



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 9, 2017 – 02:54 pm GMT

PDB ID : 5TGM  
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.; Yusupov, M.  
Deposited on : 2016-09-28  
Resolution : 3.50 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 : recal28906  
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) : recal28906

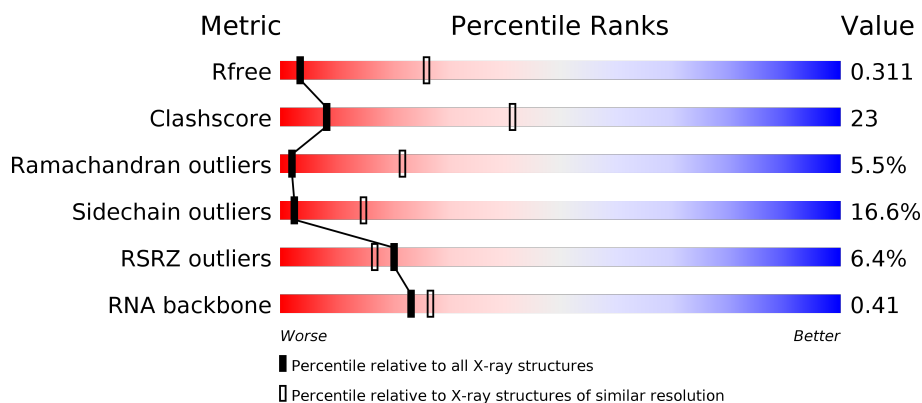
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)
RNA backbone	2435	1024 (4.10-2.86)

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	1812	<div> <div>7%</div> <div>7% 32% 45% 14%</div> </div>
2	S0	206	<div> <div>25%</div> <div>18% 69% 12%</div> </div>
2	s0	206	<div> <div>8%</div> <div>78% 20%</div> </div>
3	S1	216	<div> <div>5%</div> <div>21% 57% 20%</div> </div>

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Mol	Chain	Length	Quality of chain
3	s1	216	
4	S2	217	
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	188	
10	s8	188	
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	

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Mol	Chain	Length	Quality of chain
16	c4	128	
17	C5	135	
17	c5	135	
18	C6	142	
18	c6	142	
19	C7	120	
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	


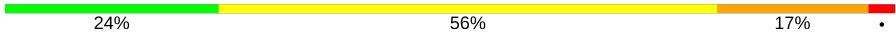

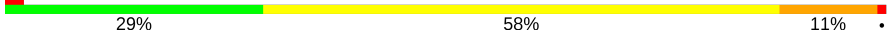
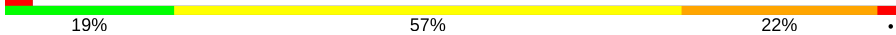

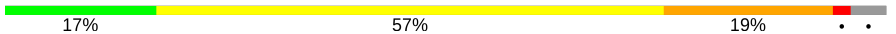

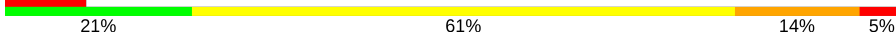

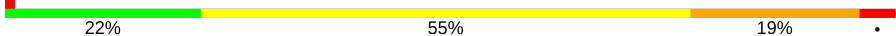

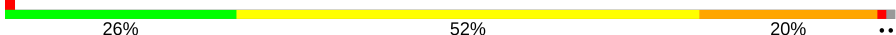

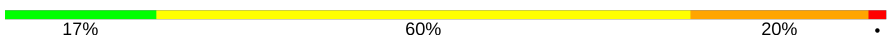





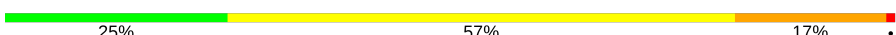




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Mol	Chain	Length	Quality of chain
29	d7	81	
30	D8	63	
30	d8	63	
31	D9	53	
31	d9	53	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
35	SM	159	
36	1	3149	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	252	
39	l2	252	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	

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Mol	Chain	Length	Quality of chain
43	l6	175	
44	L7	223	
44	l7	223	
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	
55	m9	188	
56	N0	172	




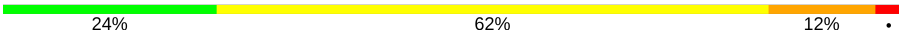

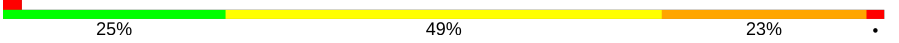

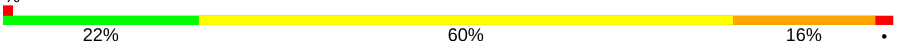

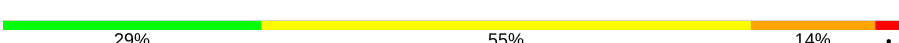



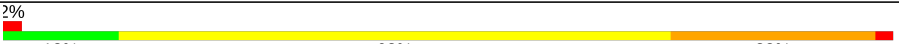



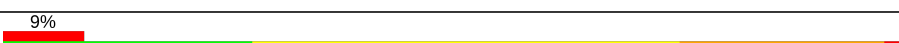
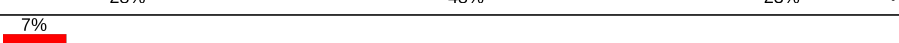

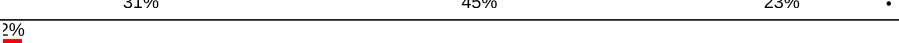
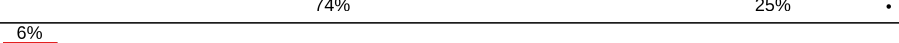



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Mol	Chain	Length	Quality of chain
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	100	
58	n2	100	
59	N3	136	
59	n3	136	
60	N4	98	
61	N5	121	
61	n5	121	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	100	
66	o0	100	
67	O1	109	
67	o1	109	
68	O2	127	
68	o2	127	
69	O3	106	

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Mol	Chain	Length	Quality of chain
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	
81	c0	96	
82	c7	121	
83	sR	318	

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Mol	Chain	Length	Quality of chain
84	sM	104	
85	5	3150	
86	l8	231	
87	m2	150	
88	n4	135	
89	p0	143	
90	p1	47	
90	p2	47	
91	P	5	
91	p	5	

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
92	OHX	1	3494	-	-	X	-
92	OHX	1	3507	-	-	X	-
92	OHX	1	3508	-	-	-	X
92	OHX	1	3511	-	-	X	-
92	OHX	1	3525	-	-	X	X
92	OHX	1	3537	-	-	-	X
92	OHX	1	3538	-	-	-	X
92	OHX	1	3560	-	-	-	X
92	OHX	1	3563	-	-	X	-
92	OHX	1	3565	-	-	X	-
92	OHX	1	3569	-	-	-	X
92	OHX	1	3576	-	-	X	X
92	OHX	1	3578	-	-	X	-
92	OHX	1	3579	-	-	-	X
92	OHX	1	3583	-	-	X	-
92	OHX	1	3585	-	-	X	-
92	OHX	1	3589	-	-	X	-
92	OHX	1	3590	-	-	X	X
92	OHX	1	3594	-	-	-	X
92	OHX	1	3597	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
92	OHX	1	3599	-	-	-	X
92	OHX	1	3600	-	-	X	-
92	OHX	1	3603	-	-	-	X
92	OHX	1	3605	-	-	-	X
92	OHX	1	3607	-	-	-	X
92	OHX	1	3612	-	-	X	-
92	OHX	1	3614	-	-	-	X
92	OHX	1	3616	-	-	X	-
92	OHX	1	3620	-	-	-	X
92	OHX	1	3621	-	-	-	X
92	OHX	1	3626	-	-	-	X
92	OHX	1	3629	-	-	-	X
92	OHX	1	3642	-	-	-	X
92	OHX	1	3643	-	-	-	X
92	OHX	1	3645	-	-	-	X
92	OHX	1	3646	-	-	-	X
92	OHX	1	3648	-	-	X	X
92	OHX	1	3649	-	-	-	X
92	OHX	1	3653	-	-	-	X
92	OHX	1	3654	-	-	-	X
92	OHX	1	3655	-	-	-	X
92	OHX	1	3660	-	-	-	X
92	OHX	1	3662	-	-	X	X
92	OHX	1	3663	-	-	-	X
92	OHX	1	3665	-	-	-	X
92	OHX	1	3667	-	-	-	X
92	OHX	1	3670	-	-	-	X
92	OHX	1	3671	-	-	-	X
92	OHX	1	3674	-	-	-	X
92	OHX	1	3675	-	-	-	X
92	OHX	1	3678	-	-	-	X
92	OHX	1	3684	-	-	X	X
92	OHX	1	3685	-	-	-	X
92	OHX	1	3687	-	-	-	X
92	OHX	1	3688	-	-	-	X
92	OHX	1	3690	-	-	X	-
92	OHX	1	3691	-	-	X	-
92	OHX	1	3693	-	-	-	X
92	OHX	1	3694	-	-	X	-
92	OHX	1	3699	-	-	-	X
92	OHX	1	3702	-	-	X	X
92	OHX	1	3703	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
92	OHX	1	3710	-	-	X	X
92	OHX	1	3711	-	-	X	-
92	OHX	1	3712	-	-	-	X
92	OHX	1	3714	-	-	-	X
92	OHX	1	3718	-	-	-	X
92	OHX	1	3721	-	-	-	X
92	OHX	1	3726	-	-	-	X
92	OHX	1	3727	-	-	-	X
92	OHX	1	3728	-	-	-	X
92	OHX	1	3729	-	-	-	X
92	OHX	2	1914	-	-	X	-
92	OHX	2	1921	-	-	X	-
92	OHX	2	1970	-	-	X	-
92	OHX	2	1976	-	-	-	X
92	OHX	2	1979	-	-	-	X
92	OHX	2	1985	-	-	X	-
92	OHX	2	1995	-	-	-	X
92	OHX	2	2021	-	-	-	X
92	OHX	2	2025	-	-	-	X
92	OHX	2	2029	-	-	-	X
92	OHX	2	2031	-	-	-	X
92	OHX	2	2040	-	-	X	-
92	OHX	2	2043	-	-	-	X
92	OHX	2	2047	-	-	-	X
92	OHX	2	2049	-	-	-	X
92	OHX	3	204	-	-	X	-
92	OHX	3	208	-	-	-	X
92	OHX	4	212	-	-	-	X
92	OHX	4	215	-	-	-	X
92	OHX	4	218	-	-	-	X
92	OHX	5	3481	-	-	X	-
92	OHX	5	3503	-	-	X	-
92	OHX	5	3506	-	-	X	-
92	OHX	5	3522	-	-	X	-
92	OHX	5	3524	-	-	X	-
92	OHX	5	3527	-	-	-	X
92	OHX	5	3531	-	-	-	X
92	OHX	5	3534	-	-	X	-
92	OHX	5	3549	-	-	-	X
92	OHX	5	3551	-	-	-	X
92	OHX	5	3554	-	-	-	X
92	OHX	5	3555	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
92	OHX	5	3565	-	-	X	X
92	OHX	5	3566	-	-	X	-
92	OHX	5	3570	-	-	-	X
92	OHX	5	3573	-	-	-	X
92	OHX	5	3574	-	-	X	-
92	OHX	5	3576	-	-	X	X
92	OHX	5	3578	-	-	-	X
92	OHX	5	3580	-	-	X	X
92	OHX	5	3582	-	-	-	X
92	OHX	5	3590	-	-	-	X
92	OHX	5	3591	-	-	X	X
92	OHX	5	3597	-	-	-	X
92	OHX	5	3598	-	-	-	X
92	OHX	5	3599	-	-	-	X
92	OHX	5	3601	-	-	-	X
92	OHX	5	3602	-	-	-	X
92	OHX	5	3606	-	-	-	X
92	OHX	5	3607	-	-	-	X
92	OHX	5	3609	-	-	-	X
92	OHX	5	3611	-	-	-	X
92	OHX	5	3617	-	-	-	X
92	OHX	5	3623	-	-	-	X
92	OHX	5	3624	-	-	-	X
92	OHX	5	3630	-	-	-	X
92	OHX	5	3632	-	-	-	X
92	OHX	5	3634	-	-	X	X
92	OHX	5	3636	-	-	-	X
92	OHX	5	3638	-	-	-	X
92	OHX	5	3640	-	-	X	-
92	OHX	5	3641	-	-	-	X
92	OHX	5	3643	-	-	-	X
92	OHX	5	3644	-	-	-	X
92	OHX	5	3645	-	-	-	X
92	OHX	5	3647	-	-	-	X
92	OHX	5	3648	-	-	-	X
92	OHX	5	3652	-	-	-	X
92	OHX	5	3658	-	-	-	X
92	OHX	5	3659	-	-	-	X
92	OHX	5	3660	-	-	-	X
92	OHX	5	3661	-	-	-	X
92	OHX	5	3662	-	-	-	X
92	OHX	5	3664	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
92	OHX	5	3670	-	-	-	X
92	OHX	5	3671	-	-	X	X
92	OHX	5	3681	-	-	-	X
92	OHX	5	3684	-	-	-	X
92	OHX	5	3687	-	-	-	X
92	OHX	5	3688	-	-	-	X
92	OHX	5	3689	-	-	-	X
92	OHX	5	3692	-	-	X	-
92	OHX	5	3693	-	-	-	X
92	OHX	5	3694	-	-	X	X
92	OHX	5	3695	-	-	-	X
92	OHX	5	3698	-	-	-	X
92	OHX	5	3700	-	-	-	X
92	OHX	5	3702	-	-	X	-
92	OHX	5	3703	-	-	X	-
92	OHX	5	3705	-	-	-	X
92	OHX	5	3706	-	-	X	X
92	OHX	5	3707	-	-	-	X
92	OHX	5	3709	-	-	-	X
92	OHX	5	3716	-	-	-	X
92	OHX	5	3718	-	-	-	X
92	OHX	5	3720	-	-	-	X
92	OHX	5	3721	-	-	X	X
92	OHX	5	3724	-	-	X	X
92	OHX	5	3729	-	-	-	X
92	OHX	5	3737	-	-	-	X
92	OHX	5	3739	-	-	-	X
92	OHX	5	3740	-	-	-	X
92	OHX	6	1914	-	-	X	-
92	OHX	6	1938	-	-	X	-
92	OHX	6	1970	-	-	-	X
92	OHX	6	1978	-	-	X	-
92	OHX	6	1990	-	-	-	X
92	OHX	6	1992	-	-	-	X
92	OHX	6	1998	-	-	X	-
92	OHX	6	2001	-	-	X	-
92	OHX	6	2009	-	-	-	X
92	OHX	6	2012	-	-	-	X
92	OHX	6	2023	-	-	-	X
92	OHX	6	2024	-	-	-	X
92	OHX	6	2026	-	-	-	X
92	OHX	6	2029	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
92	OHX	6	2032	-	-	-	X
92	OHX	6	2033	-	-	-	X
92	OHX	6	2035	-	-	-	X
92	OHX	6	2037	-	-	-	X
92	OHX	6	2042	-	-	-	X
92	OHX	6	2048	-	-	X	-
92	OHX	6	2051	-	-	-	X
92	OHX	6	2054	-	-	-	X
92	OHX	6	2057	-	-	-	X
92	OHX	6	2058	-	-	X	X
92	OHX	7	209	-	-	X	X
92	OHX	7	211	-	-	-	X
92	OHX	8	210	-	-	-	X
92	OHX	8	211	-	-	-	X
92	OHX	8	212	-	-	-	X
92	OHX	8	213	-	-	-	X
92	OHX	8	214	-	-	-	X
92	OHX	C3	201	-	-	X	-
92	OHX	C5	201	-	-	X	-
92	OHX	O4	201	-	-	-	X
92	OHX	O7	102	-	-	X	-
92	OHX	Q2	502	-	-	X	-
92	OHX	S9	201	-	-	X	X
92	OHX	l3	402	-	-	-	X
92	OHX	m0	303	-	-	-	X
93	MG	1	3737	-	-	-	X
93	MG	1	3739	-	-	-	X
93	MG	1	3741	-	-	-	X
93	MG	1	3745	-	-	-	X
93	MG	1	3763	-	-	-	X
93	MG	1	3767	-	-	-	X
93	MG	1	3784	-	-	-	X
93	MG	1	3786	-	-	-	X
93	MG	1	3790	-	-	-	X
93	MG	1	3800	-	-	-	X
93	MG	1	3801	-	-	-	X
93	MG	1	3807	-	-	-	X
93	MG	1	3809	-	-	-	X
93	MG	1	3812	-	-	-	X
93	MG	1	3814	-	-	-	X
93	MG	1	3816	-	-	-	X
93	MG	1	3820	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	MG	1	3822	-	-	-	X
93	MG	1	3824	-	-	-	X
93	MG	1	3825	-	-	-	X
93	MG	1	3826	-	-	-	X
93	MG	1	3831	-	-	-	X
93	MG	1	3832	-	-	-	X
93	MG	1	3835	-	-	-	X
93	MG	1	3836	-	-	-	X
93	MG	1	3840	-	-	-	X
93	MG	1	3841	-	-	-	X
93	MG	1	3844	-	-	-	X
93	MG	1	3845	-	-	-	X
93	MG	1	3851	-	-	-	X
93	MG	1	3852	-	-	-	X
93	MG	1	3853	-	-	-	X
93	MG	1	3859	-	-	-	X
93	MG	1	3864	-	-	-	X
93	MG	1	3867	-	-	-	X
93	MG	1	3868	-	-	-	X
93	MG	1	3875	-	-	-	X
93	MG	1	3876	-	-	-	X
93	MG	1	3877	-	-	-	X
93	MG	1	3882	-	-	-	X
93	MG	1	3883	-	-	-	X
93	MG	1	3889	-	-	-	X
93	MG	1	3892	-	-	-	X
93	MG	1	3894	-	-	-	X
93	MG	1	3896	-	-	-	X
93	MG	1	3897	-	-	-	X
93	MG	1	3898	-	-	-	X
93	MG	1	3899	-	-	-	X
93	MG	1	3904	-	-	-	X
93	MG	1	3907	-	-	-	X
93	MG	1	3909	-	-	-	X
93	MG	1	3911	-	-	-	X
93	MG	1	3912	-	-	-	X
93	MG	1	3914	-	-	-	X
93	MG	1	3916	-	-	-	X
93	MG	1	3918	-	-	-	X
93	MG	1	3919	-	-	-	X
93	MG	1	3921	-	-	-	X
93	MG	1	3922	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	MG	1	3923	-	-	-	X
93	MG	1	3925	-	-	-	X
93	MG	1	3932	-	-	-	X
93	MG	1	3937	-	-	-	X
93	MG	1	3944	-	-	-	X
93	MG	1	3949	-	-	-	X
93	MG	1	3952	-	-	-	X
93	MG	1	3966	-	-	-	X
93	MG	1	3969	-	-	-	X
93	MG	1	3971	-	-	-	X
93	MG	1	3977	-	-	-	X
93	MG	1	3983	-	-	-	X
93	MG	1	3984	-	-	-	X
93	MG	1	3989	-	-	-	X
93	MG	1	4002	-	-	-	X
93	MG	1	4014	-	-	-	X
93	MG	1	4027	-	-	-	X
93	MG	1	4030	-	-	-	X
93	MG	1	4033	-	-	-	X
93	MG	1	4034	-	-	-	X
93	MG	1	4036	-	-	-	X
93	MG	1	4045	-	-	-	X
93	MG	1	4052	-	-	-	X
93	MG	1	4055	-	-	-	X
93	MG	1	4056	-	-	-	X
93	MG	1	4071	-	-	-	X
93	MG	1	4072	-	-	-	X
93	MG	1	4073	-	-	-	X
93	MG	1	4074	-	-	-	X
93	MG	1	4077	-	-	-	X
93	MG	1	4082	-	-	-	X
93	MG	1	4088	-	-	-	X
93	MG	1	4091	-	-	-	X
93	MG	1	4093	-	-	-	X
93	MG	1	4097	-	-	-	X
93	MG	1	4098	-	-	-	X
93	MG	1	4099	-	-	-	X
93	MG	1	4100	-	-	-	X
93	MG	1	4102	-	-	-	X
93	MG	1	4104	-	-	-	X
93	MG	1	4107	-	-	-	X
93	MG	1	4108	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	MG	1	4123	-	-	-	X
93	MG	2	2060	-	-	-	X
93	MG	2	2061	-	-	-	X
93	MG	2	2062	-	-	-	X
93	MG	2	2065	-	-	-	X
93	MG	2	2069	-	-	-	X
93	MG	2	2071	-	-	-	X
93	MG	2	2076	-	-	-	X
93	MG	2	2080	-	-	-	X
93	MG	2	2087	-	-	-	X
93	MG	2	2089	-	-	-	X
93	MG	2	2095	-	-	-	X
93	MG	2	2099	-	-	-	X
93	MG	2	2109	-	-	-	X
93	MG	2	2110	-	-	-	X
93	MG	2	2115	-	-	-	X
93	MG	2	2123	-	-	-	X
93	MG	2	2126	-	-	-	X
93	MG	2	2131	-	-	-	X
93	MG	2	2141	-	-	-	X
93	MG	4	227	-	-	-	X
93	MG	4	228	-	-	-	X
93	MG	4	233	-	-	-	X
93	MG	5	3752	-	-	-	X
93	MG	5	3753	-	-	-	X
93	MG	5	3754	-	-	-	X
93	MG	5	3755	-	-	-	X
93	MG	5	3759	-	-	-	X
93	MG	5	3766	-	-	-	X
93	MG	5	3768	-	-	-	X
93	MG	5	3773	-	-	-	X
93	MG	5	3775	-	-	-	X
93	MG	5	3780	-	-	-	X
93	MG	5	3785	-	-	-	X
93	MG	5	3789	-	-	-	X
93	MG	5	3793	-	-	-	X
93	MG	5	3801	-	-	-	X
93	MG	5	3804	-	-	-	X
93	MG	5	3811	-	-	-	X
93	MG	5	3813	-	-	-	X
93	MG	5	3820	-	-	-	X
93	MG	5	3837	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	MG	5	3840	-	-	-	X
93	MG	5	3844	-	-	-	X
93	MG	5	3847	-	-	-	X
93	MG	5	3851	-	-	-	X
93	MG	5	3853	-	-	-	X
93	MG	5	3854	-	-	-	X
93	MG	5	3858	-	-	-	X
93	MG	5	3859	-	-	-	X
93	MG	5	3865	-	-	-	X
93	MG	5	3867	-	-	-	X
93	MG	5	3868	-	-	-	X
93	MG	5	3869	-	-	-	X
93	MG	5	3871	-	-	-	X
93	MG	5	3874	-	-	-	X
93	MG	5	3885	-	-	-	X
93	MG	5	3890	-	-	-	X
93	MG	5	3892	-	-	-	X
93	MG	5	3893	-	-	-	X
93	MG	5	3894	-	-	-	X
93	MG	5	3895	-	-	-	X
93	MG	5	3897	-	-	-	X
93	MG	5	3898	-	-	-	X
93	MG	5	3901	-	-	-	X
93	MG	5	3903	-	-	-	X
93	MG	5	3906	-	-	-	X
93	MG	5	3908	-	-	-	X
93	MG	5	3911	-	-	-	X
93	MG	5	3912	-	-	-	X
93	MG	5	3913	-	-	-	X
93	MG	5	3916	-	-	-	X
93	MG	5	3917	-	-	-	X
93	MG	5	3918	-	-	-	X
93	MG	5	3925	-	-	-	X
93	MG	5	3928	-	-	-	X
93	MG	5	3929	-	-	-	X
93	MG	5	3930	-	-	-	X
93	MG	5	3932	-	-	-	X
93	MG	5	3933	-	-	-	X
93	MG	5	3934	-	-	-	X
93	MG	5	3937	-	-	-	X
93	MG	5	3941	-	-	-	X
93	MG	5	3942	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	MG	5	3944	-	-	-	X
93	MG	5	3945	-	-	-	X
93	MG	5	3961	-	-	-	X
93	MG	5	3962	-	-	-	X
93	MG	5	3974	-	-	-	X
93	MG	5	3983	-	-	-	X
93	MG	5	3990	-	-	-	X
93	MG	5	4005	-	-	-	X
93	MG	5	4013	-	-	-	X
93	MG	5	4022	-	-	-	X
93	MG	5	4023	-	-	-	X
93	MG	5	4025	-	-	-	X
93	MG	5	4030	-	-	-	X
93	MG	5	4034	-	-	-	X
93	MG	5	4053	-	-	-	X
93	MG	5	4054	-	-	-	X
93	MG	5	4069	-	-	-	X
93	MG	5	4070	-	-	-	X
93	MG	5	4071	-	-	-	X
93	MG	5	4078	-	-	-	X
93	MG	5	4079	-	-	-	X
93	MG	5	4082	-	-	-	X
93	MG	5	4094	-	-	-	X
93	MG	5	4098	-	-	-	X
93	MG	5	4100	-	-	-	X
93	MG	5	4110	-	-	-	X
93	MG	5	4112	-	-	-	X
93	MG	5	4113	-	-	-	X
93	MG	5	4115	-	-	-	X
93	MG	5	4119	-	-	-	X
93	MG	5	4140	-	-	-	X
93	MG	5	4145	-	-	-	X
93	MG	5	4159	-	-	-	X
93	MG	5	4168	-	-	-	X
93	MG	5	4169	-	-	-	X
93	MG	5	4170	-	-	-	X
93	MG	5	4174	-	-	-	X
93	MG	6	2064	-	-	-	X
93	MG	6	2068	-	-	-	X
93	MG	6	2069	-	-	-	X
93	MG	6	2071	-	-	-	X
93	MG	6	2074	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	MG	6	2079	-	-	-	X
93	MG	6	2080	-	-	-	X
93	MG	6	2083	-	-	-	X
93	MG	6	2084	-	-	-	X
93	MG	6	2090	-	-	-	X
93	MG	6	2100	-	-	-	X
93	MG	6	2105	-	-	-	X
93	MG	6	2107	-	-	-	X
93	MG	6	2109	-	-	-	X
93	MG	6	2113	-	-	-	X
93	MG	6	2118	-	-	-	X
93	MG	6	2126	-	-	-	X
93	MG	6	2128	-	-	-	X
93	MG	6	2131	-	-	-	X
93	MG	6	2134	-	-	-	X
93	MG	6	2139	-	-	-	X
93	MG	6	2170	-	-	-	X
93	MG	6	2171	-	-	-	X
93	MG	6	2175	-	-	-	X
93	MG	7	221	-	-	-	X
93	MG	7	222	-	-	-	X
93	MG	7	223	-	-	-	X
93	MG	8	218	-	-	-	X
93	MG	C1	201	-	-	-	X
93	MG	C9	201	-	-	-	X
93	MG	L3	403	-	-	-	X
93	MG	L3	405	-	-	-	X
93	MG	L4	405	-	-	-	X
93	MG	L4	406	-	-	-	X
93	MG	L7	302	-	-	-	X
93	MG	M7	202	-	-	-	X
93	MG	M7	204	-	-	-	X
93	MG	M7	205	-	-	-	X
93	MG	M7	206	-	-	-	X
93	MG	N0	201	-	-	-	X
93	MG	N3	201	-	-	-	X
93	MG	N3	203	-	-	-	X
93	MG	N5	201	-	-	-	X
93	MG	N6	201	-	-	-	X
93	MG	N8	203	-	-	-	X
93	MG	O5	201	-	-	-	X
93	MG	O7	105	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	MG	P	102	-	-	-	X
93	MG	c6	201	-	-	-	X
93	MG	d3	201	-	-	-	X
93	MG	d6	102	-	-	-	X
93	MG	l2	303	-	-	-	X
93	MG	l3	405	-	-	-	X
93	MG	l3	406	-	-	-	X
93	MG	l7	301	-	-	-	X
93	MG	m5	303	-	-	-	X
93	MG	m7	201	-	-	-	X
93	MG	n0	202	-	-	-	X
93	MG	n3	201	-	-	-	X
93	MG	n8	203	-	-	-	X
93	MG	o3	203	-	-	-	X
93	MG	s6	301	-	-	-	X
93	MG	sM	202	-	-	-	X
94	ZN	D9	101	-	-	X	-
94	ZN	Q2	501	-	-	X	-
95	PHE	5	3401	-	-	-	X
96	LEU	5	3402	-	-	-	X
97	SPS	1	3403	-	-	X	-
98	8AN	P	101	-	-	X	X

## 2 Entry composition

There are 98 unique types of molecules in this entry. The entry contains 411589 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.

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,40S Ribosomal Protein S10.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 14 is a protein called 40S Ribosomal Protein S12,40S 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-A.

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

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C4	127	ARG	-	expression tag	UNP P06367
C4	128	LYS	-	expression tag	UNP P06367
C4	129	LYS	-	expression tag	UNP P06367
C4	130	GLY	-	expression tag	UNP P06367
C4	131	GLY	-	expression tag	UNP P06367
C4	132	ARG	-	expression tag	UNP P06367
C4	133	ARG	-	expression tag	UNP P06367
C4	134	GLY	-	expression tag	UNP P06367
C4	135	ARG	-	expression tag	UNP P06367
C4	136	ARG	-	expression tag	UNP P06367
C4	137	LEU	-	expression tag	UNP P06367
c4	127	ARG	-	expression tag	UNP P06367
c4	128	LYS	-	expression tag	UNP P06367
c4	129	LYS	-	expression tag	UNP P06367
c4	130	GLY	-	expression tag	UNP P06367
c4	131	GLY	-	expression tag	UNP P06367
c4	132	ARG	-	expression tag	UNP P06367
c4	133	ARG	-	expression tag	UNP P06367
c4	134	GLY	-	expression tag	UNP P06367
c4	135	ARG	-	expression tag	UNP P06367
c4	136	ARG	-	expression tag	UNP P06367
c4	137	LEU	-	expression tag	UNP P06367

- Molecule 17 is a protein called 40S Ribosomal Protein S15,40S ribosomal protein S15,40S 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	0	0	0
			1105	708	203	194			
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 19 is a protein called ES17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	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			
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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SR	161	ALA	LYS	conflict	UNP P38011

- Molecule 35 is a protein called Ribosome-bound 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
			1105	655	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			

- 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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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.

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 ES17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c7	90	ALA	-	insertion	UNP A0A0J9X224

- Molecule 83 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 84 is a protein called Suppressor protein STM1,Ribosome-bound protein Stm1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
84	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 85 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
85	5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

- Molecule 86 is a protein called 60S ribosomal protein L8-A,60S Ribosomal Protein L8.

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

- Molecule 87 is a protein called 60S Ribosomal Protein L12.

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

- Molecule 88 is a protein called 60S ribosomal protein L24-A.

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

- Molecule 89 is a protein called 60S Ribosomal Protein P0.

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

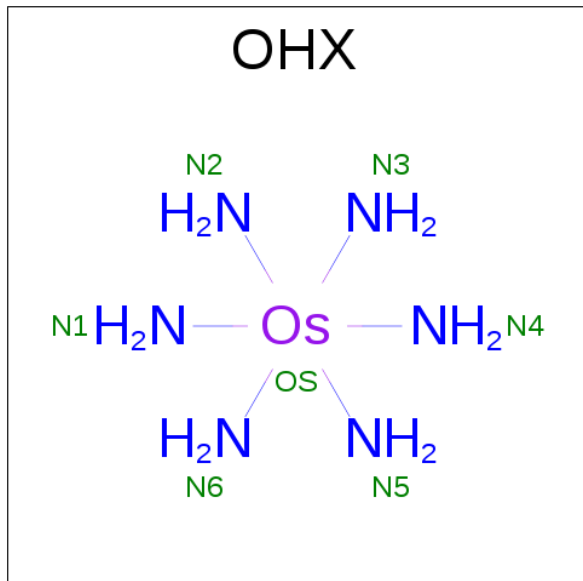
- Molecule 90 is a protein called 60S Ribosomal Protein P1/2.

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

- Molecule 91 is a RNA chain called Peptidyl-tRNA analog ACCA-Leu-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
91	P	2	Total	C	N	O	P	0	0	0
			37	18	6	12	1			
91	p	2	Total	C	N	O	P	0	0	0
			40	18	6	14	2			

- Molecule 92 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
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92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
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			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
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92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	2	1	Total 7	N 6	Os 1	0	0
92	S8	1	Total 7	N 6	Os 1	0	0
92	S9	1	Total 7	N 6	Os 1	0	0
92	C3	1	Total 7	N 6	Os 1	0	0
92	C5	1	Total 7	N 6	Os 1	0	0
92	C7	1	Total 7	N 6	Os 1	0	0
92	C8	1	Total 7	N 6	Os 1	0	0
92	D9	1	Total 7	N 6	Os 1	0	0
92	SR	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0
92	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	1	1	Total	N	Os	0	0
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			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	L3	1	Total 7	N 6	Os 1	0	0
92	L3	1	Total 7	N 6	Os 1	0	0
92	L4	1	Total 7	N 6	Os 1	0	0
92	L6	1	Total 7	N 6	Os 1	0	0
92	L6	1	Total 7	N 6	Os 1	0	0
92	M0	1	Total 7	N 6	Os 1	0	0
92	M5	1	Total 7	N 6	Os 1	0	0
92	M5	1	Total 7	N 6	Os 1	0	0
92	M6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	M7	1	Total	N	Os	0	0
			7	6	1		
92	M8	1	Total	N	Os	0	0
			7	6	1		
92	M9	1	Total	N	Os	0	0
			7	6	1		
92	N9	1	Total	N	Os	0	0
			7	6	1		
92	O3	1	Total	N	Os	0	0
			7	6	1		
92	O4	1	Total	N	Os	0	0
			7	6	1		
92	O7	1	Total	N	Os	0	0
			7	6	1		
92	O9	1	Total	N	Os	0	0
			7	6	1		
92	Q2	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	6	1	Total	N	Os	0	0
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92	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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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	s4	1	Total	N	Os	0	0
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92	s8	1	Total	N	Os	0	0
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92	s9	1	Total	N	Os	0	0
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92	c3	1	Total	N	Os	0	0
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92	c5	1	Total	N	Os	0	0
			7	6	1		
92	c8	1	Total	N	Os	0	0
			7	6	1		
92	d4	1	Total	N	Os	0	0
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92	sR	1	Total	N	Os	0	0
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92	5	1	Total	N	Os	0	0
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92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	l3	1	Total 7	N 6	Os 1	0	0
92	l3	1	Total 7	N 6	Os 1	0	0
92	l5	1	Total 7	N 6	Os 1	0	0
92	l5	1	Total 7	N 6	Os 1	0	0
92	l9	1	Total 7	N 6	Os 1	0	0
92	m0	1	Total 7	N 6	Os 1	0	0
92	m0	1	Total 7	N 6	Os 1	0	0
92	m0	1	Total 7	N 6	Os 1	0	0
92	m5	1	Total 7	N 6	Os 1	0	0
92	m5	1	Total 7	N 6	Os 1	0	0
92	m6	1	Total 7	N 6	Os 1	0	0
92	m8	1	Total 7	N 6	Os 1	0	0
92	m9	1	Total 7	N 6	Os 1	0	0
92	n9	1	Total 7	N 6	Os 1	0	0
92	o3	1	Total 7	N 6	Os 1	0	0
92	o7	1	Total 7	N 6	Os 1	0	0
92	o7	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 93 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	L7	2	Total	Mg	0	0
			2	2		
93	m6	4	Total	Mg	0	0
			4	4		
93	l6	1	Total	Mg	0	0
			1	1		
93	N5	1	Total	Mg	0	0
			1	1		
93	6	126	Total	Mg	0	0
			126	126		
93	sM	2	Total	Mg	0	0
			2	2		
93	O4	1	Total	Mg	0	0
			1	1		
93	m5	2	Total	Mg	0	0
			2	2		
93	l3	4	Total	Mg	0	0
			4	4		
93	C1	1	Total	Mg	0	0
			1	1		
93	d6	1	Total	Mg	0	0
			1	1		
93	C8	1	Total	Mg	0	0
			1	1		
93	n0	2	Total	Mg	0	0
			2	2		
93	L4	5	Total	Mg	0	0
			5	5		
93	l7	1	Total	Mg	0	0
			1	1		
93	M5	1	Total	Mg	0	0
			1	1		
93	o9	1	Total	Mg	0	0
			1	1		
93	N6	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	c9	1	Total 1	Mg 1	0	0
93	o4	1	Total 1	Mg 1	0	0
93	M0	1	Total 1	Mg 1	0	0
93	p	2	Total 2	Mg 2	0	0
93	5	427	Total 427	Mg 427	0	0
93	c8	2	Total 2	Mg 2	0	0
93	O7	4	Total 4	Mg 4	0	0
93	s6	1	Total 1	Mg 1	0	0
93	d4	1	Total 1	Mg 1	0	0
93	n9	2	Total 2	Mg 2	0	0
93	1	394	Total 394	Mg 394	0	0
93	s4	1	Total 1	Mg 1	0	0
93	c6	1	Total 1	Mg 1	0	0
93	Q2	1	Total 1	Mg 1	0	0
93	d3	1	Total 1	Mg 1	0	0
93	D9	2	Total 2	Mg 2	0	0
93	o3	2	Total 2	Mg 2	0	0
93	M3	1	Total 1	Mg 1	0	0
93	N3	3	Total 3	Mg 3	0	0
93	4	17	Total 17	Mg 17	0	0
93	n6	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	S4	1	Total 1	Mg 1	0	0
93	L2	2	Total 2	Mg 2	0	0
93	d7	1	Total 1	Mg 1	0	0
93	l5	1	Total 1	Mg 1	0	0
93	m7	3	Total 3	Mg 3	0	0
93	M7	5	Total 5	Mg 5	0	0
93	m4	1	Total 1	Mg 1	0	0
93	P	1	Total 1	Mg 1	0	0
93	N8	6	Total 6	Mg 6	0	0
93	l9	1	Total 1	Mg 1	0	0
93	o2	2	Total 2	Mg 2	0	0
93	3	7	Total 7	Mg 7	0	0
93	n8	3	Total 3	Mg 3	0	0
93	7	15	Total 15	Mg 15	0	0
93	n3	1	Total 1	Mg 1	0	0
93	q1	1	Total 1	Mg 1	0	0
93	L3	3	Total 3	Mg 3	0	0
93	O5	1	Total 1	Mg 1	0	0
93	2	90	Total 90	Mg 90	0	0
93	l2	3	Total 3	Mg 3	0	0
93	8	14	Total 14	Mg 14	0	0

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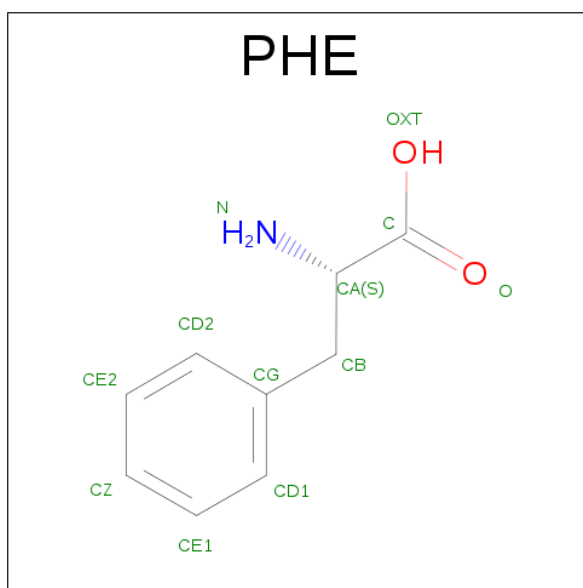
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	m0	1	Total 1	Mg 1	0	0
93	N0	2	Total 2	Mg 2	0	0
93	C9	1	Total 1	Mg 1	0	0

- Molecule 94 is ZINC ION (three-letter code: ZN) (formula: Zn).

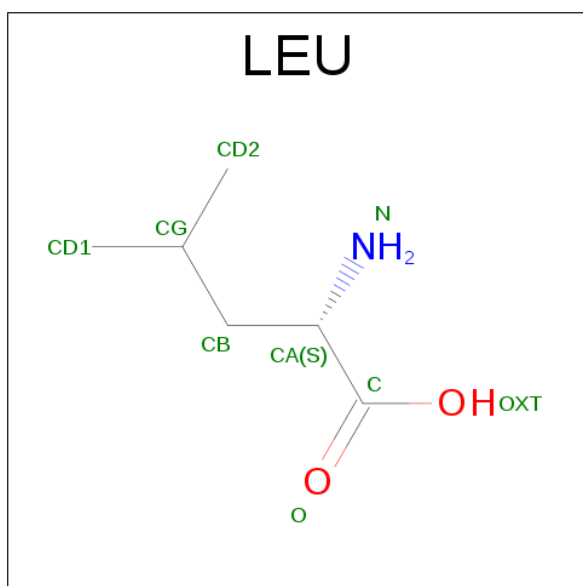
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
94	q0	1	Total 1	Zn 1	0	0
94	D6	1	Total 1	Zn 1	0	0
94	Q2	1	Total 1	Zn 1	0	0
94	e1	1	Total 1	Zn 1	0	0
94	Q3	1	Total 1	Zn 1	0	0
94	D9	1	Total 1	Zn 1	0	0
94	E1	1	Total 1	Zn 1	0	0
94	Q0	1	Total 1	Zn 1	0	0
94	d7	1	Total 1	Zn 1	0	0
94	q3	1	Total 1	Zn 1	0	0
94	d9	1	Total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

- Molecule 95 is PHENYLALANINE (three-letter code: PHE) (formula:  $C_9H_{11}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
95	1	1	Total	C	N	O	0	0
			11	9	1	1		
95	5	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 96 is LEUCINE (three-letter code: LEU) (formula:  $C_6H_{13}NO_2$ ).



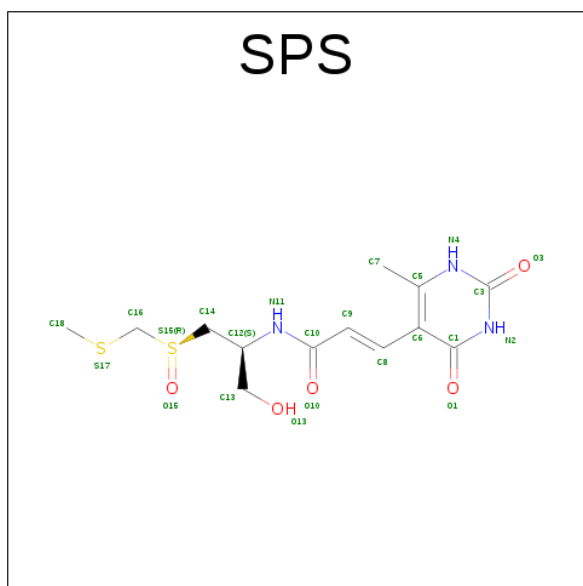
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
96	1	1	Total	C	N	O	0	0
			8	6	1	1		

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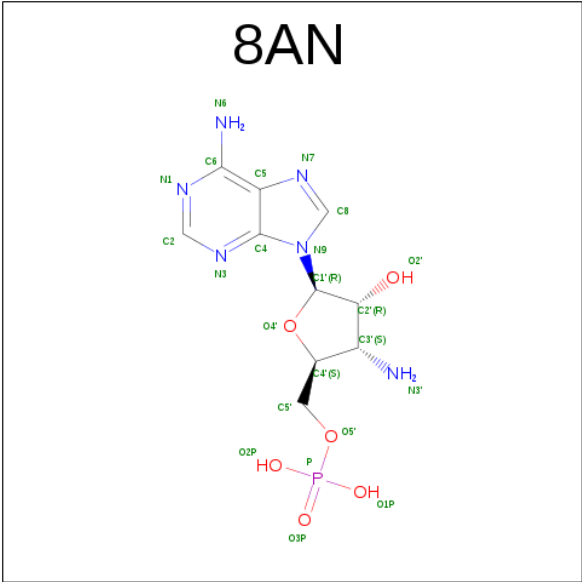
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
96	5	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 97 is SPARSOMYCIN (three-letter code: SPS) (formula:  $C_{13}H_{19}N_3O_5S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
97	1	1	Total 23	C 13	N 3	O 5	S 2	0	0
97	5	1	Total 23	C 13	N 3	O 5	S 2	0	0

- Molecule 98 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (three-letter code: 8AN) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_6\text{O}_6\text{P}$ ).

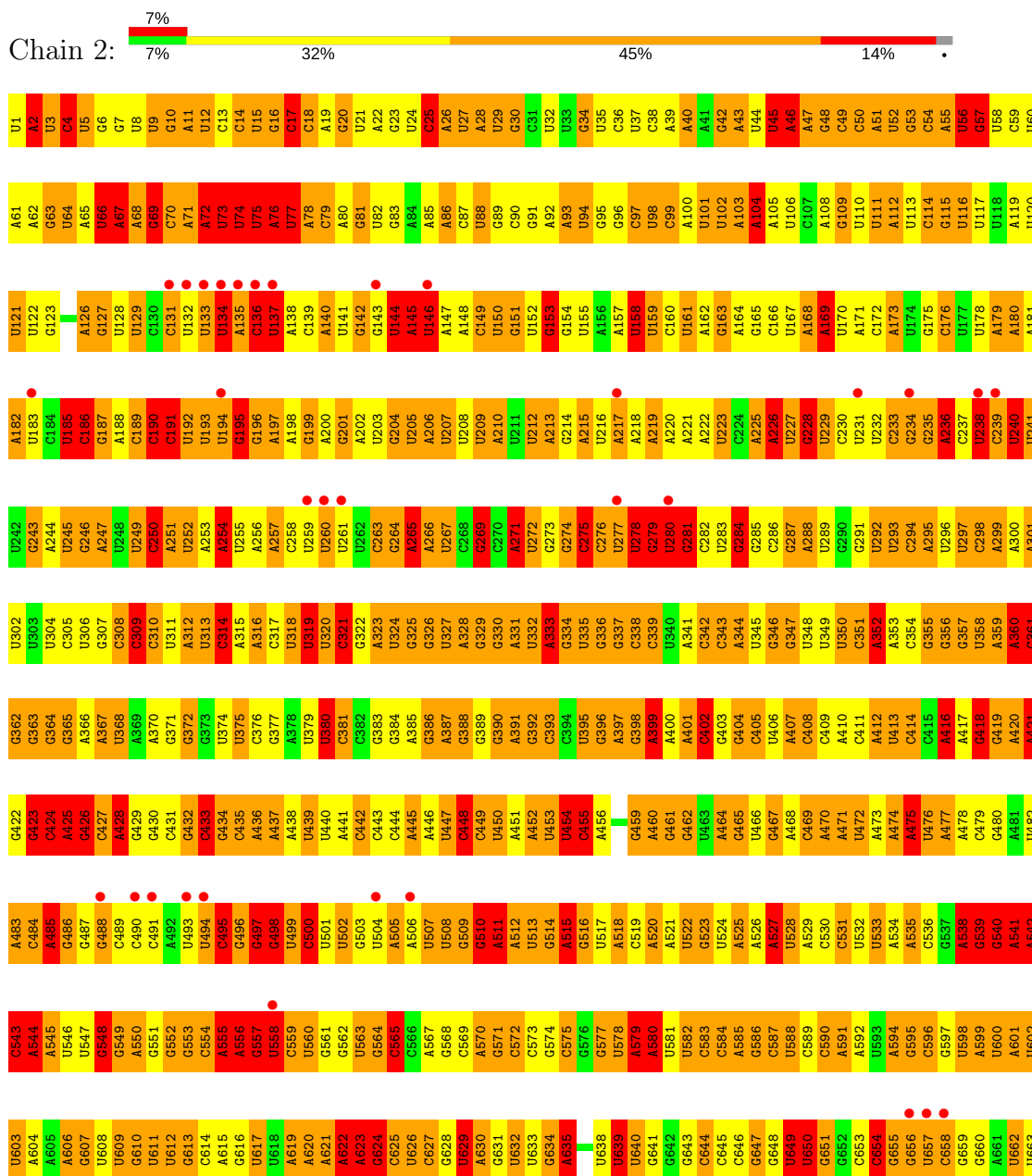


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
98	P	1	Total	C	N	O	P	0	0
			22	10	6	5	1		
98	p	1	Total	C	N	O	P	0	0
			22	10	6	5	1		

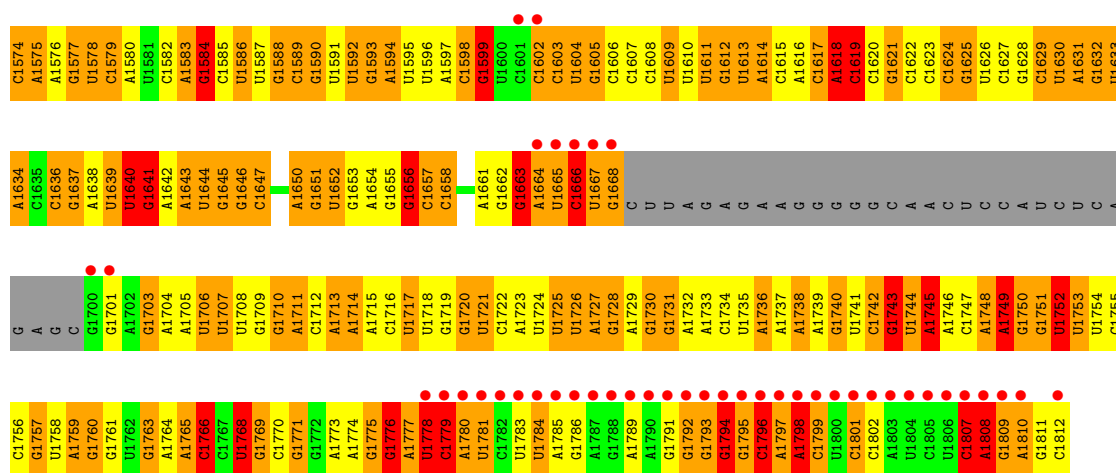
### 3 Residue-property plots

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.

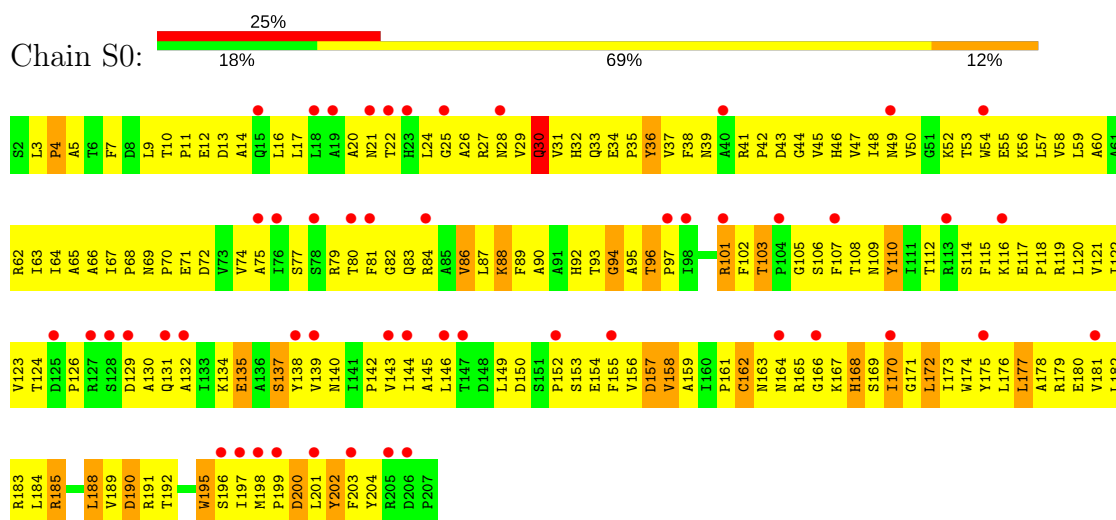
- Molecule 1: 18S ribosomal RNA



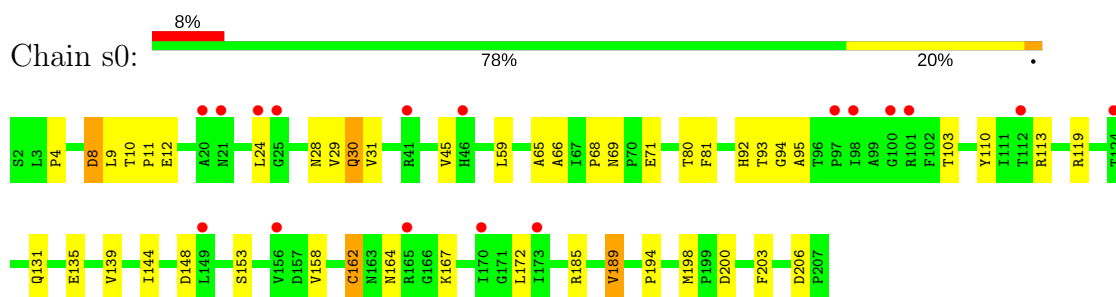
G1514	A1454	A1393	G1332	U1272	G1211	U1151	G1091	U1027	U965	U934	U844	G784	G724	U864
U1515	C1455	A1394	U1333	U1273	G1212	G1152	G1092	C1028	A966	G905	A845	G785	U725	C865
C1516	U1456	G1395	G1334	G1274	A1213	A1153	G1093	G1029	G967	A906	A846	A786	U726	C866
G1517	G1457	U1396	G1335	G1275	U1214	A1154	G1094	G968	U967	A907	U847	A787	U727	C867
U1518	A1458	U1397	U1336	U1276	U1215	C1155	G1095	G969	G968	G908	A848	U788	U728	A668
G1519	C1459	U1398	G1337	G1277	G1216	C1156	A1096	U849	G970	A909	G849	A789	U729	C868
C1520	G1460	G1399	U1338	G1278	A1217	C1157	G1097	U850	A971	C910	G850	C730	U730	G670
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G1522	A1462	G1401	U1340	G1280	U1219	U1159	A1099	U1040	U973	A912	A852	U792	U732	G672
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G1525	C1465	A1404	A1283	A1283	U1223	G1162	G1102	U1042	A976	U915	G855	A795	A735	C675
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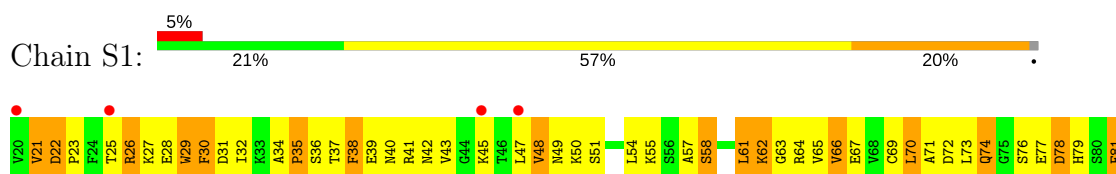
• Molecule 2: 40S ribosomal protein S0-A



• Molecule 2: 40S ribosomal protein S0-A

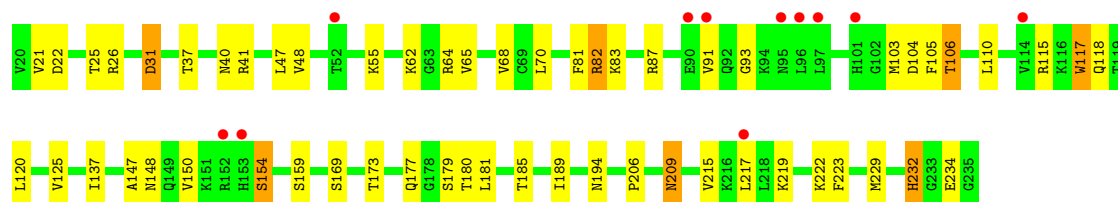
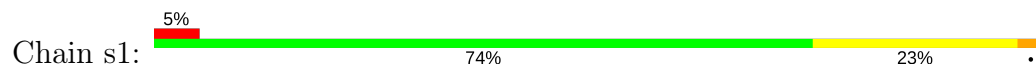


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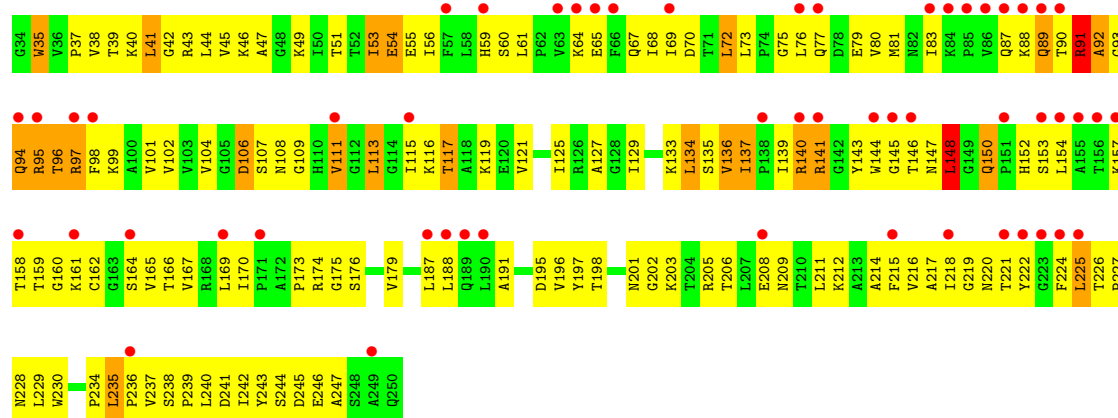




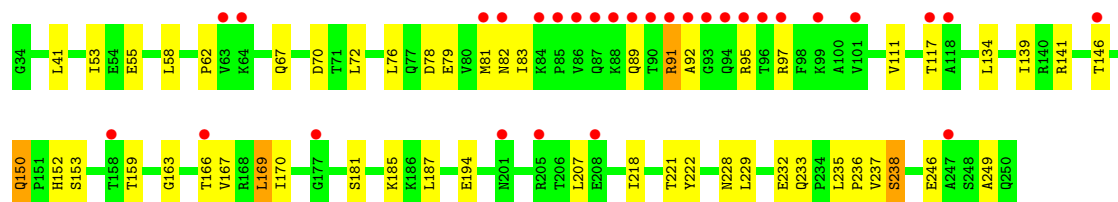
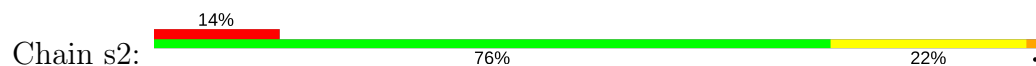
• Molecule 3: 40S ribosomal protein S1-A



