,75	7
87	MG	1	4070	1/1	0.86	0.14	-	70,70,70,70	0
87	MG	1	4278	1/1	0.76	0.65	-	46,46,46,46	1
86	OHX	6	1976	7/7	0.96	0.14	-	95,95,95,95	7
87	MG	1	4439	1/1	0.79	0.09	-	200,200,200,200	0
87	MG	5	4069	1/1	0.91	0.27	-	50,50,50,50	0
87	MG	5	4217	1/1	0.84	0.54	-	66,66,66,66	0
86	OHX	1	3630	7/7	0.95	0.28	-	57,57,57,57	7
87	MG	5	4557	1/1	1.00	0.17	-	50,50,50,50	0
87	MG	5	3927	1/1	0.94	0.37	-	38,38,38,38	0
86	OHX	2	2058	7/7	0.86	0.24	-	193,193,193,193	7
87	MG	1	3851	1/1	0.94	0.28	-	53,53,53,53	0
87	MG	6	2114	1/1	0.86	0.81	-	49,49,49,49	0
87	MG	1	4417	1/1	0.89	0.47	-	44,44,44,44	1
87	MG	5	3892	1/1	0.96	0.26	-	46,46,46,46	0
86	OHX	5	3573	7/7	0.99	0.31	-	64,64,64,64	7
87	MG	1	4425	1/1	0.91	0.25	-	46,46,46,46	1
86	OHX	1	3780	7/7	0.89	0.31	-	45,45,45,45	7
86	OHX	1	3796	7/7	0.92	0.46	-	71,71,71,71	7
87	MG	5	4233	1/1	0.80	0.35	-	58,58,58,58	1
87	MG	6	2307	1/1	0.97	0.19	-	68,68,68,68	0
87	MG	8	229	1/1	0.95	0.30	-	52,52,52,52	0
87	MG	2	2224	1/1	0.78	0.46	-	99,99,99,99	0
87	MG	5	4243	1/1	0.92	0.28	-	58,58,58,58	0
87	MG	2	2208	1/1	0.75	0.43	-	72,72,72,72	0
87	MG	1	4272	1/1	0.96	0.17	-	46,46,46,46	1
87	MG	5	4532	1/1	0.97	0.17	-	43,43,43,43	0
87	MG	6	2134	1/1	0.99	0.43	-	42,42,42,42	0
86	OHX	5	3494	7/7	0.98	0.29	-	89,89,89,89	7
87	MG	2	2220	1/1	0.94	0.29	-	70,70,70,70	1
86	OHX	6	1975	7/7	0.97	0.20	-	61,61,61,61	7
87	MG	5	4359	1/1	0.91	0.39	-	73,73,73,73	0
87	MG	5	3890	1/1	0.94	0.40	-	46,46,46,46	0
86	OHX	1	3622	7/7	0.91	0.29	-	56,56,56,56	7
87	MG	1	3937	1/1	0.92	0.56	-	33,33,33,33	0
87	MG	5	3883	1/1	0.95	0.34	-	41,41,41,41	0
87	MG	6	2267	1/1	0.85	0.31	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4401	1/1	0.36	0.40	-	36,36,36,36	1
87	MG	2	2152	1/1	0.91	0.35	-	88,88,88,88	0
87	MG	1	4414	1/1	0.97	0.29	-	50,50,50,50	1
87	MG	1	4334	1/1	0.99	0.22	-	56,56,56,56	0
86	OHX	1	3754	7/7	0.83	0.28	-	99,99,99,99	7
87	MG	5	4098	1/1	0.81	0.39	-	50,50,50,50	0
87	MG	2	2180	1/1	0.77	0.50	-	68,68,68,68	0
87	MG	4	227	1/1	0.95	0.23	-	58,58,58,58	0
87	MG	2	2145	1/1	0.89	0.57	-	97,97,97,97	0
87	MG	5	4493	1/1	0.83	0.37	-	38,38,38,38	0
87	MG	6	2325	1/1	0.89	0.40	-	59,59,59,59	0
87	MG	5	3862	1/1	0.99	0.53	-	35,35,35,35	0
87	MG	1	4161	1/1	0.94	0.40	-	47,47,47,47	0
87	MG	5	4213	1/1	0.79	0.20	-	59,59,59,59	0
87	MG	1	4504	1/1	0.99	0.16	-	60,60,60,60	0
87	MG	6	2199	1/1	0.64	0.53	-	83,83,83,83	0
87	MG	q0	202	1/1	0.97	0.14	-	42,42,42,42	0
87	MG	1	4259	1/1	0.85	0.16	-	61,61,61,61	0
87	MG	5	4558	1/1	0.95	0.41	-	50,50,50,50	1
