



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 24, 2017 – 06:15 AM EDT

PDB ID : 5DGE
Title : Coping with proline stalling: structural basis of hypusine-induced protein synthesis by the eukaryotic ribosome
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.; Dever, T.E.; Yusupov, M.
Deposited on : unknown
Resolution : 3.45 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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	:	rb-20029824
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)	:	rb-20029824

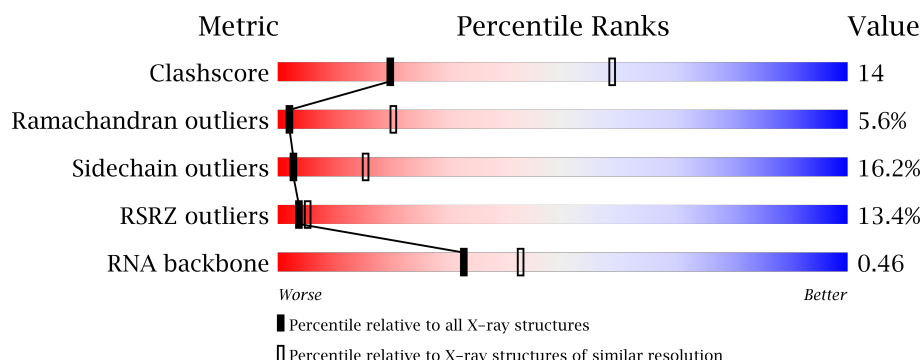
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1040 (3.52-3.40)
Ramachandran outliers	110173	1009 (3.52-3.40)
Sidechain outliers	110143	1010 (3.52-3.40)
RSRZ outliers	101464	1017 (3.54-3.38)
RNA backbone	2435	1020 (4.02-2.86)

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 ≥ 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	1800	<div> <div>6%</div> <div>38% 46% 14% ..</div> </div>
1	6	1800	<div> <div>3%</div> <div>39% 45% 15% .</div> </div>
2	S0	251	<div> <div>25%</div> <div>26% 45% 10% 18%</div> </div>
2	s0	251	<div> <div>8%</div> <div>63% 18% . 18%</div> </div>
3	S1	254	<div> <div>31%</div> <div>24% 46% 13% . 16%</div> </div>

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Mol	Chain	Length	Quality of chain
3	s1	254	
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	

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Mol	Chain	Length	Quality of chain
16	C4	136	
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	

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Mol	Chain	Length	Quality of chain
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	





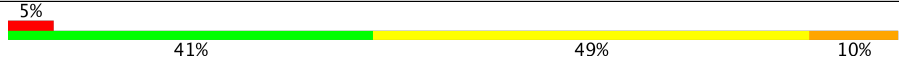
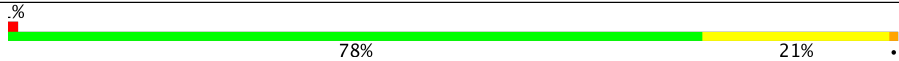
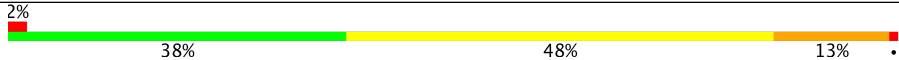
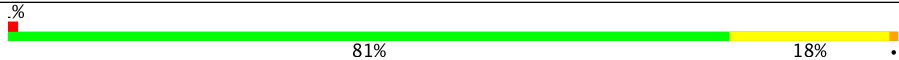
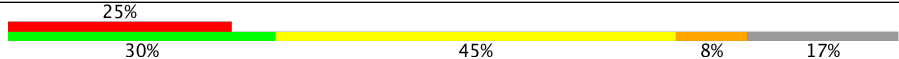
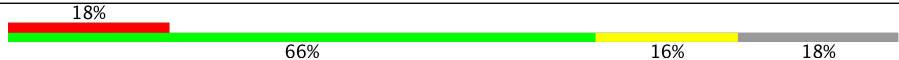
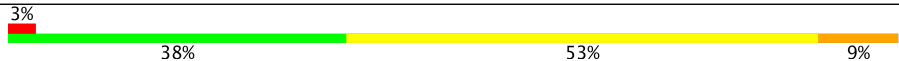
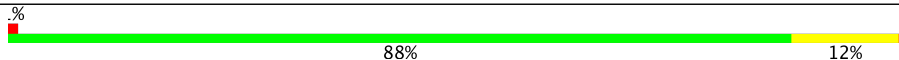
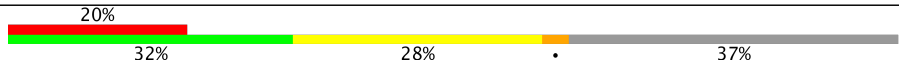

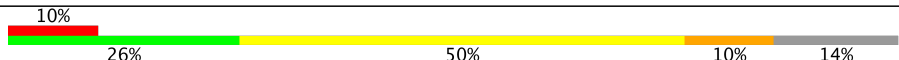
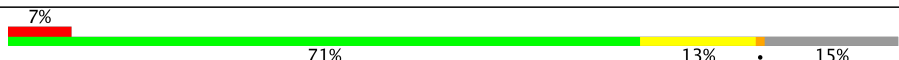
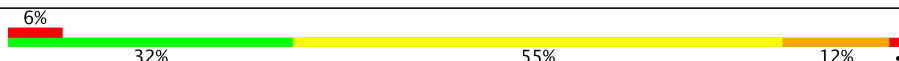
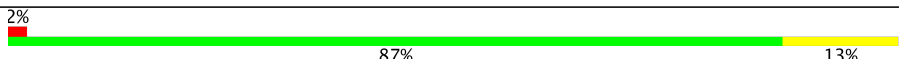


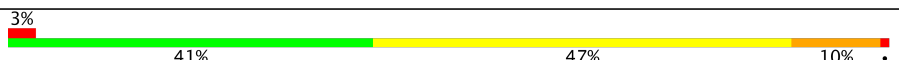
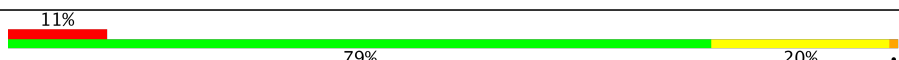
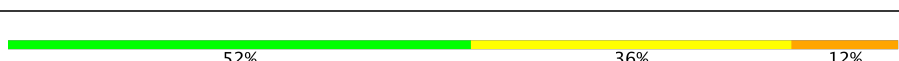
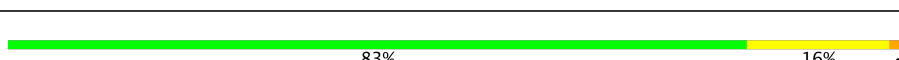
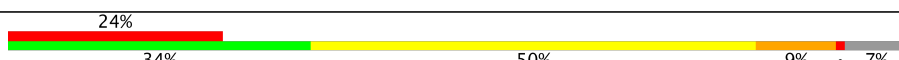
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Mol	Chain	Length	Quality of chain
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	

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Mol	Chain	Length	Quality of chain
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	

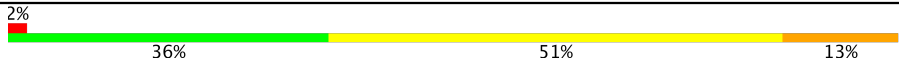


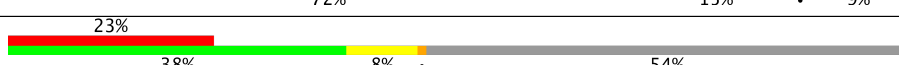



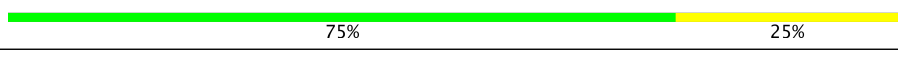
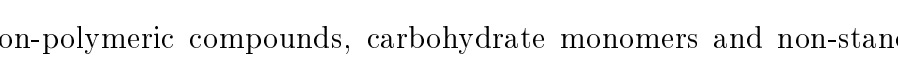

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Mol	Chain	Length	Quality of chain
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	

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Mol	Chain	Length	Quality of chain
79	Q3	91	
79	q3	91	
80	e0	62	
81	m2	165	
82	p0	311	
83	p1	106	
83	p2	106	
84	f	157	
85	B	4	
85	C	4	

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
84	5CT	f	51	X	-	-	-
86	MG	1	3401	-	-	-	X
86	MG	1	3403	-	-	-	X
86	MG	1	3406	-	-	-	X
86	MG	1	3407	-	-	-	X
86	MG	1	3413	-	-	-	X
86	MG	1	3414	-	-	-	X
86	MG	1	3415	-	-	-	X
86	MG	1	3419	-	-	-	X
86	MG	1	3422	-	-	-	X
86	MG	1	3426	-	-	-	X
86	MG	1	3429	-	-	-	X
86	MG	1	3433	-	-	-	X
86	MG	1	3437	-	-	-	X
86	MG	1	3440	-	-	-	X
86	MG	1	3441	-	-	-	X
86	MG	1	3448	-	-	-	X
86	MG	1	3454	-	-	-	X
86	MG	1	3464	-	-	-	X
86	MG	1	3465	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	1	3466	-	-	-	X
86	MG	1	3467	-	-	-	X
86	MG	1	3469	-	-	-	X
86	MG	1	3472	-	-	-	X
86	MG	1	3476	-	-	-	X
86	MG	1	3477	-	-	-	X
86	MG	1	3479	-	-	-	X
86	MG	1	3481	-	-	-	X
86	MG	1	3482	-	-	-	X
86	MG	1	3488	-	-	-	X
86	MG	1	3490	-	-	-	X
86	MG	1	3495	-	-	-	X
86	MG	1	3496	-	-	-	X
86	MG	1	3497	-	-	-	X
86	MG	1	3498	-	-	-	X
86	MG	1	3501	-	-	-	X
86	MG	1	3506	-	-	-	X
86	MG	1	3507	-	-	-	X
86	MG	1	3509	-	-	-	X
86	MG	1	3511	-	-	-	X
86	MG	1	3516	-	-	-	X
86	MG	1	3517	-	-	-	X
86	MG	1	3523	-	-	-	X
86	MG	1	3524	-	-	-	X
86	MG	1	3527	-	-	-	X
86	MG	1	3530	-	-	-	X
86	MG	1	3531	-	-	-	X
86	MG	1	3538	-	-	-	X
86	MG	1	3539	-	-	-	X
86	MG	1	3540	-	-	-	X
86	MG	1	3545	-	-	-	X
86	MG	1	3546	-	-	-	X
86	MG	1	3554	-	-	-	X
86	MG	1	3555	-	-	-	X
86	MG	1	3556	-	-	-	X
86	MG	1	3557	-	-	-	X
86	MG	1	3559	-	-	-	X
86	MG	1	3560	-	-	-	X
86	MG	1	3561	-	-	-	X
86	MG	1	3562	-	-	-	X
86	MG	1	3563	-	-	-	X
86	MG	1	3567	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	1	3570	-	-	-	X
86	MG	1	3572	-	-	-	X
86	MG	1	3573	-	-	-	X
86	MG	1	3575	-	-	-	X
86	MG	1	3576	-	-	-	X
86	MG	1	3578	-	-	-	X
86	MG	1	3580	-	-	-	X
86	MG	1	3582	-	-	-	X
86	MG	1	3583	-	-	-	X
86	MG	1	3585	-	-	-	X
86	MG	1	3586	-	-	-	X
86	MG	1	3587	-	-	-	X
86	MG	1	3588	-	-	-	X
86	MG	1	3589	-	-	-	X
86	MG	1	3609	-	-	-	X
86	MG	1	3618	-	-	-	X
86	MG	1	3627	-	-	-	X
86	MG	1	3642	-	-	-	X
86	MG	1	3653	-	-	-	X
86	MG	1	3661	-	-	-	X
86	MG	1	3664	-	-	-	X
86	MG	1	3668	-	-	-	X
86	MG	1	3670	-	-	-	X
86	MG	1	3681	-	-	-	X
86	MG	1	3687	-	-	-	X
86	MG	1	3696	-	-	-	X
86	MG	1	3705	-	-	-	X
86	MG	1	3715	-	-	-	X
86	MG	1	3719	-	-	-	X
86	MG	1	3732	-	-	-	X
86	MG	1	3735	-	-	-	X
86	MG	1	3737	-	-	-	X
86	MG	1	3738	-	-	-	X
86	MG	1	3739	-	-	-	X
86	MG	1	3742	-	-	-	X
86	MG	1	3743	-	-	-	X
86	MG	1	3756	-	-	-	X
86	MG	1	3757	-	-	-	X
86	MG	1	4112	-	-	-	X
86	MG	1	4115	-	-	-	X
86	MG	1	4116	-	-	-	X
86	MG	2	1909	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	2	1910	-	-	-	X
86	MG	2	1911	-	-	-	X
86	MG	2	1912	-	-	-	X
86	MG	2	1920	-	-	-	X
86	MG	2	1922	-	-	-	X
86	MG	2	1926	-	-	-	X
86	MG	2	1931	-	-	-	X
86	MG	2	1932	-	-	-	X
86	MG	2	1937	-	-	-	X
86	MG	2	1938	-	-	-	X
86	MG	2	1950	-	-	-	X
86	MG	2	1962	-	-	-	X
86	MG	2	1975	-	-	-	X
86	MG	2	1981	-	-	-	X
86	MG	2	1989	-	-	-	X
86	MG	3	204	-	-	-	X
86	MG	4	207	-	-	-	X
86	MG	4	233	-	-	-	X
86	MG	5	3403	-	-	-	X
86	MG	5	3405	-	-	-	X
86	MG	5	3407	-	-	-	X
86	MG	5	3409	-	-	-	X
86	MG	5	3412	-	-	-	X
86	MG	5	3413	-	-	-	X
86	MG	5	3416	-	-	-	X
86	MG	5	3419	-	-	-	X
86	MG	5	3420	-	-	-	X
86	MG	5	3421	-	-	-	X
86	MG	5	3426	-	-	-	X
86	MG	5	3428	-	-	-	X
86	MG	5	3436	-	-	-	X
86	MG	5	3440	-	-	-	X
86	MG	5	3451	-	-	-	X
86	MG	5	3455	-	-	-	X
86	MG	5	3456	-	-	-	X
86	MG	5	3457	-	-	-	X
86	MG	5	3462	-	-	-	X
86	MG	5	3465	-	-	-	X
86	MG	5	3471	-	-	-	X
86	MG	5	3472	-	-	-	X
86	MG	5	3491	-	-	-	X
86	MG	5	3493	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	5	3495	-	-	-	X
86	MG	5	3497	-	-	-	X
86	MG	5	3501	-	-	-	X
86	MG	5	3505	-	-	-	X
86	MG	5	3506	-	-	-	X
86	MG	5	3507	-	-	-	X
86	MG	5	3508	-	-	-	X
86	MG	5	3512	-	-	-	X
86	MG	5	3513	-	-	-	X
86	MG	5	3517	-	-	-	X
86	MG	5	3519	-	-	-	X
86	MG	5	3521	-	-	-	X
86	MG	5	3522	-	-	-	X
86	MG	5	3527	-	-	-	X
86	MG	5	3530	-	-	-	X
86	MG	5	3537	-	-	-	X
86	MG	5	3541	-	-	-	X
86	MG	5	3543	-	-	-	X
86	MG	5	3544	-	-	-	X
86	MG	5	3545	-	-	-	X
86	MG	5	3546	-	-	-	X
86	MG	5	3550	-	-	-	X
86	MG	5	3553	-	-	-	X
86	MG	5	3555	-	-	-	X
86	MG	5	3556	-	-	-	X
86	MG	5	3560	-	-	-	X
86	MG	5	3561	-	-	-	X
86	MG	5	3563	-	-	-	X
86	MG	5	3564	-	-	-	X
86	MG	5	3565	-	-	-	X
86	MG	5	3566	-	-	-	X
86	MG	5	3569	-	-	-	X
86	MG	5	3570	-	-	-	X
86	MG	5	3577	-	-	-	X
86	MG	5	3581	-	-	-	X
86	MG	5	3582	-	-	-	X
86	MG	5	3584	-	-	-	X
86	MG	5	3585	-	-	-	X
86	MG	5	3586	-	-	-	X
86	MG	5	3588	-	-	-	X
86	MG	5	3589	-	-	-	X
86	MG	5	3590	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	5	3591	-	-	-	X
86	MG	5	3592	-	-	-	X
86	MG	5	3593	-	-	-	X
86	MG	5	3594	-	-	-	X
86	MG	5	3596	-	-	-	X
86	MG	5	3597	-	-	-	X
86	MG	5	3599	-	-	-	X
86	MG	5	3601	-	-	-	X
86	MG	5	3606	-	-	-	X
86	MG	5	3617	-	-	-	X
86	MG	5	3638	-	-	-	X
86	MG	5	3643	-	-	-	X
86	MG	5	3644	-	-	-	X
86	MG	5	3651	-	-	-	X
86	MG	5	3654	-	-	-	X
86	MG	5	3656	-	-	-	X
86	MG	5	3672	-	-	-	X
86	MG	5	3674	-	-	-	X
86	MG	5	3677	-	-	-	X
86	MG	5	3678	-	-	-	X
86	MG	5	3680	-	-	-	X
86	MG	5	3682	-	-	-	X
86	MG	5	3686	-	-	-	X
86	MG	5	3705	-	-	-	X
86	MG	5	3717	-	-	-	X
86	MG	5	3719	-	-	-	X
86	MG	5	3720	-	-	-	X
86	MG	5	3729	-	-	-	X
86	MG	5	3735	-	-	-	X
86	MG	5	3737	-	-	-	X
86	MG	5	3741	-	-	-	X
86	MG	5	3744	-	-	-	X
86	MG	5	3767	-	-	-	X
86	MG	5	3769	-	-	-	X
86	MG	5	3774	-	-	-	X
86	MG	5	3779	-	-	-	X
86	MG	5	3783	-	-	-	X
86	MG	5	3785	-	-	-	X
86	MG	5	3794	-	-	-	X
86	MG	5	3796	-	-	-	X
86	MG	5	3800	-	-	-	X
86	MG	5	4172	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	5	4174	-	-	-	X
86	MG	5	4175	-	-	-	X
86	MG	5	4176	-	-	-	X
86	MG	6	1901	-	-	-	X
86	MG	6	1904	-	-	-	X
86	MG	6	1906	-	-	-	X
86	MG	6	1910	-	-	-	X
86	MG	6	1915	-	-	-	X
86	MG	6	1918	-	-	-	X
86	MG	6	1923	-	-	-	X
86	MG	6	1925	-	-	-	X
86	MG	6	1929	-	-	-	X
86	MG	6	1933	-	-	-	X
86	MG	6	1938	-	-	-	X
86	MG	6	1943	-	-	-	X
86	MG	6	1944	-	-	-	X
86	MG	6	1951	-	-	-	X
86	MG	6	1952	-	-	-	X
86	MG	6	1966	-	-	-	X
86	MG	6	1968	-	-	-	X
86	MG	6	1974	-	-	-	X
86	MG	6	1975	-	-	-	X
86	MG	6	1978	-	-	-	X
86	MG	6	1981	-	-	-	X
86	MG	6	1990	-	-	-	X
86	MG	6	2005	-	-	-	X
86	MG	6	2006	-	-	-	X
86	MG	6	2010	-	-	-	X
86	MG	7	203	-	-	-	X
86	MG	8	203	-	-	-	X
86	MG	8	206	-	-	-	X
86	MG	B	103	-	-	-	X
86	MG	C	102	-	-	-	X
86	MG	L2	302	-	-	-	X
86	MG	L7	302	-	-	-	X
86	MG	M7	202	-	-	-	X
86	MG	N3	201	-	-	-	X
86	MG	O7	102	-	-	-	X
86	MG	d2	201	-	-	-	X
86	MG	d6	102	-	-	-	X
86	MG	l2	301	-	-	-	X
86	MG	l2	302	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	l3	402	-	-	-	X
86	MG	m5	301	-	-	-	X
86	MG	m7	201	-	-	-	X
86	MG	n3	201	-	-	-	X
86	MG	n6	201	-	-	-	X
86	MG	n8	201	-	-	-	X
86	MG	s8	302	-	-	-	X
87	OHX	1	3778	-	-	-	X
87	OHX	1	3782	-	-	-	X
87	OHX	1	3784	-	-	-	X
87	OHX	1	3786	-	-	-	X
87	OHX	1	3791	-	-	-	X
87	OHX	1	3793	-	-	-	X
87	OHX	1	3794	-	-	-	X
87	OHX	1	3798	-	-	-	X
87	OHX	1	3800	-	-	-	X
87	OHX	1	3807	-	-	-	X
87	OHX	1	3808	-	-	-	X
87	OHX	1	3815	-	-	-	X
87	OHX	1	3820	-	-	-	X
87	OHX	1	3822	-	-	-	X
87	OHX	1	3825	-	-	-	X
87	OHX	1	3830	-	-	-	X
87	OHX	1	3834	-	-	-	X
87	OHX	1	3835	-	-	-	X
87	OHX	1	3838	-	-	-	X
87	OHX	1	3841	-	-	-	X
87	OHX	1	3843	-	-	-	X
87	OHX	1	3846	-	-	-	X
87	OHX	1	3849	-	-	-	X
87	OHX	1	3853	-	-	-	X
87	OHX	1	3854	-	-	X	-
87	OHX	1	3856	-	-	-	X
87	OHX	1	3859	-	-	-	X
87	OHX	1	3871	-	-	-	X
87	OHX	1	3874	-	-	-	X
87	OHX	1	3875	-	-	-	X
87	OHX	1	3876	-	-	-	X
87	OHX	1	3879	-	-	-	X
87	OHX	1	3883	-	-	-	X
87	OHX	1	3884	-	-	-	X
87	OHX	1	3885	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	1	3886	-	-	-	X
87	OHX	1	3887	-	-	-	X
87	OHX	1	3888	-	-	-	X
87	OHX	1	3889	-	-	X	-
87	OHX	1	3890	-	-	-	X
87	OHX	1	3896	-	-	-	X
87	OHX	1	3897	-	-	-	X
87	OHX	1	3898	-	-	-	X
87	OHX	1	3899	-	-	-	X
87	OHX	1	3903	-	-	-	X
87	OHX	1	3906	-	-	-	X
87	OHX	1	3911	-	-	-	X
87	OHX	1	3915	-	-	-	X
87	OHX	1	3920	-	-	-	X
87	OHX	1	3923	-	-	-	X
87	OHX	1	3936	-	-	-	X
87	OHX	1	3938	-	-	-	X
87	OHX	1	3939	-	-	-	X
87	OHX	1	3940	-	-	X	-
87	OHX	1	3947	-	-	-	X
87	OHX	1	3955	-	-	-	X
87	OHX	1	3962	-	-	-	X
87	OHX	1	3963	-	-	-	X
87	OHX	1	3966	-	-	-	X
87	OHX	1	3968	-	-	-	X
87	OHX	1	3971	-	-	-	X
87	OHX	1	3976	-	-	-	X
87	OHX	1	3983	-	-	-	X
87	OHX	1	3985	-	-	-	X
87	OHX	1	3992	-	-	-	X
87	OHX	1	3993	-	-	-	X
87	OHX	1	4000	-	-	-	X
87	OHX	1	4003	-	-	-	X
87	OHX	1	4004	-	-	-	X
87	OHX	1	4005	-	-	-	X
87	OHX	1	4006	-	-	-	X
87	OHX	1	4008	-	-	-	X
87	OHX	1	4010	-	-	-	X
87	OHX	1	4015	-	-	-	X
87	OHX	1	4016	-	-	-	X
87	OHX	1	4024	-	-	-	X
87	OHX	1	4027	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	1	4030	-	-	-	X
87	OHX	1	4032	-	-	-	X
87	OHX	1	4038	-	-	-	X
87	OHX	1	4043	-	-	-	X
87	OHX	1	4048	-	-	-	X
87	OHX	1	4058	-	-	-	X
87	OHX	1	4062	-	-	-	X
87	OHX	1	4064	-	-	-	X
87	OHX	1	4066	-	-	-	X
87	OHX	1	4071	-	-	X	X
87	OHX	1	4072	-	-	-	X
87	OHX	1	4074	-	-	-	X
87	OHX	1	4082	-	-	X	-
87	OHX	1	4083	-	-	-	X
87	OHX	1	4084	-	-	-	X
87	OHX	1	4085	-	-	X	-
87	OHX	1	4095	-	-	-	X
87	OHX	1	4105	-	-	-	X
87	OHX	1	4107	-	-	-	X
87	OHX	2	1995	-	-	-	X
87	OHX	2	1998	-	-	-	X
87	OHX	2	2008	-	-	-	X
87	OHX	2	2010	-	-	-	X
87	OHX	2	2011	-	-	-	X
87	OHX	2	2022	-	-	-	X
87	OHX	2	2027	-	-	-	X
87	OHX	2	2032	-	-	-	X
87	OHX	2	2037	-	-	-	X
87	OHX	2	2047	-	-	-	X
87	OHX	2	2051	-	-	-	X
87	OHX	2	2056	-	-	-	X
87	OHX	2	2057	-	-	-	X
87	OHX	2	2058	-	-	X	-
87	OHX	2	2091	-	-	-	X
87	OHX	2	2095	-	-	-	X
87	OHX	2	2097	-	-	-	X
87	OHX	2	2099	-	-	X	-
87	OHX	2	2106	-	-	-	X
87	OHX	2	2108	-	-	-	X
87	OHX	2	2117	-	-	-	X
87	OHX	2	2119	-	-	-	X
87	OHX	2	2120	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	2	2121	-	-	-	X
87	OHX	2	2125	-	-	-	X
87	OHX	2	2129	-	-	-	X
87	OHX	2	2131	-	-	X	-
87	OHX	2	2132	-	-	-	X
87	OHX	2	2134	-	-	-	X
87	OHX	2	2136	-	-	-	X
87	OHX	2	2141	-	-	-	X
87	OHX	2	2144	-	-	-	X
87	OHX	2	2148	-	-	-	X
87	OHX	2	2151	-	-	-	X
87	OHX	3	210	-	-	-	X
87	OHX	3	211	-	-	-	X
87	OHX	3	212	-	-	-	X
87	OHX	3	214	-	-	-	X
87	OHX	3	219	-	-	-	X
87	OHX	4	216	-	-	-	X
87	OHX	4	224	-	-	-	X
87	OHX	4	231	-	-	-	X
87	OHX	5	3818	-	-	-	X
87	OHX	5	3822	-	-	-	X
87	OHX	5	3833	-	-	-	X
87	OHX	5	3839	-	-	-	X
87	OHX	5	3843	-	-	-	X
87	OHX	5	3844	-	-	-	X
87	OHX	5	3845	-	-	-	X
87	OHX	5	3851	-	-	-	X
87	OHX	5	3854	-	-	-	X
87	OHX	5	3855	-	-	-	X
87	OHX	5	3862	-	-	-	X
87	OHX	5	3865	-	-	-	X
87	OHX	5	3868	-	-	-	X
87	OHX	5	3873	-	-	-	X
87	OHX	5	3875	-	-	-	X
87	OHX	5	3877	-	-	-	X
87	OHX	5	3881	-	-	-	X
87	OHX	5	3888	-	-	-	X
87	OHX	5	3893	-	-	-	X
87	OHX	5	3894	-	-	-	X
87	OHX	5	3899	-	-	-	X
87	OHX	5	3900	-	-	-	X
87	OHX	5	3903	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	5	3904	-	-	-	X
87	OHX	5	3909	-	-	-	X
87	OHX	5	3910	-	-	-	X
87	OHX	5	3911	-	-	-	X
87	OHX	5	3912	-	-	-	X
87	OHX	5	3914	-	-	X	X
87	OHX	5	3915	-	-	-	X
87	OHX	5	3916	-	-	-	X
87	OHX	5	3917	-	-	X	-
87	OHX	5	3922	-	-	-	X
87	OHX	5	3923	-	-	-	X
87	OHX	5	3928	-	-	-	X
87	OHX	5	3931	-	-	-	X
87	OHX	5	3935	-	-	-	X
87	OHX	5	3937	-	-	-	X
87	OHX	5	3939	-	-	-	X
87	OHX	5	3940	-	-	-	X
87	OHX	5	3941	-	-	-	X
87	OHX	5	3942	-	-	-	X
87	OHX	5	3943	-	-	-	X
87	OHX	5	3947	-	-	-	X
87	OHX	5	3948	-	-	-	X
87	OHX	5	3949	-	-	-	X
87	OHX	5	3954	-	-	X	-
87	OHX	5	3956	-	-	-	X
87	OHX	5	3962	-	-	-	X
87	OHX	5	3964	-	-	-	X
87	OHX	5	3965	-	-	-	X
87	OHX	5	3966	-	-	-	X
87	OHX	5	3974	-	-	-	X
87	OHX	5	3976	-	-	-	X
87	OHX	5	3984	-	-	-	X
87	OHX	5	3986	-	-	-	X
87	OHX	5	3989	-	-	-	X
87	OHX	5	3995	-	-	-	X
87	OHX	5	3998	-	-	-	X
87	OHX	5	4000	-	-	X	-
87	OHX	5	4001	-	-	X	-
87	OHX	5	4007	-	-	-	X
87	OHX	5	4008	-	-	-	X
87	OHX	5	4010	-	-	-	X
87	OHX	5	4011	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	5	4012	-	-	-	X
87	OHX	5	4019	-	-	-	X
87	OHX	5	4024	-	-	-	X
87	OHX	5	4025	-	-	-	X
87	OHX	5	4027	-	-	-	X
87	OHX	5	4033	-	-	-	X
87	OHX	5	4038	-	-	-	X
87	OHX	5	4042	-	-	-	X
87	OHX	5	4046	-	-	-	X
87	OHX	5	4048	-	-	-	X
87	OHX	5	4049	-	-	-	X
87	OHX	5	4052	-	-	-	X
87	OHX	5	4053	-	-	-	X
87	OHX	5	4054	-	-	-	X
87	OHX	5	4072	-	-	-	X
87	OHX	5	4076	-	-	-	X
87	OHX	5	4077	-	-	-	X
87	OHX	5	4082	-	-	-	X
87	OHX	5	4083	-	-	X	X
87	OHX	5	4086	-	-	-	X
87	OHX	5	4088	-	-	-	X
87	OHX	5	4093	-	-	-	X
87	OHX	5	4099	-	-	-	X
87	OHX	5	4101	-	-	-	X
87	OHX	5	4103	-	-	-	X
87	OHX	5	4106	-	-	-	X
87	OHX	5	4115	-	-	-	X
87	OHX	5	4117	-	-	-	X
87	OHX	5	4120	-	-	-	X
87	OHX	5	4123	-	-	-	X
87	OHX	5	4124	-	-	-	X
87	OHX	5	4126	-	-	-	X
87	OHX	5	4132	-	-	-	X
87	OHX	5	4134	-	-	-	X
87	OHX	5	4142	-	-	-	X
87	OHX	5	4158	-	-	-	X
87	OHX	5	4159	-	-	-	X
87	OHX	5	4162	-	-	-	X
87	OHX	5	4164	-	-	-	X
87	OHX	5	4169	-	-	-	X
87	OHX	6	2020	-	-	-	X
87	OHX	6	2025	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	6	2029	-	-	-	X
87	OHX	6	2032	-	-	-	X
87	OHX	6	2041	-	-	-	X
87	OHX	6	2043	-	-	-	X
87	OHX	6	2044	-	-	-	X
87	OHX	6	2045	-	-	-	X
87	OHX	6	2051	-	-	-	X
87	OHX	6	2058	-	-	-	X
87	OHX	6	2065	-	-	-	X
87	OHX	6	2067	-	-	X	-
87	OHX	6	2072	-	-	-	X
87	OHX	6	2073	-	-	-	X
87	OHX	6	2088	-	-	-	X
87	OHX	6	2089	-	-	-	X
87	OHX	6	2092	-	-	-	X
87	OHX	6	2097	-	-	-	X
87	OHX	6	2102	-	-	-	X
87	OHX	6	2106	-	-	-	X
87	OHX	6	2107	-	-	-	X
87	OHX	6	2110	-	-	-	X
87	OHX	6	2122	-	-	-	X
87	OHX	6	2124	-	-	X	-
87	OHX	6	2126	-	-	-	X
87	OHX	6	2127	-	-	-	X
87	OHX	6	2128	-	-	-	X
87	OHX	6	2131	-	-	-	X
87	OHX	6	2137	-	-	-	X
87	OHX	6	2146	-	-	-	X
87	OHX	6	2150	-	-	-	X
87	OHX	6	2153	-	-	-	X
87	OHX	6	2155	-	-	-	X
87	OHX	6	2158	-	-	-	X
87	OHX	6	2161	-	-	-	X
87	OHX	6	2162	-	-	-	X
87	OHX	6	2164	-	-	-	X
87	OHX	6	2178	-	-	-	X
87	OHX	7	216	-	-	-	X
87	OHX	7	218	-	-	-	X
87	OHX	7	219	-	-	-	X
87	OHX	7	220	-	-	-	X
87	OHX	7	221	-	-	-	X
87	OHX	7	222	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	7	224	-	-	-	X
87	OHX	8	214	-	-	-	X
87	OHX	8	218	-	-	-	X
87	OHX	8	220	-	-	-	X
87	OHX	8	222	-	-	-	X
87	OHX	8	224	-	-	-	X
87	OHX	8	225	-	-	-	X
87	OHX	C5	201	-	-	X	-
87	OHX	M0	302	-	-	-	X
87	OHX	M0	303	-	-	X	-
87	OHX	N9	101	-	-	-	X
87	OHX	O7	103	-	-	X	-
87	OHX	O9	101	-	-	-	X
87	OHX	S9	201	-	-	X	-
87	OHX	SR	401	-	-	X	-
87	OHX	c5	202	-	-	-	X
87	OHX	l9	201	-	-	-	X
87	OHX	o7	503	-	-	-	X
88	ZN	d7	101	-	-	-	X
89	SPS	5	3402	-	-	-	X

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 413121 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			
1	6	1795	Total	C	N	O	P	0	1	0
			38260	17105	6763	12596	1796			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

- 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				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	c6	142	Total	C	N	O			
			1111	711	204	196	0	0	0

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

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

- 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		
			1192	743	237	210	2	0	0
20	c8	145	Total	C	N	O	S		
			1192	743	237	210	2	0	0

- 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		
			1112	694	208	208	2	0	0
21	c9	143	Total	C	N	O	S		
			1112	694	208	208	2	0	0

- 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		
			855	539	156	159	1	0	0
22	d0	110	Total	C	N	O	S		
			882	554	161	166	1	0	0

- 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		
			684	420	125	137	2	0	0
23	d1	87	Total	C	N	O	S		
			684	420	125	137	2	0	0

- 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-A.

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			

- 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
			2436	1541	418	469	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2441	1544	418	471	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			
35	sM	104	Total	C	N	O	0	0	0
			680	403	140	137			

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

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

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	12	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	l8	231	Total	C	N	O	S	0	0	0
			1764	1131	316	314	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L8	119	ALA	GLY	conflict	UNP P17076
l8	119	ALA	GLY	conflict	UNP P17076

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

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

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

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

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

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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M1	3	THR	ALA	conflict	UNP P0C0W9
m1	3	THR	ALA	conflict	UNP P0C0W9

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			742	479	124	138	1			
66	o0	100	Total	C	N	O	S	0	0	0
			766	492	128	145	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			

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

There are 22 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
81	m2	150	Total	C	N	O	0	0	0
			739	439	150	150			

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

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

- Molecule 83 is a protein called 60S acidic ribosomal protein P1-alpha.

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

- Molecule 84 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
84	f	148	Total	C	N	O	S	0	0	0
			1122	696	189	228	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	51	5CT	LYS	conflict	UNP P23301

- Molecule 85 is a RNA chain called DNA (5'-R(*CP*CP*(NA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
85	B	4	Total	C	N	O	P	0	0	0
			66	33	13	18	2			
85	C	4	Total	C	N	O	P	0	0	0
			69	33	13	20	3			

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	3	Total	Mg	0	0
			3	3		
86	n8	2	Total	Mg	0	0
			2	2		
86	B	1	Total	Mg	0	0
			1	1		
86	6	113	Total	Mg	0	0
			113	113		
86	sM	1	Total	Mg	0	0
			1	1		
86	O4	1	Total	Mg	0	0
			1	1		
86	m5	2	Total	Mg	0	0
			2	2		
86	l3	2	Total	Mg	0	0
			2	2		
86	n0	1	Total	Mg	0	0
			1	1		
86	d6	1	Total	Mg	0	0
			1	1		
86	2	90	Total	Mg	0	0
			90	90		
86	O3	1	Total	Mg	0	0
			1	1		

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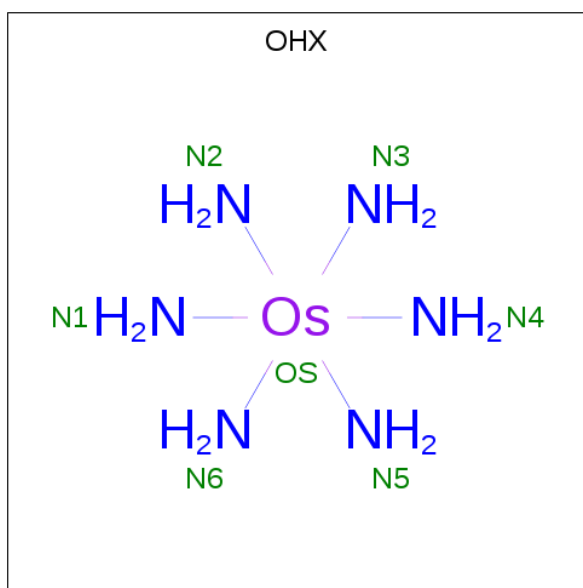
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	f	1	Total 1	Mg 1	0	0
86	l7	2	Total 2	Mg 2	0	0
86	M5	1	Total 1	Mg 1	0	0
86	m3	1	Total 1	Mg 1	0	0
86	S2	1	Total 1	Mg 1	0	0
86	N6	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	M9	1	Total 1	Mg 1	0	0
86	SM	1	Total 1	Mg 1	0	0
86	o4	1	Total 1	Mg 1	0	0
86	M0	1	Total 1	Mg 1	0	0
86	5	419	Total 419	Mg 419	0	0
86	c8	1	Total 1	Mg 1	0	0
86	O7	1	Total 1	Mg 1	0	0
86	l4	1	Total 1	Mg 1	0	0
86	1	366	Total 366	Mg 366	0	0
86	d2	1	Total 1	Mg 1	0	0
86	n6	1	Total 1	Mg 1	0	0
86	Q2	1	Total 1	Mg 1	0	0
86	d3	1	Total 1	Mg 1	0	0
86	q3	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	o3	1	Total 1	Mg 1	0	0
86	N3	1	Total 1	Mg 1	0	0
86	N8	1	Total 1	Mg 1	0	0
86	4	15	Total 15	Mg 15	0	0
86	L2	2	Total 2	Mg 2	0	0
86	l5	1	Total 1	Mg 1	0	0
86	M7	4	Total 4	Mg 4	0	0
86	L6	1	Total 1	Mg 1	0	0
86	s8	2	Total 2	Mg 2	0	0
86	o2	1	Total 1	Mg 1	0	0
86	C	1	Total 1	Mg 1	0	0
86	m7	2	Total 2	Mg 2	0	0
86	7	13	Total 13	Mg 13	0	0
86	n3	1	Total 1	Mg 1	0	0
86	q1	1	Total 1	Mg 1	0	0
86	L3	1	Total 1	Mg 1	0	0
86	s4	1	Total 1	Mg 1	0	0
86	l2	2	Total 2	Mg 2	0	0
86	8	9	Total 9	Mg 9	0	0
86	M6	2	Total 2	Mg 2	0	0
86	3	8	Total 8	Mg 8	0	0

- Molecule 87 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	1	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	1	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	1	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	1	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	1	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	1	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	1	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total 7	N 6	Os 1	0	0
87	2	1	Total 7	N 6	Os 1	0	0
87	S1	1	Total 7	N 6	Os 1	0	0
87	S6	1	Total 7	N 6	Os 1	0	0
87	S8	1	Total 7	N 6	Os 1	0	0
87	S9	1	Total 7	N 6	Os 1	0	0
87	C3	1	Total 7	N 6	Os 1	0	0
87	C5	1	Total 7	N 6	Os 1	0	0
87	C8	1	Total 7	N 6	Os 1	0	0
87	D9	1	Total 7	N 6	Os 1	0	0
87	SR	1	Total 7	N 6	Os 1	0	0
87	1	1	Total 7	N 6	Os 1	1	0
87	1	1	Total 7	N 6	Os 1	1	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	2	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	3	1	Total	N	Os	0	0
			7	6	1		
87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
			7	6	1		
87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
			7	6	1		
87	4	1	Total	N	Os	0	0
			7	6	1		
87	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	1	0
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	1	0
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	0	0
87	L3	1	Total 7	N 6	Os 1	0	0
87	L3	1	Total 7	N 6	Os 1	0	0
87	L3	1	Total 7	N 6	Os 1	0	0
87	L4	1	Total 7	N 6	Os 1	0	0
87	L5	1	Total 7	N 6	Os 1	0	0
87	M0	1	Total 7	N 6	Os 1	0	0
87	M0	1	Total 7	N 6	Os 1	0	0
87	M5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	M6	1	Total	N	Os	0	0
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87	M7	1	Total	N	Os	0	0
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87	M8	1	Total	N	Os	0	0
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87	M9	1	Total	N	Os	0	0
			7	6	1		
87	N8	1	Total	N	Os	0	0
			7	6	1		
87	N9	1	Total	N	Os	0	0
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87	O1	1	Total	N	Os	0	0
			7	6	1		
87	O3	1	Total	N	Os	0	0
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87	O4	1	Total	N	Os	0	0
			7	6	1		
87	O7	1	Total	N	Os	0	0
			7	6	1		
87	O9	1	Total	N	Os	0	0
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87	Q2	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	2	0
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	1	0
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			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	2	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	1	0
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			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total 7	N 6	Os 1	1	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
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87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	s1	1	Total 7	N 6	Os 1	0	0
87	s1	1	Total 7	N 6	Os 1	0	0
87	s4	1	Total 7	N 6	Os 1	0	0
87	s8	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	s9	1	Total 7	N 6	Os 1	0	0
87	c3	1	Total 7	N 6	Os 1	0	0
87	c5	1	Total 7	N 6	Os 1	0	0
87	c5	1	Total 7	N 6	Os 1	0	0
87	c8	1	Total 7	N 6	Os 1	0	0
87	d4	1	Total 7	N 6	Os 1	0	0
87	d9	1	Total 7	N 6	Os 1	0	0
87	sR	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	1	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	1	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
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87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	1	0
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87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
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87	7	1	Total 7	N 6	Os 1	0	0
87	7	1	Total 7	N 6	Os 1	0	0
87	7	1	Total 7	N 6	Os 1	0	0
87	7	1	Total 7	N 6	Os 1	0	0
87	7	1	Total 7	N 6	Os 1	0	0
87	7	1	Total 7	N 6	Os 1	1	0
87	7	1	Total 7	N 6	Os 1	1	0
87	7	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	8	1	Total	N	Os	0	0
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87	8	1	Total	N	Os	1	0
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87	8	1	Total	N	Os	0	0
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87	8	1	Total	N	Os	0	0
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87	8	1	Total	N	Os	0	0
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87	13	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	l4	1	Total 7	N 6	Os 1	0	0
87	l5	1	Total 7	N 6	Os 1	0	0
87	l5	1	Total 7	N 6	Os 1	1	0
87	l9	1	Total 7	N 6	Os 1	0	0
87	m0	1	Total 7	N 6	Os 1	0	0
87	m0	1	Total 7	N 6	Os 1	0	0
87	m1	1	Total 7	N 6	Os 1	0	0
87	m4	1	Total 7	N 6	Os 1	0	0
87	m5	1	Total 7	N 6	Os 1	0	0
87	m5	1	Total 7	N 6	Os 1	0	0
87	m5	1	Total 7	N 6	Os 1	0	0
87	m5	1	Total 7	N 6	Os 1	0	0
87	m6	1	Total 7	N 6	Os 1	0	0
87	m7	1	Total 7	N 6	Os 1	0	0
87	m8	1	Total 7	N 6	Os 1	0	0
87	m9	1	Total 7	N 6	Os 1	0	0
87	n3	1	Total 7	N 6	Os 1	0	0
87	n9	1	Total 7	N 6	Os 1	0	0
87	o3	1	Total 7	N 6	Os 1	0	0
87	o6	1	Total 7	N 6	Os 1	0	0
87	o7	1	Total 7	N 6	Os 1	0	0
87	o7	1	Total 7	N 6	Os 1	0	0

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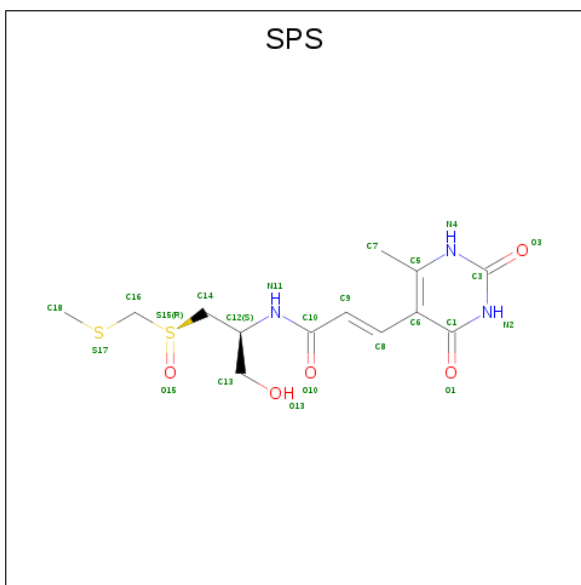
Continued from previous page...