• Molecule 4: 40S ribosomal protein S2

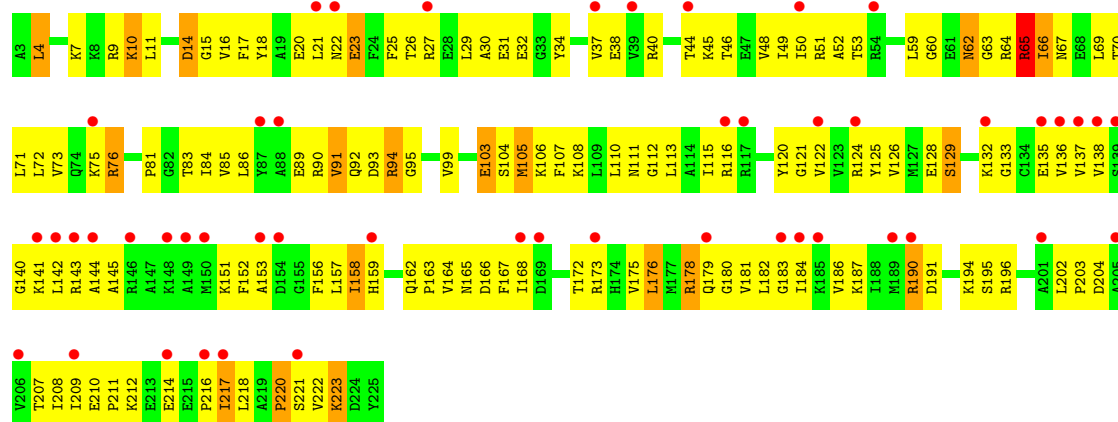


• Molecule 4: 40S ribosomal protein S2

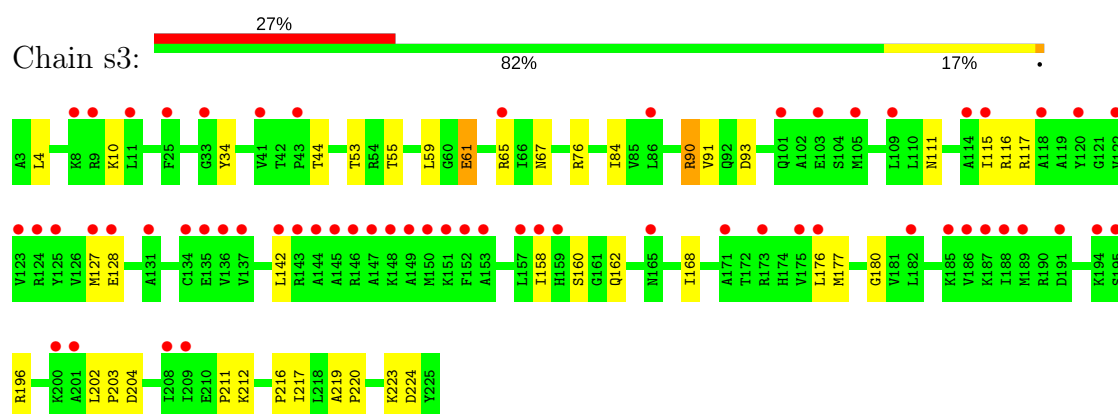


• Molecule 5: 40S ribosomal protein S3

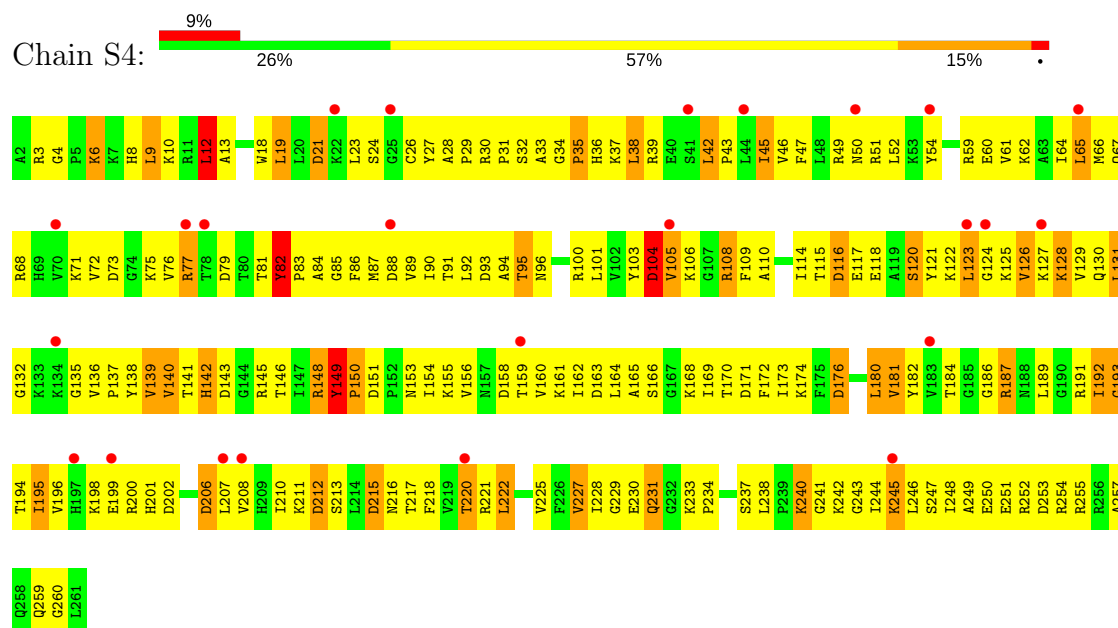




• Molecule 5: 40S ribosomal protein S3

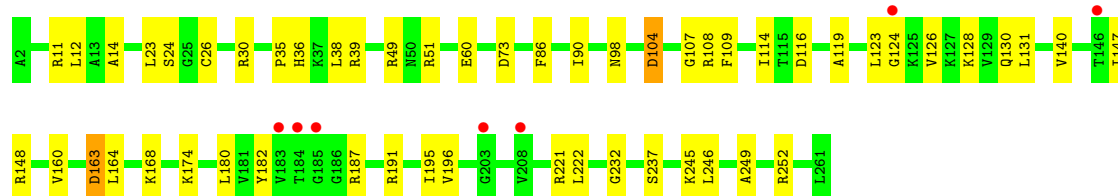


• Molecule 6: 40S ribosomal protein S4-A

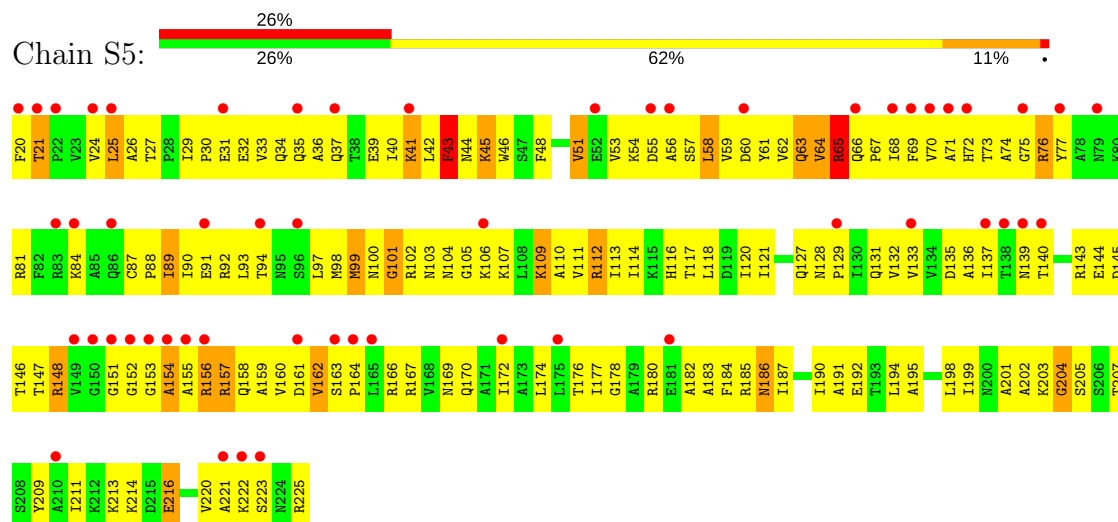


• Molecule 6: 40S ribosomal protein S4-A

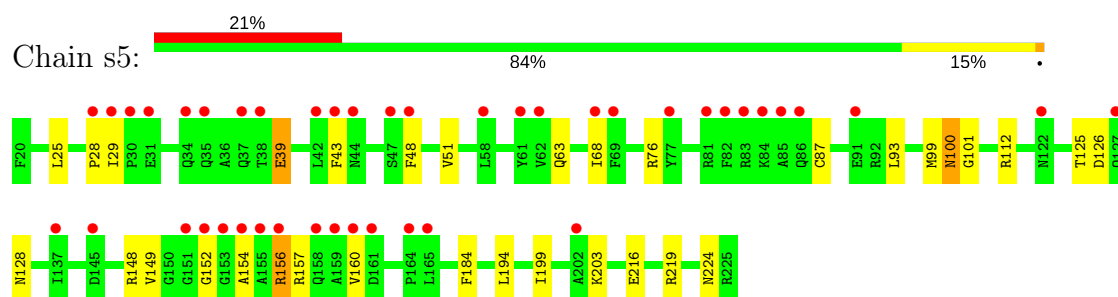




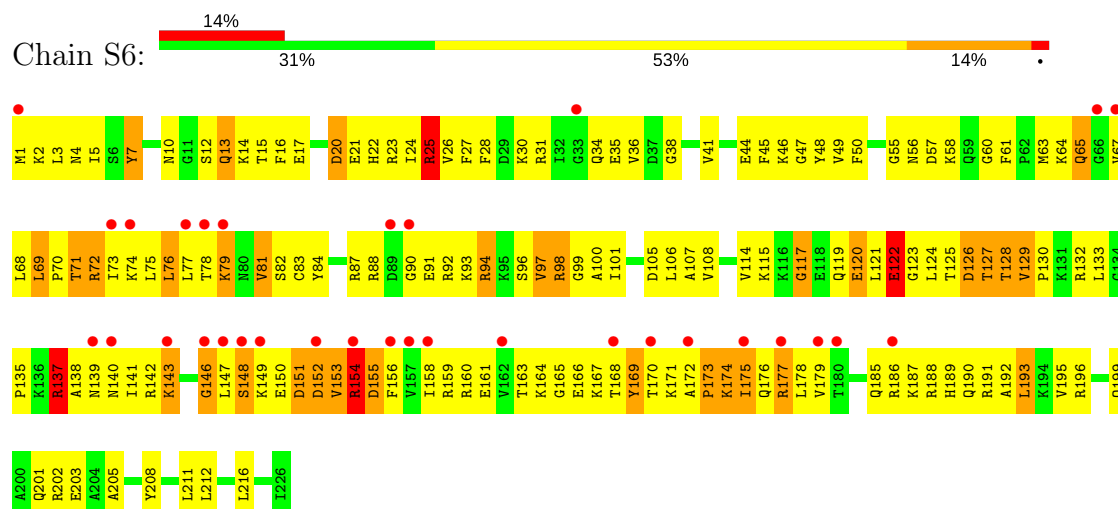
• Molecule 7: 40S ribosomal protein S5



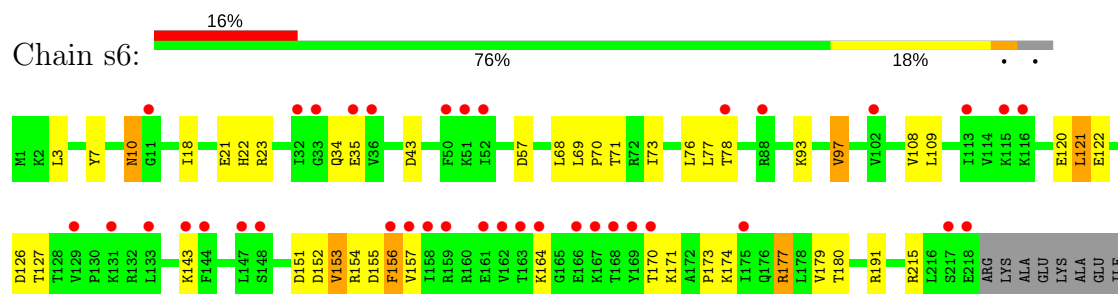
• Molecule 7: 40S ribosomal protein S5



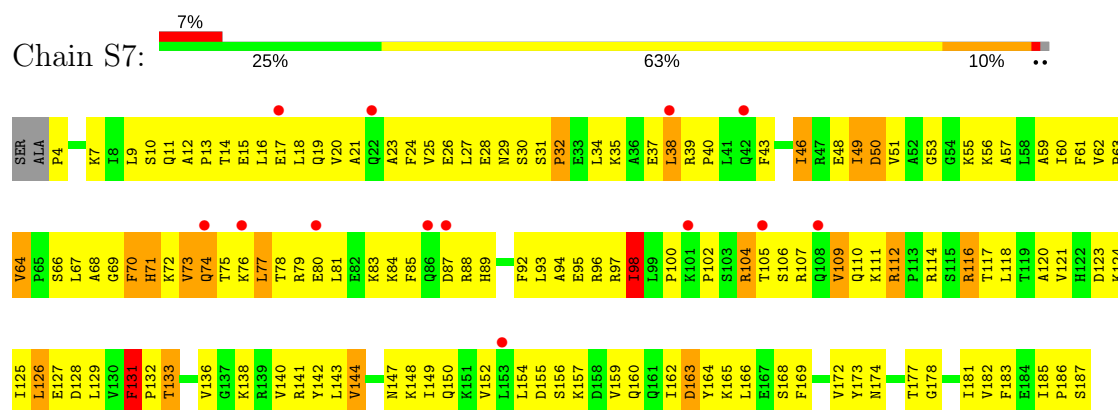
• Molecule 8: 40S ribosomal protein S6-A



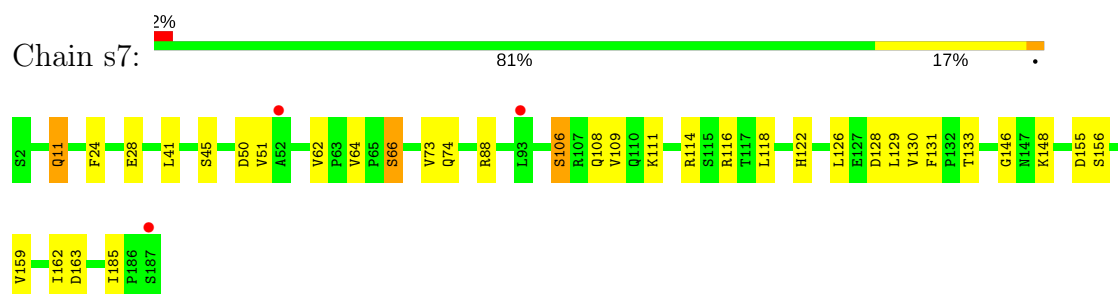
- Molecule 8: 40S ribosomal protein S6-A



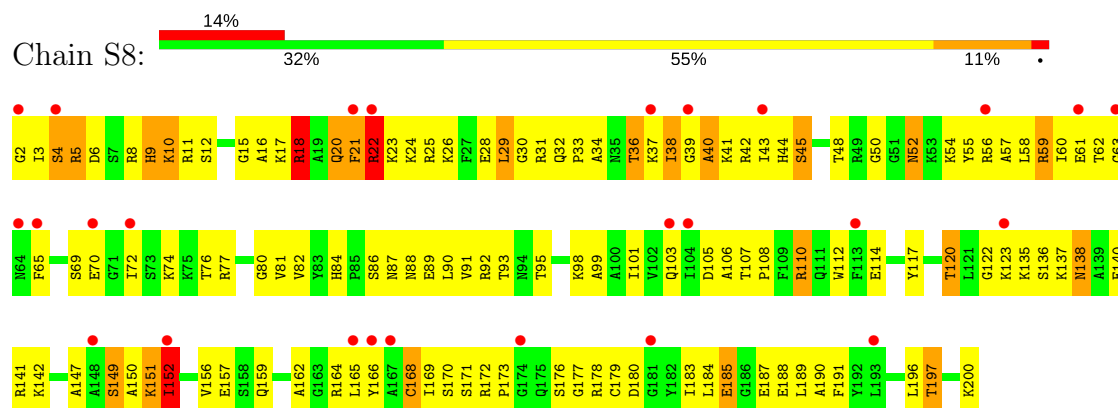
- Molecule 9: 40S ribosomal protein S7-A



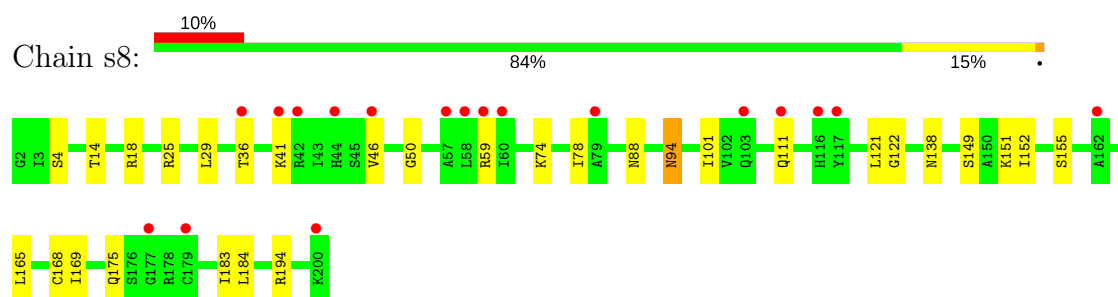
- Molecule 9: 40S ribosomal protein S7-A



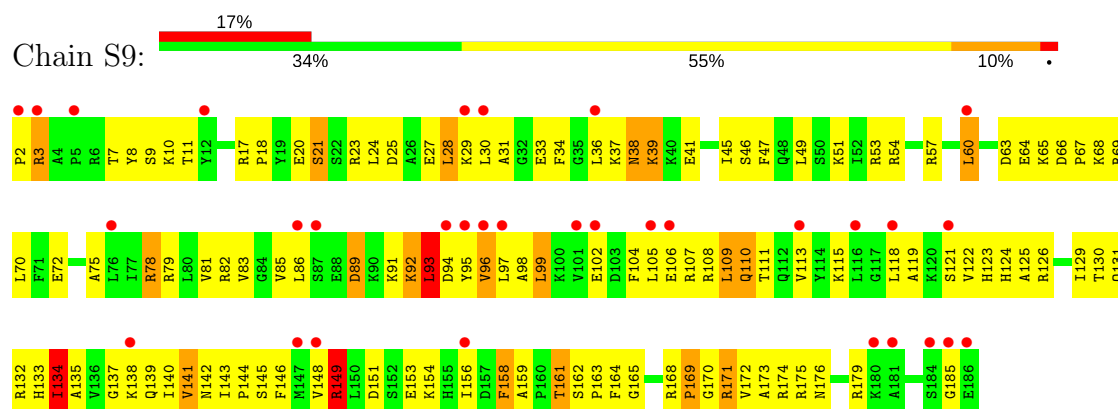
- Molecule 10: 40S ribosomal protein S8



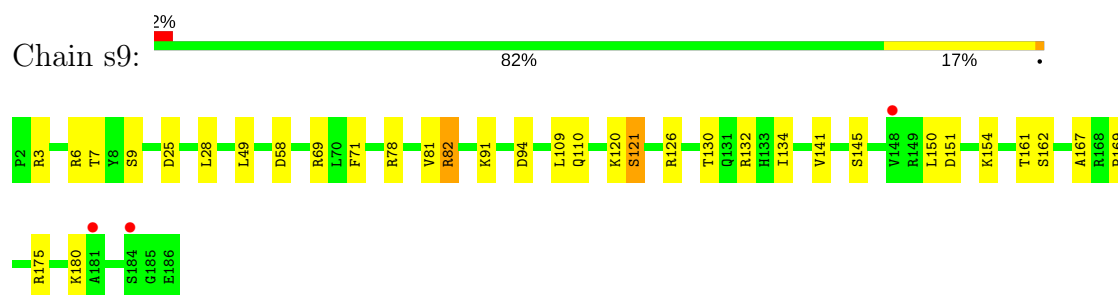
- Molecule 10: 40S ribosomal protein S8



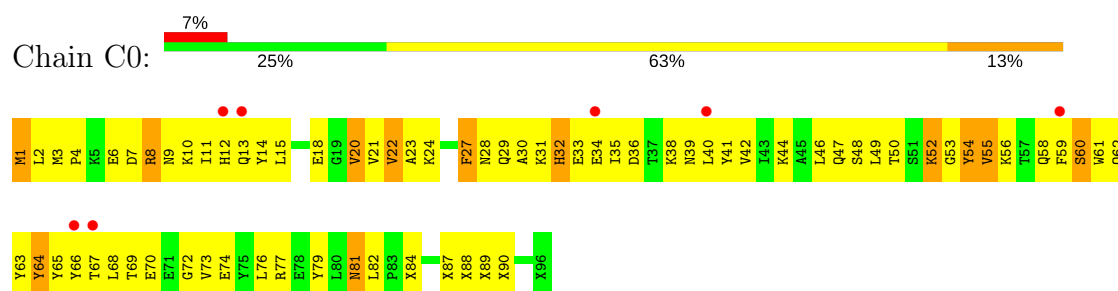
• Molecule 11: 40S ribosomal protein S9-A



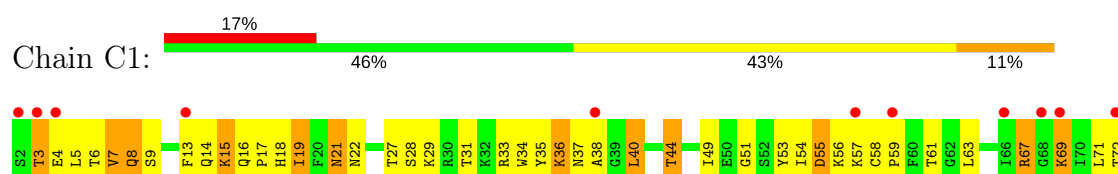
• Molecule 11: 40S ribosomal protein S9-A

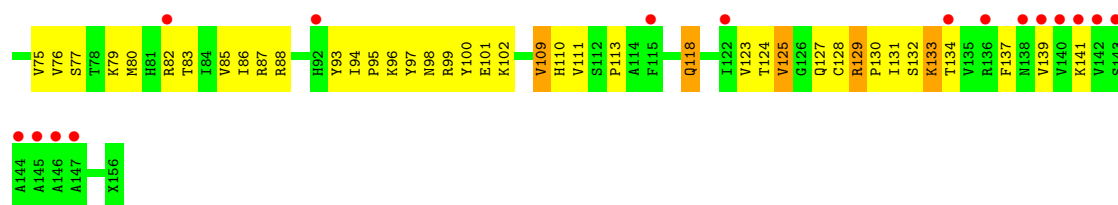


• Molecule 12: 40S ribosomal protein S10-A, 40S Ribosomal Protein S10

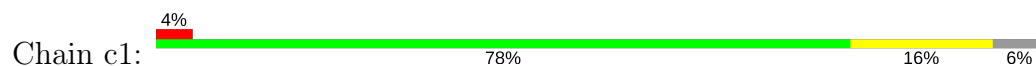


• Molecule 13: 40S ribosomal protein S11-A, 40S Ribosomal Protein S11





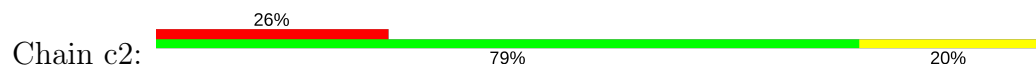
- Molecule 13: 40S ribosomal protein S11-A,40S Ribosomal Protein S11



- Molecule 14: 40S Ribosomal Protein S12,40S ribosomal protein S12



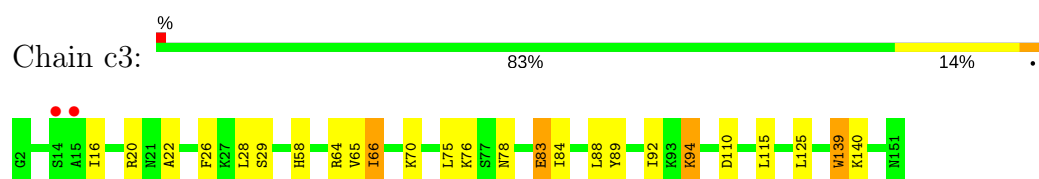
- Molecule 14: 40S Ribosomal Protein S12,40S ribosomal protein S12



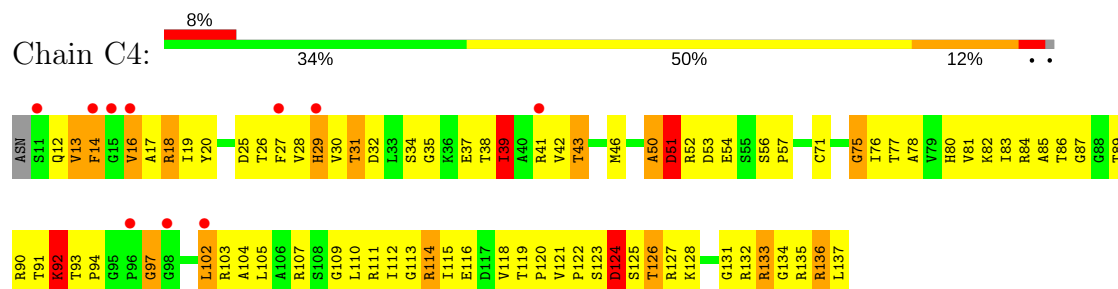
- Molecule 15: 40S ribosomal protein S13



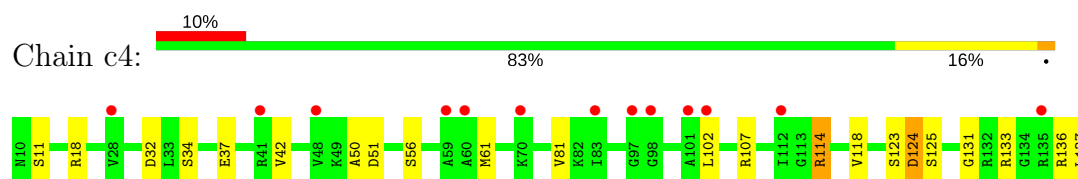
- Molecule 15: 40S ribosomal protein S13



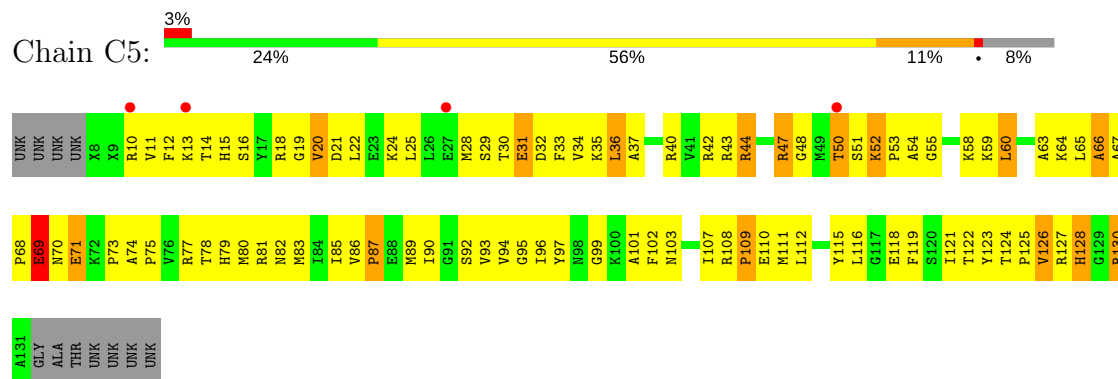
- Molecule 16: 40S ribosomal protein S14-A



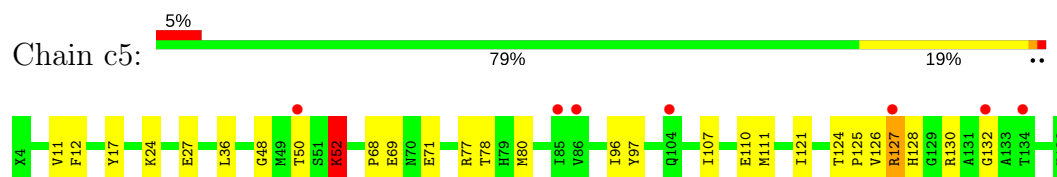
- Molecule 16: 40S ribosomal protein S14-A



- Molecule 17: 40S Ribosomal Protein S15,40S ribosomal protein S15,40S Ribosomal Protein S15

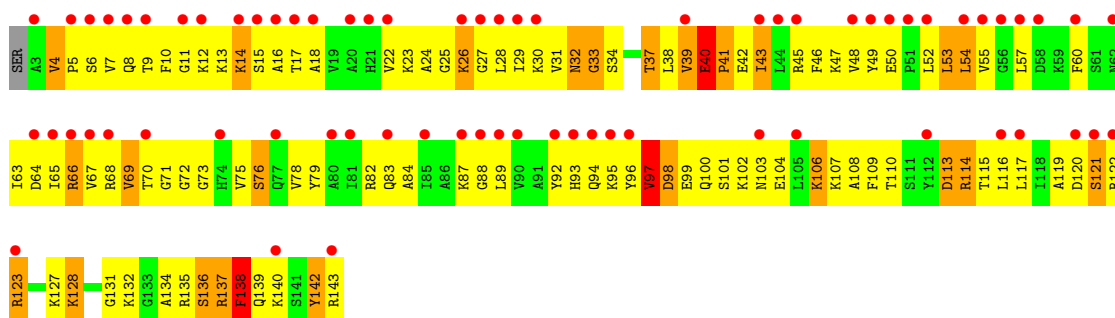


- Molecule 17: 40S Ribosomal Protein S15,40S ribosomal protein S15,40S Ribosomal Protein S15

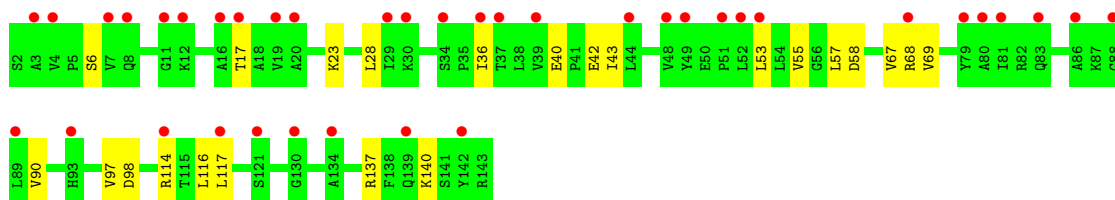
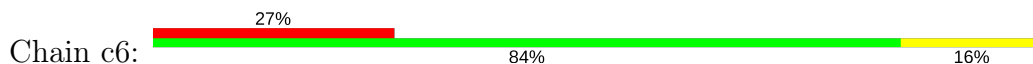


- Molecule 18: 40S ribosomal protein S16-A

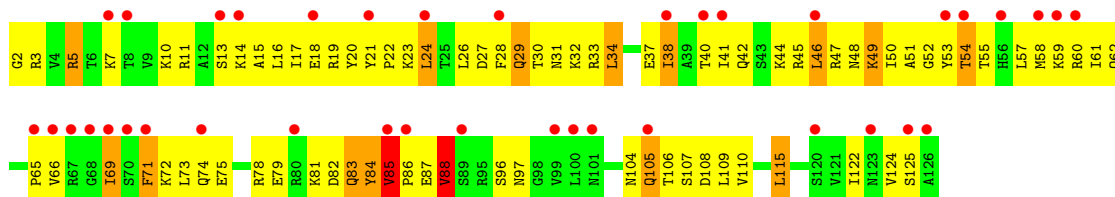




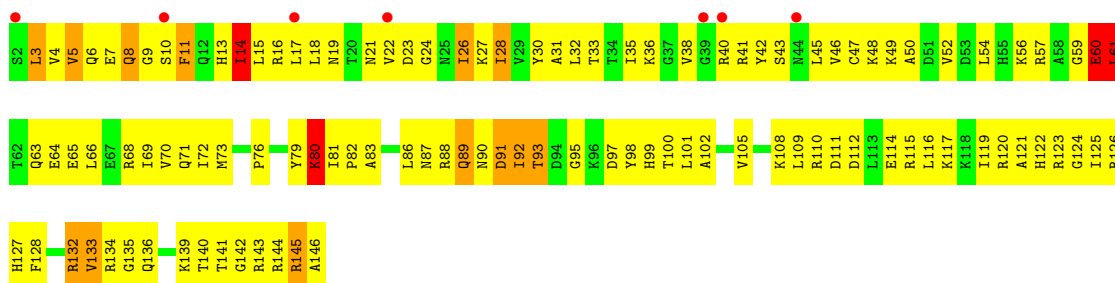
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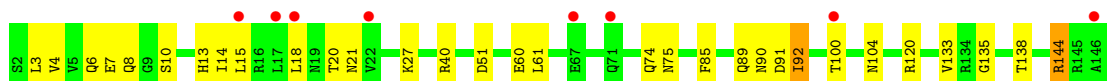
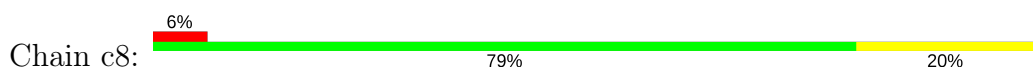
• Molecule 19: ES17



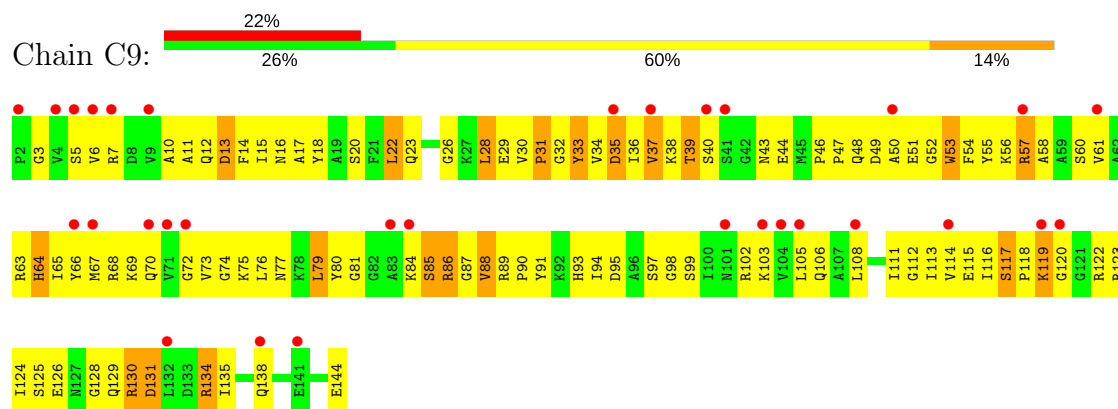
• Molecule 20: 40S ribosomal protein S18-A



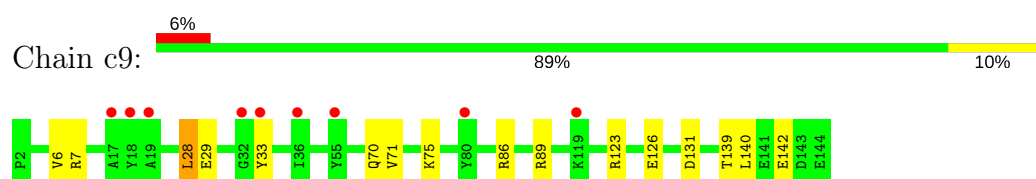
• Molecule 20: 40S ribosomal protein S18-A



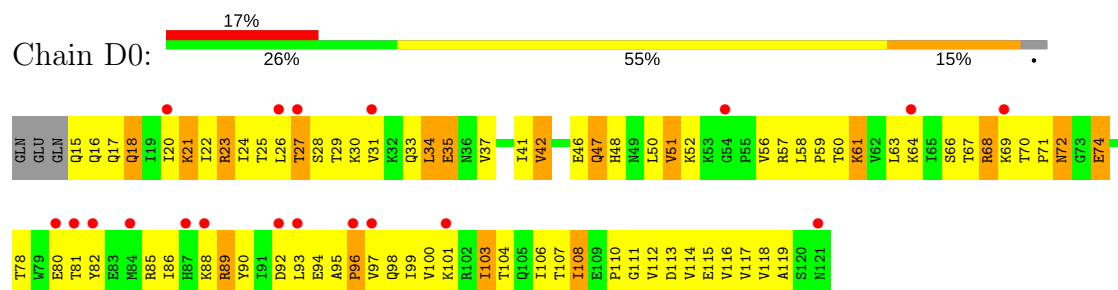
- Molecule 21: 40S ribosomal protein S19-A

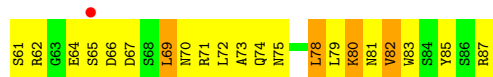


- Molecule 21: 40S ribosomal protein S19-A

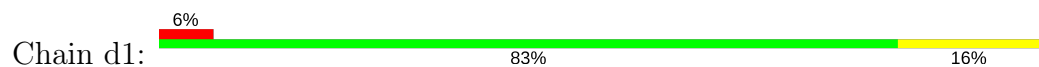


- Molecule 22: 40S ribosomal protein S20

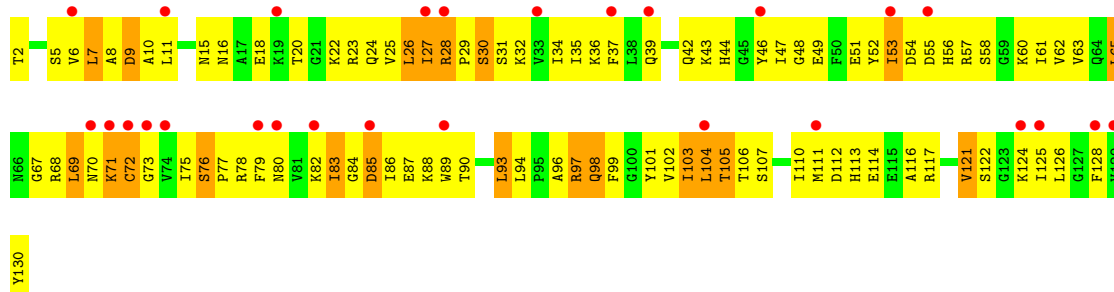




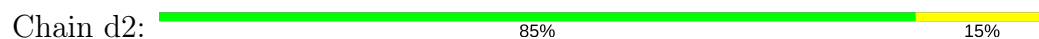
- Molecule 23: 40S ribosomal protein S21-A



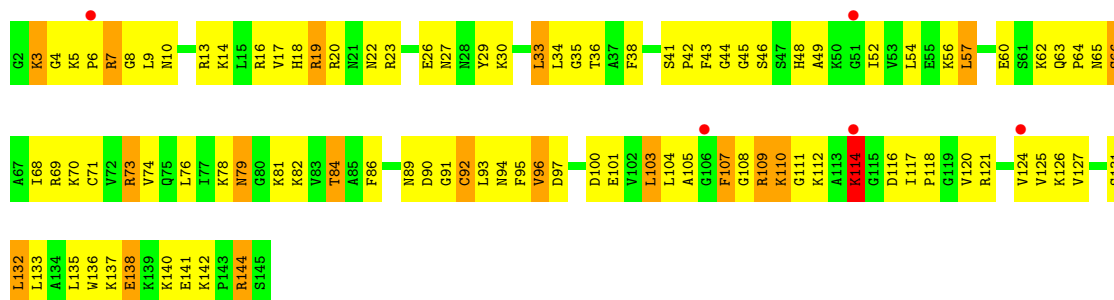
- Molecule 24: 40S ribosomal protein S22-A



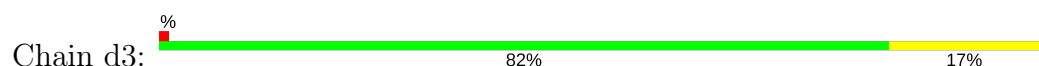
- Molecule 24: 40S ribosomal protein S22-A



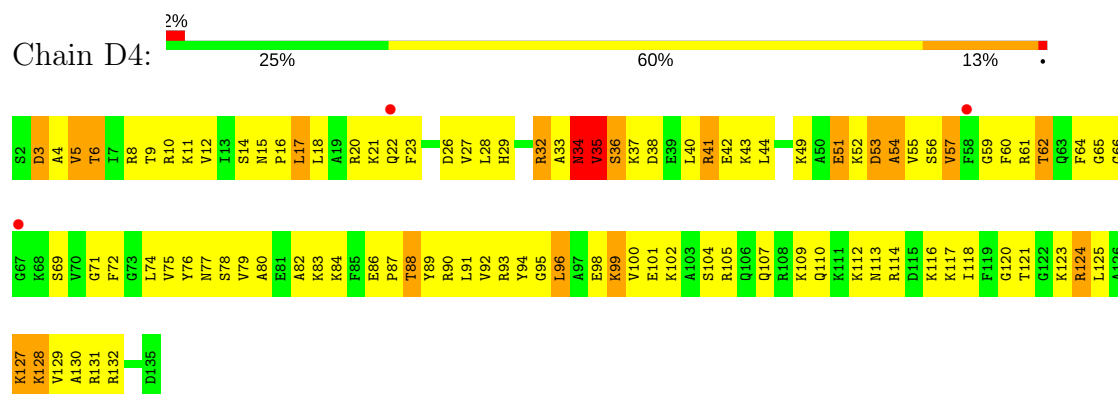
- Molecule 25: 40S ribosomal protein S23-A



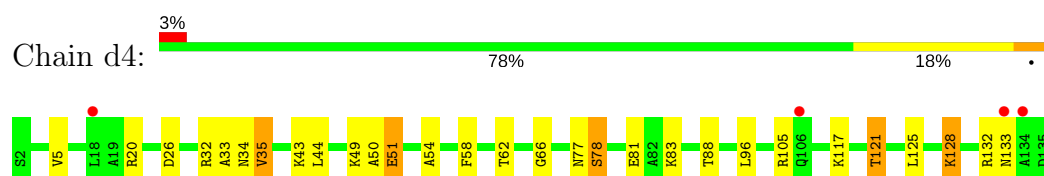
- Molecule 25: 40S ribosomal protein S23-A



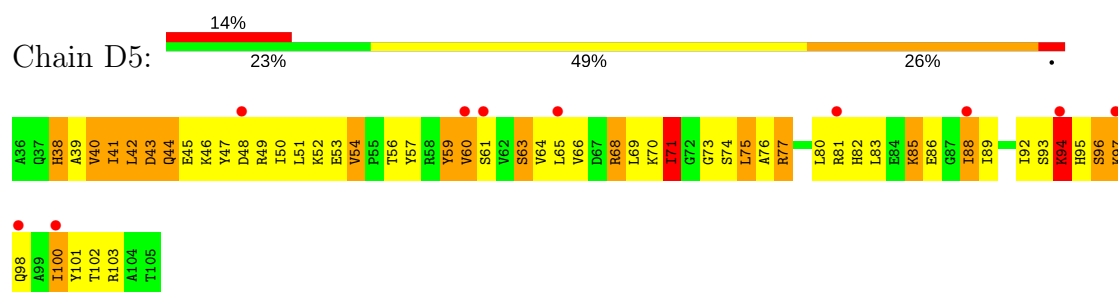
- Molecule 26: 40S ribosomal protein S24-A



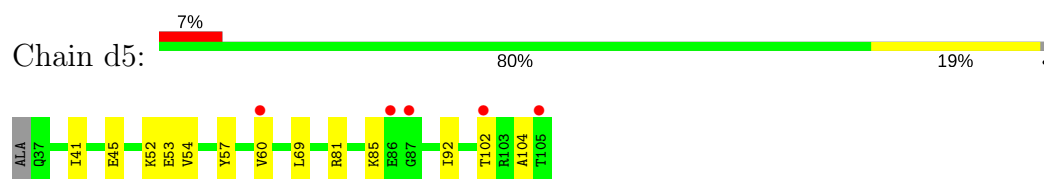
- Molecule 26: 40S ribosomal protein S24-A



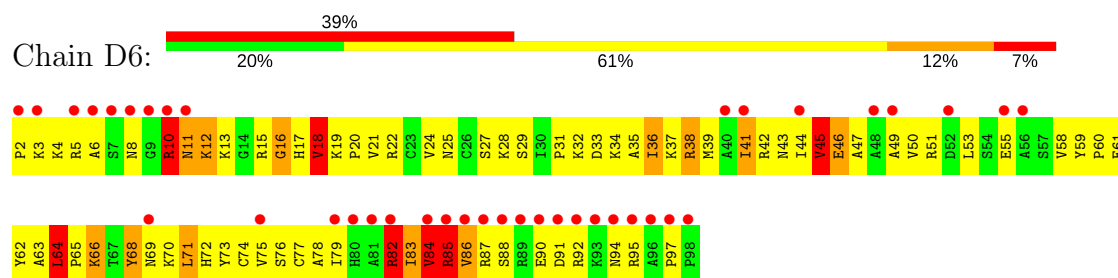
- Molecule 27: 40S ribosomal protein S25-A



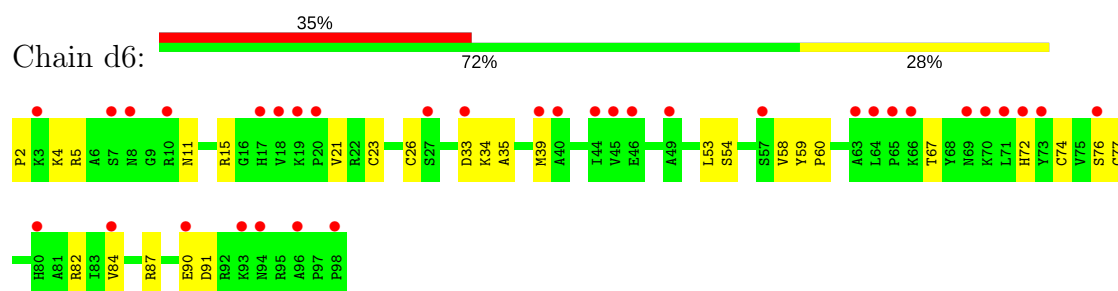
- Molecule 27: 40S ribosomal protein S25-A



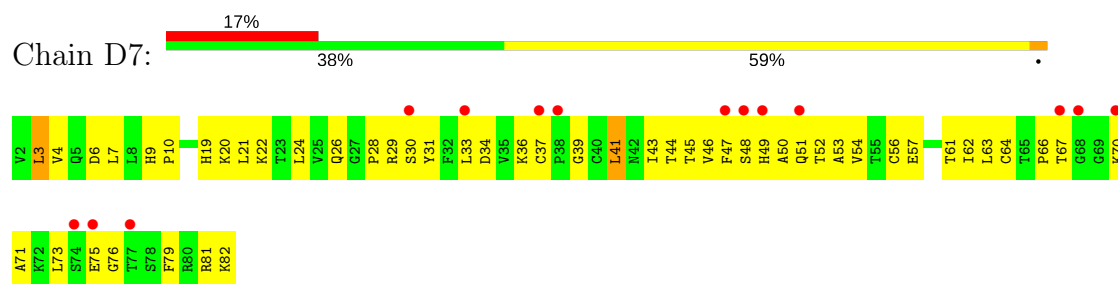
- Molecule 28: 40S ribosomal protein S26-B



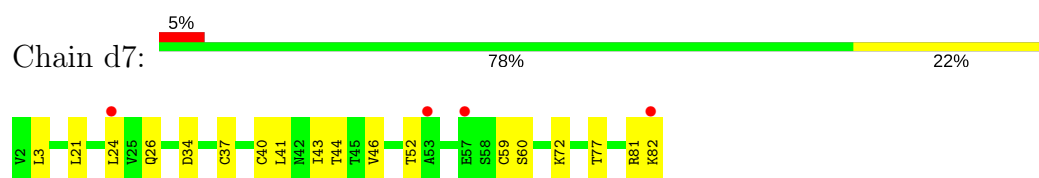
- Molecule 28: 40S ribosomal protein S26-B



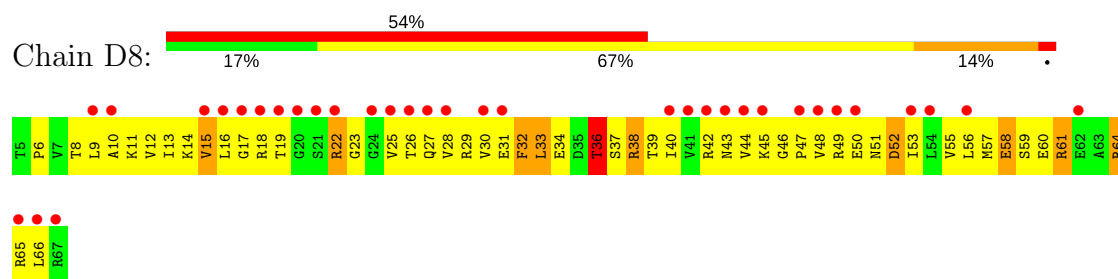
- Molecule 29: 40S ribosomal protein S27-A



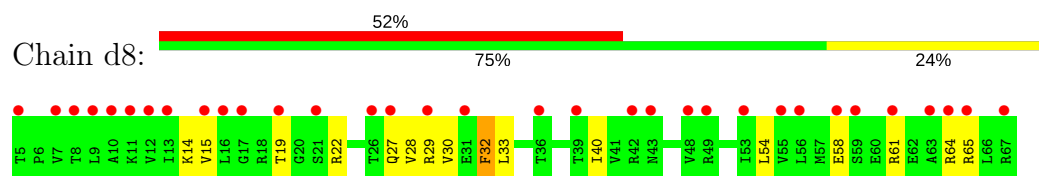
- Molecule 29: 40S ribosomal protein S27-A



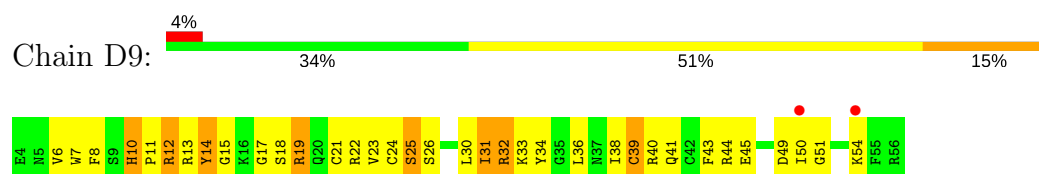
- Molecule 30: 40S ribosomal protein S28-A



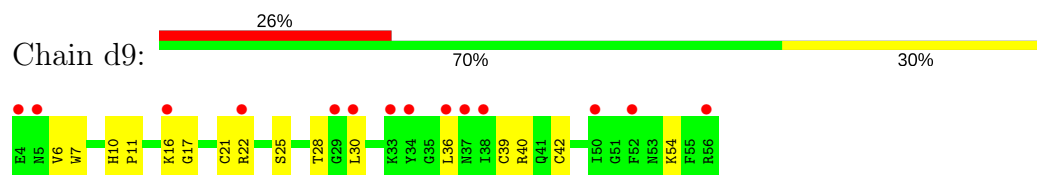
- Molecule 30: 40S ribosomal protein S28-A



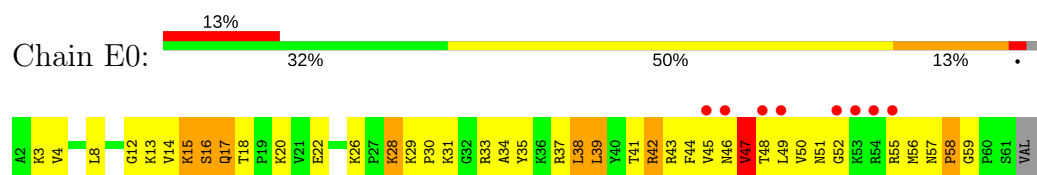
- Molecule 31: 40S ribosomal protein S29-A



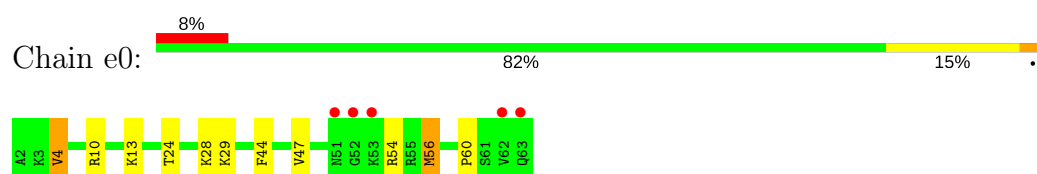
- Molecule 31: 40S ribosomal protein S29-A



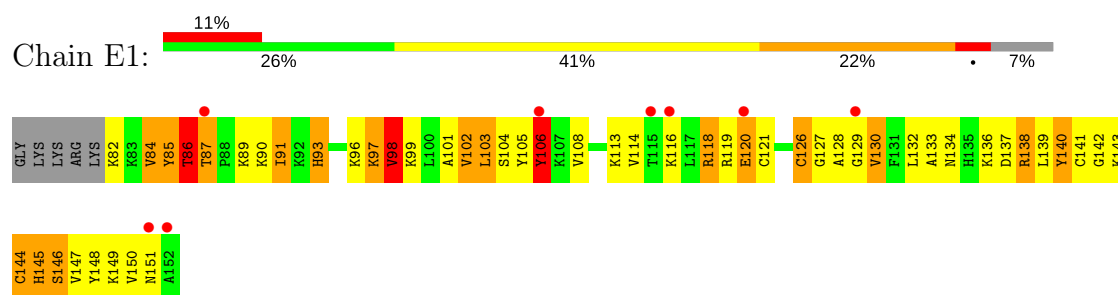
- Molecule 32: 40S ribosomal protein S30-A



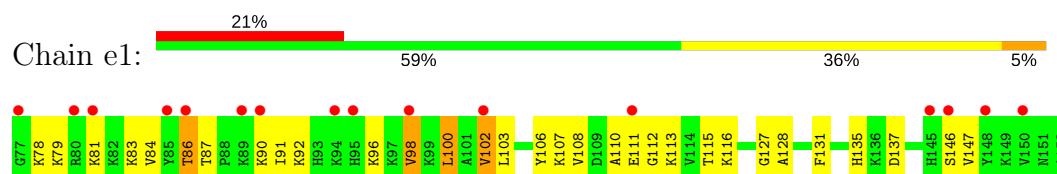
- Molecule 32: 40S ribosomal protein S30-A



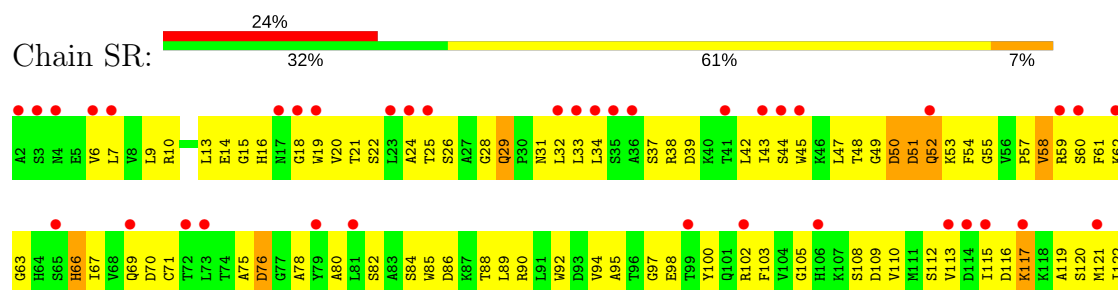
- Molecule 33: Ubiquitin-40S ribosomal protein S31

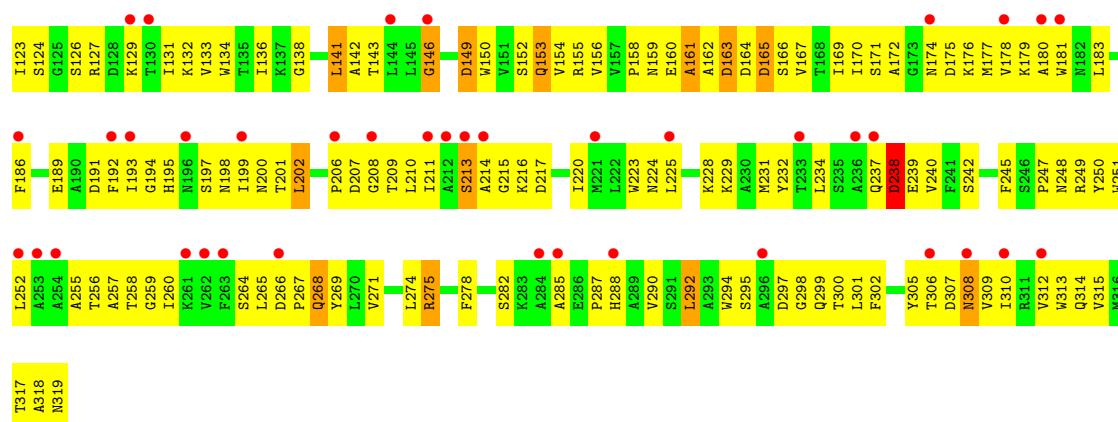


- Molecule 33: Ubiquitin-40S ribosomal protein S31

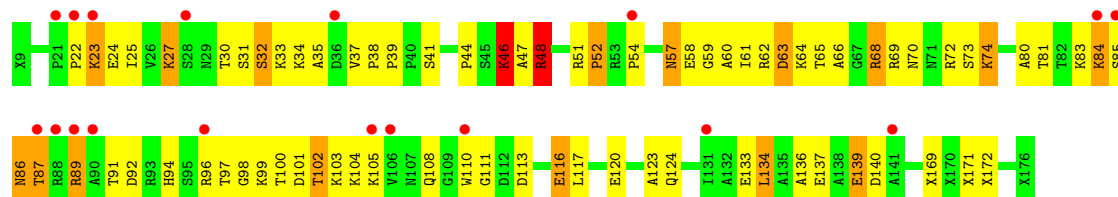


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

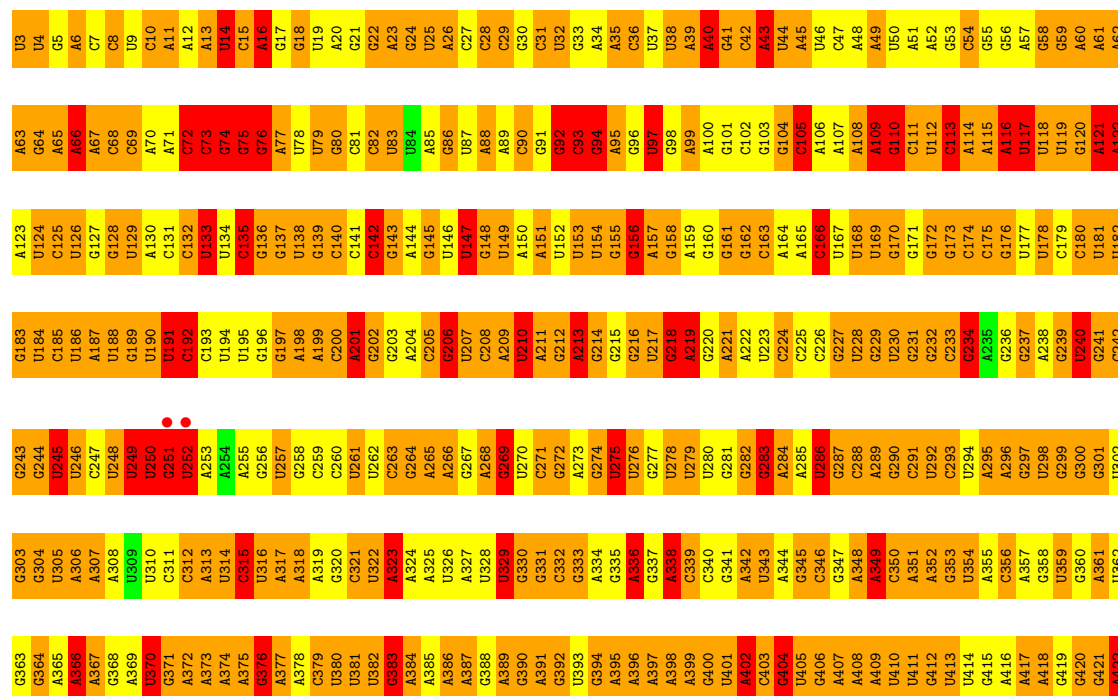




- Molecule 35: Ribosome-bound protein Stm1,Suppressor protein STM1,Ribosome-bound protein Stm1



- Molecule 36: 25S ribosomal RNA





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A3307	G3247	A3187	A3127	C3067	G2947	A2887	U2827	U2767	C2707	A2647	U2587
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U3309	G3249	A3189	A3129	G3069	U2949	C2889	U2829	A2769	C2709	A2649	G2589
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• Molecule 37: 5S ribosomal RNA

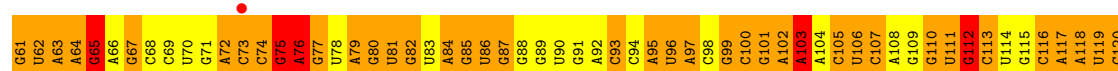
Chain 3:  28% 61% 10%



U121

• Molecule 37: 5S ribosomal RNA

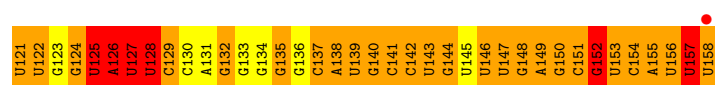
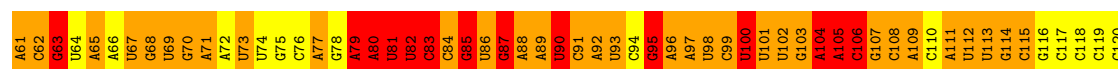
Chain 7:  34% 56% 10%



U121

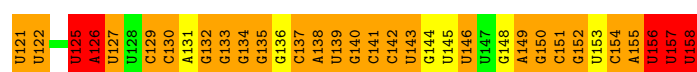
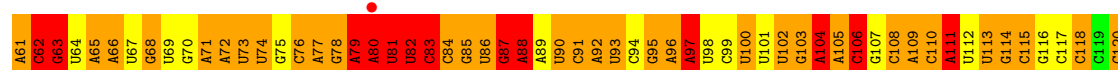
• Molecule 38: 5.8S ribosomal RNA

Chain 4:  23% 59% 17%

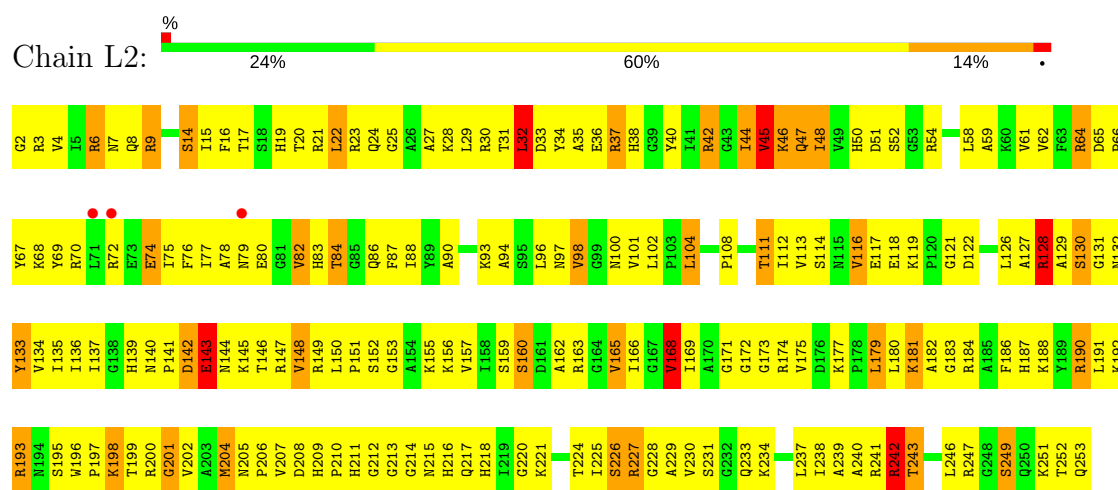


• Molecule 38: 5.8S ribosomal RNA

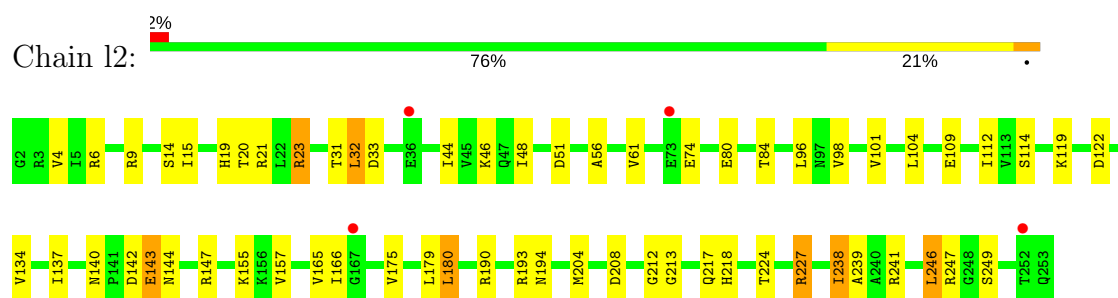
Chain 8:  22% 60% 15%



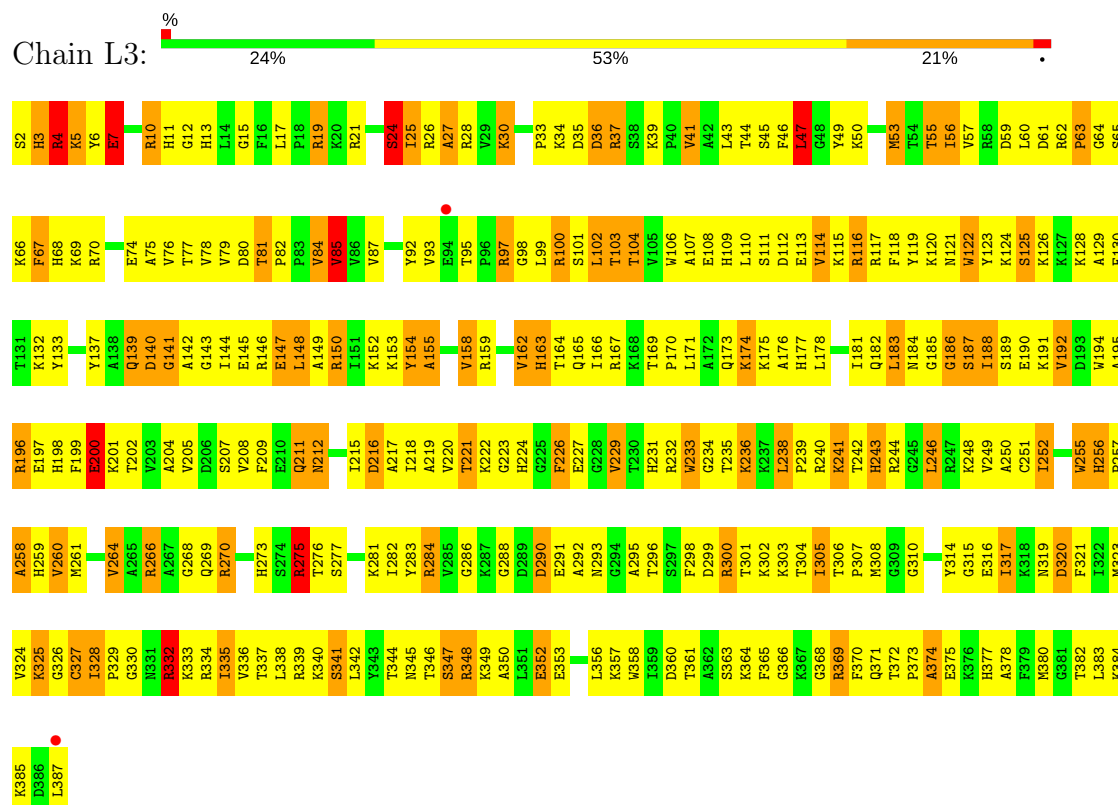
• Molecule 39: 60S ribosomal protein L2-A