87	MG	m3	201	1/1	0.95	0.48	-	55,55,55,55	1
87	MG	5	3920	1/1	0.94	0.27	-	41,41,41,41	0
87	MG	5	4271	1/1	0.96	0.48	-	40,40,40,40	1
87	MG	1	4216	1/1	0.80	0.26	-	52,52,52,52	1
87	MG	5	4451	1/1	0.99	0.23	-	39,39,39,39	1
87	MG	6	2163	1/1	0.95	0.47	-	40,40,40,40	0
86	OHX	1	3525	7/7	0.99	0.31	-	44,44,44,44	7
87	MG	5	4038	1/1	0.95	0.58	-	29,29,29,29	0
86	OHX	2	2066	7/7	0.86	0.35	-	80,80,80,80	7
87	MG	2	2181	1/1	0.92	0.42	-	80,80,80,80	0
87	MG	5	4494	1/1	0.61	0.33	-	69,69,69,69	0
87	MG	1	4219	1/1	0.90	0.10	-	54,54,54,54	0
87	MG	1	4098	1/1	0.95	0.51	-	46,46,46,46	0
87	MG	1	4171	1/1	0.91	0.34	-	46,46,46,46	0
87	MG	1	4270	1/1	0.94	0.15	-	77,77,77,77	0
87	MG	2	2107	1/1	0.85	0.37	-	60,60,60,60	0
87	MG	1	4501	1/1	0.80	0.37	-	66,66,66,66	0
87	MG	5	4091	1/1	0.90	0.60	-	53,53,53,53	0
87	MG	6	2326	1/1	0.89	0.16	-	79,79,79,79	0
86	OHX	5	3550	7/7	0.98	0.26	-	47,47,47,47	7
87	MG	6	2119	1/1	0.86	0.55	-	59,59,59,59	0
86	OHX	2	1931	7/7	0.96	0.16	-	116,116,116,116	7
87	MG	6	2161	1/1	0.92	0.47	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3915	1/1	0.91	0.40	-	48,48,48,48	0
86	OHX	5	3697	7/7	0.96	0.46	-	44,44,44,44	7
87	MG	6	2196	1/1	0.97	0.31	-	45,45,45,45	1
87	MG	5	4513	1/1	0.78	0.18	-	97,97,97,97	0
87	MG	5	3979	1/1	0.92	0.35	-	48,48,48,48	0
87	MG	1	3865	1/1	0.95	0.37	-	42,42,42,42	0
87	MG	5	3855	1/1	0.98	0.42	-	36,36,36,36	0
87	MG	m4	202	1/1	0.83	0.55	-	53,53,53,53	1
86	OHX	C8	201	7/7	0.99	0.14	-	94,94,94,94	7
86	OHX	5	3817	7/7	0.96	0.17	-	85,85,85,85	7
86	OHX	5	3739	7/7	0.78	0.44	-	72,72,72,72	7
86	OHX	5	3818	7/7	0.89	0.33	-	63,63,63,63	7
87	MG	5	4073	1/1	0.90	0.25	-	36,36,36,36	0
87	MG	1	4081	1/1	0.84	0.72	-	46,46,46,46	0
87	MG	3	228	1/1	0.91	0.12	-	78,78,78,78	0
86	OHX	1	3637	7/7	0.97	0.33	-	76,76,76,76	7
87	MG	5	4492	1/1	0.63	0.43	-	41,41,41,41	1
87	MG	1	4384	1/1	0.91	0.28	-	64,64,64,64	0
86	OHX	5	3679	7/7	0.95	0.30	-	47,47,47,47	7
86	OHX	6	1930	7/7	0.97	0.29	-	59,59,59,59	7
87	MG	1	4297	1/1	0.86	0.32	-	46,46,46,46	0
87	MG	2	2161	1/1	0.90	0.38	-	63,63,63,63	0
87	MG	6	2321	1/1	0.82	0.37	-	72,72,72,72	0
87	MG	1	4497	1/1	0.79	0.23	-	51,51,51,51	0
87	MG	1	4199	1/1	0.90	0.34	-	46,46,46,46	0
87	MG	1	4128	1/1	0.82	0.34	-	55,55,55,55	0
87	MG	5	4178	1/1	0.80	0.53	-	38,38,38,38	1
87	MG	1	4062	1/1	0.91	0.29	-	33,33,33,33	1
87	MG	5	3968	1/1	0.92	0.64	-	27,27,27,27	0
87	MG	6	2293	1/1	0.88	0.84	-	46,46,46,46	1
87	MG	5	4556	1/1	0.77	0.45	-	43,43,43,43	0