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

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

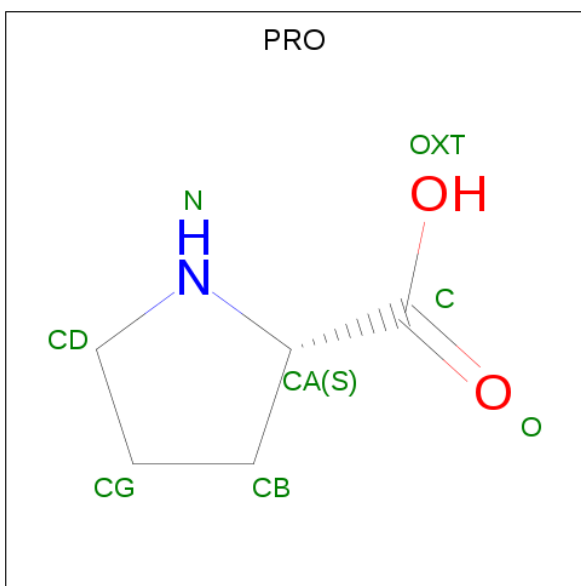
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total	Zn	0	0
			1	1		
88	D6	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		
88	Q3	1	Total	Zn	0	0
			1	1		
88	D9	1	Total	Zn	0	0
			1	1		
88	E1	1	Total	Zn	0	0
			1	1		
88	Q0	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0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

- Molecule 89 is SPARSOMYCIN (three-letter code: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
89	5	1	Total	C	N	O	S	0	0
			23	13	3	5	2		
89	B	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 90 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



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

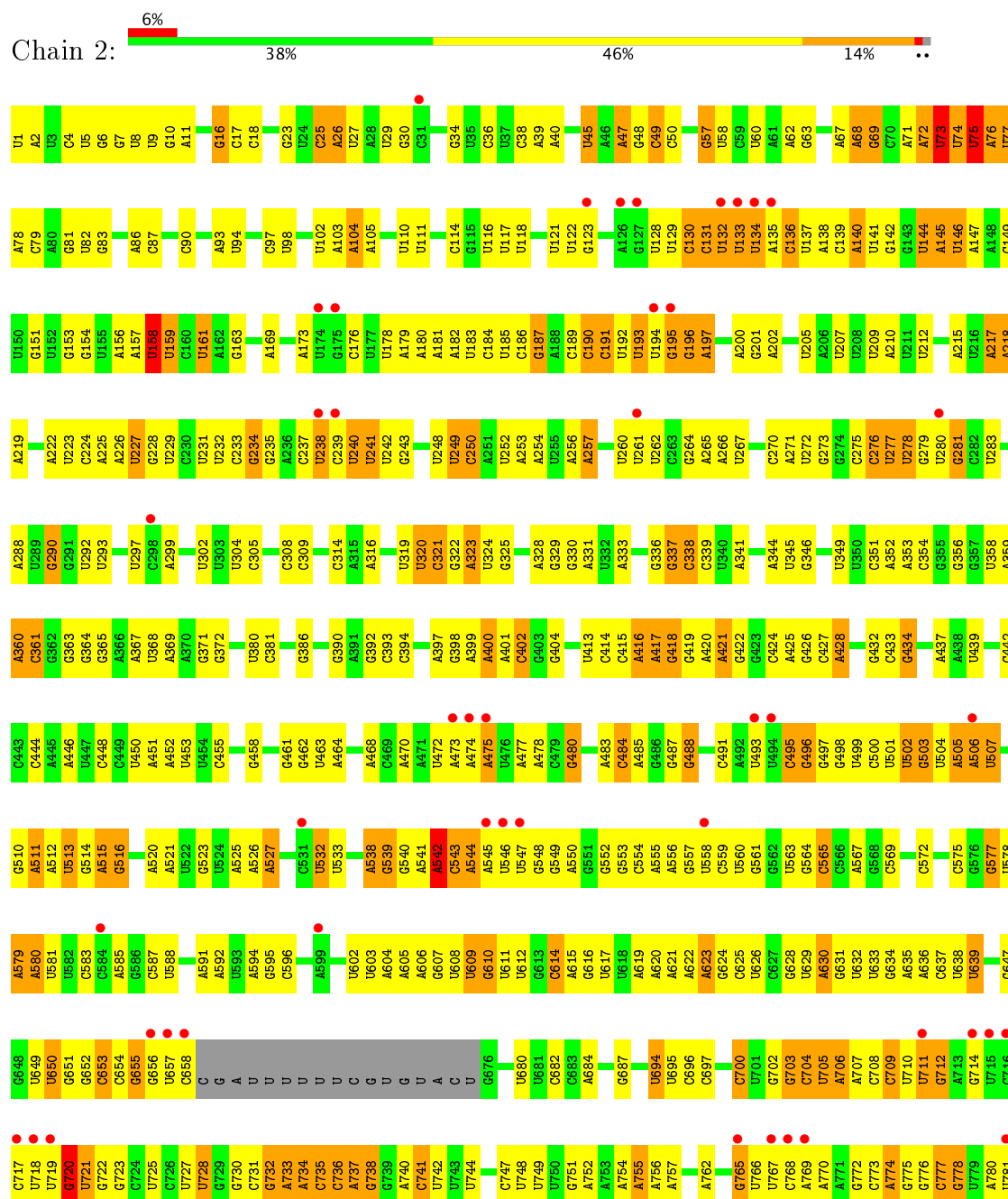
- Molecule 91 is water.

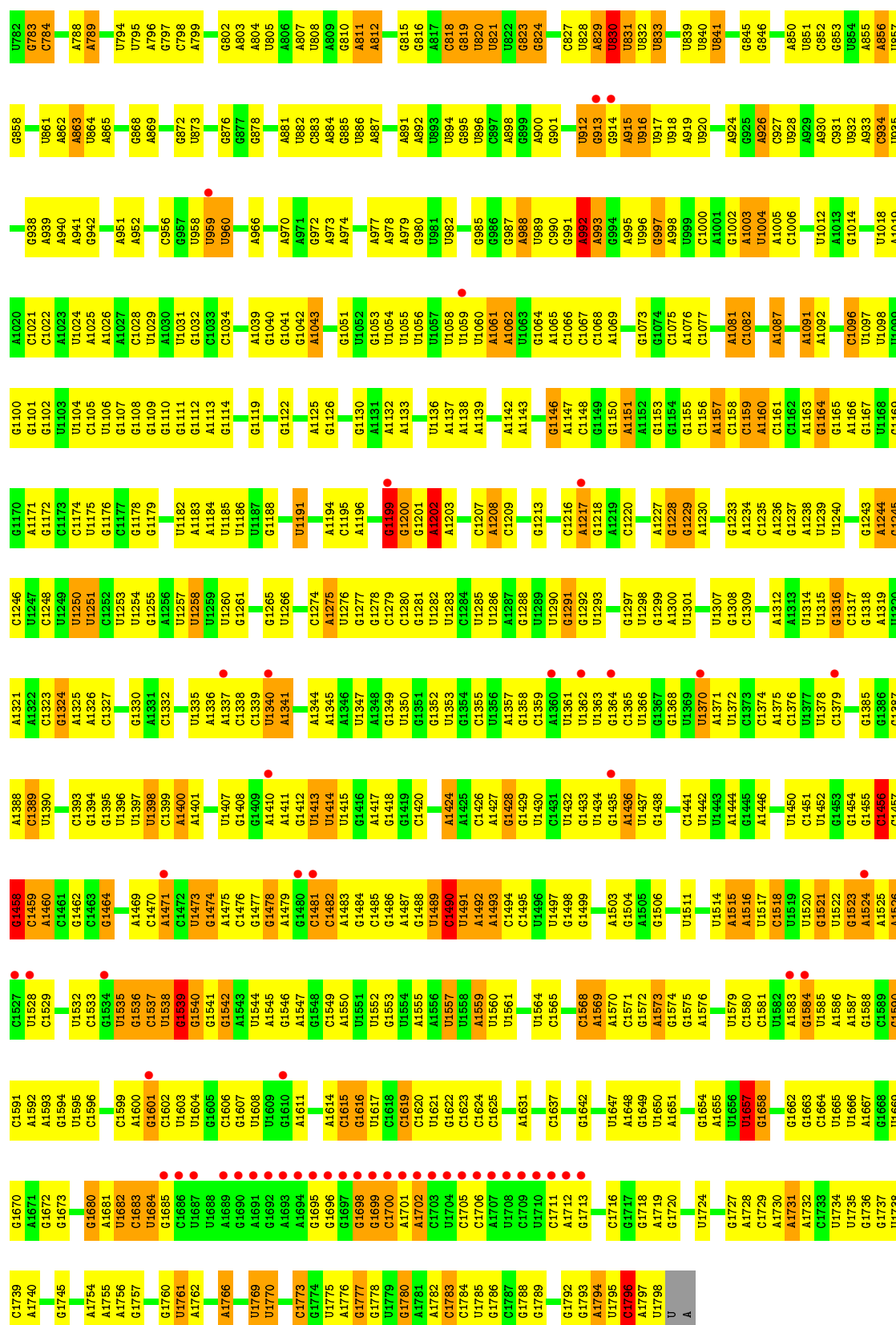
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
91	5	6	Total 6	O 6	0	0
91	f	6	Total 6	O 6	0	0

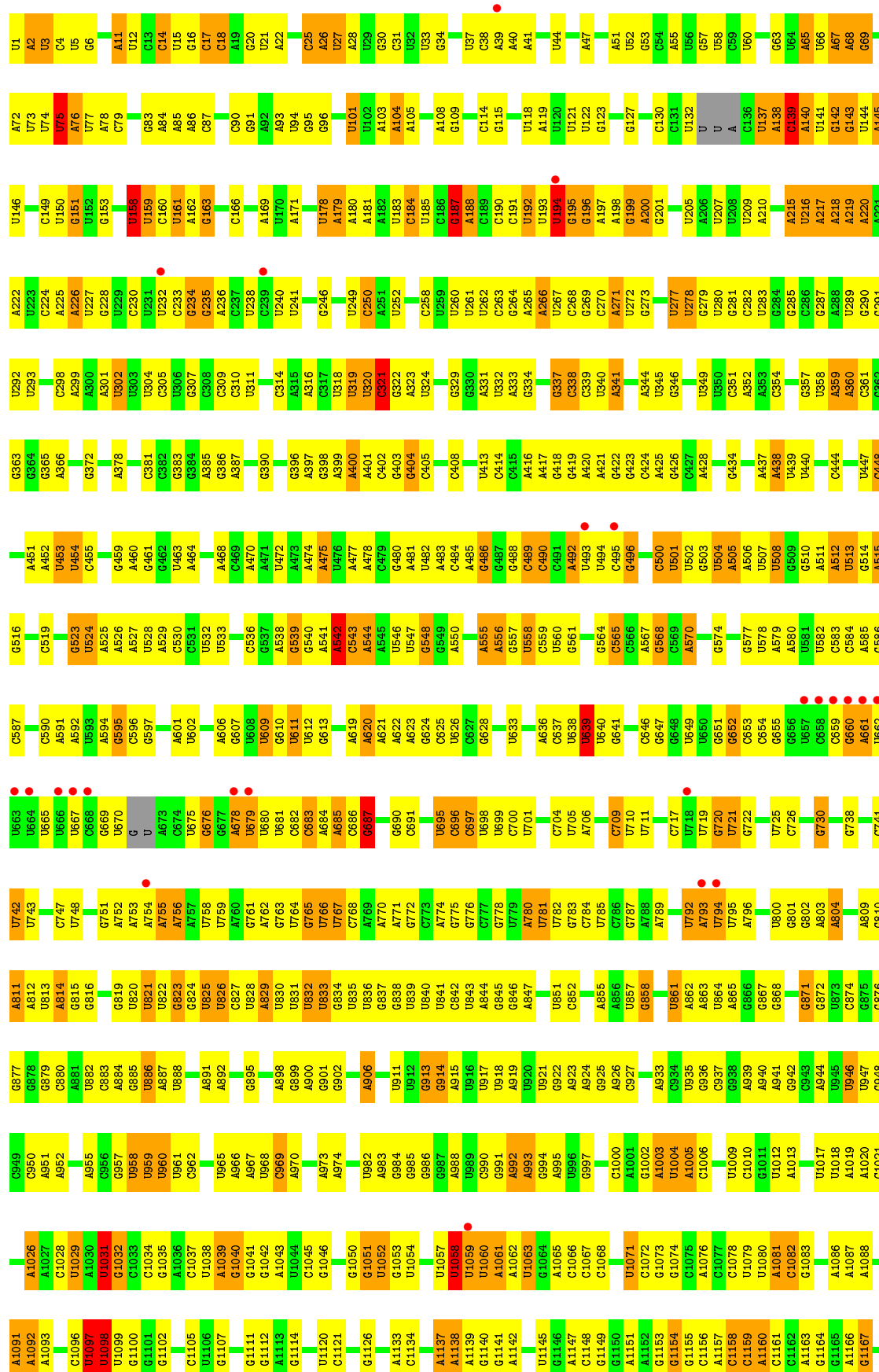
3 Residue-property plots

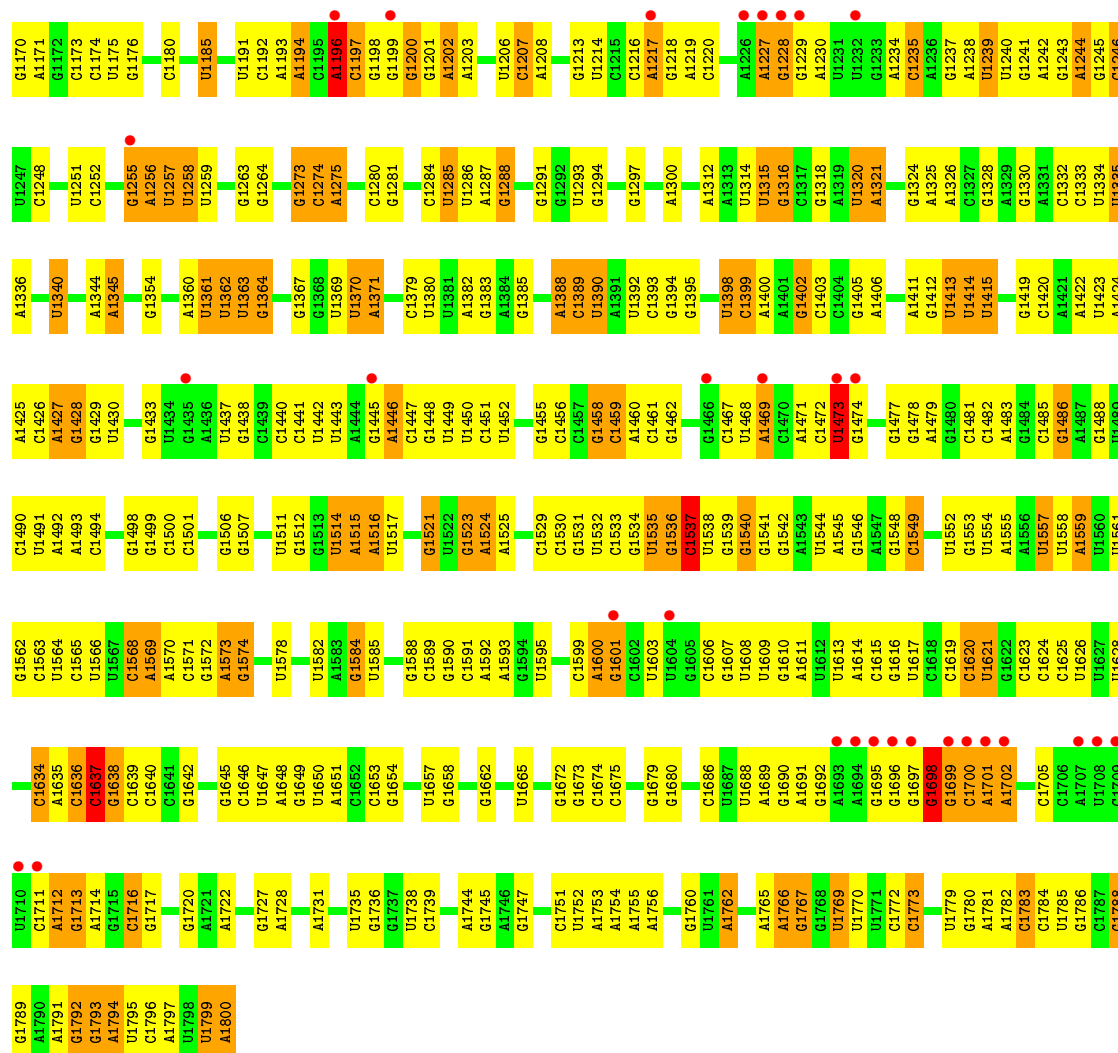
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

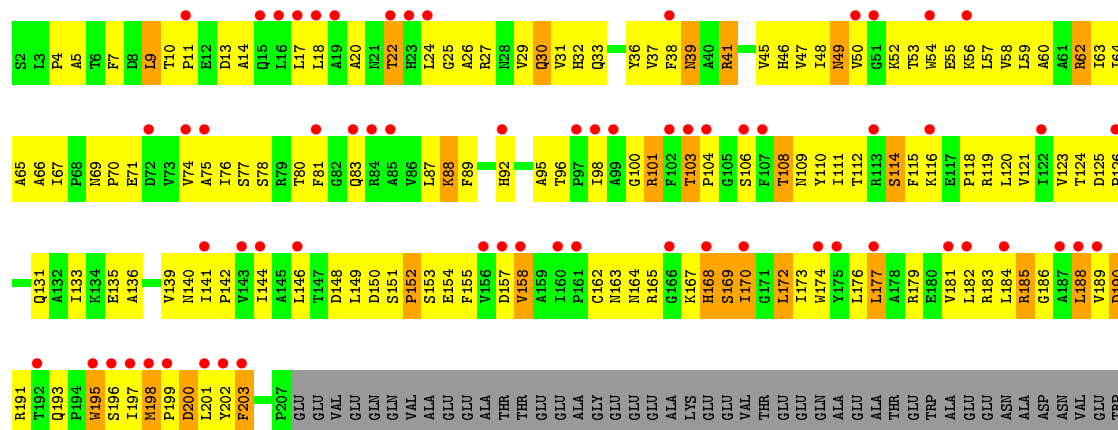




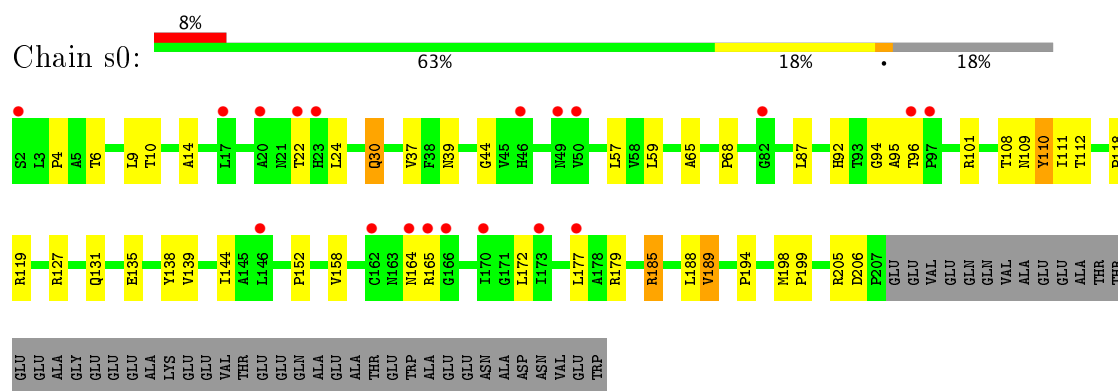




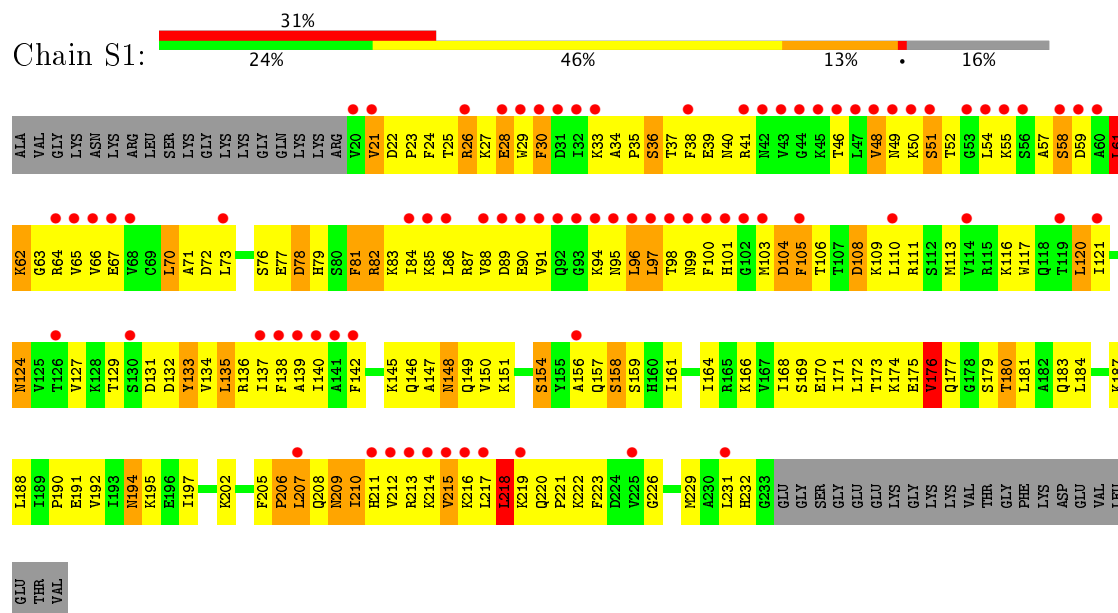
• Molecule 2: 40S ribosomal protein S0-A



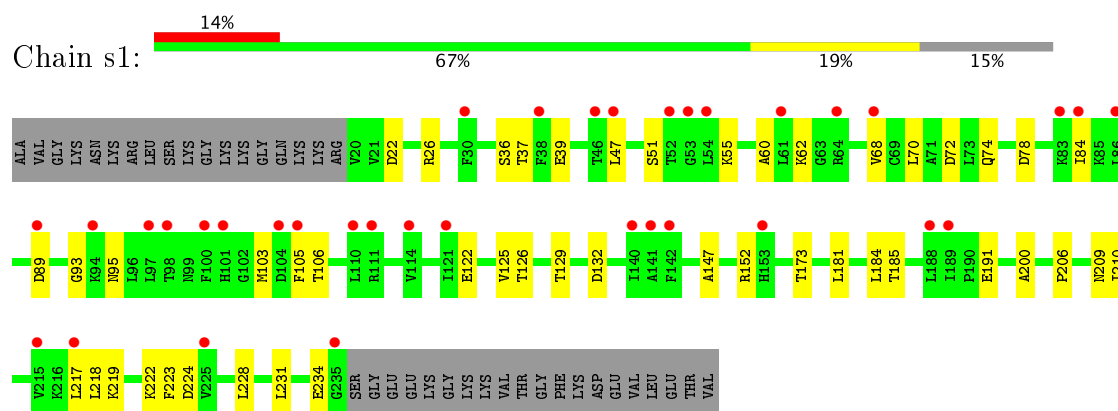
• Molecule 2: 40S ribosomal protein S0-A



• Molecule 3: 40S ribosomal protein S1-A

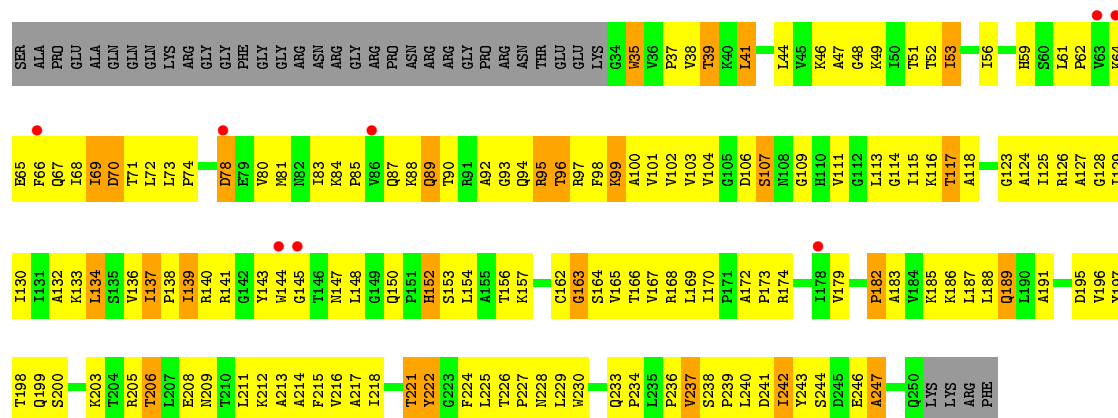


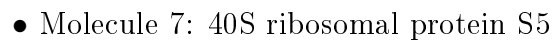
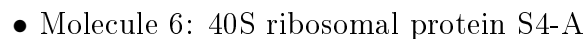
• Molecule 3: 40S ribosomal protein S1-A

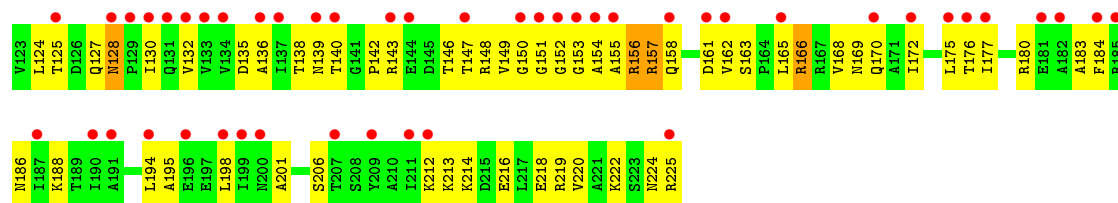


• Molecule 4: 40S ribosomal protein S2

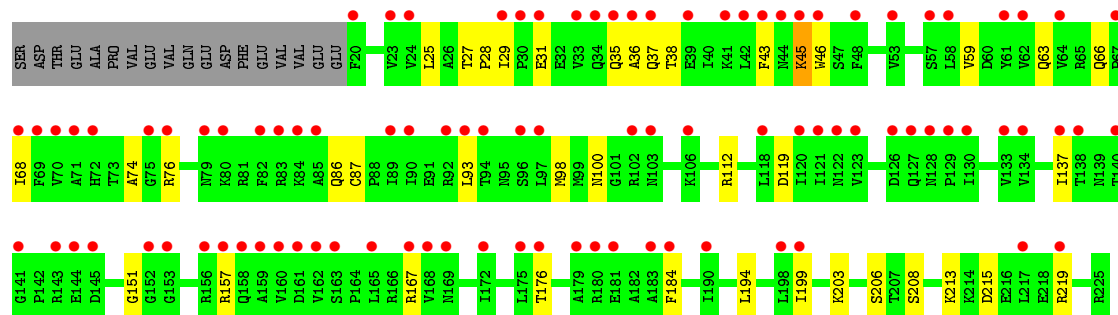
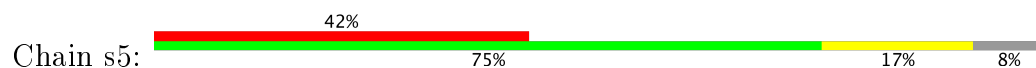




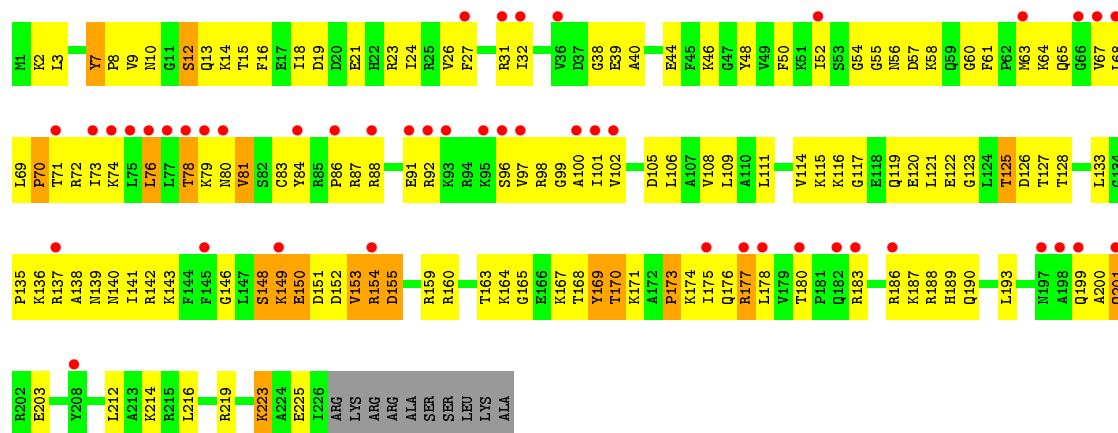




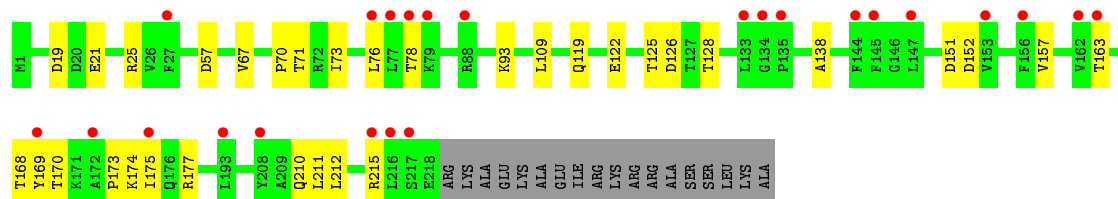
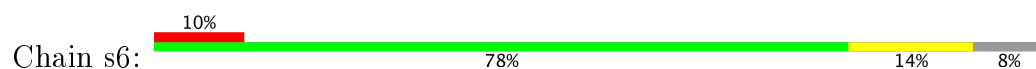
• Molecule 7: 40S ribosomal protein S5



• Molecule 8: 40S ribosomal protein S6-A



• Molecule 8: 40S ribosomal protein S6-A



• Molecule 9: 40S ribosomal protein S7-A

Chain S9:

Category	Value
P2	1
R3	1
A4	1
P5	1
R6	1
T7	1
Y8	1
K10	1
S9	1
T11	1
Y12	1
S13	1
T14	1
P15	1
K16	1
R17	1
P18	1
Y19	1
E20	1
S21	1
R22	1
S23	1
L24	1
E27	1
L28	1
K29	1
L30	1
A31	1
G32	1
E33	1
F34	1
G35	1
L36	1
K37	1
N38	1
K39	1
K40	1
E41	1
I42	1
Y43	1
R44	1
S46	1
F47	1
K51	1
I52	1
R53	1
R54	1
R57	1
D58	1
L59	1
L60	1
T61	1
R62	1
D63	1
E64	1
K65	1
R69	1
L70	1
F71	1
A75	1
L76	1
I77	1
R78	1
R79	1
L80	1
V81	1
R82	1
V83	1
G84	1
V85	1
L86	1
S87	1
E88	1
D89	1
K90	1
R91	1
K92	1
L93	1
D94	1
Y95	1
Y96	1
L97	1
A98	1
L99	1
K100	1
V101	1
E102	1
G103	1
D103	1
F104	1
L105	1
E106	1
R107	1
R108	1
L109	1
T110	1
T111	1
Q112	1
V113	1
Y114	1
K115	1
L116	1
G117	1
L118	1
A119	1
K120	1
S121	1
V122	1
H123	1
H124	1
A125	1
R126	1
V127	1
L128	1
T129	1
T130	1
A131	1
R132	1
GLU	1
H133	1
A134	1
A135	1
V136	1
G137	1
K138	1
Q139	1
L140	1
V141	1
L143	1
P144	1
S145	1
F146	1
M147	1
V148	1
L149	1
D151	1
S152	1
E153	1
K154	1
H155	1
L156	1
D157	1
F158	1
A159	1
P160	1
T161	1
S162	1
G163	1
F164	1
G165	1
P166	1
A167	1
R168	1
P169	1
G170	1
R171	1
V172	1
R173	1
R174	1
R175	1
M176	1
A177	1
A178	1
R179	1
K180	1
A181	1
E182	1
A183	1
S184	1
G185	1
E186	1
ALA	1
ALA	1

Chain s9:

State	Category
F2	Red
R3	Red
A4	Red
P5	Yellow
R6	Yellow
T7	Yellow
R8	Yellow
S9	Yellow
T10	Red
T11	Red
V12	Red
S13	Red
T14	Red
P15	Green
R16	Green
R17	Green
P18	Green
V19	Green
E20	Green
S21	Green
L28	Green
X29	Green
E33	Green
X37	Green
T45	Green
S46	Green
F47	Green
Q48	Green
L49	Yellow
S50	Yellow
X51	Yellow
S52	Yellow
R53	Yellow
R57	Yellow
F71	Yellow
R74	Red
A75	Red
L76	Red
I77	Red
R78	Yellow
R79	Yellow
L80	Yellow
R81	Yellow
R82	Yellow
R83	Red
A84	Red
R85	Red
L86	Yellow
S87	Yellow
E88	Yellow
D89	Yellow
X90	Yellow
R91	Red
R92	Red
L93	Yellow
V101	Red
D103	Yellow
F104	Yellow
L105	Yellow
L109	Red
Q110	Red
L118	Yellow
T130	Yellow
H133	Yellow
I134	Red
V141	Red
M142	Green
I143	Yellow
P144	Yellow
S145	Red
F146	Red
M147	Red
V148	Green
R149	Yellow
L150	Red
D151	Yellow
S152	Red
I156	Red
S162	Yellow
A167	Yellow
R168	Yellow
P169	Yellow
V172	Yellow
R175	Yellow
K180	Yellow
A181	Yellow
E182	Red
A183	Red
S184	Yellow
G185	Yellow
E186	Yellow
ALA	Grey
ALA	Grey
ASP	Grey
GLU	Grey
ALA	Grey
ASP	Grey
GLU	Grey
ALA	Grey

Chain C0:

Sequence logo for Chain C0. The y-axis represents frequency in bits. The x-axis lists amino acids. A pie chart at the top shows the overall composition: 42% red, 32% green, 49% yellow, 10% orange, and 9% grey.

Amino Acid	Frequency (bits)
M1	0.15
L2	0.10
M3	0.10
P4	0.15
K5	0.15
E6	0.15
D7	0.10
R8	0.10
I11	0.15
H12	0.10
G13	0.10
L14	0.10
L15	0.10
E18	0.10
G19	0.10
V20	0.10
V21	0.10
V22	0.10
A23	0.10
K24	0.10
K25	0.10
D26	0.10
F27	0.10
M28	0.10
Q29	0.10
A30	0.10
K31	0.10
H32	0.10
E33	0.10
E34	0.10
I35	0.10
D36	0.10
T37	0.10
K38	0.10
N39	0.10
L40	0.10
Y41	0.10
V42	0.10
I43	0.10
K44	0.10
A45	0.10
L46	0.10
Q47	0.10
S48	0.10
I49	0.10
T50	0.10
S51	0.10
K52	0.10
G53	0.10
Y54	0.10
V55	0.10
K56	0.10
I57	0.10
Q58	0.10
F59	0.10
S60	0.10
W61	0.10
G62	0.10
F63	0.10
Y64	0.10
Y65	0.10
Y66	0.10
T67	0.10
L68	0.10
T69	0.10
G72	0.10
Y75	0.10
L76	0.10
R77	0.10
E78	0.10
Y79	0.10
L80	0.10
N81	0.10
L82	0.10
V87	0.10
P88	0.10
A89	0.10
T90	0.10
Y91	0.10
I92	0.10
Q93	0.10
N96	0.10
PRQ	0.10
THR	0.10
GLN	0.10
ARG	0.10
PRQ	0.10
GLN	0.10
ARG	0.10
ARG	0.10
TYR	0.10

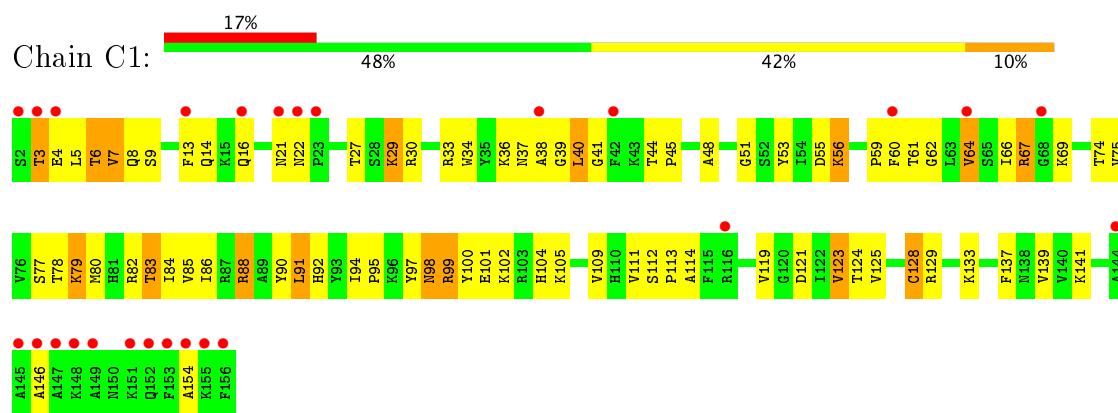
Chain c0:

Sequence logo for Chain c0. The y-axis represents information content in bits. The x-axis shows positions 1 to 200. A color scale at the top indicates conservation levels: 40% (red), 69% (green), 20% (yellow), and 9% (grey).