• Molecule 39: 60S ribosomal protein L2-A



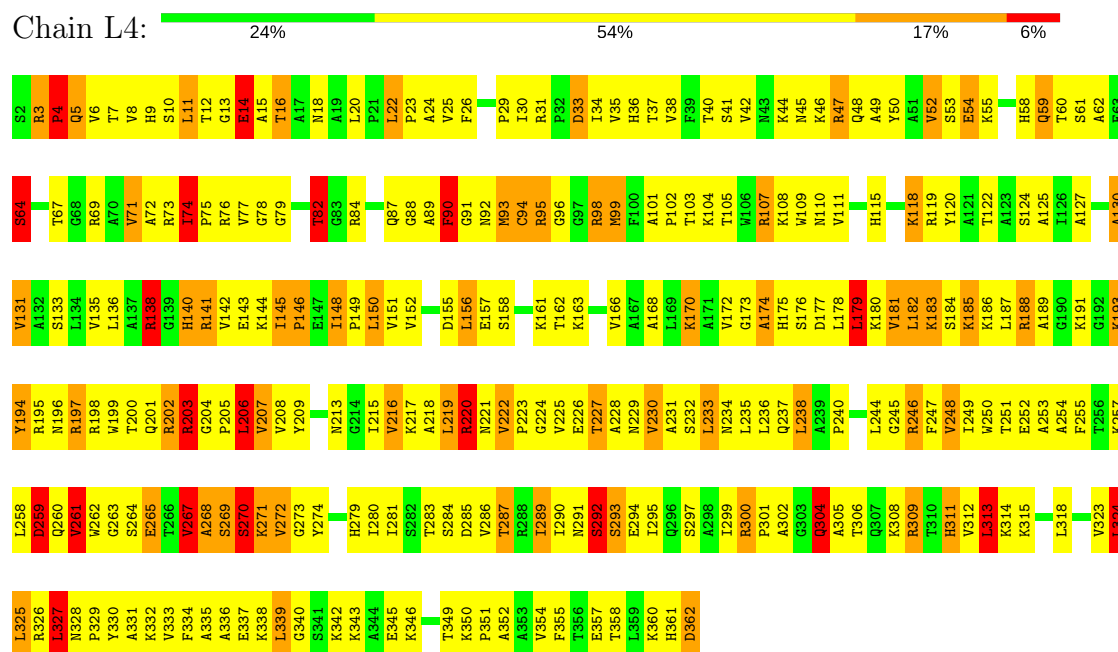
• Molecule 40: 60S ribosomal protein L3



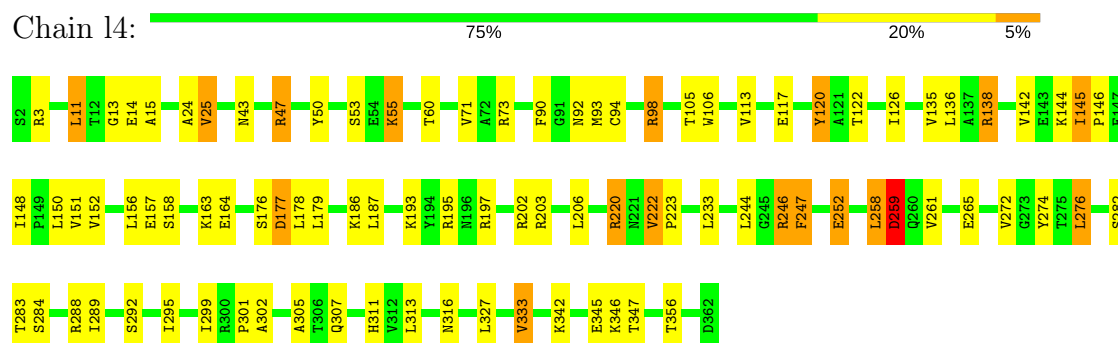
• Molecule 40: 60S ribosomal protein L3



• Molecule 41: 60S ribosomal protein L4-A



• Molecule 41: 60S ribosomal protein L4-A



• Molecule 42: 60S ribosomal protein L5

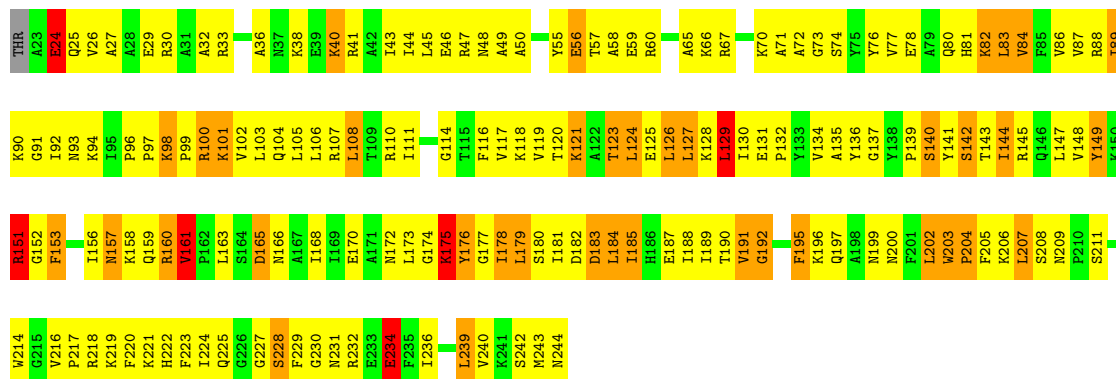






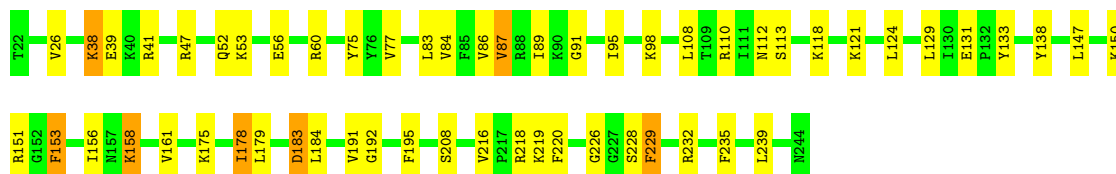
• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 24% 56% 17%



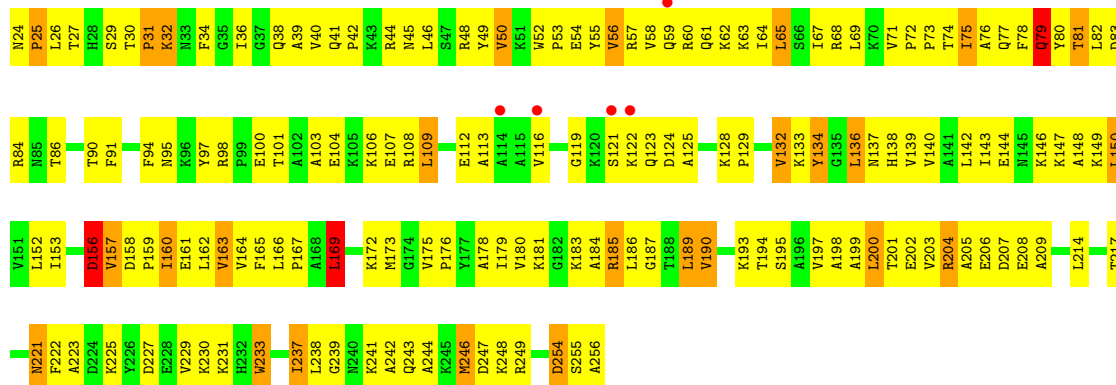
• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 75% 22%



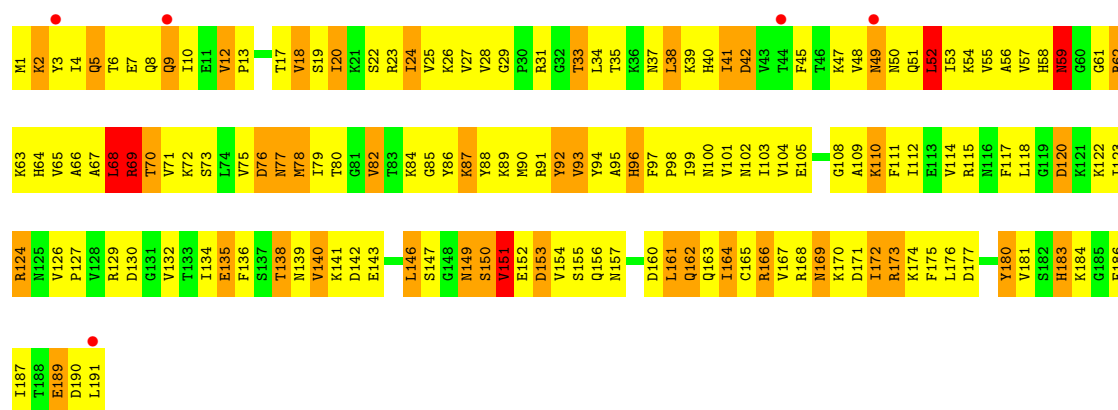
• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 2% 29% 58% 11%

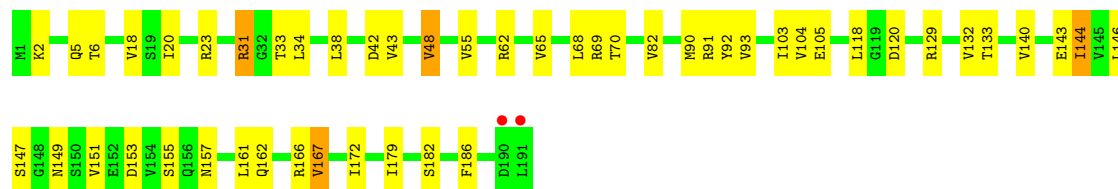
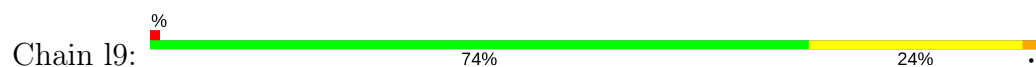


• Molecule 46: 60S ribosomal protein L9-A

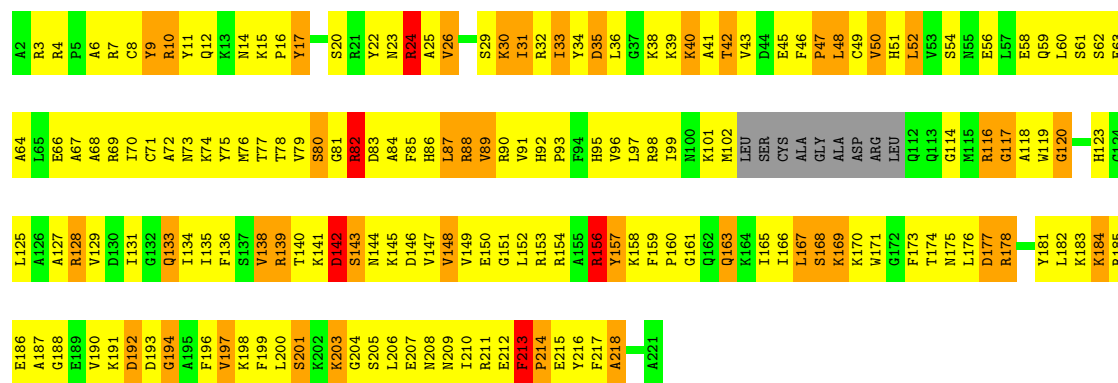
Chain L9: 3% 19% 57% 22%



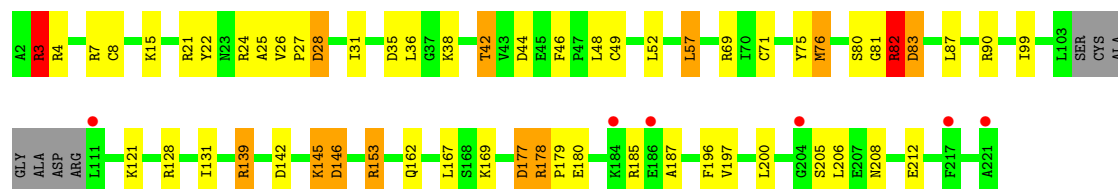
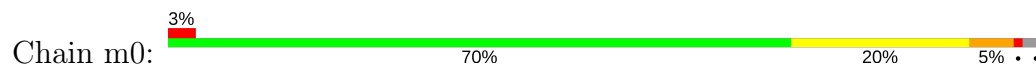
• Molecule 46: 60S ribosomal protein L9-A



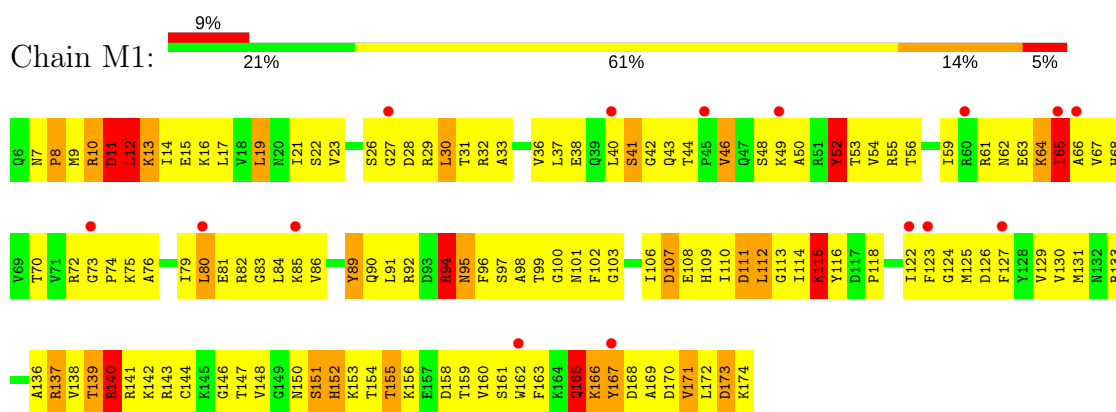
• Molecule 47: 60S ribosomal protein L10



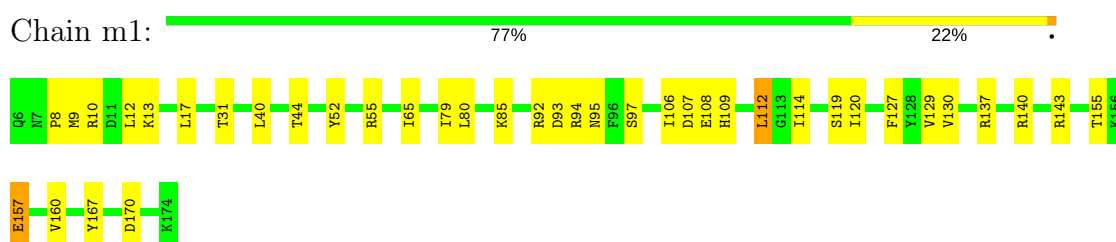
• Molecule 47: 60S ribosomal protein L10



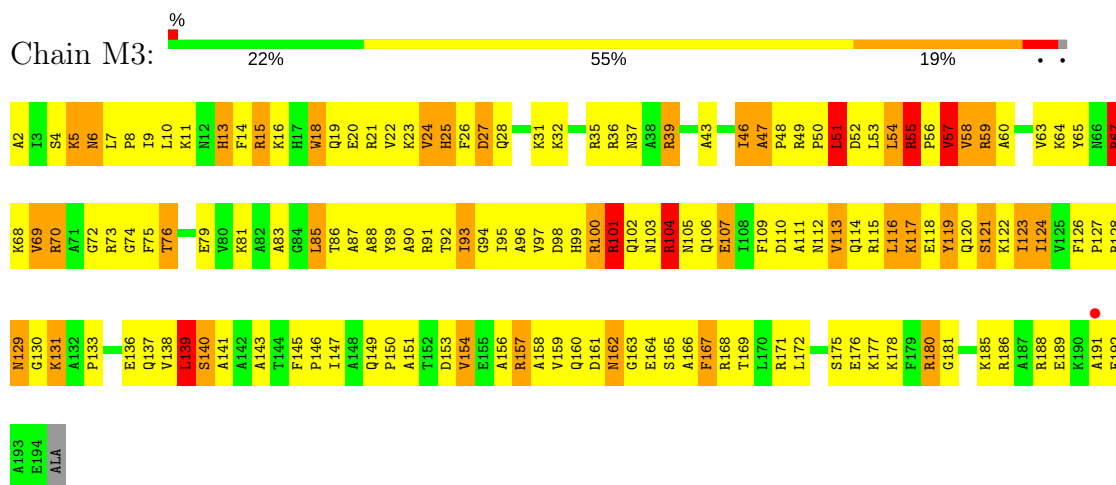
• Molecule 48: 60S ribosomal protein L11-B



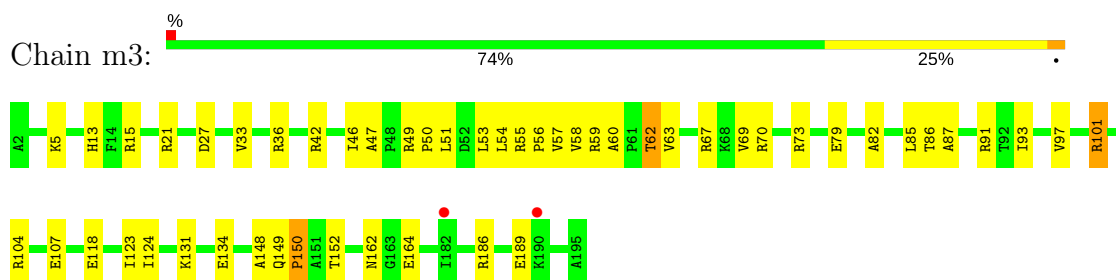
• Molecule 48: 60S ribosomal protein L11-B



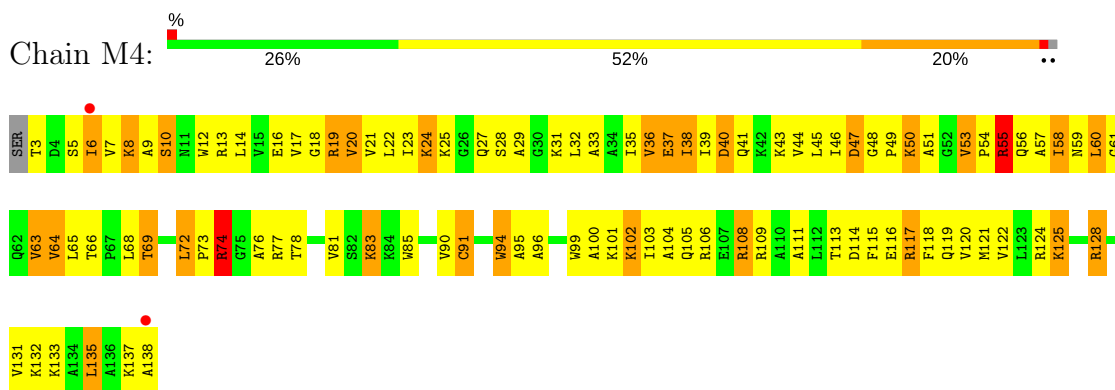
• Molecule 49: 60S ribosomal protein L13-A



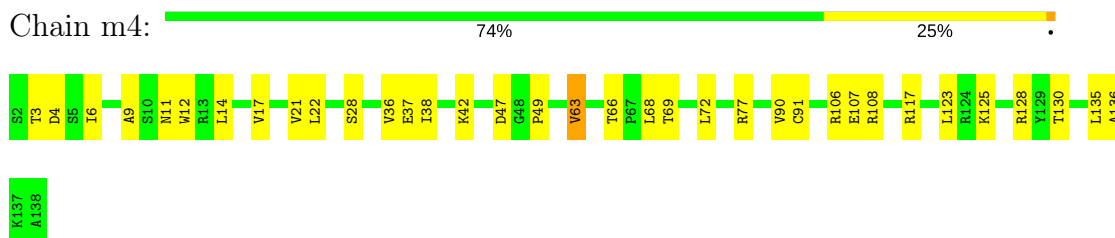
• Molecule 49: 60S ribosomal protein L13-A



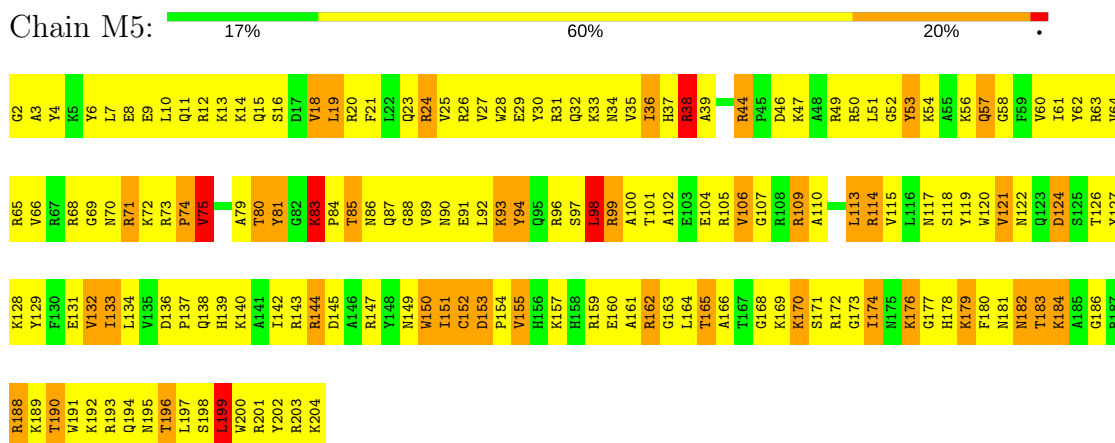
• Molecule 50: 60S ribosomal protein L14-A



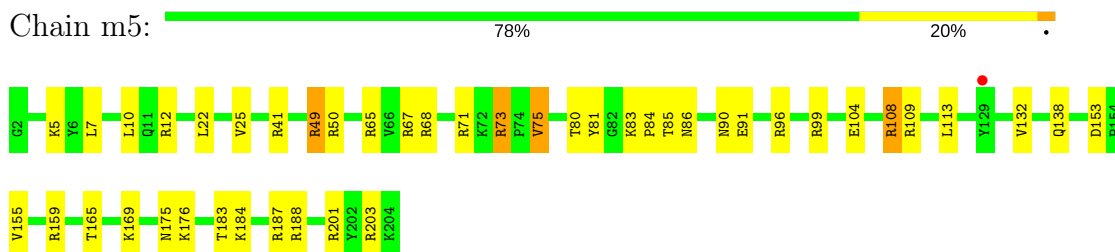
- Molecule 50: 60S ribosomal protein L14-A



- Molecule 51: 60S ribosomal protein L15-A

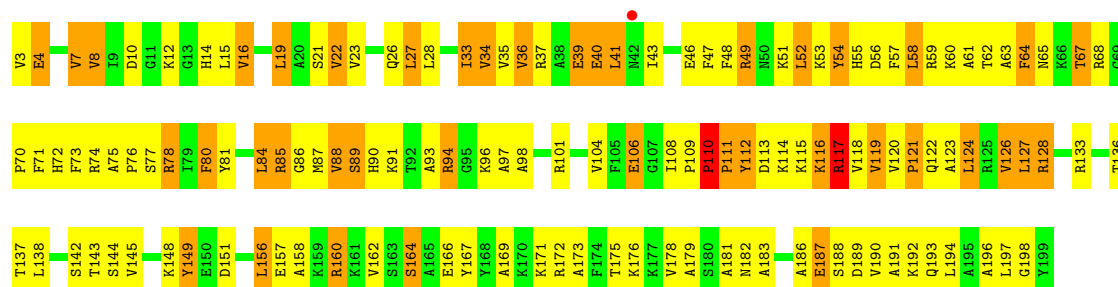


- Molecule 51: 60S ribosomal protein L15-A



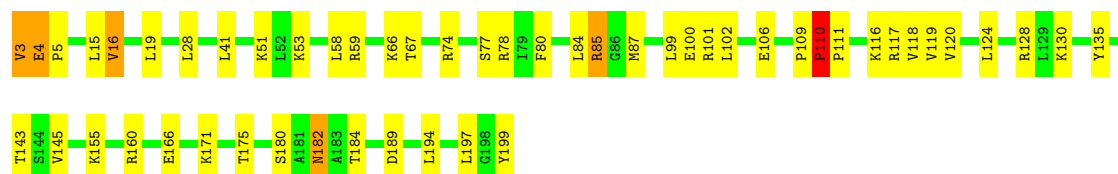
- Molecule 52: 60S ribosomal protein L16-A





• Molecule 52: 60S ribosomal protein L16-A

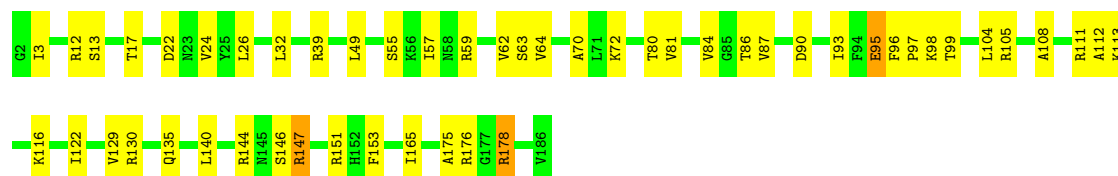
Chain m6: 74% 23%





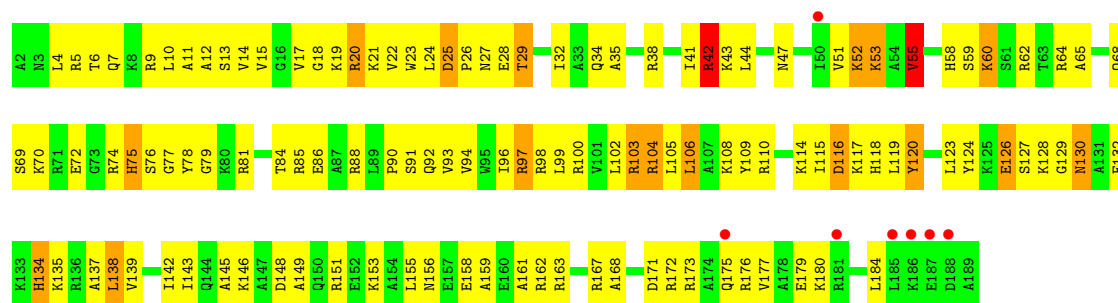
• Molecule 54: 60S ribosomal protein L18-A

Chain m8: 72% 26%



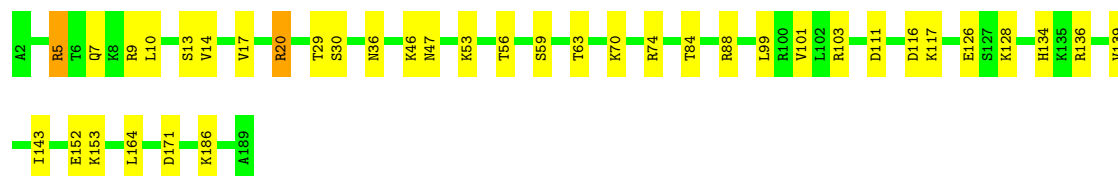
• Molecule 55: 60S ribosomal protein L19-A

Chain M9: 4% 35% 55% 9%



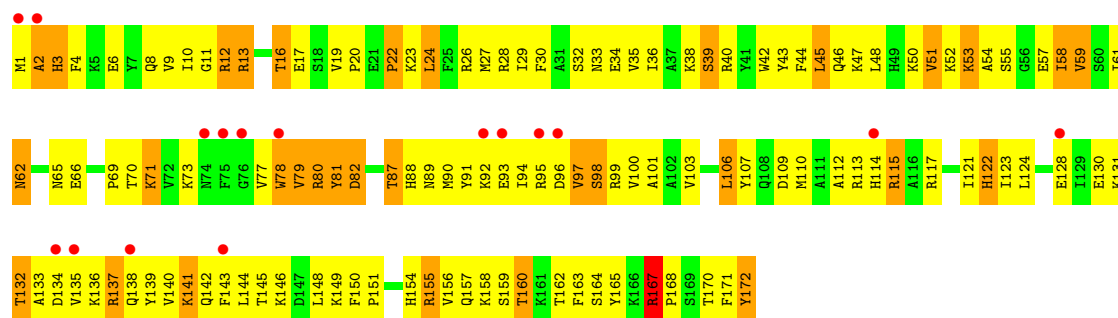
• Molecule 55: 60S ribosomal protein L19-A

Chain m9: 80% 19%



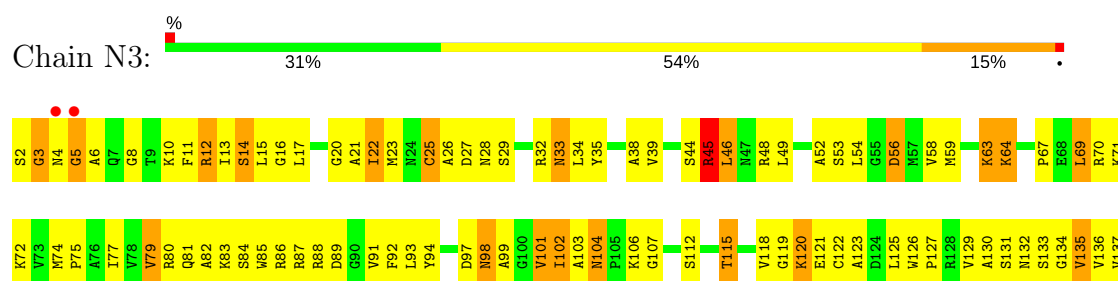
• Molecule 56: 60S ribosomal protein L20-A

Chain N0: 9% 26% 55% 19%

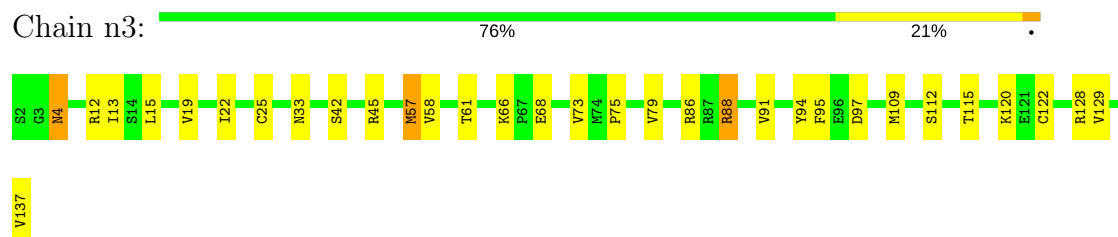


• Molecule 56: 60S ribosomal protein L20-A

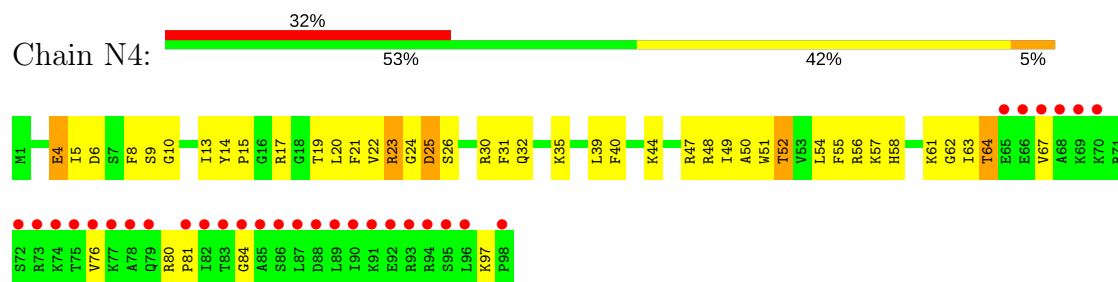




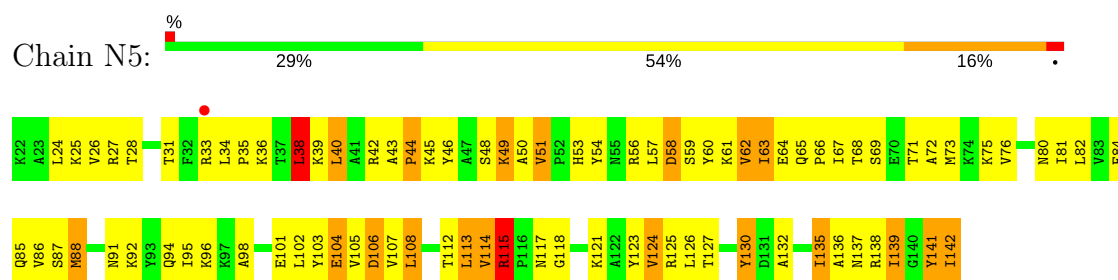
- Molecule 59: 60S ribosomal protein L23-A



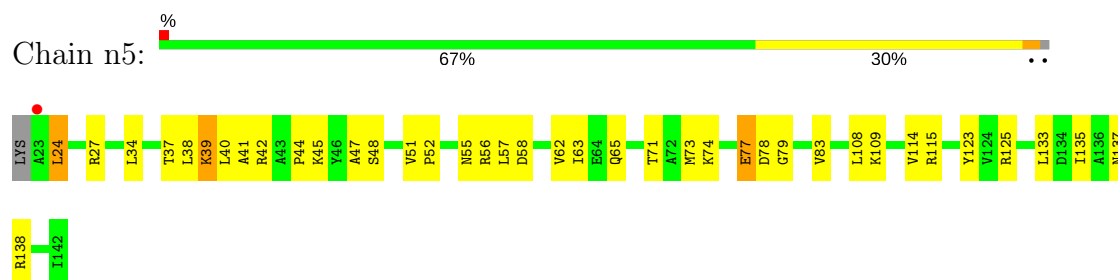
- Molecule 60: 60S ribosomal protein L24-A



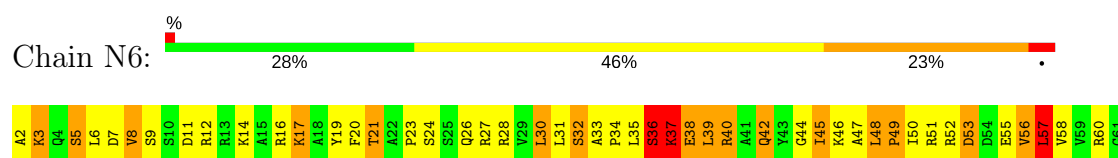
- Molecule 61: 60S ribosomal protein L25



- Molecule 61: 60S ribosomal protein L25

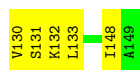
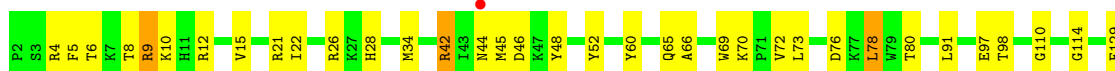
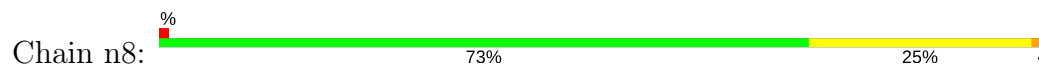


- Molecule 62: 60S ribosomal protein L26-A

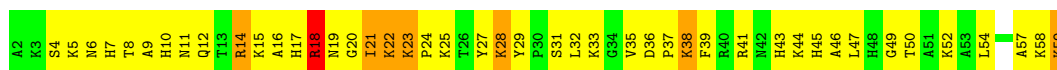




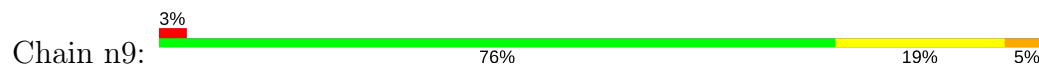
- Molecule 64: 60S ribosomal protein L28



- Molecule 65: 60S ribosomal protein L29



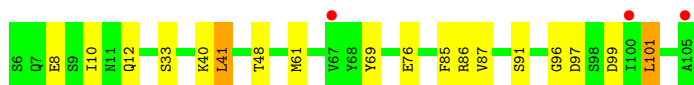
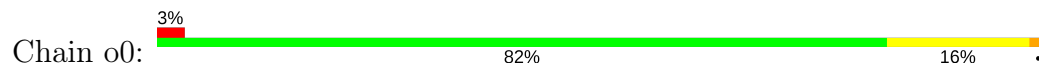
- Molecule 65: 60S ribosomal protein L29



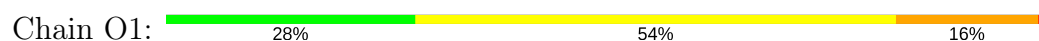
- Molecule 66: 60S ribosomal protein L30

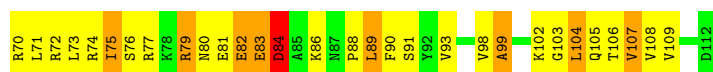


- Molecule 66: 60S ribosomal protein L30

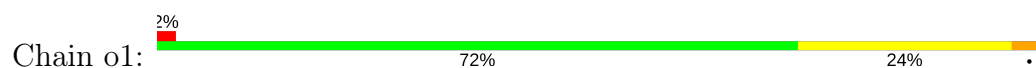


- Molecule 67: 60S ribosomal protein L31-A

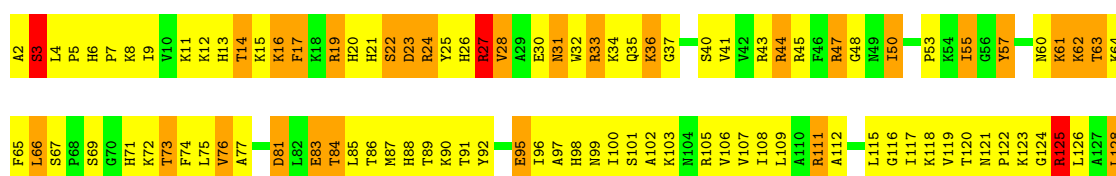




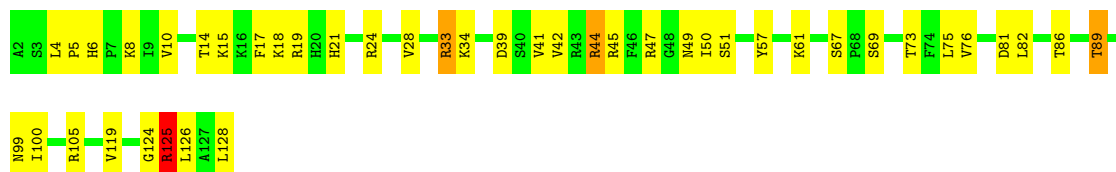
- Molecule 67: 60S ribosomal protein L31-A



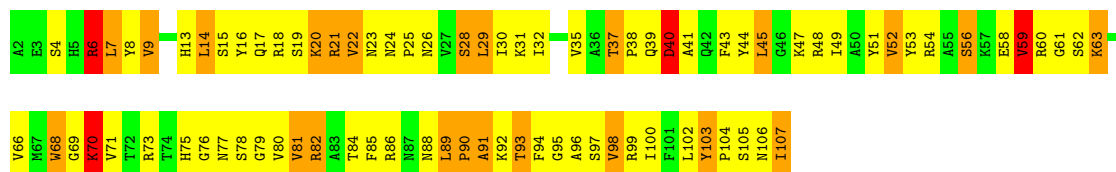
- Molecule 68: 60S ribosomal protein L32



- Molecule 68: 60S ribosomal protein L32



- Molecule 69: 60S ribosomal protein L33-A

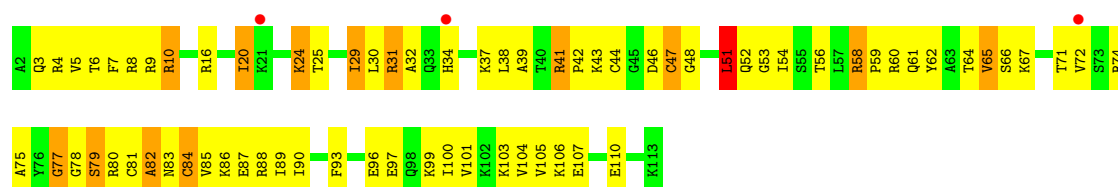


- Molecule 69: 60S ribosomal protein L33-A

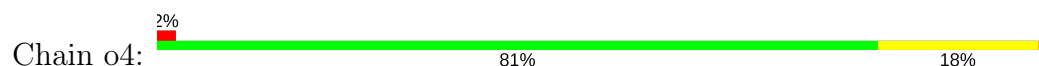


- Molecule 70: 60S ribosomal protein L34-A





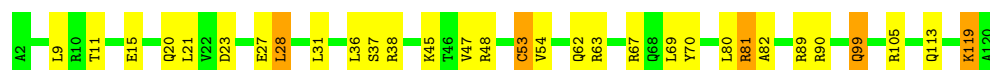
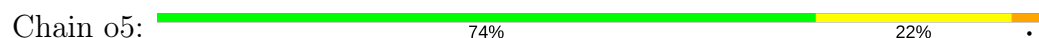
- Molecule 70: 60S ribosomal protein L34-A



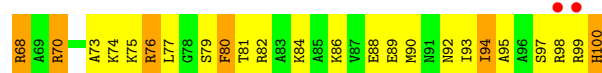
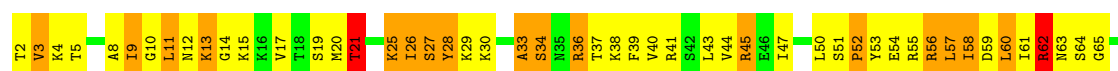
- Molecule 71: 60S ribosomal protein L35-A



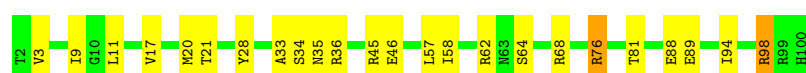
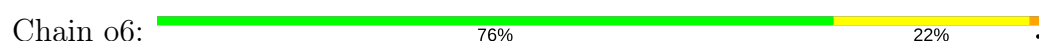
- Molecule 71: 60S ribosomal protein L35-A



- Molecule 72: 60S ribosomal protein L36-A

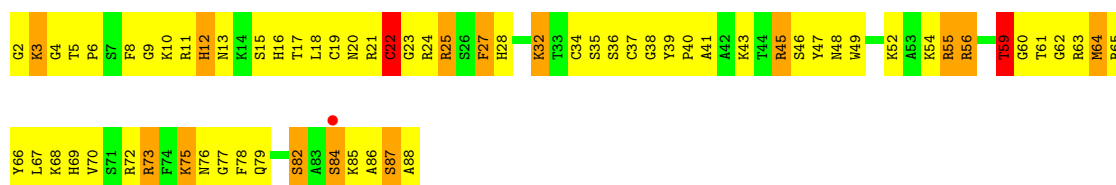


- Molecule 72: 60S ribosomal protein L36-A

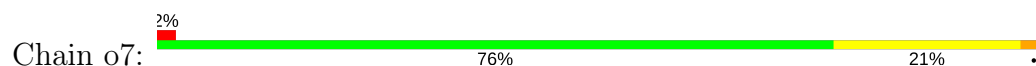


- Molecule 73: 60S ribosomal protein L37-A





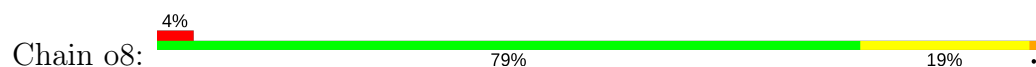
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38



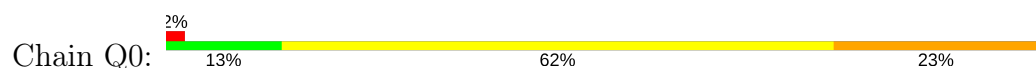
- Molecule 75: 60S ribosomal protein L39



- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40

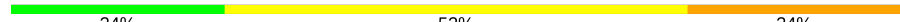


- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  71% 29%



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  24% 52% 24%



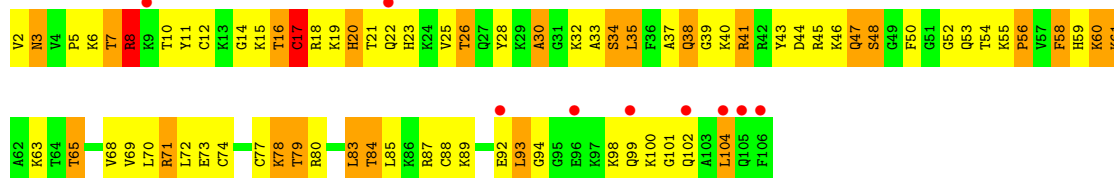
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  64% 32% .




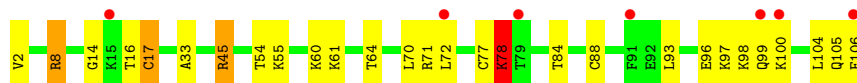
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  9% 28% 48% 23% .



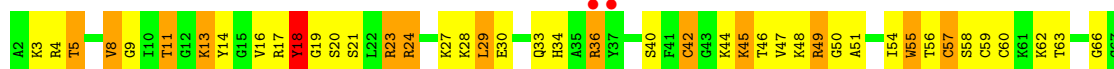
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  7% 73% 23% . .



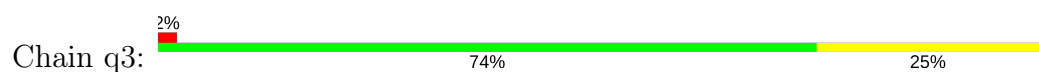
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  2% 31% 45% 23% .

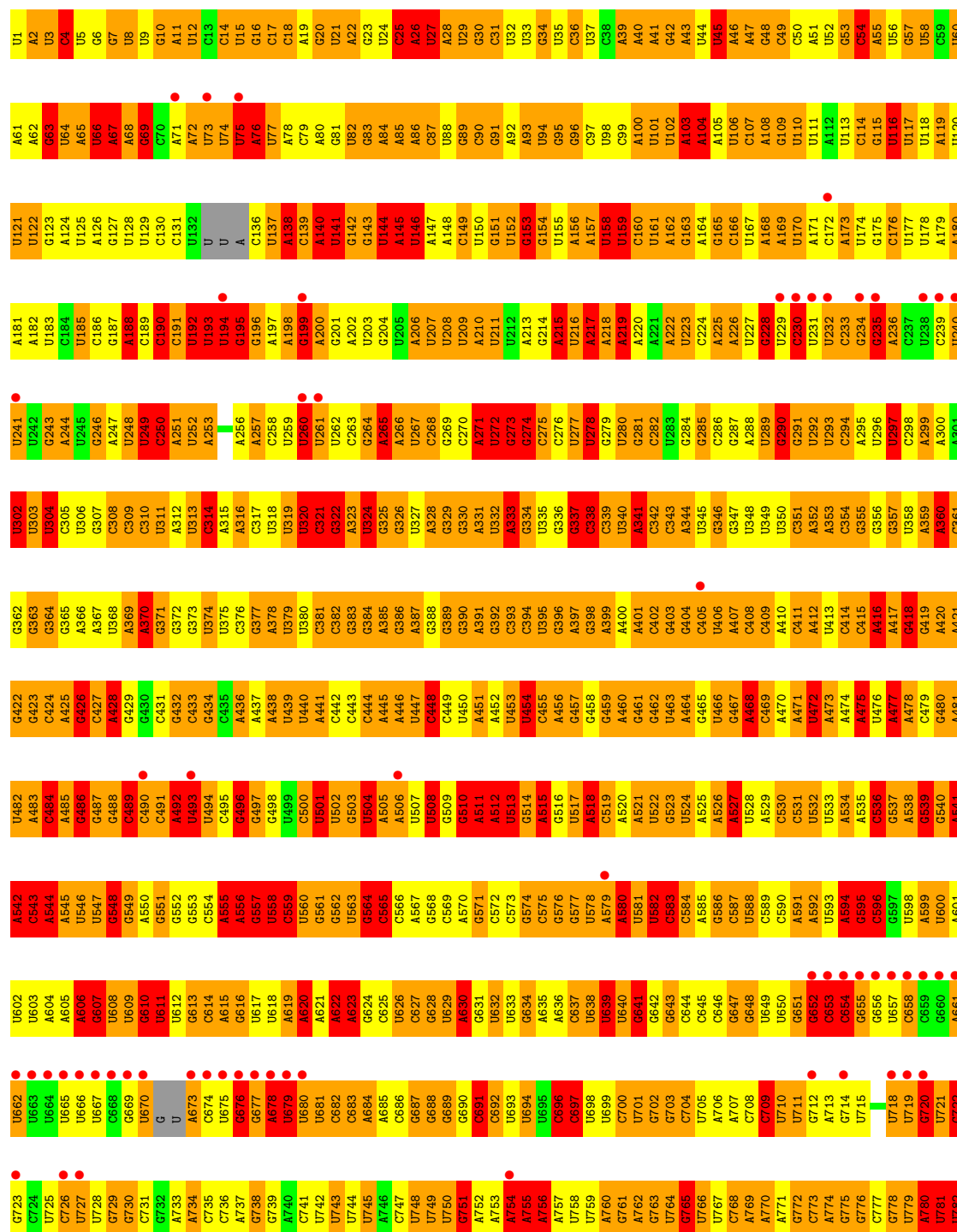


- Molecule 79: 60S ribosomal protein L43-A

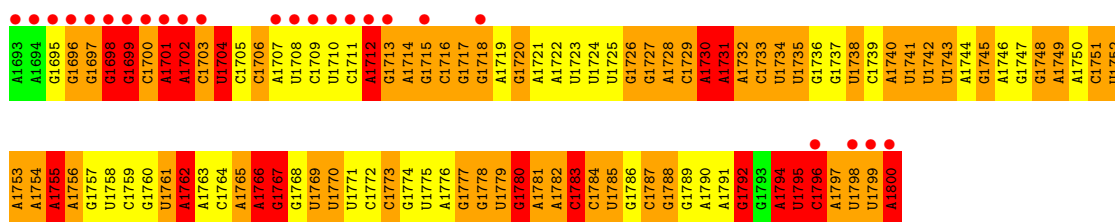




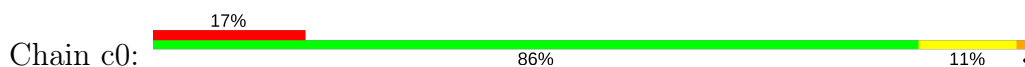
## ● Molecule 80: 18S ribosomal RNA



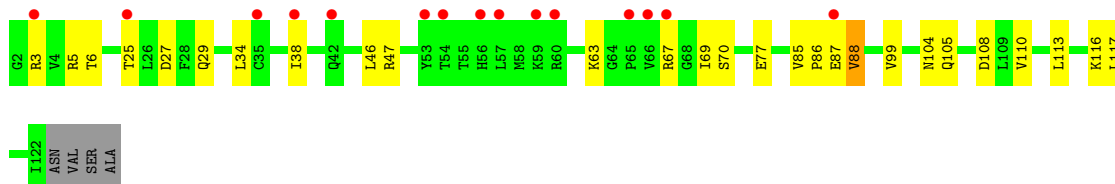
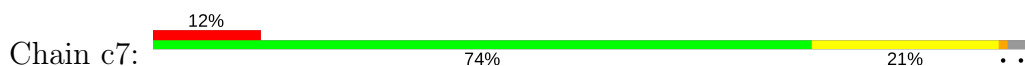
A1633	A1573	G1513	U1452	A1391	A1331	G1270	U1206	G1146	A1086	A1026	A966	A906	U843	G783
C1634	G1574	U1514	G1453	U1392	C1332	G1271	C1207	A1147	A1087	A1027	A967	A907	A844	C784
A1635	G1575	A1515	G1454	C1393	C1333	U1272	A1208	C1148	A1088	C1028	U968	U908	G845	C785
C1636	A1576	A1516	G1455	G1394	U1334	U1273	C1209	G1149	U1089	U1029	C969	U909	G846	C786
G1637	A1577	U1517	C1456	G1395	U1335	C1274	C1210	G1150	C1090	A1030	A970	C910	A847	C787
C1638	U1578	U1518	C1457	G1396	U1336	A1275	A1211	A1151	A1091	U1031	A971	U911	G848	C788
A1639	U1579	U1519	G1458	U1397	A1337	U1276	G1212	A1152	A1092	G1032	C972	U912	C849	A789
C1640	C1580	U1520	C1459	U1398	C1338	G1277	G1213	G1153	A1093	C1033	A973	G913	A850	U790
C1641	U1581	G1521	A1460	U1399	C1339	U1278	U1214	G1154	A1094	C1034	A974	G914	U851	A791
U1642	A1582	U1522	C1461	A1400	U1340	C1279	C1215	G1155	C975	A1035	C976	U915	A856	U792
U1643	A1583	G1523	G1462	A1401	A1341	C1280	C1216	C1156	C1096	A1036	A977	U916	A857	A793
C1644	U1584	A1524	C1463	C1402	C1342	G1281	U1217	A1157	U1097	C1037	U977	U917	U857	U794
G1645	U1585	A1525	G1464	C1403	U1343	U1282	G1218	C1158	U1098	U1038	A978	U918	G858	U795
C1646	A1586	A1526	C1465	C1404	A1344	U1283	A1219	C1159	U1099	A1039	A979	U919	A859	A796
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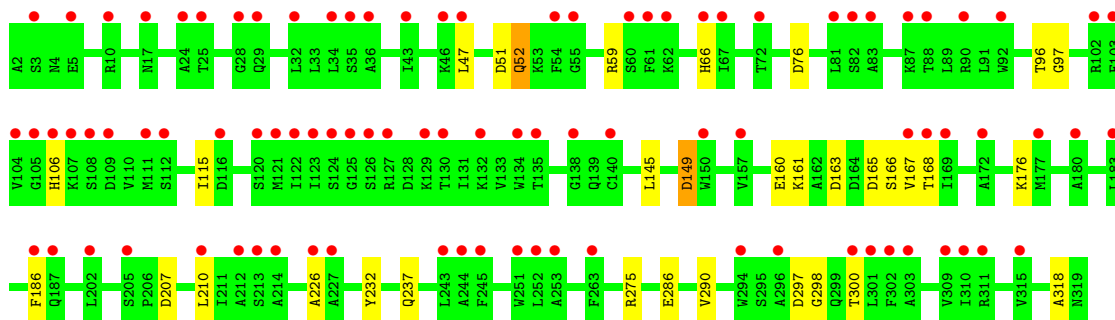
- Molecule 81: 40S ribosomal protein S10-A,40S Ribosomal Protein S10



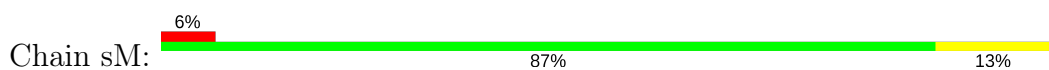
- Molecule 82: ES17



- Molecule 83: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 84: Suppressor protein STM1,Ribosome-bound protein Stm1



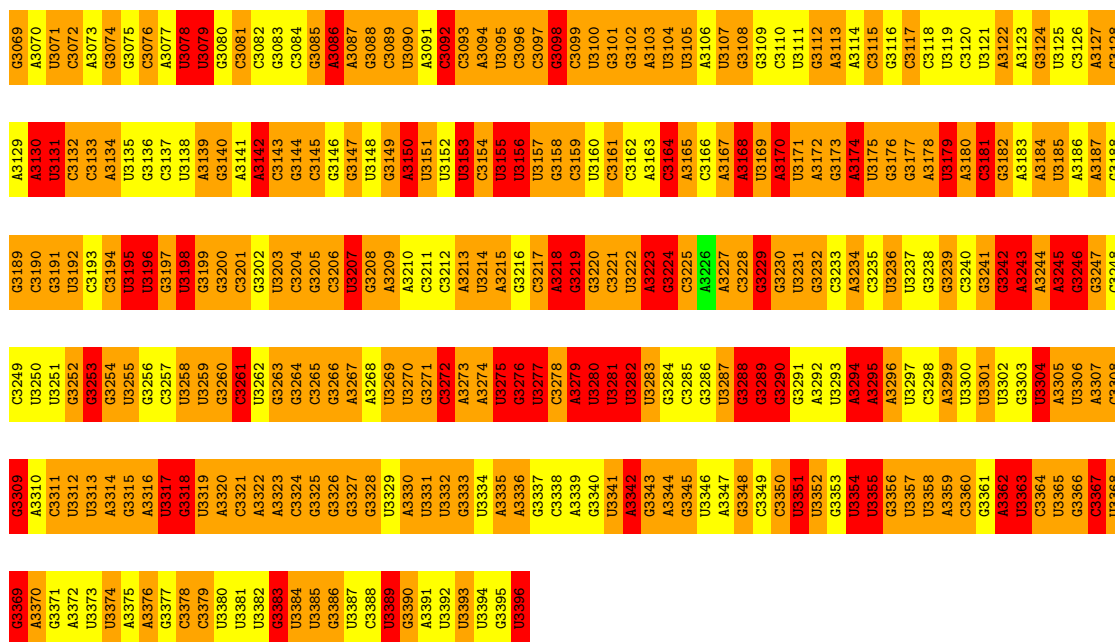
- Molecule 85: 25S ribosomal RNA



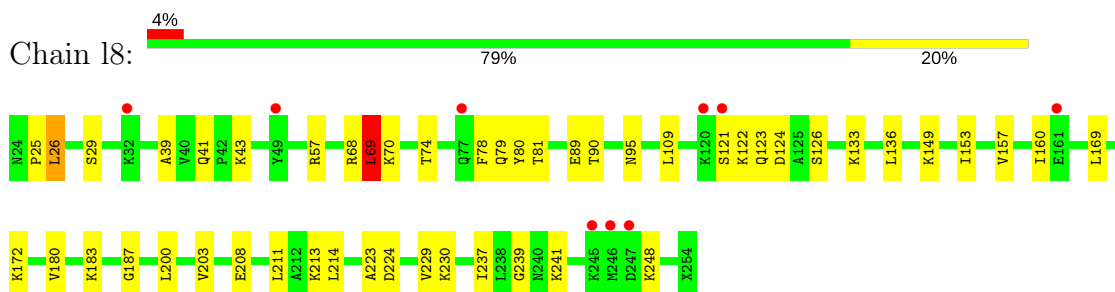
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A1884	U1824	U1764	A1704	C1644	U1584	A1524	G1464	G1404	G1344	G1284	C1224	G1164	C1104	U1044
U1885	C1825	U1765	U1705	U1645	C1585	G1525	A1465	A1405	G1345	G1285	A1225	A1165	A1105	C1045
A1886	C1826	G1766	C1706	G1646	U1586	U1526	G1466	A1406	G1346	A1286	G1226	G1166	G1106	A1046
A1887	G1827	G1767	A1707	A1647	A1587	G1527	A1467	A1407	U1347	U1287	C1227	U1167	C1107	A1047
U1888	A1828	U1768	C1708	A1648	A1588	G1528	A1468	G1408	U1348	U1288	C1228	U1168	U1108	A1048
G1889	G1829	G1769	C1709	U1649	A1589	U1529	C1469	G1409	G1349	G1289	G1229	A1169	U1109	C1049
A1890	U1830	G1770	C1710	G1650	G1590	U1530	U1470	U1410	A1350	A1290	G1230	A1170	U1110	U1050
A1891	C1831	C1771	C1711	U1651	G1591	C1531	U1471	C1411	U1351	A1291	A1231	G1171	U1111	U1051
G1892	G1832	U1772	G1712	G1652	G1592	C1532	U1472	G1412	A1352	C1292	G1232	G1172	A1112	U1052
A1893	C1833	C1773	G1713	G1653	A1593	U1533	G1473	G1413	U1353	U1293	G1233	U1173	G1113	A1053
U1894	A1834	C1774	A1714	A1654	A1594	A1534	A1474	G1414	G1354	A1294	G1234	G1174	U1114	A1054
A1895	A1835	G1775	A1715	G1655	U1595	A1535	A1475	U1415	A1355	G1295	U1235	C1175	G1115	A1055
A1896	C1836	G1776	U1716	A1656	C1596	G1536	G1476	C1416	U1356	C1296	G1236	G1176	U1056	U1056
G1897	U1837	U1777	U1717	C1657	C1597	A1537	A1477	G1417	G1357	C1297	G1237	G1177	A1057	G1057
G1898	G1838	G1778	G1718	G1658	G1598	C1538	G1478	A1418	C1358	C1298	C1238	G1178	C1118	U1058
A1899	A1839	C1779	G1719	U1659	U1599	A1539	U1479	A1419	C1359	U1299	G1239	A1179	G1059	C1059
A1900	U1840	G1780	U1720	C1660	U1600	U1540	G1480	C1420	C1360	G1300	A1240	A1180	U1120	U1060
A1901	A1841	C1781	U1721	G1661	U1601	G1541	A1481	G1421	U1361	A1301	U1241	A1181	U1121	A1061
G1902	U1842	U1782	U1722	G1662	A1602	G1542	A1482	G1422	G1362	A1302	U1242	A1182	U1122	A1062
U1903	C1843	U1783	C1723	C1663	A1603	G1543	G1483	C1423	A1363	A1303	G1243	C1183	U1123	G1063
C1904	C1844	G1784	U1724	G1664	G1604	G1544	U1484	C1424	C1364	A1304	A1244	A1184	U1124	A1064
G1905	G1845	U1785	C1725	G1665	A1605	A1545	G1485	U1425	G1365	U1305	A1245	C1185	U1125	A1065
A1906	U1846	G1786	C1726	G1666	A1606	A1546	G1486	C1426	A1366	G1306	G1246	G1186	G1126	G1066
C1907	A1847	A1787	G1727	A1667	U1607	G1547	G1487	U1427	G1367	G1307	U1247	C1187	G1127	U1067
A1908	G1848	C1788	G1728	G1668	C1608	C1548	G1488	A1428	U1368	A1308	G1248	C1188	U1128	C1068
U1909	C1849	G1789	A1729	C1669	G1609	U1549	A1489	G1429	A1369	U1309	G1249	C1189	A1129	G1069
A1910	A1850	G1790	G1730	C1670	G1610	C1550	A1490	U1430	G1370	G1310	G1250	A1190	A1130	U1070