86	OHX	c8	201	7/7	0.97	0.16	-	95,95,95,95	7
87	MG	1	4056	1/1	0.99	0.54	-	44,44,44,44	0
86	OHX	6	2081	7/7	0.74	0.42	-	91,91,91,91	7
87	MG	n6	201	1/1	0.90	0.23	-	54,54,54,54	0
87	MG	l5	304	1/1	0.73	0.16	-	61,61,61,61	0
87	MG	l4	403	1/1	0.91	0.36	-	39,39,39,39	0
87	MG	1	4286	1/1	0.88	0.41	-	40,40,40,40	0
87	MG	1	3826	1/1	0.92	0.33	-	43,43,43,43	0
87	MG	4	245	1/1	0.97	0.39	-	95,95,95,95	0
87	MG	5	4420	1/1	0.92	0.31	-	40,40,40,40	1
87	MG	5	4074	1/1	0.67	0.24	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3694	7/7	0.94	0.23	-	85,85,85,85	7
87	MG	1	3817	1/1	0.94	0.40	-	40,40,40,40	0
87	MG	6	2183	1/1	0.74	1.15	-	54,54,54,54	1
87	MG	1	4319	1/1	0.99	0.19	-	59,59,59,59	0
87	MG	1	4435	1/1	0.88	0.28	-	41,41,41,41	1
86	OHX	1	3678	7/7	0.98	0.27	-	44,44,44,44	7
86	OHX	1	3705	7/7	0.97	0.23	-	64,64,64,64	7
86	OHX	5	3809	7/7	0.96	0.33	-	86,86,86,86	7
87	MG	1	4422	1/1	0.95	0.25	-	60,60,60,60	0
87	MG	5	4324	1/1	0.73	0.61	-	42,42,42,42	1
86	OHX	1	3604	7/7	0.96	0.37	-	62,62,62,62	7
86	OHX	2	2087	7/7	0.97	0.25	-	71,71,71,71	7
87	MG	2	2132	1/1	0.88	0.48	-	70,70,70,70	0
87	MG	1	4088	1/1	0.71	0.29	-	52,52,52,52	0
87	MG	5	3853	1/1	0.87	0.47	-	43,43,43,43	0
87	MG	6	2226	1/1	0.99	0.14	-	107,107,107,107	0
87	MG	2	2174	1/1	0.97	0.62	-	68,68,68,68	0
87	MG	7	228	1/1	0.85	0.29	-	41,41,41,41	1
87	MG	5	3983	1/1	0.95	0.71	-	35,35,35,35	0
87	MG	1	4394	1/1	0.93	0.54	-	41,41,41,41	1
87	MG	5	4522	1/1	0.99	0.21	-	35,35,35,35	1
87	MG	1	4130	1/1	0.89	0.45	-	58,58,58,58	0
87	MG	1	4218	1/1	0.78	0.29	-	50,50,50,50	0
86	OHX	2	2053	7/7	0.94	0.32	-	80,80,80,80	7
86	OHX	1	3577	7/7	0.98	0.25	-	114,114,114,114	7
87	MG	5	3913	1/1	0.96	0.26	-	55,55,55,55	0
87	MG	3	217	1/1	0.92	0.49	-	36,36,36,36	0
87	MG	5	4256	1/1	0.91	0.44	-	44,44,44,44	0
87	MG	5	4503	1/1	0.83	0.23	-	46,46,46,46	0
87	MG	1	4124	1/1	0.85	0.35	-	46,46,46,46	0
87	MG	1	4148	1/1	0.62	0.38	-	69,69,69,69	0
87	MG	1	3984	1/1	0.98	0.70	-	37,37,37,37	0
87	MG	2	2184	1/1	0.94	0.32	-	59,59,59,59	0
86	OHX	5	3540	7/7	0.97	0.24	-	54,54,54,54	7
87	MG	5	4457	1/1	0.77	0.64	-	54,54,54,54	0
87	MG	1	4122	1/1	0.87	0.33	-	45,45,45,45	0
87	MG	5	4052	1/1	0.91	0.40	-	39,39,39,39	0
87	MG	6	2277	1/1	0.80	0.37	-	48,48,48,48	0
87	MG	L4	402	1/1	0.99	0.30	-	43,43,43,43	0
87	MG	5	3860	1/1	0.85	0.42	-	39,39,39,39	0
87	MG	5	4548	1/1	0.97	0.24	-	42,42,42,42	1
87	MG	7	241	1/1	0.97	0.66	-	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3954	1/1	0.98	0.58	-	47,47,47,47	0