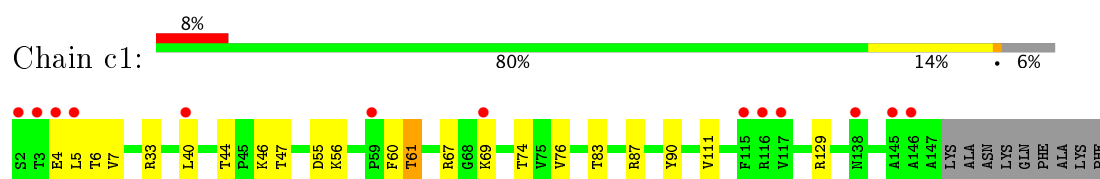
Key residues (positions and amino acids) are highlighted:

- Position 1: R1 (Red)
- Position 2: L2 (Red)
- Position 3: K3 (Red)
- Position 4: P4 (Green)
- Position 5: K5 (Yellow)
- Position 11: I11 (Green)
- Position 12: H12 (Red)
- Position 13: Q13 (Red)
- Position 14: I14 (Green)
- Position 15: L15 (Yellow)
- Position 16: F16 (Red)
- Position 17: Q17 (Green)
- Position 20: V20 (Green)
- Position 21: V21 (Green)
- Position 22: V22 (Green)
- Position 23: A23 (Red)
- Position 24: K24 (Red)
- Position 25: K25 (Red)
- Position 26: D26 (Red)
- Position 27: F27 (Red)
- Position 28: I28 (Red)
- Position 29: Q29 (Red)
- Position 30: A30 (Yellow)
- Position 31: K31 (Red)
- Position 32: H32 (Red)
- Position 33: E33 (Yellow)
- Position 34: E34 (Yellow)
- Position 35: L35 (Red)
- Position 36: D36 (Green)
- Position 41: V41 (Red)
- Position 42: V42 (Red)
- Position 43: I43 (Red)
- Position 44: A44 (Red)
- Position 45: A45 (Red)
- Position 46: L46 (Yellow)
- Position 47: Q47 (Yellow)
- Position 48: S48 (Red)
- Position 49: L49 (Red)
- Position 54: T54 (Red)
- Position 55: V55 (Red)
- Position 56: K56 (Red)
- Position 57: T57 (Red)
- Position 58: O58 (Red)
- Position 59: F59 (Red)
- Position 60: S60 (Red)
- Position 61: W61 (Red)
- Position 62: Q62 (Red)
- Position 63: V63 (Red)
- Position 64: V64 (Red)
- Position 65: V65 (Red)
- Position 66: T66 (Red)
- Position 67: T67 (Yellow)
- Position 68: L68 (Green)
- Position 74: E74 (Red)

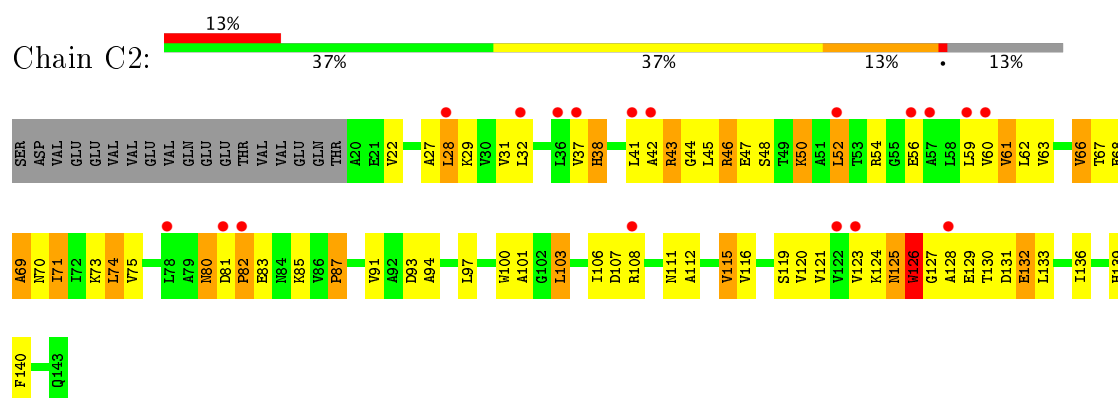
- Molecule 13: 40S ribosomal protein S11-A



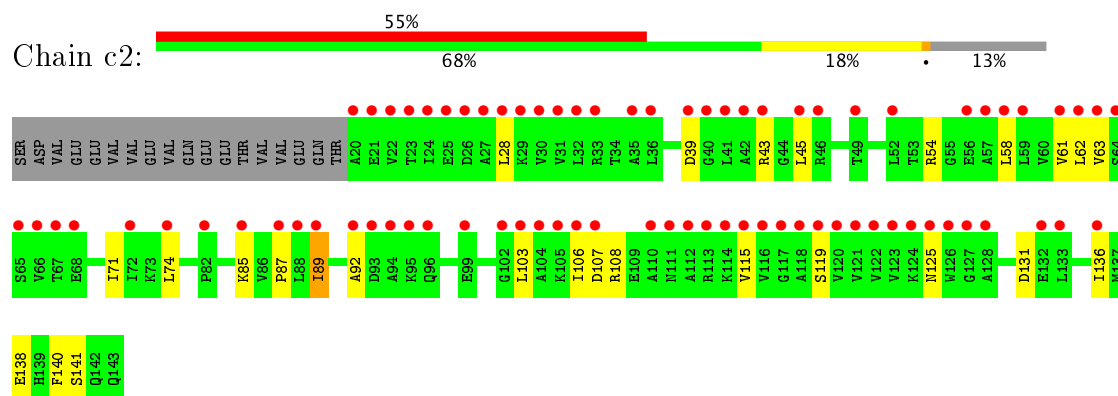
- Molecule 13: 40S ribosomal protein S11-A



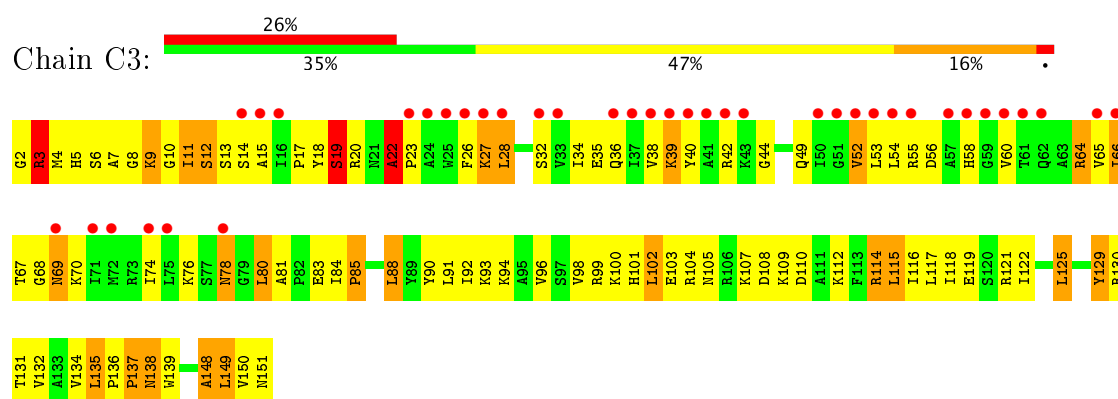
- Molecule 14: 40S ribosomal protein S12



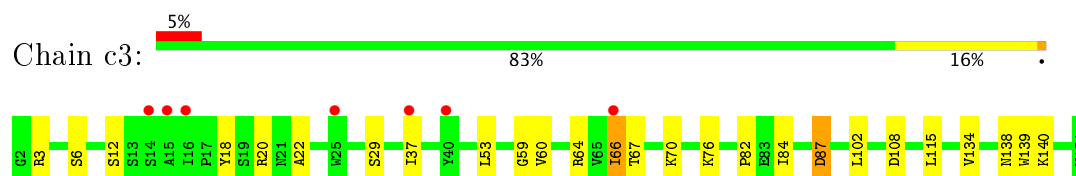
- Molecule 14: 40S ribosomal protein S12



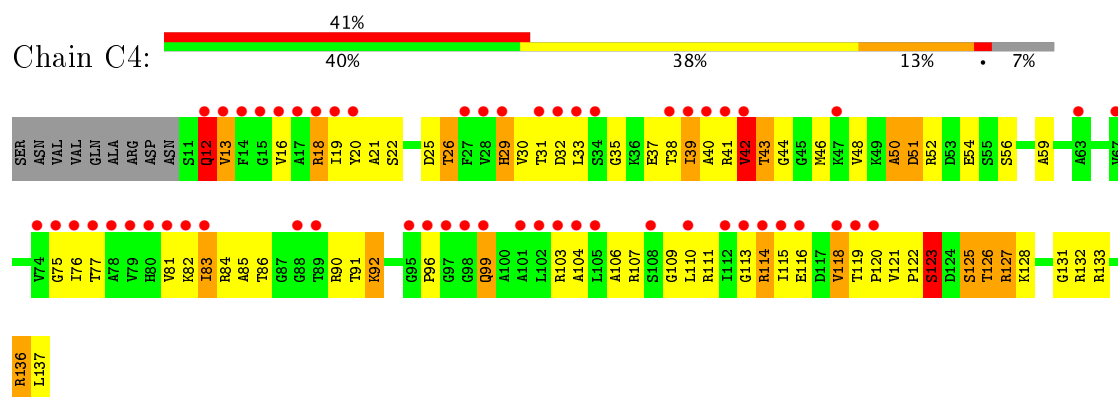
- Molecule 15: 40S ribosomal protein S13



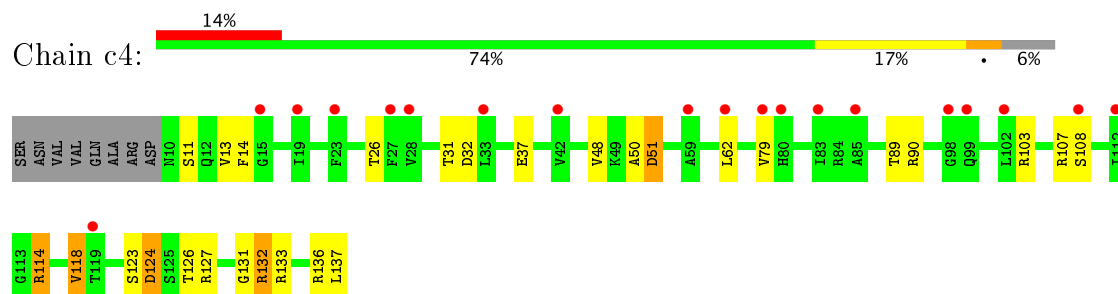
• Molecule 15: 40S ribosomal protein S13



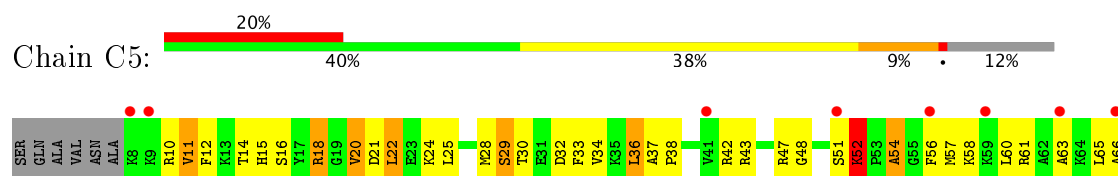
• Molecule 16: 40S ribosomal protein S14-A

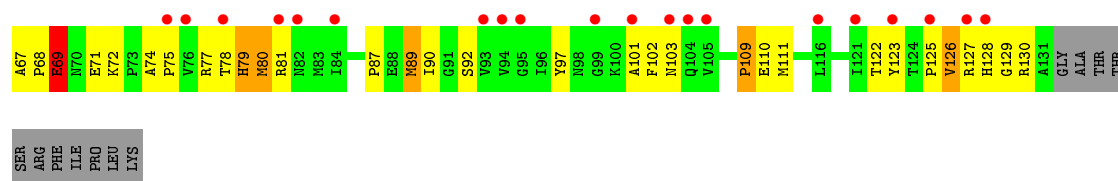


• Molecule 16: 40S ribosomal protein S14-A

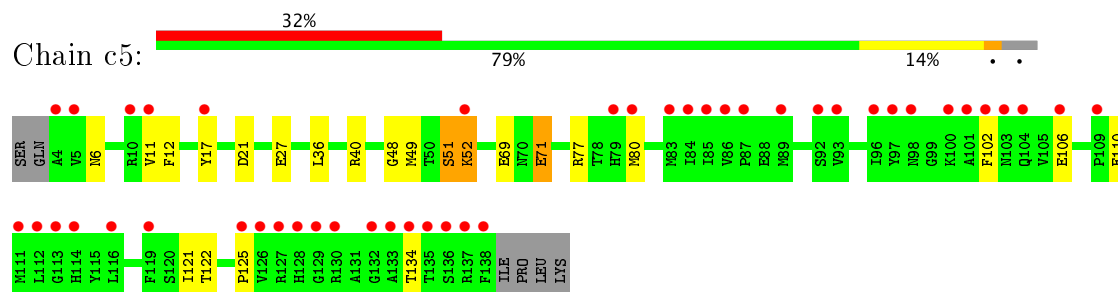


• Molecule 17: 40S ribosomal protein S15

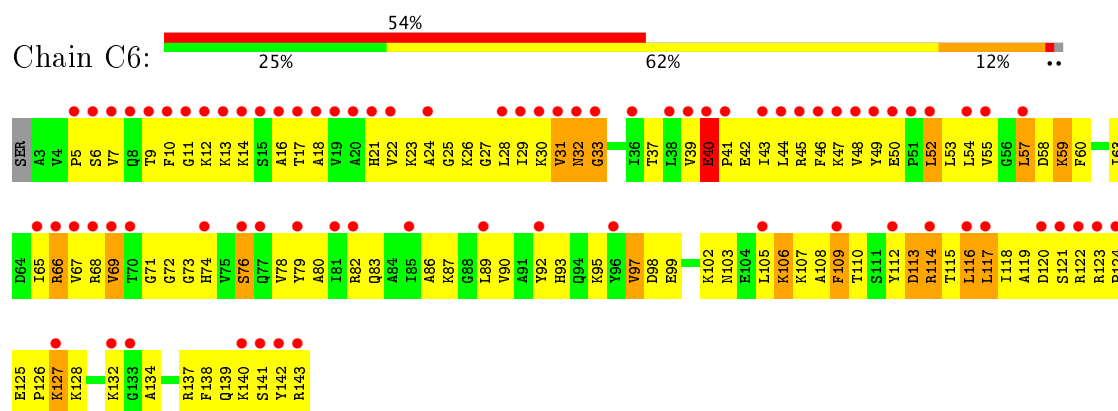




- Molecule 17: 40S ribosomal protein S15

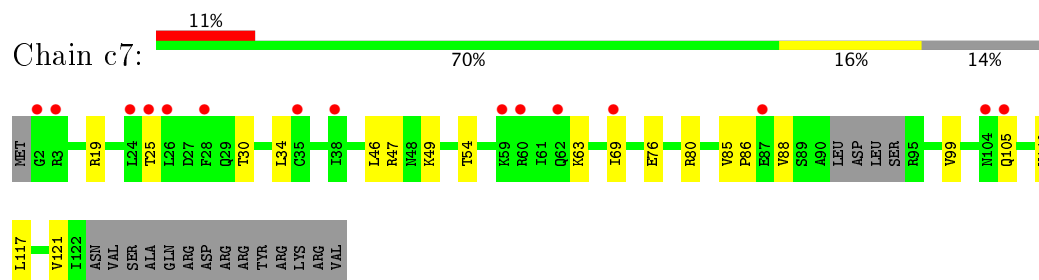


- Molecule 18: 40S ribosomal protein S16-A

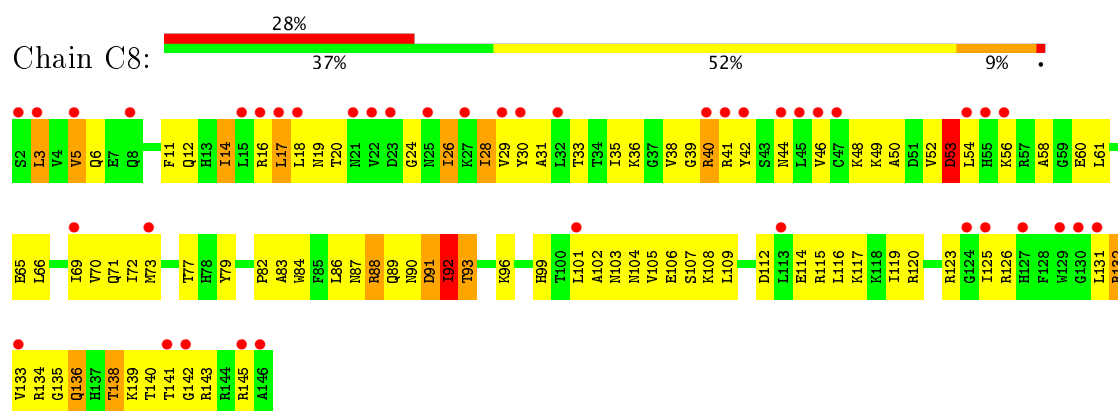


LYS
ARG
VAL

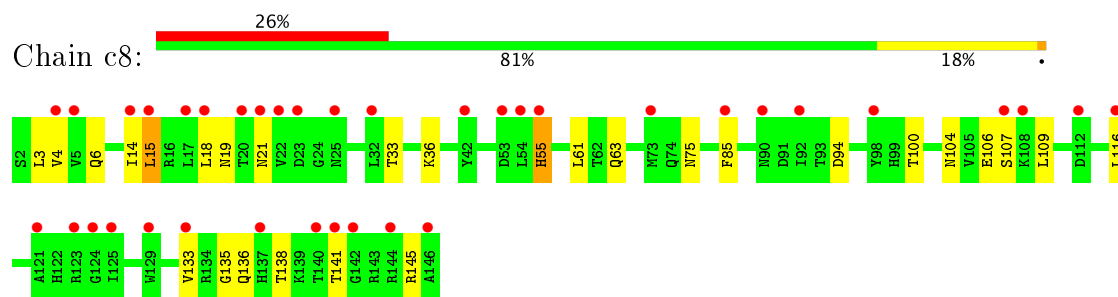
• Molecule 19: 40S ribosomal protein S17-A



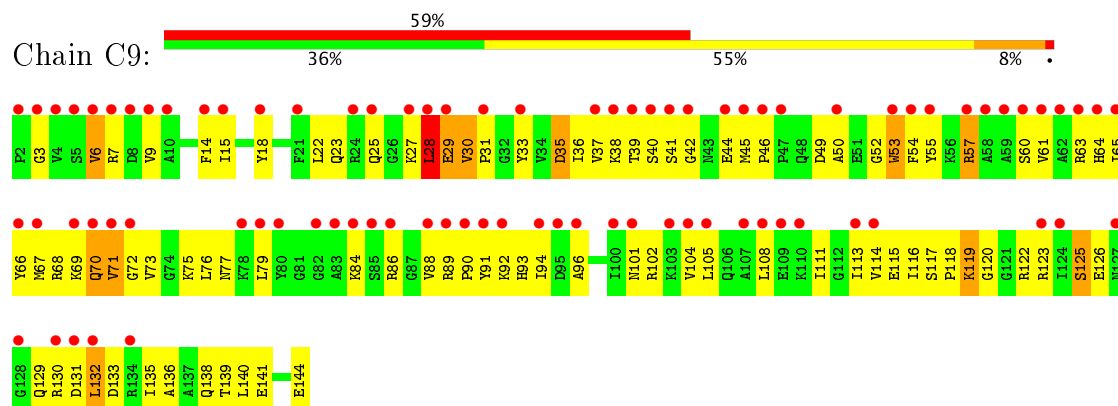
• Molecule 20: 40S ribosomal protein S18-A



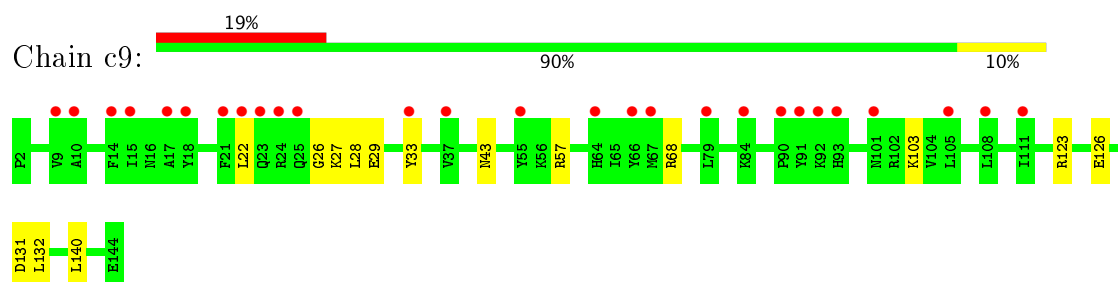
• Molecule 20: 40S ribosomal protein S18-A



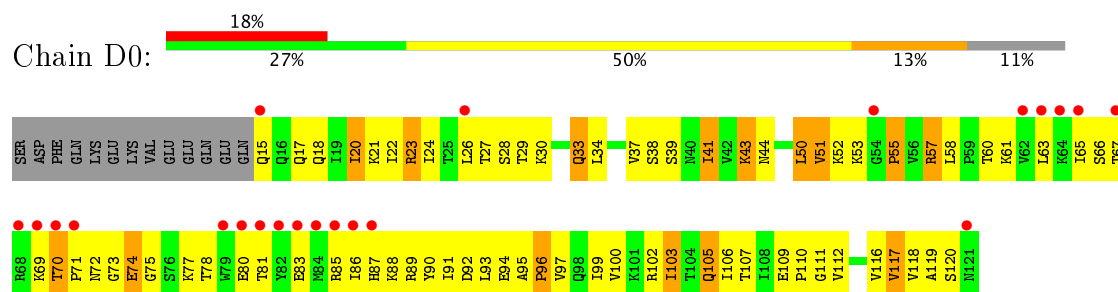
• Molecule 21: 40S ribosomal protein S19-A



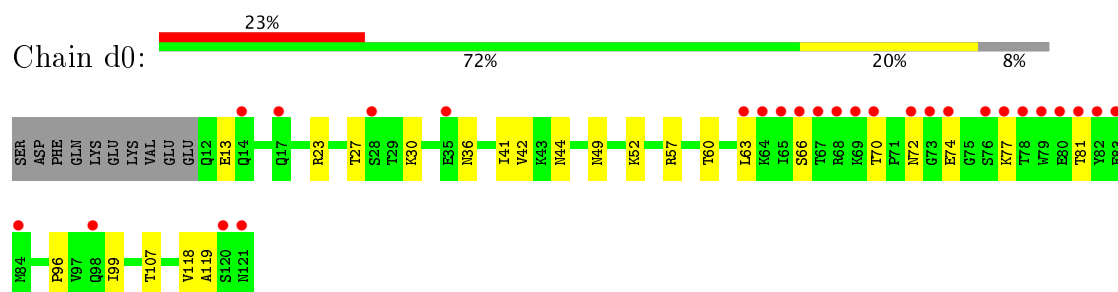
- Molecule 21: 40S ribosomal protein S19-A



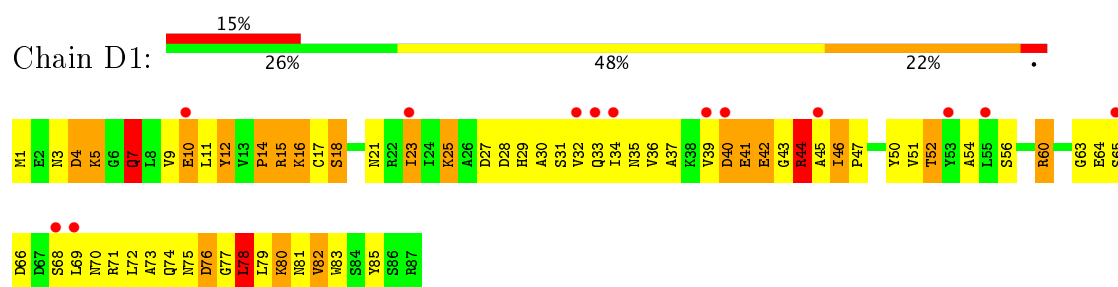
- Molecule 22: 40S ribosomal protein S20



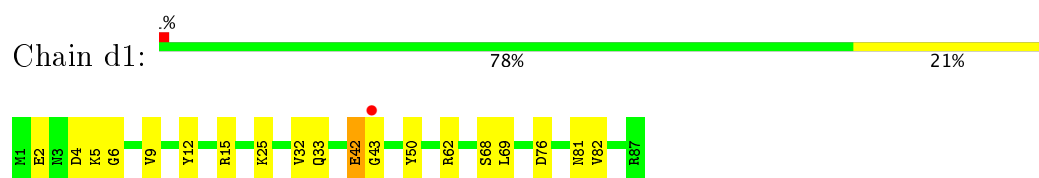
- Molecule 22: 40S ribosomal protein S20



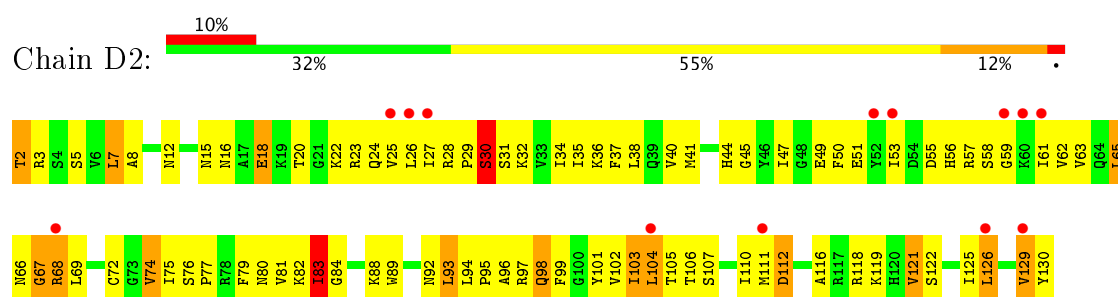
- Molecule 23: 40S ribosomal protein S21-A



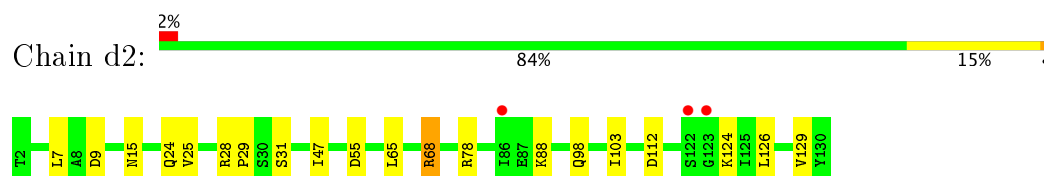
- Molecule 23: 40S ribosomal protein S21-A



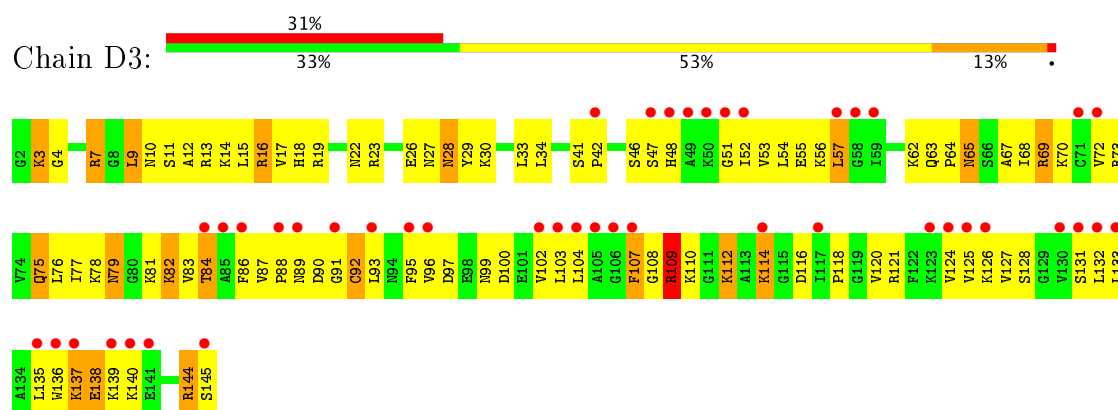
- Molecule 24: 40S ribosomal protein S22-A



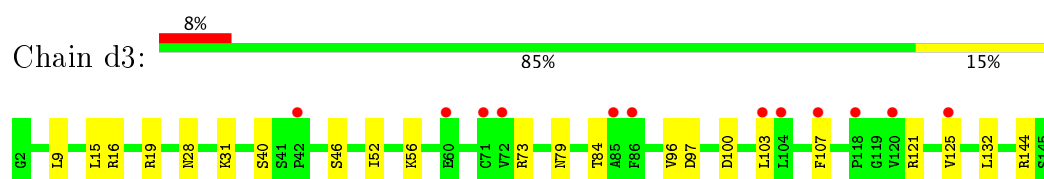
- Molecule 24: 40S ribosomal protein S22-A



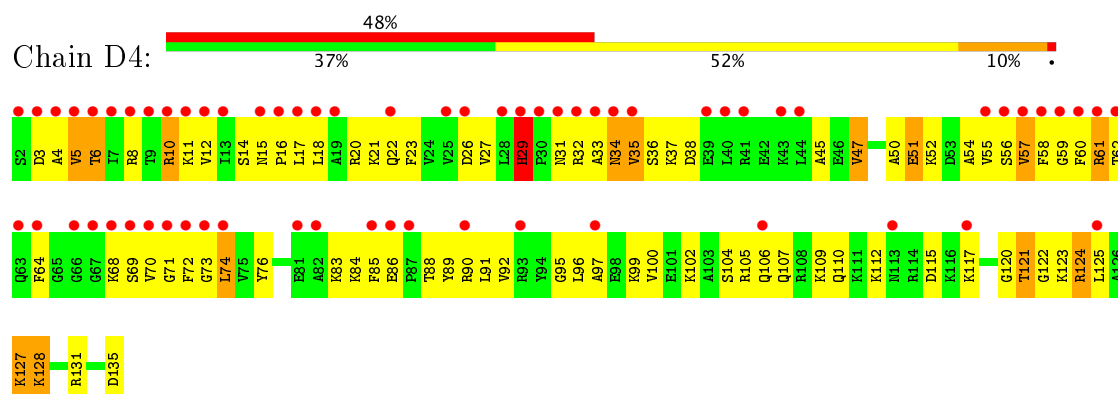
- Molecule 25: 40S ribosomal protein S23-A



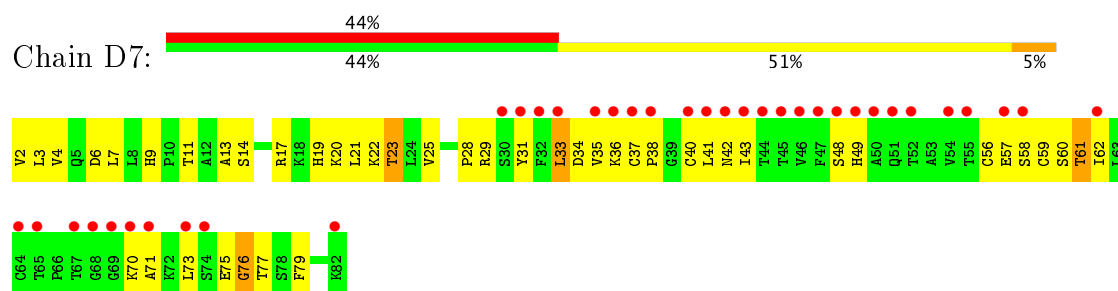
- Molecule 25: 40S ribosomal protein S23-A



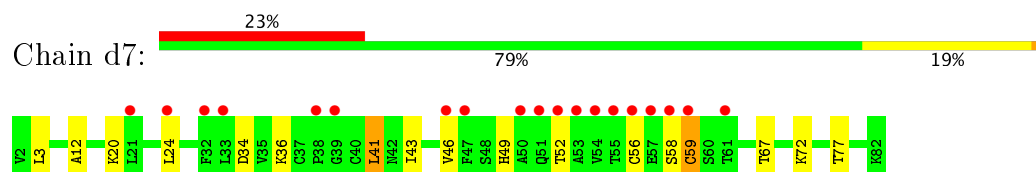
- Molecule 26: 40S ribosomal protein S24-A



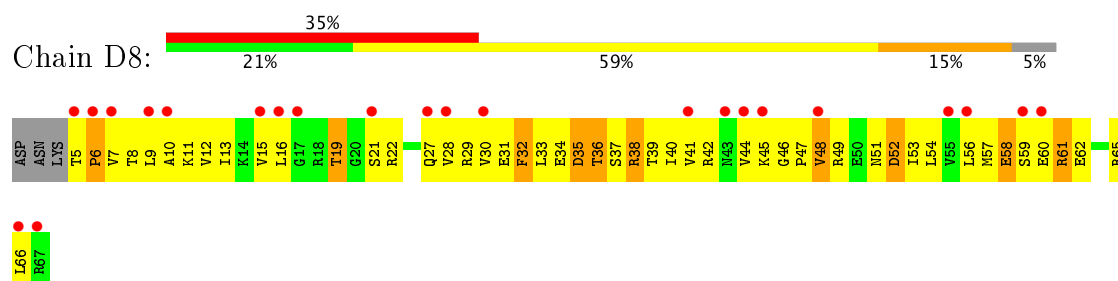
- Molecule 29: 40S ribosomal protein S27-A



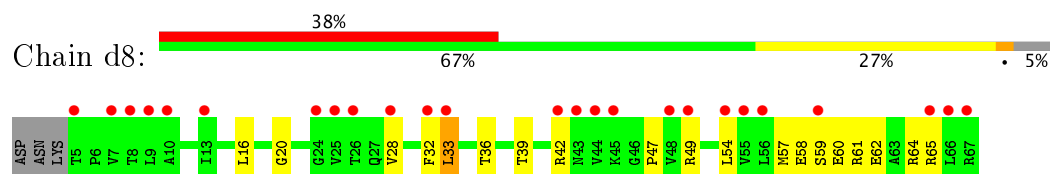
- Molecule 29: 40S ribosomal protein S27-A



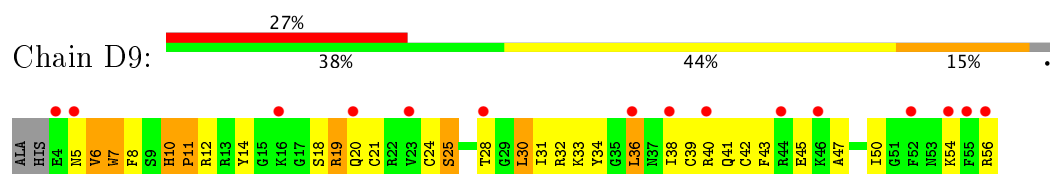
- Molecule 30: 40S ribosomal protein S28-A



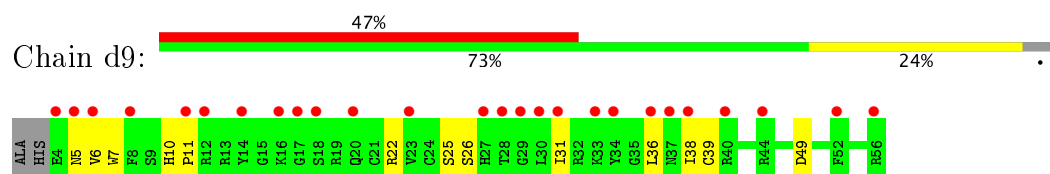
- Molecule 30: 40S ribosomal protein S28-A



- Molecule 31: 40S ribosomal protein S29-A

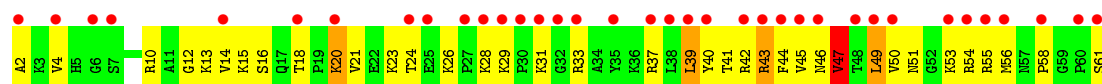


- Molecule 31: 40S ribosomal protein S29-A

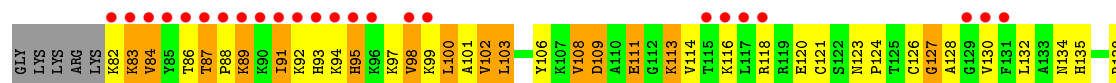


- Molecule 32: 40S ribosomal protein S30-A

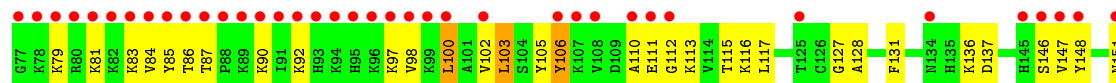




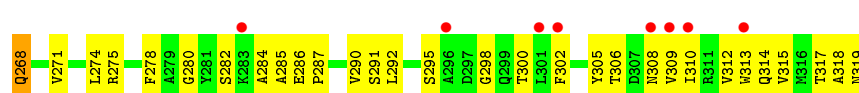
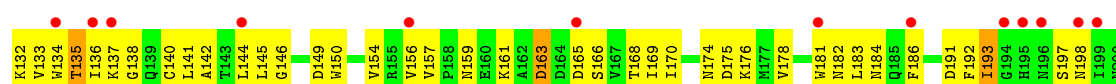
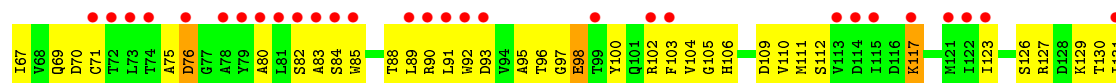
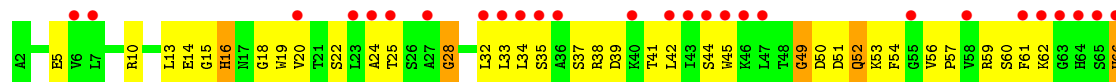
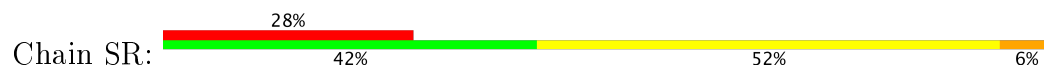
• Molecule 33: Ubiquitin-40S ribosomal protein S31



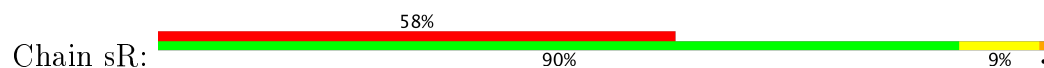
• Molecule 33: Ubiquitin-40S ribosomal protein S31

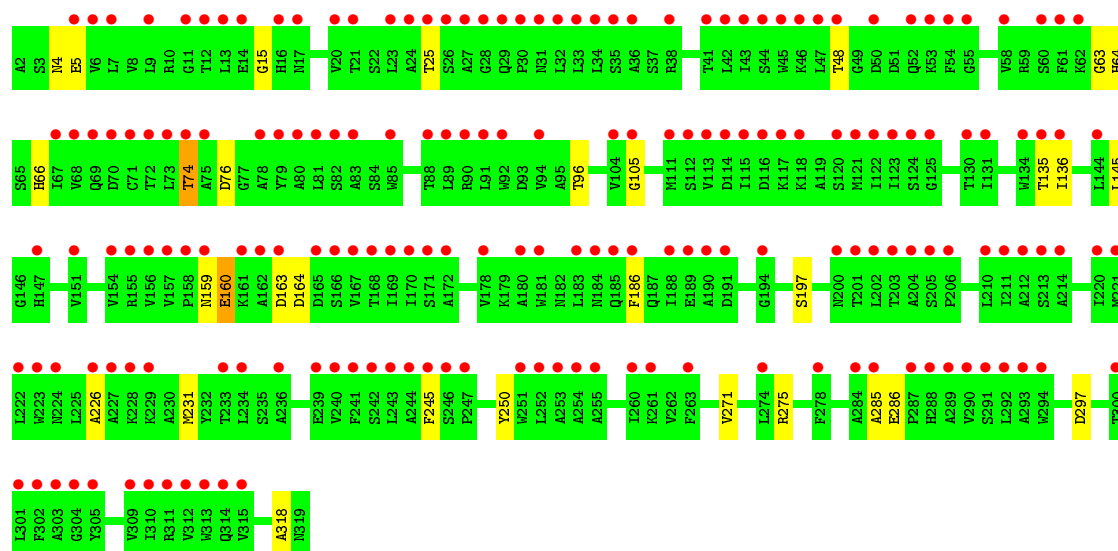


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

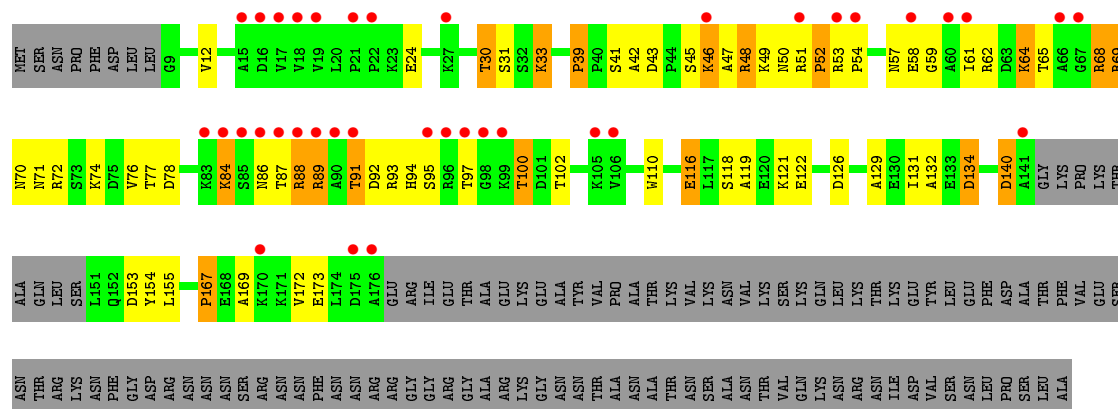
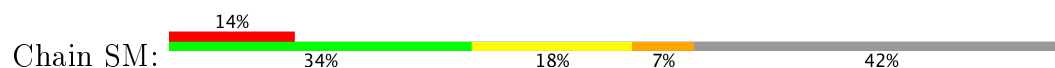