G3009	U2949	C2869	U2829	A2769	C2709	A2649	G2589	U2410	C2360	C2290	C2230	G2110	A1911
U3010	G2950	A2890	G2830	G2770	C2710	U2650	A2590	U2411	U2351	A2291	C2231	G2111	U1912
A3011	G2951	U2891	G2831	G2771	C2711	G2651	A2591	G2412	A2352	U2292	C2232	U2112	A1913
A3012	G2952	A2892	C2832	C2772	U2712	U2652	G2592	A2413	G2353	C2293	A2233	A2113	G1914
U3013	U2953	C2893	A2833	C2773	U2713	G2653	A2593	G2414	C2354	U2294	G2234	C2114	A1915
U3014	U2954	G2894	G2834	C2774	G2714	C2654	A2594	G2415	G2355	A2295	G2235	G2115	U1916
G3015	U2955	G2895	U2835	U2775	A2715	U2655	A2595	U2416	A2356	U2296	G2236	G2116	C1917
A3016	A2956	A2896	G2836	G2776	U2716	A2656	A2596	U2417	A2357	U2297	C2237	A2117	C1918
A3017	G2957	G2897	A2837	G2777	U2717	A2657	U2597	U2418	A2358	U2298	G2238	G2118	G1919
G3018	A2958	G2898	A2838	G2778	U2718	G2658	U2598	A2419	C2359	A2299	G2239	C2179	U1920
U3019	C2959	G2899	G2839	U2779	U2719	G2659	U2599	G2420	C2360	G2300	G2240	A2120	A1921
U3020	G2960	A2900	G2840	U2780	G2720	G2660	C2600	G2421	A2361	U2301	A2241	G2121	A1922
A3021	U2961	G2901	G2841	U2781	A2721	G2661	A2601	U2422	C2362	G2302	A2242	G2122	G1923
G3022	U2962	A2902	U2842	U2782	U2722	G2662	G2602	U2423	A2363	A2303	A2243	G2123	U1924
U3023	C2963	G2903	U2843	U2783	U2723	G2663	G2603	A2424	G2364	C2304	A2244	G2124	U1925
A3024	U2964	U2904	G2844	G2784	U2724	G2664	U2604	G2425	C2365	G2305	A2245	G2125	G1926
G3025	U2965	A2905	A2845	U2785	U2725	G2665	G2605	U2426	C2366	C2306	G2246	A2126	G1927
C3026	G2966	G2906	U2846	G2786	C2726	G2666	G2606	U2427	A2367	G2307	G2247	U2127	G1928
A3027	A2967	G2907	U2847	G2787	A2727	A2667	G2607	U2428	C2368	C2308	C2248	C2128	G1929
G3028	G2968	C2908	G2848	C2788	G2728	U2668	G2608	U2429	G2369	A2309	G2249	U2129	A1930
A3029	A2969	U2909	U2849	U2789	U2729	G2669	A2609	A2430	G2370	U2310	G2250	G2130	U1931
G3030	C2970	A2910	G2850	G2790	G2730	G2670	G2610	C2431	G2371	G2311	G2251	A2131	A1932
U3031	A2971	A2911	A2851	G2791	U2731	A2671	U2611	A2432	A2372	A2312	A2252	C2132	A1933
A3032	G2972	G2912	C2852	A2792	G2732	G2672	U2612	A2433	A2373	A2313	G2253	U2133	G1934
G3033	G2973	C2913	A2853	G2793	A2733	G2673	U2613	U2434	C2374	U2314	U2254	G2134	G1935
C3034	U2974	G2914	U2854	G2794	A2734	A2674	G2614	G2435	G2375	G2315	A2255	U2135	A1936
A3035	U2975	U2915	U2855	U2795	U2735	G2675	G2615	U2436	G2376	G2316	A2256	C2136	U1937
G3036	A2976	U2916	G2856	G2796	A2736	G2676	C2616	G2437	A2377	A2317	G2257	U2137	U1938
U3037	G2977	G2917	G2857	C2797	G2737	A2677	U2617	A2438	C2378	U2318	G2258	A2138	G1939
G3038	U3038	G2978	U2858	G2798	A2738	G2678	G2618	U2439	U2379	U2319	A2259	A2139	G1940
C3039	U2979	A2919	U2859	A2799	A2739	U2679	G2619	G2440	U2380	A2320	U2260	U2140	C1941
A3040	U2980	U2920	U2860	G2800	A2740	A2680	G2620	A2441	G2381	A2321	G2261	U2141	U1942
U3041	U2981	A2921	U2861	A2801	C2741	U2681	G2621	G2442	G2382	C2322	A2262	A2142	C1943
A2982	U2982	G2922	U2862	A2802	C2742	G2682	G2622	A2443	C2383	G2323	A2263	A2143	U1944
C3043	C2983	U2923	G2863	A2803	A2743	U2683	G2623	G2444	A2384	A2324	U2264	A2144	A1945
G3044	G2984	U2924	A2864	A2804	U2744	C2684	G2624	G2503	G2385	G2325	C2265	A2145	A1946
G3045	G2985	G2925	U2865	G2805	G2745	C2685	C2625	U2504	A2386	A2326	U2266	C2146	G1947
A3046	U2986	A2926	U2866	U2806	A2746	A2686	A2626	U2505	A2387	U2327	C2267	A2147	G1948
U3047	A2987	G2927	G2867	U2807	U2747	G2687	C2627	U2506	C2388	U2328	U2268	A2148	G1949
A3048	C2988	C2928	U2868	A2808	A2748	U2688	A2628	C2507	C2389	C2329	U2269	A2149	U1950
U3049	U2989	G2929	U2869	C2809	G2749	A2689	U2629	U2508	A2390	G2330	A2270	G2150	C1951
C3050	G2990	A2930	C2870	C2810	U2750	G2690	C2630	U2509	G2391	C2331	A2271	C2151	G1952
U3051	A2991	G2931	G2871	C2811	G2751	A2691	U2631	U2510	G2392	A2332	G2272	C2152	G1953
G3052	U2992	U2932	A2872	C2812	U2752	A2692	G2632	A2511	G2393	C2333	G2273	U2153	A2093
C3053	G2993	A2933	U2873	A2813	G2753	C2693	U2633	G2512	G2394	U2334	U2274	A2154	C2094
U3054	A2994	U2934	G2874	G2814	G2754	A2694	U2634	U2513	G2395	G2335	A2275	G2155	G2095
G3055	A2995	U2935	U2875	G2815	C2755	A2695	A2635	U2514	G2396	G2336	G2276	C2156	A2096
U3056	U2996	A2936	C2876	G2816	C2756	A2696	A2636	A2515	A2397	C2337	G2277	G2157	U2097
G3057	G2997	G2937	G2877	A2817	U2757	A2697	A2637	U2516	A2398	C2338	C2278	A2158	C2098
U3058	U2998	G2938	G2878	U2818	A2758	G2698	A2638	U2517	A2399	C2339	A2279	U2159	A2099
G3059	U2999	G2939	C2879	A2819	U2759	G2699	G2639	G2518	G2400	U2340	A2280	G2160	A2100
C3060	A3000	A2940	U2880	A2820	G2760	G2700	A2640	A2519	A2401	A2341	A2281	G2161	C2101
G3061	G3001	A2941	C2881	C2821	U2761	U2701	U2641	A2520	A2402	U2342	A2282	U2162	U2102
C3062	C3002	C2942	U2882	A2702	A2762	C2702	U2642	A2521	G2403	C2343	G2283	C2163	U2103
G3063	G3003	G2943	G2883	G2823	U2763	A2703	A2643	G2522	U2404	U2344	A2284	A2164	A2104
U3064	A3004	U2944	G2884	G2824	C2764	A2704	C2644	A2523	C2405	C2345	C2285	G2165	G2105
G3065	A3005	G2945	C2885	C2825	G2765	A2705	G2645	A2524	C2406	C2346	U2286	A2166	A2106
U3066	A3006	A2946	U2886	U2826	U2766	G2706	G2646	G2525	U2407	U2347	C2287	A2167	A2107
C3067	U3007	G2947	A2887	C2707	U2767	U2707	A2647	G2526	U2408	A2348	G2288	A2168	C2108
U3068	A3008	C2948	U2888	G2828	U2768	C2708	U2648	G2527	G2409	U2349	U2289	G2169	U2109



- Molecule 86: 60S ribosomal protein L8-A, 60S Ribosomal Protein L8

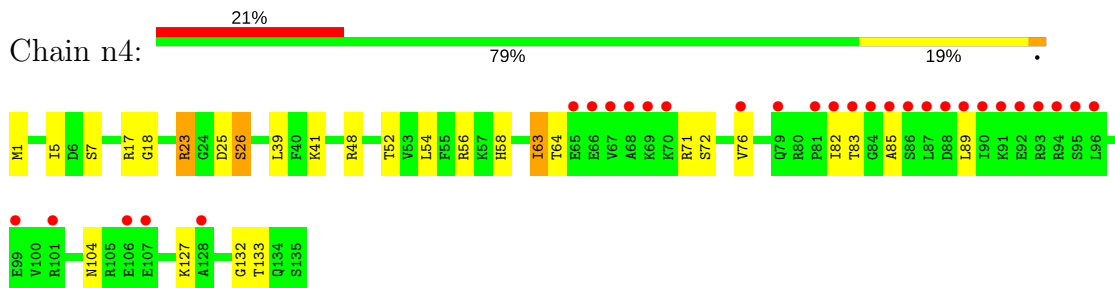


- Molecule 87: 60S Ribosomal Protein L12

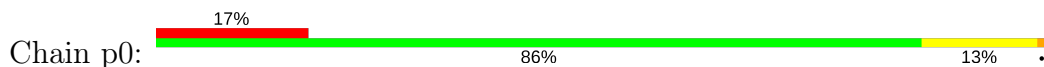


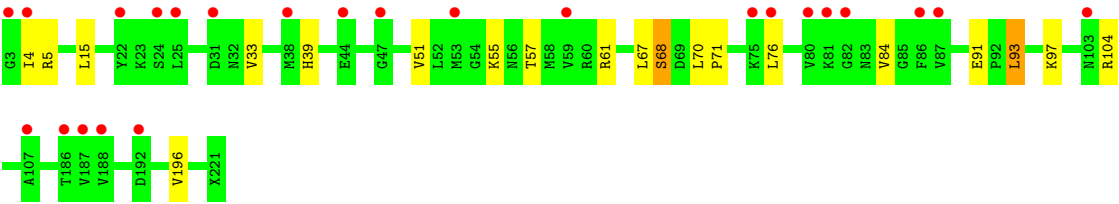
There are no outlier residues recorded for this chain.

- Molecule 88: 60S ribosomal protein L24-A



- Molecule 89: 60S Ribosomal Protein P0





- Molecule 90: 60S Ribosomal Protein P1/2



There are no outlier residues recorded for this chain.

- Molecule 90: 60S Ribosomal Protein P1/2



- Molecule 91: Peptidyl-tRNA analog ACCA-Leu-Phe



- Molecule 91: Peptidyl-tRNA analog ACCA-Leu-Phe



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	434.73Å 286.77Å 303.15Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	148.72 – 3.50 149.76 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (148.72-3.50) 99.7 (149.76-3.50)	Depositor EDS
$R_{merge}$	0.61	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.261 , 0.312 0.261 , 0.311	Depositor DCC
$R_{free}$ test set	18368 reflections (2.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.6	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	411589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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, SPS, 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	1.53	426/42467 (1.0%)	2.41	4031/66169 (6.1%)
2	S0	0.67	0/1617	0.76	0/2215
2	s0	0.78	0/1623	0.86	1/2222 (0.0%)
3	S1	0.59	0/1735	0.75	1/2335 (0.0%)
3	s1	0.82	2/1748 (0.1%)	0.95	5/2352 (0.2%)
4	S2	0.73	0/1665	0.81	0/2263
4	s2	0.86	2/1665 (0.1%)	0.96	4/2263 (0.2%)
5	S3	0.68	0/1759	0.78	0/2368
5	s3	0.70	0/1759	0.79	0/2368
6	S4	0.85	2/2109 (0.1%)	0.91	2/2839 (0.1%)
6	s4	0.84	1/2109 (0.0%)	0.98	1/2839 (0.0%)
7	S5	0.66	0/1629	0.76	0/2202
7	s5	0.65	1/1629 (0.1%)	0.76	1/2202 (0.0%)
8	S6	0.84	3/1823 (0.2%)	0.92	5/2439 (0.2%)
8	s6	0.93	1/1779 (0.1%)	1.01	6/2379 (0.3%)
9	S7	0.73	2/1506 (0.1%)	0.79	0/2028
9	s7	0.78	0/1516	0.85	2/2043 (0.1%)
10	S8	0.79	1/1514 (0.1%)	0.90	2/2021 (0.1%)
10	s8	0.94	2/1514 (0.1%)	1.00	5/2021 (0.2%)
11	S9	0.75	2/1519 (0.1%)	0.88	1/2035 (0.0%)
11	s9	0.84	1/1519 (0.1%)	0.97	4/2035 (0.2%)
12	C0	0.62	0/725	0.72	0/978
13	C1	0.86	1/1195 (0.1%)	0.84	0/1612
13	c1	0.94	1/1194 (0.1%)	0.96	1/1610 (0.1%)
14	C2	0.59	0/873	0.72	0/1185
14	c2	0.47	0/873	0.63	0/1185
15	C3	0.75	0/1215	0.86	1/1638 (0.1%)
15	c3	0.86	1/1215 (0.1%)	0.93	0/1638
16	C4	0.59	0/901	0.75	0/1217
16	c4	0.85	0/960	0.97	0/1290
17	C5	0.85	2/988 (0.2%)	0.85	0/1327
17	c5	0.74	0/1010	0.85	1/1356 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	C6	0.65	0/1125	0.80	2/1510 (0.1%)
18	c6	0.69	0/1131	0.74	0/1518
19	C7	0.66	0/935	0.76	0/1254
20	C8	0.70	0/1211	0.82	0/1628
20	c8	0.76	1/1211 (0.1%)	0.87	0/1628
21	C9	0.66	0/1130	0.75	0/1517
21	c9	0.70	0/1130	0.79	1/1517 (0.1%)
22	D0	0.64	0/865	0.80	1/1169 (0.1%)
22	d0	0.72	0/892	0.75	0/1205
23	D1	0.72	0/693	0.83	0/935
23	d1	0.87	0/693	0.96	1/935 (0.1%)
24	D2	0.81	0/1038	0.90	2/1395 (0.1%)
24	d2	0.90	2/1038 (0.2%)	0.95	2/1395 (0.1%)
25	D3	0.85	1/1139 (0.1%)	0.90	1/1518 (0.1%)
25	d3	1.05	1/1139 (0.1%)	1.07	4/1518 (0.3%)
26	D4	0.79	0/1087	0.85	0/1449
26	d4	0.93	0/1087	1.04	5/1449 (0.3%)
27	D5	0.66	0/571	0.78	0/768
27	d5	0.78	1/566 (0.2%)	0.76	0/761
28	D6	0.68	0/782	0.78	1/1047 (0.1%)
28	d6	0.84	2/782 (0.3%)	0.99	1/1047 (0.1%)
29	D7	0.76	0/620	0.80	0/838
29	d7	0.82	2/620 (0.3%)	0.89	0/838
30	D8	0.69	0/499	0.82	1/670 (0.1%)
30	d8	0.69	0/499	0.91	0/670
31	D9	0.76	1/452 (0.2%)	0.80	0/600
31	d9	0.78	1/452 (0.2%)	0.80	0/600
32	E0	0.74	0/483	0.78	0/643
32	e0	0.94	1/499 (0.2%)	0.94	1/665 (0.2%)
33	E1	0.72	0/577	0.80	0/770
33	e1	0.66	0/619	0.77	0/822
34	SR	0.57	0/2490	0.71	0/3389
35	SM	0.77	1/925 (0.1%)	0.87	1/1240 (0.1%)
36	1	2.49	4418/75394 (5.9%)	3.49	15681/117545 (13.3%)
37	3	2.00	80/2883 (2.8%)	3.26	543/4491 (12.1%)
37	7	2.57	171/2883 (5.9%)	3.80	680/4491 (15.1%)
38	4	2.46	206/3746 (5.5%)	3.78	898/5832 (15.4%)
38	8	2.34	182/3746 (4.9%)	3.37	707/5832 (12.1%)
39	L2	1.18	7/1948 (0.4%)	1.22	16/2617 (0.6%)
39	l2	1.09	6/1946 (0.3%)	1.23	16/2614 (0.6%)
40	L3	1.18	16/3146 (0.5%)	1.19	19/4228 (0.4%)
40	l3	1.33	19/3146 (0.6%)	1.32	33/4228 (0.8%)
41	L4	1.29	18/2800 (0.6%)	1.30	28/3790 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
41	l4	1.26	14/2800 (0.5%)	1.22	18/3790 (0.5%)
42	L5	1.02	5/2425 (0.2%)	1.04	10/3271 (0.3%)
42	l5	1.23	14/2408 (0.6%)	1.22	17/3248 (0.5%)
43	L6	1.21	2/1260 (0.2%)	1.15	3/1694 (0.2%)
43	l6	1.16	4/1269 (0.3%)	1.26	12/1705 (0.7%)
44	L7	1.32	12/1821 (0.7%)	1.23	14/2451 (0.6%)
44	l7	1.44	19/1828 (1.0%)	1.23	15/2461 (0.6%)
45	L8	0.98	2/1836 (0.1%)	0.99	3/2481 (0.1%)
46	L9	1.10	6/1539 (0.4%)	1.11	10/2073 (0.5%)
46	l9	1.19	4/1539 (0.3%)	1.21	13/2073 (0.6%)
47	M0	1.15	9/1741 (0.5%)	1.18	14/2335 (0.6%)
47	m0	1.24	5/1758 (0.3%)	1.37	21/2358 (0.9%)
48	M1	0.93	3/1374 (0.2%)	0.97	2/1842 (0.1%)
48	m1	1.05	4/1374 (0.3%)	1.17	10/1842 (0.5%)
49	M3	1.20	10/1568 (0.6%)	1.23	13/2106 (0.6%)
49	m3	1.05	3/1573 (0.2%)	1.20	13/2113 (0.6%)
50	M4	1.11	5/1068 (0.5%)	1.15	6/1438 (0.4%)
50	m4	1.21	7/1074 (0.7%)	1.27	10/1446 (0.7%)
51	M5	1.19	7/1757 (0.4%)	1.28	19/2354 (0.8%)
51	m5	1.10	5/1757 (0.3%)	1.16	10/2354 (0.4%)
52	M6	1.40	18/1585 (1.1%)	1.37	22/2128 (1.0%)
52	m6	1.50	13/1585 (0.8%)	1.35	22/2128 (1.0%)
53	M7	1.29	4/1443 (0.3%)	1.14	10/1944 (0.5%)
53	m7	1.47	17/1250 (1.4%)	1.29	13/1683 (0.8%)
54	M8	1.26	11/1465 (0.8%)	1.22	11/1965 (0.6%)
54	m8	1.23	10/1465 (0.7%)	1.30	11/1965 (0.6%)
55	M9	0.93	0/1538	0.98	2/2050 (0.1%)
55	m9	0.96	2/1538 (0.1%)	1.05	8/2050 (0.4%)
56	N0	1.20	4/1481 (0.3%)	1.15	6/1990 (0.3%)
56	n0	1.35	11/1481 (0.7%)	1.23	9/1990 (0.5%)
57	N1	1.16	3/1300 (0.2%)	1.13	5/1743 (0.3%)
57	n1	1.32	10/1300 (0.8%)	1.20	10/1743 (0.6%)
58	N2	0.95	0/812	0.90	1/1099 (0.1%)
58	n2	0.94	0/794	1.00	2/1076 (0.2%)
59	N3	1.16	5/1018 (0.5%)	1.21	8/1369 (0.6%)
59	n3	1.39	11/1018 (1.1%)	1.34	13/1369 (0.9%)
60	N4	0.94	1/712 (0.1%)	0.97	3/958 (0.3%)
61	N5	1.14	3/979 (0.3%)	1.16	7/1321 (0.5%)
61	n5	1.11	4/974 (0.4%)	1.19	4/1314 (0.3%)
62	N6	1.17	7/1004 (0.7%)	1.33	12/1341 (0.9%)
62	n6	1.17	5/1004 (0.5%)	1.34	15/1341 (1.1%)
63	N7	0.91	0/1118	0.91	1/1497 (0.1%)
63	n7	0.96	2/1118 (0.2%)	0.95	3/1497 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
64	N8	1.22	4/1204 (0.3%)	1.24	11/1612 (0.7%)
64	n8	1.25	10/1204 (0.8%)	1.26	10/1612 (0.6%)
65	N9	1.08	1/473 (0.2%)	1.14	2/629 (0.3%)
65	n9	1.17	2/473 (0.4%)	1.16	2/629 (0.3%)
66	O0	0.81	0/751	0.91	0/1008
66	o0	0.94	1/775 (0.1%)	0.99	2/1040 (0.2%)
67	O1	1.07	3/890 (0.3%)	1.07	4/1196 (0.3%)
67	o1	1.23	5/897 (0.6%)	1.22	5/1205 (0.4%)
68	O2	1.40	13/1041 (1.2%)	1.34	14/1394 (1.0%)
68	o2	1.24	6/1041 (0.6%)	1.33	11/1394 (0.8%)
69	O3	1.50	10/868 (1.2%)	1.22	7/1168 (0.6%)
69	o3	1.54	13/868 (1.5%)	1.32	7/1168 (0.6%)
70	O4	1.01	1/890 (0.1%)	1.14	7/1189 (0.6%)
70	o4	1.03	2/890 (0.2%)	1.11	6/1189 (0.5%)
71	O5	1.18	5/978 (0.5%)	1.26	11/1301 (0.8%)
71	o5	0.96	2/974 (0.2%)	1.13	6/1297 (0.5%)
72	O6	0.99	0/778	1.15	3/1034 (0.3%)
72	o6	1.03	2/777 (0.3%)	1.16	3/1033 (0.3%)
73	O7	1.30	2/696 (0.3%)	1.29	7/923 (0.8%)
73	o7	1.25	4/696 (0.6%)	1.16	3/923 (0.3%)
74	O8	0.96	2/618 (0.3%)	1.08	3/826 (0.4%)
74	o8	0.83	0/614	1.01	3/822 (0.4%)
75	O9	1.09	1/443 (0.2%)	1.31	7/588 (1.2%)
75	o9	1.02	0/443	1.26	6/588 (1.0%)
76	Q0	1.15	3/423 (0.7%)	1.21	4/562 (0.7%)
76	q0	1.33	6/423 (1.4%)	1.22	3/562 (0.5%)
77	Q1	0.79	0/234	1.15	3/300 (1.0%)
77	q1	0.96	0/234	1.40	2/300 (0.7%)
78	Q2	1.22	3/860 (0.3%)	1.23	7/1136 (0.6%)
78	q2	1.32	4/860 (0.5%)	1.33	9/1136 (0.8%)
79	Q3	1.26	9/701 (1.3%)	1.31	7/934 (0.7%)
79	q3	1.22	6/701 (0.9%)	1.10	3/934 (0.3%)
80	6	1.94	1088/42790 (2.5%)	2.88	5446/66673 (8.2%)
81	c0	0.60	0/693	0.62	0/933
82	c7	0.69	0/914	0.83	1/1224 (0.1%)
83	sR	0.61	0/2495	0.72	0/3395
84	sM	0.87	1/481 (0.2%)	0.90	0/644
85	5	2.61	4902/75414 (6.5%)	3.71	16861/117575 (14.3%)
86	l8	0.92	1/1765 (0.1%)	0.95	3/2387 (0.1%)
88	n4	1.08	0/1052	1.10	7/1398 (0.5%)
89	p0	0.82	0/977	0.84	2/1313 (0.2%)
91	P	2.37	2/40 (5.0%)	4.21	9/60 (15.0%)
91	p	13.84	3/43 (7.0%)	5.74	11/64 (17.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	1.87	11986/430104 (2.8%)	2.68	45668/631544 (7.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S4	0	2
9	s7	0	1
11	S9	0	1
17	c5	0	1
19	C7	0	1
22	d0	0	1
25	d3	0	1
27	D5	0	1
33	E1	0	2
39	L2	0	1
40	L3	0	1
40	l3	0	1
41	L4	0	2
41	l4	0	1
42	l5	0	2
44	L7	0	1
44	l7	0	2
47	M0	0	1
49	m3	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	2
56	n0	0	2
57	N1	0	1
64	n8	0	1
65	N9	0	1
65	n9	0	1
68	o2	0	1
75	o9	0	1
80	6	0	1
81	c0	0	1
85	5	0	1
All	All	0	39

The worst 5 of 11986 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	p	74	C	P-O5'	89.50	2.49	1.59
37	7	63	A	C6-N6	27.75	1.56	1.33
80	6	1498	G	C8-N7	24.00	1.45	1.30
85	5	748	U	C4-O4	23.12	1.42	1.23
80	6	54	C	C4-N4	22.95	1.54	1.33

The worst 5 of 45668 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	5	2707	C	N3-C4-C5	-50.63	101.65	121.90
80	6	54	C	N3-C4-C5	-49.41	102.13	121.90
80	6	1070	C	N3-C4-C5	-42.39	104.94	121.90
80	6	818	C	N3-C4-C5	-42.29	104.98	121.90
80	6	1498	G	C5-N7-C8	-42.11	83.24	104.30

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
6	S4	148	ARG	Peptide
6	S4	193	GLY	Peptide
11	S9	38	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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	19104	1323	0
2	S0	1577	0	1567	211	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	189	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	145	0
5	s3	1734	0	1817	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S4	2068	0	2154	238	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	170	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	181	0
8	s6	1755	0	1845	0	0
9	S7	1481	0	1572	166	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	135	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	153	0
11	s9	1494	0	1573	0	0
12	C0	773	0	716	70	0
13	C1	1214	0	1244	89	0
13	c1	1168	0	1231	0	0
14	C2	890	0	885	71	0
14	c2	890	0	884	0	0
15	C3	1192	0	1255	121	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	125	0
16	c4	949	0	985	0	0
17	C5	977	0	1004	115	0
17	c5	1039	0	1038	0	0
18	C6	1105	0	1166	136	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	94	0
20	C8	1192	0	1222	149	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	135	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	96	0
22	d0	882	0	939	0	0
23	D1	684	0	672	86	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	126	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	108	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	123	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	72	0
27	d5	558	0	598	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D6	769	0	815	110	0
28	d6	769	0	815	0	0
29	D7	610	0	632	48	0
29	d7	610	0	633	0	0
30	D8	497	0	535	52	0
30	d8	497	0	535	0	0
31	D9	442	0	427	42	0
31	d9	442	0	429	0	0
32	E0	475	0	525	47	0
32	e0	491	0	542	0	0
33	E1	566	0	602	65	0
33	e1	608	0	657	0	0
34	SR	2437	0	2389	195	0
35	SM	1105	0	966	82	0
36	1	67355	0	33710	2364	0
37	3	2579	0	1302	133	0
37	7	2579	0	1293	96	0
38	4	3353	0	1692	139	0
38	8	3353	0	1692	139	0
39	L2	1914	0	1981	250	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	361	0
40	l3	3075	0	3141	0	0
41	L4	2748	0	2858	382	0
41	l4	2748	0	2858	0	0
42	L5	2375	0	2325	323	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	119	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	228	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	214	0
46	L9	1518	0	1587	194	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1735	252	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	165	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	206	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	125	0
50	m4	1059	0	1154	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	M5	1720	0	1779	264	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	165	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	169	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	173	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	153	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1486	173	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	155	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	89	0
58	n2	778	0	791	0	0
59	N3	1003	0	1047	116	0
59	n3	1003	0	1047	0	0
60	N4	699	0	640	49	0
61	N5	964	0	1025	107	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	133	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	140	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1214	186	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	67	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	912	97	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	125	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	97	0
69	o3	850	0	880	0	0
70	O4	880	0	945	98	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	119	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	o6	770	0	846	0	0
73	O7	681	0	682	86	0
73	o7	681	0	685	0	0
74	O8	612	0	682	50	0
74	o8	608	0	671	0	0
75	O9	436	0	475	59	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	56	0
76	q0	417	0	458	0	0
77	Q1	233	0	284	21	0
77	q1	233	0	284	0	0
78	Q2	847	0	915	103	0
78	q2	847	0	915	0	0
79	Q3	694	0	734	86	0
79	q3	694	0	736	0	0
80	6	38260	0	19230	1390	0
81	c0	762	0	688	0	0
82	c7	906	0	909	0	0
83	sR	2442	0	2392	0	0
84	sM	681	0	542	0	0
85	5	67376	0	33690	2427	0
86	l8	1763	0	1811	0	0
87	m2	750	0	174	0	0
88	n4	1038	0	1071	0	0
89	p0	1077	0	1013	0	0
90	p1	235	0	52	0	0
90	p2	230	0	49	0	0
91	P	37	0	23	15	0
91	p	40	0	23	0	0
92	1	2296	0	0	258	0
92	2	1057	0	0	102	0
92	3	70	0	0	11	0
92	4	147	0	0	18	0
92	5	2422	0	0	260	0
92	6	1113	0	0	106	0
92	7	77	0	0	10	0
92	8	112	0	0	12	0
92	C3	7	0	0	6	0
92	C5	7	0	0	4	0
92	C7	7	0	0	2	0
92	C8	7	0	0	0	0
92	D9	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	L3	14	0	0	3	0
92	L4	7	0	0	3	0
92	L6	14	0	0	2	0
92	M0	7	0	0	2	0
92	M5	14	0	0	2	0
92	M6	7	0	0	1	0
92	M7	7	0	0	1	0
92	M8	7	0	0	1	0
92	M9	7	0	0	2	0
92	N9	7	0	0	0	0
92	O3	7	0	0	3	0
92	O4	7	0	0	0	0
92	O7	7	0	0	7	0
92	O9	7	0	0	2	0
92	Q2	7	0	0	4	0
92	S8	7	0	0	3	0
92	S9	7	0	0	4	0
92	SR	7	0	0	0	0
92	c3	7	0	0	0	0
92	c5	7	0	0	0	0
92	c8	7	0	0	0	0
92	d4	7	0	0	0	0
92	l3	14	0	0	0	0
92	l5	14	0	0	0	0
92	l9	7	0	0	0	0
92	m0	21	0	0	0	0
92	m5	14	0	0	0	0
92	m6	7	0	0	0	0
92	m8	7	0	0	0	0
92	m9	7	0	0	0	0
92	n9	7	0	0	0	0
92	o3	7	0	0	0	0
92	o7	14	0	0	0	0
92	q2	7	0	0	0	0
92	s1	7	0	0	0	0
92	s4	7	0	0	0	0
92	s8	7	0	0	0	0
92	s9	7	0	0	0	0
92	sR	7	0	0	0	0
93	1	394	0	0	1	0
93	2	90	0	0	0	0
93	3	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	4	17	0	0	0	0
93	5	427	0	0	0	0
93	6	126	0	0	0	0
93	7	15	0	0	0	0
93	8	14	0	0	0	0
93	C1	1	0	0	0	0
93	C8	1	0	0	0	0
93	C9	1	0	0	0	0
93	D9	2	0	0	0	0
93	L2	2	0	0	0	0
93	L3	3	0	0	0	0
93	L4	5	0	0	0	0
93	L7	2	0	0	0	0
93	M0	1	0	0	0	0
93	M3	1	0	0	0	0
93	M5	1	0	0	0	0
93	M7	5	0	0	0	0
93	N0	2	0	0	0	0
93	N3	3	0	0	0	0
93	N5	1	0	0	0	0
93	N6	2	0	0	0	0
93	N8	6	0	0	0	0
93	O4	1	0	0	0	0
93	O5	1	0	0	0	0
93	O7	4	0	0	0	0
93	P	1	0	0	0	0
93	Q2	1	0	0	0	0
93	S4	1	0	0	0	0
93	c6	1	0	0	0	0
93	c8	2	0	0	0	0
93	c9	1	0	0	0	0
93	d3	1	0	0	0	0
93	d4	1	0	0	0	0
93	d6	1	0	0	0	0
93	d7	1	0	0	0	0
93	l2	3	0	0	0	0
93	l3	4	0	0	0	0
93	l5	1	0	0	0	0
93	l6	1	0	0	0	0
93	l7	1	0	0	0	0
93	l9	1	0	0	0	0
93	m0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	m4	1	0	0	0	0
93	m5	2	0	0	0	0
93	m6	4	0	0	0	0
93	m7	3	0	0	0	0
93	n0	2	0	0	0	0
93	n3	1	0	0	0	0
93	n6	2	0	0	0	0
93	n8	3	0	0	0	0
93	n9	2	0	0	0	0
93	o2	2	0	0	0	0
93	o3	2	0	0	0	0
93	o4	1	0	0	0	0
93	o9	1	0	0	0	0
93	p	2	0	0	0	0
93	q1	1	0	0	0	0
93	s4	1	0	0	0	0
93	s6	1	0	0	0	0
93	sM	2	0	0	0	0
94	D6	1	0	0	0	0
94	D7	1	0	0	0	0
94	D9	1	0	0	2	0
94	E1	1	0	0	0	0
94	O7	1	0	0	0	0
94	Q0	1	0	0	0	0
94	Q2	1	0	0	3	0
94	Q3	1	0	0	0	0
94	d6	1	0	0	0	0
94	d7	1	0	0	0	0
94	d9	1	0	0	0	0
94	e1	1	0	0	0	0
94	o7	1	0	0	0	0
94	q0	1	0	0	0	0
94	q2	1	0	0	0	0
94	q3	1	0	0	0	0
95	1	11	0	8	0	0
95	5	11	0	8	5	0
96	1	8	0	11	3	0
96	5	8	0	11	3	0
97	1	23	0	18	13	0
97	5	23	0	18	7	0
98	P	22	0	12	28	0
98	p	22	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	411589	0	297245	16026	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 23.

The worst 5 of 16026 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)
17:C5:50:THR:CB	17:C5:50:THR:CA	1.74	1.62
96:1:3402:LEU:C	98:P:101:8AN:N3'	1.69	1.45
96:5:3402:LEU:C	98:P:101:8AN:N3'	212.18	1.41
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	2.09	1.40
78:Q2:17:CYS:CB	94:Q2:501:ZN:ZN	1.20	1.36

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%)	151 (74%)	38 (19%)	15 (7%)	1	14
2	s0	204/206 (99%)	151 (74%)	34 (17%)	19 (9%)	1	9
3	S1	212/216 (98%)	154 (73%)	34 (16%)	24 (11%)	0	6
3	s1	214/216 (99%)	166 (78%)	32 (15%)	16 (8%)	1	13
4	S2	215/217 (99%)	182 (85%)	24 (11%)	9 (4%)	3	28
4	s2	215/217 (99%)	172 (80%)	34 (16%)	9 (4%)	3	28
5	S3	221/223 (99%)	186 (84%)	24 (11%)	11 (5%)	2	24
5	s3	221/223 (99%)	176 (80%)	30 (14%)	15 (7%)	1	17
6	S4	258/260 (99%)	197 (76%)	45 (17%)	16 (6%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	s4	258/260 (99%)	197 (76%)	42 (16%)	19 (7%)	1	14
7	S5	204/206 (99%)	169 (83%)	20 (10%)	15 (7%)	1	14
7	s5	204/206 (99%)	159 (78%)	35 (17%)	10 (5%)	2	24
8	S6	224/226 (99%)	186 (83%)	23 (10%)	15 (7%)	1	17
8	s6	216/226 (96%)	182 (84%)	22 (10%)	12 (6%)	2	21
9	S7	182/186 (98%)	134 (74%)	36 (20%)	12 (7%)	1	17
9	s7	184/186 (99%)	143 (78%)	28 (15%)	13 (7%)	1	15
10	S8	184/188 (98%)	150 (82%)	25 (14%)	9 (5%)	2	24
10	s8	184/188 (98%)	156 (85%)	23 (12%)	5 (3%)	6	40
11	S9	183/185 (99%)	143 (78%)	33 (18%)	7 (4%)	4	31
11	s9	183/185 (99%)	149 (81%)	26 (14%)	8 (4%)	3	27
12	C0	82/96 (85%)	69 (84%)	10 (12%)	3 (4%)	4	32
13	C1	145/155 (94%)	113 (78%)	28 (19%)	4 (3%)	6	39
13	c1	144/155 (93%)	115 (80%)	25 (17%)	4 (3%)	6	39
14	C2	118/124 (95%)	76 (64%)	26 (22%)	16 (14%)	0	4
14	c2	118/124 (95%)	77 (65%)	30 (25%)	11 (9%)	1	9
15	C3	148/150 (99%)	125 (84%)	17 (12%)	6 (4%)	3	29
15	c3	148/150 (99%)	122 (82%)	18 (12%)	8 (5%)	2	22
16	C4	125/128 (98%)	90 (72%)	23 (18%)	12 (10%)	1	9
16	c4	126/128 (98%)	101 (80%)	15 (12%)	10 (8%)	1	12
17	C5	121/135 (90%)	90 (74%)	20 (16%)	11 (9%)	1	9
17	c5	125/135 (93%)	89 (71%)	23 (18%)	13 (10%)	0	7
18	C6	139/142 (98%)	115 (83%)	13 (9%)	11 (8%)	1	12
18	c6	140/142 (99%)	121 (86%)	15 (11%)	4 (3%)	5	38
19	C7	116/120 (97%)	90 (78%)	16 (14%)	10 (9%)	1	11
20	C8	143/145 (99%)	113 (79%)	22 (15%)	8 (6%)	2	21
20	c8	143/145 (99%)	113 (79%)	19 (13%)	11 (8%)	1	13
21	C9	141/143 (99%)	121 (86%)	10 (7%)	10 (7%)	1	15
21	c9	141/143 (99%)	124 (88%)	13 (9%)	4 (3%)	6	39
22	D0	105/110 (96%)	89 (85%)	13 (12%)	3 (3%)	5	38
22	d0	108/110 (98%)	86 (80%)	15 (14%)	7 (6%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	D1	85/87 (98%)	62 (73%)	11 (13%)	12 (14%)	0	4
23	d1	85/87 (98%)	64 (75%)	13 (15%)	8 (9%)	1	9
24	D2	127/129 (98%)	109 (86%)	14 (11%)	4 (3%)	5	37
24	d2	127/129 (98%)	105 (83%)	19 (15%)	3 (2%)	7	42
25	D3	142/144 (99%)	109 (77%)	26 (18%)	7 (5%)	2	24
25	d3	142/144 (99%)	116 (82%)	23 (16%)	3 (2%)	8	45
26	D4	132/134 (98%)	103 (78%)	20 (15%)	9 (7%)	1	17
26	d4	132/134 (98%)	109 (83%)	14 (11%)	9 (7%)	1	17
27	D5	68/70 (97%)	46 (68%)	13 (19%)	9 (13%)	0	4
27	d5	67/70 (96%)	53 (79%)	10 (15%)	4 (6%)	2	19
28	D6	95/97 (98%)	53 (56%)	26 (27%)	16 (17%)	0	2
28	d6	95/97 (98%)	75 (79%)	13 (14%)	7 (7%)	1	14
29	D7	79/81 (98%)	59 (75%)	20 (25%)	0	100	100
29	d7	79/81 (98%)	58 (73%)	18 (23%)	3 (4%)	4	31
30	D8	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	2	24
30	d8	61/63 (97%)	45 (74%)	14 (23%)	2 (3%)	4	35
31	D9	51/53 (96%)	40 (78%)	9 (18%)	2 (4%)	3	31
31	d9	51/53 (96%)	42 (82%)	2 (4%)	7 (14%)	0	4
32	E0	58/62 (94%)	46 (79%)	8 (14%)	4 (7%)	1	16
32	e0	60/62 (97%)	46 (77%)	11 (18%)	3 (5%)	2	24
33	E1	69/76 (91%)	38 (55%)	22 (32%)	9 (13%)	0	5
33	e1	74/76 (97%)	36 (49%)	19 (26%)	19 (26%)	0	0
34	SR	316/318 (99%)	262 (83%)	41 (13%)	13 (4%)	3	29
35	SM	120/159 (76%)	94 (78%)	15 (12%)	11 (9%)	1	9
39	L2	250/252 (99%)	218 (87%)	25 (10%)	7 (3%)	6	39
39	l2	250/252 (99%)	200 (80%)	32 (13%)	18 (7%)	1	15
40	L3	384/386 (100%)	323 (84%)	44 (12%)	17 (4%)	3	27
40	l3	384/386 (100%)	329 (86%)	36 (9%)	19 (5%)	2	24
41	L4	359/361 (99%)	288 (80%)	44 (12%)	27 (8%)	1	13
41	l4	359/361 (99%)	284 (79%)	48 (13%)	27 (8%)	1	13
42	L5	294/296 (99%)	232 (79%)	43 (15%)	19 (6%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	l5	292/296 (99%)	236 (81%)	41 (14%)	15 (5%)	2	23
43	L6	152/175 (87%)	130 (86%)	19 (12%)	3 (2%)	9	46
43	l6	153/175 (87%)	128 (84%)	22 (14%)	3 (2%)	9	46
44	L7	220/223 (99%)	184 (84%)	27 (12%)	9 (4%)	3	29
44	l7	221/223 (99%)	185 (84%)	30 (14%)	6 (3%)	6	40
45	L8	231/233 (99%)	180 (78%)	34 (15%)	17 (7%)	1	14
46	L9	189/191 (99%)	155 (82%)	22 (12%)	12 (6%)	1	18
46	l9	189/191 (99%)	161 (85%)	24 (13%)	4 (2%)	8	45
47	M0	207/220 (94%)	157 (76%)	39 (19%)	11 (5%)	2	22
47	m0	209/220 (95%)	162 (78%)	33 (16%)	14 (7%)	1	17
48	M1	167/169 (99%)	125 (75%)	22 (13%)	20 (12%)	0	6
48	m1	167/169 (99%)	132 (79%)	27 (16%)	8 (5%)	2	25
49	M3	191/194 (98%)	150 (78%)	31 (16%)	10 (5%)	2	23
49	m3	192/194 (99%)	150 (78%)	29 (15%)	13 (7%)	1	17
50	M4	134/137 (98%)	112 (84%)	15 (11%)	7 (5%)	2	23
50	m4	135/137 (98%)	107 (79%)	24 (18%)	4 (3%)	5	37
51	M5	201/203 (99%)	162 (81%)	33 (16%)	6 (3%)	5	37
51	m5	201/203 (99%)	164 (82%)	30 (15%)	7 (4%)	4	34
52	M6	195/197 (99%)	173 (89%)	19 (10%)	3 (2%)	12	52
52	m6	195/197 (99%)	176 (90%)	13 (7%)	6 (3%)	5	37
53	M7	181/183 (99%)	141 (78%)	29 (16%)	11 (6%)	2	19
53	m7	153/183 (84%)	128 (84%)	20 (13%)	5 (3%)	4	35
54	M8	183/185 (99%)	155 (85%)	22 (12%)	6 (3%)	4	35
54	m8	183/185 (99%)	152 (83%)	21 (12%)	10 (6%)	2	22
55	M9	186/188 (99%)	161 (87%)	19 (10%)	6 (3%)	5	36
55	m9	186/188 (99%)	163 (88%)	23 (12%)	0	100	100
56	N0	170/172 (99%)	139 (82%)	27 (16%)	4 (2%)	7	42
56	n0	170/172 (99%)	149 (88%)	20 (12%)	1 (1%)	28	70
57	N1	157/159 (99%)	129 (82%)	22 (14%)	6 (4%)	4	31
57	n1	157/159 (99%)	138 (88%)	15 (10%)	4 (2%)	6	41
58	N2	98/100 (98%)	72 (74%)	19 (19%)	7 (7%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	n2	96/100 (96%)	70 (73%)	23 (24%)	3 (3%)	5	37
59	N3	134/136 (98%)	108 (81%)	21 (16%)	5 (4%)	4	32
59	n3	134/136 (98%)	113 (84%)	19 (14%)	2 (2%)	12	52
60	N4	96/98 (98%)	75 (78%)	16 (17%)	5 (5%)	2	23
61	N5	119/121 (98%)	99 (83%)	17 (14%)	3 (2%)	6	41
61	n5	118/121 (98%)	90 (76%)	16 (14%)	12 (10%)	1	8
62	N6	124/126 (98%)	109 (88%)	12 (10%)	3 (2%)	7	42
62	n6	124/126 (98%)	104 (84%)	15 (12%)	5 (4%)	3	30
63	N7	133/135 (98%)	106 (80%)	17 (13%)	10 (8%)	1	13
63	n7	133/135 (98%)	93 (70%)	26 (20%)	14 (10%)	0	7
64	N8	146/148 (99%)	112 (77%)	28 (19%)	6 (4%)	3	29
64	n8	146/148 (99%)	118 (81%)	17 (12%)	11 (8%)	1	13
65	N9	56/58 (97%)	47 (84%)	8 (14%)	1 (2%)	10	48
65	n9	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	7
66	O0	95/100 (95%)	87 (92%)	7 (7%)	1 (1%)	17	59
66	o0	98/100 (98%)	83 (85%)	11 (11%)	4 (4%)	3	29
67	O1	107/109 (98%)	90 (84%)	10 (9%)	7 (6%)	1	18
67	o1	107/109 (98%)	84 (78%)	16 (15%)	7 (6%)	1	18
68	O2	125/127 (98%)	112 (90%)	11 (9%)	2 (2%)	11	50
68	o2	125/127 (98%)	100 (80%)	18 (14%)	7 (6%)	2	21
69	O3	104/106 (98%)	90 (86%)	8 (8%)	6 (6%)	2	20
69	o3	104/106 (98%)	92 (88%)	10 (10%)	2 (2%)	9	47
70	O4	110/112 (98%)	91 (83%)	17 (16%)	2 (2%)	10	48
70	o4	110/112 (98%)	92 (84%)	15 (14%)	3 (3%)	6	40
71	O5	117/119 (98%)	105 (90%)	9 (8%)	3 (3%)	6	40
71	o5	117/119 (98%)	93 (80%)	17 (14%)	7 (6%)	2	19
72	O6	97/99 (98%)	76 (78%)	11 (11%)	10 (10%)	0	8
72	o6	97/99 (98%)	84 (87%)	7 (7%)	6 (6%)	2	19
73	O7	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	4	34
73	o7	85/87 (98%)	66 (78%)	17 (20%)	2 (2%)	7	42
74	O8	75/77 (97%)	61 (81%)	11 (15%)	3 (4%)	3	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	o8	75/77 (97%)	59 (79%)	11 (15%)	5 (7%)	1	17
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	8	45
75	o9	48/50 (96%)	43 (90%)	2 (4%)	3 (6%)	1	18
76	Q0	50/52 (96%)	41 (82%)	4 (8%)	5 (10%)	1	8
76	q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	9	46
77	Q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
78	Q2	103/105 (98%)	76 (74%)	20 (19%)	7 (7%)	1	17
78	q2	103/105 (98%)	89 (86%)	9 (9%)	5 (5%)	2	24
79	Q3	89/91 (98%)	71 (80%)	16 (18%)	2 (2%)	8	44
79	q3	89/91 (98%)	70 (79%)	15 (17%)	4 (4%)	3	27
81	c0	78/96 (81%)	63 (81%)	8 (10%)	7 (9%)	1	10
82	c7	113/121 (93%)	87 (77%)	19 (17%)	7 (6%)	2	19
83	sR	316/318 (99%)	252 (80%)	51 (16%)	13 (4%)	3	29
84	sM	61/104 (59%)	45 (74%)	12 (20%)	4 (7%)	1	17
86	l8	224/231 (97%)	178 (80%)	28 (12%)	18 (8%)	1	12
88	n4	133/135 (98%)	109 (82%)	12 (9%)	12 (9%)	1	10
89	p0	117/143 (82%)	98 (84%)	15 (13%)	4 (3%)	4	35
All	All	22183/22802 (97%)	17856 (80%)	3104 (14%)	1223 (6%)	2	22

5 of 1223 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	158	VAL
2	S0	191	ARG
2	S0	195	TRP

### 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%)	144 (88%)	20 (12%)	6	27
2	s0	165/173 (95%)	135 (82%)	30 (18%)	2	11
3	S1	191/192 (100%)	157 (82%)	34 (18%)	2	12
3	s1	192/192 (100%)	151 (79%)	41 (21%)	1	6
4	S2	176/176 (100%)	150 (85%)	26 (15%)	3	20
4	s2	176/176 (100%)	135 (77%)	41 (23%)	1	4
5	S3	182/182 (100%)	158 (87%)	24 (13%)	5	24
5	s3	182/182 (100%)	154 (85%)	28 (15%)	3	18
6	S4	221/221 (100%)	184 (83%)	37 (17%)	2	14
6	s4	221/221 (100%)	187 (85%)	34 (15%)	3	18
7	S5	173/173 (100%)	153 (88%)	20 (12%)	6	30
7	s5	173/173 (100%)	149 (86%)	24 (14%)	4	23
8	S6	188/193 (97%)	157 (84%)	31 (16%)	2	15
8	s6	187/193 (97%)	154 (82%)	33 (18%)	2	12
9	S7	165/166 (99%)	147 (89%)	18 (11%)	7	33
9	s7	165/166 (99%)	143 (87%)	22 (13%)	4	24
10	S8	150/150 (100%)	128 (85%)	22 (15%)	3	20
10	s8	150/150 (100%)	131 (87%)	19 (13%)	5	25
11	S9	158/158 (100%)	137 (87%)	21 (13%)	4	24
11	s9	158/158 (100%)	134 (85%)	24 (15%)	3	19
12	C0	77/77 (100%)	66 (86%)	11 (14%)	4	22
13	C1	129/129 (100%)	112 (87%)	17 (13%)	5	24
13	c1	129/129 (100%)	110 (85%)	19 (15%)	3	20
14	C2	88/96 (92%)	75 (85%)	13 (15%)	3	20
14	c2	88/96 (92%)	72 (82%)	16 (18%)	2	11
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	7
15	c3	127/127 (100%)	107 (84%)	20 (16%)	3	18
16	C4	81/97 (84%)	67 (83%)	14 (17%)	2	13
16	c4	97/97 (100%)	83 (86%)	14 (14%)	4	21
17	C5	101/103 (98%)	90 (89%)	11 (11%)	7	33
17	c5	103/103 (100%)	87 (84%)	16 (16%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C6	117/118 (99%)	96 (82%)	21 (18%)	2	11
18	c6	118/118 (100%)	99 (84%)	19 (16%)	3	16
19	C7	94/109 (86%)	77 (82%)	17 (18%)	2	11
20	C8	128/128 (100%)	108 (84%)	20 (16%)	3	18
20	c8	128/128 (100%)	107 (84%)	21 (16%)	2	15
21	C9	115/115 (100%)	98 (85%)	17 (15%)	3	20
21	c9	115/115 (100%)	103 (90%)	12 (10%)	8	36
22	D0	100/103 (97%)	84 (84%)	16 (16%)	3	16
22	d0	103/103 (100%)	82 (80%)	21 (20%)	1	7
23	D1	74/74 (100%)	65 (88%)	9 (12%)	6	27
23	d1	74/74 (100%)	67 (90%)	7 (10%)	10	40
24	D2	110/110 (100%)	91 (83%)	19 (17%)	2	13
24	d2	110/110 (100%)	98 (89%)	12 (11%)	7	33
25	D3	119/119 (100%)	102 (86%)	17 (14%)	4	22
25	d3	119/119 (100%)	98 (82%)	21 (18%)	2	12
26	D4	112/112 (100%)	94 (84%)	18 (16%)	3	16
26	d4	112/112 (100%)	92 (82%)	20 (18%)	2	11
27	D5	61/61 (100%)	46 (75%)	15 (25%)	1	4
27	d5	61/61 (100%)	53 (87%)	8 (13%)	5	25
28	D6	83/83 (100%)	64 (77%)	19 (23%)	1	5
28	d6	83/83 (100%)	66 (80%)	17 (20%)	1	7
29	D7	70/70 (100%)	66 (94%)	4 (6%)	24	61
29	d7	70/70 (100%)	57 (81%)	13 (19%)	2	10
30	D8	56/56 (100%)	46 (82%)	10 (18%)	2	11
30	d8	56/56 (100%)	41 (73%)	15 (27%)	0	3
31	D9	47/47 (100%)	37 (79%)	10 (21%)	1	6
31	d9	47/47 (100%)	39 (83%)	8 (17%)	2	14
32	E0	51/53 (96%)	39 (76%)	12 (24%)	1	4
32	e0	53/53 (100%)	45 (85%)	8 (15%)	3	19
33	E1	62/66 (94%)	43 (69%)	19 (31%)	0	3
33	e1	66/66 (100%)	50 (76%)	16 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	SR	259/260 (100%)	233 (90%)	26 (10%)	9	37
35	SM	97/97 (100%)	78 (80%)	19 (20%)	1	8
39	L2	193/194 (100%)	162 (84%)	31 (16%)	3	16
39	l2	192/194 (99%)	159 (83%)	33 (17%)	2	13
40	L3	320/322 (99%)	252 (79%)	68 (21%)	1	6
40	l3	319/322 (99%)	268 (84%)	51 (16%)	3	16
41	L4	288/288 (100%)	239 (83%)	49 (17%)	2	14
41	l4	288/288 (100%)	231 (80%)	57 (20%)	1	8
42	L5	244/244 (100%)	205 (84%)	39 (16%)	3	16
42	l5	243/244 (100%)	201 (83%)	42 (17%)	2	13
43	L6	134/152 (88%)	114 (85%)	20 (15%)	3	20
43	l6	135/152 (89%)	119 (88%)	16 (12%)	6	28
44	L7	186/187 (100%)	156 (84%)	30 (16%)	3	16
44	l7	187/187 (100%)	155 (83%)	32 (17%)	2	14
45	L8	187/191 (98%)	166 (89%)	21 (11%)	7	32
46	L9	171/171 (100%)	134 (78%)	37 (22%)	1	6
46	l9	171/171 (100%)	134 (78%)	37 (22%)	1	6
47	M0	177/186 (95%)	147 (83%)	30 (17%)	2	14
47	m0	179/186 (96%)	139 (78%)	40 (22%)	1	5
48	M1	147/147 (100%)	120 (82%)	27 (18%)	2	10
48	m1	147/147 (100%)	126 (86%)	21 (14%)	4	22
49	M3	154/154 (100%)	125 (81%)	29 (19%)	2	9
49	m3	154/154 (100%)	127 (82%)	27 (18%)	2	13
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1	8
50	m4	108/108 (100%)	91 (84%)	17 (16%)	3	18
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	14
51	m5	175/175 (100%)	148 (85%)	27 (15%)	3	18
52	M6	160/160 (100%)	141 (88%)	19 (12%)	6	28
52	m6	160/160 (100%)	135 (84%)	25 (16%)	3	18
53	M7	140/145 (97%)	114 (81%)	26 (19%)	2	10
53	m7	125/145 (86%)	99 (79%)	26 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	M8	150/150 (100%)	126 (84%)	24 (16%)	3	16
54	m8	150/150 (100%)	122 (81%)	28 (19%)	2	9
55	M9	153/153 (100%)	133 (87%)	20 (13%)	5	25
55	m9	153/153 (100%)	121 (79%)	32 (21%)	1	7
56	N0	156/156 (100%)	129 (83%)	27 (17%)	2	13
56	n0	156/156 (100%)	130 (83%)	26 (17%)	2	14
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	6
57	n1	136/136 (100%)	112 (82%)	24 (18%)	2	12
58	N2	87/87 (100%)	73 (84%)	14 (16%)	3	16
58	n2	85/87 (98%)	70 (82%)	15 (18%)	2	12
59	N3	104/104 (100%)	89 (86%)	15 (14%)	4	21
59	n3	104/104 (100%)	93 (89%)	11 (11%)	8	35
60	N4	57/86 (66%)	53 (93%)	4 (7%)	18	55
61	N5	104/105 (99%)	89 (86%)	15 (14%)	4	21
61	n5	104/105 (99%)	80 (77%)	24 (23%)	1	5
62	N6	109/109 (100%)	85 (78%)	24 (22%)	1	6
62	n6	109/109 (100%)	88 (81%)	21 (19%)	1	9
63	N7	115/115 (100%)	97 (84%)	18 (16%)	3	18
63	n7	115/115 (100%)	96 (84%)	19 (16%)	2	15
64	N8	118/118 (100%)	99 (84%)	19 (16%)	3	16
64	n8	118/118 (100%)	101 (86%)	17 (14%)	4	21
65	N9	46/46 (100%)	39 (85%)	7 (15%)	3	19
65	n9	46/46 (100%)	39 (85%)	7 (15%)	3	19
66	O0	81/84 (96%)	64 (79%)	17 (21%)	1	7
66	o0	84/84 (100%)	71 (84%)	13 (16%)	3	18
67	O1	92/96 (96%)	79 (86%)	13 (14%)	4	22
67	o1	94/96 (98%)	74 (79%)	20 (21%)	1	6
68	O2	109/109 (100%)	88 (81%)	21 (19%)	1	9
68	o2	109/109 (100%)	83 (76%)	26 (24%)	1	4
69	O3	90/90 (100%)	72 (80%)	18 (20%)	1	8
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	O4	95/95 (100%)	82 (86%)	13 (14%)	4	23
70	o4	95/95 (100%)	83 (87%)	12 (13%)	5	26
71	O5	104/104 (100%)	93 (89%)	11 (11%)	8	35
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1	7
72	O6	81/81 (100%)	63 (78%)	18 (22%)	1	6
72	o6	80/81 (99%)	64 (80%)	16 (20%)	1	8
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	14
73	o7	70/70 (100%)	54 (77%)	16 (23%)	1	5
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	4
74	o8	67/68 (98%)	58 (87%)	9 (13%)	4	24
75	O9	45/45 (100%)	37 (82%)	8 (18%)	2	12
75	o9	45/45 (100%)	40 (89%)	5 (11%)	7	32
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3	20
76	q0	47/47 (100%)	40 (85%)	7 (15%)	3	20
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	13
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	1
78	Q2	90/90 (100%)	65 (72%)	25 (28%)	0	3
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1	7
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	14
79	q3	71/71 (100%)	58 (82%)	13 (18%)	2	10
81	c0	73/73 (100%)	66 (90%)	7 (10%)	10	39
82	c7	92/109 (84%)	72 (78%)	20 (22%)	1	6
83	sR	260/261 (100%)	238 (92%)	22 (8%)	12	45
84	sM	54/54 (100%)	44 (82%)	10 (18%)	2	10
86	l8	177/185 (96%)	147 (83%)	30 (17%)	2	14
88	n4	100/114 (88%)	87 (87%)	13 (13%)	5	25
89	p0	105/105 (100%)	89 (85%)	16 (15%)	3	19
All	All	18726/18993 (99%)	15610 (83%)	3116 (17%)	2	15

5 of 3116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
71	O5	13	SER

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Mol	Chain	Res	Type
8	s6	156	PHE
64	n8	26	ARG
74	O8	5	ILE
3	s1	185	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
68	O2	35	GLN
3	s1	118	GLN
71	o5	99	GLN
69	O3	106	ASN
78	Q2	47	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1812 (98%)	474 (26%)	0
36	1	3145/3149 (99%)	753 (23%)	0
37	3	120/121 (99%)	16 (13%)	0
37	7	120/121 (99%)	21 (17%)	0
38	4	157/158 (99%)	46 (29%)	0
38	8	157/158 (99%)	39 (24%)	0
80	6	1791/1800 (99%)	461 (25%)	0
85	5	3145/3150 (99%)	767 (24%)	0
91	P	1/5 (20%)	0	0
91	p	1/5 (20%)	0	0
All	All	10413/10479 (99%)	2577 (24%)	0