87	MG	1	4358	1/1	0.97	0.45	-	51,51,51,51	0
87	MG	1	4132	1/1	0.81	0.29	-	51,51,51,51	0
87	MG	5	4414	1/1	0.82	0.34	-	38,38,38,38	1
86	OHX	8	218	7/7	0.78	0.56	-	48,48,48,48	7
87	MG	1	4074	1/1	0.90	0.49	-	50,50,50,50	0
87	MG	1	4420	1/1	1.00	0.22	-	56,56,56,56	0
87	MG	6	2223	1/1	0.58	0.65	-	52,52,52,52	0
86	OHX	5	3799	7/7	0.92	0.34	-	72,72,72,72	7
86	OHX	5	3583	7/7	0.98	0.15	-	148,148,148,148	7
87	MG	5	4212	1/1	0.95	0.24	-	41,41,41,41	0
87	MG	8	238	1/1	0.89	0.47	-	45,45,45,45	0
86	OHX	6	2031	7/7	0.93	0.17	-	81,81,81,81	7
87	MG	2	2211	1/1	0.85	0.16	-	106,106,106,106	0
86	OHX	1	3696	7/7	0.97	0.30	-	63,63,63,63	7
87	MG	1	3866	1/1	0.97	0.50	-	49,49,49,49	0
87	MG	1	3890	1/1	0.98	0.39	-	49,49,49,49	0
87	MG	5	4531	1/1	0.99	0.29	-	39,39,39,39	0
87	MG	1	4123	1/1	0.92	0.91	-	56,56,56,56	0
87	MG	5	4186	1/1	0.79	0.76	-	123,123,123,123	0
87	MG	5	4280	1/1	0.89	0.18	-	39,39,39,39	0
86	OHX	1	3639	7/7	0.95	0.16	-	85,85,85,85	7
87	MG	6	2165	1/1	0.98	0.28	-	45,45,45,45	0
87	MG	5	4008	1/1	0.97	0.53	-	48,48,48,48	0
86	OHX	6	2064	7/7	0.56	0.59	-	68,68,68,68	7
86	OHX	6	1948	7/7	0.98	0.18	-	86,86,86,86	7
87	MG	1	3987	1/1	0.87	0.58	-	40,40,40,40	0
87	MG	1	4165	1/1	0.99	0.28	-	54,54,54,54	0
87	MG	1	4498	1/1	0.86	0.31	-	41,41,41,41	0
87	MG	1	4277	1/1	0.89	0.36	-	37,37,37,37	0
86	OHX	1	3701	7/7	0.95	0.34	-	68,68,68,68	7
87	MG	5	4553	1/1	0.68	0.42	-	50,50,50,50	1
87	MG	5	3903	1/1	0.90	0.38	-	61,61,61,61	0
87	MG	1	4479	1/1	0.92	0.20	-	41,41,41,41	1
86	OHX	5	3669	7/7	0.97	0.35	-	37,37,37,37	7
87	MG	5	3943	1/1	0.92	0.21	-	48,48,48,48	0
86	OHX	1	3556	7/7	0.98	0.25	-	70,70,70,70	7
87	MG	2	2243	1/1	0.82	0.37	-	61,61,61,61	0
87	MG	5	4100	1/1	0.92	0.43	-	32,32,32,32	0
86	OHX	5	3525	7/7	0.98	0.32	-	42,42,42,42	7
87	MG	d4	201	1/1	0.93	0.16	-	68,68,68,68	0
86	OHX	1	3574	7/7	0.97	0.25	-	56,56,56,56	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3711	7/7	0.96	0.24	-	67,67,67,67	7
87	MG	5	4153	1/1	0.93	0.43	-	41,41,41,41	0
87	MG	n8	205	1/1	0.90	0.27	-	39,39,39,39	0
86	OHX	1	3462	7/7	0.99	0.24	-	59,59,59,59	7
87	MG	5	4329	1/1	0.96	0.38	-	47,47,47,47	0
87	MG	1	3923	1/1	0.82	0.71	-	75,75,75,75	0
87	MG	5	4173	1/1	0.90	0.21	-	82,82,82,82	0
87	MG	1	4241	1/1	0.80	0.30	-	57,57,57,57	0
86	OHX	1	3811	7/7	0.97	0.18	-	89,89,89,89	7
87	MG	5	4331	1/1	0.89	0.21	-	62,62,62,62	0
87	MG	1	4440	1/1	0.87	0.32	-	43,43,43,43	0
87	MG	5	4141	1/1	0.77	0.42	-	54,54,54,54	0
87	MG	1	4298	1/1	0.94	0.28	-	53,53,53,53	0
87	MG	1	4449	1/1	0.89	0.35	-	49,49,49,49	1