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

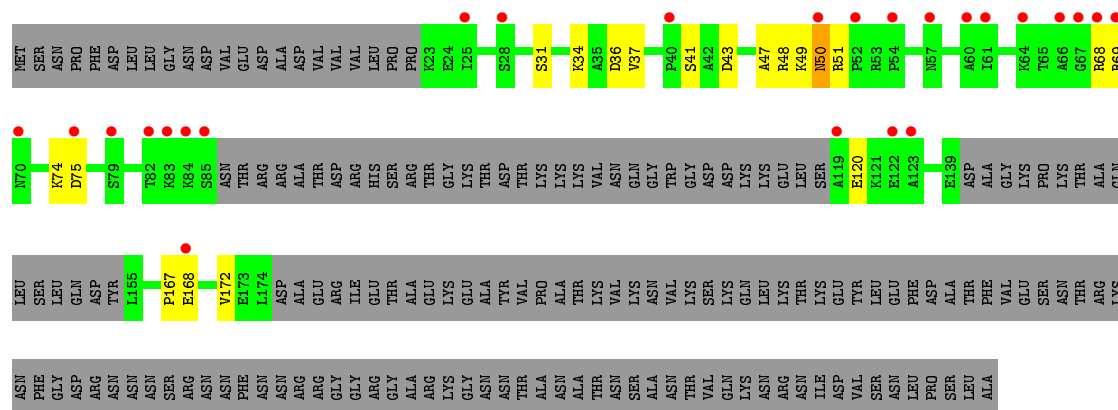




• Molecule 35: Suppressor protein STM1



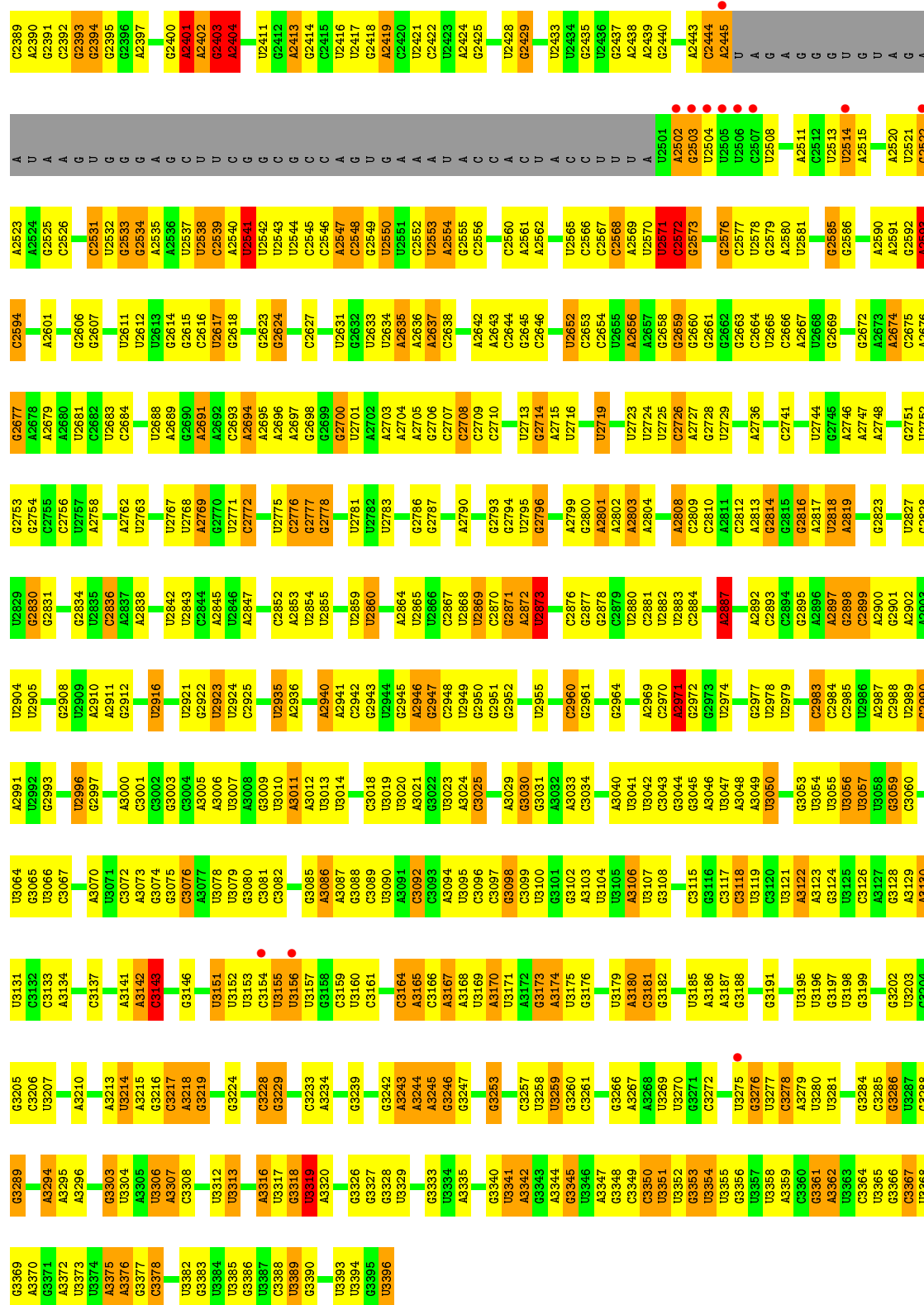
• Molecule 35: Suppressor protein STM1



• Molecule 36: 25S ribosomal RNA

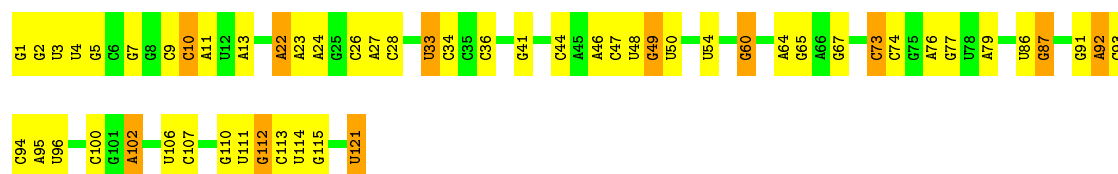


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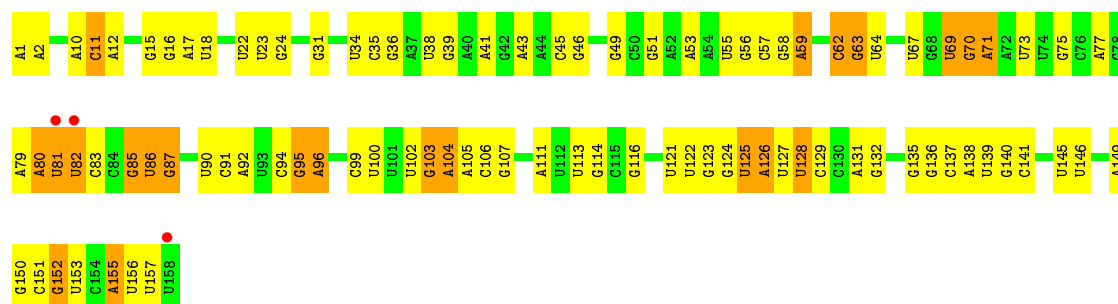


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A1278	C1193	U1028	U955	U955	A684	G754	A684	U602	U462	C206	U285	C213	A136	A65
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U1284	A1200	G1117	U960	U960	A693	G758	A693	U606	U466	C210	U289	C217	A140	C73
G1285	C1201	U1033	C961	C961	C694	G759	C694	U607	U467	C211	U290	C218	A141	G74
A1287	A1202	U1034	G962	G962	A695	G760	A695	U608	U468	C212	U291	C219	A142	G75
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G1289	A1204	U1036	A964	A964	U699	G762	U699	U610	U470	C214	U293	C221	A144	G77
U1290	C1205	G1037	G965	G965	U699	G763	U699	U611	U471	C215	U294	C222	A145	C78
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U1296	C1211	G1043	A970	A970	U699	G769	U699	U617	U477	C221	U300	C228	A151	G84
G1298	A1212	U1044	U970	U970	U699	G770	U699	U618	U478	C222	U301	C229	A152	G85
U1299	C1213	G1045	A971	A971	U699	G771	U699	U619	U479	C223	U302	C230	A153	G86
G1300	A1214	U1046	A972	A972	U699	G772	U699	U620	U480	C224	U303	C231	A154	G87
U1301	C1215	G1047	A973	A973	U699	G773	U699	U621	U481	C225	U304	C232	A155	G88
G1302	A1216	U1048	A974	A974	U699	G774	U699	U622	U482	C226	U305	C233	A156	G89
U1303	C1217	G1049	A975	A975	U699	G775	U699	U623	U483	C227	U306	C234	A157	G90
G1304	A1218	U1050	A976	A976	U699	G776	U699	U624	U484	C228	U307	C235	A158	G91
U1305	C1219	G1051	A977	A977	U699	G777	U699	U625	U485	C229	U308	C236	A159	G92
G1306	A1220	U1052	A978	A978	U699	G778	U699	U626	U486	C230	U309	C237	A160	G93
U1307	C1221	G1053	A979	A979	U699	G779	U699	U627	U487	C231	U310	C238	A161	G94
G1308	A1222	U1054	A980	A980	U699	G780	U699	U628	U488	C232	U311	C239	A162	G95
U1309	C1223	G1055	A981	A981	U699	G781	U699	U629	U489	C233	U312	C240	A163	G96
G1310	A1224	U1056	A982	A982	U699	G782	U699	U630	U490	C234	U313	C241	A164	G97
U1311	C1225	G1057	A983	A983	U699	G783	U699	U631	U491	C235	U314	C242	A165	G98
G1312	A1226	U1058	A984	A984	U699	G784	U699	U632	U492	C236	U315	C243	A166	G99
U1313	C1227	G1059	A985	A985	U699	G785	U699	U633	U493	C237	U316	C244	A167	G100
G1314	A1228	U1060	A986	A986	U699	G786	U699	U634	U494	C238	U317	C245	A168	G101
U1315	C1229	G1061	A987	A987	U699	G787	U699	U635	U495	C239	U318	C246	A169	G102
G1316	A1230	U1062	A988	A988	U699	G788	U699	U636	U496	C240	U319	C247	A170	G103
U1317	C1231	G1063	A989	A989	U699	G789	U699	U637	U497	C241	U320	C248	A171	G104
G1318	A1232	U1064	A990	A990	U699	G790	U699	U638	U498	C242	U321	C249	A172	G105
U1319	C1233	G1065	A991	A991	U699	G791	U699	U639	U499	C243	U322	C250	A173	G106
G1320	A1234	U1066	A992	A992	U699	G792	U699	U640	U500	C244	U323	C251	A174	G107
U1321	C1235	G1067	A993	A993	U699	G793	U699	U641	U501	C245	U324	C252	A175	G108
G1322	A1236	U1068	A994	A994	U699	G794	U699	U642	U502	C246	U325	C253	A176	G109
U1323	C1237	G1069	A995	A995	U699	G795	U699	U643	U503	C247	U326	C254	A177	G110
G1324	A1238	U1070	A996	A996	U699	G796	U699	U644	U504	C248	U327	C255	A178	G111
U1325	C1239	G1071	A997	A997	U699	G797	U699	U645	U505	C249	U328	C256	A179	G112
G1326	A1240	U1072	A998	A998	U699	G798	U699	U646	U506	C250	U329	C257	A180	G113
U1327	C1241	G1073	A999	A999	U699	G799	U699	U647	U507	C251	U330	C258	A181	G114
G1328	A1242	U1074	A1000	A1000	U699	G800	U699	U648	U508	C252	U331	C259	A182	G115
U1329	C1243	G1075	C1000	C1000	U699	G801	U699	U649	U509	C253	U332	C260	A183	G116
G1330	A1244	U1076	C1001	C1001	U699	G802	U699	U650	U510	C254	U333	C261	A184	G117
U1331	C1245	G1077	A1002	A1002	U699	G803	U699	U651	U511	C255	U334	C262	A185	G118
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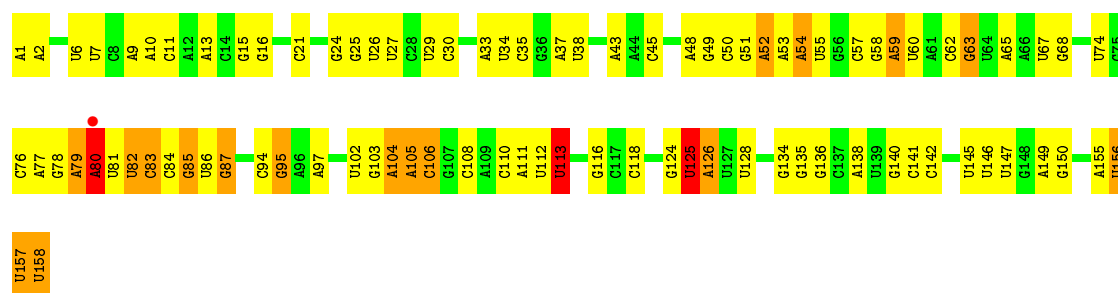
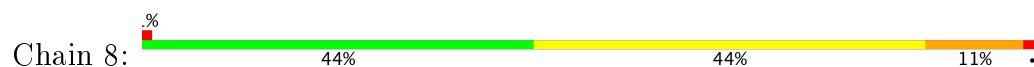
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A	U2411	A2317	A2244	C	G1868	C1781	U1702	A1559	U1472		A1302
C	G2412	U2318	G2169	C	A1874	U1782	G1713	G1560	U1473		A1303
G	A2413	U2319	U2170	C	G1875	G1790	A1714	G1561	A1474		A1304
U	G2418	A2326	G2250	C	U1876	C1791	A1715	G1562	G1473		A1305
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A			A2252	C	G1878	C1793	U1717	G1565			G1307
A			U2175	C	A1879	G1794	G1718	U1566			A1308
A			U2176	U	U1880	U1795	G1719	U1567			U1309
A			G2177	A	U1881	G1796	U1720	A1481			G1310
A			A2093	G	A1882	A1797	U1721	U1568	A1482		G1311
A			A2100	G	G1889	A1797	U1722	U1569	A1393		G1312
A			C2101	G	A1890	A1806	A1723	U1570	A1393		G1313
C			U2102	C	A1893	G1807	U1724	A1571	U1484		G1314
C			U2103	C	A1894	G1808	C1725	U1572	A1399		C1314
C			A2104	C	A1895	A1809	G1726	G1573	G1485		U1315
C			C2105	C	A1896	A1810	G1727	C1574	G1486		C1316
C			A2106	U	G1897	A1811	G1728	A1575	G1488		A1317
C				U	G1898	A1812	A1729	G1576	A1489		A1318
C			U2109	G	G1899	A1813	G1730	G1577	G1490		G1323
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A				U	U1912	U1820	A1741	U1659	U1427		A1332
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A			G2122	C	G1919	A1828	G1748	G1510	A1433		C1338
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A			C2132	A	G1934	U1840		G1598	C1437		A1343
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A			A2147	U	G1947	C1849	C1762	A1535	U1445		A1351
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A			A2158	C	U		G1770	A1613	A1453		
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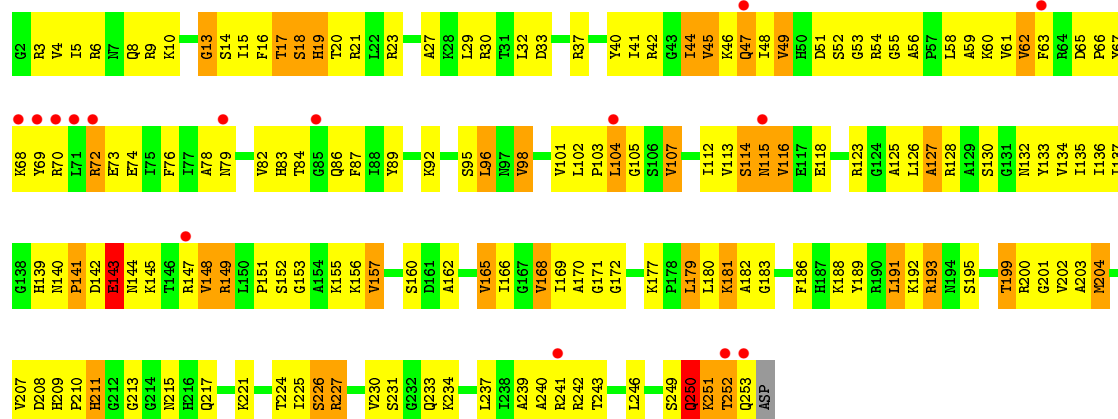
- Molecule 38: 5.8S ribosomal RNA



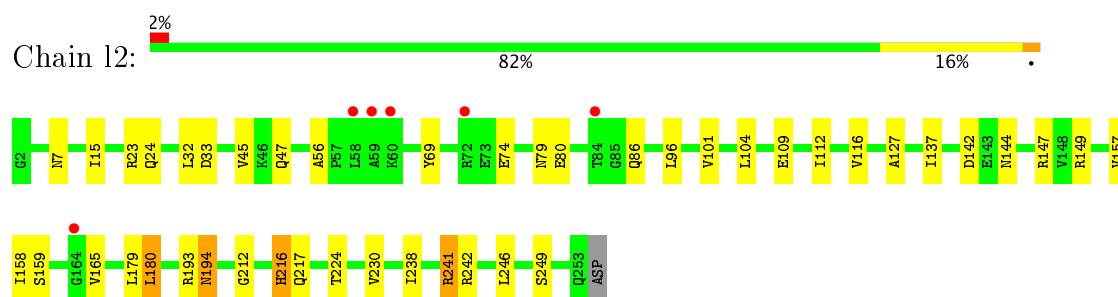
- Molecule 38: 5.8S ribosomal RNA



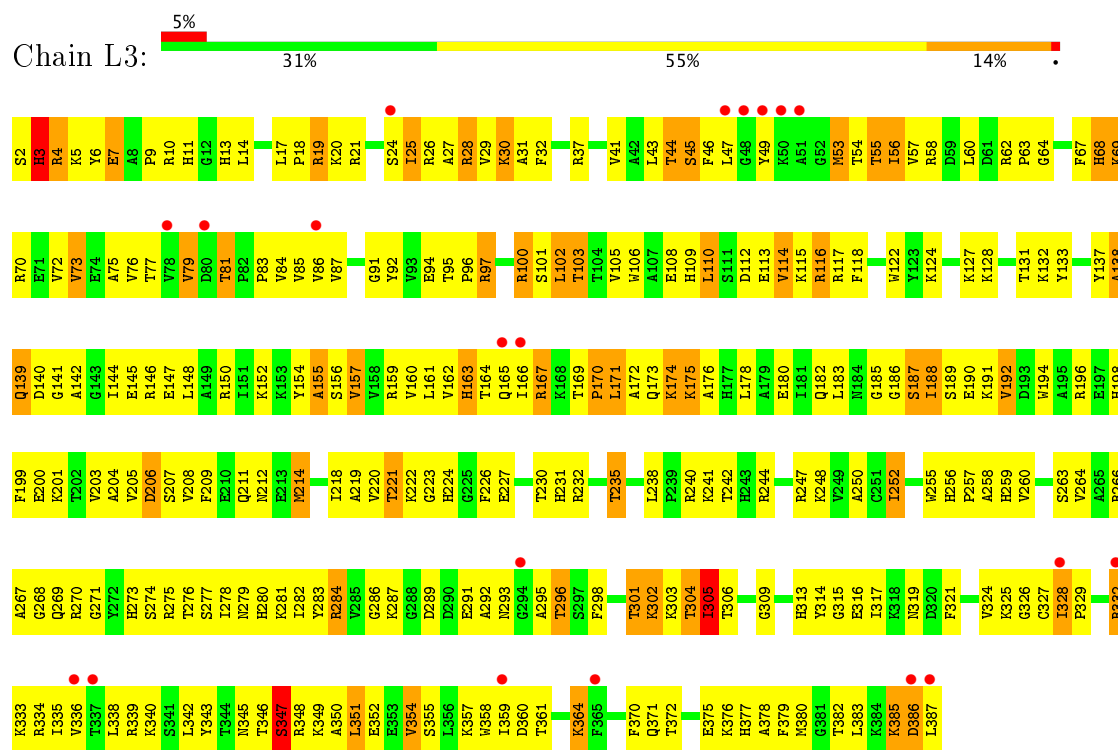
- Molecule 39: 60S ribosomal protein L2-A

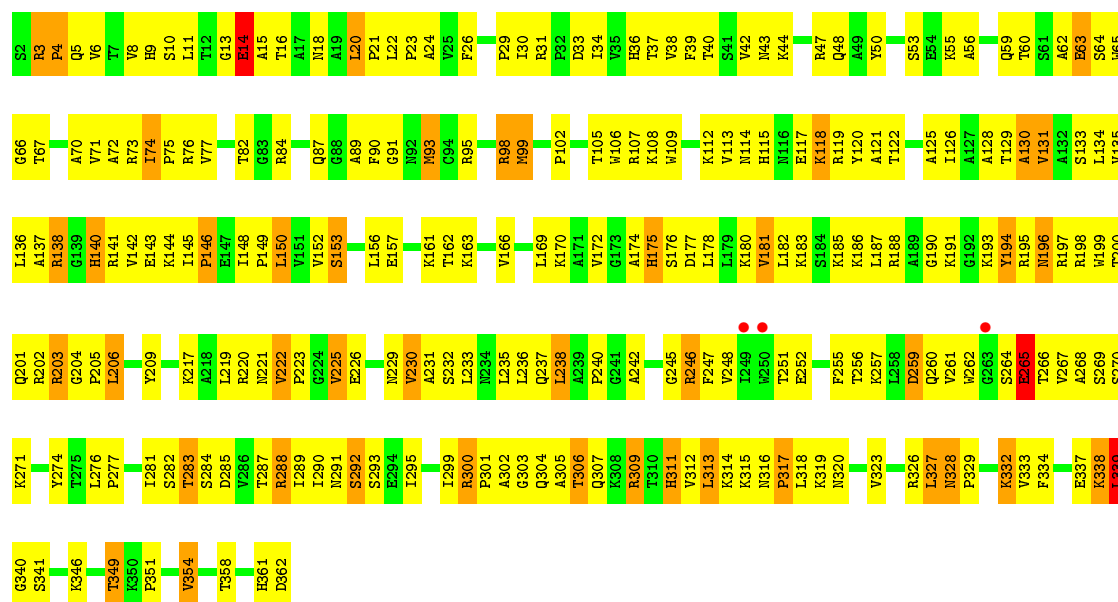


- Molecule 39: 60S ribosomal protein L2-A

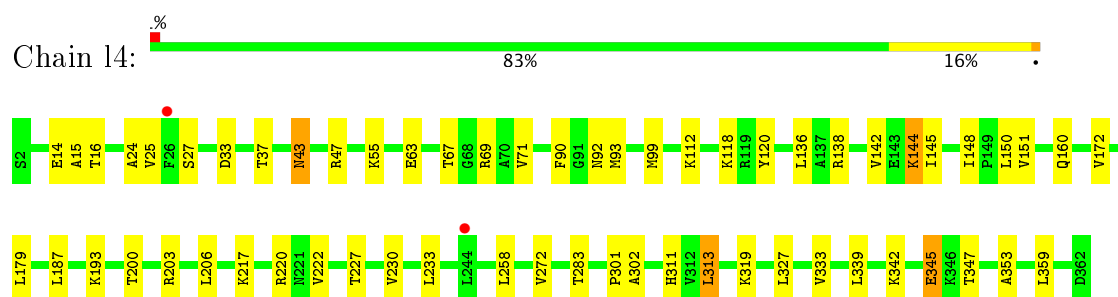


• Molecule 40: 60S ribosomal protein L3

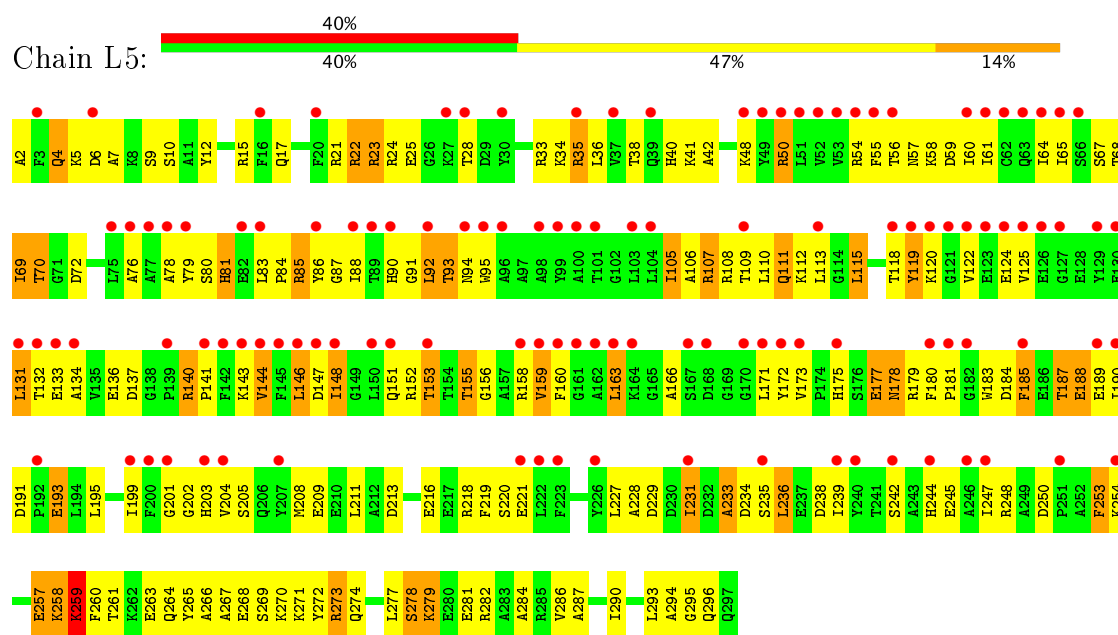




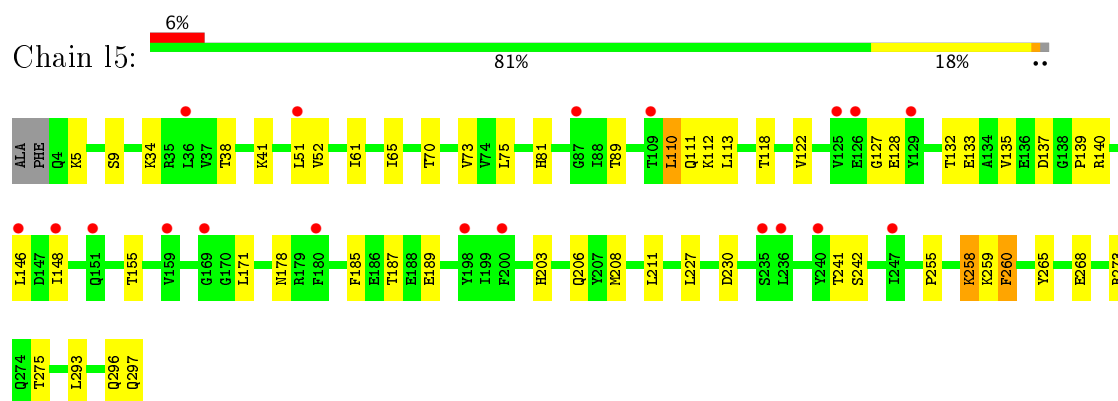
• Molecule 41: 60S ribosomal protein L4-A



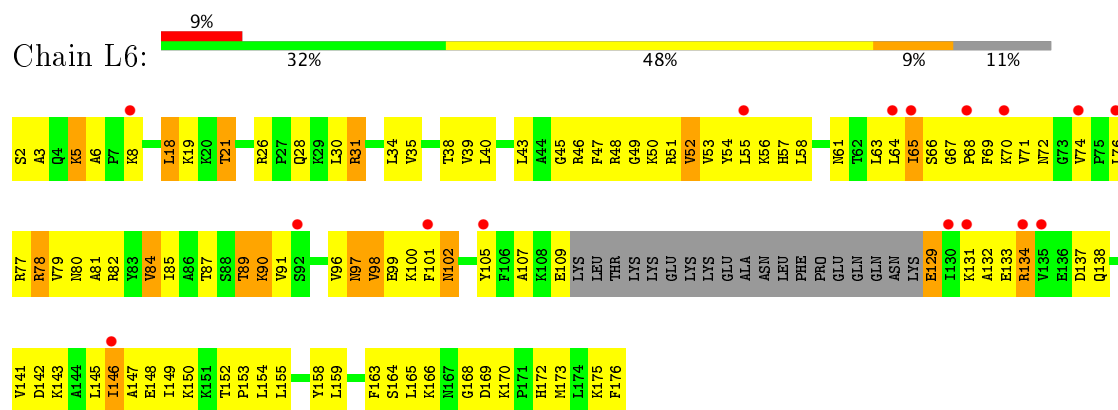
• Molecule 42: 60S ribosomal protein L5



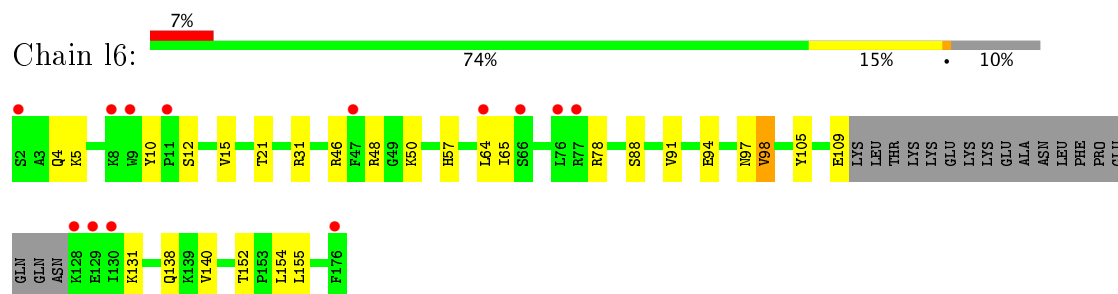
• Molecule 42: 60S ribosomal protein L5



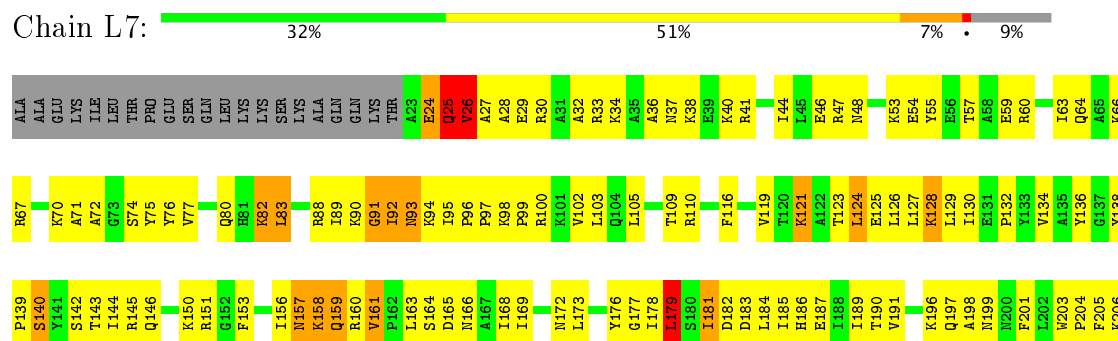
- Molecule 43: 60S ribosomal protein L6-A

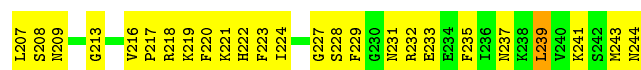


- Molecule 43: 60S ribosomal protein L6-A



- Molecule 44: 60S ribosomal protein L7-A





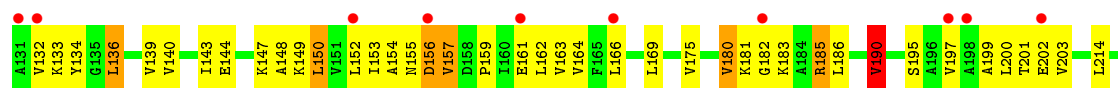
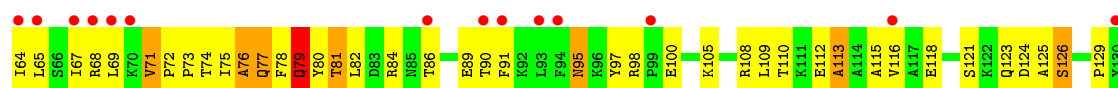
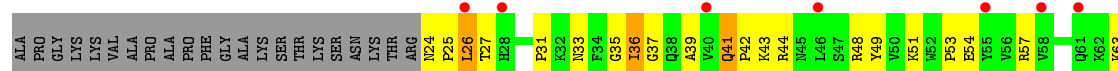
- Molecule 44: 60S ribosomal protein L7-A

Chain L7: 80% 10% 8%



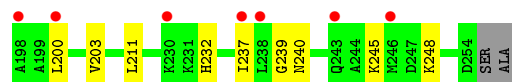
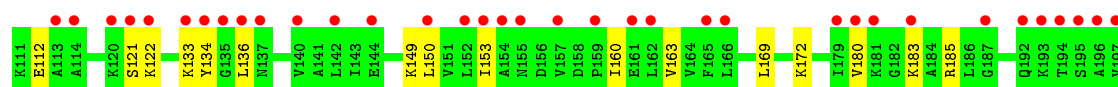
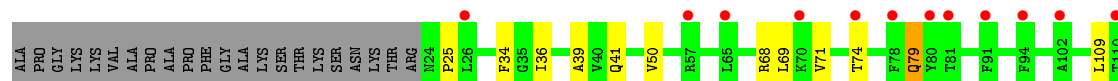
- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 15% 44% 40% 7% 9%



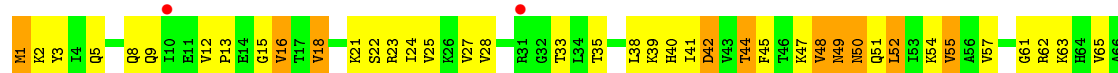
- Molecule 45: 60S ribosomal protein L8-A

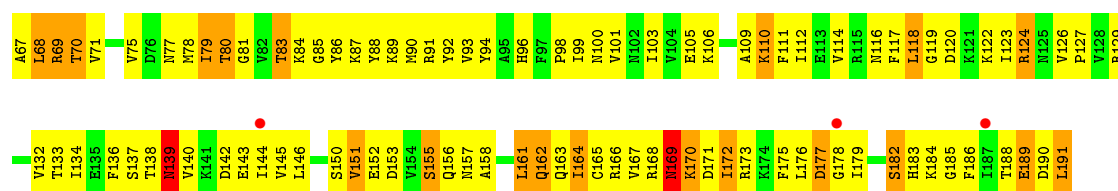
Chain L8: 21% 76% 14% 9%



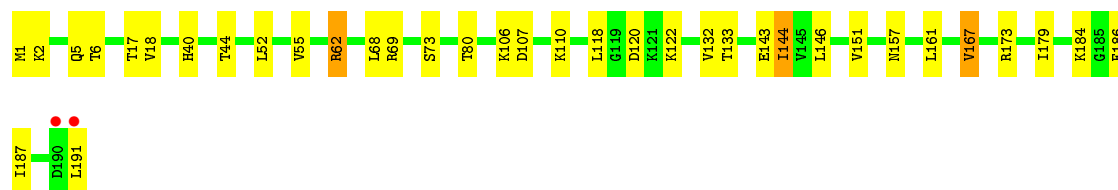
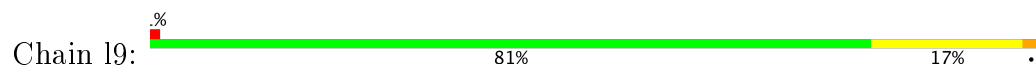
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 3% 29% 54% 16%

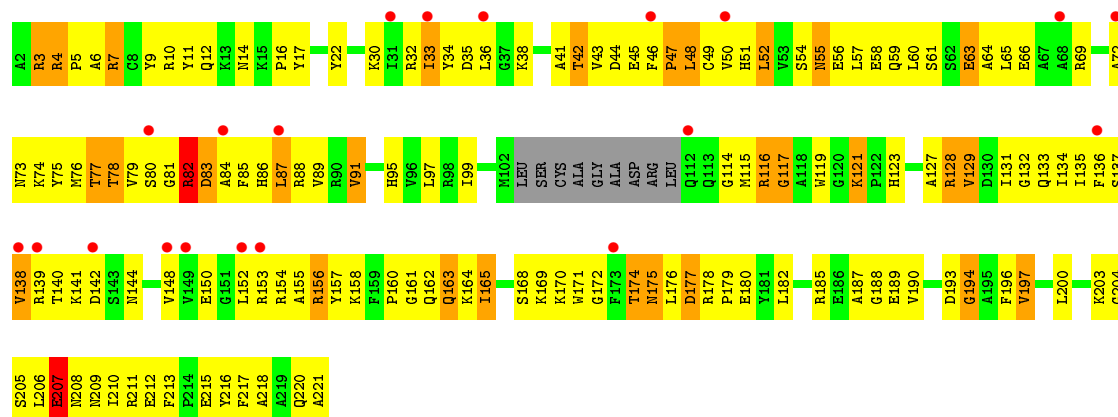




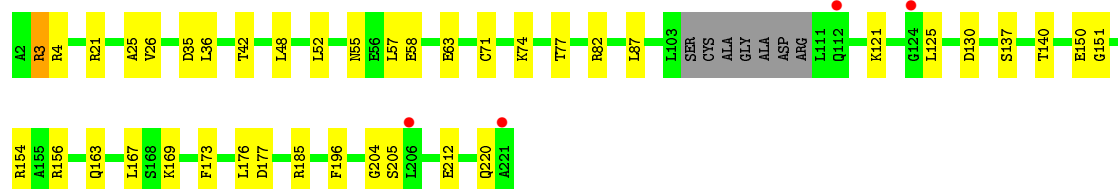
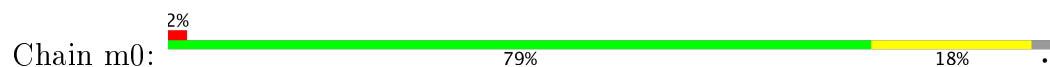
- Molecule 46: 60S ribosomal protein L9-A



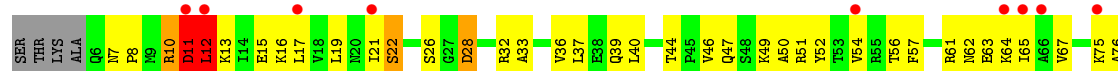
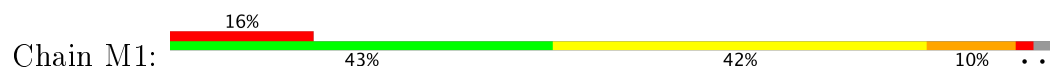
- Molecule 47: 60S ribosomal protein L10

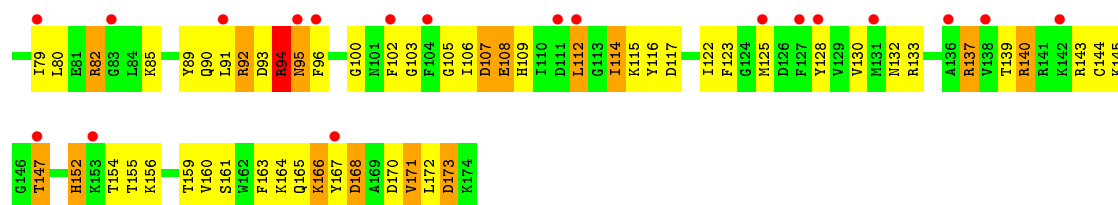


- Molecule 47: 60S ribosomal protein L10

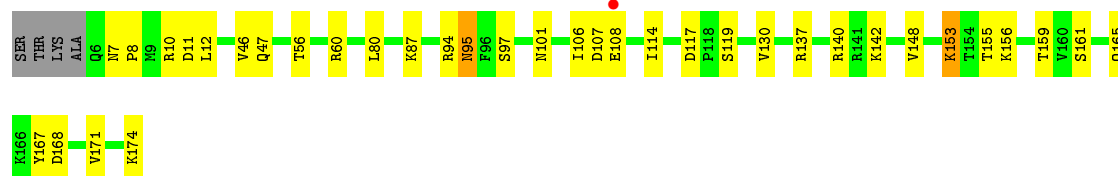
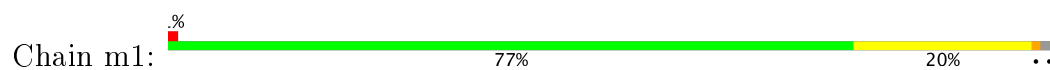


- Molecule 48: 60S ribosomal protein L11-A

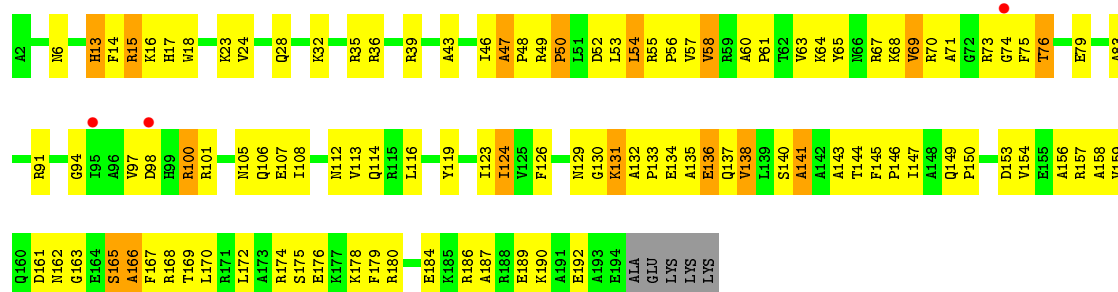
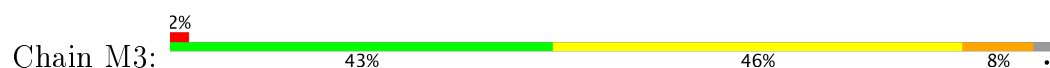




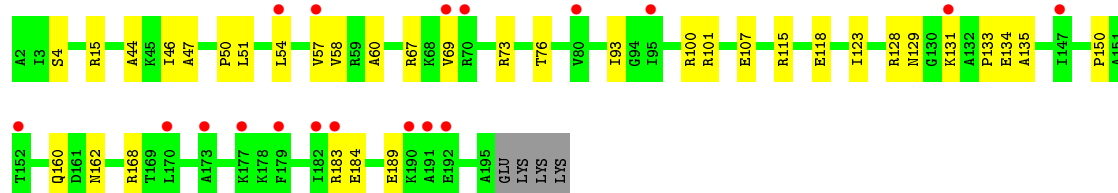
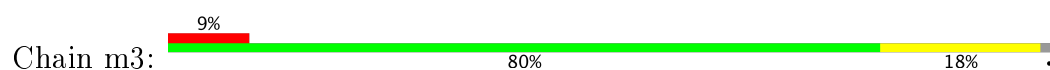
• Molecule 48: 60S ribosomal protein L11-A



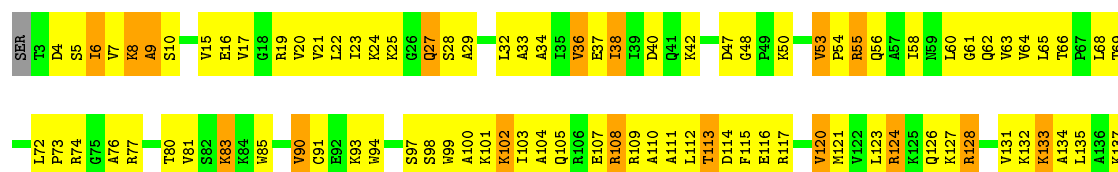
• Molecule 49: 60S ribosomal protein L13-A



• Molecule 49: 60S ribosomal protein L13-A




• Molecule 50: 60S ribosomal protein L14-A

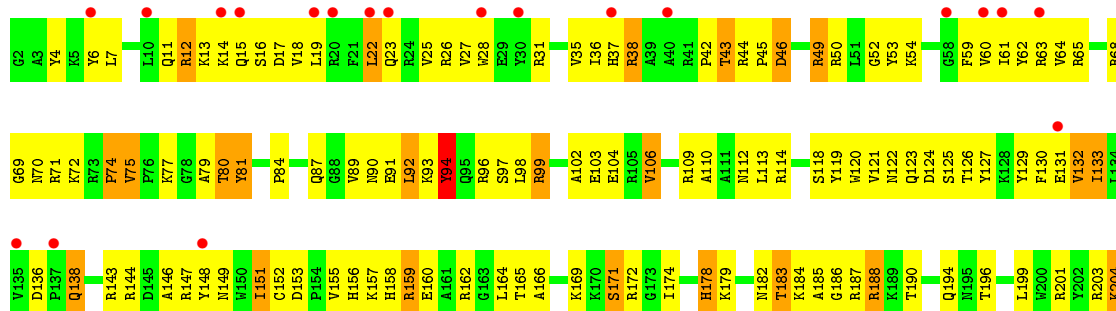


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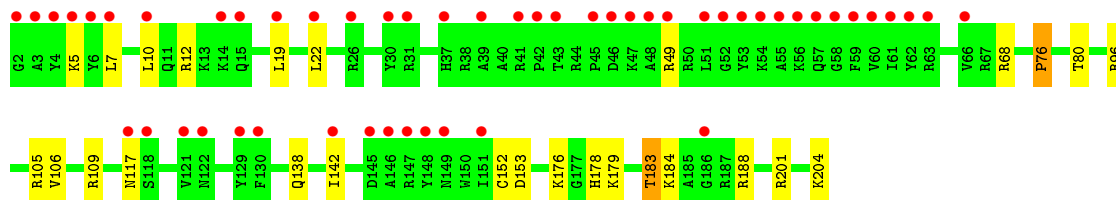
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:  83% 16% .