5 of 2577 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
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 2310 ligands modelled in this entry, 1207 are monoatomic - leaving 1103 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	$\# Z  > 2$
95	PHE	1	3401	-	11,11,12	2.33	3 (27%)	12,13,15	0.79	0
96	LEU	1	3402	-	7,7,8	1.36	1 (14%)	6,8,10	0.81	0
97	SPS	1	3403	93	20,23,23	3.45	9 (45%)	18,30,30	5.11	12 (66%)
92	OHX	1	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3420	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3422	-	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
92	OHX	1	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3428	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3449	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3450	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3465	-	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
92	OHX	1	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3494	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3495	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3499	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3508	-	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
92	OHX	1	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3510	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3513	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3530	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3531	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3551	-	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
92	OHX	1	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3565	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3567	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3573	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3574	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3577	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3583	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3589	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3594	-	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
92	OHX	1	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3617	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3622	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3628	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3630	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3637	-	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
92	OHX	1	3638	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3679	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3680	-	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
92	OHX	1	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3684	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3689	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3696	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3697	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3698	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3699	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3702	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3711	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3713	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3715	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3716	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3719	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3721	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3722	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3723	-	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
92	OHX	1	3724	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3725	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3726	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3727	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3728	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3729	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3730	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	1	3731	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1904	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1923	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1935	-	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
92	OHX	2	1936	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1950	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1952	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1963	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1966	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1969	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1972	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1978	-	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
92	OHX	2	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1986	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1987	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2009	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2011	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2012	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	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
92	OHX	2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2030	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2033	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2035	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2037	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2039	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2043	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2047	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2050	1	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	3	205	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	3	206	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	3	207	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	3	208	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	3	209	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	3	210	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	203	-	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
92	OHX	4	204	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	205	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	206	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	207	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	208	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	209	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	210	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	211	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	212	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	213	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	214	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	215	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	216	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	217	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	218	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	219	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	220	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	4	221	-	0,6,6	0.00	-	0,15,15	0.00	-
95	PHE	5	3401	-	11,11,12	2.33	3 (27%)	12,13,15	0.79	0
96	LEU	5	3402	-	7,7,8	1.37	1 (14%)	6,8,10	0.81	0
97	SPS	5	3403	93	20,23,23	3.53	10 (50%)	18,30,30	5.05	12 (66%)
92	OHX	5	3404	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3406	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3409	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3417	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3420	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3423	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3424	85	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
92	OHX	5	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3429	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3430	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3432	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3437	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3438	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3442	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3444	37	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3448	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3451	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3454	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3457	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3459	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3460	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3461	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3462	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3465	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3467	-	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
92	OHX	5	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3470	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3472	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3473	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3474	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3475	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3476	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3478	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3481	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3483	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3485	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3486	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3489	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3491	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3494	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3496	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3498	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3499	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3500	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3502	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3510	85	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
92	OHX	5	3511	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3512	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3514	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3515	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3517	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3522	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3525	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3526	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3528	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3530	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3532	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3533	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3534	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3535	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3536	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3540	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3541	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3543	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3544	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3545	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3549	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3551	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3552	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3553	85	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
92	OHX	5	3554	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3557	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3562	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3564	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3565	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3566	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3573	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3578	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3579	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3585	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3586	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3587	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3589	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3590	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3591	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3593	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3596	85	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
92	OHX	5	3597	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3598	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3599	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3600	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3601	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3605	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3607	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3616	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3623	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3626	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3627	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3630	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3632	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3636	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3638	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3639	85	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
92	OHX	5	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3641	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3643	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3644	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3654	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3658	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3659	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3661	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3666	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3667	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3669	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3670	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3671	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3672	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3674	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3675	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3678	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3679	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3682	85	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
92	OHX	5	3683	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3684	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3685	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3696	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3697	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3701	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3705	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3713	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3714	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3715	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3716	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3718	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3719	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3721	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3722	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3723	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3724	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3725	85	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
92	OHX	5	3726	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3727	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3728	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3729	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3730	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3731	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3732	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3733	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3734	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3735	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3736	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3737	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3738	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3739	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3740	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3741	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3742	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3743	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3744	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3745	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3746	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3747	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3748	85	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	5	3749	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1902	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1907	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1908	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1909	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1913	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1914	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1915	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1917	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1918	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1919	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
92	OHX	6	1920	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1921	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1922	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1923	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1924	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1926	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1927	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1928	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1929	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1930	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1931	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1932	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1935	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1939	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1940	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1941	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1942	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1944	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1945	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1948	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1951	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1952	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1953	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1955	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1957	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1958	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1960	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1962	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
92	OHX	6	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1964	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1966	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1967	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1968	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1970	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1971	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1972	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1973	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1974	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1976	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1977	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1981	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1982	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1987	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1989	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1991	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1993	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1996	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1998	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	1999	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2000	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2002	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2005	-	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
92	OHX	6	2006	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2007	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2010	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2013	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2014	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2016	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2017	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2018	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2019	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2023	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2025	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2026	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2028	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2029	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2030	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2031	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2033	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2036	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2037	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2039	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2040	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2042	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2048	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
92	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2050	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2051	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2052	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2053	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2055	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2056	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2057	80	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	202	37	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	203	37	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	204	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	205	37	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	206	37	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	207	37	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	209	37	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	210	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	7	211	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	202	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	204	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	205	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	206	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	207	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	208	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	209	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	210	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	211	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	212	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	213	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	214	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	215	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	8	216	38	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	C7	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	C8	201	36	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
92	OHX	L3	401	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	L3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	L4	401	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	L6	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	L6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	M0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	M5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	M5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	M6	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	M7	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	M9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	O4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	O7	102	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
98	8AN	P	101	91,93	17,24,25	1.15	1 (5%)	14,35,38	2.25	5 (35%)
92	OHX	Q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	S8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	S9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	c8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	d4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	l3	401	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	l5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	l5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	l9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	m0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	m5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	m5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	m6	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	m9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	o3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	o7	503	-	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
98	8AN	p	101	91,93	17,24,25	1.14	1 (5%)	14,35,38	2.27	5 (35%)
92	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	s1	301	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	s8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
92	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
92	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
95	PHE	1	3401	-	-	0/4/6/8	0/1/1/1
96	LEU	1	3402	-	-	0/4/6/8	0/0/0/0
97	SPS	1	3403	93	-	0/15/18/18	0/1/1/1
92	OHX	1	3404	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3405	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3406	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3407	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3408	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3409	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3410	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3411	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3412	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3413	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3414	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3415	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3416	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3417	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3418	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3419	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3420	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3421	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3422	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3423	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3424	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3425	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3426	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3427	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3428	36	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	1	3429	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3430	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3431	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3432	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3433	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3434	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3435	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3436	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3437	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3438	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3439	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3440	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3441	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3442	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3443	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3444	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3445	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3446	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3447	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3448	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3449	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3450	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3451	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3452	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3453	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3454	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3455	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3456	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3457	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3458	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3459	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3460	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3461	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3462	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3463	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3464	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3465	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3466	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3467	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3468	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3469	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3470	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	1	3471	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3472	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3473	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3474	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3475	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3476	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3477	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3478	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3479	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3480	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3481	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3482	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3483	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3484	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3485	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3486	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3487	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3488	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3489	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3490	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3491	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3492	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3493	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3494	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3495	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3496	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3497	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3498	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3499	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3500	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3501	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3502	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3503	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3504	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3505	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3506	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3507	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3508	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3509	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3510	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3511	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3512	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	1	3513	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3514	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3515	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3516	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3517	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3518	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3519	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3520	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3521	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3522	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3523	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3524	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3525	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3526	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3527	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3528	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3529	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3530	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3531	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3532	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3533	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3534	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3535	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3536	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3537	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3538	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3539	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3540	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3541	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3542	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3543	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3544	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3545	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3546	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3547	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3548	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3549	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3550	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3551	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3552	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3553	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3554	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	1	3555	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3556	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3557	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3558	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3559	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3560	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3561	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3562	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3563	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3564	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3565	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3566	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3567	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3568	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3569	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3570	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3571	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3572	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3573	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3574	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3575	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3576	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3577	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3578	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3579	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3580	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3581	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3582	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3583	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3584	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3585	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3586	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3587	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3588	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3589	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3590	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3591	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3592	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3593	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3594	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3595	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3596	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	1	3597	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3598	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3599	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3600	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3601	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3602	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3603	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3604	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3605	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3606	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3607	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3608	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3609	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3610	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3611	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3612	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3613	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3614	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3615	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3616	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3617	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3618	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3619	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3620	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3621	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3622	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3623	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3624	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3625	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3626	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3627	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3628	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3629	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3630	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3631	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3632	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3633	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3634	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3635	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3636	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3637	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3638	36	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	1	3639	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3640	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3641	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3642	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3643	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3644	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3645	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3646	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3647	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3648	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3649	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3650	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3651	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3652	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3653	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3654	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3655	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3656	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3657	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3658	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3659	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3660	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3661	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3662	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3663	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3664	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3665	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3666	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3667	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3668	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3669	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3670	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3671	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3672	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3673	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3674	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3675	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3676	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3677	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3678	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3679	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3680	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	1	3681	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3682	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3683	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3684	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3685	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3686	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3687	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3688	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3689	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3690	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3691	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3692	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3693	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3694	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3695	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3696	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3697	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3698	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3699	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3700	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3701	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3702	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3703	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3704	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3705	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3706	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3707	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3708	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3709	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3710	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3711	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3712	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3713	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3714	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3715	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3716	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3717	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3718	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3719	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3720	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3721	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3722	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	1	3723	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3724	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3725	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3726	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3727	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3728	36	-	0/0/0/0	0/0/0/0
92	OHX	1	3729	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3730	-	-	0/0/0/0	0/0/0/0
92	OHX	1	3731	36	-	0/0/0/0	0/0/0/0
92	OHX	2	1901	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1902	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1903	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1904	1	-	0/0/0/0	0/0/0/0
92	OHX	2	1905	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1906	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1907	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1908	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1909	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1910	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1911	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1912	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1913	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1914	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1915	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1916	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1917	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1918	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1919	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1920	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1921	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1922	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1923	1	-	0/0/0/0	0/0/0/0
92	OHX	2	1924	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1925	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1926	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1927	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1928	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1929	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1930	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1931	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1932	-	-	0/0/0/0	0/0/0/0
92	OHX	2	1933	-	-	0/0/0/0	0/0/0/0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	2	2018	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2019	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2020	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2021	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2022	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2030	1	-	0/0/0/0	0/0/0/0
92	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2033	1	-	0/0/0/0	0/0/0/0
92	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2035	1	-	0/0/0/0	0/0/0/0
92	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2037	1	-	0/0/0/0	0/0/0/0
92	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2039	1	-	0/0/0/0	0/0/0/0
92	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2043	1	-	0/0/0/0	0/0/0/0
92	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2047	1	-	0/0/0/0	0/0/0/0
92	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
92	OHX	2	2050	1	-	0/0/0/0	0/0/0/0
92	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
92	OHX	3	201	-	-	0/0/0/0	0/0/0/0
92	OHX	3	202	-	-	0/0/0/0	0/0/0/0
92	OHX	3	203	-	-	0/0/0/0	0/0/0/0
92	OHX	3	204	-	-	0/0/0/0	0/0/0/0
92	OHX	3	205	-	-	0/0/0/0	0/0/0/0
92	OHX	3	206	-	-	0/0/0/0	0/0/0/0
92	OHX	3	207	-	-	0/0/0/0	0/0/0/0
92	OHX	3	208	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	3	209	-	-	0/0/0/0	0/0/0/0
92	OHX	3	210	-	-	0/0/0/0	0/0/0/0
92	OHX	4	201	-	-	0/0/0/0	0/0/0/0
92	OHX	4	202	-	-	0/0/0/0	0/0/0/0
92	OHX	4	203	-	-	0/0/0/0	0/0/0/0
92	OHX	4	204	-	-	0/0/0/0	0/0/0/0
92	OHX	4	205	38	-	0/0/0/0	0/0/0/0
92	OHX	4	206	38	-	0/0/0/0	0/0/0/0
92	OHX	4	207	-	-	0/0/0/0	0/0/0/0
92	OHX	4	208	-	-	0/0/0/0	0/0/0/0
92	OHX	4	209	-	-	0/0/0/0	0/0/0/0
92	OHX	4	210	-	-	0/0/0/0	0/0/0/0
92	OHX	4	211	-	-	0/0/0/0	0/0/0/0
92	OHX	4	212	-	-	0/0/0/0	0/0/0/0
92	OHX	4	213	-	-	0/0/0/0	0/0/0/0
92	OHX	4	214	-	-	0/0/0/0	0/0/0/0
92	OHX	4	215	38	-	0/0/0/0	0/0/0/0
92	OHX	4	216	-	-	0/0/0/0	0/0/0/0
92	OHX	4	217	-	-	0/0/0/0	0/0/0/0
92	OHX	4	218	-	-	0/0/0/0	0/0/0/0
92	OHX	4	219	-	-	0/0/0/0	0/0/0/0
92	OHX	4	220	-	-	0/0/0/0	0/0/0/0
92	OHX	4	221	-	-	0/0/0/0	0/0/0/0
95	PHE	5	3401	-	-	0/4/6/8	0/1/1/1
96	LEU	5	3402	-	-	0/4/6/8	0/0/0/0
97	SPS	5	3403	93	-	0/15/18/18	0/1/1/1
92	OHX	5	3404	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3405	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3406	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3407	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3408	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3409	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3410	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3411	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3412	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3413	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3414	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3415	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3416	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3417	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3418	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3419	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	5	3420	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3421	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3422	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3423	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3424	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3425	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3426	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3427	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3428	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3429	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3430	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3431	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3432	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3433	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3434	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3435	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3436	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3437	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3438	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3439	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3440	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3441	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3442	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3443	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3444	37	-	0/0/0/0	0/0/0/0
92	OHX	5	3445	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3446	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3447	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3448	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3449	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3450	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3451	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3452	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3453	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3454	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3455	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3456	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3457	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3458	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3459	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3460	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3461	85	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	5	3462	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3463	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3464	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3465	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3466	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3467	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3468	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3469	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3470	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3471	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3472	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3473	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3474	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3475	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3476	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3477	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3478	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3479	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3480	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3481	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3482	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3483	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3484	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3485	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3486	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3487	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3488	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3489	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3490	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3491	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3492	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3493	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3494	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3495	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3496	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3497	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3498	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3499	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3500	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3501	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3502	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3503	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	5	3504	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3505	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3506	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3507	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3508	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3509	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3510	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3511	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3512	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3513	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3514	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3515	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3516	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3517	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3518	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3519	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3520	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3521	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3522	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3523	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3524	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3525	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3526	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3527	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3528	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3529	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3530	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3531	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3532	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3533	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3534	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3535	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3536	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3537	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3538	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3539	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3540	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3541	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3542	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3543	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3544	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3545	85	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	5	3546	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3547	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3548	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3549	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3550	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3551	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3552	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3553	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3554	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3555	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3556	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3557	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3558	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3559	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3560	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3561	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3562	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3563	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3564	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3565	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3566	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3567	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3568	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3569	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3570	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3571	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3572	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3573	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3574	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3575	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3576	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3577	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3578	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3579	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3580	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3581	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3582	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3583	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3584	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3585	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3586	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3587	85	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	5	3588	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3589	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3590	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3591	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3592	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3593	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3594	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3595	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3596	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3597	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3598	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3599	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3600	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3601	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3602	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3603	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3604	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3605	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3606	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3607	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3608	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3609	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3610	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3611	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3612	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3613	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3614	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3615	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3616	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3617	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3618	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3619	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3620	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3621	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3622	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3623	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3624	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3625	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3626	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3627	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3628	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3629	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	5	3630	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3631	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3632	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3633	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3634	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3635	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3636	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3637	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3638	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3639	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3640	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3641	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3642	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3643	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3644	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3645	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3646	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3647	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3648	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3649	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3650	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3651	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3652	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3653	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3654	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3655	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3656	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3657	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3658	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3659	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3660	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3661	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3662	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3663	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3664	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3665	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3666	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3667	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3668	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3669	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3670	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3671	85	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	5	3672	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3673	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3674	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3675	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3676	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3677	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3678	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3679	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3680	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3681	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3682	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3683	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3684	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3685	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3686	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3687	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3688	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3689	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3690	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3691	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3692	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3693	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3694	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3695	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3696	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3697	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3698	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3699	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3700	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3701	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3702	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3703	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3704	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3705	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3706	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3707	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3708	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3709	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3710	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3711	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3712	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3713	85	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	5	3714	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3715	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3716	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3717	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3718	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3719	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3720	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3721	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3722	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3723	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3724	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3725	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3726	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3727	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3728	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3729	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3730	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3731	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3732	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3733	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3734	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3735	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3736	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3737	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3738	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3739	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3740	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3741	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3742	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3743	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3744	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3745	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3746	-	-	0/0/0/0	0/0/0/0
92	OHX	5	3747	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3748	85	-	0/0/0/0	0/0/0/0
92	OHX	5	3749	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1901	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1902	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1903	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1904	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1905	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1906	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	6	1907	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1908	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1909	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1910	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1911	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1912	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1913	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1914	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1915	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1916	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1917	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1918	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1919	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1920	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1921	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1922	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1923	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1924	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1925	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1926	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1927	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1928	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1929	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1930	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1931	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1932	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1933	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1934	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1935	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1936	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1937	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1938	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1939	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1940	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1941	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1942	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1943	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1944	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1945	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1946	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1947	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1948	80	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	6	1949	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1950	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1951	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1952	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1953	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1954	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1955	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1956	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1957	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1958	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1959	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1960	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1961	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1962	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1963	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1964	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1965	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1966	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1967	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1968	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1969	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1970	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1971	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1972	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1973	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1974	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1975	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1976	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1977	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1978	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1979	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1980	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1981	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1982	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1983	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1984	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1985	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1986	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1987	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1988	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1989	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1990	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	6	1991	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1992	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1993	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1994	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1995	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1996	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1997	-	-	0/0/0/0	0/0/0/0
92	OHX	6	1998	80	-	0/0/0/0	0/0/0/0
92	OHX	6	1999	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2000	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2001	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2002	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2003	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2004	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2005	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2006	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2007	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2008	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2009	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2010	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2011	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2012	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2013	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2014	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2015	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2016	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2017	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2018	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2019	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2020	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2021	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2022	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2023	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2024	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2025	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2026	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2027	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2028	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2029	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2030	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2031	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2032	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	6	2033	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2034	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2035	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2036	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2037	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2038	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2039	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2040	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2041	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2042	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2043	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2048	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2050	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2051	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2052	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2053	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2055	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2056	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2057	80	-	0/0/0/0	0/0/0/0
92	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
92	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
92	OHX	7	201	-	-	0/0/0/0	0/0/0/0
92	OHX	7	202	37	-	0/0/0/0	0/0/0/0
92	OHX	7	203	37	-	0/0/0/0	0/0/0/0
92	OHX	7	204	-	-	0/0/0/0	0/0/0/0
92	OHX	7	205	37	-	0/0/0/0	0/0/0/0
92	OHX	7	206	37	-	0/0/0/0	0/0/0/0
92	OHX	7	207	37	-	0/0/0/0	0/0/0/0
92	OHX	7	208	-	-	0/0/0/0	0/0/0/0
92	OHX	7	209	37	-	0/0/0/0	0/0/0/0
92	OHX	7	210	-	-	0/0/0/0	0/0/0/0
92	OHX	7	211	-	-	0/0/0/0	0/0/0/0
92	OHX	8	201	-	-	0/0/0/0	0/0/0/0
92	OHX	8	202	38	-	0/0/0/0	0/0/0/0
92	OHX	8	203	-	-	0/0/0/0	0/0/0/0
92	OHX	8	204	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	8	205	-	-	0/0/0/0	0/0/0/0
92	OHX	8	206	38	-	0/0/0/0	0/0/0/0
92	OHX	8	207	38	-	0/0/0/0	0/0/0/0
92	OHX	8	208	-	-	0/0/0/0	0/0/0/0
92	OHX	8	209	38	-	0/0/0/0	0/0/0/0
92	OHX	8	210	38	-	0/0/0/0	0/0/0/0
92	OHX	8	211	-	-	0/0/0/0	0/0/0/0
92	OHX	8	212	38	-	0/0/0/0	0/0/0/0
92	OHX	8	213	-	-	0/0/0/0	0/0/0/0
92	OHX	8	214	38	-	0/0/0/0	0/0/0/0
92	OHX	8	215	38	-	0/0/0/0	0/0/0/0
92	OHX	8	216	38	-	0/0/0/0	0/0/0/0
92	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
92	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
92	OHX	C7	201	-	-	0/0/0/0	0/0/0/0
92	OHX	C8	201	36	-	0/0/0/0	0/0/0/0
92	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
92	OHX	L3	401	-	-	0/0/0/0	0/0/0/0
92	OHX	L3	402	-	-	0/0/0/0	0/0/0/0
92	OHX	L4	401	-	-	0/0/0/0	0/0/0/0
92	OHX	L6	201	-	-	0/0/0/0	0/0/0/0
92	OHX	L6	202	-	-	0/0/0/0	0/0/0/0
92	OHX	M0	301	-	-	0/0/0/0	0/0/0/0
92	OHX	M5	301	-	-	0/0/0/0	0/0/0/0
92	OHX	M5	302	-	-	0/0/0/0	0/0/0/0
92	OHX	M6	201	-	-	0/0/0/0	0/0/0/0
92	OHX	M7	201	-	-	0/0/0/0	0/0/0/0
92	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
92	OHX	M9	201	-	-	0/0/0/0	0/0/0/0
92	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
92	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
92	OHX	O4	201	-	-	0/0/0/0	0/0/0/0
92	OHX	O7	102	-	-	0/0/0/0	0/0/0/0
92	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
98	8AN	P	101	91,93	-	0/3/25/26	0/3/3/3
92	OHX	Q2	502	-	-	0/0/0/0	0/0/0/0
92	OHX	S8	301	-	-	0/0/0/0	0/0/0/0
92	OHX	S9	201	-	-	0/0/0/0	0/0/0/0
92	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
92	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
92	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
92	OHX	c8	201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
92	OHX	l3	401	-	-	0/0/0/0	0/0/0/0
92	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
92	OHX	l5	301	-	-	0/0/0/0	0/0/0/0
92	OHX	l5	302	-	-	0/0/0/0	0/0/0/0
92	OHX	l9	201	-	-	0/0/0/0	0/0/0/0
92	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
92	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
92	OHX	m0	303	-	-	0/0/0/0	0/0/0/0
92	OHX	m5	301	-	-	0/0/0/0	0/0/0/0
92	OHX	m5	302	-	-	0/0/0/0	0/0/0/0
92	OHX	m6	201	-	-	0/0/0/0	0/0/0/0
92	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
92	OHX	m9	201	-	-	0/0/0/0	0/0/0/0
92	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
92	OHX	o3	201	-	-	0/0/0/0	0/0/0/0
92	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
92	OHX	o7	503	-	-	0/0/0/0	0/0/0/0
98	8AN	p	101	91,93	-	0/3/25/26	0/3/3/3
92	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
92	OHX	s1	301	-	-	0/0/0/0	0/0/0/0
92	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
92	OHX	s8	301	-	-	0/0/0/0	0/0/0/0
92	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
92	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	5	3403	SPS	C9-C10	-8.22	1.32	1.48
97	1	3403	SPS	C9-C10	-6.63	1.35	1.48
97	1	3403	SPS	O13-C13	-5.02	1.21	1.42
97	5	3403	SPS	O13-C13	-4.91	1.21	1.42
97	5	3403	SPS	C6-C5	-4.66	1.33	1.41

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	5	3403	SPS	C7-C5-C6	-11.29	112.86	122.69
97	1	3403	SPS	C6-C1-N2	-9.45	117.79	124.45
97	1	3403	SPS	C7-C5-C6	-7.98	115.75	122.69
97	5	3403	SPS	C6-C1-N2	-6.65	119.76	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	5	3403	SPS	O15-S15-C14	-5.96	97.53	106.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

500 monomers are involved in 860 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
96	1	3402	LEU	3	0
97	1	3403	SPS	13	0
92	1	3407	OHX	1	0
92	1	3408	OHX	2	0
92	1	3414	OHX	1	0
92	1	3415	OHX	2	0
92	1	3417	OHX	1	0
92	1	3418	OHX	2	0
92	1	3419	OHX	2	0
92	1	3420	OHX	1	0
92	1	3422	OHX	1	0
92	1	3425	OHX	1	0
92	1	3429	OHX	1	0
92	1	3430	OHX	1	0
92	1	3431	OHX	1	0
92	1	3438	OHX	1	0
92	1	3441	OHX	1	0
92	1	3443	OHX	2	0
92	1	3446	OHX	2	0
92	1	3447	OHX	1	0
92	1	3449	OHX	2	0
92	1	3451	OHX	1	0
92	1	3455	OHX	1	0
92	1	3458	OHX	1	0
92	1	3460	OHX	1	0
92	1	3463	OHX	1	0
92	1	3464	OHX	1	0
92	1	3466	OHX	1	0
92	1	3467	OHX	1	0
92	1	3468	OHX	1	0
92	1	3470	OHX	1	0
92	1	3471	OHX	1	0
92	1	3474	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	1	3475	OHX	1	0
92	1	3476	OHX	1	0
92	1	3477	OHX	1	0
92	1	3479	OHX	1	0
92	1	3480	OHX	1	0
92	1	3484	OHX	2	0
92	1	3487	OHX	1	0
92	1	3489	OHX	1	0
92	1	3490	OHX	1	0
92	1	3493	OHX	1	0
92	1	3494	OHX	6	0
92	1	3496	OHX	1	0
92	1	3500	OHX	3	0
92	1	3501	OHX	2	0
92	1	3502	OHX	2	0
92	1	3507	OHX	8	0
92	1	3508	OHX	2	0
92	1	3511	OHX	6	0
92	1	3513	OHX	3	0
92	1	3515	OHX	2	0
92	1	3516	OHX	1	0
92	1	3517	OHX	1	0
92	1	3518	OHX	2	0
92	1	3521	OHX	1	0
92	1	3523	OHX	1	0
92	1	3525	OHX	4	0
92	1	3526	OHX	2	0
92	1	3528	OHX	1	0
92	1	3531	OHX	1	0
92	1	3532	OHX	2	0
92	1	3534	OHX	3	0
92	1	3536	OHX	1	0
92	1	3537	OHX	2	0
92	1	3540	OHX	1	0
92	1	3542	OHX	1	0
92	1	3543	OHX	1	0
92	1	3547	OHX	1	0
92	1	3552	OHX	1	0
92	1	3558	OHX	1	0
92	1	3560	OHX	2	0
92	1	3562	OHX	1	0
92	1	3563	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	1	3565	OHX	7	0
92	1	3566	OHX	2	0
92	1	3568	OHX	2	0
92	1	3571	OHX	2	0
92	1	3572	OHX	2	0
92	1	3574	OHX	1	0
92	1	3575	OHX	1	0
92	1	3576	OHX	4	0
92	1	3577	OHX	3	0
92	1	3578	OHX	5	0
92	1	3580	OHX	2	0
92	1	3583	OHX	4	0
92	1	3585	OHX	4	0
92	1	3586	OHX	2	0
92	1	3589	OHX	4	0
92	1	3590	OHX	4	0
92	1	3591	OHX	1	0
92	1	3597	OHX	1	0
92	1	3599	OHX	1	0
92	1	3600	OHX	6	0
92	1	3603	OHX	2	0
92	1	3604	OHX	1	0
92	1	3605	OHX	2	0
92	1	3606	OHX	1	0
92	1	3607	OHX	1	0
92	1	3609	OHX	1	0
92	1	3611	OHX	1	0
92	1	3612	OHX	5	0
92	1	3616	OHX	4	0
92	1	3620	OHX	1	0
92	1	3624	OHX	1	0
92	1	3626	OHX	2	0
92	1	3627	OHX	1	0
92	1	3631	OHX	1	0
92	1	3635	OHX	1	0
92	1	3638	OHX	2	0
92	1	3640	OHX	1	0
92	1	3641	OHX	1	0
92	1	3644	OHX	1	0
92	1	3648	OHX	7	0
92	1	3651	OHX	2	0
92	1	3652	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	1	3654	OHX	2	0
92	1	3655	OHX	1	0
92	1	3657	OHX	1	0
92	1	3660	OHX	1	0
92	1	3662	OHX	4	0
92	1	3665	OHX	2	0
92	1	3668	OHX	2	0
92	1	3670	OHX	3	0
92	1	3671	OHX	1	0
92	1	3674	OHX	2	0
92	1	3675	OHX	1	0
92	1	3677	OHX	1	0
92	1	3679	OHX	1	0
92	1	3683	OHX	1	0
92	1	3684	OHX	4	0
92	1	3687	OHX	1	0
92	1	3689	OHX	2	0
92	1	3690	OHX	6	0
92	1	3691	OHX	7	0
92	1	3694	OHX	6	0
92	1	3697	OHX	1	0
92	1	3698	OHX	1	0
92	1	3699	OHX	2	0
92	1	3702	OHX	5	0
92	1	3703	OHX	1	0
92	1	3705	OHX	2	0
92	1	3707	OHX	1	0
92	1	3709	OHX	1	0
92	1	3710	OHX	4	0
92	1	3711	OHX	5	0
92	1	3713	OHX	2	0
92	1	3714	OHX	1	0
92	1	3715	OHX	1	0
92	1	3720	OHX	1	0
92	1	3721	OHX	1	0
92	1	3728	OHX	2	0
92	1	3729	OHX	3	0
92	1	3731	OHX	1	0
92	2	1909	OHX	1	0
92	2	1911	OHX	1	0
92	2	1912	OHX	1	0
92	2	1913	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	2	1914	OHX	4	0
92	2	1916	OHX	1	0
92	2	1917	OHX	2	0
92	2	1919	OHX	1	0
92	2	1920	OHX	2	0
92	2	1921	OHX	6	0
92	2	1922	OHX	1	0
92	2	1924	OHX	1	0
92	2	1928	OHX	1	0
92	2	1929	OHX	1	0
92	2	1931	OHX	1	0
92	2	1938	OHX	3	0
92	2	1940	OHX	2	0
92	2	1942	OHX	1	0
92	2	1944	OHX	2	0
92	2	1949	OHX	2	0
92	2	1952	OHX	1	0
92	2	1955	OHX	2	0
92	2	1956	OHX	2	0
92	2	1960	OHX	2	0
92	2	1961	OHX	2	0
92	2	1962	OHX	1	0
92	2	1966	OHX	3	0
92	2	1967	OHX	3	0
92	2	1969	OHX	1	0
92	2	1970	OHX	5	0
92	2	1971	OHX	1	0
92	2	1972	OHX	3	0
92	2	1973	OHX	1	0
92	2	1974	OHX	1	0
92	2	1976	OHX	1	0
92	2	1977	OHX	1	0
92	2	1980	OHX	1	0
92	2	1982	OHX	2	0
92	2	1983	OHX	1	0
92	2	1985	OHX	5	0
92	2	1986	OHX	2	0
92	2	1988	OHX	2	0
92	2	1989	OHX	3	0
92	2	1993	OHX	1	0
92	2	1994	OHX	1	0
92	2	1997	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	2	1999	OHX	1	0
92	2	2005	OHX	2	0
92	2	2006	OHX	1	0
92	2	2009	OHX	2	0
92	2	2013	OHX	2	0
92	2	2020	OHX	1	0
92	2	2023	OHX	2	0
92	2	2026	OHX	1	0
92	2	2027	OHX	1	0
92	2	2028	OHX	1	0
92	2	2029	OHX	2	0
92	2	2035	OHX	2	0
92	2	2038	OHX	2	0
92	2	2040	OHX	7	0
92	2	2043	OHX	1	0
92	2	2046	OHX	1	0
92	2	2050	OHX	1	0
92	2	2051	OHX	1	0
92	3	203	OHX	1	0
92	3	204	OHX	8	0
92	3	206	OHX	1	0
92	3	207	OHX	1	0
92	4	201	OHX	1	0
92	4	202	OHX	1	0
92	4	203	OHX	1	0
92	4	204	OHX	1	0
92	4	206	OHX	1	0
92	4	207	OHX	1	0
92	4	208	OHX	2	0
92	4	209	OHX	1	0
92	4	210	OHX	2	0
92	4	211	OHX	1	0
92	4	213	OHX	1	0
92	4	215	OHX	1	0
92	4	216	OHX	1	0
92	4	217	OHX	2	0
92	4	218	OHX	2	0
92	4	220	OHX	1	0
95	5	3401	PHE	5	0
96	5	3402	LEU	3	0
97	5	3403	SPS	7	0
92	5	3404	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	5	3406	OHX	2	0
92	5	3407	OHX	1	0
92	5	3412	OHX	1	0
92	5	3413	OHX	1	0
92	5	3415	OHX	1	0
92	5	3422	OHX	1	0
92	5	3428	OHX	1	0
92	5	3430	OHX	1	0
92	5	3431	OHX	1	0
92	5	3433	OHX	2	0
92	5	3435	OHX	1	0
92	5	3437	OHX	1	0
92	5	3438	OHX	1	0
92	5	3440	OHX	1	0
92	5	3446	OHX	1	0
92	5	3447	OHX	1	0
92	5	3450	OHX	1	0
92	5	3453	OHX	1	0
92	5	3456	OHX	3	0
92	5	3457	OHX	2	0
92	5	3459	OHX	1	0
92	5	3460	OHX	2	0
92	5	3463	OHX	1	0
92	5	3464	OHX	1	0
92	5	3465	OHX	2	0
92	5	3467	OHX	1	0
92	5	3470	OHX	1	0
92	5	3472	OHX	2	0
92	5	3475	OHX	3	0
92	5	3477	OHX	1	0
92	5	3479	OHX	1	0
92	5	3480	OHX	1	0
92	5	3481	OHX	4	0
92	5	3485	OHX	1	0
92	5	3487	OHX	1	0
92	5	3488	OHX	1	0
92	5	3489	OHX	1	0
92	5	3493	OHX	1	0
92	5	3498	OHX	1	0
92	5	3500	OHX	1	0
92	5	3503	OHX	6	0
92	5	3505	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	5	3506	OHX	8	0
92	5	3509	OHX	1	0
92	5	3511	OHX	2	0
92	5	3512	OHX	2	0
92	5	3518	OHX	1	0
92	5	3519	OHX	1	0
92	5	3521	OHX	1	0
92	5	3522	OHX	6	0
92	5	3524	OHX	4	0
92	5	3525	OHX	1	0
92	5	3527	OHX	1	0
92	5	3528	OHX	1	0
92	5	3529	OHX	1	0
92	5	3530	OHX	2	0
92	5	3531	OHX	1	0
92	5	3532	OHX	1	0
92	5	3533	OHX	1	0
92	5	3534	OHX	6	0
92	5	3539	OHX	1	0
92	5	3541	OHX	1	0
92	5	3542	OHX	1	0
92	5	3544	OHX	1	0
92	5	3545	OHX	1	0
92	5	3550	OHX	1	0
92	5	3551	OHX	1	0
92	5	3555	OHX	11	0
92	5	3565	OHX	4	0
92	5	3566	OHX	5	0
92	5	3570	OHX	1	0
92	5	3571	OHX	1	0
92	5	3572	OHX	1	0
92	5	3574	OHX	4	0
92	5	3576	OHX	5	0
92	5	3578	OHX	1	0
92	5	3579	OHX	1	0
92	5	3580	OHX	7	0
92	5	3583	OHX	1	0
92	5	3588	OHX	2	0
92	5	3589	OHX	1	0
92	5	3590	OHX	1	0
92	5	3591	OHX	4	0
92	5	3592	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	5	3594	OHX	1	0
92	5	3600	OHX	2	0
92	5	3601	OHX	2	0
92	5	3602	OHX	1	0
92	5	3604	OHX	2	0
92	5	3605	OHX	2	0
92	5	3606	OHX	2	0
92	5	3608	OHX	1	0
92	5	3609	OHX	2	0
92	5	3612	OHX	1	0
92	5	3617	OHX	1	0
92	5	3622	OHX	1	0
92	5	3625	OHX	3	0
92	5	3627	OHX	3	0
92	5	3628	OHX	2	0
92	5	3633	OHX	1	0
92	5	3634	OHX	4	0
92	5	3635	OHX	1	0
92	5	3637	OHX	2	0
92	5	3638	OHX	1	0
92	5	3640	OHX	4	0
92	5	3641	OHX	1	0
92	5	3643	OHX	3	0
92	5	3645	OHX	1	0
92	5	3646	OHX	2	0
92	5	3649	OHX	2	0
92	5	3652	OHX	1	0
92	5	3653	OHX	1	0
92	5	3655	OHX	1	0
92	5	3656	OHX	1	0
92	5	3658	OHX	2	0
92	5	3659	OHX	1	0
92	5	3660	OHX	1	0
92	5	3662	OHX	2	0
92	5	3663	OHX	1	0
92	5	3670	OHX	1	0
92	5	3671	OHX	6	0
92	5	3675	OHX	2	0
92	5	3677	OHX	1	0
92	5	3681	OHX	1	0
92	5	3683	OHX	2	0
92	5	3686	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	5	3687	OHX	2	0
92	5	3688	OHX	2	0
92	5	3692	OHX	5	0
92	5	3694	OHX	5	0
92	5	3696	OHX	1	0
92	5	3698	OHX	1	0
92	5	3700	OHX	2	0
92	5	3702	OHX	8	0
92	5	3703	OHX	7	0
92	5	3705	OHX	3	0
92	5	3706	OHX	5	0
92	5	3712	OHX	1	0
92	5	3718	OHX	3	0
92	5	3721	OHX	8	0
92	5	3724	OHX	4	0
92	5	3725	OHX	1	0
92	5	3727	OHX	1	0
92	5	3729	OHX	2	0
92	5	3730	OHX	3	0
92	5	3731	OHX	1	0
92	5	3732	OHX	1	0
92	5	3733	OHX	1	0
92	5	3734	OHX	1	0
92	5	3738	OHX	1	0
92	5	3740	OHX	3	0
92	5	3742	OHX	1	0
92	5	3744	OHX	1	0
92	5	3745	OHX	1	0
92	5	3746	OHX	1	0
92	5	3747	OHX	2	0
92	6	1906	OHX	1	0
92	6	1908	OHX	1	0
92	6	1910	OHX	1	0
92	6	1911	OHX	2	0
92	6	1913	OHX	1	0
92	6	1914	OHX	4	0
92	6	1915	OHX	1	0
92	6	1916	OHX	1	0
92	6	1917	OHX	1	0
92	6	1920	OHX	3	0
92	6	1921	OHX	3	0
92	6	1923	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	6	1925	OHX	1	0
92	6	1927	OHX	3	0
92	6	1929	OHX	2	0
92	6	1934	OHX	1	0
92	6	1938	OHX	4	0
92	6	1939	OHX	1	0
92	6	1943	OHX	1	0
92	6	1944	OHX	1	0
92	6	1948	OHX	2	0
92	6	1949	OHX	1	0
92	6	1950	OHX	1	0
92	6	1951	OHX	3	0
92	6	1952	OHX	2	0
92	6	1953	OHX	1	0
92	6	1955	OHX	3	0
92	6	1956	OHX	2	0
92	6	1957	OHX	1	0
92	6	1960	OHX	1	0
92	6	1962	OHX	3	0
92	6	1965	OHX	1	0
92	6	1968	OHX	1	0
92	6	1970	OHX	2	0
92	6	1973	OHX	1	0
92	6	1976	OHX	2	0
92	6	1978	OHX	4	0
92	6	1982	OHX	1	0
92	6	1988	OHX	1	0
92	6	1990	OHX	1	0
92	6	1994	OHX	2	0
92	6	1995	OHX	1	0
92	6	1996	OHX	2	0
92	6	1998	OHX	4	0
92	6	1999	OHX	1	0
92	6	2000	OHX	1	0
92	6	2001	OHX	4	0
92	6	2005	OHX	3	0
92	6	2007	OHX	1	0
92	6	2012	OHX	2	0
92	6	2016	OHX	3	0
92	6	2017	OHX	1	0
92	6	2018	OHX	3	0
92	6	2022	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	6	2023	OHX	1	0
92	6	2030	OHX	2	0
92	6	2031	OHX	2	0
92	6	2032	OHX	1	0
92	6	2033	OHX	2	0
92	6	2034	OHX	2	0
92	6	2038	OHX	2	0
92	6	2039	OHX	3	0
92	6	2046	OHX	1	0
92	6	2048	OHX	4	0
92	6	2049	OHX	3	0
92	6	2052	OHX	1	0
92	6	2053	OHX	1	0
92	6	2058	OHX	4	0
92	7	202	OHX	1	0
92	7	205	OHX	2	0
92	7	208	OHX	1	0
92	7	209	OHX	6	0
92	8	201	OHX	2	0
92	8	202	OHX	1	0
92	8	203	OHX	1	0
92	8	205	OHX	1	0
92	8	206	OHX	1	0
92	8	208	OHX	2	0
92	8	210	OHX	3	0
92	8	216	OHX	1	0
92	C3	201	OHX	6	0
92	C5	201	OHX	4	0
92	C7	201	OHX	2	0
92	D9	102	OHX	1	0
92	L3	402	OHX	3	0
92	L4	401	OHX	3	0
92	L6	202	OHX	2	0
92	M0	301	OHX	2	0
92	M5	301	OHX	1	0
92	M5	302	OHX	1	0
92	M6	201	OHX	1	0
92	M7	201	OHX	1	0
92	M8	201	OHX	1	0
92	M9	201	OHX	2	0
92	O3	201	OHX	3	0
92	O7	102	OHX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	O9	101	OHX	2	0
98	P	101	8AN	28	0
92	Q2	502	OHX	4	0
92	S8	301	OHX	3	0
92	S9	201	OHX	4	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
36	1	3
85	5	3
87	m2	2
84	sM	2
41	l4	2
1	2	2
35	SM	1
10	S8	1
68	O2	1
89	p0	1
19	C7	1
81	c0	1
40	l3	1
13	C1	1
6	S4	1
57	n1	1
82	c7	1
10	s8	1

The worst 5 of 26 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1781:U	O3'	1782:C	P	145.43
1	sM	85:SER	C	119:UNK	N	43.83
1	sM	139:UNK	C	155:UNK	N	38.91
1	1	1955:U	O3'	2093:A	P	25.58

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SM	141:ALA	C	151:UNK	N	25.40

## 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	1781/1812 (98%)	0.53	125 (7%) 17 15	60, 89, 120, 149	0
2	S0	206/206 (100%)	1.31	51 (24%) 1 1	93, 99, 105, 107	0
2	s0	206/206 (100%)	0.53	17 (8%) 12 12	77, 83, 89, 90	0
3	S1	214/216 (99%)	0.52	10 (4%) 32 26	95, 106, 113, 113	0
3	s1	216/216 (100%)	0.56	11 (5%) 29 23	70, 75, 81, 84	0
4	S2	217/217 (100%)	1.26	54 (24%) 1 1	81, 88, 96, 99	0
4	s2	217/217 (100%)	0.85	30 (13%) 3 4	67, 73, 79, 81	0
5	S3	223/223 (100%)	1.26	49 (21%) 1 1	85, 96, 110, 115	0
5	s3	223/223 (100%)	1.36	61 (27%) 1 1	91, 102, 113, 114	0
6	S4	260/260 (100%)	0.85	24 (9%) 10 10	75, 88, 91, 93	0
6	s4	260/260 (100%)	0.42	7 (2%) 55 46	59, 73, 78, 80	0
7	S5	206/206 (100%)	1.35	54 (26%) 1 1	97, 105, 111, 113	0
7	s5	206/206 (100%)	0.87	43 (20%) 1 1	90, 95, 101, 103	0
8	S6	226/226 (100%)	0.82	32 (14%) 3 4	62, 76, 96, 101	0
8	s6	218/226 (96%)	0.90	37 (16%) 2 2	55, 63, 82, 86	0
9	S7	184/186 (98%)	0.49	13 (7%) 17 15	92, 102, 108, 109	0
9	s7	186/186 (100%)	0.02	3 (1%) 72 64	75, 90, 101, 104	0
10	S8	188/188 (100%)	1.02	26 (13%) 3 4	72, 78, 92, 95	0
10	s8	188/188 (100%)	0.66	18 (9%) 9 9	57, 68, 89, 95	0
11	S9	185/185 (100%)	1.02	32 (17%) 2 2	81, 89, 99, 103	0
11	s9	185/185 (100%)	0.10	3 (1%) 72 64	63, 74, 82, 84	0
12	C0	83/96 (86%)	0.60	7 (8%) 12 12	94, 100, 105, 107	0
13	C1	146/155 (94%)	1.14	27 (18%) 1 2	75, 79, 85, 89	0
13	c1	146/155 (94%)	0.38	6 (4%) 38 31	62, 67, 81, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	C2	119/124 (95%)	1.43	35 (29%) 1 1	111, 116, 118, 119	0
14	c2	119/124 (95%)	1.47	32 (26%) 1 1	133, 142, 148, 149	0
15	C3	150/150 (100%)	0.38	9 (6%) 23 19	80, 88, 92, 94	0
15	c3	150/150 (100%)	-0.01	2 (1%) 77 69	65, 75, 80, 82	0
16	C4	127/128 (99%)	0.34	10 (7%) 13 13	82, 105, 111, 112	0
16	c4	128/128 (100%)	0.78	13 (10%) 7 8	63, 74, 79, 80	0
17	C5	122/135 (90%)	0.43	4 (3%) 47 39	80, 90, 96, 101	0
17	c5	125/135 (92%)	0.30	7 (5%) 25 21	65, 91, 98, 100	0
18	C6	141/142 (99%)	2.04	69 (48%) 0 0	88, 105, 109, 110	0
18	c6	142/142 (100%)	1.40	38 (26%) 1 1	90, 98, 102, 104	0
19	C7	120/120 (100%)	1.42	38 (31%) 0 0	98, 104, 108, 109	0
20	C8	145/145 (100%)	0.55	7 (4%) 31 25	83, 95, 107, 110	0
20	c8	145/145 (100%)	0.36	8 (5%) 26 21	69, 86, 93, 97	0
21	C9	143/143 (100%)	1.25	31 (21%) 1 1	92, 101, 106, 108	0
21	c9	143/143 (100%)	0.42	9 (6%) 21 17	87, 92, 96, 98	0
22	D0	107/110 (97%)	0.94	19 (17%) 2 2	87, 100, 105, 106	0
22	d0	110/110 (100%)	1.86	43 (39%) 0 0	92, 104, 110, 111	0
23	D1	87/87 (100%)	0.79	16 (18%) 1 2	90, 94, 102, 106	0
23	d1	87/87 (100%)	0.53	5 (5%) 24 20	74, 78, 86, 89	0
24	D2	129/129 (100%)	1.23	27 (20%) 1 1	82, 88, 92, 98	0
24	d2	129/129 (100%)	0.22	0 100 100	67, 73, 75, 76	0
25	D3	144/144 (100%)	0.29	5 (3%) 44 38	71, 76, 79, 80	0
25	d3	144/144 (100%)	0.07	2 (1%) 75 67	57, 59, 64, 66	0
26	D4	134/134 (100%)	0.27	3 (2%) 62 53	76, 88, 92, 94	0
26	d4	134/134 (100%)	0.04	4 (2%) 51 42	60, 71, 74, 76	0
27	D5	70/70 (100%)	0.68	10 (14%) 3 4	104, 108, 111, 112	0
27	d5	69/70 (98%)	0.45	5 (7%) 16 14	93, 97, 100, 101	0
28	D6	97/97 (100%)	1.75	38 (39%) 0 0	84, 91, 112, 113	0
28	d6	97/97 (100%)	1.67	34 (35%) 0 0	65, 72, 81, 83	0
29	D7	81/81 (100%)	1.13	14 (17%) 2 2	90, 94, 99, 100	0
29	d7	81/81 (100%)	0.67	4 (4%) 30 24	74, 80, 88, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	D8	63/63 (100%)	2.13	34 (53%) 0 0	98, 107, 112, 113	0
30	d8	63/63 (100%)	2.20	33 (52%) 0 0	90, 95, 99, 100	0
31	D9	53/53 (100%)	0.32	2 (3%) 41 35	89, 91, 96, 97	0
31	d9	53/53 (100%)	1.23	14 (26%) 1 1	93, 97, 113, 120	0
32	E0	60/62 (96%)	0.85	8 (13%) 4 5	72, 87, 97, 101	0
32	e0	62/62 (100%)	0.24	5 (8%) 13 12	58, 72, 77, 80	0
33	E1	71/76 (93%)	0.61	8 (11%) 6 7	92, 108, 113, 113	0
33	e1	76/76 (100%)	1.04	16 (21%) 1 1	99, 127, 139, 140	0
34	SR	318/318 (100%)	1.24	77 (24%) 1 1	104, 111, 118, 122	0
35	SM	121/159 (76%)	1.02	18 (14%) 3 3	55, 83, 96, 98	0
36	1	3149/3149 (100%)	0.08	53 (1%) 70 62	31, 49, 82, 154	0
37	3	121/121 (100%)	-0.23	0 100 100	41, 59, 64, 65	0
37	7	121/121 (100%)	-0.30	1 (0%) 86 79	36, 47, 51, 54	0
38	4	158/158 (100%)	-0.09	1 (0%) 89 84	33, 45, 63, 84	0
38	8	158/158 (100%)	-0.05	1 (0%) 89 84	37, 49, 68, 76	0
39	L2	252/252 (100%)	0.24	3 (1%) 79 71	40, 52, 61, 73	0
39	l2	252/252 (100%)	0.08	4 (1%) 72 64	39, 53, 62, 66	0
40	L3	386/386 (100%)	-0.25	2 (0%) 90 86	38, 50, 58, 62	0
40	l3	386/386 (100%)	-0.37	1 (0%) 93 90	32, 39, 47, 58	0
41	L4	361/361 (100%)	-0.35	0 100 100	31, 37, 47, 51	0
41	l4	361/361 (100%)	-0.30	0 100 100	33, 41, 48, 58	0
42	L5	296/296 (100%)	0.56	26 (8%) 11 11	50, 60, 67, 69	0
42	l5	294/296 (99%)	-0.03	3 (1%) 82 75	43, 49, 57, 66	0
43	L6	156/175 (89%)	-0.38	0 100 100	38, 46, 49, 55	0
43	l6	157/175 (89%)	-0.34	0 100 100	40, 46, 49, 52	0
44	L7	222/223 (99%)	-0.16	0 100 100	36, 40, 48, 50	0
44	l7	223/223 (100%)	-0.34	0 100 100	34, 38, 48, 54	0
45	L8	233/233 (100%)	0.19	5 (2%) 64 55	54, 60, 74, 77	0
46	L9	191/191 (100%)	0.19	5 (2%) 56 47	48, 51, 53, 59	0
46	l9	191/191 (100%)	0.12	2 (1%) 82 75	39, 44, 52, 63	0
47	M0	211/220 (95%)	-0.16	0 100 100	39, 48, 61, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
47	m0	213/220 (96%)	0.08	6 (2%) 53 45	36, 42, 57, 67	0
48	M1	169/169 (100%)	0.71	15 (8%) 10 10	57, 67, 73, 76	0
48	m1	169/169 (100%)	-0.29	0 100 100	44, 54, 59, 63	0
49	M3	193/194 (99%)	-0.06	1 (0%) 90 86	33, 46, 59, 74	0
49	m3	194/194 (100%)	-0.11	2 (1%) 82 75	35, 50, 61, 70	0
50	M4	136/137 (99%)	-0.27	2 (1%) 74 66	45, 49, 54, 56	0
50	m4	137/137 (100%)	-0.40	0 100 100	39, 43, 53, 60	0
51	M5	203/203 (100%)	0.03	0 100 100	35, 46, 54, 56	0
51	m5	203/203 (100%)	-0.03	1 (0%) 90 86	38, 50, 57, 59	0
52	M6	197/197 (100%)	-0.17	1 (0%) 90 86	39, 42, 50, 52	0
52	m6	197/197 (100%)	-0.37	0 100 100	32, 36, 49, 50	0
53	M7	183/183 (100%)	0.00	9 (4%) 30 24	38, 43, 58, 62	0
53	m7	155/183 (84%)	-0.38	0 100 100	34, 37, 40, 43	0
54	M8	185/185 (100%)	-0.00	0 100 100	36, 44, 54, 61	0
54	m8	185/185 (100%)	-0.05	0 100 100	35, 44, 48, 50	0
55	M9	188/188 (100%)	0.14	7 (3%) 42 35	49, 61, 103, 111	0
55	m9	188/188 (100%)	-0.09	0 100 100	43, 55, 98, 106	0
56	N0	172/172 (100%)	0.58	16 (9%) 9 10	42, 46, 51, 53	0
56	n0	172/172 (100%)	-0.17	1 (0%) 89 84	36, 39, 44, 48	0
57	N1	159/159 (100%)	0.30	4 (2%) 58 48	40, 47, 56, 57	0
57	n1	159/159 (100%)	0.28	1 (0%) 89 84	36, 42, 53, 55	0
58	N2	100/100 (100%)	0.36	6 (6%) 23 19	65, 69, 72, 73	0
58	n2	98/100 (98%)	0.14	3 (3%) 49 41	56, 59, 60, 61	0
59	N3	136/136 (100%)	-0.01	2 (1%) 74 66	43, 49, 52, 54	0
59	n3	136/136 (100%)	-0.05	0 100 100	33, 37, 41, 43	0
60	N4	98/98 (100%)	1.74	31 (31%) 0 0	49, 59, 89, 91	0
61	N5	121/121 (100%)	0.11	1 (0%) 86 79	43, 45, 62, 72	0
61	n5	120/121 (99%)	0.02	1 (0%) 86 79	44, 48, 65, 67	0
62	N6	126/126 (100%)	-0.10	1 (0%) 86 79	35, 41, 44, 45	0
62	n6	126/126 (100%)	-0.25	0 100 100	38, 45, 49, 50	0
63	N7	135/135 (100%)	0.48	7 (5%) 28 23	62, 67, 76, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
63	n7	135/135 (100%)	0.40	6 (4%) 35 28	65, 71, 78, 83	0
64	N8	148/148 (100%)	-0.08	0 100 100	31, 43, 50, 57	0
64	n8	148/148 (100%)	-0.05	1 (0%) 87 82	31, 45, 48, 50	0
65	N9	58/58 (100%)	0.14	0 100 100	36, 49, 66, 71	0
65	n9	58/58 (100%)	0.17	2 (3%) 46 38	34, 45, 52, 53	0
66	O0	97/100 (97%)	0.05	3 (3%) 49 41	60, 64, 70, 71	0
66	o0	100/100 (100%)	0.36	3 (3%) 51 42	61, 66, 73, 75	0
67	O1	109/109 (100%)	0.17	0 100 100	51, 55, 59, 67	0
67	o1	109/109 (100%)	0.08	2 (1%) 69 60	41, 43, 47, 49	0
68	O2	127/127 (100%)	-0.28	0 100 100	32, 39, 41, 43	0
68	o2	127/127 (100%)	-0.26	0 100 100	31, 40, 43, 45	0
69	O3	106/106 (100%)	-0.26	0 100 100	37, 42, 50, 52	0
69	o3	106/106 (100%)	-0.15	0 100 100	34, 40, 50, 51	0
70	O4	112/112 (100%)	0.45	3 (2%) 55 46	47, 60, 70, 73	0
70	o4	112/112 (100%)	0.45	2 (1%) 69 60	46, 62, 70, 72	0
71	O5	119/119 (100%)	-0.07	0 100 100	42, 44, 56, 58	0
71	o5	119/119 (100%)	-0.25	0 100 100	46, 48, 60, 64	0
72	O6	99/99 (100%)	-0.18	2 (2%) 65 57	44, 54, 62, 66	0
72	o6	99/99 (100%)	-0.32	0 100 100	48, 57, 62, 66	0
73	O7	87/87 (100%)	0.02	1 (1%) 80 72	35, 41, 46, 49	0
73	o7	87/87 (100%)	0.14	2 (2%) 61 51	37, 42, 51, 58	0
74	O8	77/77 (100%)	-0.40	0 100 100	57, 60, 66, 66	0
74	o8	77/77 (100%)	0.49	3 (3%) 40 33	59, 63, 66, 68	0
75	O9	50/50 (100%)	-0.03	0 100 100	40, 42, 44, 45	0
75	o9	50/50 (100%)	0.12	0 100 100	40, 44, 46, 49	0
76	Q0	52/52 (100%)	-0.16	1 (1%) 67 59	46, 49, 50, 52	0
76	q0	52/52 (100%)	-0.35	0 100 100	38, 39, 43, 45	0
77	Q1	25/25 (100%)	-0.14	0 100 100	60, 70, 78, 78	0
77	q1	25/25 (100%)	-0.39	0 100 100	49, 56, 59, 60	0
78	Q2	105/105 (100%)	0.55	9 (8%) 11 11	38, 49, 58, 66	0
78	q2	105/105 (100%)	0.55	7 (6%) 19 16	37, 44, 49, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
79	Q3	91/91 (100%)	0.22	2 (2%) 62 53	49, 53, 57, 58	0
79	q3	91/91 (100%)	0.04	2 (2%) 62 53	45, 53, 60, 64	0
80	6	1795/1800 (99%)	0.39	114 (6%) 20 17	46, 75, 111, 134	0
81	c0	79/96 (82%)	1.21	16 (20%) 1 1	105, 116, 121, 122	0
82	c7	117/121 (96%)	0.73	15 (12%) 4 5	86, 94, 99, 100	0
83	sR	318/318 (100%)	1.40	92 (28%) 1 1	90, 107, 111, 114	0
84	sM	63/104 (60%)	0.46	6 (9%) 9 9	45, 78, 89, 91	0
85	5	3150/3150 (100%)	0.08	44 (1%) 75 67	31, 45, 82, 107	0
86	l8	225/231 (97%)	0.18	9 (4%) 39 32	58, 64, 78, 81	0
87	m2	0/150	-	-	-	-
88	n4	135/135 (100%)	0.85	29 (21%) 1 1	37, 62, 81, 82	0
89	p0	120/143 (83%)	1.18	24 (20%) 1 1	78, 91, 98, 104	0
90	p1	0/47	-	-	-	-
90	p2	0/47	-	-	-	-
91	P	2/5 (40%)	-0.07	0 100 100	38, 38, 38, 40	0
91	p	2/5 (40%)	0.79	0 100 100	34, 34, 34, 38	0
All	All	32929/33525 (98%)	0.32	2121 (6%) 20 17	31, 60, 107, 154	0

The worst 5 of 2121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	88	ASP	11.4
1	2	1807	C	11.2
1	2	1805	C	10.2
1	2	1789	A	9.6
60	N4	75	THR	9.5