87	MG	5	4428	1/1	0.98	0.09	-	69,69,69,69	0
86	OHX	5	3634	7/7	0.96	0.26	-	42,42,42,42	7
87	MG	2	2233	1/1	0.96	0.20	-	72,72,72,72	0
87	MG	5	4099	1/1	0.78	0.31	-	61,61,61,61	0
87	MG	5	4282	1/1	0.87	0.35	-	39,39,39,39	0
87	MG	1	4021	1/1	0.98	0.62	-	37,37,37,37	0
87	MG	5	4094	1/1	0.98	0.28	-	52,52,52,52	0
87	MG	5	4134	1/1	0.95	0.49	-	37,37,37,37	0
87	MG	2	2140	1/1	0.92	0.55	-	81,81,81,81	0
86	OHX	5	3512	7/7	0.98	0.19	-	69,69,69,69	7
87	MG	2	2252	1/1	0.64	0.29	-	126,126,126,126	0
87	MG	5	4228	1/1	0.86	0.28	-	44,44,44,44	0
87	MG	5	4169	1/1	0.92	0.57	-	43,43,43,43	0
87	MG	2	2246	1/1	0.98	0.21	-	77,77,77,77	0
86	OHX	5	3732	7/7	0.98	0.23	-	49,49,49,49	7
87	MG	8	227	1/1	0.88	0.32	-	61,61,61,61	0
87	MG	1	4228	1/1	0.84	0.19	-	62,62,62,62	0
87	MG	5	3990	1/1	0.91	0.21	-	57,57,57,57	0
87	MG	6	2287	1/1	0.81	0.15	-	62,62,62,62	0
86	OHX	1	3552	7/7	0.98	0.36	-	60,60,60,60	7
87	MG	5	4112	1/1	0.91	0.34	-	28,28,28,28	0
87	MG	6	2330	1/1	0.90	0.27	-	55,55,55,55	1
87	MG	5	3914	1/1	0.94	0.56	-	33,33,33,33	0
87	MG	1	4117	1/1	0.99	0.34	-	59,59,59,59	0
87	MG	1	4477	1/1	0.62	0.77	-	47,47,47,47	0
87	MG	2	2163	1/1	0.84	0.60	-	70,70,70,70	0
87	MG	1	4244	1/1	0.77	0.22	-	72,72,72,72	0
87	MG	5	4435	1/1	0.99	0.26	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4109	1/1	0.95	0.23	-	46,46,46,46	0
87	MG	1	3922	1/1	0.81	0.45	-	58,58,58,58	0
87	MG	6	2257	1/1	0.75	0.73	-	72,72,72,72	0
86	OHX	2	2011	7/7	0.97	0.28	-	69,69,69,69	7
86	OHX	1	3619	7/7	0.95	0.35	-	70,70,70,70	7
87	MG	1	3913	1/1	0.92	0.26	-	49,49,49,49	0
86	OHX	5	3777	7/7	0.96	0.41	-	38,38,38,38	7
87	MG	5	3852	1/1	0.91	0.35	-	40,40,40,40	0
87	MG	1	4185	1/1	0.89	0.79	-	40,40,40,40	1
87	MG	1	3856	1/1	0.75	0.45	-	63,63,63,63	0
86	OHX	5	3784	7/7	0.95	0.53	-	55,55,55,55	7
87	MG	6	2158	1/1	0.96	0.52	-	40,40,40,40	0
86	OHX	5	3675	7/7	0.92	0.26	-	49,49,49,49	7
86	OHX	1	3623	7/7	0.97	0.21	-	51,51,51,51	7
87	MG	1	4063	1/1	0.92	0.33	-	53,53,53,53	0
86	OHX	1	3654	7/7	0.96	0.36	-	65,65,65,65	7
87	MG	1	4303	1/1	0.94	0.82	-	41,41,41,41	1
87	MG	2	2134	1/1	0.91	0.61	-	76,76,76,76	0
87	MG	6	2129	1/1	0.95	0.24	-	59,59,59,59	0
87	MG	2	2142	1/1	0.92	0.60	-	61,61,61,61	0
87	MG	5	4085	1/1	0.77	0.26	-	57,57,57,57	0
87	MG	5	3887	1/1	0.93	0.30	-	34,34,34,34	0
87	MG	1	4207	1/1	0.91	0.19	-	58,58,58,58	0
86	OHX	1	3621	7/7	0.97	0.17	-	73,73,73,73	7
86	OHX	1	3555	7/7	0.95	0.17	-	89,89,89,89	7
86	OHX	1	3769	7/7	0.91	0.58	-	49,49,49,49	7