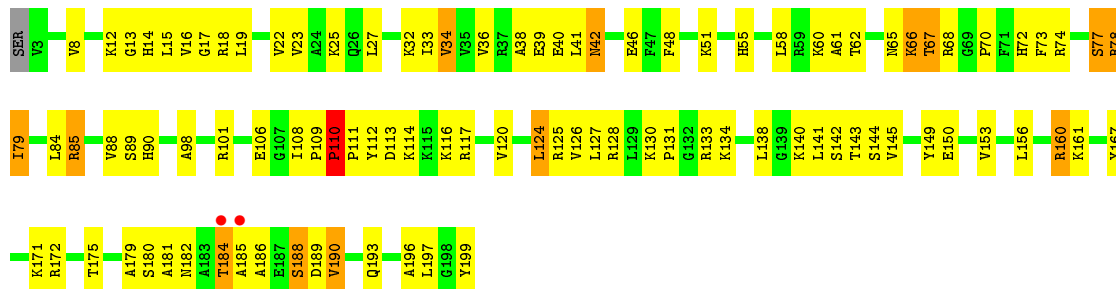
- Molecule 51: 60S ribosomal protein L15-A

Chain M5:  10% 37% 51% 11%

- Molecule 51: 60S ribosomal protein L15-A

Chain m5:  26% 87% 12% .

- Molecule 52: 60S ribosomal protein L16-A

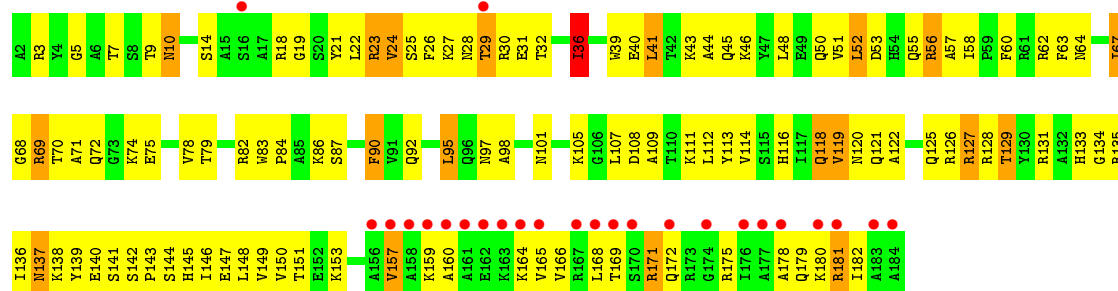
Chain M6:  % 49% 43% 7% ..

- Molecule 52: 60S ribosomal protein L16-A

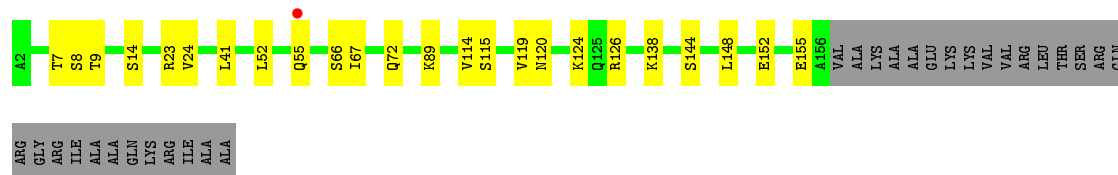
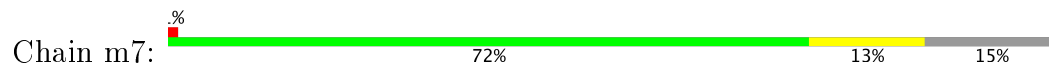
Chain m6:  90% 10% .



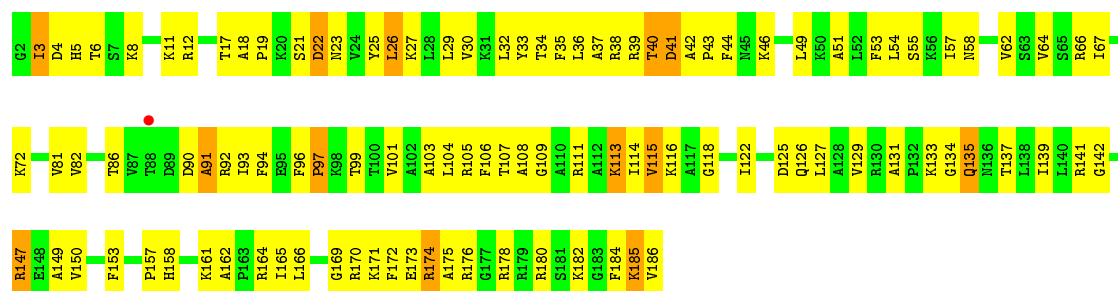
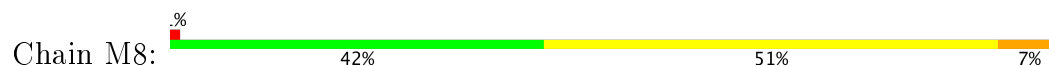
- Molecule 53: 60S ribosomal protein L17-A



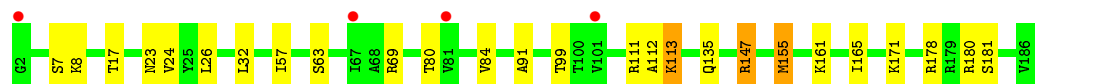
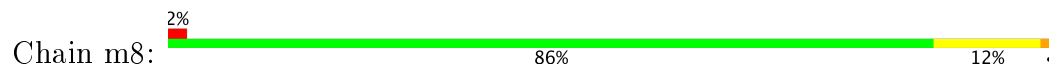
- Molecule 53: 60S ribosomal protein L17-A



- Molecule 54: 60S ribosomal protein L18-A

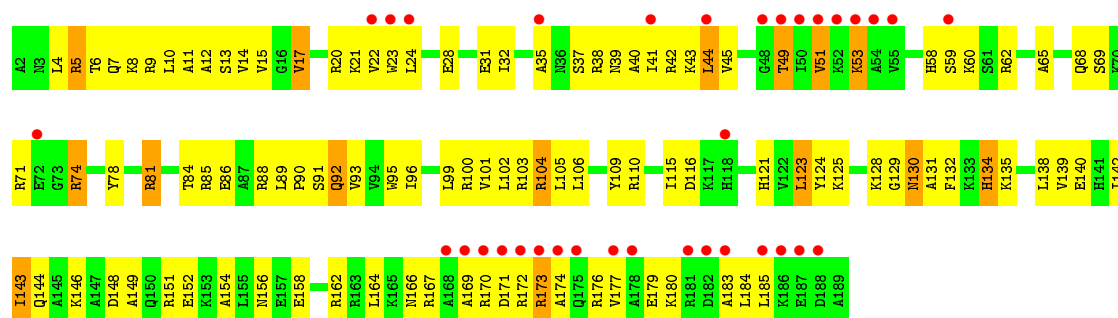


- Molecule 54: 60S ribosomal protein L18-A

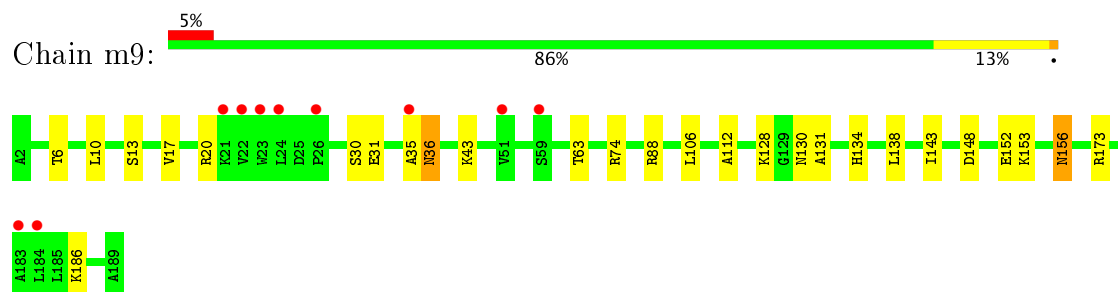


- Molecule 55: 60S ribosomal protein L19-A

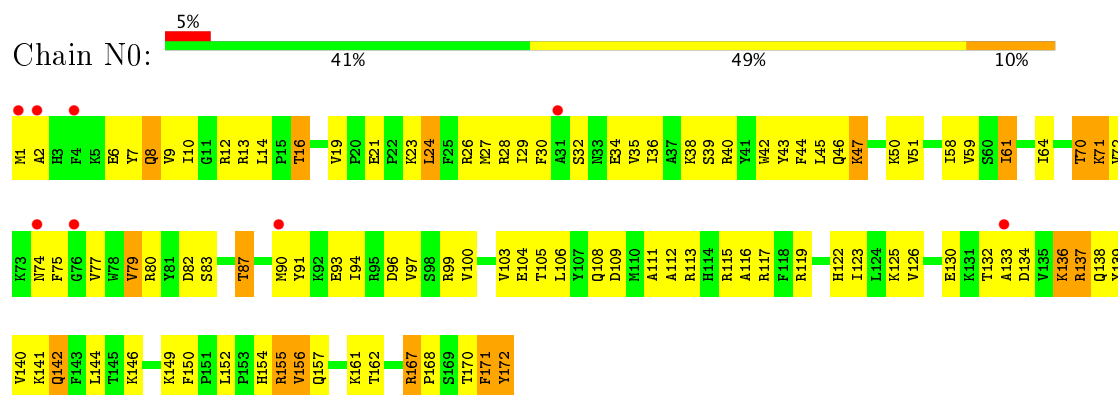




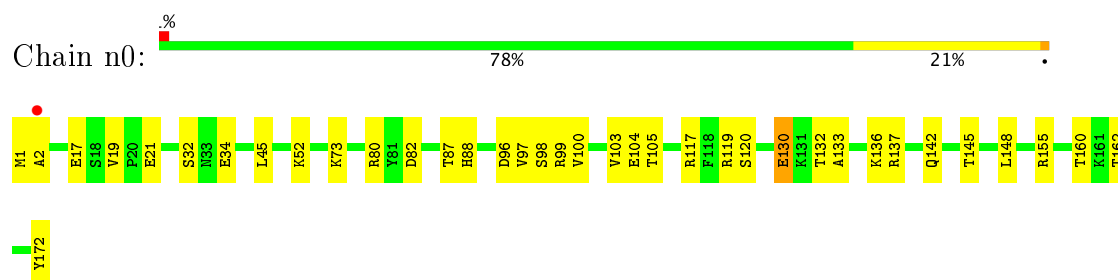
- Molecule 55: 60S ribosomal protein L19-A



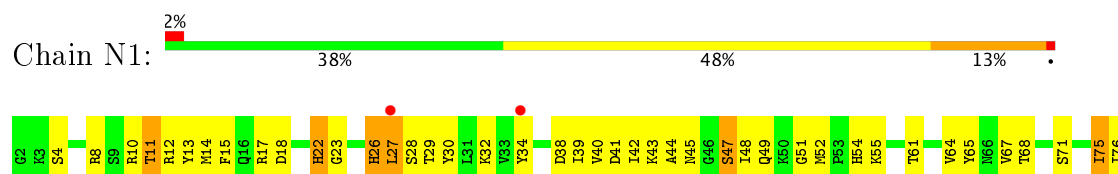
- Molecule 56: 60S ribosomal protein L20-A

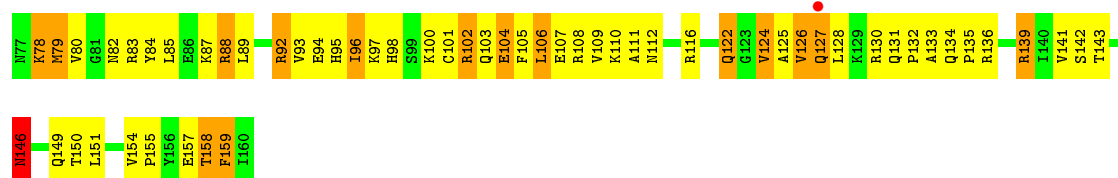


- Molecule 56: 60S ribosomal protein L20-A

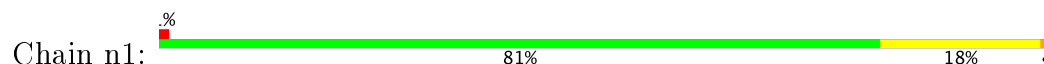


- Molecule 57: 60S ribosomal protein L21-A

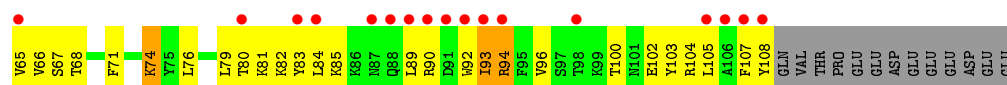




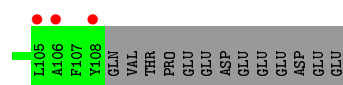
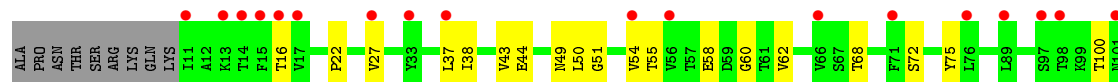
- Molecule 57: 60S ribosomal protein L21-A



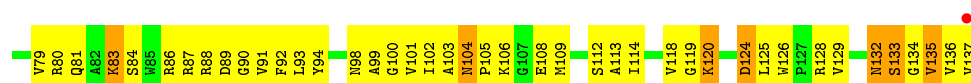
- Molecule 58: 60S ribosomal protein L22-A



- Molecule 58: 60S ribosomal protein L22-A

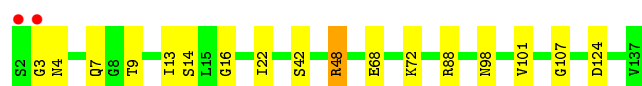


- Molecule 59: 60S ribosomal protein L23-A

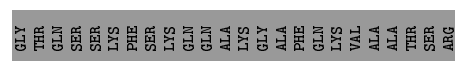
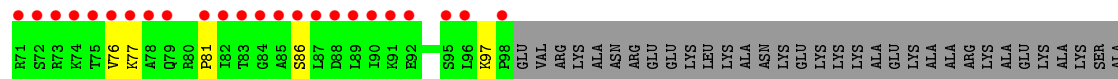
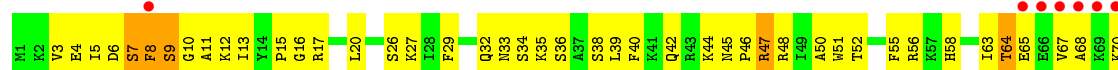


- Molecule 59: 60S ribosomal protein L23-A

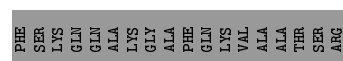
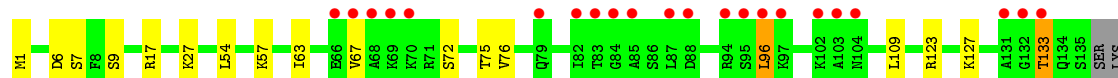
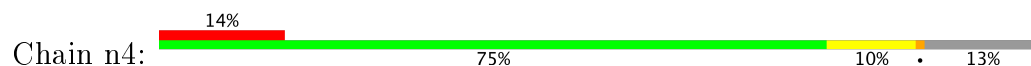




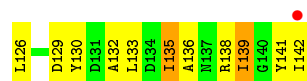
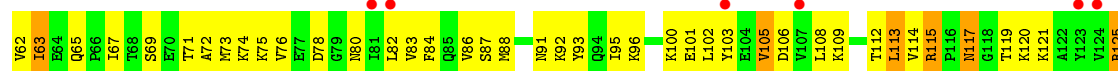
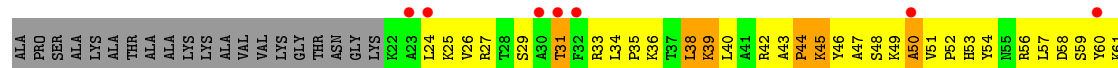
- Molecule 60: 60S ribosomal protein L24-A



- Molecule 60: 60S ribosomal protein L24-A



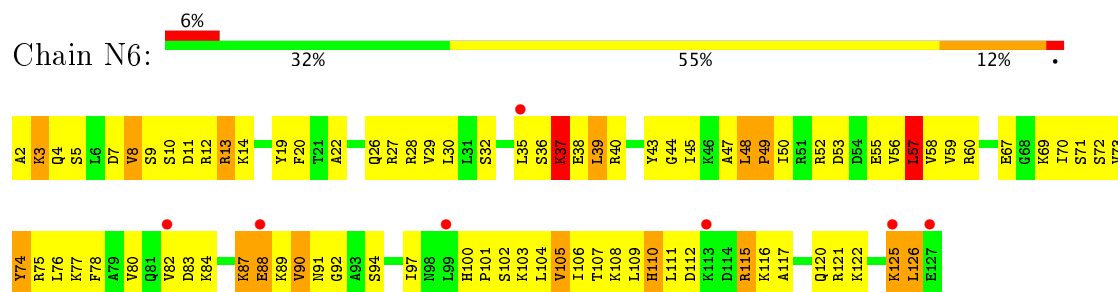
- Molecule 61: 60S ribosomal protein L25



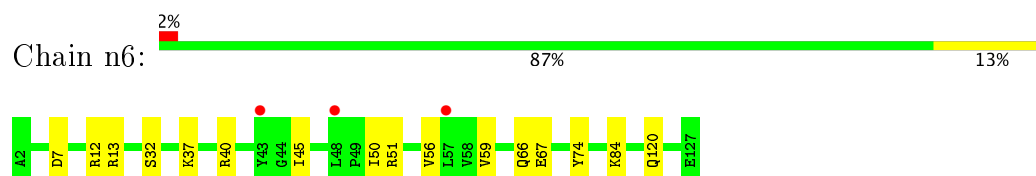
- Molecule 61: 60S ribosomal protein L25



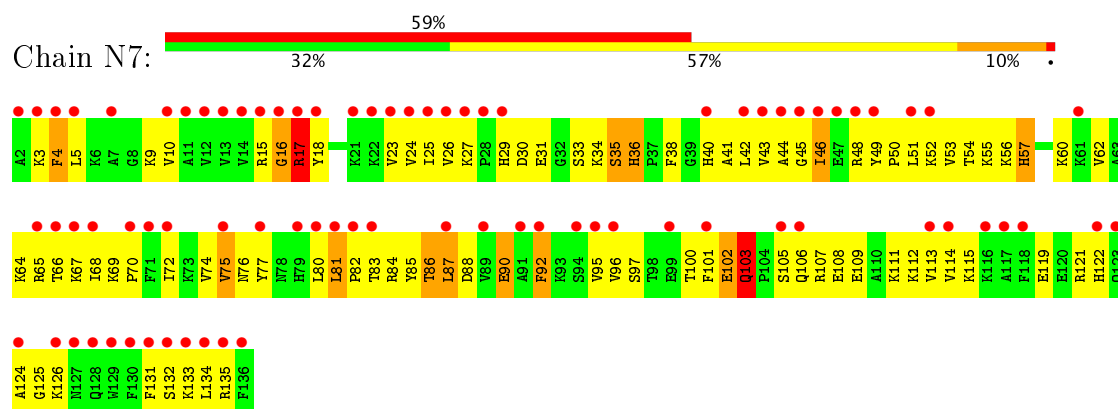
- Molecule 62: 60S ribosomal protein L26-A



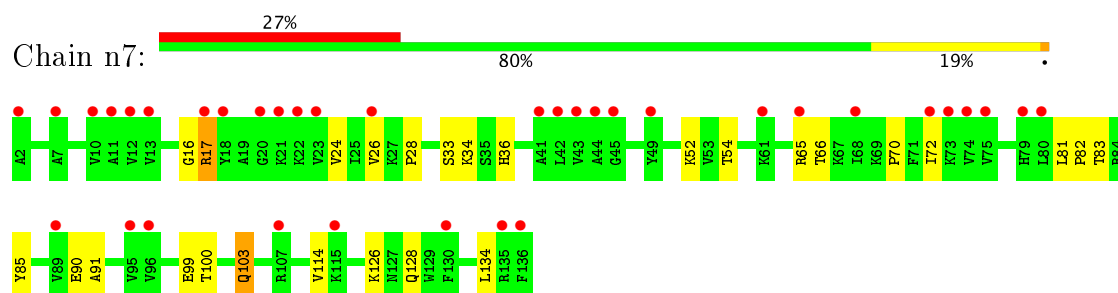
- Molecule 62: 60S ribosomal protein L26-A



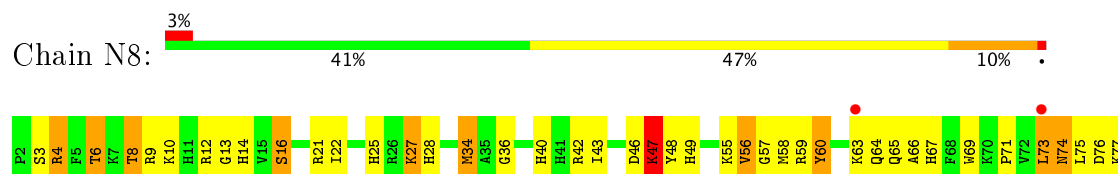
- Molecule 63: 60S ribosomal protein L27-A

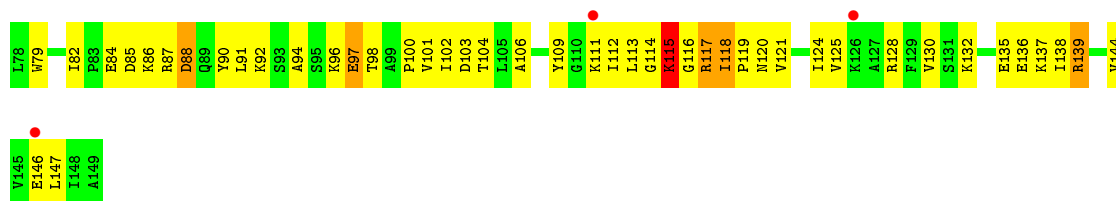


- Molecule 63: 60S ribosomal protein L27-A

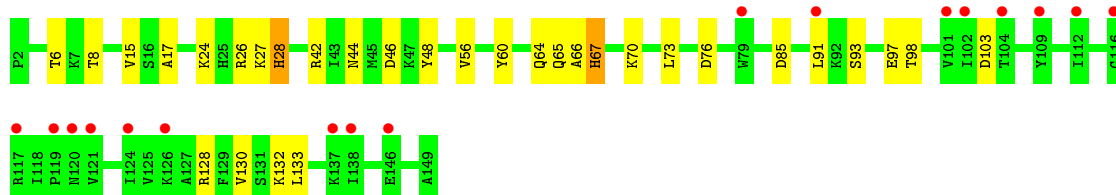
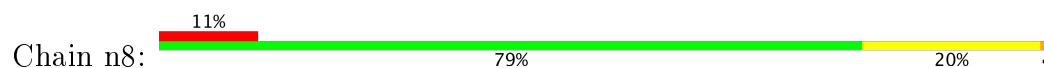


- Molecule 64: 60S ribosomal protein L28

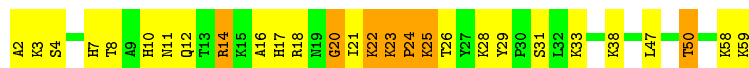




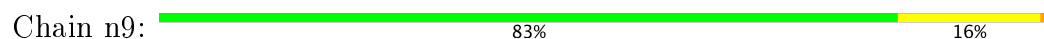
- Molecule 64: 60S ribosomal protein L28



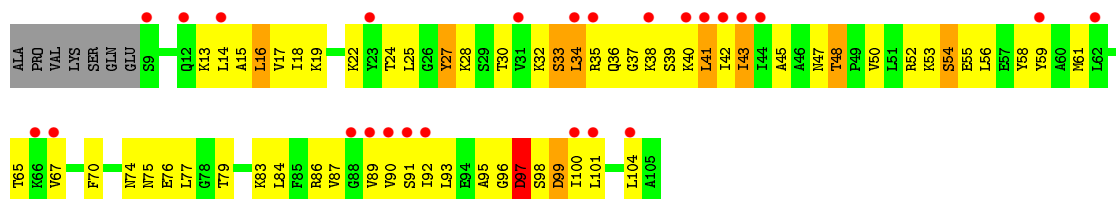
- Molecule 65: 60S ribosomal protein L29



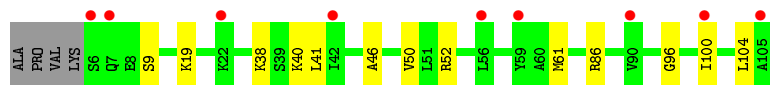
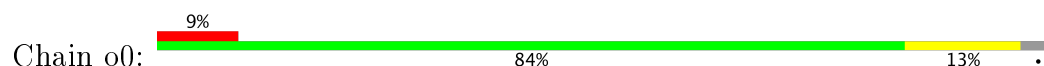
- Molecule 65: 60S ribosomal protein L29



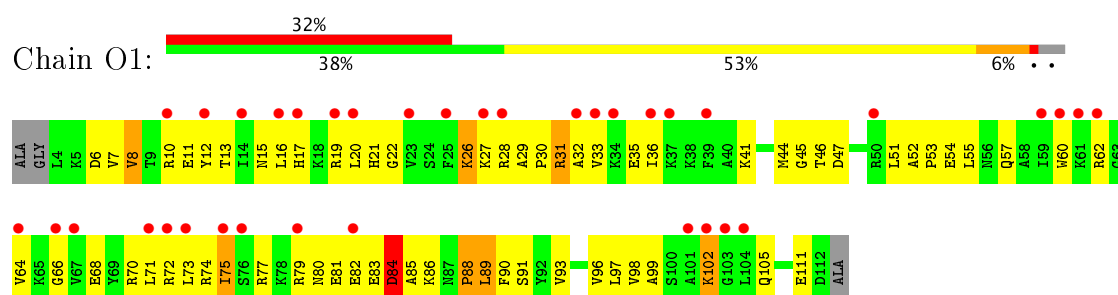
- Molecule 66: 60S ribosomal protein L30



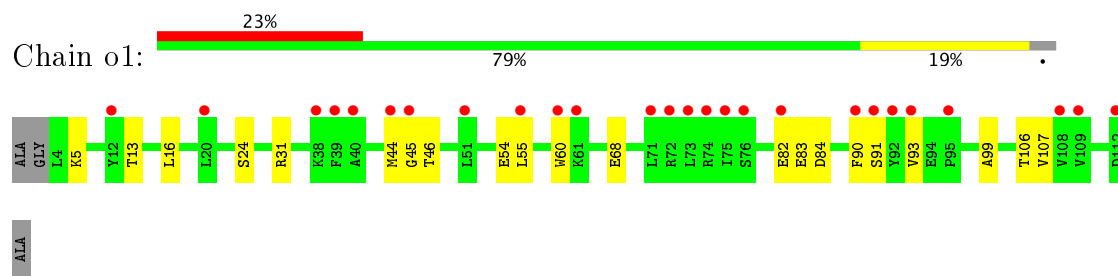
- Molecule 66: 60S ribosomal protein L30



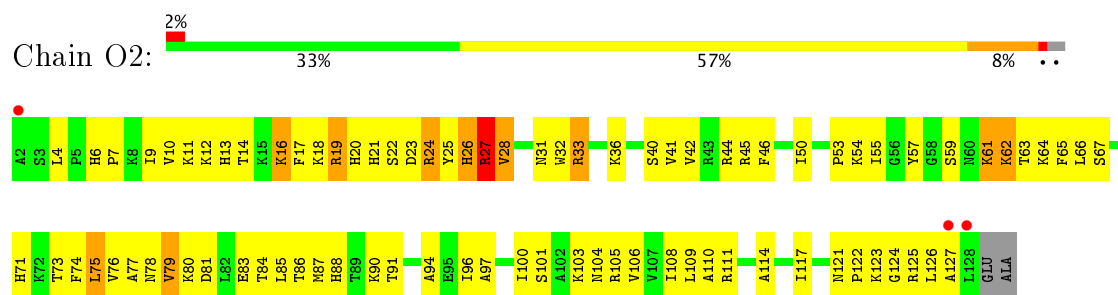
- Molecule 67: 60S ribosomal protein L31-A



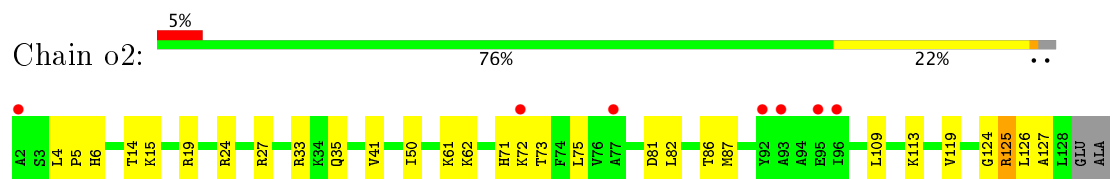
- Molecule 67: 60S ribosomal protein L31-A



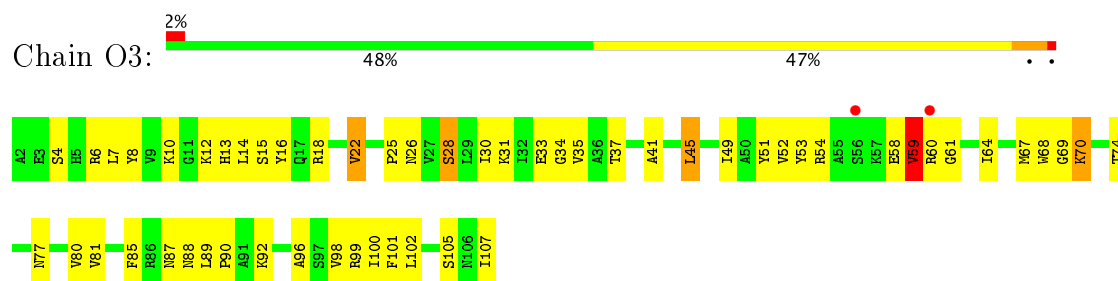
- Molecule 68: 60S ribosomal protein L32



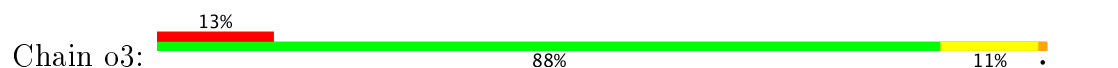
- Molecule 68: 60S ribosomal protein L32

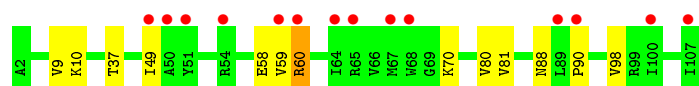


- Molecule 69: 60S ribosomal protein L33-A

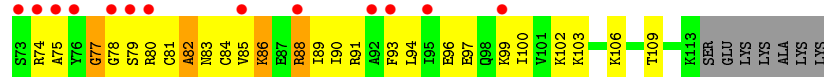
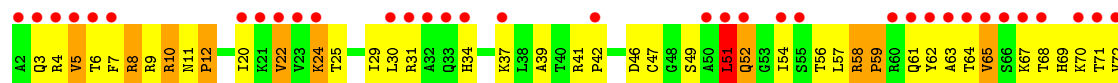


- Molecule 69: 60S ribosomal protein L33-A

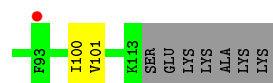
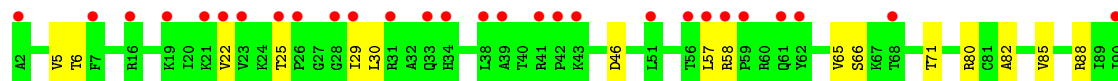
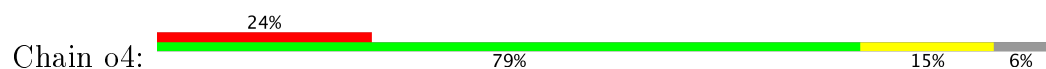




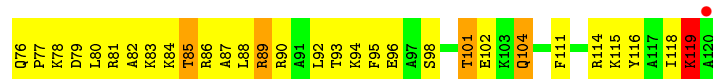
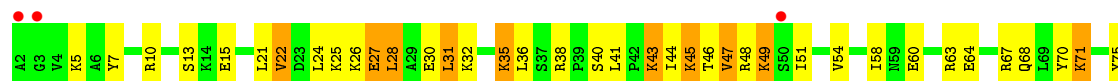
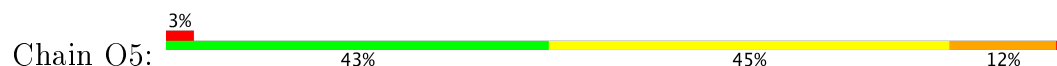
- Molecule 70: 60S ribosomal protein L34-A



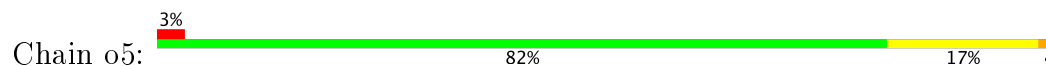
- Molecule 70: 60S ribosomal protein L34-A



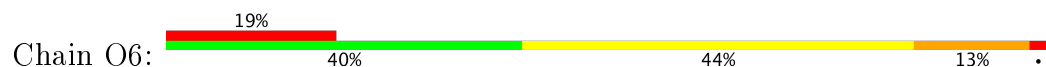
- Molecule 71: 60S ribosomal protein L35-A

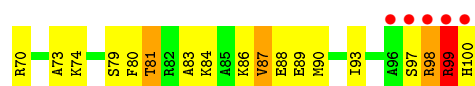


- Molecule 71: 60S ribosomal protein L35-A

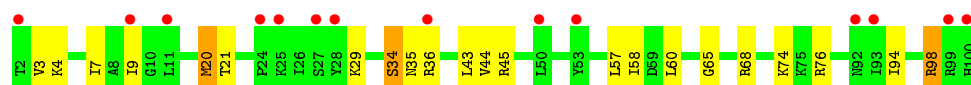
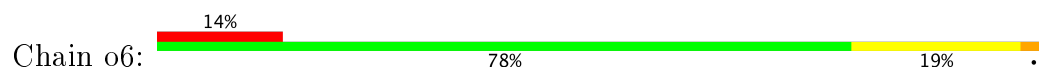


- Molecule 72: 60S ribosomal protein L36-A





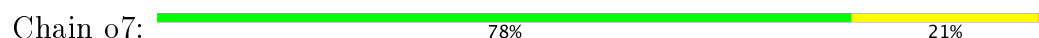
- Molecule 72: 60S ribosomal protein L36-A



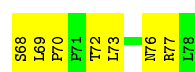
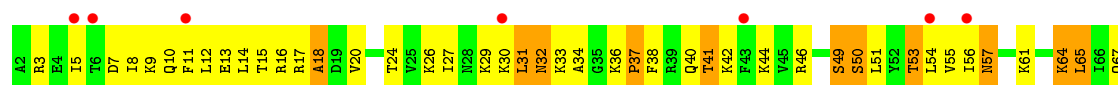
- Molecule 73: 60S ribosomal protein L37-A



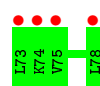
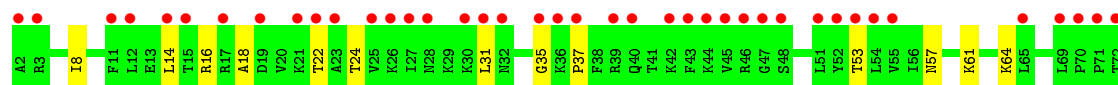
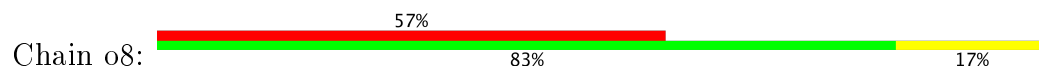
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38

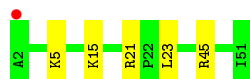
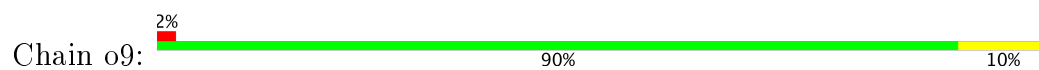


- Molecule 75: 60S ribosomal protein L39

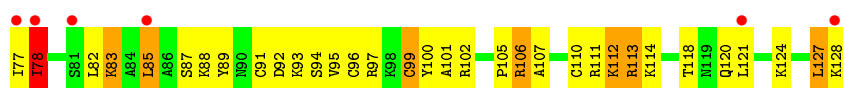




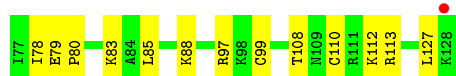
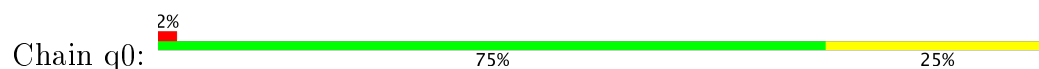
- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40



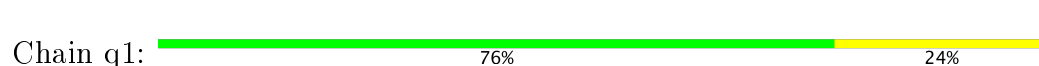
- Molecule 76: Ubiquitin-60S ribosomal protein L40



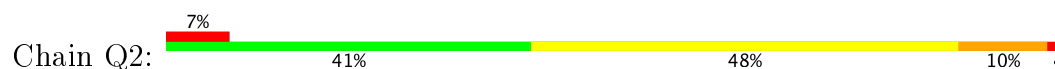
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 77: 60S ribosomal protein L41-A



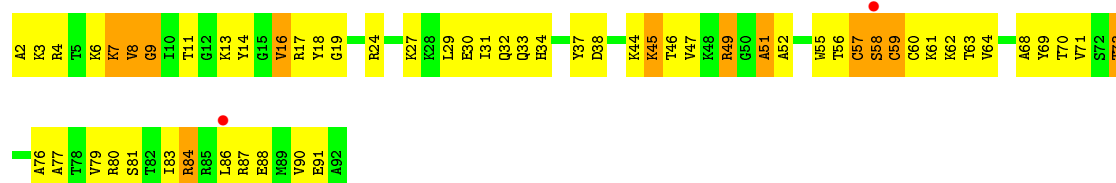
- Molecule 78: 60S ribosomal protein L42-A

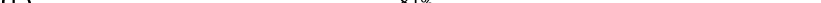


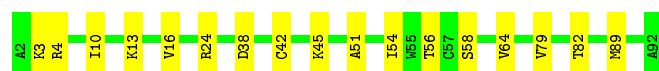
- Molecule 78: 60S ribosomal protein L42-A