## 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
93	MG	1	3897	1/1	0.94	0.67	65.16	44,44,44,44	0
93	MG	5	4100	1/1	0.94	1.47	60.36	32,32,32,32	0
93	MG	1	3921	1/1	0.95	0.91	58.20	34,34,34,34	0
93	MG	5	3847	1/1	0.97	0.64	44.76	32,32,32,32	0
93	MG	1	3876	1/1	0.96	0.63	41.06	45,45,45,45	0
93	MG	1	4056	1/1	0.88	0.97	39.52	32,32,32,32	0
93	MG	5	3928	1/1	0.97	0.73	39.39	32,32,32,32	0
93	MG	1	4102	1/1	0.93	0.94	38.75	43,43,43,43	0
93	MG	6	2083	1/1	0.92	0.76	37.29	56,56,56,56	0
93	MG	5	3911	1/1	0.92	0.58	36.82	31,31,31,31	0
93	MG	6	2074	1/1	0.84	0.62	36.13	88,88,88,88	0
93	MG	1	3898	1/1	0.98	0.67	34.58	30,30,30,30	0
93	MG	5	3903	1/1	0.96	0.75	32.05	39,39,39,39	0
93	MG	5	3974	1/1	0.90	0.43	31.32	37,37,37,37	0
93	MG	1	3852	1/1	0.95	0.63	31.14	36,36,36,36	0
93	MG	5	3918	1/1	0.93	0.72	29.72	44,44,44,44	0
93	MG	5	3874	1/1	0.98	0.56	29.42	31,31,31,31	0
93	MG	1	4027	1/1	0.82	0.69	29.20	39,39,39,39	0
93	MG	1	3859	1/1	0.95	0.62	28.59	32,32,32,32	0
93	MG	5	4082	1/1	0.95	0.88	27.21	40,40,40,40	0
93	MG	5	4023	1/1	0.73	0.78	26.90	33,33,33,33	0
93	MG	6	2109	1/1	0.89	0.82	25.82	90,90,90,90	0
93	MG	1	3784	1/1	0.85	0.76	25.59	39,39,39,39	0
93	MG	5	3906	1/1	0.96	0.65	25.48	32,32,32,32	0
93	MG	1	3983	1/1	0.85	0.57	25.21	48,48,48,48	0
93	MG	5	3895	1/1	0.88	0.61	24.97	47,47,47,47	0
93	MG	5	3990	1/1	0.67	0.79	24.95	35,35,35,35	0
93	MG	1	3877	1/1	0.91	0.70	24.80	43,43,43,43	0
93	MG	1	3889	1/1	0.97	0.75	24.77	39,39,39,39	0
93	MG	5	3908	1/1	0.90	0.62	24.50	33,33,33,33	0
93	MG	5	3929	1/1	0.97	0.53	24.34	34,34,34,34	0
93	MG	N8	203	1/1	0.88	0.89	24.23	32,32,32,32	0
93	MG	6	2100	1/1	0.94	0.84	24.21	45,45,45,45	0
92	OHX	1	3710	7/7	0.96	0.45	23.47	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
93	MG	5	3913	1/1	0.97	0.69	23.34	37,37,37,37	0
93	MG	1	3911	1/1	0.95	0.43	23.34	38,38,38,38	0
93	MG	1	3912	1/1	0.91	0.81	22.86	52,52,52,52	0
93	MG	5	3945	1/1	0.70	0.60	22.68	44,44,44,44	0
93	MG	5	3898	1/1	0.96	0.63	22.59	44,44,44,44	0
93	MG	1	3840	1/1	0.92	0.55	22.48	42,42,42,42	0
93	MG	1	4055	1/1	0.95	0.51	22.31	38,38,38,38	0
93	MG	1	3825	1/1	0.90	0.60	22.24	38,38,38,38	0
93	MG	5	4115	1/1	0.97	0.57	22.21	35,35,35,35	0
93	MG	5	3853	1/1	0.98	0.85	22.18	40,40,40,40	0
93	MG	5	4170	1/1	0.96	0.50	21.87	33,33,33,33	0
93	MG	5	3759	1/1	0.89	0.54	21.26	43,43,43,43	0
93	MG	o3	203	1/1	0.90	0.65	21.02	36,36,36,36	0
93	MG	1	3836	1/1	0.90	0.73	20.77	32,32,32,32	0
93	MG	5	3917	1/1	0.97	0.55	20.64	36,36,36,36	0
93	MG	6	2131	1/1	0.94	0.47	20.26	60,60,60,60	0
93	MG	1	3790	1/1	0.91	0.50	19.98	33,33,33,33	0
93	MG	5	3811	1/1	0.70	0.48	19.81	39,39,39,39	0
93	MG	1	3984	1/1	0.98	0.47	19.58	37,37,37,37	0
93	MG	5	3851	1/1	0.88	0.62	19.45	31,31,31,31	0
93	MG	5	3865	1/1	0.91	0.54	19.35	38,38,38,38	0
93	MG	5	3942	1/1	0.88	0.44	18.94	34,34,34,34	0
93	MG	1	3909	1/1	0.93	0.58	18.92	41,41,41,41	0
93	MG	1	4036	1/1	0.94	0.56	18.80	37,37,37,37	0
93	MG	1	3914	1/1	0.97	0.56	18.23	49,49,49,49	0
93	MG	5	4034	1/1	0.97	0.61	18.16	34,34,34,34	0
93	MG	2	2126	1/1	0.89	0.57	17.78	78,78,78,78	0
93	MG	1	3989	1/1	0.94	0.69	17.63	59,59,59,59	0
93	MG	1	4072	1/1	0.93	0.65	17.51	34,34,34,34	0
93	MG	1	3739	1/1	0.86	0.47	17.40	37,37,37,37	0
95	PHE	5	3401	11/12	0.68	0.49	17.21	31,31,41,41	0
93	MG	L4	406	1/1	0.96	0.73	17.20	33,33,33,33	0
93	MG	5	3962	1/1	0.97	0.48	17.09	39,39,39,39	0
93	MG	5	3840	1/1	0.69	0.50	16.55	45,45,45,45	0
93	MG	1	3919	1/1	0.97	0.50	16.36	32,32,32,32	0
93	MG	1	3845	1/1	0.94	0.64	16.00	39,39,39,39	0
93	MG	5	3912	1/1	0.99	0.42	15.96	34,34,34,34	0
93	MG	5	3755	1/1	0.71	0.53	15.78	45,45,45,45	0
93	MG	1	3896	1/1	0.96	0.62	15.70	37,37,37,37	0
93	MG	1	4104	1/1	0.94	0.40	15.44	39,39,39,39	0
93	MG	5	3820	1/1	0.97	0.49	15.23	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	1	3851	1/1	0.95	0.45	15.22	33,33,33,33	0
93	MG	1	4045	1/1	0.97	0.40	15.17	35,35,35,35	0
93	MG	N3	201	1/1	0.94	0.50	14.40	41,41,41,41	0
93	MG	5	3894	1/1	0.88	0.60	14.06	43,43,43,43	0
93	MG	1	3894	1/1	0.95	0.50	14.01	46,46,46,46	0
93	MG	1	3971	1/1	0.96	0.52	14.00	37,37,37,37	0
93	MG	1	3867	1/1	0.99	0.54	13.98	40,40,40,40	0
92	OHX	5	3718	7/7	0.97	0.39	13.75	48,48,48,48	0
93	MG	1	4077	1/1	0.78	0.52	13.49	51,51,51,51	0
93	MG	5	3858	1/1	0.84	0.45	13.49	42,42,42,42	0
93	MG	5	4094	1/1	0.79	0.38	13.29	34,34,34,34	0
93	MG	N0	201	1/1	0.93	0.93	13.15	43,43,43,43	0
93	MG	6	2084	1/1	0.83	0.42	13.15	60,60,60,60	0
93	MG	5	3930	1/1	0.98	0.58	13.11	29,29,29,29	0
92	OHX	1	3727	7/7	0.95	0.37	13.06	69,69,69,69	0
93	MG	5	3754	1/1	0.93	0.38	12.73	43,43,43,43	0
92	OHX	5	3658	7/7	0.96	0.27	12.61	50,50,50,50	0
92	OHX	1	3729	7/7	0.97	0.35	12.60	55,55,55,55	0
92	OHX	5	3617	7/7	0.97	0.34	12.32	63,63,63,63	0
92	OHX	1	3703	7/7	0.98	0.33	12.31	49,49,49,49	0
93	MG	1	3786	1/1	0.77	0.49	12.19	51,51,51,51	0
93	MG	5	3934	1/1	0.97	0.72	12.14	41,41,41,41	0
93	MG	5	3766	1/1	0.95	0.49	12.02	31,31,31,31	0
93	MG	5	3868	1/1	0.82	0.40	11.97	33,33,33,33	0
93	MG	1	3844	1/1	0.99	0.45	11.95	36,36,36,36	0
93	MG	2	2060	1/1	0.92	0.71	11.89	74,74,74,74	0
93	MG	5	3937	1/1	0.96	0.50	11.82	34,34,34,34	0
93	MG	5	4013	1/1	0.91	0.46	11.51	32,32,32,32	0
93	MG	5	3925	1/1	0.92	0.48	11.50	38,38,38,38	0
92	OHX	1	3599	7/7	0.98	0.32	11.43	50,50,50,50	0
93	MG	5	3941	1/1	0.86	0.53	11.38	38,38,38,38	0
93	MG	5	3844	1/1	0.92	0.61	11.35	38,38,38,38	0
93	MG	1	3944	1/1	0.84	0.34	11.27	47,47,47,47	0
93	MG	2	2076	1/1	0.73	0.42	11.25	86,86,86,86	0
92	OHX	4	215	7/7	0.98	0.32	11.19	48,48,48,48	0
92	OHX	5	3707	7/7	0.98	0.44	11.17	76,76,76,76	0
93	MG	5	4071	1/1	0.93	0.41	10.92	33,33,33,33	0
93	MG	L3	405	1/1	0.93	0.79	10.91	41,41,41,41	0
93	MG	1	4074	1/1	0.96	0.60	10.84	41,41,41,41	0
93	MG	5	4169	1/1	0.93	1.01	10.83	44,44,44,44	0
93	MG	1	4014	1/1	0.92	0.38	10.78	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
93	MG	5	4140	1/1	0.93	0.45	10.78	38,38,38,38	0
92	OHX	1	3712	7/7	0.99	0.30	10.66	58,58,58,58	0
93	MG	2	2071	1/1	0.96	0.51	10.66	79,79,79,79	0
93	MG	5	3933	1/1	0.96	0.39	10.63	31,31,31,31	0
93	MG	1	3853	1/1	0.89	0.63	10.60	52,52,52,52	0
92	OHX	5	3609	7/7	0.99	0.36	10.57	67,67,67,67	0
93	MG	5	3854	1/1	0.96	0.59	10.48	31,31,31,31	0
93	MG	5	4119	1/1	0.73	0.44	10.42	43,43,43,43	0
93	MG	1	4123	1/1	0.98	0.27	10.14	37,37,37,37	0
93	MG	1	3949	1/1	0.94	0.45	10.06	48,48,48,48	0
93	MG	6	2068	1/1	0.90	0.45	9.93	105,105,105,105	0
93	MG	5	4078	1/1	0.98	0.32	9.81	61,61,61,61	0
93	MG	5	4110	1/1	0.95	0.39	9.74	32,32,32,32	0
93	MG	1	3824	1/1	0.97	0.31	9.70	37,37,37,37	0
93	MG	6	2079	1/1	0.85	0.41	9.69	72,72,72,72	0
93	MG	1	3918	1/1	0.98	0.56	9.55	32,32,32,32	0
93	MG	5	4025	1/1	0.93	0.55	9.55	41,41,41,41	0
92	OHX	6	2029	7/7	0.97	0.44	9.53	69,69,69,69	0
93	MG	l3	406	1/1	0.92	0.77	9.52	34,34,34,34	0
93	MG	1	3907	1/1	0.91	0.45	9.41	49,49,49,49	0
93	MG	1	3800	1/1	0.96	0.41	9.25	39,39,39,39	0
93	MG	1	3966	1/1	0.90	0.34	9.14	44,44,44,44	0
93	MG	6	2105	1/1	0.83	0.56	9.04	65,65,65,65	0
92	OHX	5	3661	7/7	0.97	0.38	8.94	58,58,58,58	0
93	MG	d3	201	1/1	0.79	0.50	8.89	55,55,55,55	0
93	MG	5	3893	1/1	0.73	0.28	8.82	43,43,43,43	0
93	MG	5	3916	1/1	0.94	0.50	8.81	48,48,48,48	0
93	MG	1	3737	1/1	0.87	0.36	8.77	47,47,47,47	0
92	OHX	1	3646	7/7	0.95	0.33	8.61	57,57,57,57	0
93	MG	5	3932	1/1	0.96	0.57	8.60	37,37,37,37	0
93	MG	1	3835	1/1	0.94	0.38	8.54	35,35,35,35	0
92	OHX	1	3648	7/7	0.99	0.33	8.51	55,55,55,55	0
93	MG	2	2110	1/1	0.74	0.45	8.51	76,76,76,76	0
93	MG	6	2128	1/1	0.82	0.36	8.27	88,88,88,88	0
93	MG	5	3768	1/1	0.97	0.55	8.25	36,36,36,36	0
93	MG	1	3937	1/1	0.90	0.33	8.23	40,40,40,40	0
93	MG	1	3841	1/1	0.96	0.39	8.17	41,41,41,41	0
93	MG	5	3867	1/1	0.90	0.46	8.09	44,44,44,44	0
92	OHX	5	3689	7/7	0.98	0.40	8.08	59,59,59,59	0
93	MG	M7	204	1/1	0.91	0.45	8.05	38,38,38,38	0
93	MG	5	3901	1/1	0.96	0.34	7.97	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	5	4159	1/1	0.93	0.32	7.91	39,39,39,39	0
92	OHX	1	3685	7/7	0.94	0.37	7.91	65,65,65,65	0
93	MG	1	3868	1/1	0.96	0.39	7.88	44,44,44,44	0
93	MG	5	3837	1/1	0.98	0.39	7.88	34,34,34,34	0
93	MG	2	2141	1/1	0.61	0.57	7.82	79,79,79,79	0
92	OHX	1	3699	7/7	0.98	0.28	7.75	60,60,60,60	0
92	OHX	5	3698	7/7	0.98	0.36	7.64	59,59,59,59	0
93	MG	1	3916	1/1	0.97	0.50	7.62	34,34,34,34	0
92	OHX	1	3654	7/7	0.98	0.31	7.59	60,60,60,60	0
92	OHX	8	210	7/7	0.98	0.30	7.47	57,57,57,57	0
93	MG	1	3882	1/1	0.98	0.30	7.44	33,33,33,33	0
92	OHX	1	3642	7/7	0.97	0.25	7.43	64,64,64,64	0
92	OHX	7	211	7/7	0.96	0.30	7.43	69,69,69,69	0
93	MG	13	405	1/1	0.87	0.37	7.42	38,38,38,38	0
92	OHX	1	3728	7/7	0.92	0.35	7.40	50,50,50,50	0
93	MG	1	3932	1/1	0.76	0.25	7.34	37,37,37,37	0
92	OHX	5	3551	7/7	0.98	0.26	7.30	49,49,49,49	0
93	MG	1	4088	1/1	0.90	0.98	7.30	34,34,34,34	0
92	OHX	5	3662	7/7	0.98	0.37	7.27	51,51,51,51	0
93	MG	5	3983	1/1	0.90	0.35	7.26	35,35,35,35	0
92	OHX	1	3579	7/7	0.97	0.30	7.25	59,59,59,59	0
93	MG	1	4097	1/1	0.82	0.30	7.25	49,49,49,49	0
93	MG	5	3961	1/1	0.94	0.31	7.23	41,41,41,41	0
92	OHX	5	3740	7/7	0.96	0.35	7.21	55,55,55,55	0
92	OHX	1	3665	7/7	0.98	0.27	7.19	66,66,66,66	0
93	MG	5	3859	1/1	0.96	0.44	7.03	32,32,32,32	0
93	MG	5	3801	1/1	0.91	0.33	7.00	31,31,31,31	0
93	MG	8	218	1/1	0.94	0.34	6.91	37,37,37,37	0
92	OHX	1	3688	7/7	0.98	0.36	6.88	58,58,58,58	0
93	MG	2	2123	1/1	0.87	0.49	6.88	96,96,96,96	0
93	MG	1	3826	1/1	0.78	0.33	6.86	49,49,49,49	0
92	OHX	4	212	7/7	0.98	0.25	6.85	50,50,50,50	0
92	OHX	5	3670	7/7	0.97	0.31	6.77	50,50,50,50	0
93	MG	1	4100	1/1	0.94	0.82	6.76	45,45,45,45	0
93	MG	5	4113	1/1	0.94	0.29	6.68	35,35,35,35	0
92	OHX	5	3623	7/7	0.95	0.24	6.66	59,59,59,59	0
92	OHX	8	211	7/7	0.96	0.27	6.59	60,60,60,60	0
93	MG	1	3899	1/1	0.97	0.44	6.57	34,34,34,34	0
92	OHX	6	2037	7/7	0.93	0.38	6.56	77,77,77,77	0
93	MG	1	3812	1/1	0.98	0.35	6.53	40,40,40,40	0
93	MG	m5	303	1/1	0.90	0.38	6.53	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
93	MG	2	2062	1/1	0.77	0.29	6.53	98,98,98,98	0
92	OHX	1	3721	7/7	0.95	0.30	6.50	61,61,61,61	0
93	MG	5	3813	1/1	0.96	0.42	6.45	44,44,44,44	0
92	OHX	5	3664	7/7	0.97	0.30	6.43	71,71,71,71	0
92	OHX	6	2051	7/7	0.96	0.36	6.41	84,84,84,84	0
92	OHX	5	3684	7/7	0.98	0.44	6.40	72,72,72,72	0
92	OHX	1	3597	7/7	0.98	0.28	6.40	56,56,56,56	0
93	MG	5	4112	1/1	0.86	0.93	6.34	45,45,45,45	0
92	OHX	8	213	7/7	0.96	0.32	6.28	62,62,62,62	0
93	MG	6	2069	1/1	0.95	0.35	6.27	61,61,61,61	0
92	OHX	5	3565	7/7	0.98	0.26	6.25	59,59,59,59	0
93	MG	n3	201	1/1	0.90	0.39	6.23	32,32,32,32	0
92	OHX	4	218	7/7	0.96	0.34	6.20	67,67,67,67	0
92	OHX	5	3573	7/7	0.98	0.22	6.19	54,54,54,54	0
92	OHX	5	3721	7/7	0.98	0.25	6.19	49,49,49,49	0
93	MG	1	3969	1/1	0.97	0.27	6.13	42,42,42,42	0
93	MG	2	2099	1/1	0.89	0.60	6.13	80,80,80,80	0
93	MG	6	2080	1/1	0.69	0.63	6.10	63,63,63,63	0
93	MG	5	4145	1/1	0.98	0.36	6.10	34,34,34,34	0
93	MG	1	3801	1/1	0.97	0.37	6.09	32,32,32,32	0
92	OHX	5	3632	7/7	0.96	0.31	6.07	51,51,51,51	0
92	OHX	1	3626	7/7	0.96	0.34	6.06	70,70,70,70	0
92	OHX	1	3621	7/7	0.96	0.25	6.05	70,70,70,70	0
92	OHX	5	3647	7/7	0.98	0.41	5.98	63,63,63,63	0
96	LEU	5	3402	8/9	0.79	0.36	5.97	36,36,36,36	0
92	OHX	2	2025	7/7	0.94	0.36	5.97	85,85,85,85	0
93	MG	2	2095	1/1	0.81	0.39	5.94	80,80,80,80	0
93	MG	5	3780	1/1	0.71	0.32	5.94	57,57,57,57	0
92	OHX	5	3705	7/7	0.98	0.34	5.92	59,59,59,59	0
92	OHX	5	3671	7/7	0.95	0.33	5.91	40,40,40,40	0
93	MG	4	227	1/1	0.97	0.35	5.91	36,36,36,36	0
93	MG	5	3785	1/1	0.97	0.27	5.87	33,33,33,33	0
93	MG	5	3773	1/1	0.98	0.31	5.77	38,38,38,38	0
92	OHX	5	3716	7/7	0.96	0.36	5.76	59,59,59,59	0
93	MG	5	4022	1/1	0.76	0.38	5.72	65,65,65,65	0
93	MG	1	3952	1/1	0.80	0.27	5.68	32,32,32,32	0
93	MG	1	4073	1/1	0.88	0.75	5.62	37,37,37,37	0
93	MG	7	222	1/1	0.95	0.31	5.59	35,35,35,35	0
92	OHX	5	3636	7/7	0.98	0.27	5.58	46,46,46,46	0
92	OHX	1	3614	7/7	0.95	0.34	5.58	58,58,58,58	0
92	OHX	5	3694	7/7	0.98	0.25	5.57	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	5	3643	7/7	0.98	0.30	5.54	49,49,49,49	0
92	OHX	1	3560	7/7	0.95	0.31	5.52	54,54,54,54	0
93	MG	1	3883	1/1	0.93	0.34	5.45	44,44,44,44	0
92	OHX	5	3659	7/7	0.96	0.30	5.42	58,58,58,58	0
92	OHX	5	3720	7/7	0.97	0.28	5.38	67,67,67,67	0
93	MG	1	3892	1/1	0.98	0.45	5.37	33,33,33,33	0
93	MG	n0	202	1/1	0.97	0.60	5.36	37,37,37,37	0
93	MG	2	2065	1/1	0.91	0.39	5.35	88,88,88,88	0
93	MG	5	4070	1/1	0.87	0.69	5.33	40,40,40,40	0
92	OHX	1	3590	7/7	0.98	0.29	5.26	53,53,53,53	0
93	MG	2	2089	1/1	0.72	0.39	5.23	85,85,85,85	0
92	OHX	1	3667	7/7	0.94	0.32	5.16	81,81,81,81	0
93	MG	N5	201	1/1	0.95	0.37	5.15	43,43,43,43	0
93	MG	4	228	1/1	0.93	0.27	5.14	32,32,32,32	0
93	MG	5	3793	1/1	0.92	0.26	5.14	42,42,42,42	0
93	MG	O5	201	1/1	0.92	0.55	5.09	42,42,42,42	0
93	MG	5	3890	1/1	0.92	0.41	5.06	48,48,48,48	0
92	OHX	1	3594	7/7	0.93	0.32	5.05	66,66,66,66	0
93	MG	1	4108	1/1	0.96	0.36	5.05	48,48,48,48	0
92	OHX	5	3695	7/7	0.98	0.30	5.05	55,55,55,55	0
92	OHX	5	3739	7/7	0.93	0.44	5.04	69,69,69,69	0
93	MG	5	4069	1/1	0.95	0.43	5.03	35,35,35,35	0
93	MG	5	3789	1/1	0.98	0.33	5.00	32,32,32,32	0
92	OHX	5	3688	7/7	0.96	0.38	4.98	66,66,66,66	0
93	MG	P	102	1/1	0.96	0.40	4.97	39,39,39,39	0
92	OHX	5	3700	7/7	0.94	0.33	4.92	63,63,63,63	0
92	OHX	1	3718	7/7	0.98	0.32	4.90	64,64,64,64	0
93	MG	M7	206	1/1	0.98	0.58	4.86	37,37,37,37	0
92	OHX	5	3570	7/7	0.97	0.23	4.86	63,63,63,63	0
92	OHX	1	3649	7/7	0.98	0.30	4.80	65,65,65,65	0
93	MG	l2	303	1/1	0.98	0.93	4.77	44,44,44,44	0
92	OHX	5	3645	7/7	0.97	0.31	4.74	53,53,53,53	0
93	MG	1	3922	1/1	0.87	0.23	4.74	42,42,42,42	0
93	MG	1	4098	1/1	0.94	0.32	4.73	41,41,41,41	0
93	MG	5	4053	1/1	0.94	0.37	4.73	34,34,34,34	0
92	OHX	2	1995	7/7	0.94	0.27	4.69	103,103,103,103	0
93	MG	2	2115	1/1	0.87	0.62	4.68	84,84,84,84	0
93	MG	n8	203	1/1	0.95	0.80	4.65	34,34,34,34	0
93	MG	1	4099	1/1	0.84	0.54	4.63	58,58,58,58	0
93	MG	5	4098	1/1	0.82	0.37	4.63	45,45,45,45	0
92	OHX	7	209	7/7	0.98	0.25	4.62	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
93	MG	1	4082	1/1	0.96	0.27	4.60	38,38,38,38	0
93	MG	1	3977	1/1	0.83	0.51	4.59	36,36,36,36	0
93	MG	1	3814	1/1	0.98	0.29	4.58	44,44,44,44	0
93	MG	5	3869	1/1	0.87	0.27	4.57	40,40,40,40	0
93	MG	1	4071	1/1	0.97	0.25	4.57	35,35,35,35	0
92	OHX	1	3653	7/7	0.98	0.26	4.56	57,57,57,57	0
92	OHX	1	3671	7/7	0.97	0.32	4.55	65,65,65,65	0
92	OHX	1	3675	7/7	0.96	0.32	4.53	61,61,61,61	0
93	MG	5	4168	1/1	0.97	0.23	4.49	32,32,32,32	0
92	OHX	5	3729	7/7	0.96	0.33	4.49	49,49,49,49	0
93	MG	1	3822	1/1	0.96	0.31	4.43	40,40,40,40	0
93	MG	1	4091	1/1	0.97	0.55	4.39	42,42,42,42	0
92	OHX	5	3531	7/7	0.97	0.25	4.35	55,55,55,55	0
92	OHX	6	2035	7/7	0.96	0.41	4.34	84,84,84,84	0
92	OHX	5	3660	7/7	0.97	0.30	4.29	70,70,70,70	0
92	OHX	5	3630	7/7	0.97	0.31	4.28	53,53,53,53	0
92	OHX	1	3660	7/7	0.98	0.32	4.26	70,70,70,70	0
92	OHX	1	3687	7/7	0.97	0.27	4.24	67,67,67,67	0
92	OHX	5	3687	7/7	0.98	0.37	4.23	58,58,58,58	0
93	MG	5	3892	1/1	0.85	0.32	4.23	40,40,40,40	0
92	OHX	5	3554	7/7	0.95	0.31	4.22	50,50,50,50	0
93	MG	5	4079	1/1	0.94	0.46	4.21	43,43,43,43	0
93	MG	4	233	1/1	0.89	0.35	4.17	45,45,45,45	0
92	OHX	2	2029	7/7	0.97	0.29	4.14	79,79,79,79	0
93	MG	1	3925	1/1	0.98	0.26	4.12	42,42,42,42	0
92	OHX	1	3662	7/7	0.98	0.32	4.11	50,50,50,50	0
92	OHX	5	3693	7/7	0.96	0.27	4.11	70,70,70,70	0
92	OHX	5	3681	7/7	0.98	0.31	4.07	45,45,45,45	0
93	MG	sM	202	1/1	0.97	0.61	4.02	45,45,45,45	0
92	OHX	5	3599	7/7	0.96	0.28	4.01	68,68,68,68	0
93	MG	1	3809	1/1	0.66	0.32	3.97	37,37,37,37	0
93	MG	L3	403	1/1	0.90	0.57	3.97	51,51,51,51	0
93	MG	5	3752	1/1	0.75	0.32	3.96	45,45,45,45	0
92	OHX	1	3508	7/7	0.99	0.20	3.93	51,51,51,51	0
92	OHX	1	3576	7/7	0.97	0.28	3.93	47,47,47,47	0
92	OHX	1	3537	7/7	0.98	0.25	3.87	61,61,61,61	0
93	MG	5	3944	1/1	0.94	0.37	3.85	40,40,40,40	0
93	MG	5	4174	1/1	0.81	0.45	3.85	31,31,31,31	0
93	MG	1	3745	1/1	0.95	0.36	3.85	41,41,41,41	0
92	OHX	1	3655	7/7	0.97	0.29	3.82	55,55,55,55	0
93	MG	L7	302	1/1	0.90	0.61	3.80	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
92	OHX	2	2031	7/7	0.93	0.31	3.79	103,103,103,103	0
92	OHX	5	3706	7/7	0.98	0.36	3.78	54,54,54,54	0
98	8AN	P	101	22/23	0.91	0.25	3.78	37,38,38,38	0
92	OHX	1	3525	7/7	0.98	0.24	3.77	57,57,57,57	0
92	OHX	5	3549	7/7	0.98	0.24	3.74	49,49,49,49	0
92	OHX	6	2032	7/7	0.95	0.26	3.74	92,92,92,92	0
92	OHX	5	3590	7/7	0.98	0.28	3.71	47,47,47,47	0
93	MG	1	4002	1/1	0.92	0.28	3.70	52,52,52,52	0
92	OHX	6	2033	7/7	0.96	0.37	3.69	78,78,78,78	0
93	MG	7	221	1/1	0.82	0.51	3.68	47,47,47,47	0
93	MG	1	4093	1/1	0.96	0.59	3.68	33,33,33,33	0
93	MG	O7	105	1/1	0.73	0.53	3.68	42,42,42,42	0
93	MG	M7	205	1/1	0.90	0.31	3.63	38,38,38,38	0
93	MG	N3	203	1/1	0.96	0.34	3.63	46,46,46,46	0
92	OHX	2	2047	7/7	0.94	0.44	3.61	105,105,105,105	0
93	MG	1	3767	1/1	0.98	0.33	3.60	36,36,36,36	0
92	OHX	5	3527	7/7	0.97	0.24	3.60	47,47,47,47	0
92	OHX	5	3607	7/7	0.98	0.31	3.56	59,59,59,59	0
93	MG	2	2069	1/1	0.97	0.35	3.54	79,79,79,79	0
92	OHX	m0	303	7/7	0.98	0.32	3.54	53,53,53,53	0
92	OHX	5	3606	7/7	0.98	0.25	3.53	61,61,61,61	0
92	OHX	5	3578	7/7	0.96	0.30	3.52	50,50,50,50	0
92	OHX	5	3652	7/7	0.95	0.37	3.51	48,48,48,48	0
92	OHX	1	3714	7/7	0.96	0.36	3.46	72,72,72,72	0
92	OHX	1	3674	7/7	0.97	0.40	3.44	73,73,73,73	0
92	OHX	1	3643	7/7	0.98	0.27	3.43	77,77,77,77	0
92	OHX	5	3644	7/7	0.96	0.26	3.42	48,48,48,48	0
92	OHX	1	3702	7/7	0.93	0.27	3.38	38,38,38,38	0
92	OHX	8	212	7/7	0.97	0.34	3.37	76,76,76,76	0
92	OHX	6	2024	7/7	0.96	0.39	3.37	103,103,103,103	0
92	OHX	1	3684	7/7	0.99	0.25	3.35	56,56,56,56	0
93	MG	6	2118	1/1	0.92	0.30	3.35	96,96,96,96	0
93	MG	1	3875	1/1	0.93	0.49	3.34	44,44,44,44	0
92	OHX	1	3670	7/7	0.98	0.25	3.32	60,60,60,60	0
92	OHX	5	3724	7/7	0.95	0.30	3.31	36,36,36,36	0
92	OHX	1	3645	7/7	0.98	0.32	3.29	61,61,61,61	0
92	OHX	1	3605	7/7	0.93	0.37	3.28	43,43,43,43	0
92	OHX	5	3582	7/7	0.99	0.23	3.28	56,56,56,56	0
92	OHX	5	3709	7/7	0.98	0.31	3.28	68,68,68,68	0
93	MG	6	2071	1/1	0.81	0.55	3.27	63,63,63,63	0
93	MG	d6	102	1/1	0.91	0.59	3.26	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	3	208	7/7	0.97	0.21	3.24	81,81,81,81	0
92	OHX	1	3693	7/7	0.98	0.26	3.23	69,69,69,69	0
92	OHX	1	3678	7/7	0.97	0.32	3.22	54,54,54,54	0
92	OHX	5	3641	7/7	0.99	0.27	3.22	59,59,59,59	0
93	MG	2	2080	1/1	0.96	0.31	3.21	82,82,82,82	0
93	MG	1	4107	1/1	0.84	0.27	3.16	39,39,39,39	0
93	MG	1	4034	1/1	0.92	0.25	3.13	34,34,34,34	0
93	MG	6	2090	1/1	0.97	0.26	3.11	56,56,56,56	0
93	MG	M7	202	1/1	0.63	0.77	3.08	52,52,52,52	0
93	MG	6	2113	1/1	0.90	0.42	3.06	55,55,55,55	0
92	OHX	6	2058	7/7	0.96	0.29	3.04	100,100,100,100	0
92	OHX	2	2021	7/7	0.96	0.31	3.04	110,110,110,110	0
93	MG	17	301	1/1	0.99	0.42	3.03	34,34,34,34	0
93	MG	5	4054	1/1	0.92	0.52	3.02	65,65,65,65	0
93	MG	2	2131	1/1	0.82	0.35	3.01	80,80,80,80	0
92	OHX	5	3648	7/7	0.91	0.34	3.01	64,64,64,64	0
93	MG	1	3832	1/1	0.75	0.39	2.95	31,31,31,31	0
92	OHX	1	3726	7/7	0.96	0.39	2.92	87,87,87,87	0
92	OHX	6	2009	7/7	0.97	0.26	2.91	88,88,88,88	0
93	MG	6	2175	1/1	0.77	0.29	2.86	64,64,64,64	0
92	OHX	5	3602	7/7	0.94	0.24	2.82	84,84,84,84	0
93	MG	7	223	1/1	0.84	0.25	2.81	36,36,36,36	0
93	MG	1	3763	1/1	0.93	0.26	2.81	34,34,34,34	0
92	OHX	1	3663	7/7	0.98	0.25	2.80	71,71,71,71	0
93	MG	1	3807	1/1	0.96	0.28	2.79	41,41,41,41	0
93	MG	6	2134	1/1	0.97	0.28	2.78	57,57,57,57	0
92	OHX	8	214	7/7	0.96	0.33	2.78	59,59,59,59	0
93	MG	1	3816	1/1	0.95	0.29	2.76	41,41,41,41	0
92	OHX	6	1992	7/7	0.98	0.26	2.72	88,88,88,88	0
92	OHX	2	2049	7/7	0.91	0.37	2.71	108,108,108,108	0
92	OHX	6	2012	7/7	0.97	0.29	2.71	76,76,76,76	0
93	MG	1	3923	1/1	0.96	0.28	2.70	34,34,34,34	0
92	OHX	5	3611	7/7	0.99	0.26	2.70	45,45,45,45	0
92	OHX	5	3598	7/7	0.96	0.30	2.66	51,51,51,51	0
93	MG	5	3753	1/1	0.88	0.29	2.65	32,32,32,32	0
93	MG	1	3741	1/1	0.92	0.27	2.64	48,48,48,48	0
92	OHX	1	3569	7/7	0.97	0.29	2.61	63,63,63,63	0
93	MG	5	3775	1/1	0.98	0.28	2.60	33,33,33,33	0
93	MG	1	4052	1/1	0.97	0.38	2.58	33,33,33,33	0
92	OHX	5	3580	7/7	0.97	0.30	2.57	53,53,53,53	0
92	OHX	5	3591	7/7	0.98	0.28	2.56	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	S9	201	7/7	0.94	0.46	2.54	93,93,93,93	0
92	OHX	6	2057	7/7	0.93	0.41	2.54	92,92,92,92	0
93	MG	5	3804	1/1	0.87	0.32	2.52	38,38,38,38	0
93	MG	6	2171	1/1	0.89	0.90	2.52	68,68,68,68	0
93	MG	2	2061	1/1	0.83	0.46	2.50	83,83,83,83	0
92	OHX	2	1976	7/7	0.93	0.40	2.49	110,110,110,110	0
93	MG	1	4030	1/1	0.96	0.52	2.47	44,44,44,44	0
93	MG	2	2109	1/1	0.93	0.27	2.45	80,80,80,80	0
92	OHX	1	3538	7/7	0.96	0.28	2.44	66,66,66,66	0
92	OHX	5	3737	7/7	0.98	0.26	2.43	85,85,85,85	0
93	MG	6	2064	1/1	0.81	0.42	2.40	68,68,68,68	0
93	MG	1	3904	1/1	0.84	0.41	2.39	48,48,48,48	0
92	OHX	6	2054	7/7	0.96	0.28	2.38	89,89,89,89	0
93	MG	5	4030	1/1	0.88	0.36	2.37	36,36,36,36	0
93	MG	6	2126	1/1	0.98	0.46	2.35	62,62,62,62	0
92	OHX	1	3607	7/7	0.98	0.21	2.35	62,62,62,62	0
92	OHX	5	3601	7/7	0.95	0.25	2.32	44,44,44,44	0
92	OHX	5	3638	7/7	0.98	0.26	2.32	41,41,41,41	0
93	MG	s6	301	1/1	0.56	0.95	2.32	67,67,67,67	0
93	MG	L4	405	1/1	0.97	0.36	2.31	37,37,37,37	0
92	OHX	1	3629	7/7	0.98	0.22	2.28	79,79,79,79	0
93	MG	1	3864	1/1	0.91	0.26	2.28	30,30,30,30	0
92	OHX	1	3603	7/7	0.97	0.23	2.27	74,74,74,74	0
93	MG	1	4033	1/1	0.98	0.26	2.26	47,47,47,47	0
92	OHX	6	1990	7/7	0.97	0.21	2.24	79,79,79,79	0
92	OHX	2	1979	7/7	0.98	0.24	2.24	82,82,82,82	0
93	MG	1	3831	1/1	0.96	0.34	2.24	38,38,38,38	0
93	MG	N6	201	1/1	0.80	0.39	2.21	40,40,40,40	0
93	MG	1	3820	1/1	0.98	0.21	2.21	43,43,43,43	0
92	OHX	5	3597	7/7	0.95	0.22	2.20	68,68,68,68	0
93	MG	6	2107	1/1	0.86	0.37	2.16	63,63,63,63	0
92	OHX	2	2043	7/7	0.97	0.33	2.16	85,85,85,85	0
93	MG	2	2087	1/1	0.90	0.29	2.12	77,77,77,77	0
92	OHX	5	3576	7/7	0.98	0.30	2.11	65,65,65,65	0
93	MG	6	2139	1/1	0.89	0.50	2.07	57,57,57,57	0
92	OHX	5	3624	7/7	0.98	0.23	2.07	58,58,58,58	0
92	OHX	1	3620	7/7	0.98	0.26	2.04	41,41,41,41	0
93	MG	m7	201	1/1	0.91	0.32	2.03	34,34,34,34	0
92	OHX	6	2042	7/7	0.94	0.26	2.03	94,94,94,94	0
93	MG	5	4005	1/1	0.96	0.23	2.02	36,36,36,36	0
92	OHX	1	3631	7/7	0.96	0.26	1.99	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
92	OHX	6	1977	7/7	0.97	0.21	1.99	97,97,97,97	0
92	OHX	5	3542	7/7	0.97	0.21	1.98	57,57,57,57	0
93	MG	8	217	1/1	0.90	0.21	1.97	36,36,36,36	0
93	MG	6	2063	1/1	0.88	0.24	1.97	89,89,89,89	0
93	MG	5	3998	1/1	0.95	0.32	1.96	35,35,35,35	0
92	OHX	2	1985	7/7	0.96	0.32	1.96	98,98,98,98	0
93	MG	1	4031	1/1	0.97	0.26	1.95	40,40,40,40	0
92	OHX	5	3676	7/7	0.98	0.25	1.94	59,59,59,59	0
92	OHX	1	3658	7/7	0.97	0.34	1.93	65,65,65,65	0
92	OHX	O4	201	7/7	0.97	0.45	1.93	73,73,73,73	0
93	MG	5	3986	1/1	0.95	0.19	1.93	49,49,49,49	0
93	MG	6	2092	1/1	0.60	0.18	1.93	88,88,88,88	0
92	OHX	5	3710	7/7	0.94	0.36	1.90	57,57,57,57	0
93	MG	m5	304	1/1	0.82	0.35	1.90	47,47,47,47	0
92	OHX	5	3604	7/7	0.98	0.26	1.89	57,57,57,57	0
92	OHX	1	3683	7/7	0.91	0.36	1.88	87,87,87,87	0
93	MG	5	3914	1/1	0.97	0.32	1.88	35,35,35,35	0
92	OHX	2	2035	7/7	0.94	0.26	1.88	107,107,107,107	0
92	OHX	3	210	7/7	0.96	0.40	1.86	85,85,85,85	0
93	MG	1	3803	1/1	0.88	0.36	1.85	36,36,36,36	0
93	MG	d4	202	1/1	0.75	0.26	1.85	65,65,65,65	0
93	MG	1	3752	1/1	0.81	0.30	1.85	38,38,38,38	0
92	OHX	6	1969	7/7	0.97	0.19	1.85	99,99,99,99	0
93	MG	6	2170	1/1	0.85	0.46	1.83	64,64,64,64	0
92	OHX	5	3528	7/7	0.97	0.23	1.83	46,46,46,46	0
92	OHX	1	3640	7/7	0.98	0.34	1.81	63,63,63,63	0
93	MG	5	3838	1/1	0.92	0.36	1.79	37,37,37,37	0
92	OHX	1	3657	7/7	0.97	0.25	1.79	50,50,50,50	0
92	OHX	1	3669	7/7	0.97	0.27	1.78	63,63,63,63	0
92	OHX	5	3562	7/7	0.98	0.22	1.78	60,60,60,60	0
92	OHX	4	209	7/7	0.98	0.27	1.75	56,56,56,56	0
92	OHX	6	2013	7/7	0.96	0.28	1.75	72,72,72,72	0
92	OHX	4	211	7/7	0.98	0.22	1.75	63,63,63,63	0
92	OHX	6	2025	7/7	0.95	0.34	1.74	70,70,70,70	0
93	MG	5	3897	1/1	0.76	0.42	1.72	48,48,48,48	0
92	OHX	1	3676	7/7	0.96	0.26	1.70	64,64,64,64	0
93	MG	5	3885	1/1	0.97	0.41	1.70	32,32,32,32	0
93	MG	6	2168	1/1	0.96	0.24	1.68	57,57,57,57	0
92	OHX	4	221	7/7	0.97	0.30	1.67	61,61,61,61	0
92	OHX	1	3542	7/7	0.97	0.22	1.67	60,60,60,60	0
93	MG	C1	201	1/1	0.47	0.61	1.63	76,76,76,76	0
92	OHX	1	3566	7/7	0.98	0.23	1.63	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	6	2094	1/1	0.83	0.26	1.63	77,77,77,77	0
92	OHX	1	3713	7/7	0.98	0.38	1.62	58,58,58,58	0
92	OHX	5	3587	7/7	0.97	0.25	1.61	47,47,47,47	0
92	OHX	2	2023	7/7	0.95	0.28	1.61	91,91,91,91	0
92	OHX	5	3619	7/7	0.97	0.30	1.60	68,68,68,68	0
92	OHX	5	3585	7/7	0.97	0.29	1.60	58,58,58,58	0
92	OHX	6	1965	7/7	0.98	0.24	1.59	77,77,77,77	0
93	MG	5	4049	1/1	0.88	0.27	1.57	36,36,36,36	0
92	OHX	2	2011	7/7	0.93	0.35	1.57	104,104,104,104	0
92	OHX	5	3628	7/7	0.97	0.17	1.54	60,60,60,60	0
92	OHX	2	1988	7/7	0.97	0.26	1.53	87,87,87,87	0
92	OHX	5	3743	7/7	0.97	0.29	1.49	70,70,70,70	0
92	OHX	1	3591	7/7	0.96	0.21	1.47	92,92,92,92	0
92	OHX	5	3634	7/7	0.97	0.45	1.46	70,70,70,70	0
92	OHX	2	1999	7/7	0.95	0.36	1.46	106,106,106,106	0
93	MG	5	3953	1/1	0.94	0.34	1.45	39,39,39,39	0
92	OHX	6	1976	7/7	0.99	0.21	1.44	58,58,58,58	0
93	MG	12	302	1/1	0.92	0.34	1.42	41,41,41,41	0
92	OHX	1	3589	7/7	0.95	0.23	1.39	45,45,45,45	0
92	OHX	2	2048	7/7	0.88	0.25	1.37	100,100,100,100	0
92	OHX	4	220	7/7	0.97	0.32	1.37	66,66,66,66	0
92	OHX	1	3644	7/7	0.97	0.27	1.36	48,48,48,48	0
92	OHX	5	3536	7/7	0.96	0.18	1.35	65,65,65,65	0
92	OHX	2	2032	7/7	0.94	0.36	1.35	106,106,106,106	0
93	MG	2	2122	1/1	0.93	0.26	1.33	74,74,74,74	0
92	OHX	2	1970	7/7	0.96	0.35	1.33	98,98,98,98	0
93	MG	5	3871	1/1	0.91	0.42	1.31	59,59,59,59	0
92	OHX	5	3646	7/7	0.96	0.32	1.29	56,56,56,56	0
93	MG	m7	203	1/1	0.89	0.29	1.28	33,33,33,33	0
92	OHX	5	3618	7/7	0.97	0.33	1.28	74,74,74,74	0
93	MG	5	4043	1/1	0.84	0.30	1.27	41,41,41,41	0
92	OHX	6	2002	7/7	0.94	0.27	1.27	71,71,71,71	0
93	MG	1	3931	1/1	0.92	0.39	1.26	60,60,60,60	0
93	MG	5	3888	1/1	0.94	0.32	1.26	61,61,61,61	0
92	OHX	6	1988	7/7	0.95	0.30	1.25	82,82,82,82	0
93	MG	n6	202	1/1	0.90	0.31	1.25	42,42,42,42	0
92	OHX	6	2044	7/7	0.95	0.29	1.25	63,63,63,63	0
92	OHX	5	3589	7/7	0.97	0.24	1.25	46,46,46,46	0
92	OHX	2	1941	7/7	0.98	0.25	1.23	93,93,93,93	0
92	OHX	1	3524	7/7	0.98	0.21	1.23	59,59,59,59	0
92	OHX	1	3528	7/7	0.98	0.28	1.21	52,52,52,52	0
92	OHX	8	216	7/7	0.97	0.38	1.18	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	2	2092	1/1	0.74	0.37	1.17	80,80,80,80	0
93	MG	5	3899	1/1	0.95	0.34	1.15	37,37,37,37	0
93	MG	6	2116	1/1	0.93	0.33	1.14	63,63,63,63	0
92	OHX	6	1970	7/7	0.92	0.52	1.14	105,105,105,105	0
92	OHX	6	1984	7/7	0.98	0.36	1.12	87,87,87,87	0
92	OHX	s9	201	7/7	0.95	0.34	1.12	77,77,77,77	0
92	OHX	1	3587	7/7	0.98	0.21	1.12	46,46,46,46	0
93	MG	6	2121	1/1	0.93	0.32	1.11	62,62,62,62	0
92	OHX	2	1986	7/7	0.93	0.33	1.10	107,107,107,107	0
92	OHX	O9	101	7/7	0.97	0.38	1.10	49,49,49,49	0
93	MG	1	3893	1/1	0.94	0.30	1.09	32,32,32,32	0
93	MG	1	3817	1/1	0.94	0.23	1.08	34,34,34,34	0
93	MG	2	2086	1/1	0.87	0.29	1.08	71,71,71,71	0
92	OHX	5	3544	7/7	0.98	0.21	1.07	45,45,45,45	0
92	OHX	1	3623	7/7	0.99	0.27	1.06	54,54,54,54	0
92	OHX	1	3696	7/7	0.94	0.31	1.06	64,64,64,64	0
93	MG	2	2130	1/1	0.89	0.20	1.06	85,85,85,85	0
92	OHX	6	2040	7/7	0.93	0.34	1.05	72,72,72,72	0
92	OHX	1	3694	7/7	0.94	0.31	1.04	80,80,80,80	0
92	OHX	5	3669	7/7	0.96	0.30	1.03	60,60,60,60	0
92	OHX	2	1963	7/7	0.97	0.24	1.02	73,73,73,73	0
92	OHX	2	2046	7/7	0.94	0.39	1.02	100,100,100,100	0
92	OHX	6	2048	7/7	0.93	0.29	0.99	77,77,77,77	0
92	OHX	1	3716	7/7	0.95	0.29	0.99	51,51,51,51	0
92	OHX	1	3611	7/7	0.98	0.29	0.99	64,64,64,64	0
92	OHX	6	1998	7/7	0.94	0.24	0.99	65,65,65,65	0
92	OHX	1	3711	7/7	0.98	0.24	0.98	56,56,56,56	0
93	MG	1	4086	1/1	0.97	0.37	0.98	39,39,39,39	0
93	MG	1	3775	1/1	0.94	0.34	0.97	44,44,44,44	0
93	MG	1	3891	1/1	0.92	0.32	0.95	40,40,40,40	0
92	OHX	2	2015	7/7	0.93	0.30	0.95	92,92,92,92	0
92	OHX	5	3574	7/7	0.99	0.19	0.95	60,60,60,60	0
92	OHX	1	3575	7/7	0.98	0.24	0.95	57,57,57,57	0
92	OHX	1	3616	7/7	0.98	0.19	0.95	64,64,64,64	0
92	OHX	1	3668	7/7	0.95	0.34	0.94	92,92,92,92	0
92	OHX	1	3723	7/7	0.95	0.37	0.93	76,76,76,76	0
92	OHX	5	3675	7/7	0.98	0.23	0.92	43,43,43,43	0
92	OHX	5	3496	7/7	0.99	0.25	0.91	47,47,47,47	0
92	OHX	1	3489	7/7	0.96	0.20	0.91	47,47,47,47	0
92	OHX	6	1993	7/7	0.96	0.20	0.90	99,99,99,99	0
92	OHX	1	3543	7/7	0.97	0.21	0.88	69,69,69,69	0
93	MG	5	3819	1/1	0.96	0.26	0.87	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	D9	102	7/7	0.96	0.37	0.87	98,98,98,98	0
93	MG	5	4074	1/1	0.98	0.30	0.87	37,37,37,37	0
93	MG	N0	202	1/1	0.82	0.37	0.86	44,44,44,44	0
92	OHX	5	3654	7/7	0.99	0.31	0.85	54,54,54,54	0
92	OHX	1	3689	7/7	0.97	0.32	0.85	65,65,65,65	0
93	MG	2	2096	1/1	0.87	0.22	0.82	75,75,75,75	0
93	MG	5	3846	1/1	0.99	0.22	0.81	45,45,45,45	0
92	OHX	1	3635	7/7	0.98	0.22	0.81	57,57,57,57	0
92	OHX	5	3605	7/7	0.97	0.26	0.81	46,46,46,46	0
93	MG	1	4057	1/1	0.98	0.22	0.80	34,34,34,34	0
92	OHX	2	1931	7/7	0.98	0.28	0.80	95,95,95,95	0
92	OHX	5	3745	7/7	0.96	0.18	0.80	59,59,59,59	0
93	MG	C9	201	1/1	0.82	0.49	0.79	96,96,96,96	0
92	OHX	6	2028	7/7	0.98	0.23	0.79	62,62,62,62	0
93	MG	1	3732	1/1	0.96	0.23	0.77	47,47,47,47	0
92	OHX	1	3619	7/7	0.97	0.28	0.74	59,59,59,59	0
93	MG	1	3813	1/1	0.99	0.23	0.74	47,47,47,47	0
93	MG	5	4105	1/1	0.92	0.31	0.74	38,38,38,38	0
93	MG	5	3765	1/1	0.94	0.23	0.74	34,34,34,34	0
93	MG	5	4132	1/1	0.99	0.21	0.71	32,32,32,32	0
92	OHX	2	1978	7/7	0.96	0.25	0.71	103,103,103,103	0
92	OHX	6	1978	7/7	0.98	0.24	0.70	90,90,90,90	0
92	OHX	1	3571	7/7	0.98	0.24	0.68	58,58,58,58	0
92	OHX	2	2020	7/7	0.95	0.27	0.68	96,96,96,96	0
92	OHX	3	206	7/7	0.97	0.15	0.68	69,69,69,69	0
92	OHX	5	3642	7/7	0.96	0.23	0.68	72,72,72,72	0
93	MG	L2	301	1/1	0.95	0.29	0.66	42,42,42,42	0
92	OHX	d4	201	7/7	0.96	0.39	0.66	84,84,84,84	0
92	OHX	1	3551	7/7	0.96	0.23	0.65	75,75,75,75	0
93	MG	5	4008	1/1	0.93	0.22	0.64	33,33,33,33	0
93	MG	L2	302	1/1	0.97	0.29	0.64	42,42,42,42	0
92	OHX	6	2019	7/7	0.94	0.34	0.64	75,75,75,75	0
93	MG	5	3750	1/1	0.96	0.22	0.62	36,36,36,36	0
92	OHX	6	2008	7/7	0.96	0.26	0.61	100,100,100,100	0
92	OHX	5	3656	7/7	0.97	0.20	0.60	71,71,71,71	0
92	OHX	1	3679	7/7	0.97	0.26	0.60	84,84,84,84	0
93	MG	5	3936	1/1	0.88	0.33	0.60	31,31,31,31	0
92	OHX	6	1996	7/7	0.97	0.31	0.59	78,78,78,78	0
92	OHX	5	3563	7/7	0.97	0.19	0.59	70,70,70,70	0
92	OHX	L6	202	7/7	0.99	0.32	0.58	62,62,62,62	0
92	OHX	6	2049	7/7	0.97	0.40	0.58	81,81,81,81	0
92	OHX	1	3695	7/7	0.96	0.27	0.57	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	6	2026	7/7	0.97	0.49	0.56	90,90,90,90	0
92	OHX	1	3612	7/7	0.98	0.25	0.54	57,57,57,57	0
92	OHX	5	3663	7/7	0.99	0.22	0.54	47,47,47,47	0
92	OHX	2	2012	7/7	0.90	0.26	0.54	108,108,108,108	0
92	OHX	M8	201	7/7	0.97	0.33	0.53	65,65,65,65	0
92	OHX	5	3616	7/7	0.98	0.21	0.53	54,54,54,54	0
92	OHX	m8	201	7/7	0.97	0.30	0.52	60,60,60,60	0
92	OHX	6	1985	7/7	0.98	0.30	0.52	91,91,91,91	0
92	OHX	5	3730	7/7	0.96	0.26	0.52	74,74,74,74	0
93	MG	D9	104	1/1	0.96	0.29	0.50	89,89,89,89	0
93	MG	1	3908	1/1	0.97	0.22	0.49	53,53,53,53	0
92	OHX	2	1994	7/7	0.90	0.30	0.49	98,98,98,98	0
92	OHX	2	1932	7/7	0.96	0.23	0.49	76,76,76,76	0
92	OHX	l3	402	7/7	0.94	0.46	0.48	67,67,67,67	0
92	OHX	1	3507	7/7	0.99	0.20	0.46	50,50,50,50	0
93	MG	5	4151	1/1	0.98	0.21	0.46	34,34,34,34	0
92	OHX	1	3608	7/7	0.97	0.20	0.46	63,63,63,63	0
93	MG	1	3924	1/1	0.98	0.23	0.44	41,41,41,41	0
92	OHX	L4	401	7/7	0.97	0.30	0.43	54,54,54,54	0
92	OHX	2	1982	7/7	0.95	0.24	0.42	94,94,94,94	0
93	MG	o2	202	1/1	0.88	0.32	0.42	32,32,32,32	0
92	OHX	1	3637	7/7	0.97	0.19	0.42	75,75,75,75	0
92	OHX	5	3692	7/7	0.98	0.27	0.41	64,64,64,64	0
92	OHX	5	3560	7/7	0.97	0.17	0.39	79,79,79,79	0
92	OHX	6	1966	7/7	0.97	0.25	0.38	69,69,69,69	0
92	OHX	5	3507	7/7	0.99	0.21	0.38	52,52,52,52	0
92	OHX	7	207	7/7	0.98	0.17	0.37	59,59,59,59	0
92	OHX	2	1972	7/7	0.97	0.26	0.37	105,105,105,105	0
92	OHX	2	1957	7/7	0.98	0.28	0.37	85,85,85,85	0
92	OHX	1	3548	7/7	0.99	0.17	0.36	58,58,58,58	0
92	OHX	5	3557	7/7	0.97	0.22	0.35	83,83,83,83	0
92	OHX	2	1962	7/7	0.98	0.20	0.33	86,86,86,86	0
92	OHX	1	3601	7/7	0.99	0.23	0.33	63,63,63,63	0
92	OHX	M0	301	7/7	0.97	0.25	0.32	55,55,55,55	0
93	MG	6	2077	1/1	0.86	0.29	0.31	55,55,55,55	0
92	OHX	1	3650	7/7	0.98	0.19	0.30	64,64,64,64	0
93	MG	5	3852	1/1	0.98	0.27	0.29	41,41,41,41	0
93	MG	N6	202	1/1	0.97	0.23	0.29	37,37,37,37	0
93	MG	c6	201	1/1	0.73	0.43	0.28	90,90,90,90	0
93	MG	1	4092	1/1	0.96	0.20	0.28	33,33,33,33	0
92	OHX	2	1993	7/7	0.97	0.24	0.27	96,96,96,96	0
93	MG	1	4076	1/1	0.78	0.29	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
92	OHX	6	1991	7/7	0.97	0.20	0.26	81,81,81,81	0
92	OHX	5	3651	7/7	0.98	0.23	0.26	50,50,50,50	0
92	OHX	6	2027	7/7	0.96	0.37	0.25	91,91,91,91	0
93	MG	N8	204	1/1	0.86	0.25	0.24	44,44,44,44	0
93	MG	1	3811	1/1	0.94	0.18	0.23	40,40,40,40	0
92	OHX	8	204	7/7	0.98	0.19	0.23	58,58,58,58	0
92	OHX	m0	302	7/7	0.99	0.26	0.22	49,49,49,49	0
92	OHX	L3	401	7/7	0.98	0.20	0.22	65,65,65,65	0
92	OHX	1	3554	7/7	0.98	0.21	0.22	63,63,63,63	0
93	MG	L4	404	1/1	0.98	0.20	0.20	33,33,33,33	0
92	OHX	2	2038	7/7	0.94	0.32	0.20	95,95,95,95	0
92	OHX	2	2001	7/7	0.97	0.22	0.18	99,99,99,99	0
92	OHX	5	3579	7/7	0.98	0.17	0.16	63,63,63,63	0
92	OHX	1	3427	7/7	0.99	0.15	0.14	58,58,58,58	0
93	MG	1	3785	1/1	0.86	0.30	0.13	57,57,57,57	0
98	8AN	p	101	22/23	0.91	0.24	0.13	33,34,35,35	0
92	OHX	8	208	7/7	0.98	0.17	0.12	66,66,66,66	0
93	MG	l3	404	1/1	0.86	0.25	0.11	32,32,32,32	0
92	OHX	2	1943	7/7	0.96	0.29	0.11	101,101,101,101	0
92	OHX	l9	201	7/7	0.98	0.21	0.10	60,60,60,60	0
92	OHX	6	2014	7/7	0.97	0.25	0.10	64,64,64,64	0
92	OHX	5	3685	7/7	0.98	0.22	0.09	73,73,73,73	0
97	SPS	1	3403	23/23	0.93	0.22	0.09	37,37,48,51	0
93	MG	6	2104	1/1	0.90	0.28	0.09	90,90,90,90	0
93	MG	5	3909	1/1	0.98	0.20	0.08	31,31,31,31	0
92	OHX	6	1957	7/7	0.96	0.20	0.08	72,72,72,72	0
92	OHX	6	1980	7/7	0.94	0.18	0.07	112,112,112,112	0
92	OHX	2	2006	7/7	0.98	0.27	0.04	98,98,98,98	0
93	MG	N8	206	1/1	0.94	0.31	0.04	37,37,37,37	0
93	MG	1	4029	1/1	0.89	0.20	0.04	43,43,43,43	0
92	OHX	6	2023	7/7	0.94	0.43	0.03	91,91,91,91	0
93	MG	2	2073	1/1	0.85	0.29	0.02	93,93,93,93	0
92	OHX	5	3712	7/7	0.98	0.29	0.01	48,48,48,48	0
93	MG	7	220	1/1	0.95	0.14	-0.00	48,48,48,48	0
93	MG	2	2105	1/1	0.90	0.22	-0.00	96,96,96,96	0
92	OHX	5	3506	7/7	0.99	0.22	-0.01	39,39,39,39	0
92	OHX	5	3530	7/7	0.97	0.23	-0.01	42,42,42,42	0
92	OHX	1	3526	7/7	0.98	0.17	-0.01	77,77,77,77	0
92	OHX	5	3501	7/7	0.98	0.17	-0.01	63,63,63,63	0
93	MG	2	2098	1/1	0.71	0.21	-0.02	87,87,87,87	0
92	OHX	1	3656	7/7	0.98	0.23	-0.02	74,74,74,74	0
92	OHX	M5	302	7/7	0.98	0.22	-0.03	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	5	3603	7/7	0.99	0.22	-0.03	64,64,64,64	0
92	OHX	15	302	7/7	0.96	0.35	-0.04	70,70,70,70	0
92	OHX	5	3524	7/7	0.98	0.20	-0.06	50,50,50,50	0
92	OHX	6	1973	7/7	0.94	0.21	-0.06	68,68,68,68	0
92	OHX	1	3588	7/7	0.96	0.17	-0.06	81,81,81,81	0
92	OHX	6	1987	7/7	0.94	0.25	-0.07	89,89,89,89	0
92	OHX	2	2004	7/7	0.96	0.30	-0.07	96,96,96,96	0
92	OHX	5	3593	7/7	0.98	0.18	-0.08	54,54,54,54	0
92	OHX	1	3523	7/7	0.98	0.16	-0.09	58,58,58,58	0
93	MG	5	3770	1/1	0.94	0.19	-0.10	51,51,51,51	0
93	MG	sM	201	1/1	0.71	0.30	-0.10	45,45,45,45	0
92	OHX	5	3673	7/7	0.97	0.24	-0.11	76,76,76,76	0
93	MG	1	3738	1/1	0.90	0.21	-0.11	48,48,48,48	0
92	OHX	4	214	7/7	0.99	0.20	-0.12	70,70,70,70	0
92	OHX	6	2006	7/7	0.96	0.24	-0.12	72,72,72,72	0
92	OHX	2	1942	7/7	0.98	0.24	-0.13	84,84,84,84	0
93	MG	1	3878	1/1	0.98	0.24	-0.13	39,39,39,39	0
97	SPS	5	3403	23/23	0.93	0.24	-0.13	33,34,45,47	0
92	OHX	6	1971	7/7	0.98	0.21	-0.14	55,55,55,55	0
92	OHX	5	3552	7/7	0.97	0.20	-0.14	46,46,46,46	0
93	MG	1	4010	1/1	0.97	0.19	-0.17	37,37,37,37	0
92	OHX	5	3514	7/7	0.98	0.19	-0.18	52,52,52,52	0
92	OHX	6	1944	7/7	0.99	0.18	-0.18	71,71,71,71	0
93	MG	s4	302	1/1	0.91	0.25	-0.18	63,63,63,63	0
92	OHX	4	208	7/7	0.98	0.21	-0.20	69,69,69,69	0
92	OHX	6	1952	7/7	0.97	0.17	-0.20	80,80,80,80	0
93	MG	5	3967	1/1	0.96	0.21	-0.20	35,35,35,35	0
92	OHX	5	3555	7/7	0.99	0.18	-0.21	52,52,52,52	0
92	OHX	3	207	7/7	0.98	0.14	-0.21	68,68,68,68	0
93	MG	4	236	1/1	0.68	0.22	-0.22	43,43,43,43	0
93	MG	5	3763	1/1	0.85	0.18	-0.23	50,50,50,50	0
93	MG	1	3755	1/1	0.89	0.25	-0.23	35,35,35,35	0
93	MG	1	4012	1/1	0.96	0.16	-0.23	50,50,50,50	0
92	OHX	2	2003	7/7	0.95	0.23	-0.26	100,100,100,100	0
92	OHX	6	1989	7/7	0.96	0.34	-0.26	97,97,97,97	0
92	OHX	1	3574	7/7	0.98	0.17	-0.26	73,73,73,73	0
92	OHX	2	2000	7/7	0.97	0.23	-0.27	95,95,95,95	0
92	OHX	6	2039	7/7	0.94	0.22	-0.28	94,94,94,94	0
93	MG	O7	104	1/1	0.93	0.20	-0.28	42,42,42,42	0
92	OHX	6	1979	7/7	0.98	0.23	-0.28	62,62,62,62	0
92	OHX	5	3627	7/7	0.96	0.16	-0.29	84,84,84,84	0
92	OHX	4	205	7/7	0.99	0.19	-0.29	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
92	OHX	6	1997	7/7	0.96	0.29	-0.29	83,83,83,83	0
93	MG	5	3756	1/1	0.94	0.18	-0.30	34,34,34,34	0
92	OHX	6	1981	7/7	0.97	0.20	-0.30	87,87,87,87	0
92	OHX	1	3532	7/7	0.99	0.20	-0.30	55,55,55,55	0
92	OHX	5	3546	7/7	0.98	0.22	-0.31	49,49,49,49	0
92	OHX	5	3517	7/7	0.99	0.17	-0.31	51,51,51,51	0
92	OHX	1	3520	7/7	0.99	0.21	-0.32	53,53,53,53	0
92	OHX	5	3508	7/7	0.98	0.20	-0.33	61,61,61,61	0
93	MG	6	2060	1/1	0.96	0.22	-0.33	63,63,63,63	0