87	MG	1	4333	1/1	0.94	0.29	-	49,49,49,49	0
87	MG	2	2102	1/1	0.62	0.39	-	84,84,84,84	0
86	OHX	2	1962	7/7	0.95	0.20	-	97,97,97,97	7
87	MG	5	3960	1/1	0.99	0.45	-	37,37,37,37	0
87	MG	2	2115	1/1	0.93	0.71	-	71,71,71,71	0
86	OHX	5	3590	7/7	0.96	0.15	-	83,83,83,83	7
87	MG	2	2222	1/1	0.78	0.20	-	80,80,80,80	0
86	OHX	5	3719	7/7	0.93	0.30	-	64,64,64,64	7
86	OHX	4	205	7/7	0.98	0.21	-	75,75,75,75	7
87	MG	5	4552	1/1	0.88	0.30	-	39,39,39,39	0
87	MG	1	3872	1/1	0.81	0.77	-	54,54,54,54	0
87	MG	7	234	1/1	0.89	0.34	-	45,45,45,45	0
86	OHX	5	3654	7/7	0.95	0.34	-	55,55,55,55	7
87	MG	1	4325	1/1	0.86	0.55	-	52,52,52,52	0
87	MG	5	3896	1/1	0.76	0.24	-	50,50,50,50	0
87	MG	1	3848	1/1	0.74	0.63	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3605	7/7	0.91	0.14	-	107,107,107,107	7
87	MG	2	2178	1/1	0.91	0.36	-	79,79,79,79	0
86	OHX	6	1934	7/7	0.98	0.30	-	57,57,57,57	7
87	MG	5	4104	1/1	0.58	0.54	-	45,45,45,45	1
86	OHX	6	2046	7/7	0.93	0.13	-	100,100,100,100	7
87	MG	5	3998	1/1	0.92	0.58	-	41,41,41,41	0
87	MG	M0	306	1/1	0.84	0.29	-	53,53,53,53	0
87	MG	8	237	1/1	0.83	0.21	-	71,71,71,71	0
87	MG	2	2137	1/1	0.85	0.46	-	126,126,126,126	0
87	MG	1	4321	1/1	0.95	0.18	-	44,44,44,44	1
87	MG	1	4398	1/1	0.83	0.23	-	72,72,72,72	0
86	OHX	2	2073	7/7	0.96	0.18	-	89,89,89,89	7
86	OHX	2	2084	7/7	0.84	0.16	-	183,183,183,183	7
87	MG	1	4405	1/1	0.91	0.19	-	44,44,44,44	0
87	MG	2	2167	1/1	0.74	0.26	-	84,84,84,84	0
87	MG	5	3967	1/1	0.95	0.80	-	28,28,28,28	0
87	MG	5	4164	1/1	0.83	0.12	-	83,83,83,83	0
87	MG	1	4369	1/1	0.90	0.23	-	43,43,43,43	0
87	MG	5	4481	1/1	0.76	0.40	-	44,44,44,44	1
87	MG	1	4499	1/1	0.88	0.16	-	60,60,60,60	0
87	MG	5	4358	1/1	0.90	0.21	-	54,54,54,54	0
87	MG	5	4132	1/1	0.87	0.27	-	33,33,33,33	1
87	MG	5	4010	1/1	0.92	0.52	-	46,46,46,46	0
87	MG	1	4282	1/1	0.63	0.54	-	47,47,47,47	1
87	MG	M7	206	1/1	0.87	0.30	-	43,43,43,43	0
87	MG	5	4175	1/1	0.98	0.23	-	86,86,86,86	0
87	MG	1	4288	1/1	0.91	0.31	-	52,52,52,52	0
86	OHX	2	1926	7/7	0.99	0.20	-	81,81,81,81	7
87	MG	5	3971	1/1	0.90	0.47	-	27,27,27,27	0
86	OHX	5	3783	7/7	0.76	0.59	-	56,56,56,56	7
87	MG	6	2294	1/1	0.98	0.17	-	43,43,43,43	0
86	OHX	5	3603	7/7	0.95	0.22	-	43,43,43,43	7
86	OHX	1	3787	7/7	0.91	0.24	-	69,69,69,69	7
87	MG	2	2205	1/1	0.76	0.67	-	76,76,76,76	0
87	MG	1	4382	1/1	0.98	0.35	-	70,70,70,70	0
87	MG	6	2256	1/1	0.75	0.38	-	73,73,73,73	0
87	MG	5	4242	1/1	0.95	0.37	-	44,44,44,44	0
86	OHX	1	3427	7/7	0.99	0.24	-	65,65,65,65	7
87	MG	1	4231	1/1	0.98	0.22	-	44,44,44,44	0