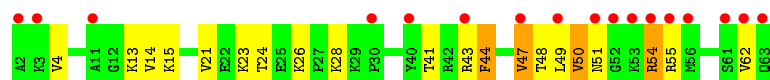
- Chain Q3: 

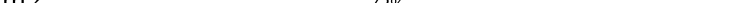


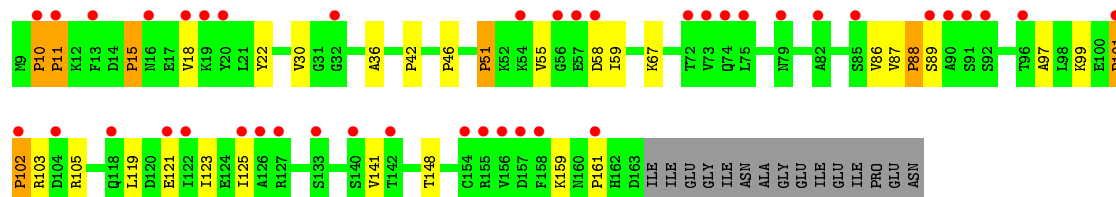
- Chain q3:  81% 19%




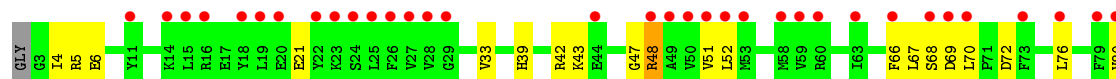
- Chain e0: 

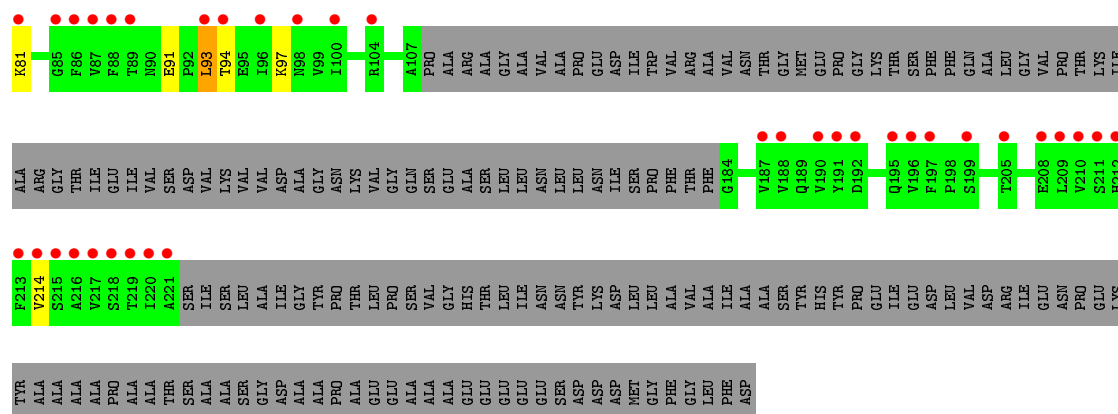


- Chain m2:  25% 72% 15% 9%

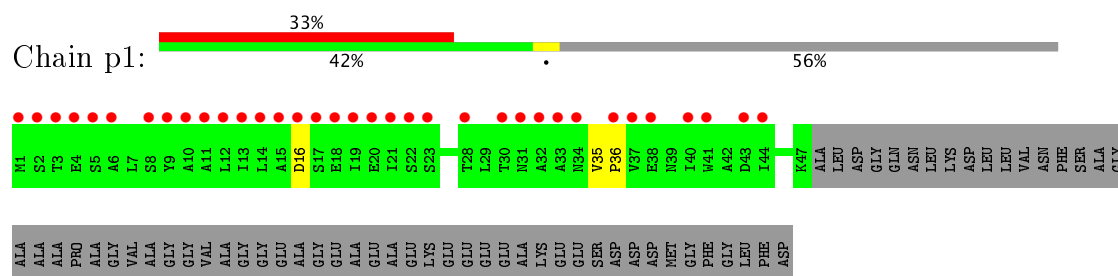


- Chain p0: 

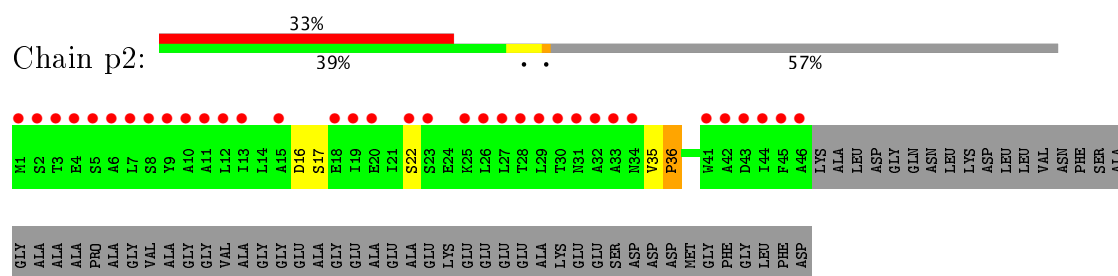




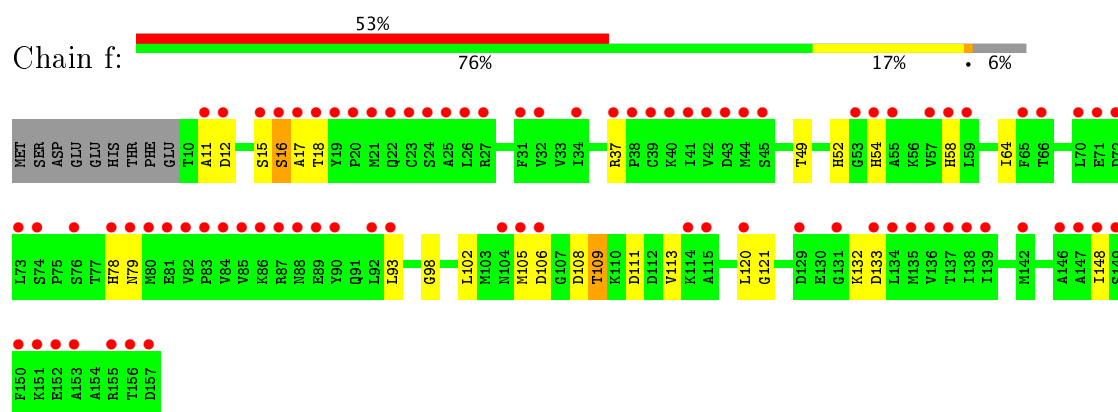
- Molecule 83: 60S acidic ribosomal protein P1-alpha



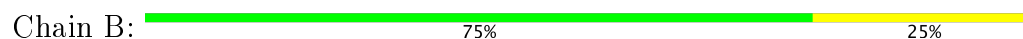
- Molecule 83: 60S acidic ribosomal protein P1-alpha



- Molecule 84: Eukaryotic translation initiation factor 5A-1




- Molecule 85: DNA (5'-R(*CP*CP*(NA))-3')





- Molecule 85: DNA (5'-R(*CP*CP*(NA))-3')

Chain C:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	438.00Å 289.05Å 305.26Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	122.88 – 3.45 123.03 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (122.88-3.45) 99.9 (123.03-3.45)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.207 , 0.263 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 92.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	413121	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 5CT, SPS, MG, OHX, 8AN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.44	0/42467	0.98	58/66169 (0.1%)
1	6	0.53	0/42790	1.04	77/66673 (0.1%)
2	S0	0.33	0/1617	0.55	0/2215
2	s0	0.36	0/1623	0.58	0/2222
3	S1	0.30	0/1735	0.53	1/2335 (0.0%)
3	s1	0.34	0/1748	0.56	0/2352
4	S2	0.34	0/1665	0.56	0/2263
4	s2	0.41	0/1665	0.63	0/2263
5	S3	0.33	0/1759	0.53	0/2368
5	s3	0.33	0/1759	0.50	0/2368
6	S4	0.34	0/2109	0.57	0/2839
6	s4	0.39	0/2109	0.62	0/2839
7	S5	0.31	0/1629	0.52	0/2202
7	s5	0.30	0/1629	0.51	0/2202
8	S6	0.34	0/1823	0.52	0/2439
8	s6	0.39	0/1779	0.61	0/2379
9	S7	0.32	0/1506	0.54	0/2028
9	s7	0.34	0/1516	0.57	0/2043
10	S8	0.36	0/1514	0.53	0/2021
10	s8	0.41	0/1514	0.58	0/2021
11	S9	0.33	0/1519	0.49	0/2035
11	s9	0.38	0/1519	0.57	0/2035
12	C0	0.31	0/790	0.54	1/1069 (0.1%)
12	c0	0.30	0/777	0.59	3/1049 (0.3%)
13	C1	0.38	0/1240	0.56	0/1675
13	c1	0.44	0/1194	0.61	0/1610
14	C2	0.29	0/900	0.51	0/1224
14	c2	0.25	0/900	0.48	0/1224
15	C3	0.35	0/1215	0.56	1/1638 (0.1%)
15	c3	0.37	0/1215	0.58	0/1638
16	C4	0.30	0/901	0.56	0/1217
16	c4	0.35	0/960	0.56	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.34	0/998	0.56	0/1341
17	c5	0.36	0/1060	0.57	0/1426
18	C6	0.32	0/1125	0.57	2/1510 (0.1%)
18	c6	0.34	0/1131	0.54	0/1518
19	C7	0.36	0/935	0.59	0/1254
19	c7	0.32	0/914	0.54	0/1224
20	C8	0.35	0/1211	0.54	1/1628 (0.1%)
20	c8	0.34	0/1211	0.57	1/1628 (0.1%)
21	C9	0.32	0/1130	0.52	0/1517
21	c9	0.33	0/1130	0.51	0/1517
22	D0	0.32	0/865	0.55	0/1169
22	d0	0.35	0/892	0.54	0/1205
23	D1	0.34	0/693	0.53	0/935
23	d1	0.37	0/693	0.61	0/935
24	D2	0.34	0/1038	0.61	1/1395 (0.1%)
24	d2	0.41	0/1038	0.62	0/1395
25	D3	0.39	0/1139	0.59	0/1518
25	d3	0.45	0/1139	0.62	0/1518
26	D4	0.34	0/1087	0.50	0/1449
26	d4	0.39	0/1087	0.62	0/1449
27	D5	0.32	0/571	0.57	0/768
27	d5	0.33	0/566	0.53	0/761
28	D6	0.33	0/782	0.54	0/1047
28	d6	0.38	0/782	0.58	0/1047
29	D7	0.32	0/620	0.52	0/838
29	d7	0.36	0/620	0.57	0/838
30	D8	0.29	0/499	0.51	0/670
30	d8	0.32	0/499	0.57	0/670
31	D9	0.40	0/452	0.57	0/600
31	d9	0.35	0/452	0.52	0/600
32	E0	0.32	0/483	0.49	0/643
33	E1	0.35	0/577	0.61	0/770
33	e1	0.34	0/619	0.61	0/822
34	SR	0.29	0/2489	0.51	0/3389
34	sR	0.28	0/2494	0.49	0/3395
35	SM	0.38	0/1113	0.57	2/1502 (0.1%)
35	sM	0.34	0/683	0.55	1/923 (0.1%)
36	1	0.66	6/75394 (0.0%)	1.15	212/117545 (0.2%)
36	5	0.71	8/75414 (0.0%)	1.18	277/117575 (0.2%)
37	3	0.57	0/2883	1.03	1/4491 (0.0%)
37	7	0.69	0/2883	1.15	7/4491 (0.2%)
38	4	0.60	0/3746	1.07	5/5832 (0.1%)
38	8	0.60	0/3746	1.08	7/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.43	0/1948	0.62	0/2617
39	l2	0.45	0/1946	0.65	0/2614
40	L3	0.46	0/3146	0.63	0/4228
40	l3	0.53	0/3146	0.63	0/4228
41	L4	0.49	0/2800	0.67	0/3790
41	l4	0.47	0/2800	0.66	0/3790
42	L5	0.41	0/2425	0.57	0/3271
42	l5	0.51	0/2408	0.64	1/3248 (0.0%)
43	L6	0.45	0/1260	0.61	0/1694
43	l6	0.47	0/1269	0.61	0/1705
44	L7	0.49	0/1821	0.64	1/2451 (0.0%)
44	l7	0.52	0/1828	0.65	1/2461 (0.0%)
45	L8	0.36	0/1836	0.54	0/2481
45	l8	0.38	0/1796	0.57	0/2431
46	L9	0.43	0/1539	0.60	0/2073
46	l9	0.51	0/1539	0.64	0/2073
47	M0	0.45	0/1741	0.58	0/2335
47	m0	0.51	0/1758	0.65	0/2358
48	M1	0.37	0/1374	0.57	0/1842
48	m1	0.45	0/1374	0.60	0/1842
49	M3	0.44	0/1568	0.65	0/2106
49	m3	0.46	0/1573	0.61	0/2113
50	M4	0.44	0/1068	0.59	0/1438
50	m4	0.49	0/1074	0.64	0/1446
51	M5	0.46	0/1757	0.59	0/2354
51	m5	0.44	0/1757	0.58	0/2354
52	M6	0.53	0/1585	0.54	0/2128
52	m6	0.62	0/1585	0.57	0/2128
53	M7	0.48	0/1443	0.62	0/1944
53	m7	0.54	0/1250	0.63	0/1683
54	M8	0.48	0/1465	0.65	0/1965
54	m8	0.47	0/1465	0.67	0/1965
55	M9	0.37	0/1538	0.54	0/2050
55	m9	0.40	0/1538	0.55	0/2050
56	N0	0.46	0/1481	0.61	1/1990 (0.1%)
56	n0	0.54	0/1481	0.65	0/1990
57	N1	0.45	0/1300	0.60	0/1743
57	n1	0.53	0/1300	0.59	0/1743
58	N2	0.35	0/812	0.55	0/1099
58	n2	0.39	0/794	0.58	0/1076
59	N3	0.46	0/1018	0.59	0/1369
59	n3	0.54	0/1018	0.69	1/1369 (0.1%)
60	N4	0.37	0/712	0.55	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.44	0/1052	0.60	0/1398
61	N5	0.40	0/979	0.59	0/1321
61	n5	0.41	0/974	0.62	0/1314
62	N6	0.43	0/1004	0.63	1/1341 (0.1%)
62	n6	0.42	0/1004	0.60	0/1341
63	N7	0.36	0/1118	0.56	0/1497
63	n7	0.38	0/1118	0.52	0/1497
64	N8	0.47	0/1204	0.68	0/1612
64	n8	0.49	0/1204	0.66	1/1612 (0.1%)
65	N9	0.45	0/473	0.67	0/629
65	n9	0.53	0/473	0.74	0/629
66	O0	0.33	0/750	0.54	0/1008
66	o0	0.38	0/774	0.59	0/1040
67	O1	0.41	0/890	0.57	0/1196
67	o1	0.49	0/897	0.67	0/1205
68	O2	0.51	0/1041	0.62	0/1394
68	o2	0.52	0/1041	0.66	0/1394
69	O3	0.55	0/868	0.63	0/1168
69	o3	0.54	0/868	0.63	0/1168
70	O4	0.39	0/890	0.60	1/1189 (0.1%)
70	o4	0.44	0/890	0.59	0/1189
71	O5	0.43	0/978	0.61	0/1301
71	o5	0.41	0/974	0.59	0/1297
72	O6	0.40	0/778	0.59	0/1034
72	o6	0.42	0/777	0.61	0/1033
73	O7	0.48	0/696	0.70	0/923
73	o7	0.46	0/696	0.65	1/923 (0.1%)
74	O8	0.34	0/618	0.52	0/826
74	o8	0.38	0/614	0.60	0/822
75	O9	0.48	0/443	0.64	0/588
75	o9	0.45	0/443	0.63	0/588
76	Q0	0.48	0/423	0.72	0/562
76	q0	0.55	0/423	0.65	0/562
77	Q1	0.43	0/234	0.55	0/300
77	q1	0.50	0/234	0.65	0/300
78	Q2	0.61	1/860 (0.1%)	0.72	1/1136 (0.1%)
78	q2	0.58	1/860 (0.1%)	0.67	1/1136 (0.1%)
79	Q3	0.46	0/701	0.65	0/934
79	q3	0.50	0/701	0.61	0/934
80	e0	0.38	0/499	0.62	0/665
81	m2	0.34	0/736	0.76	10/1019 (1.0%)
82	p0	0.30	0/1092	0.52	0/1474
83	p1	0.29	0/234	0.49	1/326 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
83	p2	0.31	0/229	0.46	1/319 (0.3%)
84	f	0.40	0/1121	0.61	0/1508
85	B	0.66	0/47	1.57	0/68
85	C	0.58	0/50	1.12	0/72
All	All	0.54	16/433278 (0.0%)	0.94	681/635910 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	s7	0	1
16	C4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	1
39	L2	0	2
40	l3	0	1
52	M6	0	1
53	m7	0	1
56	n0	0	1
65	N9	0	1
84	f	1	0
All	All	1	12

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	9.97	1.99	1.82
78	q2	17	CYS	CB-SG	8.34	1.96	1.82
36	5	1152	G	N9-C4	-6.27	1.32	1.38
36	5	2401	A	N9-C4	6.26	1.41	1.37
36	5	2860	U	N1-C2	5.96	1.44	1.38

The worst 5 of 681 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-11.84	118.90	126.00
36	5	2355	G	N1-C6-O6	11.18	126.61	119.90
1	6	321	C	N1-C2-O2	11.14	125.58	118.90
36	5	1152	G	N3-C4-C5	11.03	134.11	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1897	G	N1-C6-O6	10.10	125.96	119.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
84	f	51	5CT	C2

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
19	C7	85	VAL	Peptide
39	L2	142	ASP	Peptide
39	L2	19	HIS	Peptide
52	M6	110	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37970	0	19106	870	0
1	6	38260	0	19250	844	0
2	S0	1577	0	1567	157	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	145	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	145	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	131	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	177	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	129	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	114	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	107	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	143	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	62	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	67	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	59	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	94	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	84	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	74	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	106	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	70	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	94	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	82	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	75	0
22	d0	882	0	939	0	0
23	D1	684	0	672	85	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	87	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	88	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	78	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	45	0
27	d5	558	0	598	0	0
28	D6	769	0	814	80	0
28	d6	769	0	814	0	0
29	D7	610	0	630	41	0
29	d7	610	0	631	0	0
30	D8	497	0	535	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d8	497	0	535	0	0
31	D9	442	0	428	28	0
31	d9	442	0	428	0	0
32	E0	475	0	525	38	0
33	E1	566	0	601	53	0
33	e1	608	0	656	0	0
34	SR	2436	0	2386	145	0
34	sR	2441	0	2392	0	0
35	SM	1104	0	996	53	0
35	sM	680	0	607	0	0
36	1	67355	0	33846	1384	0
36	5	67376	0	33856	1308	0
37	3	2579	0	1304	58	0
37	7	2579	0	1304	51	0
38	4	3353	0	1695	81	0
38	8	3353	0	1695	77	0
39	L2	1914	0	1981	167	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	262	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	227	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	201	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	95	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	139	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1875	110	0
45	l8	1764	0	1821	0	0
46	L9	1518	0	1587	113	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	176	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	85	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	107	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	104	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	143	0
51	m5	1720	0	1779	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	M6	1555	0	1659	90	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	113	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	90	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1616	121	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	104	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	93	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	50	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	81	0
59	n3	1003	0	1047	0	0
60	N4	699	0	640	31	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	75	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	93	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	96	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	96	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	29	0
65	n9	462	0	491	0	0
66	O0	742	0	797	50	0
66	o0	766	0	816	0	0
67	O1	876	0	912	49	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	70	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	48	0
69	o3	850	0	880	0	0
70	O4	880	0	945	78	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	80	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	55	0
72	o6	770	0	846	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	O7	681	0	683	53	0
73	o7	681	0	683	0	0
74	O8	612	0	682	43	0
74	o8	608	0	671	0	0
75	O9	436	0	475	49	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	28	0
76	q0	417	0	456	0	0
77	Q1	233	0	284	23	0
77	q1	233	0	284	0	0
78	Q2	847	0	914	54	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	69	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	739	0	343	0	0
82	p0	1077	0	1041	0	0
83	p1	235	0	119	0	0
83	p2	230	0	117	0	0
84	f	1122	0	1115	0	0
85	B	66	0	41	0	0
85	C	69	0	40	1	0
86	1	366	0	0	0	0
86	2	90	0	0	0	0
86	3	8	0	0	0	0
86	4	15	0	0	0	0
86	5	419	0	0	0	0
86	6	113	0	0	0	0
86	7	13	0	0	0	0
86	8	9	0	0	0	0
86	B	1	0	0	0	0
86	C	1	0	0	0	0
86	D3	1	0	0	0	0
86	L2	2	0	0	0	0
86	L3	1	0	0	0	0
86	L6	1	0	0	0	0
86	L7	3	0	0	0	0
86	M0	1	0	0	0	0
86	M5	1	0	0	0	0
86	M6	2	0	0	0	0
86	M7	4	0	0	0	0
86	M9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	N3	1	0	0	0	0
86	N6	1	0	0	0	0
86	N8	1	0	0	0	0
86	O3	1	0	0	0	0
86	O4	1	0	0	0	0
86	O7	1	0	0	0	0
86	Q2	1	0	0	0	0
86	S2	1	0	0	0	0
86	SM	1	0	0	0	0
86	c8	1	0	0	0	0
86	d2	1	0	0	0	0
86	d3	1	0	0	0	0
86	d6	1	0	0	0	0
86	f	1	0	0	0	0
86	l2	2	0	0	0	0
86	l3	2	0	0	0	0
86	l4	1	0	0	0	0
86	l5	1	0	0	0	0
86	l7	2	0	0	0	0
86	m3	1	0	0	0	0
86	m5	2	0	0	0	0
86	m7	2	0	0	0	0
86	n0	1	0	0	0	0
86	n3	1	0	0	0	0
86	n6	1	0	0	0	0
86	n8	2	0	0	0	0
86	o2	1	0	0	0	0
86	o3	1	0	0	0	0
86	o4	1	0	0	0	0
86	q1	1	0	0	0	0
86	q3	1	0	0	0	0
86	s4	1	0	0	0	0
86	s8	2	0	0	0	0
86	sM	1	0	0	0	0
87	1	2457	0	0	236	0
87	2	1134	0	0	124	0
87	3	77	0	0	3	0
87	4	126	0	0	14	0
87	5	2492	0	0	243	0
87	6	1204	0	0	118	0
87	7	77	0	0	4	0
87	8	147	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	C3	7	0	0	3	0
87	C5	7	0	0	5	0
87	C8	7	0	0	0	0
87	D9	7	0	0	0	0
87	L3	21	0	0	3	0
87	L4	7	0	0	3	0
87	L5	7	0	0	1	0
87	M0	14	0	0	7	0
87	M5	14	0	0	2	0
87	M6	7	0	0	0	0
87	M7	7	0	0	1	0
87	M8	7	0	0	0	0
87	M9	7	0	0	1	0
87	N8	7	0	0	0	0
87	N9	7	0	0	2	0
87	O1	7	0	0	2	0
87	O3	7	0	0	1	0
87	O4	7	0	0	2	0
87	O7	7	0	0	6	0
87	O9	7	0	0	1	0
87	Q2	7	0	0	2	0
87	S1	7	0	0	3	0
87	S6	7	0	0	3	0
87	S8	7	0	0	1	0
87	S9	7	0	0	4	0
87	SR	7	0	0	5	0
87	c3	7	0	0	0	0
87	c5	14	0	0	0	0
87	c8	7	0	0	0	0
87	d4	7	0	0	0	0
87	d9	7	0	0	0	0
87	l3	14	0	0	0	0
87	l4	14	0	0	0	0
87	l5	14	0	0	0	0
87	l9	7	0	0	0	0
87	m0	14	0	0	0	0
87	m1	7	0	0	0	0
87	m4	7	0	0	0	0
87	m5	21	0	0	0	0
87	m6	7	0	0	0	0
87	m7	7	0	0	0	0
87	m8	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	m9	7	0	0	0	0
87	n3	7	0	0	0	0
87	n9	7	0	0	0	0
87	o3	7	0	0	0	0
87	o6	7	0	0	0	0
87	o7	14	0	0	0	0
87	q2	7	0	0	0	0
87	s1	14	0	0	0	0
87	s4	7	0	0	0	0
87	s8	7	0	0	0	0
87	s9	7	0	0	0	0
87	sR	7	0	0	0	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	1	0
88	Q2	1	0	0	0	0
88	Q3	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
89	5	23	0	18	6	0
89	B	23	0	18	2	0
90	B	7	0	7	0	0
90	C	7	0	7	0	0
91	5	6	0	0	0	0
91	f	6	0	0	0	0
All	All	413121	0	299176	9881	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 14.

The worst 5 of 9881 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)
36:1:2208:A:N1	87:1:3940:OHX:N6	2.03	1.05
36:1:2403:G:OP2	87:1:4071:OHX:N5	1.95	0.99
73:O7:87:SER:O	87:O7:103:OHX:N3	1.96	0.98
36:1:860:G:OP1	79:Q3:17:ARG:NH1	1.98	0.96
36:1:2392:C:O2'	40:L3:266:ARG:NH2	1.98	0.96

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	204/251 (81%)	157 (77%)	34 (17%)	13 (6%)	1	17
2	s0	204/251 (81%)	148 (72%)	31 (15%)	25 (12%)	0	5
3	S1	212/254 (84%)	154 (73%)	38 (18%)	20 (9%)	1	9
3	s1	214/254 (84%)	169 (79%)	30 (14%)	15 (7%)	1	14
4	S2	215/253 (85%)	169 (79%)	36 (17%)	10 (5%)	3	25
4	s2	215/253 (85%)	172 (80%)	25 (12%)	18 (8%)	1	11
5	S3	221/239 (92%)	186 (84%)	24 (11%)	11 (5%)	2	23
5	s3	221/239 (92%)	172 (78%)	36 (16%)	13 (6%)	2	19
6	S4	258/260 (99%)	197 (76%)	44 (17%)	17 (7%)	1	16
6	s4	258/260 (99%)	200 (78%)	42 (16%)	16 (6%)	2	18
7	S5	204/224 (91%)	153 (75%)	35 (17%)	16 (8%)	1	12
7	s5	204/224 (91%)	150 (74%)	41 (20%)	13 (6%)	1	17
8	S6	224/236 (95%)	189 (84%)	23 (10%)	12 (5%)	2	21
8	s6	216/236 (92%)	176 (82%)	32 (15%)	8 (4%)	4	32
9	S7	182/189 (96%)	127 (70%)	39 (21%)	16 (9%)	1	10
9	s7	184/189 (97%)	141 (77%)	29 (16%)	14 (8%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	S8	184/200 (92%)	150 (82%)	25 (14%)	9 (5%)	2	23
10	s8	184/200 (92%)	151 (82%)	27 (15%)	6 (3%)	4	34
11	S9	183/196 (93%)	148 (81%)	27 (15%)	8 (4%)	3	27
11	s9	183/196 (93%)	141 (77%)	33 (18%)	9 (5%)	2	23
12	C0	94/105 (90%)	69 (73%)	16 (17%)	9 (10%)	1	9
12	c0	92/105 (88%)	63 (68%)	14 (15%)	15 (16%)	0	2
13	C1	153/155 (99%)	122 (80%)	21 (14%)	10 (6%)	1	16
13	c1	144/155 (93%)	120 (83%)	19 (13%)	5 (4%)	4	33
14	C2	122/142 (86%)	71 (58%)	33 (27%)	18 (15%)	0	3
14	c2	122/142 (86%)	78 (64%)	30 (25%)	14 (12%)	0	6
15	C3	148/150 (99%)	120 (81%)	17 (12%)	11 (7%)	1	13
15	c3	148/150 (99%)	116 (78%)	20 (14%)	12 (8%)	1	11
16	C4	125/136 (92%)	89 (71%)	24 (19%)	12 (10%)	1	9
16	c4	126/136 (93%)	96 (76%)	16 (13%)	14 (11%)	0	7
17	C5	122/141 (86%)	99 (81%)	13 (11%)	10 (8%)	1	11
17	c5	133/141 (94%)	86 (65%)	38 (29%)	9 (7%)	1	16
18	C6	139/142 (98%)	118 (85%)	13 (9%)	8 (6%)	2	19
18	c6	140/142 (99%)	118 (84%)	13 (9%)	9 (6%)	1	17
19	C7	116/136 (85%)	90 (78%)	18 (16%)	8 (7%)	1	15
19	c7	113/136 (83%)	86 (76%)	18 (16%)	9 (8%)	1	12
20	C8	143/145 (99%)	111 (78%)	25 (18%)	7 (5%)	2	23
20	c8	143/145 (99%)	117 (82%)	19 (13%)	7 (5%)	2	23
21	C9	141/143 (99%)	116 (82%)	18 (13%)	7 (5%)	2	23
21	c9	141/143 (99%)	116 (82%)	21 (15%)	4 (3%)	6	38
22	D0	105/120 (88%)	89 (85%)	12 (11%)	4 (4%)	4	30
22	d0	108/120 (90%)	90 (83%)	13 (12%)	5 (5%)	3	25
23	D1	85/87 (98%)	64 (75%)	8 (9%)	13 (15%)	0	3
23	d1	85/87 (98%)	61 (72%)	17 (20%)	7 (8%)	1	11
24	D2	127/129 (98%)	106 (84%)	16 (13%)	5 (4%)	3	30
24	d2	127/129 (98%)	107 (84%)	17 (13%)	3 (2%)	7	42
25	D3	142/144 (99%)	104 (73%)	22 (16%)	16 (11%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	d3	142/144 (99%)	117 (82%)	24 (17%)	1 (1%)	25	67
26	D4	132/134 (98%)	106 (80%)	16 (12%)	10 (8%)	1	12
26	d4	132/134 (98%)	101 (76%)	20 (15%)	11 (8%)	1	11
27	D5	68/107 (64%)	50 (74%)	12 (18%)	6 (9%)	1	10
27	d5	67/107 (63%)	49 (73%)	16 (24%)	2 (3%)	5	36
28	D6	95/97 (98%)	57 (60%)	24 (25%)	14 (15%)	0	3
28	d6	95/97 (98%)	69 (73%)	14 (15%)	12 (13%)	0	5
29	D7	79/81 (98%)	69 (87%)	7 (9%)	3 (4%)	4	30
29	d7	79/81 (98%)	57 (72%)	16 (20%)	6 (8%)	1	12
30	D8	61/66 (92%)	47 (77%)	10 (16%)	4 (7%)	1	16
30	d8	61/66 (92%)	41 (67%)	11 (18%)	9 (15%)	0	3
31	D9	51/55 (93%)	37 (72%)	11 (22%)	3 (6%)	2	19
31	d9	51/55 (93%)	40 (78%)	8 (16%)	3 (6%)	2	19
32	E0	58/60 (97%)	41 (71%)	15 (26%)	2 (3%)	4	34
33	E1	69/76 (91%)	38 (55%)	19 (28%)	12 (17%)	0	2
33	e1	74/76 (97%)	39 (53%)	12 (16%)	23 (31%)	0	0
34	SR	316/318 (99%)	260 (82%)	43 (14%)	13 (4%)	3	29
34	sR	316/318 (99%)	264 (84%)	38 (12%)	14 (4%)	3	27
35	SM	155/273 (57%)	107 (69%)	32 (21%)	16 (10%)	0	8
35	sM	98/273 (36%)	66 (67%)	23 (24%)	9 (9%)	1	9
39	L2	250/253 (99%)	217 (87%)	23 (9%)	10 (4%)	3	29
39	l2	250/253 (99%)	204 (82%)	33 (13%)	13 (5%)	2	21
40	L3	384/386 (100%)	315 (82%)	46 (12%)	23 (6%)	2	18
40	l3	384/386 (100%)	337 (88%)	35 (9%)	12 (3%)	5	36
41	L4	359/361 (99%)	285 (79%)	52 (14%)	22 (6%)	2	18
41	l4	359/361 (99%)	288 (80%)	53 (15%)	18 (5%)	2	23
42	L5	294/296 (99%)	229 (78%)	42 (14%)	23 (8%)	1	12
42	l5	292/296 (99%)	250 (86%)	35 (12%)	7 (2%)	7	42
43	L6	152/175 (87%)	132 (87%)	17 (11%)	3 (2%)	9	45
43	l6	153/175 (87%)	123 (80%)	25 (16%)	5 (3%)	4	34
44	L7	220/243 (90%)	173 (79%)	39 (18%)	8 (4%)	4	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	l7	221/243 (91%)	193 (87%)	23 (10%)	5 (2%)	7	43
45	L8	231/255 (91%)	184 (80%)	38 (16%)	9 (4%)	3	30
45	l8	229/255 (90%)	167 (73%)	48 (21%)	14 (6%)	2	18
46	L9	189/191 (99%)	159 (84%)	19 (10%)	11 (6%)	2	19
46	l9	189/191 (99%)	163 (86%)	21 (11%)	5 (3%)	6	39
47	M0	207/220 (94%)	167 (81%)	31 (15%)	9 (4%)	3	27
47	m0	209/220 (95%)	165 (79%)	33 (16%)	11 (5%)	2	21
48	M1	167/173 (96%)	134 (80%)	19 (11%)	14 (8%)	1	11
48	m1	167/173 (96%)	137 (82%)	19 (11%)	11 (7%)	1	16
49	M3	191/198 (96%)	153 (80%)	27 (14%)	11 (6%)	2	19
49	m3	192/198 (97%)	153 (80%)	24 (12%)	15 (8%)	1	12
50	M4	134/137 (98%)	114 (85%)	15 (11%)	5 (4%)	4	32
50	m4	135/137 (98%)	115 (85%)	16 (12%)	4 (3%)	5	36
51	M5	201/203 (99%)	176 (88%)	19 (10%)	6 (3%)	5	36
51	m5	201/203 (99%)	174 (87%)	23 (11%)	4 (2%)	9	45
52	M6	195/198 (98%)	173 (89%)	16 (8%)	6 (3%)	5	36
52	m6	195/198 (98%)	182 (93%)	9 (5%)	4 (2%)	8	44
53	M7	181/183 (99%)	150 (83%)	25 (14%)	6 (3%)	4	34
53	m7	153/183 (84%)	127 (83%)	25 (16%)	1 (1%)	25	67
54	M8	183/185 (99%)	151 (82%)	24 (13%)	8 (4%)	3	27
54	m8	183/185 (99%)	154 (84%)	20 (11%)	9 (5%)	2	23
55	M9	186/188 (99%)	160 (86%)	23 (12%)	3 (2%)	11	50
55	m9	186/188 (99%)	166 (89%)	13 (7%)	7 (4%)	4	30
56	N0	170/172 (99%)	155 (91%)	12 (7%)	3 (2%)	10	47
56	n0	170/172 (99%)	152 (89%)	15 (9%)	3 (2%)	10	47
57	N1	157/159 (99%)	137 (87%)	15 (10%)	5 (3%)	5	35
57	n1	157/159 (99%)	131 (83%)	24 (15%)	2 (1%)	14	54
58	N2	98/120 (82%)	72 (74%)	23 (24%)	3 (3%)	5	36
58	n2	96/120 (80%)	80 (83%)	11 (12%)	5 (5%)	2	21
59	N3	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	12	51
59	n3	134/136 (98%)	122 (91%)	7 (5%)	5 (4%)	4	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	N4	96/155 (62%)	68 (71%)	18 (19%)	10 (10%)	0	7
60	n4	133/155 (86%)	102 (77%)	22 (16%)	9 (7%)	1	16
61	N5	119/141 (84%)	99 (83%)	14 (12%)	6 (5%)	2	23
61	n5	118/141 (84%)	94 (80%)	19 (16%)	5 (4%)	3	28
62	N6	124/126 (98%)	107 (86%)	13 (10%)	4 (3%)	5	35
62	n6	124/126 (98%)	102 (82%)	21 (17%)	1 (1%)	22	65
63	N7	133/135 (98%)	114 (86%)	10 (8%)	9 (7%)	1	16
63	n7	133/135 (98%)	112 (84%)	12 (9%)	9 (7%)	1	16
64	N8	146/148 (99%)	118 (81%)	22 (15%)	6 (4%)	3	29
64	n8	146/148 (99%)	111 (76%)	24 (16%)	11 (8%)	1	13
65	N9	56/58 (97%)	41 (73%)	12 (21%)	3 (5%)	2	21
65	n9	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	10
66	O0	95/104 (91%)	80 (84%)	11 (12%)	4 (4%)	3	28
66	o0	98/104 (94%)	84 (86%)	11 (11%)	3 (3%)	5	36
67	O1	107/112 (96%)	89 (83%)	8 (8%)	10 (9%)	1	9
67	o1	107/112 (96%)	83 (78%)	18 (17%)	6 (6%)	2	20
68	O2	125/129 (97%)	104 (83%)	18 (14%)	3 (2%)	7	42
68	o2	125/129 (97%)	103 (82%)	16 (13%)	6 (5%)	2	24
69	O3	104/106 (98%)	96 (92%)	7 (7%)	1 (1%)	18	60
69	o3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	5	37
70	O4	110/119 (92%)	88 (80%)	17 (16%)	5 (4%)	3	26
70	o4	110/119 (92%)	98 (89%)	11 (10%)	1 (1%)	20	63
71	O5	117/119 (98%)	93 (80%)	22 (19%)	2 (2%)	11	49
71	o5	117/119 (98%)	98 (84%)	14 (12%)	5 (4%)	3	27
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	2	18
72	o6	97/99 (98%)	78 (80%)	14 (14%)	5 (5%)	2	21
73	O7	85/87 (98%)	64 (75%)	16 (19%)	5 (6%)	2	19
73	o7	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	7	42
74	O8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	2	21
74	o8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	3	29
75	O9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	8	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	o9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
76	Q0	50/52 (96%)	42 (84%)	7 (14%)	1 (2%)	9	45
76	q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	29
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	80 (78%)	17 (16%)	6 (6%)	2	19
78	q2	103/105 (98%)	95 (92%)	7 (7%)	1 (1%)	18	60
79	Q3	89/91 (98%)	71 (80%)	10 (11%)	8 (9%)	1	9
79	q3	89/91 (98%)	74 (83%)	12 (14%)	3 (3%)	4	34
80	e0	60/62 (97%)	38 (63%)	15 (25%)	7 (12%)	0	6
81	m2	144/165 (87%)	67 (46%)	48 (33%)	29 (20%)	0	2
82	p0	139/311 (45%)	110 (79%)	20 (14%)	9 (6%)	1	16
83	p1	45/106 (42%)	26 (58%)	17 (38%)	2 (4%)	3	27
83	p2	44/106 (42%)	33 (75%)	6 (14%)	5 (11%)	0	6
84	f	145/157 (92%)	97 (67%)	34 (23%)	14 (10%)	1	9
All	All	22711/24675 (92%)	18197 (80%)	3231 (14%)	1283 (6%)	2	20