92	OHX	1	3563	7/7	0.98	0.19	-0.34	58,58,58,58	0
92	OHX	5	3621	7/7	0.98	0.18	-0.34	76,76,76,76	0
92	OHX	1	3496	7/7	0.97	0.14	-0.34	56,56,56,56	0
92	OHX	1	3530	7/7	0.97	0.21	-0.35	60,60,60,60	0
92	OHX	5	3409	7/7	0.99	0.17	-0.35	47,47,47,47	0
92	OHX	5	3566	7/7	0.99	0.16	-0.36	55,55,55,55	0
92	OHX	1	3535	7/7	0.98	0.13	-0.37	70,70,70,70	0
93	MG	6	2122	1/1	0.95	0.16	-0.37	74,74,74,74	0
92	OHX	5	3444	7/7	0.97	0.16	-0.37	51,51,51,51	0
92	OHX	5	3408	7/7	1.00	0.20	-0.38	44,44,44,44	0
93	MG	6	2112	1/1	0.96	0.22	-0.39	63,63,63,63	0
92	OHX	5	3495	7/7	0.97	0.17	-0.39	57,57,57,57	0
93	MG	5	3878	1/1	0.96	0.15	-0.39	45,45,45,45	0
93	MG	6	2149	1/1	0.94	0.20	-0.40	73,73,73,73	0
92	OHX	O7	102	7/7	0.96	0.20	-0.41	52,52,52,52	0
92	OHX	L3	402	7/7	0.97	0.19	-0.41	62,62,62,62	0
92	OHX	5	3497	7/7	0.99	0.19	-0.41	71,71,71,71	0
92	OHX	2	2022	7/7	0.97	0.24	-0.42	105,105,105,105	0
92	OHX	C7	201	7/7	0.96	0.25	-0.42	106,106,106,106	0
92	OHX	1	3503	7/7	0.98	0.19	-0.42	46,46,46,46	0
92	OHX	1	3690	7/7	0.97	0.20	-0.43	57,57,57,57	0
93	MG	1	4020	1/1	0.92	0.14	-0.43	49,49,49,49	0
92	OHX	2	1934	7/7	0.99	0.24	-0.43	94,94,94,94	0
92	OHX	5	3714	7/7	0.96	0.18	-0.44	39,39,39,39	0
92	OHX	1	3572	7/7	0.98	0.18	-0.44	64,64,64,64	0
92	OHX	2	1974	7/7	0.93	0.23	-0.44	112,112,112,112	0
92	OHX	1	3502	7/7	0.94	0.16	-0.45	66,66,66,66	0
92	OHX	1	3580	7/7	0.99	0.15	-0.46	67,67,67,67	0
92	OHX	1	3581	7/7	0.98	0.14	-0.46	79,79,79,79	0
92	OHX	5	3586	7/7	0.99	0.18	-0.47	51,51,51,51	0
92	OHX	5	3543	7/7	0.96	0.20	-0.48	53,53,53,53	0
92	OHX	s4	301	7/7	0.97	0.29	-0.49	90,90,90,90	0
92	OHX	O3	201	7/7	0.99	0.20	-0.49	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
93	MG	O4	202	1/1	0.85	0.20	-0.50	61,61,61,61	0
92	OHX	2	2050	7/7	0.93	0.20	-0.52	115,115,115,115	0
92	OHX	5	3612	7/7	0.97	0.21	-0.52	49,49,49,49	0
92	OHX	2	1983	7/7	0.98	0.20	-0.53	81,81,81,81	0
92	OHX	3	205	7/7	0.99	0.12	-0.53	69,69,69,69	0
92	OHX	5	3498	7/7	0.96	0.17	-0.56	62,62,62,62	0
92	OHX	1	3549	7/7	0.95	0.17	-0.57	91,91,91,91	0
92	OHX	5	3534	7/7	0.98	0.20	-0.58	51,51,51,51	0
92	OHX	1	3562	7/7	0.98	0.20	-0.58	64,64,64,64	0
93	MG	6	2146	1/1	0.92	0.18	-0.59	75,75,75,75	0
92	OHX	5	3584	7/7	0.99	0.16	-0.59	52,52,52,52	0
92	OHX	5	3550	7/7	0.98	0.14	-0.59	79,79,79,79	0
92	OHX	5	3476	7/7	0.96	0.20	-0.59	42,42,42,42	0
92	OHX	5	3672	7/7	0.94	0.22	-0.60	103,103,103,103	0
94	ZN	D7	101	1/1	0.71	0.28	-0.61	100,100,100,100	0
93	MG	6	2110	1/1	0.94	0.21	-0.61	91,91,91,91	0
93	MG	1	3746	1/1	0.96	0.17	-0.61	40,40,40,40	0
92	OHX	3	202	7/7	0.99	0.19	-0.61	54,54,54,54	0
92	OHX	1	3568	7/7	0.98	0.20	-0.63	45,45,45,45	0
92	OHX	2	2010	7/7	0.98	0.21	-0.63	85,85,85,85	0
93	MG	2	2090	1/1	0.95	0.17	-0.65	83,83,83,83	0
92	OHX	2	1987	7/7	0.98	0.17	-0.65	94,94,94,94	0
93	MG	6	2140	1/1	0.70	0.11	-0.65	71,71,71,71	0
92	OHX	2	1956	7/7	0.97	0.21	-0.65	92,92,92,92	0
92	OHX	5	3521	7/7	0.99	0.16	-0.65	60,60,60,60	0
92	OHX	2	2040	7/7	0.97	0.22	-0.66	97,97,97,97	0
92	OHX	1	3518	7/7	0.97	0.18	-0.66	57,57,57,57	0
92	OHX	5	3595	7/7	0.97	0.17	-0.67	76,76,76,76	0
92	OHX	1	3407	7/7	0.99	0.14	-0.68	52,52,52,52	0
92	OHX	1	3506	7/7	0.98	0.19	-0.69	66,66,66,66	0
93	MG	c9	201	1/1	0.85	0.16	-0.69	90,90,90,90	0
92	OHX	5	3456	7/7	0.98	0.20	-0.69	41,41,41,41	0
92	OHX	5	3588	7/7	0.99	0.18	-0.70	44,44,44,44	0
92	OHX	sR	401	7/7	0.95	0.21	-0.70	116,116,116,116	0
92	OHX	6	2018	7/7	0.94	0.20	-0.71	114,114,114,114	0
92	OHX	5	3722	7/7	0.95	0.26	-0.71	99,99,99,99	0
92	OHX	1	3585	7/7	0.98	0.19	-0.71	80,80,80,80	0
92	OHX	3	204	7/7	0.98	0.19	-0.72	49,49,49,49	0
92	OHX	1	3409	7/7	0.99	0.12	-0.72	41,41,41,41	0
92	OHX	2	1946	7/7	0.96	0.17	-0.72	99,99,99,99	0
92	OHX	4	204	7/7	0.98	0.15	-0.72	51,51,51,51	0
93	MG	5	4051	1/1	0.98	0.14	-0.74	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	1	3730	7/7	0.98	0.13	-0.74	60,60,60,60	0
92	OHX	6	1962	7/7	0.99	0.17	-0.75	69,69,69,69	0
92	OHX	2	1967	7/7	0.97	0.16	-0.76	85,85,85,85	0
92	OHX	5	3715	7/7	0.97	0.24	-0.76	95,95,95,95	0
93	MG	5	3960	1/1	0.96	0.19	-0.77	39,39,39,39	0
92	OHX	2	1950	7/7	0.95	0.27	-0.77	101,101,101,101	0
92	OHX	1	3517	7/7	0.98	0.13	-0.78	73,73,73,73	0
92	OHX	5	3696	7/7	0.96	0.22	-0.79	92,92,92,92	0
92	OHX	C5	201	7/7	0.93	0.24	-0.79	105,105,105,105	0
93	MG	5	4014	1/1	0.98	0.18	-0.81	35,35,35,35	0
92	OHX	6	2059	7/7	0.94	0.28	-0.81	103,103,103,103	0
92	OHX	6	1960	7/7	0.96	0.17	-0.82	77,77,77,77	0
93	MG	6	2173	1/1	0.96	0.23	-0.82	70,70,70,70	0
93	MG	6	2089	1/1	0.91	0.24	-0.83	70,70,70,70	0
93	MG	5	3979	1/1	0.91	0.15	-0.84	48,48,48,48	0
92	OHX	1	3539	7/7	0.99	0.15	-0.84	54,54,54,54	0
92	OHX	5	3486	7/7	0.99	0.17	-0.85	52,52,52,52	0
93	MG	1	3995	1/1	0.99	0.19	-0.85	46,46,46,46	0
92	OHX	1	3433	7/7	0.98	0.15	-0.85	55,55,55,55	0
92	OHX	1	3552	7/7	0.97	0.20	-0.86	60,60,60,60	0
93	MG	2	2137	1/1	0.96	0.11	-0.86	85,85,85,85	0
92	OHX	5	3538	7/7	0.98	0.18	-0.86	73,73,73,73	0
93	MG	6	2097	1/1	0.89	0.18	-0.86	92,92,92,92	0
94	ZN	d7	101	1/1	0.86	0.21	-0.86	89,89,89,89	0
92	OHX	6	1958	7/7	0.96	0.19	-0.90	89,89,89,89	0
92	OHX	6	1919	7/7	0.97	0.16	-0.90	74,74,74,74	0
92	OHX	2	2005	7/7	0.98	0.21	-0.91	84,84,84,84	0
92	OHX	7	206	7/7	0.99	0.13	-0.91	56,56,56,56	0
92	OHX	1	3565	7/7	0.99	0.16	-0.92	50,50,50,50	0
92	OHX	2	1955	7/7	0.98	0.20	-0.93	96,96,96,96	0
93	MG	2	2129	1/1	0.95	0.14	-0.93	80,80,80,80	0
92	OHX	2	1971	7/7	0.95	0.17	-0.93	108,108,108,108	0
93	MG	5	4072	1/1	0.95	0.18	-0.94	40,40,40,40	0
93	MG	2	2116	1/1	0.91	0.14	-0.94	85,85,85,85	0
92	OHX	5	3540	7/7	0.98	0.18	-0.94	55,55,55,55	0
92	OHX	3	203	7/7	0.97	0.16	-0.95	59,59,59,59	0
92	OHX	5	3483	7/7	0.98	0.14	-0.95	57,57,57,57	0
92	OHX	1	3545	7/7	0.98	0.12	-0.98	77,77,77,77	0
93	MG	o4	201	1/1	0.89	0.14	-0.98	63,63,63,63	0
92	OHX	1	3522	7/7	0.99	0.13	-0.98	62,62,62,62	0
92	OHX	5	3608	7/7	0.99	0.19	-0.98	40,40,40,40	0
92	OHX	5	3414	7/7	0.99	0.15	-1.00	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
92	OHX	2	1925	7/7	0.96	0.15	-1.00	85,85,85,85	0
92	OHX	6	1953	7/7	0.96	0.14	-1.00	109,109,109,109	0
92	OHX	1	3536	7/7	0.96	0.18	-1.01	50,50,50,50	0
92	OHX	6	1949	7/7	0.96	0.19	-1.01	81,81,81,81	0
92	OHX	5	3553	7/7	0.98	0.17	-1.02	54,54,54,54	0
92	OHX	2	1945	7/7	0.95	0.16	-1.04	90,90,90,90	0
93	MG	5	3776	1/1	0.93	0.18	-1.05	33,33,33,33	0
93	MG	5	4036	1/1	0.76	0.23	-1.05	89,89,89,89	0
92	OHX	1	3586	7/7	0.98	0.16	-1.06	74,74,74,74	0
92	OHX	1	3405	7/7	0.99	0.18	-1.07	43,43,43,43	0
92	OHX	5	3520	7/7	0.99	0.19	-1.08	48,48,48,48	0
93	MG	1	3821	1/1	0.95	0.19	-1.08	49,49,49,49	0
94	ZN	q3	501	1/1	0.99	0.12	-1.08	55,55,55,55	0
92	OHX	1	3534	7/7	0.97	0.21	-1.09	55,55,55,55	0
92	OHX	o7	503	7/7	0.97	0.12	-1.10	59,59,59,59	0
92	OHX	S8	301	7/7	0.94	0.30	-1.10	96,96,96,96	0
92	OHX	l5	301	7/7	0.98	0.17	-1.11	77,77,77,77	0
92	OHX	2	1901	7/7	0.99	0.19	-1.11	78,78,78,78	0
92	OHX	2	1926	7/7	0.95	0.14	-1.11	91,91,91,91	0
92	OHX	2	1938	7/7	0.97	0.21	-1.11	79,79,79,79	0
92	OHX	8	203	7/7	0.98	0.15	-1.12	56,56,56,56	0
92	OHX	2	1921	7/7	0.98	0.21	-1.12	97,97,97,97	0
92	OHX	5	3532	7/7	0.97	0.15	-1.12	84,84,84,84	0
92	OHX	1	3686	7/7	0.98	0.20	-1.12	65,65,65,65	0
92	OHX	o7	502	7/7	0.99	0.13	-1.15	54,54,54,54	0
92	OHX	5	3469	7/7	0.97	0.11	-1.15	63,63,63,63	0
92	OHX	2	1948	7/7	0.96	0.18	-1.16	80,80,80,80	0
93	MG	2	2102	1/1	0.93	0.20	-1.16	98,98,98,98	0
92	OHX	6	1908	7/7	0.99	0.13	-1.17	65,65,65,65	0
92	OHX	1	3484	7/7	0.99	0.11	-1.17	72,72,72,72	0
92	OHX	1	3511	7/7	0.98	0.20	-1.17	58,58,58,58	0
94	ZN	d9	101	1/1	0.99	0.10	-1.18	97,97,97,97	0
92	OHX	6	1912	7/7	0.99	0.10	-1.20	74,74,74,74	0
92	OHX	m0	301	7/7	0.96	0.21	-1.20	68,68,68,68	0
92	OHX	6	1938	7/7	0.98	0.12	-1.20	76,76,76,76	0
92	OHX	1	3513	7/7	0.98	0.19	-1.20	48,48,48,48	0
92	OHX	5	3404	7/7	0.99	0.13	-1.21	43,43,43,43	0
93	MG	8	223	1/1	0.98	0.13	-1.23	47,47,47,47	0
92	OHX	M5	301	7/7	0.99	0.12	-1.24	46,46,46,46	0
92	OHX	2	1913	7/7	0.99	0.14	-1.24	84,84,84,84	0
92	OHX	1	3457	7/7	0.98	0.11	-1.24	73,73,73,73	0
92	OHX	1	3638	7/7	0.94	0.18	-1.24	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	1	3901	1/1	0.90	0.19	-1.25	31,31,31,31	0
92	OHX	1	3531	7/7	0.99	0.15	-1.25	89,89,89,89	0
92	OHX	s8	301	7/7	0.97	0.27	-1.25	96,96,96,96	0
92	OHX	5	3478	7/7	0.97	0.13	-1.25	56,56,56,56	0
92	OHX	5	3519	7/7	0.96	0.14	-1.25	78,78,78,78	0
93	MG	1	3972	1/1	0.98	0.21	-1.26	44,44,44,44	0
92	OHX	6	1921	7/7	0.98	0.17	-1.26	64,64,64,64	0
92	OHX	6	1956	7/7	0.98	0.12	-1.27	79,79,79,79	0
92	OHX	5	3504	7/7	0.96	0.14	-1.27	61,61,61,61	0
92	OHX	6	1920	7/7	0.96	0.15	-1.28	95,95,95,95	0
92	OHX	5	3430	7/7	0.99	0.14	-1.30	47,47,47,47	0
93	MG	M0	302	1/1	0.86	0.12	-1.30	46,46,46,46	0
92	OHX	2	1910	7/7	0.98	0.10	-1.30	89,89,89,89	0
92	OHX	2	1915	7/7	0.95	0.13	-1.31	99,99,99,99	0
92	OHX	1	3582	7/7	0.98	0.18	-1.31	53,53,53,53	0
93	MG	6	2099	1/1	0.94	0.21	-1.34	65,65,65,65	0
92	OHX	7	202	7/7	0.98	0.12	-1.34	52,52,52,52	0
92	OHX	1	3533	7/7	0.99	0.14	-1.37	48,48,48,48	0
93	MG	2	2113	1/1	0.78	0.26	-1.37	101,101,101,101	0
92	OHX	1	3472	7/7	0.98	0.10	-1.39	62,62,62,62	0
93	MG	1	3754	1/1	0.97	0.14	-1.39	45,45,45,45	0
94	ZN	Q3	501	1/1	0.99	0.07	-1.40	55,55,55,55	0
92	OHX	5	3411	7/7	0.99	0.15	-1.40	45,45,45,45	0
92	OHX	5	3738	7/7	0.95	0.15	-1.41	56,56,56,56	0
92	OHX	1	3443	7/7	0.99	0.12	-1.44	58,58,58,58	0
92	OHX	6	1939	7/7	0.95	0.14	-1.46	102,102,102,102	0
92	OHX	1	3463	7/7	0.98	0.10	-1.47	80,80,80,80	0
93	MG	2	2093	1/1	0.88	0.14	-1.47	81,81,81,81	0
92	OHX	6	2000	7/7	0.99	0.19	-1.49	69,69,69,69	0
92	OHX	4	206	7/7	0.98	0.13	-1.49	49,49,49,49	0
92	OHX	1	3460	7/7	0.99	0.11	-1.50	44,44,44,44	0
92	OHX	1	3606	7/7	0.98	0.12	-1.51	63,63,63,63	0
92	OHX	2	1924	7/7	0.99	0.08	-1.55	103,103,103,103	0
93	MG	C8	202	1/1	0.91	0.06	-1.56	94,94,94,94	0
94	ZN	d6	101	1/1	0.99	0.07	-1.56	67,67,67,67	0
93	MG	6	2179	1/1	0.99	0.12	-1.56	93,93,93,93	0
92	OHX	2	2039	7/7	0.93	0.21	-1.58	133,133,133,133	0
93	MG	5	4153	1/1	1.00	0.13	-1.59	37,37,37,37	0
92	OHX	1	3512	7/7	0.99	0.13	-1.61	45,45,45,45	0
92	OHX	6	1972	7/7	0.99	0.12	-1.61	67,67,67,67	0
94	ZN	Q0	500	1/1	0.98	0.10	-1.61	47,47,47,47	0
92	OHX	1	3697	7/7	0.98	0.14	-1.61	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
92	OHX	2	1966	7/7	0.98	0.17	-1.62	65,65,65,65	0
92	OHX	1	3441	7/7	0.98	0.18	-1.62	44,44,44,44	0
94	ZN	D9	101	1/1	0.98	0.07	-1.62	90,90,90,90	0
92	OHX	5	3541	7/7	0.97	0.10	-1.63	93,93,93,93	0
92	OHX	m5	302	7/7	0.99	0.17	-1.64	66,66,66,66	0
93	MG	1	3776	1/1	0.98	0.12	-1.64	44,44,44,44	0
92	OHX	6	1975	7/7	0.96	0.15	-1.64	93,93,93,93	0
92	OHX	6	1926	7/7	0.99	0.17	-1.65	67,67,67,67	0
93	MG	5	3769	1/1	0.92	0.16	-1.66	43,43,43,43	0
92	OHX	1	3498	7/7	0.98	0.15	-1.67	74,74,74,74	0
92	OHX	1	3529	7/7	0.98	0.12	-1.67	79,79,79,79	0
92	OHX	5	3450	7/7	0.99	0.11	-1.68	58,58,58,58	0
92	OHX	6	1927	7/7	0.95	0.11	-1.68	109,109,109,109	0
92	OHX	1	3482	7/7	0.97	0.15	-1.69	66,66,66,66	0
92	OHX	2	1917	7/7	0.98	0.15	-1.70	83,83,83,83	0
93	MG	5	3842	1/1	0.98	0.17	-1.70	35,35,35,35	0
92	OHX	5	3443	7/7	0.99	0.12	-1.71	59,59,59,59	0
92	OHX	1	3493	7/7	0.97	0.21	-1.72	61,61,61,61	0
92	OHX	l3	401	7/7	0.99	0.11	-1.73	52,52,52,52	0
92	OHX	6	1907	7/7	0.98	0.13	-1.73	77,77,77,77	0
92	OHX	2	1973	7/7	0.96	0.13	-1.74	112,112,112,112	0
93	MG	1	3747	1/1	0.94	0.13	-1.75	48,48,48,48	0
92	OHX	6	2056	7/7	0.94	0.16	-1.75	99,99,99,99	0
92	OHX	5	3525	7/7	0.97	0.12	-1.76	75,75,75,75	0
92	OHX	5	3516	7/7	0.98	0.17	-1.76	47,47,47,47	0
92	OHX	5	3600	7/7	0.97	0.15	-1.76	83,83,83,83	0
93	MG	O7	106	1/1	0.97	0.12	-1.77	46,46,46,46	0
92	OHX	2	1923	7/7	0.98	0.11	-1.79	84,84,84,84	0
92	OHX	o3	201	7/7	0.98	0.16	-1.81	54,54,54,54	0
92	OHX	6	1951	7/7	0.96	0.14	-1.82	119,119,119,119	0
92	OHX	1	3426	7/7	0.99	0.10	-1.82	50,50,50,50	0
93	MG	6	2159	1/1	0.80	0.15	-1.82	88,88,88,88	0
94	ZN	O7	101	1/1	0.99	0.07	-1.83	39,39,39,39	0
92	OHX	1	3428	7/7	0.98	0.09	-1.84	52,52,52,52	0
92	OHX	7	201	7/7	0.99	0.07	-1.85	49,49,49,49	0
93	MG	5	4012	1/1	0.75	0.12	-1.86	44,44,44,44	0
93	MG	n8	201	1/1	0.90	0.12	-1.86	43,43,43,43	0
93	MG	5	3985	1/1	0.87	0.14	-1.87	41,41,41,41	0
92	OHX	5	3512	7/7	0.98	0.17	-1.87	42,42,42,42	0
92	OHX	6	1931	7/7	0.94	0.18	-1.87	86,86,86,86	0
92	OHX	L6	201	7/7	0.99	0.15	-1.87	44,44,44,44	0
92	OHX	1	3453	7/7	0.98	0.12	-1.88	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
92	OHX	5	3464	7/7	0.99	0.09	-1.89	50,50,50,50	0
92	OHX	2	1949	7/7	0.98	0.10	-1.89	94,94,94,94	0
93	MG	L7	301	1/1	0.98	0.16	-1.91	37,37,37,37	0
92	OHX	6	1902	7/7	0.97	0.14	-1.92	91,91,91,91	0
92	OHX	5	3436	7/7	0.99	0.10	-1.96	64,64,64,64	0
93	MG	5	3826	1/1	0.97	0.16	-1.97	45,45,45,45	0
92	OHX	1	3486	7/7	0.98	0.12	-1.98	69,69,69,69	0
92	OHX	5	3458	7/7	0.98	0.13	-1.98	57,57,57,57	0
94	ZN	q2	501	1/1	0.95	0.09	-1.99	47,47,47,47	0
93	MG	2	2120	1/1	0.96	0.05	-2.02	95,95,95,95	0
92	OHX	1	3577	7/7	0.99	0.13	-2.02	60,60,60,60	0
92	OHX	1	3540	7/7	0.99	0.16	-2.03	52,52,52,52	0
92	OHX	6	1955	7/7	0.99	0.08	-2.04	108,108,108,108	0
94	ZN	o7	501	1/1	0.99	0.09	-2.06	41,41,41,41	0
92	OHX	s1	301	7/7	0.98	0.14	-2.07	77,77,77,77	0
92	OHX	1	3494	7/7	0.99	0.14	-2.07	42,42,42,42	0
92	OHX	6	1901	7/7	0.99	0.15	-2.08	59,59,59,59	0
92	OHX	1	3418	7/7	0.99	0.18	-2.08	52,52,52,52	0
92	OHX	2	1907	7/7	0.98	0.12	-2.09	93,93,93,93	0
92	OHX	7	205	7/7	0.98	0.12	-2.09	55,55,55,55	0
92	OHX	m5	301	7/7	0.99	0.13	-2.09	48,48,48,48	0
94	ZN	q0	500	1/1	0.99	0.13	-2.10	37,37,37,37	0
92	OHX	2	1911	7/7	0.98	0.10	-2.10	98,98,98,98	0
92	OHX	5	3417	7/7	0.99	0.11	-2.11	43,43,43,43	0
92	OHX	6	1945	7/7	0.98	0.15	-2.14	72,72,72,72	0
92	OHX	2	1903	7/7	0.96	0.14	-2.17	95,95,95,95	0
92	OHX	5	3500	7/7	0.98	0.11	-2.20	72,72,72,72	0
92	OHX	2	1975	7/7	0.95	0.13	-2.21	77,77,77,77	0
92	OHX	1	3731	7/7	0.95	0.16	-2.22	94,94,94,94	0
92	OHX	6	1922	7/7	0.99	0.14	-2.22	60,60,60,60	0
93	MG	5	4044	1/1	0.98	0.15	-2.22	35,35,35,35	0
92	OHX	5	3515	7/7	0.98	0.11	-2.23	85,85,85,85	0
92	OHX	5	3472	7/7	0.98	0.10	-2.23	66,66,66,66	0
93	MG	5	3943	1/1	0.98	0.16	-2.23	41,41,41,41	0
92	OHX	Q2	502	7/7	1.00	0.05	-2.24	41,41,41,41	0
92	OHX	2	1902	7/7	0.99	0.13	-2.25	81,81,81,81	0
92	OHX	6	1923	7/7	0.97	0.12	-2.26	81,81,81,81	0
92	OHX	2	1914	7/7	0.99	0.09	-2.26	78,78,78,78	0
92	OHX	1	3471	7/7	0.99	0.12	-2.30	48,48,48,48	0
92	OHX	6	1946	7/7	0.98	0.14	-2.31	79,79,79,79	0
92	OHX	5	3482	7/7	0.99	0.08	-2.31	49,49,49,49	0
93	MG	6	2177	1/1	0.93	0.10	-2.32	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	5	3433	7/7	0.99	0.17	-2.34	45,45,45,45	0
92	OHX	5	3529	7/7	0.99	0.14	-2.34	42,42,42,42	0
92	OHX	6	1950	7/7	0.99	0.14	-2.34	90,90,90,90	0
92	OHX	1	3422	7/7	0.99	0.13	-2.35	57,57,57,57	0
92	OHX	5	3490	7/7	0.99	0.11	-2.35	53,53,53,53	0
94	ZN	E1	501	1/1	0.93	0.06	-2.36	109,109,109,109	0
92	OHX	6	2052	7/7	0.97	0.13	-2.36	65,65,65,65	0
92	OHX	m6	201	7/7	0.98	0.10	-2.39	48,48,48,48	0
93	MG	5	3812	1/1	0.95	0.14	-2.39	89,89,89,89	0
92	OHX	1	3516	7/7	0.99	0.14	-2.42	39,39,39,39	0
92	OHX	5	3418	7/7	0.99	0.12	-2.42	41,41,41,41	0
94	ZN	Q2	501	1/1	0.99	0.03	-2.44	51,51,51,51	0
92	OHX	2	1951	7/7	0.97	0.13	-2.46	82,82,82,82	0
92	OHX	6	1918	7/7	0.99	0.08	-2.46	49,49,49,49	0
92	OHX	6	1911	7/7	0.99	0.08	-2.50	57,57,57,57	0
92	OHX	5	3460	7/7	0.99	0.08	-2.51	46,46,46,46	0
92	OHX	5	3452	7/7	0.98	0.11	-2.52	63,63,63,63	0
92	OHX	M6	201	7/7	0.99	0.12	-2.53	54,54,54,54	0
92	OHX	5	3457	7/7	0.98	0.09	-2.54	58,58,58,58	0
92	OHX	5	3502	7/7	0.96	0.14	-2.56	59,59,59,59	0
92	OHX	5	3575	7/7	0.98	0.16	-2.58	55,55,55,55	0
92	OHX	5	3465	7/7	0.99	0.06	-2.60	57,57,57,57	0
92	OHX	5	3451	7/7	0.99	0.10	-2.60	65,65,65,65	0
92	OHX	1	3500	7/7	0.99	0.10	-2.61	40,40,40,40	0
92	OHX	1	3573	7/7	0.98	0.19	-2.63	60,60,60,60	0
93	MG	5	4093	1/1	1.00	0.12	-2.63	32,32,32,32	0
92	OHX	1	3411	7/7	0.99	0.14	-2.66	48,48,48,48	0
92	OHX	5	3503	7/7	0.98	0.16	-2.66	44,44,44,44	0
92	OHX	SR	401	7/7	0.92	0.21	-2.68	121,121,121,121	0
92	OHX	5	3748	7/7	0.97	0.14	-2.69	92,92,92,92	0
92	OHX	1	3514	7/7	0.99	0.14	-2.69	52,52,52,52	0
92	OHX	6	1906	7/7	0.99	0.13	-2.71	60,60,60,60	0
92	OHX	1	3416	7/7	0.99	0.11	-2.73	53,53,53,53	0
92	OHX	1	3447	7/7	0.97	0.15	-2.73	53,53,53,53	0
92	OHX	1	3404	7/7	1.00	0.14	-2.73	37,37,37,37	0
92	OHX	5	3474	7/7	0.98	0.15	-2.74	46,46,46,46	0
92	OHX	6	1954	7/7	0.98	0.10	-2.76	116,116,116,116	0
92	OHX	5	3511	7/7	0.99	0.07	-2.80	35,35,35,35	0
92	OHX	1	3434	7/7	0.98	0.14	-2.81	52,52,52,52	0
93	MG	c8	203	1/1	0.98	0.07	-2.81	86,86,86,86	0
92	OHX	5	3475	7/7	0.97	0.14	-2.86	47,47,47,47	0
92	OHX	2	1969	7/7	0.98	0.08	-2.90	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	2	1916	7/7	0.98	0.10	-2.91	84,84,84,84	0
92	OHX	6	1943	7/7	0.98	0.11	-2.93	102,102,102,102	0
92	OHX	5	3494	7/7	0.99	0.12	-2.95	51,51,51,51	0
92	OHX	5	3412	7/7	0.99	0.10	-2.96	44,44,44,44	0
92	OHX	6	1904	7/7	0.99	0.09	-2.99	68,68,68,68	0
93	MG	5	3955	1/1	0.96	0.16	-2.99	41,41,41,41	0
92	OHX	1	3449	7/7	0.99	0.06	-3.01	54,54,54,54	0
92	OHX	5	3462	7/7	0.98	0.10	-3.02	44,44,44,44	0
92	OHX	1	3448	7/7	0.99	0.13	-3.03	54,54,54,54	0
93	MG	M5	303	1/1	0.94	0.13	-3.05	37,37,37,37	0
92	OHX	6	1947	7/7	0.98	0.15	-3.06	71,71,71,71	0
92	OHX	2	2008	7/7	0.98	0.12	-3.08	106,106,106,106	0
92	OHX	6	1928	7/7	0.97	0.15	-3.10	105,105,105,105	0
92	OHX	5	3561	7/7	0.99	0.12	-3.11	41,41,41,41	0
92	OHX	5	3415	7/7	1.00	0.10	-3.12	42,42,42,42	0
93	MG	1	3927	1/1	0.95	0.12	-3.13	38,38,38,38	0
92	OHX	N9	101	7/7	0.99	0.11	-3.15	42,42,42,42	0
92	OHX	5	3406	7/7	0.99	0.18	-3.16	36,36,36,36	0
92	OHX	1	3452	7/7	0.98	0.09	-3.17	65,65,65,65	0
92	OHX	7	203	7/7	0.98	0.12	-3.17	48,48,48,48	0
92	OHX	5	3422	7/7	0.99	0.09	-3.18	44,44,44,44	0
92	OHX	1	3432	7/7	0.98	0.18	-3.19	46,46,46,46	0
92	OHX	6	1913	7/7	0.99	0.07	-3.21	80,80,80,80	0
92	OHX	1	3490	7/7	0.98	0.16	-3.24	51,51,51,51	0
92	OHX	1	3455	7/7	0.98	0.10	-3.27	65,65,65,65	0
92	OHX	5	3461	7/7	0.98	0.09	-3.27	48,48,48,48	0
92	OHX	2	1909	7/7	0.95	0.13	-3.28	97,97,97,97	0
92	OHX	1	3473	7/7	0.99	0.09	-3.34	62,62,62,62	0
94	ZN	e1	501	1/1	0.80	0.06	-3.35	130,130,130,130	0
92	OHX	4	201	7/7	1.00	0.13	-3.35	41,41,41,41	0
92	OHX	1	3466	7/7	0.98	0.12	-3.40	70,70,70,70	0
92	OHX	2	1981	7/7	0.98	0.16	-3.40	75,75,75,75	0
92	OHX	5	3442	7/7	0.99	0.07	-3.40	57,57,57,57	0
92	OHX	5	3702	7/7	0.98	0.15	-3.40	50,50,50,50	0
92	OHX	7	204	7/7	0.99	0.14	-3.44	45,45,45,45	0
92	OHX	1	3479	7/7	0.99	0.15	-3.45	51,51,51,51	0
92	OHX	2	1905	7/7	0.99	0.14	-3.45	76,76,76,76	0
92	OHX	5	3505	7/7	0.99	0.09	-3.49	52,52,52,52	0
92	OHX	2	1964	7/7	0.98	0.14	-3.50	97,97,97,97	0
92	OHX	1	3488	7/7	0.98	0.11	-3.53	68,68,68,68	0
92	OHX	1	3481	7/7	0.98	0.10	-3.54	48,48,48,48	0
92	OHX	6	1910	7/7	0.99	0.12	-3.54	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
92	OHX	1	3470	7/7	0.99	0.16	-3.57	82,82,82,82	0
92	OHX	1	3406	7/7	0.99	0.13	-3.57	43,43,43,43	0
92	OHX	1	3435	7/7	0.99	0.12	-3.57	58,58,58,58	0
92	OHX	1	3419	7/7	0.99	0.16	-3.58	52,52,52,52	0
92	OHX	6	1924	7/7	0.98	0.09	-3.58	63,63,63,63	0
92	OHX	5	3484	7/7	0.99	0.13	-3.61	43,43,43,43	0
92	OHX	1	3478	7/7	0.99	0.14	-3.63	51,51,51,51	0
92	OHX	n9	101	7/7	0.99	0.07	-3.63	41,41,41,41	0
92	OHX	5	3480	7/7	0.98	0.09	-3.66	52,52,52,52	0
92	OHX	1	3430	7/7	0.99	0.10	-3.66	55,55,55,55	0
92	OHX	1	3412	7/7	0.99	0.09	-3.66	43,43,43,43	0
92	OHX	1	3515	7/7	0.98	0.16	-3.67	56,56,56,56	0
92	OHX	5	3405	7/7	0.99	0.14	-3.68	36,36,36,36	0
92	OHX	5	3454	7/7	0.99	0.07	-3.68	91,91,91,91	0
92	OHX	1	3485	7/7	0.98	0.10	-3.72	78,78,78,78	0
92	OHX	2	1904	7/7	0.98	0.08	-3.73	83,83,83,83	0
92	OHX	1	3501	7/7	0.98	0.14	-3.73	62,62,62,62	0
92	OHX	5	3499	7/7	0.98	0.15	-3.74	50,50,50,50	0
92	OHX	1	3461	7/7	0.98	0.10	-3.75	58,58,58,58	0
92	OHX	6	1932	7/7	0.97	0.14	-3.76	59,59,59,59	0
92	OHX	1	3425	7/7	0.99	0.12	-3.77	55,55,55,55	0
92	OHX	2	1940	7/7	0.98	0.08	-3.81	94,94,94,94	0
92	OHX	5	3610	7/7	0.99	0.14	-3.81	57,57,57,57	0
92	OHX	5	3407	7/7	1.00	0.13	-3.83	38,38,38,38	0
92	OHX	2	1918	7/7	0.96	0.14	-3.85	83,83,83,83	0
92	OHX	5	3446	7/7	0.99	0.12	-3.86	45,45,45,45	0
92	OHX	2	1908	7/7	0.97	0.10	-3.86	95,95,95,95	0
94	ZN	D6	500	1/1	0.98	0.03	-3.87	87,87,87,87	0
92	OHX	2	1935	7/7	0.97	0.12	-3.94	82,82,82,82	0
92	OHX	6	1914	7/7	0.97	0.12	-3.94	61,61,61,61	0
92	OHX	1	3444	7/7	0.99	0.07	-4.03	53,53,53,53	0
92	OHX	5	3439	7/7	0.99	0.08	-4.04	46,46,46,46	0
92	OHX	5	3489	7/7	0.99	0.11	-4.16	41,41,41,41	0
92	OHX	2	1936	7/7	0.97	0.12	-4.16	102,102,102,102	0
92	OHX	1	3439	7/7	0.99	0.11	-4.16	56,56,56,56	0
92	OHX	1	3408	7/7	1.00	0.10	-4.17	41,41,41,41	0
92	OHX	1	3544	7/7	0.99	0.14	-4.17	72,72,72,72	0
92	OHX	5	3426	7/7	1.00	0.06	-4.21	52,52,52,52	0
92	OHX	8	202	7/7	0.99	0.11	-4.21	40,40,40,40	0
92	OHX	2	1912	7/7	0.99	0.07	-4.21	93,93,93,93	0
93	MG	1	4060	1/1	0.97	0.09	-4.31	46,46,46,46	0
92	OHX	6	1929	7/7	0.98	0.11	-4.32	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	5	3438	7/7	0.99	0.09	-4.33	46,46,46,46	0
92	OHX	1	3417	7/7	1.00	0.07	-4.41	38,38,38,38	0
92	OHX	1	3465	7/7	0.96	0.12	-4.42	66,66,66,66	0
92	OHX	1	3483	7/7	0.98	0.12	-4.45	57,57,57,57	0
92	OHX	1	3415	7/7	0.99	0.07	-4.47	47,47,47,47	0
92	OHX	1	3424	7/7	0.99	0.10	-4.49	61,61,61,61	0
92	OHX	1	3630	7/7	0.99	0.12	-4.58	50,50,50,50	0
92	OHX	5	3427	7/7	0.99	0.14	-4.60	51,51,51,51	0
92	OHX	5	3424	7/7	0.99	0.10	-4.62	54,54,54,54	0
92	OHX	5	3440	7/7	0.99	0.09	-4.63	43,43,43,43	0
92	OHX	1	3469	7/7	0.98	0.11	-4.65	56,56,56,56	0
92	OHX	1	3429	7/7	1.00	0.07	-4.70	47,47,47,47	0
92	OHX	1	3446	7/7	0.98	0.09	-4.70	47,47,47,47	0
92	OHX	5	3463	7/7	0.97	0.14	-4.77	48,48,48,48	0
92	OHX	6	1903	7/7	0.99	0.12	-4.77	61,61,61,61	0
92	OHX	5	3445	7/7	0.99	0.08	-4.78	51,51,51,51	0
92	OHX	1	3431	7/7	0.99	0.08	-4.85	43,43,43,43	0
92	OHX	2	1922	7/7	0.99	0.06	-4.88	83,83,83,83	0
93	MG	1	3802	1/1	0.99	0.13	-4.90	37,37,37,37	0
92	OHX	5	3615	7/7	0.99	0.11	-4.90	47,47,47,47	0
92	OHX	q2	502	7/7	0.99	0.08	-4.94	45,45,45,45	0
92	OHX	1	3438	7/7	0.99	0.06	-4.99	47,47,47,47	0
92	OHX	1	3462	7/7	0.99	0.08	-5.01	43,43,43,43	0
92	OHX	5	3420	7/7	0.99	0.10	-5.04	50,50,50,50	0
93	MG	6	2158	1/1	0.96	0.05	-5.06	54,54,54,54	0
92	OHX	5	3487	7/7	0.98	0.12	-5.09	53,53,53,53	0
92	OHX	5	3453	7/7	0.99	0.09	-5.11	55,55,55,55	0
92	OHX	5	3493	7/7	0.99	0.10	-5.16	48,48,48,48	0
92	OHX	6	1933	7/7	0.98	0.11	-5.19	98,98,98,98	0
92	OHX	4	203	7/7	0.98	0.10	-5.20	49,49,49,49	0
92	OHX	2	1919	7/7	0.99	0.07	-5.21	73,73,73,73	0
92	OHX	5	3577	7/7	0.99	0.13	-5.26	50,50,50,50	0
92	OHX	1	3421	7/7	0.99	0.10	-5.29	59,59,59,59	0
92	OHX	5	3432	7/7	0.99	0.10	-5.42	46,46,46,46	0
92	OHX	1	3499	7/7	0.98	0.12	-5.61	50,50,50,50	0
92	OHX	5	3523	7/7	0.99	0.12	-5.63	61,61,61,61	0
92	OHX	5	3481	7/7	0.98	0.10	-5.74	49,49,49,49	0
93	MG	1	3764	1/1	0.98	0.07	-5.78	50,50,50,50	0
92	OHX	1	3527	7/7	0.98	0.14	-5.78	69,69,69,69	0
92	OHX	5	3467	7/7	0.99	0.10	-5.80	45,45,45,45	0
92	OHX	1	3451	7/7	0.98	0.10	-5.84	62,62,62,62	0
92	OHX	5	3485	7/7	0.99	0.11	-5.84	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	5	3421	7/7	0.98	0.14	-5.85	44,44,44,44	0
92	OHX	1	3475	7/7	0.97	0.11	-5.98	51,51,51,51	0
92	OHX	5	3466	7/7	0.99	0.08	-6.06	56,56,56,56	0
92	OHX	1	3467	7/7	0.99	0.11	-6.41	43,43,43,43	0
92	OHX	5	3434	7/7	1.00	0.06	-6.54	39,39,39,39	0
92	OHX	6	1909	7/7	0.99	0.09	-6.55	91,91,91,91	0
92	OHX	5	3522	7/7	0.99	0.15	-6.67	47,47,47,47	0
92	OHX	1	3420	7/7	1.00	0.06	-6.67	38,38,38,38	0
92	OHX	6	1917	7/7	0.99	0.07	-6.87	55,55,55,55	0
92	OHX	1	3487	7/7	0.99	0.09	-6.88	57,57,57,57	0
92	OHX	5	3429	7/7	1.00	0.06	-6.95	37,37,37,37	0
92	OHX	5	3419	7/7	1.00	0.12	-7.01	40,40,40,40	0
92	OHX	1	3414	7/7	0.99	0.09	-7.09	45,45,45,45	0
92	OHX	6	1915	7/7	0.99	0.09	-7.17	62,62,62,62	0
92	OHX	5	3488	7/7	0.99	0.10	-7.30	47,47,47,47	0
93	MG	1	3928	1/1	0.94	0.15	-7.37	56,56,56,56	0
92	OHX	5	3441	7/7	0.99	0.06	-7.76	45,45,45,45	0
92	OHX	1	3413	7/7	0.99	0.09	-7.89	51,51,51,51	0
92	OHX	5	3416	7/7	0.99	0.09	-7.95	42,42,42,42	0
92	OHX	5	3492	7/7	1.00	0.06	-8.19	46,46,46,46	0
92	OHX	5	3428	7/7	0.99	0.05	-8.24	41,41,41,41	0
92	OHX	5	3410	7/7	0.99	0.13	-8.61	43,43,43,43	0
92	OHX	5	3473	7/7	0.98	0.09	-9.49	63,63,63,63	0
92	OHX	1	3474	7/7	0.99	0.09	-9.87	55,55,55,55	0
92	OHX	1	3423	7/7	0.99	0.10	-10.60	55,55,55,55	0
92	OHX	5	3431	7/7	1.00	0.08	-10.98	53,53,53,53	0
93	MG	5	3751	1/1	0.88	0.70	-	60,60,60,60	0
92	OHX	1	3584	7/7	0.98	0.36	-	78,78,78,78	0
93	MG	6	2157	1/1	0.96	0.29	-	57,57,57,57	0
93	MG	5	4136	1/1	0.93	0.24	-	36,36,36,36	0
93	MG	3	214	1/1	0.96	0.42	-	59,59,59,59	0
93	MG	2	2106	1/1	0.63	0.24	-	96,96,96,96	0
92	OHX	2	1997	7/7	0.97	0.22	-	96,96,96,96	0
92	OHX	2	2013	7/7	0.95	0.22	-	104,104,104,104	0
93	MG	N3	202	1/1	0.96	0.16	-	51,51,51,51	0
92	OHX	5	3614	7/7	0.96	0.17	-	71,71,71,71	0
92	OHX	5	3708	7/7	0.97	0.41	-	67,67,67,67	0
92	OHX	5	3728	7/7	0.97	0.30	-	71,71,71,71	0
92	OHX	1	3595	7/7	0.94	0.39	-	68,68,68,68	0
92	OHX	5	3677	7/7	0.98	0.25	-	66,66,66,66	0
93	MG	1	3926	1/1	0.94	0.35	-	39,39,39,39	0
93	MG	1	3973	1/1	0.92	0.34	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	5	3880	1/1	0.93	0.86	-	37,37,37,37	0
92	OHX	6	2020	7/7	0.97	0.28	-	94,94,94,94	0
93	MG	1	3963	1/1	0.91	0.63	-	54,54,54,54	0
92	OHX	6	1982	7/7	0.97	0.18	-	96,96,96,96	0
93	MG	5	4137	1/1	0.88	0.46	-	38,38,38,38	0
93	MG	1	4122	1/1	0.90	0.31	-	39,39,39,39	0
93	MG	6	2138	1/1	0.88	0.12	-	82,82,82,82	0
92	OHX	1	3553	7/7	0.95	0.26	-	58,58,58,58	0
93	MG	1	3871	1/1	0.89	0.46	-	52,52,52,52	0
92	OHX	5	3572	7/7	0.98	0.22	-	61,61,61,61	0
93	MG	5	4121	1/1	0.95	0.14	-	41,41,41,41	0
93	MG	2	2097	1/1	0.94	0.17	-	118,118,118,118	0
93	MG	1	3818	1/1	0.75	0.42	-	51,51,51,51	0
93	MG	5	3907	1/1	0.95	0.82	-	38,38,38,38	0
93	MG	1	3771	1/1	0.94	0.49	-	41,41,41,41	0
93	MG	1	4058	1/1	0.94	0.78	-	38,38,38,38	0
92	OHX	4	202	7/7	0.99	0.13	-	47,47,47,47	0
93	MG	5	3841	1/1	0.95	0.24	-	35,35,35,35	0
92	OHX	1	3632	7/7	0.98	0.28	-	88,88,88,88	0
93	MG	5	4154	1/1	0.83	0.27	-	46,46,46,46	0
92	OHX	1	3567	7/7	0.99	0.15	-	71,71,71,71	0
92	OHX	5	3448	7/7	0.99	0.08	-	41,41,41,41	0
92	OHX	1	3541	7/7	0.96	0.22	-	66,66,66,66	0
92	OHX	6	2001	7/7	0.96	0.26	-	93,93,93,93	0
93	MG	5	3919	1/1	0.86	0.59	-	32,32,32,32	0
93	MG	O7	103	1/1	0.94	0.20	-	40,40,40,40	0
93	MG	5	3843	1/1	0.97	0.53	-	43,43,43,43	0
93	MG	1	3873	1/1	0.94	0.48	-	41,41,41,41	0
93	MG	5	3795	1/1	0.94	0.27	-	62,62,62,62	0
93	MG	5	4144	1/1	0.94	0.15	-	38,38,38,38	0
93	MG	1	3756	1/1	0.95	0.42	-	54,54,54,54	0
93	MG	1	3953	1/1	0.64	0.37	-	48,48,48,48	0
93	MG	1	4050	1/1	0.92	0.37	-	47,47,47,47	0
93	MG	1	3895	1/1	0.96	0.63	-	42,42,42,42	0
92	OHX	2	1958	7/7	0.96	0.19	-	109,109,109,109	0
92	OHX	5	3731	7/7	0.95	0.29	-	97,97,97,97	0
93	MG	5	3977	1/1	0.97	0.32	-	35,35,35,35	0
92	OHX	1	3666	7/7	0.97	0.25	-	87,87,87,87	0
93	MG	6	2086	1/1	0.41	0.26	-	75,75,75,75	0
93	MG	5	4065	1/1	0.97	0.16	-	38,38,38,38	0
93	MG	M3	1000	1/1	0.87	0.35	-	64,64,64,64	0
92	OHX	6	2022	7/7	0.97	0.39	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	2	2112	1/1	0.80	0.58	-	83,83,83,83	0
93	MG	5	4046	1/1	0.95	0.52	-	47,47,47,47	0
93	MG	1	3744	1/1	0.69	0.41	-	52,52,52,52	0
93	MG	1	3805	1/1	0.88	0.14	-	58,58,58,58	0
93	MG	5	4109	1/1	0.81	0.70	-	42,42,42,42	0
92	OHX	5	3736	7/7	0.97	0.37	-	81,81,81,81	0
93	MG	5	3891	1/1	0.91	0.51	-	39,39,39,39	0
93	MG	5	4149	1/1	0.91	0.22	-	37,37,37,37	0
92	OHX	2	1989	7/7	0.96	0.17	-	93,93,93,93	0
93	MG	4	226	1/1	0.89	0.54	-	40,40,40,40	0
92	OHX	1	3708	7/7	0.95	0.24	-	114,114,114,114	0
93	MG	2	2066	1/1	0.93	0.75	-	72,72,72,72	0
93	MG	2	2094	1/1	0.29	0.71	-	81,81,81,81	0
93	MG	1	4094	1/1	0.70	0.63	-	55,55,55,55	0
93	MG	1	3862	1/1	0.96	0.72	-	38,38,38,38	0
92	OHX	1	3557	7/7	0.99	0.16	-	56,56,56,56	0
93	MG	5	4095	1/1	0.92	0.37	-	35,35,35,35	0
96	LEU	1	3402	8/9	0.95	0.28	-	39,40,40,40	0
93	MG	1	3860	1/1	0.86	0.65	-	41,41,41,41	0
93	MG	1	4084	1/1	0.92	0.25	-	56,56,56,56	0
93	MG	1	3934	1/1	0.93	0.20	-	51,51,51,51	0
93	MG	5	4058	1/1	0.87	0.20	-	40,40,40,40	0
93	MG	1	4112	1/1	0.94	0.32	-	45,45,45,45	0
93	MG	5	3848	1/1	0.84	0.43	-	50,50,50,50	0
93	MG	5	4009	1/1	0.81	0.60	-	48,48,48,48	0
92	OHX	6	2010	7/7	0.95	0.24	-	91,91,91,91	0
93	MG	5	4047	1/1	0.88	0.35	-	41,41,41,41	0
93	MG	1	3869	1/1	0.78	0.41	-	41,41,41,41	0
92	OHX	1	3647	7/7	0.96	0.27	-	93,93,93,93	0
93	MG	6	2167	1/1	0.60	0.95	-	55,55,55,55	0
92	OHX	1	3459	7/7	0.99	0.08	-	72,72,72,72	0
93	MG	5	4117	1/1	0.68	0.28	-	63,63,63,63	0
93	MG	4	230	1/1	0.86	0.34	-	46,46,46,46	0
93	MG	5	4171	1/1	0.72	0.51	-	41,41,41,41	0
93	MG	5	3882	1/1	0.93	0.39	-	37,37,37,37	0
92	OHX	5	3437	7/7	0.99	0.11	-	41,41,41,41	0
93	MG	n8	202	1/1	0.93	0.18	-	34,34,34,34	0
92	OHX	1	3476	7/7	0.98	0.16	-	62,62,62,62	0
93	MG	1	3976	1/1	0.98	0.14	-	53,53,53,53	0
93	MG	1	3819	1/1	0.81	0.31	-	62,62,62,62	0
92	OHX	1	3715	7/7	0.98	0.25	-	82,82,82,82	0
93	MG	5	4131	1/1	0.91	0.27	-	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
93	MG	1	4096	1/1	0.97	0.11	-	52,52,52,52	0
93	MG	5	4084	1/1	0.88	0.55	-	42,42,42,42	0
93	MG	1	3843	1/1	0.94	0.57	-	38,38,38,38	0
93	MG	4	225	1/1	0.83	0.47	-	47,47,47,47	0
92	OHX	5	3639	7/7	0.96	0.27	-	56,56,56,56	0
93	MG	5	3999	1/1	0.94	0.23	-	31,31,31,31	0
92	OHX	1	3546	7/7	0.98	0.19	-	68,68,68,68	0
93	MG	6	2148	1/1	0.89	0.23	-	58,58,58,58	0
92	OHX	1	3442	7/7	0.97	0.12	-	55,55,55,55	0
93	MG	1	3750	1/1	0.87	0.52	-	55,55,55,55	0
93	MG	1	4101	1/1	0.87	0.19	-	37,37,37,37	0
93	MG	1	3829	1/1	0.97	0.59	-	43,43,43,43	0
93	MG	1	4049	1/1	0.89	0.16	-	44,44,44,44	0
93	MG	5	3884	1/1	0.96	0.25	-	30,30,30,30	0
92	OHX	5	3479	7/7	0.99	0.10	-	58,58,58,58	0
93	MG	5	3954	1/1	0.97	0.33	-	41,41,41,41	0
93	MG	5	3762	1/1	0.92	0.42	-	33,33,33,33	0
92	OHX	2	2037	7/7	0.96	0.26	-	98,98,98,98	0
93	MG	5	4160	1/1	0.98	0.33	-	33,33,33,33	0
92	OHX	5	3449	7/7	0.98	0.14	-	48,48,48,48	0
93	MG	6	2101	1/1	0.89	0.40	-	53,53,53,53	0
92	OHX	5	3526	7/7	0.98	0.15	-	58,58,58,58	0
93	MG	2	2053	1/1	0.94	0.81	-	70,70,70,70	0
93	MG	5	4102	1/1	0.97	0.20	-	40,40,40,40	0
93	MG	n0	201	1/1	0.95	0.31	-	37,37,37,37	0
93	MG	1	4035	1/1	0.95	0.27	-	47,47,47,47	0
92	OHX	1	3725	7/7	0.96	0.30	-	75,75,75,75	0
93	MG	1	3804	1/1	0.86	0.38	-	46,46,46,46	0
93	MG	5	4018	1/1	0.97	0.19	-	31,31,31,31	0
93	MG	6	2165	1/1	0.91	0.25	-	69,69,69,69	0
93	MG	7	225	1/1	0.64	1.51	-	44,44,44,44	0
93	MG	5	4130	1/1	0.87	0.29	-	33,33,33,33	0
92	OHX	5	3690	7/7	0.94	0.30	-	79,79,79,79	0
93	MG	5	3778	1/1	0.98	0.47	-	40,40,40,40	0
92	OHX	5	3744	7/7	0.98	0.30	-	72,72,72,72	0
93	MG	5	4163	1/1	0.94	0.20	-	44,44,44,44	0
92	OHX	2	2051	7/7	0.93	0.35	-	105,105,105,105	0
93	MG	8	227	1/1	0.85	0.18	-	51,51,51,51	0
93	MG	1	4019	1/1	0.98	0.16	-	36,36,36,36	0
92	OHX	1	3510	7/7	0.97	0.17	-	60,60,60,60	0
93	MG	2	2085	1/1	0.93	0.64	-	76,76,76,76	0
93	MG	6	2067	1/1	0.80	0.35	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
92	OHX	5	3447	7/7	0.99	0.07	-	56,56,56,56	0
92	OHX	2	2027	7/7	0.95	0.29	-	93,93,93,93	0
92	OHX	5	3723	7/7	0.97	0.32	-	62,62,62,62	0
93	MG	4	235	1/1	0.96	0.35	-	42,42,42,42	0
93	MG	1	4039	1/1	0.87	0.68	-	52,52,52,52	0
92	OHX	6	1941	7/7	0.97	0.19	-	96,96,96,96	0
92	OHX	5	3674	7/7	0.98	0.34	-	56,56,56,56	0
93	MG	13	403	1/1	0.95	0.70	-	31,31,31,31	0
93	MG	1	3903	1/1	0.87	0.46	-	40,40,40,40	0
93	MG	5	4076	1/1	0.95	0.50	-	47,47,47,47	0
93	MG	1	3781	1/1	0.96	0.44	-	52,52,52,52	0
92	OHX	1	3691	7/7	0.99	0.18	-	52,52,52,52	0
93	MG	5	3920	1/1	0.90	0.48	-	42,42,42,42	0
92	OHX	1	3578	7/7	0.98	0.21	-	51,51,51,51	0
93	MG	5	4165	1/1	0.84	0.65	-	49,49,49,49	0
93	MG	1	4106	1/1	0.82	0.29	-	54,54,54,54	0
93	MG	2	2111	1/1	0.90	0.38	-	78,78,78,78	0
93	MG	6	2070	1/1	0.87	0.30	-	94,94,94,94	0
93	MG	1	3945	1/1	0.74	0.54	-	45,45,45,45	0
93	MG	5	3815	1/1	0.76	0.31	-	40,40,40,40	0
92	OHX	5	3735	7/7	0.97	0.35	-	70,70,70,70	0
92	OHX	5	3631	7/7	0.99	0.20	-	65,65,65,65	0
92	OHX	5	3622	7/7	0.98	0.17	-	73,73,73,73	0
93	MG	4	229	1/1	0.99	0.09	-	46,46,46,46	0
93	MG	6	2085	1/1	0.85	0.53	-	58,58,58,58	0
93	MG	1	3993	1/1	0.98	0.29	-	44,44,44,44	0
93	MG	6	2117	1/1	0.91	0.48	-	55,55,55,55	0
93	MG	5	3938	1/1	0.85	0.52	-	38,38,38,38	0
92	OHX	M7	201	7/7	0.97	0.32	-	62,62,62,62	0
92	OHX	2	1944	7/7	0.98	0.15	-	83,83,83,83	0
93	MG	5	3824	1/1	0.90	0.33	-	42,42,42,42	0
93	MG	5	3866	1/1	0.97	0.52	-	39,39,39,39	0
92	OHX	2	2024	7/7	0.94	0.23	-	103,103,103,103	0
93	MG	6	2183	1/1	0.77	0.41	-	72,72,72,72	0
93	MG	q1	101	1/1	0.92	0.32	-	58,58,58,58	0
92	OHX	5	3459	7/7	0.98	0.15	-	64,64,64,64	0
92	OHX	5	3699	7/7	0.97	0.25	-	70,70,70,70	0
93	MG	5	3924	1/1	0.85	0.41	-	36,36,36,36	0
93	MG	5	3951	1/1	0.94	0.50	-	33,33,33,33	0
93	MG	1	4032	1/1	0.61	0.49	-	34,34,34,34	0
93	MG	1	4015	1/1	0.87	0.34	-	36,36,36,36	0
93	MG	5	4120	1/1	0.88	0.47	-	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
92	OHX	1	3570	7/7	0.98	0.18	-	75,75,75,75	0
93	MG	2	2103	1/1	0.90	0.54	-	74,74,74,74	0
93	MG	6	2145	1/1	0.73	0.13	-	89,89,89,89	0
93	MG	c8	202	1/1	0.58	0.38	-	84,84,84,84	0
93	MG	6	2180	1/1	0.58	0.90	-	98,98,98,98	0
93	MG	1	3858	1/1	0.87	0.46	-	35,35,35,35	0
93	MG	5	4124	1/1	0.66	0.40	-	37,37,37,37	0
93	MG	8	228	1/1	0.94	0.20	-	47,47,47,47	0
92	OHX	6	2046	7/7	0.97	0.30	-	93,93,93,93	0
93	MG	1	4067	1/1	0.96	0.77	-	38,38,38,38	0
92	OHX	2	2030	7/7	0.92	0.40	-	95,95,95,95	0
93	MG	1	3938	1/1	0.78	0.19	-	57,57,57,57	0
93	MG	1	4078	1/1	0.68	0.45	-	40,40,40,40	0
92	OHX	1	3698	7/7	0.94	0.27	-	58,58,58,58	0
92	OHX	6	1968	7/7	0.96	0.31	-	74,74,74,74	0
93	MG	5	3947	1/1	0.84	0.67	-	32,32,32,32	0
93	MG	1	4044	1/1	0.29	0.32	-	52,52,52,52	0
92	OHX	1	3547	7/7	0.98	0.22	-	65,65,65,65	0
93	MG	N8	202	1/1	0.94	0.23	-	31,31,31,31	0
93	MG	1	4080	1/1	0.78	0.34	-	54,54,54,54	0
92	OHX	1	3550	7/7	0.99	0.22	-	63,63,63,63	0
93	MG	1	3890	1/1	0.93	0.90	-	36,36,36,36	0
93	MG	5	3833	1/1	0.66	0.73	-	44,44,44,44	0
92	OHX	5	3509	7/7	0.97	0.21	-	63,63,63,63	0
92	OHX	2	1992	7/7	0.99	0.16	-	95,95,95,95	0
92	OHX	5	3620	7/7	0.93	0.26	-	73,73,73,73	0
93	MG	1	3939	1/1	0.40	0.39	-	54,54,54,54	0
92	OHX	6	1925	7/7	0.97	0.12	-	76,76,76,76	0
92	OHX	5	3678	7/7	0.97	0.28	-	60,60,60,60	0
92	OHX	1	3492	7/7	0.98	0.14	-	66,66,66,66	0
93	MG	1	4064	1/1	0.54	0.45	-	43,43,43,43	0
93	MG	1	3796	1/1	0.89	0.25	-	39,39,39,39	0
93	MG	1	3902	1/1	0.90	0.77	-	37,37,37,37	0
92	OHX	1	3437	7/7	0.99	0.09	-	52,52,52,52	0
92	OHX	6	1959	7/7	0.94	0.20	-	67,67,67,67	0
93	MG	6	2082	1/1	0.62	0.38	-	87,87,87,87	0
93	MG	5	4147	1/1	0.96	0.17	-	33,33,33,33	0
92	OHX	6	1935	7/7	0.98	0.17	-	68,68,68,68	0
92	OHX	1	3707	7/7	0.98	0.08	-	97,97,97,97	0
92	OHX	5	3713	7/7	0.97	0.24	-	53,53,53,53	0
93	MG	6	2153	1/1	0.78	0.30	-	86,86,86,86	0
93	MG	1	3978	1/1	0.91	0.31	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	1	3874	1/1	0.84	0.40	-	33,33,33,33	0
93	MG	2	2078	1/1	0.81	0.44	-	92,92,92,92	0
93	MG	1	3753	1/1	0.95	0.16	-	40,40,40,40	0
92	OHX	1	3440	7/7	0.98	0.10	-	59,59,59,59	0
92	OHX	1	3598	7/7	0.99	0.15	-	78,78,78,78	0
93	MG	5	3959	1/1	0.90	0.28	-	38,38,38,38	0
93	MG	16	201	1/1	0.80	0.38	-	44,44,44,44	0
93	MG	1	3789	1/1	0.94	0.87	-	39,39,39,39	0
92	OHX	1	3596	7/7	0.98	0.39	-	60,60,60,60	0
92	OHX	2	2007	7/7	0.97	0.33	-	88,88,88,88	0
92	OHX	5	3567	7/7	0.99	0.13	-	58,58,58,58	0
92	OHX	5	3665	7/7	0.95	0.27	-	92,92,92,92	0
92	OHX	6	2030	7/7	0.97	0.25	-	74,74,74,74	0
93	MG	5	4048	1/1	0.97	0.19	-	40,40,40,40	0
93	MG	5	4031	1/1	0.88	0.16	-	56,56,56,56	0
93	MG	4	237	1/1	0.87	0.31	-	31,31,31,31	0
92	OHX	M9	201	7/7	0.97	0.33	-	74,74,74,74	0
93	MG	n9	102	1/1	0.97	0.86	-	29,29,29,29	0
93	MG	2	2132	1/1	0.77	0.46	-	76,76,76,76	0
93	MG	5	4032	1/1	0.90	0.39	-	33,33,33,33	0
93	MG	5	3997	1/1	0.90	0.20	-	34,34,34,34	0
93	MG	5	3994	1/1	0.90	0.67	-	40,40,40,40	0
93	MG	5	3818	1/1	0.98	0.26	-	43,43,43,43	0
93	MG	1	3740	1/1	0.96	0.43	-	33,33,33,33	0
93	MG	4	234	1/1	0.88	0.23	-	41,41,41,41	0
93	MG	5	3969	1/1	0.93	0.28	-	40,40,40,40	0
93	MG	1	3815	1/1	0.95	0.38	-	50,50,50,50	0
93	MG	5	3870	1/1	0.93	0.50	-	32,32,32,32	0
92	OHX	6	1986	7/7	0.98	0.24	-	77,77,77,77	0
93	MG	2	2138	1/1	0.75	0.62	-	87,87,87,87	0
93	MG	5	4024	1/1	0.91	0.26	-	37,37,37,37	0
92	OHX	5	3558	7/7	0.98	0.18	-	78,78,78,78	0
93	MG	1	4028	1/1	0.91	0.18	-	41,41,41,41	0
92	OHX	2	2033	7/7	0.95	0.19	-	123,123,123,123	0
93	MG	5	3791	1/1	0.84	0.51	-	36,36,36,36	0
93	MG	1	3970	1/1	0.91	0.63	-	42,42,42,42	0
93	MG	5	4007	1/1	0.96	0.64	-	37,37,37,37	0
92	OHX	4	210	7/7	0.98	0.22	-	53,53,53,53	0
93	MG	1	3910	1/1	0.98	0.54	-	29,29,29,29	0
93	MG	1	4089	1/1	0.92	0.60	-	44,44,44,44	0
93	MG	n6	201	1/1	0.67	0.43	-	46,46,46,46	0
93	MG	1	4048	1/1	0.94	0.52	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	5	3993	1/1	0.92	0.52	-	38,38,38,38	0
93	MG	5	4080	1/1	0.92	0.20	-	32,32,32,32	0
93	MG	1	4070	1/1	0.90	0.20	-	46,46,46,46	0
93	MG	1	3870	1/1	0.82	0.40	-	49,49,49,49	0
93	MG	m6	205	1/1	0.86	0.47	-	36,36,36,36	0
93	MG	5	3790	1/1	0.91	0.79	-	34,34,34,34	0
93	MG	1	3967	1/1	0.89	0.24	-	32,32,32,32	0
93	MG	1	3766	1/1	0.97	0.49	-	47,47,47,47	0
93	MG	2	2070	1/1	0.80	0.72	-	71,71,71,71	0
93	MG	5	4086	1/1	0.51	0.46	-	34,34,34,34	0