87	MG	5	4051	1/1	0.84	0.42	-	33,33,33,33	0
87	MG	5	3936	1/1	0.92	0.55	-	28,28,28,28	0
87	MG	5	4283	1/1	0.99	0.24	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3812	7/7	0.85	0.59	-	54,54,54,54	7
87	MG	1	4363	1/1	0.87	0.31	-	45,45,45,45	1
87	MG	6	2245	1/1	0.93	0.12	-	60,60,60,60	0
87	MG	2	2129	1/1	0.94	0.26	-	66,66,66,66	0
87	MG	1	4438	1/1	0.97	0.37	-	64,64,64,64	0
87	MG	1	4253	1/1	0.96	0.32	-	66,66,66,66	0
87	MG	5	4560	1/1	0.88	0.27	-	40,40,40,40	0
87	MG	2	2095	1/1	0.83	0.38	-	63,63,63,63	0
87	MG	1	4110	1/1	0.87	0.71	-	51,51,51,51	0
87	MG	3	224	1/1	0.90	0.71	-	47,47,47,47	0
87	MG	5	4423	1/1	0.57	0.51	-	59,59,59,59	0
87	MG	1	4349	1/1	0.83	0.20	-	69,69,69,69	0
87	MG	5	4129	1/1	0.75	0.58	-	82,82,82,82	0
86	OHX	1	3444	7/7	0.99	0.25	-	61,61,61,61	7
87	MG	1	4494	1/1	0.89	0.47	-	58,58,58,58	0
87	MG	1	4176	1/1	0.94	0.24	-	72,72,72,72	0
87	MG	6	2324	1/1	0.82	0.52	-	47,47,47,47	1
87	MG	6	2124	1/1	0.64	0.41	-	71,71,71,71	0
87	MG	1	4330	1/1	0.79	0.44	-	59,59,59,59	0
87	MG	m7	205	1/1	0.74	0.36	-	50,50,50,50	0
87	MG	6	2116	1/1	0.93	0.37	-	61,61,61,61	0
87	MG	1	4043	1/1	0.88	0.15	-	66,66,66,66	0
87	MG	5	4418	1/1	0.92	0.32	-	64,64,64,64	0
87	MG	5	4416	1/1	0.89	0.44	-	38,38,38,38	0
86	OHX	6	1984	7/7	0.75	0.29	-	82,82,82,82	7
87	MG	4	234	1/1	0.82	0.26	-	67,67,67,67	0
86	OHX	1	3646	7/7	0.97	0.32	-	54,54,54,54	7
86	OHX	1	3468	7/7	0.98	0.23	-	65,65,65,65	7
87	MG	6	2100	1/1	0.96	0.13	-	60,60,60,60	0
86	OHX	5	3575	7/7	0.97	0.23	-	66,66,66,66	7
87	MG	1	4351	1/1	0.89	0.26	-	43,43,43,43	0
87	MG	4	237	1/1	0.72	0.47	-	67,67,67,67	0
87	MG	7	221	1/1	0.92	0.20	-	41,41,41,41	0
86	OHX	2	2000	7/7	0.93	0.36	-	110,110,110,110	7
87	MG	1	4027	1/1	0.96	0.32	-	43,43,43,43	0
87	MG	3	216	1/1	0.92	0.36	-	55,55,55,55	0
87	MG	2	2227	1/1	0.86	0.34	-	63,63,63,63	0
86	OHX	6	1964	7/7	0.96	0.26	-	49,49,49,49	7
87	MG	5	4499	1/1	0.93	0.32	-	55,55,55,55	0
86	OHX	5	3794	7/7	0.97	0.23	-	57,57,57,57	7
87	MG	6	2265	1/1	0.91	0.46	-	48,48,48,48	0
87	MG	2	2191	1/1	0.81	0.58	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	7	238	1/1	0.94	0.81	-	51,51,51,51	1
87	MG	1	4014	1/1	0.77	0.50	-	49,49,49,49	0
87	MG	5	4564	1/1	0.92	0.43	-	34,34,34,34	1
87	MG	1	4354	1/1	0.92	0.15	-	62,62,62,62	0
86	OHX	7	212	7/7	0.84	0.44	-	61,61,61,61	7
87	MG	1	4121	1/1	0.92	0.42	-	37,37,37,37	0
87	MG	5	4110	1/1	0.79	0.42	-	50,50,50,50	0
87	MG	5	4417	1/1	0.92	0.31	-	56,56,56,56	0
87	MG	4	229	1/1	0.90	0.39	-	66,66,66,66	0