5 of 1283 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	158	VAL
2	S0	169	SER
2	S0	191	ARG
3	S1	82	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	140 (85%)	24 (15%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	s0	165/209 (79%)	137 (83%)	28 (17%)	2	13
3	S1	191/223 (86%)	157 (82%)	34 (18%)	2	11
3	s1	192/223 (86%)	160 (83%)	32 (17%)	2	14
4	S2	176/204 (86%)	147 (84%)	29 (16%)	2	14
4	s2	176/204 (86%)	134 (76%)	42 (24%)	1	4
5	S3	182/194 (94%)	146 (80%)	36 (20%)	1	7
5	s3	182/194 (94%)	158 (87%)	24 (13%)	5	24
6	S4	221/221 (100%)	194 (88%)	27 (12%)	6	27
6	s4	221/221 (100%)	192 (87%)	29 (13%)	5	24
7	S5	173/190 (91%)	146 (84%)	27 (16%)	3	17
7	s5	173/190 (91%)	146 (84%)	27 (16%)	3	17
8	S6	188/201 (94%)	162 (86%)	26 (14%)	4	22
8	s6	187/201 (93%)	162 (87%)	25 (13%)	4	23
9	S7	165/169 (98%)	144 (87%)	21 (13%)	5	25
9	s7	165/169 (98%)	138 (84%)	27 (16%)	2	15
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3	20
10	s8	150/161 (93%)	128 (85%)	22 (15%)	3	20
11	S9	158/165 (96%)	128 (81%)	30 (19%)	2	9
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	9
12	C0	77/98 (79%)	69 (90%)	8 (10%)	8	35
12	c0	73/98 (74%)	64 (88%)	9 (12%)	5	27
13	C1	129/136 (95%)	110 (85%)	19 (15%)	3	20
13	c1	129/136 (95%)	111 (86%)	18 (14%)	4	21
14	C2	88/118 (75%)	73 (83%)	15 (17%)	2	13
14	c2	88/118 (75%)	74 (84%)	14 (16%)	3	16
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	7
15	c3	127/127 (100%)	111 (87%)	16 (13%)	5	26
16	C4	81/104 (78%)	65 (80%)	16 (20%)	1	7
16	c4	97/104 (93%)	78 (80%)	19 (20%)	1	8
17	C5	101/117 (86%)	89 (88%)	12 (12%)	6	27
17	c5	103/117 (88%)	87 (84%)	16 (16%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C6	117/118 (99%)	98 (84%)	19 (16%)	3	15
18	c6	118/118 (100%)	101 (86%)	17 (14%)	4	20
19	C7	94/124 (76%)	77 (82%)	17 (18%)	2	10
19	c7	92/124 (74%)	79 (86%)	13 (14%)	4	21
20	C8	128/128 (100%)	106 (83%)	22 (17%)	2	13
20	c8	128/128 (100%)	106 (83%)	22 (17%)	2	13
21	C9	115/115 (100%)	95 (83%)	20 (17%)	2	12
21	c9	115/115 (100%)	104 (90%)	11 (10%)	10	38
22	D0	100/113 (88%)	83 (83%)	17 (17%)	2	13
22	d0	103/113 (91%)	84 (82%)	19 (18%)	2	10
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1	7
23	d1	74/74 (100%)	61 (82%)	13 (18%)	2	11
24	D2	110/110 (100%)	89 (81%)	21 (19%)	2	8
24	d2	110/110 (100%)	92 (84%)	18 (16%)	2	15
25	D3	119/119 (100%)	100 (84%)	19 (16%)	3	16
25	d3	119/119 (100%)	98 (82%)	21 (18%)	2	11
26	D4	112/112 (100%)	98 (88%)	14 (12%)	5	26
26	d4	112/112 (100%)	92 (82%)	20 (18%)	2	11
27	D5	61/88 (69%)	50 (82%)	11 (18%)	2	11
27	d5	61/88 (69%)	53 (87%)	8 (13%)	5	24
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	7
28	d6	83/83 (100%)	74 (89%)	9 (11%)	7	33
29	D7	70/70 (100%)	66 (94%)	4 (6%)	24	61
29	d7	70/70 (100%)	57 (81%)	13 (19%)	2	9
30	D8	56/59 (95%)	45 (80%)	11 (20%)	1	8
30	d8	56/59 (95%)	45 (80%)	11 (20%)	1	8
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	13
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	6
32	E0	51/51 (100%)	43 (84%)	8 (16%)	3	17
33	E1	62/66 (94%)	53 (86%)	9 (14%)	4	20
33	e1	66/66 (100%)	54 (82%)	12 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	SR	259/261 (99%)	236 (91%)	23 (9%)	11	42
34	sR	260/261 (100%)	241 (93%)	19 (7%)	16	53
35	SM	97/228 (42%)	78 (80%)	19 (20%)	1	8
35	sM	54/228 (24%)	44 (82%)	10 (18%)	2	9
39	L2	193/195 (99%)	157 (81%)	36 (19%)	2	9
39	l2	192/195 (98%)	157 (82%)	35 (18%)	2	10
40	L3	319/322 (99%)	256 (80%)	63 (20%)	1	7
40	l3	320/322 (99%)	263 (82%)	57 (18%)	2	11
41	L4	288/288 (100%)	242 (84%)	46 (16%)	3	16
41	l4	288/288 (100%)	242 (84%)	46 (16%)	3	16
42	L5	244/244 (100%)	206 (84%)	38 (16%)	3	17
42	l5	243/244 (100%)	193 (79%)	50 (21%)	1	6
43	L6	134/152 (88%)	116 (87%)	18 (13%)	4	23
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	13
44	L7	186/204 (91%)	162 (87%)	24 (13%)	5	25
44	l7	187/204 (92%)	162 (87%)	25 (13%)	4	23
45	L8	187/207 (90%)	160 (86%)	27 (14%)	4	20
45	l8	177/207 (86%)	153 (86%)	24 (14%)	4	23
46	L9	171/171 (100%)	135 (79%)	36 (21%)	1	6
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	7
47	M0	177/186 (95%)	146 (82%)	31 (18%)	2	12
47	m0	179/186 (96%)	149 (83%)	30 (17%)	2	14
48	M1	147/150 (98%)	122 (83%)	25 (17%)	2	13
48	m1	147/150 (98%)	120 (82%)	27 (18%)	2	10
49	M3	154/158 (98%)	136 (88%)	18 (12%)	6	28
49	m3	154/158 (98%)	134 (87%)	20 (13%)	5	24
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	11
50	m4	108/108 (100%)	88 (82%)	20 (18%)	2	9
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	13
51	m5	175/175 (100%)	150 (86%)	25 (14%)	4	21
52	M6	160/161 (99%)	141 (88%)	19 (12%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	m6	160/161 (99%)	145 (91%)	15 (9%)	10	39
53	M7	140/145 (97%)	108 (77%)	32 (23%)	1	4
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	11
54	M8	150/150 (100%)	130 (87%)	20 (13%)	4	24
54	m8	150/150 (100%)	130 (87%)	20 (13%)	4	24
55	M9	153/153 (100%)	135 (88%)	18 (12%)	6	28
55	m9	153/153 (100%)	131 (86%)	22 (14%)	4	20
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	11
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1	5
57	N1	136/136 (100%)	109 (80%)	27 (20%)	1	7
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	6
58	N2	87/106 (82%)	74 (85%)	13 (15%)	3	19
58	n2	85/106 (80%)	71 (84%)	14 (16%)	2	14
59	N3	104/104 (100%)	90 (86%)	14 (14%)	4	23
59	n3	104/104 (100%)	92 (88%)	12 (12%)	6	29
60	N4	57/129 (44%)	54 (95%)	3 (5%)	26	62
60	n4	100/129 (78%)	89 (89%)	11 (11%)	7	32
61	N5	104/117 (89%)	82 (79%)	22 (21%)	1	6
61	n5	104/117 (89%)	88 (85%)	16 (15%)	3	17
62	N6	109/109 (100%)	88 (81%)	21 (19%)	1	8
62	n6	109/109 (100%)	94 (86%)	15 (14%)	4	22
63	N7	115/115 (100%)	102 (89%)	13 (11%)	7	30
63	n7	115/115 (100%)	95 (83%)	20 (17%)	2	12
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	11
64	n8	118/118 (100%)	97 (82%)	21 (18%)	2	11
65	N9	46/46 (100%)	39 (85%)	7 (15%)	3	18
65	n9	46/46 (100%)	40 (87%)	6 (13%)	5	24
66	O0	81/87 (93%)	65 (80%)	16 (20%)	1	7
66	o0	84/87 (97%)	74 (88%)	10 (12%)	6	27
67	O1	92/96 (96%)	79 (86%)	13 (14%)	4	21
67	o1	94/96 (98%)	79 (84%)	15 (16%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	O2	109/110 (99%)	88 (81%)	21 (19%)	1	8
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	5
69	O3	90/90 (100%)	80 (89%)	10 (11%)	7	31
69	o3	90/90 (100%)	79 (88%)	11 (12%)	6	27
70	O4	95/101 (94%)	82 (86%)	13 (14%)	4	22
70	o4	95/101 (94%)	78 (82%)	17 (18%)	2	11
71	O5	104/104 (100%)	85 (82%)	19 (18%)	2	10
71	o5	103/104 (99%)	84 (82%)	19 (18%)	2	10
72	O6	81/81 (100%)	62 (76%)	19 (24%)	1	4
72	o6	80/81 (99%)	60 (75%)	20 (25%)	1	4
73	O7	70/70 (100%)	57 (81%)	13 (19%)	2	9
73	o7	70/70 (100%)	53 (76%)	17 (24%)	1	4
74	O8	68/68 (100%)	55 (81%)	13 (19%)	2	8
74	o8	67/68 (98%)	57 (85%)	10 (15%)	3	19
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	7
75	o9	45/45 (100%)	40 (89%)	5 (11%)	7	31
76	Q0	47/47 (100%)	38 (81%)	9 (19%)	2	8
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1	4
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	0	3
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	3
78	Q2	90/90 (100%)	73 (81%)	17 (19%)	2	9
78	q2	90/90 (100%)	66 (73%)	24 (27%)	0	3
79	Q3	71/71 (100%)	63 (89%)	8 (11%)	7	30
79	q3	71/71 (100%)	57 (80%)	14 (20%)	1	7
80	e0	53/53 (100%)	36 (68%)	17 (32%)	0	2
82	p0	105/253 (42%)	86 (82%)	19 (18%)	2	10
84	f	123/132 (93%)	107 (87%)	16 (13%)	5	24
All	All	18849/20371 (92%)	15796 (84%)	3053 (16%)	3	15

5 of 3053 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	O4	52	GLN

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Mol	Chain	Res	Type
9	s7	11	GLN
66	o0	61	MET
72	O6	68	ARG
3	s1	181	LEU

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

Mol	Chain	Res	Type
56	N0	138	GLN
7	s5	72	HIS
61	n5	65	GLN
57	N1	146	ASN
70	O4	18	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1800 (98%)	463 (26%)	42 (2%)
1	6	1791/1800 (99%)	450 (25%)	35 (1%)
36	1	3145/3396 (92%)	683 (21%)	65 (2%)
36	5	3145/3396 (92%)	661 (21%)	65 (2%)
37	3	120/121 (99%)	20 (16%)	1 (0%)
37	7	120/121 (99%)	15 (12%)	1 (0%)
38	4	157/158 (99%)	33 (21%)	3 (1%)
38	8	157/158 (99%)	32 (20%)	1 (0%)
85	B	1/4 (25%)	1 (100%)	0
85	C	1/4 (25%)	0	0
All	All	10413/10958 (95%)	2358 (22%)	213 (2%)

5 of 2358 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	23	G
1	2	25	C
1	2	26	A

5 of 213 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3078	U
1	6	272	U
36	5	2818	U
36	1	3218	A
38	4	80	A

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
85	8AN	B	76	86,85	17,24,25	1.08	1 (5%)	14,35,38	2.02	3 (21%)
85	8AN	C	76	86,85	17,24,25	1.15	1 (5%)	14,35,38	1.92	3 (21%)
84	5CT	f	51	84	14,14,15	2.59	4 (28%)	11,15,17	3.65	5 (45%)

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
85	8AN	B	76	86,85	-	0/3/25/26	0/3/3/3
85	8AN	C	76	86,85	-	0/3/25/26	0/3/3/3
84	5CT	f	51	84	1/1/2/4	0/12/14/16	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	f	51	5CT	O1-C2	-6.94	1.22	1.43
84	f	51	5CT	C1-NZ	-3.43	1.41	1.47
85	B	76	8AN	C5-C4	2.83	1.46	1.40
85	C	76	8AN	C5-C4	3.06	1.47	1.40
84	f	51	5CT	CA-C	3.63	1.55	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	C	76	8AN	N3-C2-N1	-5.65	123.94	128.86
85	B	76	8AN	N3-C2-N1	-5.48	124.09	128.86
85	B	76	8AN	C4-C5-N7	-3.35	106.17	109.41
84	f	51	5CT	CB-CA-C	-2.89	106.89	111.65
85	C	76	8AN	C4-C5-N7	-2.60	106.90	109.41

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
84	f	51	5CT	C2

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	C	76	8AN	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2282 ligands modelled in this entry, 1109 are monoatomic - leaving 1173 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	$\# Z > 2$
87	OHX	1	3761	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3762	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3763	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3764	-	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
87	OHX	1	3765	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3766	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3767	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3768	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3769	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3770	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3771	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3772	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3773	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3774	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3775	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3776	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3777	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3778	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3779	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3780	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3781	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3782	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3783	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3784	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3785	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3786	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3787	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3788	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3789	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3790	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3791	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3792	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3793	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3794	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3795	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3796	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3797	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3798	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3799	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3800	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3801	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3802	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3803	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3804	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3805	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3806	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3807	-	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
87	OHX	1	3808	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3809	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3810	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3811	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3812	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3813	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3814	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3815	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3816	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3817	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3818	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3819	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3820	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3821	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3822	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3823	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3824	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3825	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3826	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3827	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3828	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3829	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3830	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3831	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3832	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3833	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3834	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3835	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3836	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3837	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3838	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3839	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3840	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3841	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3842	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3843	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3844	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3845	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3846	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3847	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3848	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3849	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3850	-	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
87	OHX	1	3851	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3852	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3853	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3854	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3855	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3856	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3857	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3858	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3859	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3860	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3861	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3862	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3863	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4071	36	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2030	-	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
87	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2073	-	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
87	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2116	-	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
87	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	215	-	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
87	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
89	SPS	5	3402	-	20,23,23	3.48	12 (60%)	18,30,30	3.19	11 (61%)
87	OHX	5	3816	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3817	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3818	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3819	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3820	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3821	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3822	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3823	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3824	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3825	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3826	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3827	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3828	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3829	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3830	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3831	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3832	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3833	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3834	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3835	-	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
87	OHX	5	3836	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3837	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3838	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3839	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3840	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3841	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3842	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3843	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3844	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3845	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3846	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3847	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3848	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3849	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3850	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3851	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3852	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3853	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3854	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3855	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3856	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3857	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3858	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3859	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3860	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3861	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3862	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3863	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3878	-	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
87	OHX	5	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3921	-	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
87	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3954	36	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3964	-	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
87	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4007	-	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
87	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4050	-	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
87	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4083	36	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4093	-	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
87	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4136	-	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
87	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2019	-	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
87	OHX	6	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2062	-	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
87	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2067	1	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2105	-	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
87	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2148	-	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
87	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
89	SPS	B	101	86	20,23,23	3.56	12 (60%)	18,30,30	3.30	7 (38%)
90	PRO	B	102	-	6,7,8	1.86	1 (16%)	7,8,10	1.13	0
90	PRO	C	101	-	6,7,8	1.09	1 (16%)	7,8,10	1.44	1 (14%)
87	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C5	201	17	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L4	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M6	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M7	205	-	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
87	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	N8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O7	103	73	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	S1	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	S6	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	S8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	S9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c5	202	17	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m6	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m7	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o6	201	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o7	503	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s1	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s4	602	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	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
87	OHX	1	3761	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3762	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3763	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3764	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3765	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3766	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3767	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3768	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3769	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3770	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3771	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3772	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3773	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3774	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3775	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3776	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3777	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3778	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3779	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3780	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3781	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3782	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3783	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3784	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3785	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3786	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3787	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3788	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3789	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3790	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3791	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3792	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3793	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3794	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3795	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3796	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3797	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3798	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3799	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3800	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3801	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3802	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3803	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3804	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3805	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3806	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3807	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3808	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3809	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3810	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3811	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3812	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3813	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3814	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3815	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3816	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3817	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3818	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3819	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3820	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3821	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3822	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3823	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3824	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3825	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3826	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3827	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3828	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3829	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3830	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3831	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3832	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3833	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3834	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3835	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3836	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3837	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3838	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3839	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3840	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3841	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3842	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3843	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3844	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3845	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3846	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3847	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3848	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3849	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3850	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3851	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3852	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3853	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3854	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3855	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3856	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3857	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3858	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3859	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3860	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3861	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3862	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3863	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3864	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3865	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3866	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3867	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3869	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3871	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3913	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3955	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3997	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4039	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4071	36	-	0/0/0/0	0/0/0/0
87	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4081	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	2	1991	-	-	0/0/0/0	0/0/0/0
87	OHX	2	1992	-	-	0/0/0/0	0/0/0/0
87	OHX	2	1993	-	-	0/0/0/0	0/0/0/0
87	OHX	2	1994	-	-	0/0/0/0	0/0/0/0
87	OHX	2	1995	-	-	0/0/0/0	0/0/0/0
87	OHX	2	1996	-	-	0/0/0/0	0/0/0/0
87	OHX	2	1997	-	-	0/0/0/0	0/0/0/0
87	OHX	2	1998	-	-	0/0/0/0	0/0/0/0
87	OHX	2	1999	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2000	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2001	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2002	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2003	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2004	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2005	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2006	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2007	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2008	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2009	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2010	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2011	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2012	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2013	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2014	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2015	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2016	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2017	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2018	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2019	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2020	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2021	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2022	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2044	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2086	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2128	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	3	209	-	-	0/0/0/0	0/0/0/0
87	OHX	3	210	-	-	0/0/0/0	0/0/0/0
87	OHX	3	211	-	-	0/0/0/0	0/0/0/0
87	OHX	3	212	-	-	0/0/0/0	0/0/0/0
87	OHX	3	213	-	-	0/0/0/0	0/0/0/0
87	OHX	3	214	-	-	0/0/0/0	0/0/0/0
87	OHX	3	215	-	-	0/0/0/0	0/0/0/0
87	OHX	3	216	-	-	0/0/0/0	0/0/0/0
87	OHX	3	217	-	-	0/0/0/0	0/0/0/0
87	OHX	3	218	-	-	0/0/0/0	0/0/0/0
87	OHX	3	219	-	-	0/0/0/0	0/0/0/0
87	OHX	4	215	-	-	0/0/0/0	0/0/0/0
87	OHX	4	216	-	-	0/0/0/0	0/0/0/0
87	OHX	4	217	-	-	0/0/0/0	0/0/0/0
87	OHX	4	218	-	-	0/0/0/0	0/0/0/0
87	OHX	4	219	-	-	0/0/0/0	0/0/0/0
87	OHX	4	220	-	-	0/0/0/0	0/0/0/0
87	OHX	4	221	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	4	222	-	-	0/0/0/0	0/0/0/0
87	OHX	4	223	-	-	0/0/0/0	0/0/0/0
87	OHX	4	224	-	-	0/0/0/0	0/0/0/0
87	OHX	4	225	-	-	0/0/0/0	0/0/0/0
87	OHX	4	226	-	-	0/0/0/0	0/0/0/0
87	OHX	4	227	-	-	0/0/0/0	0/0/0/0
87	OHX	4	228	-	-	0/0/0/0	0/0/0/0
87	OHX	4	229	-	-	0/0/0/0	0/0/0/0
87	OHX	4	230	-	-	0/0/0/0	0/0/0/0
87	OHX	4	231	-	-	0/0/0/0	0/0/0/0
87	OHX	4	232	-	-	0/0/0/0	0/0/0/0
89	SPS	5	3402	-	-	0/15/18/18	0/1/1/1
87	OHX	5	3816	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3817	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3818	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3819	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3820	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3821	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3822	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3823	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3824	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3825	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3826	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3827	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3828	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3829	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3830	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3831	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3832	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3833	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3834	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3835	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3836	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3837	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3838	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3839	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3840	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3841	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3842	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3843	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3844	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3845	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3846	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3847	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3848	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3849	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3850	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3851	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3852	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3853	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3854	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3855	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3856	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3857	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3858	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3859	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3860	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3861	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3862	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3863	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3864	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3865	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3866	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3867	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3868	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3869	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3870	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3871	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3872	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3873	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3874	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3875	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3876	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3877	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3878	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3879	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3880	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3881	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3882	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3883	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3884	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3885	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3886	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3887	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3888	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3889	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3890	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3891	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3892	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3893	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3894	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3895	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3896	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3897	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3899	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3929	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3954	36	-	0/0/0/0	0/0/0/0
87	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3971	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4013	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4055	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4083	36	-	0/0/0/0	0/0/0/0
87	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4097	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4139	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2012	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2013	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2014	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2015	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2016	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2017	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2018	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2019	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2020	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2021	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2022	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2023	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2024	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2025	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2026	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2027	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2028	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2029	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2030	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2031	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2032	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2033	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2034	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2035	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2036	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2037	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2038	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2039	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2040	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2041	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2042	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2043	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2063	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2067	1	-	0/0/0/0	0/0/0/0
87	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2105	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2147	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
87	OHX	7	214	-	-	0/0/0/0	0/0/0/0
87	OHX	7	215	-	-	0/0/0/0	0/0/0/0
87	OHX	7	216	-	-	0/0/0/0	0/0/0/0
87	OHX	7	217	-	-	0/0/0/0	0/0/0/0
87	OHX	7	218	-	-	0/0/0/0	0/0/0/0
87	OHX	7	219	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	7	220	-	-	0/0/0/0	0/0/0/0
87	OHX	7	221	-	-	0/0/0/0	0/0/0/0
87	OHX	7	222	-	-	0/0/0/0	0/0/0/0
87	OHX	7	223	-	-	0/0/0/0	0/0/0/0
87	OHX	7	224	-	-	0/0/0/0	0/0/0/0
87	OHX	8	210	-	-	0/0/0/0	0/0/0/0
87	OHX	8	211	-	-	0/0/0/0	0/0/0/0
87	OHX	8	212	-	-	0/0/0/0	0/0/0/0
87	OHX	8	213	-	-	0/0/0/0	0/0/0/0
87	OHX	8	214	-	-	0/0/0/0	0/0/0/0
87	OHX	8	215	-	-	0/0/0/0	0/0/0/0
87	OHX	8	216	-	-	0/0/0/0	0/0/0/0
87	OHX	8	217	-	-	0/0/0/0	0/0/0/0
87	OHX	8	218	-	-	0/0/0/0	0/0/0/0
87	OHX	8	219	-	-	0/0/0/0	0/0/0/0
87	OHX	8	220	-	-	0/0/0/0	0/0/0/0
87	OHX	8	221	-	-	0/0/0/0	0/0/0/0
87	OHX	8	222	-	-	0/0/0/0	0/0/0/0
87	OHX	8	223	-	-	0/0/0/0	0/0/0/0
87	OHX	8	224	-	-	0/0/0/0	0/0/0/0
87	OHX	8	225	-	-	0/0/0/0	0/0/0/0
87	OHX	8	226	-	-	0/0/0/0	0/0/0/0
87	OHX	8	227	-	-	0/0/0/0	0/0/0/0
87	OHX	8	228	-	-	0/0/0/0	0/0/0/0
87	OHX	8	229	-	-	0/0/0/0	0/0/0/0
87	OHX	8	230	-	-	0/0/0/0	0/0/0/0
89	SPS	B	101	86	-	0/15/18/18	0/1/1/1
90	PRO	B	102	-	-	0/0/9/11	0/1/1/1
90	PRO	C	101	-	-	0/0/9/11	0/1/1/1
87	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	C5	201	17	-	0/0/0/0	0/0/0/0
87	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	402	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	L4	401	-	-	0/0/0/0	0/0/0/0
87	OHX	L5	301	-	-	0/0/0/0	0/0/0/0
87	OHX	M0	302	-	-	0/0/0/0	0/0/0/0
87	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
87	OHX	M5	302	-	-	0/0/0/0	0/0/0/0
87	OHX	M5	303	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	M6	203	-	-	0/0/0/0	0/0/0/0
87	OHX	M7	205	-	-	0/0/0/0	0/0/0/0
87	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
87	OHX	N8	202	-	-	0/0/0/0	0/0/0/0
87	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	O1	201	-	-	0/0/0/0	0/0/0/0
87	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	O4	202	-	-	0/0/0/0	0/0/0/0
87	OHX	O7	103	73	-	0/0/0/0	0/0/0/0
87	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
87	OHX	S1	301	-	-	0/0/0/0	0/0/0/0
87	OHX	S6	301	-	-	0/0/0/0	0/0/0/0
87	OHX	S8	301	-	-	0/0/0/0	0/0/0/0
87	OHX	S9	201	-	-	0/0/0/0	0/0/0/0
87	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
87	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c5	202	17	-	0/0/0/0	0/0/0/0
87	OHX	c8	202	-	-	0/0/0/0	0/0/0/0
87	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
87	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	302	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	l9	201	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
87	OHX	m1	201	-	-	0/0/0/0	0/0/0/0
87	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
87	OHX	m5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	m5	304	-	-	0/0/0/0	0/0/0/0
87	OHX	m5	305	-	-	0/0/0/0	0/0/0/0
87	OHX	m6	201	-	-	0/0/0/0	0/0/0/0
87	OHX	m7	203	-	-	0/0/0/0	0/0/0/0
87	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	m9	201	-	-	0/0/0/0	0/0/0/0
87	OHX	n3	202	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	o6	201	-	-	0/0/0/0	0/0/0/0
87	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
87	OHX	o7	503	-	-	0/0/0/0	0/0/0/0
87	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
87	OHX	s1	301	-	-	0/0/0/0	0/0/0/0
87	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
87	OHX	s4	602	-	-	0/0/0/0	0/0/0/0
87	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
87	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
87	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	B	101	SPS	C9-C10	-9.16	1.31	1.48
89	5	3402	SPS	C9-C10	-8.98	1.31	1.48
89	5	3402	SPS	O13-C13	-5.40	1.19	1.42
89	B	101	SPS	O13-C13	-5.33	1.19	1.42
89	B	101	SPS	C3-N4	-2.97	1.32	1.38

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	B	101	SPS	C6-C1-N2	-7.92	118.86	124.45
89	5	3402	SPS	C6-C1-N2	-6.34	119.98	124.45
89	5	3402	SPS	C12-N11-C10	-4.83	116.01	122.63
89	B	101	SPS	C7-C5-C6	-3.93	119.27	122.69
89	5	3402	SPS	C6-C8-C9	-3.47	116.62	127.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

560 monomers are involved in 816 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3763	OHX	1	0
87	1	3765	OHX	1	0
87	1	3766	OHX	2	0
87	1	3768	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3769	OHX	2	0
87	1	3770	OHX	2	0
87	1	3771	OHX	1	0
87	1	3774	OHX	2	0
87	1	3775	OHX	1	0
87	1	3776	OHX	1	0
87	1	3777	OHX	2	0
87	1	3779	OHX	2	0
87	1	3781	OHX	1	0
87	1	3782	OHX	1	0
87	1	3783	OHX	1	0
87	1	3785	OHX	1	0
87	1	3787	OHX	1	0
87	1	3788	OHX	1	0
87	1	3789	OHX	1	0
87	1	3790	OHX	1	0
87	1	3794	OHX	1	0
87	1	3796	OHX	1	0
87	1	3800	OHX	1	0
87	1	3803	OHX	1	0
87	1	3806	OHX	1	0
87	1	3809	OHX	3	0
87	1	3810	OHX	1	0
87	1	3811	OHX	1	0
87	1	3812	OHX	2	0
87	1	3813	OHX	1	0
87	1	3815	OHX	1	0
87	1	3816	OHX	1	0
87	1	3819	OHX	1	0
87	1	3821	OHX	1	0
87	1	3823	OHX	1	0
87	1	3824	OHX	1	0
87	1	3825	OHX	1	0
87	1	3826	OHX	1	0
87	1	3828	OHX	1	0
87	1	3830	OHX	2	0
87	1	3831	OHX	1	0
87	1	3833	OHX	1	0
87	1	3834	OHX	1	0
87	1	3837	OHX	1	0
87	1	3838	OHX	1	0
87	1	3839	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3840	OHX	1	0
87	1	3844	OHX	1	0
87	1	3847	OHX	1	0
87	1	3849	OHX	1	0
87	1	3850	OHX	1	0
87	1	3853	OHX	2	0
87	1	3854	OHX	4	0
87	1	3855	OHX	1	0
87	1	3856	OHX	1	0
87	1	3858	OHX	2	0
87	1	3859	OHX	1	0
87	1	3860	OHX	1	0
87	1	3863	OHX	1	0
87	1	3868	OHX	1	0
87	1	3870	OHX	2	0
87	1	3872	OHX	1	0
87	1	3873	OHX	1	0
87	1	3875	OHX	1	0
87	1	3877	OHX	2	0
87	1	3878	OHX	1	0
87	1	3881	OHX	2	0
87	1	3884	OHX	3	0
87	1	3887	OHX	1	0
87	1	3889	OHX	4	0
87	1	3893	OHX	2	0
87	1	3894	OHX	1	0
87	1	3897	OHX	3	0
87	1	3898	OHX	1	0
87	1	3899	OHX	1	0
87	1	3900	OHX	1	0
87	1	3904	OHX	1	0
87	1	3906	OHX	1	0
87	1	3911	OHX	1	0
87	1	3913	OHX	1	0
87	1	3915	OHX	1	0
87	1	3919	OHX	1	0
87	1	3920	OHX	1	0
87	1	3921	OHX	1	0
87	1	3930	OHX	1	0
87	1	3932	OHX	1	0
87	1	3934	OHX	1	0
87	1	3935	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3936	OHX	1	0
87	1	3937	OHX	2	0
87	1	3938	OHX	2	0
87	1	3939	OHX	1	0
87	1	3940	OHX	5	0
87	1	3942	OHX	2	0
87	1	3943	OHX	1	0
87	1	3945	OHX	3	0
87	1	3949	OHX	1	0
87	1	3950	OHX	3	0
87	1	3951	OHX	3	0
87	1	3952	OHX	1	0
87	1	3956	OHX	1	0
87	1	3957	OHX	1	0
87	1	3958	OHX	1	0
87	1	3960	OHX	1	0
87	1	3963	OHX	1	0
87	1	3964	OHX	1	0
87	1	3967	OHX	2	0
87	1	3974	OHX	1	0
87	1	3978	OHX	1	0
87	1	3979	OHX	1	0
87	1	3981	OHX	1	0
87	1	3984	OHX	1	0
87	1	3986	OHX	1	0
87	1	3991	OHX	1	0
87	1	3993	OHX	1	0
87	1	3996	OHX	1	0
87	1	3997	OHX	1	0
87	1	3999	OHX	2	0
87	1	4000	OHX	1	0
87	1	4001	OHX	1	0
87	1	4003	OHX	1	0
87	1	4014	OHX	1	0
87	1	4018	OHX	1	0
87	1	4019	OHX	1	0
87	1	4027	OHX	2	0
87	1	4029	OHX	1	0
87	1	4030	OHX	2	0
87	1	4032	OHX	1	0
87	1	4033	OHX	2	0
87	1	4034	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4036	OHX	1	0
87	1	4037	OHX	2	0
87	1	4038	OHX	2	0
87	1	4040	OHX	1	0
87	1	4043	OHX	1	0
87	1	4044	OHX	2	0
87	1	4046	OHX	1	0
87	1	4048	OHX	1	0
87	1	4049	OHX	1	0
87	1	4050	OHX	1	0
87	1	4055	OHX	1	0
87	1	4058	OHX	1	0
87	1	4060	OHX	3	0
87	1	4061	OHX	3	0
87	1	4065	OHX	1	0
87	1	4066	OHX	2	0
87	1	4067	OHX	1	0
87	1	4070	OHX	1	0
87	1	4071	OHX	8	0
87	1	4072	OHX	1	0
87	1	4076	OHX	3	0
87	1	4077	OHX	1	0
87	1	4081	OHX	1	0
87	1	4082	OHX	6	0
87	1	4083	OHX	1	0
87	1	4085	OHX	4	0
87	1	4087	OHX	1	0
87	1	4096	OHX	1	0
87	1	4097	OHX	2	0
87	1	4098	OHX	1	0
87	1	4100	OHX	2	0
87	1	4102	OHX	1	0
87	1	4106	OHX	1	0
87	1	4107	OHX	1	0
87	1	4110	OHX	1	0
87	2	1991	OHX	1	0
87	2	1992	OHX	1	0
87	2	1993	OHX	1	0
87	2	1994	OHX	2	0
87	2	1995	OHX	1	0
87	2	1997	OHX	1	0
87	2	2000	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2001	OHX	2	0
87	2	2002	OHX	2	0
87	2	2003	OHX	1	0
87	2	2005	OHX	1	0
87	2	2006	OHX	1	0
87	2	2008	OHX	3	0
87	2	2012	OHX	1	0
87	2	2013	OHX	1	0
87	2	2014	OHX	1	0
87	2	2015	OHX	1	0
87	2	2016	OHX	1	0
87	2	2018	OHX	1	0
87	2	2019	OHX	1	0
87	2	2020	OHX	1	0
87	2	2026	OHX	1	0
87	2	2027	OHX	1	0
87	2	2032	OHX	1	0
87	2	2033	OHX	1	0
87	2	2034	OHX	2	0
87	2	2035	OHX	1	0
87	2	2036	OHX	1	0
87	2	2038	OHX	2	0
87	2	2039	OHX	3	0
87	2	2041	OHX	3	0
87	2	2042	OHX	1	0
87	2	2046	OHX	1	0
87	2	2049	OHX	1	0
87	2	2050	OHX	1	0
87	2	2051	OHX	1	0
87	2	2052	OHX	2	0
87	2	2055	OHX	1	0
87	2	2057	OHX	1	0
87	2	2058	OHX	5	0
87	2	2059	OHX	1	0
87	2	2061	OHX	1	0
87	2	2064	OHX	1	0
87	2	2066	OHX	2	0
87	2	2072	OHX	1	0
87	2	2074	OHX	2	0
87	2	2075	OHX	1	0
87	2	2076	OHX	1	0
87	2	2078	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2079	OHX	1	0
87	2	2080	OHX	3	0
87	2	2082	OHX	1	0
87	2	2083	OHX	1	0
87	2	2084	OHX	2	0
87	2	2089	OHX	3	0
87	2	2092	OHX	2	0
87	2	2095	OHX	1	0
87	2	2097	OHX	1	0
87	2	2099	OHX	4	0
87	2	2101	OHX	2	0
87	2	2102	OHX	1	0
87	2	2105	OHX	1	0
87	2	2106	OHX	1	0
87	2	2108	OHX	2	0
87	2	2109	OHX	1	0
87	2	2110	OHX	1	0
87	2	2112	OHX	1	0
87	2	2116	OHX	2	0
87	2	2117	OHX	1	0
87	2	2119	OHX	1	0
87	2	2120	OHX	1	0
87	2	2122	OHX	1	0
87	2	2123	OHX	2	0
87	2	2124	OHX	1	0
87	2	2127	OHX	3	0
87	2	2128	OHX	1	0
87	2	2130	OHX	1	0
87	2	2131	OHX	4	0
87	2	2132	OHX	1	0
87	2	2133	OHX	1	0
87	2	2136	OHX	1	0
87	2	2138	OHX	1	0
87	2	2142	OHX	1	0
87	2	2143	OHX	1	0
87	2	2145	OHX	1	0
87	2	2150	OHX	2	0
87	2	2151	OHX	1	0
87	3	209	OHX	1	0
87	3	214	OHX	1	0
87	3	216	OHX	1	0
87	4	216	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	4	217	OHX	1	0
87	4	218	OHX	2	0
87	4	219	OHX	1	0
87	4	220	OHX	1	0
87	4	222	OHX	2	0
87	4	223	OHX	1	0
87	4	224	OHX	1	0
87	4	226	OHX	1	0
87	4	227	OHX	1	0
87	4	228	OHX	1	0
87	4	229	OHX	1	0
89	5	3402	SPS	6	0
87	5	3816	OHX	1	0
87	5	3818	OHX	2	0
87	5	3820	OHX	1	0
87	5	3822	OHX	1	0
87	5	3824	OHX	1	0
87	5	3825	OHX	2	0
87	5	3827	OHX	1	0
87	5	3829	OHX	2	0
87	5	3832	OHX	1	0
87	5	3833	OHX	2	0
87	5	3834	OHX	2	0
87	5	3835	OHX	1	0
87	5	3836	OHX	1	0
87	5	3838	OHX	2	0
87	5	3840	OHX	1	0
87	5	3841	OHX	1	0
87	5	3845	OHX	1	0
87	5	3848	OHX	1	0
87	5	3849	OHX	1	0
87	5	3854	OHX	1	0
87	5	3855	OHX	1	0
87	5	3857	OHX	1	0
87	5	3858	OHX	1	0
87	5	3860	OHX	1	0
87	5	3861	OHX	1	0
87	5	3868	OHX	1	0
87	5	3869	OHX	2	0
87	5	3872	OHX	3	0
87	5	3874	OHX	1	0
87	5	3875	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	3876	OHX	1	0
87	5	3877	OHX	3	0
87	5	3878	OHX	2	0
87	5	3879	OHX	1	0
87	5	3880	OHX	1	0
87	5	3884	OHX	1	0
87	5	3885	OHX	1	0
87	5	3887	OHX	1	0
87	5	3889	OHX	1	0
87	5	3890	OHX	1	0
87	5	3893	OHX	3	0
87	5	3894	OHX	1	0
87	5	3895	OHX	1	0
87	5	3898	OHX	1	0
87	5	3899	OHX	1	0
87	5	3900	OHX	1	0
87	5	3901	OHX	2	0
87	5	3903	OHX	2	0
87	5	3904	OHX	1	0
87	5	3905	OHX	2	0
87	5	3906	OHX	1	0
87	5	3909	OHX	1	0
87	5	3910	OHX	1	0
87	5	3911	OHX	1	0
87	5	3914	OHX	4	0
87	5	3917	OHX	4	0
87	5	3918	OHX	1	0
87	5	3920	OHX	1	0
87	5	3921	OHX	3	0
87	5	3922	OHX	1	0
87	5	3924	OHX	1	0
87	5	3925	OHX	1	0
87	5	3927	OHX	1	0
87	5	3928	OHX	2	0
87	5	3929	OHX	1	0
87	5	3932	OHX	2	0
87	5	3934	OHX	1	0
87	5	3935	OHX	2	0
87	5	3938	OHX	2	0
87	5	3940	OHX	1	0
87	5	3942	OHX	1	0
87	5	3943	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	3944	OHX	1	0
87	5	3945	OHX	1	0
87	5	3947	OHX	1	0
87	5	3948	OHX	1	0
87	5	3952	OHX	1	0
87	5	3954	OHX	4	0
87	5	3955	OHX	1	0
87	5	3956	OHX	1	0
87	5	3958	OHX	1	0
87	5	3959	OHX	1	0
87	5	3960	OHX	1	0
87	5	3961	OHX	1	0
87	5	3962	OHX	1	0
87	5	3963	OHX	1	0
87	5	3964	OHX	1	0
87	5	3965	OHX	1	0
87	5	3966	OHX	1	0
87	5	3969	OHX	1	0
87	5	3976	OHX	2	0
87	5	3977	OHX	3	0
87	5	3981	OHX	1	0
87	5	3983	OHX	1	0
87	5	3985	OHX	1	0
87	5	3987	OHX	1	0
87	5	3988	OHX	2	0
87	5	3991	OHX	1	0
87	5	3995	OHX	2	0
87	5	3996	OHX	1	0
87	5	3997	OHX	1	0
87	5	3999	OHX	1	0
87	5	4000	OHX	5	0
87	5	4001	OHX	5	0
87	5	4004	OHX	1	0
87	5	4008	OHX	1	0
87	5	4009	OHX	1	0
87	5	4010	OHX	2	0
87	5	4011	OHX	1	0
87	5	4012	OHX	1	0
87	5	4013	OHX	3	0
87	5	4014	OHX	2	0
87	5	4016	OHX	1	0
87	5	4018	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4023	OHX	1	0
87	5	4026	OHX	1	0
87	5	4036	OHX	1	0
87	5	4037	OHX	1	0
87	5	4040	OHX	1	0
87	5	4045	OHX	1	0
87	5	4046	OHX	2	0
87	5	4047	OHX	1	0
87	5	4048	OHX	1	0
87	5	4051	OHX	3	0
87	5	4052	OHX	3	0
87	5	4053	OHX	1	0
87	5	4055	OHX	1	0
87	5	4057	OHX	2	0
87	5	4059	OHX	1	0
87	5	4060	OHX	2	0
87	5	4065	OHX	1	0
87	5	4068	OHX	1	0
87	5	4069	OHX	1	0
87	5	4071	OHX	1	0
87	5	4075	OHX	1	0
87	5	4081	OHX	1	0
87	5	4083	OHX	5	0
87	5	4086	OHX	1	0
87	5	4087	OHX	1	0
87	5	4092	OHX	2	0
87	5	4095	OHX	3	0
87	5	4096	OHX	1	0
87	5	4100	OHX	1	0
87	5	4101	OHX	1	0
87	5	4102	OHX	2	0
87	5	4103	OHX	1	0
87	5	4104	OHX	1	0
87	5	4111	OHX	1	0
87	5	4113	OHX	3	0
87	5	4116	OHX	2	0
87	5	4117	OHX	3	0
87	5	4119	OHX	3	0
87	5	4120	OHX	1	0
87	5	4124	OHX	1	0
87	5	4128	OHX	1	0
87	5	4129	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4130	OHX	1	0
87	5	4132	OHX	1	0
87	5	4137	OHX	1	0
87	5	4139	OHX	2	0
87	5	4140	OHX	1	0
87	5	4143	OHX	2	0
87	5	4147	OHX	1	0
87	5	4148	OHX	1	0
87	5	4151	OHX	1	0
87	5	4152	OHX	1	0
87	5	4153	OHX	2	0
87	5	4156	OHX	1	0
87	5	4158	OHX	1	0
87	5	4163	OHX	1	0
87	5	4165	OHX	1	0
87	5	4169	OHX	2	0
87	5	4170	OHX	2	0
87	5	4171	OHX	1	0
87	6	2014	OHX	2	0
87	6	2015	OHX	1	0
87	6	2018	OHX	1	0
87	6	2020	OHX	1	0
87	6	2022	OHX	2	0
87	6	2023	OHX	1	0
87	6	2024	OHX	1	0
87	6	2027	OHX	2	0
87	6	2028	OHX	2	0
87	6	2031	OHX	1	0
87	6	2032	OHX	1	0
87	6	2033	OHX	1	0
87	6	2034	OHX	1	0
87	6	2036	OHX	1	0
87	6	2037	OHX	1	0
87	6	2038	OHX	2	0
87	6	2039	OHX	2	0
87	6	2040	OHX	2	0
87	6	2041	OHX	2	0
87	6	2044	OHX	1	0
87	6	2050	OHX	1	0
87	6	2053	OHX	1	0
87	6	2054	OHX	1	0
87	6	2055	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2056	OHX	1	0
87	6	2057	OHX	1	0
87	6	2058	OHX	1	0
87	6	2060	OHX	1	0
87	6	2063	OHX	3	0
87	6	2064	OHX	1	0
87	6	2067	OHX	4	0
87	6	2069	OHX	2	0
87	6	2070	OHX	1	0
87	6	2074	OHX	2	0
87	6	2078	OHX	1	0
87	6	2081	OHX	1	0
87	6	2083	OHX	2	0
87	6	2085	OHX	1	0
87	6	2086	OHX	1	0
87	6	2087	OHX	1	0
87	6	2089	OHX	2	0
87	6	2092	OHX	2	0
87	6	2094	OHX	2	0
87	6	2095	OHX	1	0
87	6	2096	OHX	3	0
87	6	2101	OHX	1	0
87	6	2103	OHX	1	0
87	6	2104	OHX	2	0
87	6	2105	OHX	1	0
87	6	2107	OHX	1	0
87	6	2108	OHX	1	0
87	6	2109	OHX	2	0
87	6	2110	OHX	3	0
87	6	2111	OHX	2	0
87	6	2112	OHX	1	0
87	6	2115	OHX	2	0
87	6	2123	OHX	2	0
87	6	2124	OHX	5	0
87	6	2127	OHX	2	0
87	6	2129	OHX	1	0
87	6	2131	OHX	1	0
87	6	2132	OHX	1	0
87	6	2134	OHX	1	0
87	6	2138	OHX	1	0
87	6	2141	OHX	1	0
87	6	2145	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2149	OHX	1	0
87	6	2150	OHX	1	0
87	6	2151	OHX	1	0
87	6	2153	OHX	1	0
87	6	2156	OHX	2	0
87	6	2157	OHX	1	0
87	6	2159	OHX	1	0
87	6	2168	OHX	1	0
87	6	2170	OHX	3	0
87	6	2172	OHX	1	0
87	6	2173	OHX	1	0
87	6	2175	OHX	1	0
87	6	2180	OHX	1	0
87	6	2181	OHX	3	0
87	6	2183	OHX	1	0
87	7	218	OHX	1	0
87	7	221	OHX	1	0
87	7	222	OHX	2	0
87	8	210	OHX	1	0
87	8	214	OHX	1	0
87	8	215	OHX	1	0
87	8	216	OHX	2	0
87	8	217	OHX	1	0
87	8	221	OHX	1	0
87	8	222	OHX	1	0
87	8	228	OHX	2	0
87	8	230	OHX	1	0
89	B	101	SPS	2	0
87	C3	201	OHX	3	0
87	C5	201	OHX	5	0
87	L3	402	OHX	1	0
87	L3	403	OHX	2	0
87	L4	401	OHX	3	0
87	L5	301	OHX	1	0
87	M0	302	OHX	2	0
87	M0	303	OHX	5	0
87	M5	302	OHX	1	0
87	M5	303	OHX	1	0
87	M7	205	OHX	1	0
87	M9	202	OHX	1	0
87	N9	101	OHX	2	0
87	O1	201	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	O3	202	OHX	1	0
87	O4	202	OHX	2	0
87	O7	103	OHX	6	0
87	O9	101	OHX	1	0
87	Q2	503	OHX	2	0
87	S1	301	OHX	3	0
87	S6	301	OHX	3	0
87	S8	301	OHX	1	0
87	S9	201	OHX	4	0
87	SR	401	OHX	5	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
1	2	2
81	m2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	5.10
1	m2	23:LEU	C	28:ARG	N	3.71
1	m2	52:LYS	C	54:LYS	N	3.25
1	2	1685:G	O3'	1686:C	P	2.98