93	MG	2	2108	1/1	0.54	0.34	-	92,92,92,92	0
93	MG	1	3872	1/1	0.99	0.23	-	41,41,41,41	0
93	MG	6	2114	1/1	0.55	0.50	-	89,89,89,89	0
93	MG	5	4011	1/1	0.95	0.69	-	43,43,43,43	0
92	OHX	5	3533	7/7	0.98	0.17	-	45,45,45,45	0
93	MG	1	4005	1/1	0.86	0.30	-	40,40,40,40	0
93	MG	m0	304	1/1	0.98	0.30	-	36,36,36,36	0
93	MG	1	3957	1/1	0.92	0.22	-	56,56,56,56	0
93	MG	1	3940	1/1	0.92	0.33	-	54,54,54,54	0
93	MG	2	2127	1/1	0.92	0.71	-	77,77,77,77	0
93	MG	6	2163	1/1	0.89	0.48	-	66,66,66,66	0
92	OHX	3	209	7/7	0.96	0.27	-	84,84,84,84	0
93	MG	5	3963	1/1	0.96	0.44	-	43,43,43,43	0
93	MG	2	2125	1/1	0.81	0.51	-	78,78,78,78	0
93	MG	6	2150	1/1	0.93	1.11	-	58,58,58,58	0
93	MG	6	2132	1/1	0.91	0.48	-	59,59,59,59	0
92	OHX	1	3583	7/7	0.97	0.22	-	53,53,53,53	0
93	MG	5	3968	1/1	0.99	0.09	-	49,49,49,49	0
92	OHX	1	3627	7/7	0.97	0.28	-	73,73,73,73	0
92	OHX	5	3518	7/7	0.99	0.13	-	55,55,55,55	0
92	OHX	2	1965	7/7	0.97	0.16	-	84,84,84,84	0
92	OHX	1	3680	7/7	0.96	0.27	-	67,67,67,67	0
92	OHX	1	3677	7/7	0.98	0.28	-	67,67,67,67	0
93	MG	5	3797	1/1	0.92	0.25	-	37,37,37,37	0
93	MG	5	3872	1/1	0.99	0.36	-	33,33,33,33	0
93	MG	D9	103	1/1	0.79	0.31	-	92,92,92,92	0
93	MG	1	3770	1/1	0.94	0.46	-	36,36,36,36	0
92	OHX	2	2034	7/7	0.97	0.26	-	87,87,87,87	0
93	MG	m6	203	1/1	0.73	0.32	-	34,34,34,34	0
92	OHX	1	3636	7/7	0.96	0.31	-	59,59,59,59	0
93	MG	5	3946	1/1	0.98	0.45	-	35,35,35,35	0
92	OHX	1	3555	7/7	0.99	0.12	-	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
93	MG	1	3865	1/1	0.91	0.69	-	49,49,49,49	0
93	MG	p	102	1/1	0.90	0.31	-	35,35,35,35	0
93	MG	5	4099	1/1	0.78	0.63	-	52,52,52,52	0
93	MG	5	3757	1/1	0.94	0.66	-	44,44,44,44	0
93	MG	6	2166	1/1	0.34	0.43	-	114,114,114,114	0
92	OHX	5	3657	7/7	0.98	0.28	-	64,64,64,64	0
93	MG	1	3964	1/1	0.80	1.09	-	45,45,45,45	0
92	OHX	5	3535	7/7	0.97	0.17	-	53,53,53,53	0
93	MG	5	3821	1/1	0.80	0.27	-	41,41,41,41	0
93	MG	6	2172	1/1	0.94	0.52	-	64,64,64,64	0
92	OHX	1	3706	7/7	0.97	0.27	-	74,74,74,74	0
93	MG	5	4148	1/1	0.86	0.33	-	48,48,48,48	0
93	MG	5	4122	1/1	0.98	0.21	-	34,34,34,34	0
93	MG	2	2104	1/1	0.86	0.47	-	97,97,97,97	0
93	MG	2	2064	1/1	0.88	0.31	-	85,85,85,85	0
93	MG	1	3954	1/1	0.83	0.25	-	55,55,55,55	0
93	MG	1	3855	1/1	0.79	0.78	-	56,56,56,56	0
93	MG	1	4121	1/1	0.95	0.24	-	38,38,38,38	0
93	MG	5	3774	1/1	0.98	0.85	-	46,46,46,46	0
93	MG	1	3768	1/1	0.87	0.43	-	46,46,46,46	0
93	MG	1	3849	1/1	0.98	0.30	-	34,34,34,34	0
93	MG	1	3990	1/1	0.80	0.45	-	40,40,40,40	0
92	OHX	6	1964	7/7	0.98	0.21	-	62,62,62,62	0
93	MG	3	212	1/1	0.95	0.53	-	59,59,59,59	0
92	OHX	2	2028	7/7	0.93	0.25	-	109,109,109,109	0
93	MG	1	4046	1/1	0.96	0.27	-	40,40,40,40	0
93	MG	5	3787	1/1	0.95	0.33	-	33,33,33,33	0
92	OHX	6	2003	7/7	0.96	0.20	-	89,89,89,89	0
92	OHX	7	208	7/7	0.98	0.23	-	61,61,61,61	0
93	MG	1	4124	1/1	0.95	0.30	-	46,46,46,46	0
92	OHX	5	3668	7/7	0.98	0.20	-	72,72,72,72	0
93	MG	1	3828	1/1	0.92	0.88	-	50,50,50,50	0
92	OHX	5	3564	7/7	0.99	0.20	-	72,72,72,72	0
93	MG	5	3981	1/1	0.85	0.20	-	50,50,50,50	0
93	MG	2	2101	1/1	0.72	0.40	-	79,79,79,79	0
92	OHX	5	3691	7/7	0.97	0.34	-	49,49,49,49	0
93	MG	L4	403	1/1	0.82	0.32	-	31,31,31,31	0
93	MG	2	2107	1/1	0.97	0.34	-	81,81,81,81	0
93	MG	5	4041	1/1	0.69	0.37	-	43,43,43,43	0
93	MG	2	2082	1/1	0.94	0.43	-	74,74,74,74	0
93	MG	m4	201	1/1	0.91	0.29	-	42,42,42,42	0
92	OHX	4	216	7/7	0.97	0.28	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	1	4085	1/1	0.90	0.28	-	33,33,33,33	0
93	MG	6	2125	1/1	0.64	0.88	-	57,57,57,57	0
93	MG	6	2133	1/1	0.57	0.34	-	94,94,94,94	0
93	MG	6	2102	1/1	0.78	0.48	-	96,96,96,96	0
93	MG	1	3782	1/1	0.96	0.36	-	41,41,41,41	0
92	OHX	6	1967	7/7	0.96	0.17	-	78,78,78,78	0
92	OHX	5	3741	7/7	0.98	0.11	-	59,59,59,59	0
93	MG	5	3786	1/1	0.89	0.38	-	37,37,37,37	0
93	MG	2	2117	1/1	0.28	0.55	-	94,94,94,94	0
92	OHX	1	3673	7/7	0.96	0.34	-	67,67,67,67	0
93	MG	1	3936	1/1	0.96	0.45	-	40,40,40,40	0
92	OHX	2	1952	7/7	0.97	0.24	-	104,104,104,104	0
92	OHX	1	3701	7/7	0.95	0.26	-	87,87,87,87	0
93	MG	1	3987	1/1	0.94	0.35	-	43,43,43,43	0
93	MG	5	3800	1/1	0.89	0.44	-	52,52,52,52	0
93	MG	1	3734	1/1	0.91	0.48	-	39,39,39,39	0
93	MG	5	4101	1/1	0.97	0.43	-	33,33,33,33	0
92	OHX	2	1939	7/7	0.97	0.14	-	92,92,92,92	0
93	MG	5	4060	1/1	0.95	0.26	-	47,47,47,47	0
93	MG	5	4108	1/1	0.85	0.50	-	37,37,37,37	0
93	MG	5	3814	1/1	0.90	0.23	-	42,42,42,42	0
92	OHX	6	1934	7/7	0.99	0.12	-	68,68,68,68	0
93	MG	5	3881	1/1	0.94	0.71	-	36,36,36,36	0
92	OHX	2	2026	7/7	0.95	0.28	-	109,109,109,109	0
93	MG	5	3828	1/1	0.89	0.28	-	43,43,43,43	0
92	OHX	1	3564	7/7	0.98	0.21	-	70,70,70,70	0
93	MG	5	3964	1/1	0.91	0.53	-	46,46,46,46	0
92	OHX	1	3600	7/7	0.99	0.30	-	58,58,58,58	0
93	MG	M7	203	1/1	0.97	0.20	-	38,38,38,38	0
92	OHX	1	3558	7/7	0.98	0.19	-	74,74,74,74	0
92	OHX	1	3458	7/7	0.99	0.10	-	53,53,53,53	0
93	MG	3	211	1/1	0.96	0.28	-	60,60,60,60	0
93	MG	1	4110	1/1	0.79	0.25	-	43,43,43,43	0
92	OHX	1	3561	7/7	0.95	0.22	-	60,60,60,60	0
92	OHX	8	205	7/7	0.98	0.12	-	75,75,75,75	0
93	MG	5	3995	1/1	0.90	0.36	-	41,41,41,41	0
93	MG	1	4113	1/1	0.99	0.19	-	59,59,59,59	0
93	MG	5	3975	1/1	0.94	0.12	-	46,46,46,46	0
93	MG	5	3764	1/1	0.77	0.38	-	34,34,34,34	0
92	OHX	2	2014	7/7	0.95	0.17	-	107,107,107,107	0
93	MG	6	2164	1/1	0.91	0.25	-	57,57,57,57	0
93	MG	1	3863	1/1	0.96	0.34	-	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
92	OHX	1	3436	7/7	0.98	0.09	-	63,63,63,63	0
93	MG	5	4026	1/1	0.93	0.28	-	49,49,49,49	0
92	OHX	2	1998	7/7	0.97	0.38	-	95,95,95,95	0
93	MG	8	221	1/1	0.94	0.51	-	39,39,39,39	0
93	MG	5	3836	1/1	0.87	0.27	-	41,41,41,41	0
93	MG	3	213	1/1	0.98	0.68	-	39,39,39,39	0
92	OHX	2	1928	7/7	0.98	0.15	-	79,79,79,79	0
92	OHX	5	3733	7/7	0.98	0.25	-	74,74,74,74	0
93	MG	6	2141	1/1	0.70	0.51	-	95,95,95,95	0
93	MG	5	3807	1/1	0.81	0.41	-	36,36,36,36	0
93	MG	5	3876	1/1	0.76	0.63	-	35,35,35,35	0
93	MG	7	224	1/1	0.95	0.17	-	36,36,36,36	0
93	MG	1	3774	1/1	0.71	0.63	-	51,51,51,51	0
92	OHX	1	3480	7/7	0.98	0.11	-	67,67,67,67	0
92	OHX	1	3652	7/7	0.98	0.25	-	64,64,64,64	0
93	MG	5	4138	1/1	0.88	0.45	-	38,38,38,38	0
93	MG	1	3847	1/1	0.96	0.30	-	33,33,33,33	0
93	MG	5	3856	1/1	0.94	0.52	-	53,53,53,53	0
93	MG	1	3961	1/1	0.77	0.35	-	40,40,40,40	0
92	OHX	5	3697	7/7	0.97	0.31	-	70,70,70,70	0
93	MG	5	4088	1/1	0.76	0.40	-	41,41,41,41	0
92	OHX	8	201	7/7	0.99	0.11	-	41,41,41,41	0
92	OHX	5	3701	7/7	0.95	0.37	-	53,53,53,53	0
93	MG	1	4111	1/1	0.89	0.60	-	41,41,41,41	0
93	MG	5	4135	1/1	0.91	0.48	-	47,47,47,47	0
93	MG	5	3989	1/1	0.97	0.14	-	38,38,38,38	0
93	MG	2	2077	1/1	0.91	1.23	-	59,59,59,59	0
93	MG	6	2154	1/1	0.85	0.30	-	94,94,94,94	0
92	OHX	m9	201	7/7	0.96	0.42	-	89,89,89,89	0
93	MG	2	2091	1/1	0.95	0.36	-	77,77,77,77	0
92	OHX	2	1927	7/7	0.98	0.12	-	85,85,85,85	0
92	OHX	5	3470	7/7	0.99	0.12	-	48,48,48,48	0
93	MG	12	301	1/1	0.96	0.62	-	42,42,42,42	0
93	MG	5	3956	1/1	0.90	0.11	-	48,48,48,48	0
92	OHX	1	3618	7/7	0.98	0.31	-	68,68,68,68	0
93	MG	5	4004	1/1	0.95	0.29	-	43,43,43,43	0
93	MG	1	3997	1/1	0.88	0.41	-	40,40,40,40	0
93	MG	2	2136	1/1	0.91	0.17	-	90,90,90,90	0
93	MG	1	3827	1/1	0.83	0.36	-	33,33,33,33	0
93	MG	1	3850	1/1	0.88	0.50	-	39,39,39,39	0
93	MG	1	3956	1/1	0.67	0.29	-	50,50,50,50	0
93	MG	5	4087	1/1	0.97	0.58	-	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
93	MG	1	3748	1/1	0.84	0.86	-	49,49,49,49	0
93	MG	5	4068	1/1	0.81	0.25	-	42,42,42,42	0
93	MG	5	3825	1/1	0.89	0.58	-	50,50,50,50	0
93	MG	5	3835	1/1	0.72	0.35	-	40,40,40,40	0
92	OHX	1	3464	7/7	0.99	0.09	-	54,54,54,54	0
93	MG	5	3796	1/1	0.97	0.31	-	37,37,37,37	0
93	MG	1	3751	1/1	0.94	0.44	-	39,39,39,39	0
93	MG	m7	202	1/1	0.89	0.27	-	36,36,36,36	0
92	OHX	2	2045	7/7	0.95	0.45	-	100,100,100,100	0
93	MG	1	3959	1/1	0.90	0.33	-	36,36,36,36	0
93	MG	5	3861	1/1	0.96	0.45	-	30,30,30,30	0
93	MG	1	3788	1/1	0.98	0.41	-	49,49,49,49	0
93	MG	1	4004	1/1	0.96	0.23	-	39,39,39,39	0
93	MG	2	2075	1/1	0.76	0.21	-	96,96,96,96	0
93	MG	N8	205	1/1	0.94	0.24	-	35,35,35,35	0
92	OHX	6	2045	7/7	0.96	0.34	-	94,94,94,94	0
92	OHX	1	3602	7/7	0.94	0.34	-	62,62,62,62	0
93	MG	5	3902	1/1	0.86	0.20	-	49,49,49,49	0
93	MG	6	2103	1/1	0.94	0.59	-	62,62,62,62	0
93	MG	5	3832	1/1	0.98	0.24	-	35,35,35,35	0
92	OHX	5	3539	7/7	0.99	0.23	-	47,47,47,47	0
92	OHX	2	1980	7/7	0.95	0.18	-	140,140,140,140	0
92	OHX	8	206	7/7	0.97	0.18	-	57,57,57,57	0
92	OHX	c8	201	7/7	0.97	0.19	-	96,96,96,96	0
93	MG	1	3778	1/1	0.87	0.32	-	31,31,31,31	0
93	MG	1	3975	1/1	0.94	0.47	-	35,35,35,35	0
92	OHX	2	1947	7/7	0.93	0.22	-	106,106,106,106	0
93	MG	6	2174	1/1	0.93	0.23	-	60,60,60,60	0
93	MG	1	3733	1/1	0.78	0.86	-	48,48,48,48	0
93	MG	1	3848	1/1	0.45	1.16	-	36,36,36,36	0
92	OHX	6	2004	7/7	0.98	0.21	-	84,84,84,84	0
93	MG	l5	303	1/1	0.82	0.14	-	50,50,50,50	0
93	MG	1	3839	1/1	0.92	0.45	-	46,46,46,46	0
93	MG	5	4061	1/1	0.81	0.63	-	33,33,33,33	0
92	OHX	5	3423	7/7	0.99	0.11	-	51,51,51,51	0
92	OHX	6	1994	7/7	0.97	0.27	-	98,98,98,98	0
92	OHX	5	3683	7/7	0.98	0.27	-	83,83,83,83	0
93	MG	5	4129	1/1	0.88	0.52	-	36,36,36,36	0
93	MG	5	4042	1/1	0.91	0.15	-	54,54,54,54	0
92	OHX	8	207	7/7	0.98	0.29	-	56,56,56,56	0
92	OHX	1	3628	7/7	0.99	0.21	-	62,62,62,62	0
93	MG	5	3799	1/1	0.94	0.18	-	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
93	MG	5	4059	1/1	0.94	0.38	-	35,35,35,35	0
92	OHX	1	3504	7/7	0.98	0.14	-	75,75,75,75	0
93	MG	5	4150	1/1	0.66	0.31	-	41,41,41,41	0
92	OHX	5	3435	7/7	0.98	0.08	-	46,46,46,46	0
93	MG	5	3830	1/1	0.88	0.30	-	35,35,35,35	0
92	OHX	5	3727	7/7	0.96	0.42	-	60,60,60,60	0
92	OHX	c3	201	7/7	0.94	0.24	-	89,89,89,89	0
93	MG	5	4073	1/1	0.93	0.28	-	35,35,35,35	0
93	MG	2	2118	1/1	0.69	0.42	-	92,92,92,92	0
93	MG	N8	201	1/1	0.91	0.21	-	31,31,31,31	0
93	MG	1	3994	1/1	0.88	0.47	-	45,45,45,45	0
93	MG	8	229	1/1	0.88	0.23	-	40,40,40,40	0
93	MG	1	4024	1/1	0.90	0.36	-	60,60,60,60	0
93	MG	1	3830	1/1	0.99	0.59	-	38,38,38,38	0
93	MG	1	3999	1/1	0.95	0.51	-	43,43,43,43	0
92	OHX	1	3624	7/7	0.98	0.21	-	81,81,81,81	0
92	OHX	6	2055	7/7	0.92	0.27	-	118,118,118,118	0
93	MG	5	4116	1/1	0.85	0.23	-	44,44,44,44	0
92	OHX	1	3659	7/7	0.97	0.26	-	73,73,73,73	0
92	OHX	1	3491	7/7	0.99	0.17	-	53,53,53,53	0
93	MG	5	3845	1/1	0.89	0.29	-	34,34,34,34	0
93	MG	7	217	1/1	0.96	0.47	-	33,33,33,33	0
93	MG	6	2144	1/1	0.93	0.23	-	94,94,94,94	0
93	MG	1	4006	1/1	0.93	0.41	-	45,45,45,45	0
93	MG	1	3736	1/1	0.67	0.46	-	125,125,125,125	0
92	OHX	5	3596	7/7	0.98	0.27	-	48,48,48,48	0
93	MG	5	3805	1/1	0.96	0.31	-	34,34,34,34	0
92	OHX	4	217	7/7	0.97	0.33	-	69,69,69,69	0
93	MG	1	4053	1/1	0.84	0.41	-	59,59,59,59	0
92	OHX	5	3633	7/7	0.96	0.31	-	65,65,65,65	0
93	MG	1	3886	1/1	0.98	0.19	-	53,53,53,53	0
92	OHX	1	3719	7/7	0.95	0.37	-	83,83,83,83	0
93	MG	5	4064	1/1	0.60	0.34	-	59,59,59,59	0
92	OHX	6	2011	7/7	0.98	0.30	-	72,72,72,72	0
93	MG	5	4038	1/1	0.91	0.32	-	41,41,41,41	0
93	MG	5	3779	1/1	0.87	0.29	-	48,48,48,48	0
93	MG	1	3793	1/1	0.92	0.42	-	38,38,38,38	0
92	OHX	5	3568	7/7	0.99	0.23	-	53,53,53,53	0
93	MG	5	3965	1/1	0.96	0.13	-	36,36,36,36	0
92	OHX	5	3592	7/7	0.98	0.23	-	62,62,62,62	0
92	OHX	8	209	7/7	0.96	0.26	-	78,78,78,78	0
93	MG	8	219	1/1	0.86	0.25	-	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
93	MG	1	3808	1/1	0.93	0.27	-	48,48,48,48	0
93	MG	5	3952	1/1	0.96	0.41	-	34,34,34,34	0
92	OHX	6	1940	7/7	0.98	0.13	-	59,59,59,59	0
93	MG	1	4043	1/1	0.74	0.46	-	43,43,43,43	0
93	MG	1	4054	1/1	0.62	0.41	-	34,34,34,34	0
93	MG	5	3875	1/1	0.93	0.38	-	51,51,51,51	0
92	OHX	1	3633	7/7	0.99	0.19	-	72,72,72,72	0
93	MG	5	3923	1/1	0.94	0.56	-	31,31,31,31	0
93	MG	5	4089	1/1	0.96	0.12	-	41,41,41,41	0
92	OHX	2	1937	7/7	0.98	0.14	-	84,84,84,84	0
93	MG	5	3935	1/1	0.98	0.59	-	31,31,31,31	0
93	MG	2	2134	1/1	0.92	0.96	-	59,59,59,59	0
93	MG	1	3905	1/1	0.78	0.62	-	38,38,38,38	0
93	MG	4	223	1/1	0.87	0.50	-	49,49,49,49	0
93	MG	1	3906	1/1	0.97	0.35	-	35,35,35,35	0
93	MG	2	2133	1/1	0.87	0.26	-	85,85,85,85	0
93	MG	5	4103	1/1	0.96	0.71	-	60,60,60,60	0
93	MG	5	4143	1/1	0.90	0.64	-	39,39,39,39	0
92	OHX	5	3725	7/7	0.96	0.37	-	55,55,55,55	0
93	MG	1	3759	1/1	0.90	1.04	-	41,41,41,41	0
93	MG	8	225	1/1	0.86	0.36	-	62,62,62,62	0
92	OHX	6	1905	7/7	0.98	0.11	-	73,73,73,73	0
93	MG	2	2100	1/1	0.74	0.29	-	102,102,102,102	0
93	MG	6	2182	1/1	0.59	0.30	-	66,66,66,66	0
93	MG	5	3782	1/1	0.91	0.23	-	35,35,35,35	0
93	MG	1	4013	1/1	0.82	0.40	-	50,50,50,50	0
92	OHX	5	3468	7/7	0.99	0.12	-	70,70,70,70	0
93	MG	5	4081	1/1	0.88	0.56	-	43,43,43,43	0
93	MG	1	3749	1/1	0.83	0.38	-	69,69,69,69	0
92	OHX	2	1977	7/7	0.97	0.21	-	99,99,99,99	0
93	MG	1	3968	1/1	0.85	0.54	-	51,51,51,51	0
93	MG	1	4018	1/1	0.86	0.29	-	61,61,61,61	0
93	MG	1	3861	1/1	0.91	0.67	-	44,44,44,44	0
92	OHX	5	3711	7/7	0.96	0.25	-	89,89,89,89	0
92	OHX	5	3653	7/7	0.98	0.28	-	59,59,59,59	0
93	MG	5	4175	1/1	0.72	0.19	-	81,81,81,81	0
93	MG	5	3834	1/1	0.97	0.76	-	41,41,41,41	0
93	MG	5	3976	1/1	0.91	0.36	-	38,38,38,38	0
93	MG	5	4066	1/1	0.97	1.00	-	31,31,31,31	0
93	MG	1	4075	1/1	0.82	0.30	-	54,54,54,54	0
93	MG	1	3955	1/1	0.86	0.22	-	57,57,57,57	0
92	OHX	1	3456	7/7	0.99	0.09	-	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
93	MG	5	4000	1/1	0.80	0.31	-	39,39,39,39	0
93	MG	1	3783	1/1	0.61	0.53	-	41,41,41,41	0
93	MG	5	4152	1/1	0.84	0.42	-	34,34,34,34	0
93	MG	5	4050	1/1	0.73	0.38	-	57,57,57,57	0
93	MG	2	2063	1/1	0.93	0.28	-	74,74,74,74	0
93	MG	19	202	1/1	0.81	0.33	-	41,41,41,41	0
92	OHX	6	1963	7/7	0.98	0.14	-	78,78,78,78	0
93	MG	1	3933	1/1	0.81	0.44	-	37,37,37,37	0
93	MG	5	3784	1/1	0.97	0.38	-	42,42,42,42	0
93	MG	5	4085	1/1	0.95	0.53	-	35,35,35,35	0
93	MG	5	4006	1/1	0.86	0.69	-	29,29,29,29	0
93	MG	5	4002	1/1	0.88	0.36	-	40,40,40,40	0
93	MG	5	3973	1/1	0.76	0.22	-	84,84,84,84	0
93	MG	n9	103	1/1	0.95	0.46	-	34,34,34,34	0
93	MG	1	3866	1/1	0.97	0.43	-	31,31,31,31	0
92	OHX	1	3521	7/7	0.98	0.15	-	64,64,64,64	0
93	MG	5	4172	1/1	0.94	0.46	-	47,47,47,47	0
92	OHX	5	3704	7/7	0.95	0.19	-	57,57,57,57	0
93	MG	1	4061	1/1	0.82	0.27	-	37,37,37,37	0
92	OHX	5	3746	7/7	0.99	0.10	-	70,70,70,70	0
93	MG	2	2074	1/1	0.93	0.68	-	80,80,80,80	0
92	OHX	1	3692	7/7	0.98	0.25	-	80,80,80,80	0
92	OHX	5	3425	7/7	0.99	0.09	-	41,41,41,41	0
92	OHX	2	1930	7/7	0.97	0.12	-	95,95,95,95	0
93	MG	6	2184	1/1	0.98	0.17	-	57,57,57,57	0
92	OHX	1	3509	7/7	0.98	0.10	-	67,67,67,67	0
93	MG	2	2079	1/1	0.98	0.37	-	85,85,85,85	0
93	MG	5	4128	1/1	0.66	0.55	-	57,57,57,57	0
93	MG	5	3926	1/1	0.90	0.54	-	36,36,36,36	0
93	MG	1	3946	1/1	0.99	0.11	-	39,39,39,39	0
93	MG	1	4069	1/1	0.91	0.23	-	43,43,43,43	0
93	MG	1	3838	1/1	0.99	0.56	-	39,39,39,39	0
93	MG	1	3930	1/1	0.94	0.49	-	51,51,51,51	0
93	MG	1	3986	1/1	0.91	0.20	-	42,42,42,42	0
93	MG	5	3817	1/1	0.77	0.29	-	46,46,46,46	0
93	MG	5	3863	1/1	0.96	0.59	-	39,39,39,39	0
93	MG	7	214	1/1	0.95	0.39	-	47,47,47,47	0
93	MG	6	2066	1/1	0.92	0.10	-	89,89,89,89	0
92	OHX	5	3547	7/7	0.98	0.19	-	68,68,68,68	0
93	MG	5	3883	1/1	0.92	0.93	-	35,35,35,35	0
93	MG	1	3943	1/1	0.87	0.26	-	33,33,33,33	0
92	OHX	5	3650	7/7	0.99	0.23	-	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
95	PHE	1	3401	11/12	0.92	0.26	-	34,34,44,44	0
93	MG	6	2152	1/1	0.20	1.10	-	62,62,62,62	0
93	MG	1	4081	1/1	0.98	0.47	-	33,33,33,33	0
92	OHX	5	3679	7/7	0.97	0.34	-	55,55,55,55	0
93	MG	5	3873	1/1	0.94	0.22	-	33,33,33,33	0
92	OHX	2	1960	7/7	0.97	0.21	-	100,100,100,100	0
93	MG	5	4083	1/1	0.84	0.36	-	32,32,32,32	0
92	OHX	6	2021	7/7	0.97	0.34	-	84,84,84,84	0
92	OHX	1	3724	7/7	0.97	0.30	-	65,65,65,65	0
92	OHX	C8	201	7/7	0.98	0.11	-	80,80,80,80	0
92	OHX	1	3704	7/7	0.94	0.33	-	82,82,82,82	0
93	MG	2	2083	1/1	0.97	0.62	-	83,83,83,83	0
93	MG	6	2178	1/1	0.63	0.29	-	67,67,67,67	0
92	OHX	1	3559	7/7	0.98	0.12	-	69,69,69,69	0
93	MG	5	3987	1/1	0.73	0.62	-	42,42,42,42	0
92	OHX	5	3655	7/7	0.98	0.39	-	62,62,62,62	0
93	MG	6	2075	1/1	0.96	0.44	-	71,71,71,71	0
93	MG	1	3980	1/1	0.75	0.45	-	48,48,48,48	0
92	OHX	2	1929	7/7	0.98	0.14	-	83,83,83,83	0
93	MG	5	3927	1/1	0.95	0.47	-	38,38,38,38	0
93	MG	4	232	1/1	0.96	0.20	-	44,44,44,44	0
93	MG	1	4021	1/1	0.96	0.29	-	39,39,39,39	0
93	MG	6	2143	1/1	0.85	0.48	-	75,75,75,75	0
93	MG	5	4126	1/1	0.95	0.40	-	40,40,40,40	0
93	MG	5	4156	1/1	0.83	0.59	-	52,52,52,52	0
93	MG	6	2176	1/1	0.91	0.36	-	58,58,58,58	0
93	MG	8	230	1/1	0.84	0.45	-	56,56,56,56	0
93	MG	5	4127	1/1	0.88	0.26	-	41,41,41,41	0
93	MG	6	2151	1/1	0.87	0.48	-	64,64,64,64	0
93	MG	5	4029	1/1	0.91	0.18	-	40,40,40,40	0
92	OHX	1	3450	7/7	0.98	0.12	-	56,56,56,56	0
93	MG	1	4051	1/1	0.92	0.96	-	53,53,53,53	0
93	MG	5	4010	1/1	0.88	0.30	-	56,56,56,56	0
92	OHX	2	2044	7/7	0.89	0.44	-	88,88,88,88	0
93	MG	1	3929	1/1	0.95	0.31	-	51,51,51,51	0
93	MG	1	3951	1/1	0.91	0.39	-	44,44,44,44	0
92	OHX	5	3477	7/7	0.97	0.12	-	56,56,56,56	0
92	OHX	5	3513	7/7	0.99	0.12	-	60,60,60,60	0
93	MG	6	2111	1/1	0.60	0.46	-	69,69,69,69	0
92	OHX	6	2043	7/7	0.97	0.40	-	81,81,81,81	0
93	MG	5	3971	1/1	0.62	0.66	-	73,73,73,73	0
92	OHX	6	1936	7/7	0.99	0.11	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	1	4003	1/1	0.95	0.24	-	41,41,41,41	0
92	OHX	1	3722	7/7	0.92	0.45	-	62,62,62,62	0
93	MG	5	3849	1/1	0.94	0.42	-	33,33,33,33	0
93	MG	5	4033	1/1	0.81	0.51	-	54,54,54,54	0
92	OHX	5	3635	7/7	0.98	0.26	-	57,57,57,57	0
93	MG	1	3950	1/1	0.93	0.48	-	36,36,36,36	0
93	MG	5	3857	1/1	0.98	0.51	-	31,31,31,31	0
93	MG	7	219	1/1	0.91	0.35	-	45,45,45,45	0
93	MG	5	3816	1/1	0.94	0.54	-	38,38,38,38	0
93	MG	5	4146	1/1	0.94	0.37	-	32,32,32,32	0
93	MG	6	2076	1/1	0.63	0.32	-	70,70,70,70	0
92	OHX	1	3445	7/7	0.99	0.10	-	66,66,66,66	0
93	MG	1	4119	1/1	0.82	0.25	-	44,44,44,44	0
93	MG	1	3913	1/1	0.79	0.53	-	43,43,43,43	0
93	MG	4	224	1/1	0.88	0.61	-	49,49,49,49	0
93	MG	5	4166	1/1	0.93	0.63	-	37,37,37,37	0
93	MG	1	3757	1/1	0.77	0.43	-	43,43,43,43	0
93	MG	1	3998	1/1	0.90	0.34	-	43,43,43,43	0
92	OHX	5	3649	7/7	0.97	0.30	-	50,50,50,50	0
93	MG	5	4096	1/1	1.00	0.12	-	32,32,32,32	0
93	MG	5	4040	1/1	0.95	0.38	-	37,37,37,37	0
92	OHX	2	1953	7/7	0.98	0.21	-	83,83,83,83	0
92	OHX	1	3700	7/7	0.97	0.41	-	80,80,80,80	0
93	MG	5	3915	1/1	0.93	0.62	-	30,30,30,30	0
93	MG	1	3962	1/1	0.91	0.41	-	31,31,31,31	0
93	MG	2	2135	1/1	0.88	0.58	-	68,68,68,68	0
93	MG	6	2137	1/1	0.77	0.45	-	85,85,85,85	0
93	MG	5	4015	1/1	0.92	0.40	-	38,38,38,38	0
93	MG	5	4111	1/1	0.96	0.19	-	49,49,49,49	0
92	OHX	6	2017	7/7	0.95	0.32	-	99,99,99,99	0
93	MG	6	2119	1/1	0.96	0.31	-	59,59,59,59	0
92	OHX	2	2041	7/7	0.95	0.35	-	83,83,83,83	0
93	MG	6	2162	1/1	0.93	0.31	-	55,55,55,55	0
93	MG	5	3803	1/1	0.98	0.20	-	32,32,32,32	0
93	MG	1	4083	1/1	0.94	0.47	-	54,54,54,54	0
93	MG	6	2091	1/1	0.65	0.73	-	66,66,66,66	0
93	MG	5	4021	1/1	0.74	0.54	-	50,50,50,50	0
93	MG	6	2065	1/1	0.96	0.32	-	61,61,61,61	0
93	MG	1	3791	1/1	0.95	0.43	-	32,32,32,32	0
92	OHX	6	1937	7/7	0.96	0.15	-	81,81,81,81	0
93	MG	6	2169	1/1	0.69	0.44	-	97,97,97,97	0
93	MG	1	3935	1/1	0.86	0.41	-	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
93	MG	5	3940	1/1	0.97	0.70	-	34,34,34,34	0
93	MG	5	4035	1/1	0.81	0.32	-	47,47,47,47	0
93	MG	2	2058	1/1	0.92	0.23	-	81,81,81,81	0
93	MG	6	2078	1/1	0.85	0.23	-	58,58,58,58	0
93	MG	5	3855	1/1	0.89	0.23	-	36,36,36,36	0
93	MG	5	3887	1/1	0.89	0.32	-	34,34,34,34	0
93	MG	5	3831	1/1	0.95	0.25	-	41,41,41,41	0
93	MG	5	4055	1/1	0.94	0.28	-	43,43,43,43	0
92	OHX	1	3593	7/7	0.98	0.17	-	86,86,86,86	0
92	OHX	5	3510	7/7	0.99	0.10	-	90,90,90,90	0
93	MG	6	2087	1/1	0.87	0.29	-	66,66,66,66	0
93	MG	5	3991	1/1	0.91	0.20	-	44,44,44,44	0
92	OHX	4	213	7/7	0.97	0.22	-	72,72,72,72	0
93	MG	3	217	1/1	0.97	0.49	-	39,39,39,39	0
92	OHX	5	3640	7/7	0.99	0.25	-	58,58,58,58	0
93	MG	1	4062	1/1	0.86	0.34	-	32,32,32,32	0
93	MG	1	4001	1/1	0.76	0.39	-	61,61,61,61	0
92	OHX	5	3455	7/7	0.98	0.12	-	58,58,58,58	0
93	MG	1	3991	1/1	0.95	0.31	-	39,39,39,39	0
92	OHX	1	3604	7/7	0.96	0.33	-	62,62,62,62	0
93	MG	5	4003	1/1	0.94	0.27	-	37,37,37,37	0
93	MG	5	4142	1/1	0.67	0.25	-	60,60,60,60	0
93	MG	5	4133	1/1	0.86	0.41	-	35,35,35,35	0
93	MG	5	4125	1/1	0.98	0.21	-	39,39,39,39	0
93	MG	5	3823	1/1	0.96	0.47	-	55,55,55,55	0
93	MG	1	3773	1/1	0.95	0.16	-	57,57,57,57	0
92	OHX	1	3454	7/7	0.98	0.11	-	59,59,59,59	0
93	MG	5	3798	1/1	0.85	0.59	-	42,42,42,42	0
93	MG	o3	202	1/1	0.92	0.42	-	44,44,44,44	0
93	MG	5	4118	1/1	0.88	0.56	-	44,44,44,44	0
92	OHX	1	3622	7/7	0.98	0.24	-	79,79,79,79	0
92	OHX	4	219	7/7	0.96	0.30	-	65,65,65,65	0
92	OHX	5	3545	7/7	0.99	0.18	-	66,66,66,66	0
93	MG	5	3980	1/1	0.90	0.28	-	56,56,56,56	0
92	OHX	2	2002	7/7	0.98	0.34	-	86,86,86,86	0
93	MG	5	4067	1/1	0.76	0.60	-	37,37,37,37	0
93	MG	1	3743	1/1	0.88	0.48	-	41,41,41,41	0
93	MG	5	3862	1/1	0.80	0.52	-	32,32,32,32	0
92	OHX	5	3734	7/7	0.98	0.25	-	91,91,91,91	0
93	MG	2	2067	1/1	0.88	0.59	-	78,78,78,78	0
92	OHX	1	3641	7/7	0.98	0.27	-	70,70,70,70	0
93	MG	5	4134	1/1	0.80	0.34	-	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
93	MG	6	2161	1/1	0.89	0.38	-	59,59,59,59	0
92	OHX	2	1961	7/7	0.97	0.24	-	103,103,103,103	0
93	MG	5	4161	1/1	0.96	0.20	-	57,57,57,57	0
92	OHX	1	3661	7/7	0.97	0.22	-	77,77,77,77	0
93	MG	2	2056	1/1	0.83	0.31	-	74,74,74,74	0
93	MG	5	3957	1/1	0.90	0.61	-	35,35,35,35	0
93	MG	5	4016	1/1	0.95	0.35	-	42,42,42,42	0
93	MG	5	3810	1/1	0.87	0.34	-	37,37,37,37	0
93	MG	1	3982	1/1	0.88	0.21	-	58,58,58,58	0
93	MG	1	3787	1/1	0.93	0.39	-	33,33,33,33	0
93	MG	5	4057	1/1	0.80	0.21	-	48,48,48,48	0
92	OHX	6	1983	7/7	0.98	0.17	-	89,89,89,89	0
92	OHX	2	1920	7/7	0.99	0.08	-	76,76,76,76	0
93	MG	6	2093	1/1	0.61	0.48	-	90,90,90,90	0
93	MG	5	3760	1/1	0.90	0.20	-	32,32,32,32	0
93	MG	1	4117	1/1	0.97	0.18	-	76,76,76,76	0
92	OHX	1	3651	7/7	0.97	0.19	-	57,57,57,57	0
93	MG	5	3996	1/1	0.95	0.45	-	31,31,31,31	0
93	MG	1	4022	1/1	0.86	0.19	-	83,83,83,83	0
93	MG	3	216	1/1	0.90	0.12	-	59,59,59,59	0
93	MG	6	2127	1/1	0.88	0.25	-	54,54,54,54	0
92	OHX	1	3497	7/7	0.99	0.10	-	53,53,53,53	0
92	OHX	5	3626	7/7	0.96	0.31	-	79,79,79,79	0
93	MG	5	4063	1/1	0.92	0.47	-	39,39,39,39	0
93	MG	1	4095	1/1	0.95	0.44	-	37,37,37,37	0
92	OHX	1	3634	7/7	0.98	0.24	-	66,66,66,66	0
93	MG	6	2115	1/1	0.84	0.37	-	69,69,69,69	0
93	MG	1	3799	1/1	0.93	0.26	-	34,34,34,34	0
93	MG	1	4065	1/1	0.90	1.04	-	54,54,54,54	0
93	MG	1	3837	1/1	0.94	0.63	-	34,34,34,34	0
93	MG	5	4123	1/1	0.94	0.24	-	33,33,33,33	0
93	MG	6	2062	1/1	0.76	0.73	-	61,61,61,61	0
93	MG	1	3735	1/1	0.96	0.48	-	53,53,53,53	0
93	MG	5	4056	1/1	0.91	0.24	-	36,36,36,36	0
93	MG	1	4120	1/1	0.93	0.31	-	58,58,58,58	0
92	OHX	5	3667	7/7	0.97	0.24	-	51,51,51,51	0
92	OHX	5	3682	7/7	0.95	0.29	-	61,61,61,61	0
93	MG	5	4155	1/1	0.93	0.31	-	40,40,40,40	0
92	OHX	2	1984	7/7	0.98	0.24	-	83,83,83,83	0
93	MG	1	3846	1/1	0.87	0.53	-	38,38,38,38	0
93	MG	1	3797	1/1	0.91	0.32	-	35,35,35,35	0
92	OHX	6	2053	7/7	0.96	0.32	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	2	2088	1/1	0.92	0.39	-	77,77,77,77	0
93	MG	1	3960	1/1	0.94	0.17	-	41,41,41,41	0
93	MG	4	222	1/1	0.88	0.50	-	48,48,48,48	0
93	MG	6	2129	1/1	0.74	0.66	-	61,61,61,61	0
92	OHX	6	2036	7/7	0.95	0.33	-	73,73,73,73	0
93	MG	1	3981	1/1	0.95	1.02	-	63,63,63,63	0
92	OHX	5	3471	7/7	0.98	0.12	-	53,53,53,53	0
93	MG	1	3834	1/1	0.93	0.44	-	39,39,39,39	0
93	MG	o9	101	1/1	0.69	0.51	-	41,41,41,41	0
93	MG	6	2185	1/1	0.94	0.40	-	92,92,92,92	0
93	MG	5	3829	1/1	0.95	0.58	-	31,31,31,31	0
93	MG	1	3885	1/1	0.95	0.55	-	35,35,35,35	0
93	MG	6	2130	1/1	0.73	0.52	-	67,67,67,67	0
93	MG	8	226	1/1	0.93	0.52	-	53,53,53,53	0
93	MG	5	4173	1/1	0.96	0.20	-	42,42,42,42	0
93	MG	1	3965	1/1	0.61	0.62	-	51,51,51,51	0
93	MG	5	3808	1/1	0.66	0.23	-	50,50,50,50	0
93	MG	1	3992	1/1	0.97	0.26	-	45,45,45,45	0
93	MG	6	2120	1/1	0.68	0.54	-	102,102,102,102	0
92	OHX	1	3495	7/7	0.99	0.12	-	67,67,67,67	0
93	MG	5	4091	1/1	0.90	0.22	-	51,51,51,51	0
93	MG	2	2068	1/1	0.83	0.83	-	75,75,75,75	0
92	OHX	1	3609	7/7	0.98	0.26	-	71,71,71,71	0
93	MG	L4	402	1/1	0.94	0.35	-	50,50,50,50	0
92	OHX	1	3613	7/7	0.95	0.28	-	87,87,87,87	0
93	MG	1	3795	1/1	0.92	0.52	-	58,58,58,58	0
93	MG	5	3982	1/1	0.92	0.49	-	43,43,43,43	0
92	OHX	5	3749	7/7	0.96	0.29	-	87,87,87,87	0
93	MG	1	3915	1/1	0.67	0.85	-	50,50,50,50	0
93	MG	5	4001	1/1	0.91	0.29	-	45,45,45,45	0
93	MG	1	3948	1/1	0.92	0.49	-	43,43,43,43	0
93	MG	2	2140	1/1	0.91	0.30	-	83,83,83,83	0
93	MG	5	4162	1/1	0.90	0.35	-	45,45,45,45	0
93	MG	6	2136	1/1	-0.02	0.45	-	75,75,75,75	0
93	MG	5	3904	1/1	0.94	0.69	-	37,37,37,37	0
93	MG	1	3760	1/1	0.86	0.58	-	45,45,45,45	0
92	OHX	1	3505	7/7	0.98	0.14	-	64,64,64,64	0
92	OHX	6	1942	7/7	0.97	0.12	-	73,73,73,73	0
93	MG	1	3947	1/1	0.67	0.57	-	98,98,98,98	0
93	MG	1	3988	1/1	0.85	0.37	-	35,35,35,35	0
93	MG	1	3857	1/1	0.92	0.67	-	36,36,36,36	0
92	OHX	2	1933	7/7	0.98	0.10	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	1	4115	1/1	0.93	0.33	-	34,34,34,34	0
93	MG	5	3966	1/1	0.91	0.26	-	55,55,55,55	0
92	OHX	5	3732	7/7	0.97	0.30	-	65,65,65,65	0
93	MG	1	3772	1/1	0.99	0.23	-	30,30,30,30	0
92	OHX	1	3556	7/7	0.98	0.21	-	81,81,81,81	0
93	MG	1	4008	1/1	0.87	0.15	-	51,51,51,51	0
93	MG	1	3856	1/1	0.94	0.27	-	32,32,32,32	0
92	OHX	5	3625	7/7	0.98	0.29	-	53,53,53,53	0
93	MG	5	3806	1/1	0.95	0.47	-	39,39,39,39	0
93	MG	5	3802	1/1	0.91	0.31	-	48,48,48,48	0
92	OHX	5	3717	7/7	0.96	0.25	-	84,84,84,84	0
93	MG	6	2081	1/1	0.96	0.22	-	70,70,70,70	0
92	OHX	6	2015	7/7	0.96	0.32	-	79,79,79,79	0
93	MG	6	2123	1/1	0.93	0.06	-	93,93,93,93	0
93	MG	1	4114	1/1	0.89	0.35	-	39,39,39,39	0
93	MG	d7	102	1/1	0.52	0.51	-	74,74,74,74	0
93	MG	1	3742	1/1	0.91	0.52	-	35,35,35,35	0
93	MG	5	3972	1/1	0.90	0.39	-	32,32,32,32	0
93	MG	5	4104	1/1	0.79	0.56	-	43,43,43,43	0
92	OHX	7	210	7/7	0.93	0.30	-	91,91,91,91	0
92	OHX	2	2042	7/7	0.94	0.21	-	126,126,126,126	0
93	MG	1	3780	1/1	0.92	0.51	-	37,37,37,37	0
93	MG	5	3761	1/1	0.93	0.21	-	42,42,42,42	0
93	MG	5	3900	1/1	0.82	0.48	-	39,39,39,39	0
92	OHX	5	3726	7/7	0.98	0.29	-	90,90,90,90	0
93	MG	1	3777	1/1	0.82	0.47	-	47,47,47,47	0
93	MG	1	4011	1/1	0.97	0.15	-	47,47,47,47	0
92	OHX	1	3672	7/7	0.97	0.15	-	60,60,60,60	0
92	OHX	C3	201	7/7	0.95	0.20	-	96,96,96,96	0
93	MG	1	3917	1/1	0.91	0.55	-	35,35,35,35	0
92	OHX	6	2050	7/7	0.96	0.41	-	68,68,68,68	0
93	MG	2	2084	1/1	0.76	0.61	-	88,88,88,88	0
93	MG	1	4118	1/1	0.62	0.30	-	43,43,43,43	0
92	OHX	1	3610	7/7	0.98	0.25	-	66,66,66,66	0
93	MG	5	3889	1/1	0.97	0.19	-	36,36,36,36	0
93	MG	1	4042	1/1	0.92	0.51	-	53,53,53,53	0
93	MG	1	4026	1/1	0.88	0.37	-	49,49,49,49	0
93	MG	5	4106	1/1	0.73	0.11	-	93,93,93,93	0
93	MG	5	3772	1/1	0.84	0.30	-	41,41,41,41	0
93	MG	1	3779	1/1	0.88	0.42	-	37,37,37,37	0
93	MG	1	3823	1/1	0.93	0.46	-	44,44,44,44	0
93	MG	5	4097	1/1	0.96	0.78	-	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
93	MG	1	3854	1/1	0.94	0.76	-	43,43,43,43	0
93	MG	1	3881	1/1	0.87	0.62	-	41,41,41,41	0
93	MG	5	3905	1/1	0.99	0.39	-	32,32,32,32	0
93	MG	1	3900	1/1	0.77	0.37	-	33,33,33,33	0
93	MG	7	215	1/1	0.92	0.42	-	36,36,36,36	0
93	MG	5	3860	1/1	0.96	0.40	-	39,39,39,39	0
92	OHX	5	3491	7/7	0.97	0.17	-	64,64,64,64	0
93	MG	1	3758	1/1	0.88	0.14	-	42,42,42,42	0
93	MG	7	213	1/1	0.89	0.73	-	33,33,33,33	0
92	OHX	6	2047	7/7	0.94	0.36	-	87,87,87,87	0
93	MG	5	4045	1/1	0.96	0.53	-	41,41,41,41	0
93	MG	5	3822	1/1	0.96	0.28	-	54,54,54,54	0
93	MG	6	2106	1/1	0.79	0.51	-	60,60,60,60	0
93	MG	1	4087	1/1	0.81	0.28	-	41,41,41,41	0
93	MG	6	2098	1/1	0.73	0.85	-	99,99,99,99	0
93	MG	5	3771	1/1	0.93	0.37	-	35,35,35,35	0
93	MG	4	231	1/1	0.84	0.26	-	72,72,72,72	0
93	MG	1	3798	1/1	0.88	0.23	-	51,51,51,51	0
93	MG	5	3794	1/1	0.81	0.50	-	39,39,39,39	0
92	OHX	5	3742	7/7	0.96	0.34	-	56,56,56,56	0
93	MG	1	4017	1/1	0.98	0.36	-	52,52,52,52	0
93	MG	6	2181	1/1	0.92	0.15	-	77,77,77,77	0
93	MG	1	3810	1/1	0.84	0.45	-	49,49,49,49	0
92	OHX	1	3410	7/7	1.00	0.09	-	39,39,39,39	0
92	OHX	2	2009	7/7	0.93	0.21	-	117,117,117,117	0
92	OHX	5	3413	7/7	1.00	0.11	-	33,33,33,33	0
93	MG	4	238	1/1	0.88	0.40	-	42,42,42,42	0
93	MG	5	4017	1/1	0.90	0.70	-	66,66,66,66	0
92	OHX	2	1991	7/7	0.98	0.32	-	96,96,96,96	0
93	MG	5	3948	1/1	0.71	0.34	-	61,61,61,61	0
93	MG	5	3921	1/1	0.91	0.49	-	34,34,34,34	0
92	OHX	5	3666	7/7	0.97	0.25	-	55,55,55,55	0
92	OHX	5	3637	7/7	0.96	0.25	-	63,63,63,63	0
93	MG	5	3992	1/1	0.95	0.14	-	50,50,50,50	0
93	MG	5	3939	1/1	0.89	0.37	-	43,43,43,43	0
92	OHX	6	1916	7/7	0.99	0.07	-	70,70,70,70	0
93	MG	1	3761	1/1	0.94	0.47	-	45,45,45,45	0
92	OHX	5	3581	7/7	0.98	0.36	-	55,55,55,55	0
93	MG	5	4157	1/1	0.72	0.41	-	50,50,50,50	0
92	OHX	1	3717	7/7	0.97	0.32	-	65,65,65,65	0
93	MG	5	3984	1/1	0.83	0.45	-	41,41,41,41	0
92	OHX	6	2005	7/7	0.97	0.20	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	2	2052	1/1	0.91	0.84	-	69,69,69,69	0
93	MG	5	4020	1/1	0.87	0.27	-	38,38,38,38	0
93	MG	1	3762	1/1	0.97	0.46	-	46,46,46,46	0
93	MG	2	2057	1/1	0.86	0.42	-	73,73,73,73	0
93	MG	5	3879	1/1	0.93	0.41	-	37,37,37,37	0
92	OHX	1	3720	7/7	0.96	0.33	-	65,65,65,65	0
93	MG	1	3879	1/1	0.95	0.58	-	33,33,33,33	0
93	MG	5	3777	1/1	0.90	0.28	-	32,32,32,32	0
92	OHX	5	3719	7/7	0.95	0.22	-	102,102,102,102	0
93	MG	6	2142	1/1	0.90	0.78	-	48,48,48,48	0
93	MG	1	4007	1/1	0.83	0.46	-	61,61,61,61	0
92	OHX	2	2016	7/7	0.97	0.26	-	84,84,84,84	0
93	MG	1	3974	1/1	0.95	0.53	-	47,47,47,47	0
93	MG	1	4068	1/1	0.92	0.37	-	39,39,39,39	0
93	MG	5	4077	1/1	0.86	0.37	-	49,49,49,49	0
93	MG	1	4000	1/1	0.80	0.44	-	43,43,43,43	0
92	OHX	2	2017	7/7	0.95	0.27	-	88,88,88,88	0
93	MG	1	4009	1/1	0.84	0.49	-	34,34,34,34	0
93	MG	5	4158	1/1	0.96	0.27	-	72,72,72,72	0
93	MG	1	4023	1/1	0.90	0.25	-	34,34,34,34	0
93	MG	1	4066	1/1	0.97	0.52	-	44,44,44,44	0
93	MG	6	2156	1/1	0.78	0.46	-	68,68,68,68	0
93	MG	1	4059	1/1	0.85	0.32	-	38,38,38,38	0
93	MG	1	4025	1/1	0.75	0.46	-	49,49,49,49	0
93	MG	1	3880	1/1	0.97	0.34	-	41,41,41,41	0
93	MG	1	4063	1/1	0.75	0.33	-	105,105,105,105	0
93	MG	1	4116	1/1	0.93	0.25	-	63,63,63,63	0
93	MG	1	3769	1/1	0.98	0.76	-	36,36,36,36	0
92	OHX	1	3625	7/7	0.97	0.22	-	69,69,69,69	0
93	MG	1	4079	1/1	0.90	0.38	-	36,36,36,36	0
92	OHX	c5	201	7/7	0.94	0.24	-	99,99,99,99	0
93	MG	1	3884	1/1	0.89	0.73	-	42,42,42,42	0
93	MG	1	3887	1/1	0.93	0.62	-	38,38,38,38	0
92	OHX	1	3681	7/7	0.98	0.27	-	76,76,76,76	0
93	MG	2	2059	1/1	0.39	0.30	-	86,86,86,86	0
93	MG	1	3920	1/1	0.98	0.53	-	36,36,36,36	0
92	OHX	5	3583	7/7	0.98	0.16	-	71,71,71,71	0
93	MG	7	218	1/1	0.95	0.20	-	37,37,37,37	0
93	MG	5	3850	1/1	0.93	0.98	-	41,41,41,41	0
93	MG	1	4125	1/1	0.91	0.91	-	49,49,49,49	0
93	MG	5	3809	1/1	0.55	0.21	-	88,88,88,88	0
92	OHX	1	3682	7/7	0.96	0.24	-	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
93	MG	1	3979	1/1	0.90	0.60	-	43,43,43,43	0
93	MG	1	3996	1/1	0.90	0.49	-	47,47,47,47	0
93	MG	5	3839	1/1	0.90	0.47	-	34,34,34,34	0
93	MG	5	3788	1/1	0.93	0.21	-	33,33,33,33	0
92	OHX	6	1948	7/7	0.97	0.23	-	82,82,82,82	0
93	MG	6	2147	1/1	0.60	0.43	-	66,66,66,66	0
93	MG	S4	301	1/1	0.58	0.73	-	83,83,83,83	0
92	OHX	2	2036	7/7	0.96	0.38	-	112,112,112,112	0
92	OHX	5	3594	7/7	0.97	0.30	-	74,74,74,74	0
93	MG	6	2095	1/1	0.94	0.42	-	55,55,55,55	0
93	MG	6	2072	1/1	0.90	0.48	-	59,59,59,59	0
93	MG	6	2160	1/1	0.98	0.51	-	73,73,73,73	0
93	MG	2	2121	1/1	0.88	0.48	-	68,68,68,68	0
93	MG	L3	404	1/1	0.95	0.12	-	41,41,41,41	0
93	MG	5	3896	1/1	0.86	0.74	-	33,33,33,33	0
92	OHX	6	2031	7/7	0.93	0.36	-	106,106,106,106	0
93	MG	1	3942	1/1	0.93	0.46	-	42,42,42,42	0
92	OHX	5	3629	7/7	0.96	0.23	-	90,90,90,90	0
92	OHX	6	2041	7/7	0.98	0.28	-	79,79,79,79	0
93	MG	5	3910	1/1	0.86	0.59	-	44,44,44,44	0
92	OHX	6	1930	7/7	0.99	0.11	-	64,64,64,64	0
93	MG	p	103	1/1	0.93	0.70	-	40,40,40,40	0
93	MG	2	2128	1/1	0.79	0.37	-	89,89,89,89	0
93	MG	2	2114	1/1	0.75	0.70	-	77,77,77,77	0
93	MG	6	2108	1/1	0.84	0.45	-	63,63,63,63	0
93	MG	5	4052	1/1	0.95	0.89	-	24,24,24,24	0
93	MG	8	222	1/1	0.94	0.34	-	43,43,43,43	0
92	OHX	1	3519	7/7	0.99	0.19	-	46,46,46,46	0
93	MG	1	3842	1/1	0.98	0.36	-	33,33,33,33	0
93	MG	1	4016	1/1	0.92	0.89	-	49,49,49,49	0
93	MG	1	4041	1/1	0.90	0.27	-	49,49,49,49	0
92	OHX	2	2018	7/7	0.97	0.32	-	84,84,84,84	0
93	MG	2	2139	1/1	0.45	0.33	-	93,93,93,93	0
93	MG	2	2055	1/1	0.90	0.75	-	75,75,75,75	0
92	OHX	6	2038	7/7	0.95	0.22	-	105,105,105,105	0
93	MG	m6	202	1/1	0.91	0.70	-	29,29,29,29	0
92	OHX	5	3569	7/7	0.98	0.20	-	62,62,62,62	0
93	MG	1	4040	1/1	0.94	0.20	-	49,49,49,49	0
92	OHX	1	3664	7/7	0.94	0.37	-	73,73,73,73	0
93	MG	5	4090	1/1	0.96	0.20	-	42,42,42,42	0
93	MG	1	3958	1/1	0.92	0.25	-	39,39,39,39	0
92	OHX	2	1996	7/7	0.95	0.22	-	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
93	MG	o2	201	1/1	0.74	0.46	-	32,32,32,32	0
92	OHX	2	1968	7/7	0.97	0.32	-	86,86,86,86	0
93	MG	Q2	503	1/1	0.93	0.23	-	48,48,48,48	0
93	MG	5	4062	1/1	0.92	0.19	-	48,48,48,48	0
93	MG	1	3941	1/1	0.87	0.28	-	51,51,51,51	0
92	OHX	6	1974	7/7	0.97	0.24	-	106,106,106,106	0
93	MG	5	3767	1/1	0.95	0.36	-	46,46,46,46	0
93	MG	5	4039	1/1	0.84	0.36	-	39,39,39,39	0
93	MG	2	2054	1/1	0.80	0.39	-	81,81,81,81	0
93	MG	1	3765	1/1	0.58	0.69	-	42,42,42,42	0
93	MG	1	4037	1/1	0.84	0.22	-	56,56,56,56	0
93	MG	1	3888	1/1	0.83	0.41	-	35,35,35,35	0
92	OHX	6	1999	7/7	0.97	0.30	-	75,75,75,75	0
92	OHX	1	3617	7/7	0.97	0.10	-	131,131,131,131	0
93	MG	5	3781	1/1	0.95	0.54	-	33,33,33,33	0
92	OHX	5	3747	7/7	0.95	0.23	-	61,61,61,61	0
93	MG	5	4167	1/1	0.91	0.22	-	33,33,33,33	0
93	MG	7	226	1/1	0.94	0.11	-	46,46,46,46	0
93	MG	5	4139	1/1	0.63	0.31	-	39,39,39,39	0
93	MG	5	3877	1/1	0.97	0.37	-	34,34,34,34	0
92	OHX	1	3639	7/7	0.98	0.27	-	67,67,67,67	0
93	MG	5	3950	1/1	0.51	0.77	-	43,43,43,43	0
93	MG	8	220	1/1	0.88	0.69	-	46,46,46,46	0
93	MG	5	3783	1/1	0.95	0.18	-	37,37,37,37	0
92	OHX	6	1995	7/7	0.98	0.31	-	79,79,79,79	0
93	MG	1	4038	1/1	0.89	0.89	-	46,46,46,46	0
93	MG	5	4028	1/1	0.88	0.31	-	33,33,33,33	0
92	OHX	6	1961	7/7	0.97	0.28	-	75,75,75,75	0
93	MG	5	3958	1/1	0.90	0.39	-	33,33,33,33	0
93	MG	m6	204	1/1	0.97	0.85	-	35,35,35,35	0
93	MG	6	2124	1/1	0.76	0.17	-	89,89,89,89	0
93	MG	6	2073	1/1	0.31	0.46	-	91,91,91,91	0
93	MG	6	2135	1/1	0.94	0.40	-	64,64,64,64	0
93	MG	5	3758	1/1	0.89	0.45	-	42,42,42,42	0
93	MG	7	216	1/1	0.96	0.69	-	34,34,34,34	0
92	OHX	1	3705	7/7	0.97	0.37	-	49,49,49,49	0
93	MG	1	3806	1/1	0.90	0.43	-	52,52,52,52	0
92	OHX	2	1954	7/7	0.97	0.12	-	89,89,89,89	0
93	MG	5	4037	1/1	0.95	0.32	-	40,40,40,40	0
93	MG	6	2096	1/1	0.88	0.60	-	59,59,59,59	0
92	OHX	1	3709	7/7	0.98	0.28	-	60,60,60,60	0
93	MG	5	4176	1/1	0.89	0.50	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
93	MG	5	3949	1/1	0.88	0.25	-	40,40,40,40	0
93	MG	5	3922	1/1	0.94	0.67	-	44,44,44,44	0
93	MG	1	4103	1/1	0.78	0.41	-	39,39,39,39	0
93	MG	1	3794	1/1	0.81	0.36	-	39,39,39,39	0
93	MG	5	4141	1/1	0.97	0.17	-	43,43,43,43	0
93	MG	5	3970	1/1	0.93	0.26	-	40,40,40,40	0
92	OHX	6	2007	7/7	0.97	0.36	-	82,82,82,82	0
93	MG	1	4047	1/1	0.90	0.58	-	43,43,43,43	0
92	OHX	5	3680	7/7	0.97	0.31	-	67,67,67,67	0
92	OHX	5	3548	7/7	0.97	0.25	-	61,61,61,61	0
92	OHX	8	215	7/7	0.91	0.41	-	55,55,55,55	0
93	MG	2	2119	1/1	0.89	0.12	-	87,87,87,87	0
93	MG	6	2155	1/1	0.85	0.21	-	76,76,76,76	0
93	MG	3	215	1/1	0.88	0.13	-	59,59,59,59	0
93	MG	2	2124	1/1	0.87	0.19	-	87,87,87,87	0
93	MG	8	224	1/1	0.87	0.33	-	53,53,53,53	0
93	MG	5	3864	1/1	0.96	0.44	-	35,35,35,35	0
93	MG	6	2088	1/1	0.85	0.35	-	65,65,65,65	0
92	OHX	5	3686	7/7	0.96	0.29	-	73,73,73,73	0
93	MG	1	4090	1/1	0.97	0.51	-	31,31,31,31	0
92	OHX	5	3613	7/7	0.98	0.25	-	54,54,54,54	0
92	OHX	5	3703	7/7	0.97	0.23	-	52,52,52,52	0
92	OHX	5	3556	7/7	0.98	0.26	-	55,55,55,55	0
92	OHX	5	3559	7/7	0.98	0.24	-	59,59,59,59	0
93	MG	5	4114	1/1	0.82	0.70	-	62,62,62,62	0
92	OHX	4	207	7/7	0.99	0.14	-	55,55,55,55	0
92	OHX	5	3537	7/7	0.97	0.21	-	73,73,73,73	0
93	MG	5	3886	1/1	0.97	0.39	-	39,39,39,39	0
92	OHX	1	3615	7/7	0.97	0.26	-	77,77,77,77	0
92	OHX	1	3592	7/7	0.97	0.24	-	65,65,65,65	0
93	MG	5	4027	1/1	0.94	0.38	-	39,39,39,39	0
93	MG	1	4109	1/1	0.89	0.38	-	44,44,44,44	0
93	MG	5	4019	1/1	0.86	0.21	-	42,42,42,42	0
93	MG	5	4075	1/1	0.94	0.27	-	34,34,34,34	0
92	OHX	3	201	7/7	0.99	0.08	-	60,60,60,60	0
92	OHX	2	1906	7/7	0.97	0.12	-	89,89,89,89	0
92	OHX	6	2034	7/7	0.97	0.26	-	99,99,99,99	0
93	MG	6	2061	1/1	0.93	0.17	-	69,69,69,69	0
93	MG	5	3827	1/1	0.91	0.60	-	35,35,35,35	0
93	MG	5	3978	1/1	0.97	0.66	-	40,40,40,40	0
93	MG	2	2081	1/1	0.87	0.41	-	87,87,87,87	0
92	OHX	1	3477	7/7	0.98	0.15	-	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
92	OHX	2	1990	7/7	0.98	0.26	-	99,99,99,99	0
93	MG	5	3792	1/1	0.99	0.39	-	31,31,31,31	0
92	OHX	6	2016	7/7	0.93	0.32	-	95,95,95,95	0
93	MG	1	3985	1/1	0.71	0.83	-	42,42,42,42	0
93	MG	5	4092	1/1	0.97	0.18	-	37,37,37,37	0
93	MG	2	2072	1/1	0.82	0.33	-	83,83,83,83	0
93	MG	5	3988	1/1	0.83	0.39	-	60,60,60,60	0
93	MG	5	4164	1/1	0.90	0.21	-	39,39,39,39	0
93	MG	5	4107	1/1	0.97	0.29	-	34,34,34,34	0
93	MG	1	4105	1/1	0.98	0.43	-	54,54,54,54	0
92	OHX	1	3468	7/7	0.99	0.09	-	54,54,54,54	0
93	MG	7	212	1/1	0.81	0.51	-	46,46,46,46	0
92	OHX	2	1959	7/7	0.95	0.19	-	98,98,98,98	0
93	MG	1	3833	1/1	0.86	0.48	-	39,39,39,39	0
92	OHX	2	2019	7/7	0.97	0.37	-	91,91,91,91	0
92	OHX	5	3571	7/7	0.96	0.26	-	61,61,61,61	0
93	MG	5	3931	1/1	0.94	0.71	-	32,32,32,32	0
93	MG	1	3792	1/1	0.98	0.32	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.