87	MG	5	4116	1/1	0.96	0.81	-	36,36,36,36	1
87	MG	5	3840	1/1	0.97	0.58	-	60,60,60,60	0
87	MG	5	4172	1/1	0.72	0.42	-	40,40,40,40	0
87	MG	6	2258	1/1	0.97	0.30	-	84,84,84,84	0
87	MG	5	3985	1/1	0.96	0.64	-	50,50,50,50	0
87	MG	1	4092	1/1	0.96	0.57	-	42,42,42,42	0
87	MG	5	3916	1/1	0.82	0.32	-	57,57,57,57	0
87	MG	M7	207	1/1	0.94	0.28	-	43,43,43,43	0
87	MG	5	4369	1/1	0.84	0.85	-	52,52,52,52	1
86	OHX	6	1998	7/7	0.94	0.27	-	64,64,64,64	7
86	OHX	5	3510	7/7	0.99	0.25	-	48,48,48,48	7
87	MG	5	4204	1/1	0.86	0.54	-	60,60,60,60	0
87	MG	2	2217	1/1	0.49	0.52	-	103,103,103,103	0
87	MG	Q2	503	1/1	0.64	0.26	-	62,62,62,62	0
87	MG	1	3857	1/1	0.87	0.28	-	51,51,51,51	0
87	MG	6	2156	1/1	0.83	0.62	-	66,66,66,66	0
87	MG	1	3938	1/1	0.93	0.61	-	36,36,36,36	0
87	MG	2	2147	1/1	0.54	0.20	-	100,100,100,100	0
87	MG	1	4490	1/1	0.97	0.73	-	100,100,100,100	0
87	MG	5	3931	1/1	0.91	0.46	-	42,42,42,42	0
87	MG	5	4059	1/1	0.96	0.44	-	39,39,39,39	0
87	MG	5	3953	1/1	0.85	0.62	-	45,45,45,45	0
87	MG	5	4229	1/1	0.85	0.46	-	43,43,43,43	0
87	MG	5	3872	1/1	0.96	0.41	-	32,32,32,32	0
86	OHX	1	3498	7/7	0.99	0.25	-	62,62,62,62	7
87	MG	5	4308	1/1	0.93	0.28	-	58,58,58,58	0
86	OHX	5	3516	7/7	0.98	0.20	-	60,60,60,60	7
87	MG	5	4471	1/1	0.95	0.35	-	55,55,55,55	0
87	MG	1	4374	1/1	0.65	0.71	-	44,44,44,44	0
87	MG	5	4102	1/1	0.94	0.53	-	44,44,44,44	0
86	OHX	5	3627	7/7	0.98	0.14	-	81,81,81,81	7
87	MG	1	4503	1/1	0.86	0.28	-	47,47,47,47	0
87	MG	2	2245	1/1	0.78	0.46	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2019	7/7	0.90	0.28	-	105,105,105,105	7
87	MG	1	3944	1/1	0.98	0.47	-	35,35,35,35	0
87	MG	1	4100	1/1	0.88	0.40	-	44,44,44,44	1
87	MG	1	4442	1/1	0.93	0.29	-	51,51,51,51	0
86	OHX	1	3704	7/7	0.94	0.48	-	55,55,55,55	7
87	MG	5	4399	1/1	0.96	0.98	-	46,46,46,46	1
86	OHX	6	1967	7/7	0.98	0.19	-	47,47,47,47	7
87	MG	6	2130	1/1	0.85	0.19	-	55,55,55,55	0
87	MG	5	4016	1/1	0.95	0.72	-	29,29,29,29	0
86	OHX	6	2049	7/7	0.79	0.40	-	70,70,70,70	7
87	MG	5	3857	1/1	0.91	0.29	-	47,47,47,47	0
87	MG	1	4047	1/1	0.69	0.21	-	83,83,83,83	0
86	OHX	5	3804	7/7	0.98	0.24	-	52,52,52,52	7
86	OHX	s4	301	7/7	0.97	0.27	-	79,79,79,79	7
87	MG	1	4229	1/1	0.89	0.16	-	64,64,64,64	0
87	MG	1	4380	1/1	0.91	0.36	-	30,30,30,30	0
87	MG	2	2255	1/1	0.78	0.18	-	88,88,88,88	0
87	MG	m0	305	1/1	0.92	0.35	-	32,32,32,32	0
86	OHX	6	2017	7/7	0.89	0.34	-	50,50,50,50	7
87	MG	1	3849	1/1	0.87	0.63	-	44,44,44,44	0

## 6.5 Other polymers

There are no such residues in this entry.