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1781/1800 (98%)	0.47	99 (5%) 25 23	58, 100, 190, 245	0
1	6	1795/1800 (99%)	0.23	55 (3%) 49 43	41, 84, 172, 231	0
2	S0	206/251 (82%)	1.44	64 (31%) 0 1	99, 112, 122, 125	0
2	s0	206/251 (82%)	0.72	19 (9%) 10 11	78, 93, 107, 115	0
3	S1	214/254 (84%)	1.78	78 (36%) 0 0	114, 152, 175, 179	0
3	s1	216/254 (85%)	0.92	35 (16%) 2 3	80, 93, 110, 126	0
4	S2	217/253 (85%)	0.31	8 (3%) 42 37	79, 95, 109, 118	0
4	s2	217/253 (85%)	0.63	24 (11%) 6 8	63, 79, 90, 99	0
5	S3	223/239 (93%)	0.92	36 (16%) 2 3	90, 103, 122, 135	0
5	s3	223/239 (93%)	0.99	45 (20%) 1 1	83, 108, 131, 139	0
6	S4	260/260 (100%)	2.36	139 (53%) 0 0	78, 101, 111, 133	0
6	s4	260/260 (100%)	1.62	86 (33%) 0 0	56, 79, 94, 113	0
7	S5	206/224 (91%)	2.20	103 (50%) 0 0	107, 122, 134, 144	0
7	s5	206/224 (91%)	1.90	95 (46%) 0 0	88, 106, 123, 134	0
8	S6	226/236 (95%)	0.98	46 (20%) 1 1	77, 113, 131, 142	0
8	s6	218/236 (92%)	0.69	24 (11%) 6 8	56, 85, 110, 123	0
9	S7	184/189 (97%)	1.14	41 (22%) 1 1	96, 127, 147, 152	0
9	s7	186/189 (98%)	0.36	8 (4%) 36 31	70, 103, 132, 139	0
10	S8	188/200 (94%)	1.30	52 (27%) 1 1	68, 88, 122, 139	0
10	s8	188/200 (94%)	0.77	25 (13%) 4 5	52, 69, 110, 129	0
11	S9	185/196 (94%)	2.38	101 (54%) 0 0	91, 107, 137, 157	0
11	s9	185/196 (94%)	1.29	45 (24%) 1 1	68, 87, 125, 146	0
12	C0	96/105 (91%)	2.05	44 (45%) 0 0	96, 121, 141, 151	0
12	c0	96/105 (91%)	2.10	42 (43%) 0 0	105, 136, 149, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	1.01	26 (16%) 2 2	71, 84, 118, 130	0
13	c1	146/155 (94%)	0.60	13 (8%) 10 12	54, 66, 94, 115	0
14	C2	124/142 (87%)	0.93	18 (14%) 3 4	149, 161, 174, 180	0
14	c2	124/142 (87%)	2.60	78 (62%) 0 0	180, 196, 211, 215	0
15	C3	150/150 (100%)	1.14	39 (26%) 1 1	79, 94, 109, 115	0
15	c3	150/150 (100%)	0.26	7 (4%) 32 28	63, 76, 93, 96	0
16	C4	127/136 (93%)	1.85	56 (44%) 0 0	83, 146, 158, 162	0
16	c4	128/136 (94%)	0.95	19 (14%) 3 4	64, 96, 104, 109	0
17	C5	124/141 (87%)	1.10	28 (22%) 1 1	87, 103, 120, 130	0
17	c5	135/141 (95%)	1.36	45 (33%) 0 0	72, 107, 122, 123	0
18	C6	141/142 (99%)	2.40	77 (54%) 0 0	92, 110, 116, 118	0
18	c6	142/142 (100%)	2.01	61 (42%) 0 0	82, 104, 118, 136	0
19	C7	120/136 (88%)	1.24	29 (24%) 1 1	95, 110, 129, 131	0
19	c7	117/136 (86%)	0.63	15 (12%) 4 6	85, 102, 114, 122	0
20	C8	145/145 (100%)	1.33	41 (28%) 1 1	85, 109, 135, 142	0
20	c8	145/145 (100%)	1.35	37 (25%) 1 1	83, 101, 117, 124	0
21	C9	143/143 (100%)	2.44	84 (58%) 0 0	95, 110, 125, 133	0
21	c9	143/143 (100%)	1.10	27 (18%) 1 2	82, 98, 115, 123	0
22	D0	107/120 (89%)	1.02	22 (20%) 1 1	86, 114, 136, 138	0
22	d0	110/120 (91%)	1.08	27 (24%) 1 1	85, 115, 144, 149	0
23	D1	87/87 (100%)	0.75	13 (14%) 3 4	96, 103, 117, 122	0
23	d1	87/87 (100%)	0.15	1 (1%) 80 74	71, 82, 104, 111	0
24	D2	129/129 (100%)	0.82	13 (10%) 8 9	80, 92, 101, 111	0
24	d2	129/129 (100%)	0.29	3 (2%) 61 54	59, 68, 75, 84	0
25	D3	144/144 (100%)	1.29	44 (30%) 0 1	70, 78, 90, 102	0
25	d3	144/144 (100%)	0.75	12 (8%) 12 13	52, 57, 70, 81	0
26	D4	134/134 (100%)	2.20	64 (47%) 0 0	89, 111, 123, 127	0
26	d4	134/134 (100%)	0.42	14 (10%) 7 9	65, 88, 100, 105	0
27	D5	70/107 (65%)	2.43	39 (55%) 0 0	118, 134, 141, 146	0
27	d5	69/107 (64%)	2.38	38 (55%) 0 0	98, 112, 124, 126	0
28	D6	97/97 (100%)	1.79	39 (40%) 0 0	86, 108, 160, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
28	d6	97/97 (100%)	0.76	13 (13%)	4	5	67, 84, 111, 116	0
29	D7	81/81 (100%)	1.77	36 (44%)	0	0	95, 113, 139, 143	0
29	d7	81/81 (100%)	1.12	19 (23%)	1	1	72, 89, 127, 128	0
30	D8	63/66 (95%)	1.69	23 (36%)	0	0	114, 131, 139, 144	0
30	d8	63/66 (95%)	1.77	25 (39%)	0	0	105, 118, 125, 128	0
31	D9	53/55 (96%)	1.47	15 (28%)	1	1	85, 90, 108, 114	0
31	d9	53/55 (96%)	2.16	26 (49%)	0	0	82, 92, 128, 145	0
32	E0	60/60 (100%)	2.37	36 (60%)	0	0	80, 110, 134, 137	0
33	E1	71/76 (93%)	1.74	28 (39%)	0	0	115, 142, 155, 157	0
33	e1	76/76 (100%)	2.68	38 (50%)	0	0	117, 168, 186, 187	0
34	SR	318/318 (100%)	1.41	90 (28%)	1	1	109, 122, 138, 156	0
34	sR	318/318 (100%)	2.74	185 (58%)	0	0	112, 127, 141, 153	0
35	SM	159/273 (58%)	1.17	37 (23%)	1	1	58, 100, 159, 163	0
35	sM	104/273 (38%)	1.33	25 (24%)	1	1	51, 115, 188, 197	0
36	1	3149/3396 (92%)	0.17	64 (2%)	65	60	33, 58, 136, 238	0
36	5	3150/3396 (92%)	0.13	35 (1%)	80	74	28, 52, 127, 213	0
37	3	121/121 (100%)	-0.02	0	100	100	42, 77, 90, 98	0
37	7	121/121 (100%)	-0.11	0	100	100	33, 55, 66, 75	0
38	4	158/158 (100%)	0.06	3 (1%)	67	61	42, 63, 102, 146	0
38	8	158/158 (100%)	0.03	1 (0%)	89	85	42, 63, 101, 131	0
39	L2	252/253 (99%)	0.59	15 (5%)	23	21	40, 60, 78, 84	0
39	l2	252/253 (99%)	0.35	6 (2%)	59	52	36, 55, 73, 80	0
40	L3	386/386 (100%)	0.40	20 (5%)	28	25	37, 62, 77, 88	0
40	l3	386/386 (100%)	0.32	17 (4%)	35	30	28, 45, 60, 81	0
41	L4	361/361 (100%)	0.09	3 (0%)	86	80	38, 54, 69, 74	0
41	l4	361/361 (100%)	0.03	2 (0%)	89	85	37, 56, 74, 82	0
42	L5	296/296 (100%)	1.67	118 (39%)	0	0	58, 80, 98, 119	0
42	l5	294/296 (99%)	0.55	19 (6%)	20	18	42, 56, 83, 97	0
43	L6	156/175 (89%)	0.76	16 (10%)	7	9	46, 56, 72, 87	0
43	l6	157/175 (89%)	0.70	13 (8%)	12	13	48, 57, 78, 93	0
44	L7	222/243 (91%)	0.20	0	100	100	38, 47, 77, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	-0.00	1 (0%) 92 89	33, 45, 82, 112	0
45	L8	233/255 (91%)	0.88	37 (15%) 2 3	68, 84, 110, 120	0
45	l8	231/255 (90%)	1.21	54 (23%) 1 1	69, 82, 107, 117	0
46	L9	191/191 (100%)	0.26	5 (2%) 56 49	59, 71, 82, 94	0
46	l9	191/191 (100%)	-0.02	2 (1%) 82 76	41, 51, 68, 78	0
47	M0	211/220 (95%)	0.58	20 (9%) 9 10	44, 63, 94, 105	0
47	m0	213/220 (96%)	0.31	4 (1%) 67 61	39, 54, 78, 94	0
48	M1	169/173 (97%)	1.06	28 (16%) 2 3	68, 85, 97, 103	0
48	m1	169/173 (97%)	0.31	1 (0%) 89 85	47, 66, 77, 81	0
49	M3	193/198 (97%)	0.34	3 (1%) 72 66	36, 63, 101, 122	0
49	m3	194/198 (97%)	0.68	18 (9%) 9 11	38, 67, 104, 119	0
50	M4	136/137 (99%)	-0.07	0 100 100	50, 59, 72, 83	0
50	m4	137/137 (100%)	-0.15	0 100 100	43, 50, 66, 84	0
51	M5	203/203 (100%)	0.66	20 (9%) 8 9	39, 56, 67, 71	0
51	m5	203/203 (100%)	1.29	52 (25%) 1 1	40, 58, 68, 73	0
52	M6	197/198 (99%)	-0.15	2 (1%) 82 76	25, 32, 46, 49	0
52	m6	197/198 (99%)	-0.13	0 100 100	18, 24, 45, 52	0
53	M7	183/183 (100%)	0.77	25 (13%) 3 5	44, 52, 105, 133	0
53	m7	155/183 (84%)	0.09	1 (0%) 89 85	36, 45, 55, 77	0
54	M8	185/185 (100%)	0.18	1 (0%) 90 87	42, 51, 68, 88	0
54	m8	185/185 (100%)	0.29	4 (2%) 62 55	39, 53, 64, 72	0
55	M9	188/188 (100%)	0.89	34 (18%) 1 2	64, 78, 147, 156	0
55	m9	188/188 (100%)	0.21	10 (5%) 27 24	50, 62, 123, 138	0
56	N0	172/172 (100%)	0.48	8 (4%) 32 28	37, 56, 70, 75	0
56	n0	172/172 (100%)	0.02	1 (0%) 89 85	32, 45, 57, 67	0
57	N1	159/159 (100%)	0.33	3 (1%) 67 61	41, 56, 99, 105	0
57	n1	159/159 (100%)	0.21	1 (0%) 89 85	37, 45, 82, 88	0
58	N2	100/120 (83%)	1.43	30 (30%) 1 1	94, 106, 112, 117	0
58	n2	98/120 (81%)	1.12	21 (21%) 1 1	74, 85, 93, 95	0
59	N3	136/136 (100%)	0.47	4 (2%) 52 45	49, 59, 73, 82	0
59	n3	136/136 (100%)	0.16	2 (1%) 74 68	31, 41, 52, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	2.28	31 (31%) 0 1	59, 74, 147, 155	0
60	n4	135/155 (87%)	0.87	22 (16%) 2 3	41, 93, 124, 142	0
61	N5	121/141 (85%)	0.89	14 (11%) 5 7	59, 71, 86, 103	0
61	n5	120/141 (85%)	0.72	10 (8%) 12 13	55, 68, 82, 97	0
62	N6	126/126 (100%)	0.62	7 (5%) 25 23	48, 64, 77, 85	0
62	n6	126/126 (100%)	0.45	3 (2%) 59 52	50, 66, 82, 85	0
63	N7	135/135 (100%)	2.30	79 (58%) 0 0	83, 96, 107, 111	0
63	n7	135/135 (100%)	1.25	36 (26%) 1 1	78, 89, 101, 109	0
64	N8	148/148 (100%)	0.46	5 (3%) 46 40	32, 54, 76, 82	0
64	n8	148/148 (100%)	0.68	17 (11%) 5 7	34, 55, 72, 75	0
65	N9	58/58 (100%)	0.08	0 100 100	36, 59, 97, 113	0
65	n9	58/58 (100%)	0.05	0 100 100	36, 55, 76, 82	0
66	O0	97/104 (93%)	1.18	25 (25%) 1 1	83, 90, 106, 111	0
66	o0	100/104 (96%)	0.54	9 (9%) 10 11	69, 79, 98, 105	0
67	O1	109/112 (97%)	1.54	36 (33%) 0 0	60, 73, 94, 101	0
67	o1	109/112 (97%)	1.37	26 (23%) 1 1	44, 56, 89, 97	0
68	O2	127/129 (98%)	0.35	3 (2%) 59 52	34, 48, 63, 79	0
68	o2	127/129 (98%)	0.67	7 (5%) 26 23	32, 52, 67, 78	0
69	O3	106/106 (100%)	0.34	2 (1%) 67 61	39, 46, 70, 82	0
69	o3	106/106 (100%)	0.85	14 (13%) 4 5	36, 44, 71, 82	0
70	O4	112/119 (94%)	1.82	48 (42%) 0 0	57, 74, 110, 117	0
70	o4	112/119 (94%)	1.17	29 (25%) 1 1	50, 66, 101, 108	0
71	O5	119/119 (100%)	0.48	4 (3%) 46 40	56, 73, 80, 83	0
71	o5	119/119 (100%)	0.16	4 (3%) 46 40	58, 71, 86, 96	0
72	O6	99/99 (100%)	1.13	19 (19%) 1 2	59, 70, 100, 111	0
72	o6	99/99 (100%)	0.91	14 (14%) 3 5	62, 72, 91, 110	0
73	O7	87/87 (100%)	0.03	0 100 100	41, 49, 70, 80	0
73	o7	87/87 (100%)	0.03	0 100 100	37, 48, 79, 85	0
74	O8	77/77 (100%)	0.91	7 (9%) 10 11	85, 97, 107, 108	0
74	o8	77/77 (100%)	2.16	44 (57%) 0 0	75, 85, 94, 97	0
75	O9	50/50 (100%)	0.19	0 100 100	51, 57, 61, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	-0.01	1 (2%) 65 60	49, 54, 63, 64	0
76	Q0	52/52 (100%)	0.87	6 (11%) 5 7	53, 59, 74, 82	0
76	q0	52/52 (100%)	-0.00	1 (1%) 67 61	38, 42, 52, 57	0
77	Q1	25/25 (100%)	0.27	0 100 100	62, 66, 72, 74	0
77	q1	25/25 (100%)	-0.20	0 100 100	49, 53, 54, 55	0
78	Q2	105/105 (100%)	0.37	7 (6%) 19 18	41, 55, 76, 97	0
78	q2	105/105 (100%)	0.11	1 (0%) 82 76	40, 53, 69, 96	0
79	Q3	91/91 (100%)	0.41	2 (2%) 62 55	49, 65, 79, 85	0
79	q3	91/91 (100%)	0.18	0 100 100	40, 55, 71, 81	0
80	e0	62/62 (100%)	1.55	17 (27%) 1 1	60, 88, 117, 120	0
81	m2	150/165 (90%)	1.38	42 (28%) 1 1	102, 138, 156, 161	0
82	p0	143/311 (45%)	2.15	70 (48%) 0 0	100, 125, 220, 229	0
83	p1	47/106 (44%)	4.36	35 (74%) 0 0	179, 224, 242, 245	0
83	p2	46/106 (43%)	4.94	35 (76%) 0 0	275, 283, 288, 289	0
84	f	147/157 (93%)	2.48	83 (56%) 0 0	47, 99, 167, 169	74 (50%)
85	B	3/4 (75%)	0.55	0 100 100	45, 45, 46, 48	0
85	C	3/4 (75%)	0.35	0 100 100	42, 42, 43, 49	0
All	All	33490/35633 (93%)	0.72	4478 (13%) 4 5	18, 74, 141, 289	74 (0%)

The worst 5 of 4478 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
83	p2	31	ASN	23.0
83	p2	30	THR	19.4
83	p1	17	SER	14.6
83	p2	12	LEU	13.6
83	p2	32	ALA	13.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	8AN	B	76	22/23	0.97	0.20	-	44,44,45,45	0
84	5CT	f	51	15/16	0.70	0.37	-	44,44,44,44	15
85	8AN	C	76	22/23	0.95	0.24	-	40,42,43,43	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3735	1/1	0.94	0.74	66.32	35,35,35,35	1
86	MG	5	3507	1/1	0.95	0.72	64.49	31,31,31,31	0
86	MG	6	1966	1/1	0.97	0.44	56.19	56,56,56,56	0
86	MG	1	3501	1/1	0.90	0.56	50.20	26,26,26,26	0
86	MG	1	3437	1/1	0.89	0.74	47.55	44,44,44,44	0
86	MG	1	3507	1/1	0.98	0.75	47.00	30,30,30,30	0
86	MG	1	3580	1/1	0.97	0.69	46.72	35,35,35,35	0
86	MG	1	3561	1/1	0.95	0.75	46.36	22,22,22,22	0
86	MG	1	3454	1/1	0.97	0.90	45.32	31,31,31,31	0
86	MG	1	3582	1/1	0.98	0.77	43.93	27,27,27,27	0
86	MG	5	3556	1/1	0.94	0.79	41.67	29,29,29,29	0
86	MG	8	203	1/1	0.94	0.84	41.49	44,44,44,44	0
86	MG	5	3505	1/1	0.92	0.76	41.43	27,27,27,27	0
86	MG	N3	201	1/1	0.96	0.61	40.76	36,36,36,36	0
86	MG	1	3495	1/1	0.94	0.84	40.55	34,34,34,34	0
86	MG	5	3560	1/1	0.93	0.65	39.81	26,26,26,26	0
86	MG	5	3563	1/1	0.96	0.68	39.31	27,27,27,27	0
86	MG	1	3465	1/1	0.93	0.69	38.93	28,28,28,28	0
86	MG	1	3557	1/1	0.88	0.67	38.60	55,55,55,55	0
86	MG	1	3448	1/1	0.93	0.89	38.49	49,49,49,49	0
86	MG	5	3582	1/1	0.99	0.62	37.74	23,23,23,23	0
86	MG	1	3681	1/1	0.95	0.91	36.09	37,37,37,37	0
86	MG	5	3527	1/1	0.96	0.77	36.04	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3467	1/1	0.83	0.58	35.05	42,42,42,42	0
86	MG	5	3656	1/1	0.97	0.54	34.78	33,33,33,33	0
86	MG	1	3560	1/1	0.96	0.69	34.52	46,46,46,46	0
86	MG	5	3593	1/1	0.93	0.64	34.17	35,35,35,35	0
86	MG	5	3501	1/1	0.85	0.86	33.90	31,31,31,31	0
86	MG	2	1911	1/1	0.88	0.84	33.82	77,77,77,77	0
87	OHX	2	2120	7/7	0.91	0.50	33.36	87,87,87,87	3
86	MG	1	3696	1/1	0.93	0.65	32.44	30,30,30,30	0
86	MG	1	3506	1/1	0.99	0.63	31.55	32,32,32,32	0
86	MG	1	3497	1/1	0.94	0.83	31.22	25,25,25,25	0
86	MG	7	203	1/1	0.96	0.54	30.55	54,54,54,54	0
86	MG	1	3414	1/1	0.96	0.74	30.37	43,43,43,43	0
86	MG	6	1901	1/1	0.98	0.59	29.70	52,52,52,52	0
86	MG	5	3686	1/1	0.87	0.67	29.21	37,37,37,37	0
86	MG	6	1981	1/1	0.92	0.61	29.20	54,54,54,54	0
86	MG	5	3537	1/1	0.97	0.70	29.14	32,32,32,32	0
86	MG	1	3477	1/1	0.96	0.62	28.92	41,41,41,41	0
86	MG	5	3508	1/1	0.96	0.57	28.24	25,25,25,25	0
86	MG	6	1933	1/1	0.84	0.64	28.20	56,56,56,56	0
86	MG	1	3509	1/1	0.99	0.64	28.02	33,33,33,33	0
86	MG	5	3581	1/1	0.97	0.56	27.95	31,31,31,31	0
86	MG	5	3541	1/1	0.94	0.64	27.66	46,46,46,46	0
86	MG	5	3599	1/1	0.80	0.45	27.64	37,37,37,37	0
86	MG	5	3522	1/1	0.90	0.51	27.17	29,29,29,29	0
86	MG	1	3498	1/1	0.93	0.67	26.99	45,45,45,45	0
86	MG	1	3516	1/1	0.91	0.62	26.23	33,33,33,33	0
86	MG	5	3513	1/1	0.94	0.59	26.07	35,35,35,35	0
86	MG	5	3457	1/1	0.96	0.76	25.91	28,28,28,28	0
86	MG	1	3407	1/1	0.61	0.56	25.80	33,33,33,33	0
86	MG	1	3562	1/1	0.94	0.91	25.71	33,33,33,33	0
86	MG	1	3538	1/1	0.95	0.64	25.19	39,39,39,39	0
86	MG	1	3422	1/1	0.91	0.45	24.81	32,32,32,32	0
87	OHX	2	2141	7/7	0.88	0.50	24.71	90,90,90,90	6
87	OHX	6	2131	7/7	0.92	0.29	24.71	89,89,89,89	6
87	OHX	5	4033	7/7	0.89	0.29	24.65	66,66,66,66	4
86	MG	1	3555	1/1	0.97	0.62	24.13	26,26,26,26	0
87	OHX	1	3939	7/7	0.95	0.26	24.09	54,54,54,54	3
86	MG	1	3587	1/1	0.97	0.63	23.51	35,35,35,35	0
86	MG	2	1910	1/1	0.83	0.61	23.01	69,69,69,69	0
86	MG	1	3573	1/1	0.81	0.71	22.98	40,40,40,40	0
86	MG	1	3585	1/1	0.97	0.81	22.85	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3756	1/1	0.88	0.77	22.68	53,53,53,53	0
86	MG	1	3546	1/1	0.95	0.61	22.64	36,36,36,36	0
86	MG	5	3585	1/1	0.94	0.48	22.35	29,29,29,29	0
86	MG	1	3530	1/1	0.96	0.60	22.14	41,41,41,41	0
86	MG	1	3464	1/1	0.94	0.50	22.14	38,38,38,38	0
86	MG	1	3469	1/1	0.94	0.59	21.76	41,41,41,41	0
87	OHX	1	3875	7/7	0.97	0.56	21.70	53,53,53,53	3
86	MG	5	3544	1/1	0.81	0.49	21.69	57,57,57,57	0
86	MG	2	1989	1/1	0.68	0.52	21.60	65,65,65,65	0
86	MG	5	3677	1/1	0.95	0.56	21.59	37,37,37,37	0
86	MG	5	3617	1/1	0.92	0.49	21.30	34,34,34,34	0
87	OHX	2	2121	7/7	0.95	0.62	21.07	94,94,94,94	4
86	MG	6	1923	1/1	0.89	0.64	21.00	46,46,46,46	0
86	MG	5	3416	1/1	0.91	0.61	20.87	64,64,64,64	0
86	MG	1	3482	1/1	0.94	0.51	20.83	33,33,33,33	0
86	MG	5	3644	1/1	0.86	0.54	20.32	31,31,31,31	0
86	MG	1	3524	1/1	0.90	0.51	20.05	44,44,44,44	0
87	OHX	5	4053	7/7	0.85	0.67	20.02	50,50,50,50	2
86	MG	5	3594	1/1	0.93	0.51	19.90	28,28,28,28	0
86	MG	5	3472	1/1	0.98	0.52	19.88	30,30,30,30	0
86	MG	1	3527	1/1	0.95	0.66	19.28	31,31,31,31	0
86	MG	5	3419	1/1	0.89	0.69	19.26	26,26,26,26	0
86	MG	5	3601	1/1	0.90	0.47	18.93	30,30,30,30	0
86	MG	1	3496	1/1	0.95	0.54	18.82	41,41,41,41	0
86	MG	1	3642	1/1	0.74	0.57	18.62	32,32,32,32	0
87	OHX	5	4132	7/7	0.85	0.53	18.43	34,34,34,34	3
87	OHX	1	4000	7/7	0.92	0.42	18.10	55,55,55,55	3
86	MG	1	3490	1/1	0.94	0.66	18.07	34,34,34,34	0
86	MG	M7	202	1/1	0.96	0.89	18.01	40,40,40,40	0
86	MG	5	3428	1/1	0.95	0.42	17.72	31,31,31,31	0
86	MG	n3	201	1/1	0.93	0.42	17.57	25,25,25,25	0
87	OHX	1	3971	7/7	0.81	0.37	17.55	47,47,47,47	4
86	MG	1	3488	1/1	0.98	0.54	17.12	37,37,37,37	0
86	MG	5	3643	1/1	0.97	0.54	16.96	34,34,34,34	0
86	MG	1	3757	1/1	0.92	0.43	16.71	55,55,55,55	0
86	MG	5	3744	1/1	0.95	0.52	16.60	34,34,34,34	0
86	MG	1	3570	1/1	0.93	0.50	16.60	46,46,46,46	0
87	OHX	6	2127	7/7	0.94	0.40	16.43	58,58,58,58	5
86	MG	5	3497	1/1	0.94	0.52	16.39	32,32,32,32	0
86	MG	5	3719	1/1	0.95	0.44	16.29	34,34,34,34	0
86	MG	5	3455	1/1	0.83	0.56	16.00	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	7	220	7/7	0.97	0.37	15.90	73,73,73,73	1
86	MG	2	1932	1/1	0.81	0.64	15.82	64,64,64,64	0
86	MG	1	3413	1/1	0.93	0.57	15.79	41,41,41,41	0
86	MG	1	3583	1/1	0.97	0.64	15.59	31,31,31,31	0
87	OHX	5	3956	7/7	0.95	0.40	15.48	46,46,46,46	3
86	MG	1	3627	1/1	0.96	0.81	15.41	41,41,41,41	0
87	OHX	6	2155	7/7	0.94	0.40	15.36	71,71,71,71	3
87	OHX	5	4076	7/7	0.97	0.36	15.34	32,32,32,32	3
86	MG	1	3415	1/1	0.90	0.37	15.31	43,43,43,43	0
86	MG	m7	201	1/1	0.97	0.63	15.26	33,33,33,33	0
86	MG	5	3545	1/1	0.90	0.59	15.20	46,46,46,46	0
86	MG	1	3559	1/1	0.94	0.50	15.13	22,22,22,22	0
86	MG	5	3550	1/1	0.97	0.48	14.93	32,32,32,32	0
86	MG	5	3451	1/1	0.95	0.41	14.89	29,29,29,29	0
86	MG	1	3575	1/1	0.98	0.46	14.80	32,32,32,32	0
86	MG	5	3440	1/1	0.95	0.48	14.46	30,30,30,30	0
86	MG	1	3588	1/1	0.92	0.40	14.38	39,39,39,39	0
86	MG	4	207	1/1	0.94	0.44	14.17	37,37,37,37	0
86	MG	5	3592	1/1	0.98	0.55	14.10	22,22,22,22	0
86	MG	5	3517	1/1	0.86	0.43	14.08	38,38,38,38	0
86	MG	5	3586	1/1	0.96	0.46	14.00	30,30,30,30	0
86	MG	5	3566	1/1	0.97	0.46	13.73	37,37,37,37	0
86	MG	O7	102	1/1	0.90	0.38	13.61	49,49,49,49	0
86	MG	2	1920	1/1	0.95	0.57	13.56	76,76,76,76	0
87	OHX	1	3985	7/7	0.97	0.40	13.51	38,38,38,38	2
86	MG	1	3705	1/1	0.98	0.46	13.49	33,33,33,33	0
86	MG	5	3651	1/1	0.98	0.44	13.46	35,35,35,35	0
87	OHX	1	3983	7/7	0.89	0.47	13.22	77,77,77,77	2
86	MG	1	3517	1/1	0.95	0.40	13.22	46,46,46,46	0
86	MG	1	3670	1/1	0.92	0.41	13.18	38,38,38,38	0
86	MG	5	3597	1/1	0.79	0.38	13.00	48,48,48,48	0
86	MG	6	2006	1/1	0.94	0.62	12.89	67,67,67,67	0
86	MG	5	3589	1/1	0.94	0.53	12.82	35,35,35,35	0
87	OHX	7	222	7/7	0.95	0.40	12.80	38,38,38,38	4
86	MG	1	3742	1/1	0.53	0.69	12.78	44,44,44,44	0
86	MG	1	3540	1/1	0.99	0.51	12.66	41,41,41,41	0
87	OHX	5	4126	7/7	0.89	0.50	12.66	44,44,44,44	3
86	MG	5	3553	1/1	0.87	0.61	12.57	32,32,32,32	0
86	MG	5	3543	1/1	0.95	0.67	12.54	48,48,48,48	0
86	MG	1	3531	1/1	0.97	0.57	12.51	40,40,40,40	0
87	OHX	5	4019	7/7	0.98	0.39	12.49	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3584	1/1	0.94	0.58	12.37	35,35,35,35	0
86	MG	5	3570	1/1	0.94	0.52	12.35	34,34,34,34	0
86	MG	5	3465	1/1	0.96	0.43	12.31	37,37,37,37	0
86	MG	5	3521	1/1	0.89	0.36	12.28	36,36,36,36	0
86	MG	5	3674	1/1	0.94	0.43	12.13	34,34,34,34	1
87	OHX	5	3940	7/7	0.91	0.41	11.96	34,34,34,34	4
86	MG	1	3609	1/1	0.96	0.47	11.90	44,44,44,44	0
86	MG	1	3732	1/1	0.94	0.38	11.76	35,35,35,35	0
87	OHX	2	2119	7/7	0.94	0.36	11.73	62,62,62,62	3
87	OHX	5	4008	7/7	0.96	0.37	11.63	41,41,41,41	3
87	OHX	1	3963	7/7	0.90	0.42	11.51	51,51,51,51	3
86	MG	5	3588	1/1	0.92	0.60	11.45	28,28,28,28	0
86	MG	1	3545	1/1	0.93	0.38	11.41	31,31,31,31	0
86	MG	5	3519	1/1	0.94	0.40	11.33	30,30,30,30	0
87	OHX	5	4088	7/7	0.95	0.28	11.32	47,47,47,47	3
87	OHX	1	3899	7/7	0.91	0.34	11.26	52,52,52,52	4
86	MG	C	102	1/1	0.94	0.58	11.17	39,39,39,39	0
86	MG	1	3433	1/1	0.89	0.45	11.15	34,34,34,34	0
87	OHX	5	3947	7/7	0.83	0.41	10.96	49,49,49,49	2
86	MG	5	3493	1/1	0.92	0.37	10.85	45,45,45,45	0
87	OHX	1	4004	7/7	0.94	0.34	10.85	75,75,75,75	5
87	OHX	5	3912	7/7	0.98	0.22	10.84	77,77,77,77	3
87	OHX	1	3856	7/7	0.90	0.34	10.83	76,76,76,76	3
87	OHX	6	2102	7/7	0.93	0.39	10.75	97,97,97,97	4
87	OHX	7	216	7/7	0.97	0.33	10.73	62,62,62,62	3
86	MG	5	3783	1/1	0.73	0.34	10.61	35,35,35,35	0
86	MG	5	3421	1/1	0.90	0.46	10.58	44,44,44,44	0
86	MG	5	3407	1/1	0.86	0.42	10.55	40,40,40,40	0
86	MG	1	3735	1/1	0.95	0.36	10.54	49,49,49,49	0
87	OHX	1	4064	7/7	0.97	0.39	10.50	39,39,39,39	3
87	OHX	1	4074	7/7	0.92	0.42	10.48	38,38,38,38	3
86	MG	5	3767	1/1	0.98	0.41	10.29	34,34,34,34	0
86	MG	5	3436	1/1	0.97	0.30	10.27	34,34,34,34	0
86	MG	5	4174	1/1	0.92	1.22	10.22	56,56,56,56	0
86	MG	5	3495	1/1	0.99	0.40	10.21	35,35,35,35	0
87	OHX	2	2010	7/7	0.95	0.30	10.19	101,101,101,101	4
86	MG	6	1990	1/1	0.48	0.53	10.17	79,79,79,79	0
86	MG	5	3413	1/1	0.86	0.33	10.14	33,33,33,33	0
87	OHX	2	2106	7/7	0.95	0.34	10.10	78,78,78,78	3
86	MG	5	3420	1/1	0.91	0.41	10.08	38,38,38,38	0
87	OHX	6	2051	7/7	0.93	0.37	10.04	131,131,131,131	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3653	1/1	0.84	1.15	9.98	55,55,55,55	0
86	MG	5	4172	1/1	0.90	0.39	9.94	43,43,43,43	0
86	MG	5	4176	1/1	0.94	0.55	9.78	43,43,43,43	1
86	MG	1	3743	1/1	0.70	0.37	9.74	50,50,50,50	0
86	MG	2	1909	1/1	0.80	0.48	9.70	83,83,83,83	0
87	OHX	5	4072	7/7	0.96	0.32	9.68	44,44,44,44	4
87	OHX	1	4058	7/7	0.91	0.31	9.54	100,100,100,100	4
86	MG	5	3720	1/1	0.90	0.29	9.50	36,36,36,36	0
86	MG	5	3737	1/1	0.85	0.31	9.45	42,42,42,42	0
87	OHX	1	3871	7/7	0.86	0.51	9.42	61,61,61,61	2
86	MG	5	3555	1/1	0.97	0.37	9.38	33,33,33,33	0
87	OHX	1	3883	7/7	0.95	0.27	9.34	71,71,71,71	1
86	MG	5	3565	1/1	0.97	0.66	9.32	31,31,31,31	0
87	OHX	1	4043	7/7	0.98	0.34	9.30	39,39,39,39	2
86	MG	1	3576	1/1	0.93	0.44	9.27	46,46,46,46	0
87	OHX	1	3879	7/7	0.97	0.39	9.24	44,44,44,44	2
87	OHX	5	4077	7/7	0.89	0.35	9.23	68,68,68,68	3
87	OHX	5	3995	7/7	0.98	0.26	9.10	52,52,52,52	3
87	OHX	5	3899	7/7	0.97	0.26	9.06	52,52,52,52	3
87	OHX	2	2022	7/7	0.96	0.36	8.98	78,78,78,78	4
87	OHX	6	2162	7/7	0.93	0.40	8.97	114,114,114,114	5
87	OHX	5	4099	7/7	0.93	0.31	8.93	46,46,46,46	5
87	OHX	3	210	7/7	0.97	0.33	8.91	51,51,51,51	5
86	MG	1	3664	1/1	0.93	0.27	8.90	39,39,39,39	0
86	MG	5	3412	1/1	0.99	0.40	8.82	36,36,36,36	0
86	MG	3	204	1/1	0.95	0.58	8.79	33,33,33,33	0
87	OHX	8	225	7/7	0.94	0.28	8.77	47,47,47,47	3
87	OHX	7	221	7/7	0.96	0.29	8.74	50,50,50,50	4
87	OHX	5	4164	7/7	0.88	0.37	8.68	51,51,51,51	3
86	MG	5	3403	1/1	0.98	0.32	8.56	33,33,33,33	0
86	MG	1	3554	1/1	0.96	0.37	8.54	37,37,37,37	0
87	OHX	1	4062	7/7	0.83	0.40	8.51	51,51,51,51	3
87	OHX	5	3974	7/7	0.94	0.46	8.49	85,85,85,85	3
86	MG	6	1943	1/1	0.91	0.55	8.44	70,70,70,70	0
87	OHX	1	4038	7/7	0.91	0.32	8.34	56,56,56,56	4
86	MG	5	3561	1/1	0.98	0.32	8.34	27,27,27,27	0
87	OHX	6	2097	7/7	0.97	0.54	8.33	49,49,49,49	1
87	OHX	3	212	7/7	0.97	0.27	8.30	86,86,86,86	3
86	MG	5	3577	1/1	0.96	0.41	8.27	35,35,35,35	0
87	OHX	6	2153	7/7	0.93	0.32	8.14	67,67,67,67	3
87	OHX	5	4025	7/7	0.93	0.30	8.08	54,54,54,54	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3654	1/1	0.93	0.31	8.08	42,42,42,42	0
86	MG	1	3466	1/1	0.98	0.37	8.07	37,37,37,37	0
86	MG	L7	302	1/1	0.91	0.74	8.06	50,50,50,50	0
87	OHX	1	3992	7/7	0.97	0.29	8.03	52,52,52,52	3
86	MG	1	3539	1/1	0.90	0.44	8.01	44,44,44,44	0
86	MG	1	3523	1/1	0.64	0.44	7.95	54,54,54,54	0
87	OHX	6	2161	7/7	0.80	0.35	7.92	84,84,84,84	6
86	MG	5	3794	1/1	0.82	0.30	7.89	41,41,41,41	0
86	MG	12	301	1/1	0.96	0.58	7.87	37,37,37,37	0
86	MG	5	3426	1/1	0.97	0.53	7.85	40,40,40,40	0
86	MG	5	3774	1/1	0.87	0.74	7.72	40,40,40,40	0
87	OHX	1	3838	7/7	0.99	0.30	7.70	52,52,52,52	3
87	OHX	2	2151	7/7	0.84	0.31	7.69	112,112,112,112	7
86	MG	5	3512	1/1	0.96	0.35	7.57	37,37,37,37	0
86	MG	2	1937	1/1	0.95	0.39	7.47	80,80,80,80	0
87	OHX	8	224	7/7	0.97	0.29	7.39	40,40,40,40	3
87	OHX	5	4158	7/7	0.77	0.37	7.29	48,48,48,48	4
86	MG	1	3715	1/1	0.97	0.49	7.28	46,46,46,46	0
87	OHX	5	3962	7/7	0.95	0.29	7.17	62,62,62,62	5
86	MG	B	103	1/1	0.98	0.55	7.17	38,38,38,38	0
87	OHX	1	4105	7/7	0.94	0.29	7.16	46,46,46,46	5
86	MG	6	1918	1/1	0.90	0.40	7.15	41,41,41,41	0
86	MG	1	3472	1/1	0.97	0.39	7.12	42,42,42,42	0
87	OHX	5	3931	7/7	0.94	0.26	7.04	139,139,139,139	5
87	OHX	5	3923	7/7	0.97	0.32	7.03	43,43,43,43	5
86	MG	1	3687	1/1	0.93	0.38	7.00	46,46,46,46	0
87	OHX	1	3968	7/7	0.96	0.27	6.99	72,72,72,72	3
87	OHX	8	218	7/7	0.96	0.22	6.98	80,80,80,80	2
86	MG	1	4112	1/1	0.80	0.34	6.90	36,36,36,36	0
86	MG	1	3419	1/1	0.89	0.25	6.89	36,36,36,36	0
87	OHX	5	3915	7/7	0.96	0.32	6.86	77,77,77,77	3
87	OHX	5	3868	7/7	0.95	0.31	6.84	35,35,35,35	4
86	MG	6	1904	1/1	0.91	0.54	6.84	59,59,59,59	0
87	OHX	1	3920	7/7	0.94	0.35	6.83	43,43,43,43	3
87	OHX	5	4042	7/7	0.88	0.36	6.79	38,38,38,38	4
87	OHX	5	4169	7/7	0.97	0.34	6.79	71,71,71,71	3
87	OHX	1	3897	7/7	0.96	0.30	6.76	49,49,49,49	5
87	OHX	5	4106	7/7	0.91	0.23	6.75	81,81,81,81	5
86	MG	2	1922	1/1	0.92	0.56	6.67	85,85,85,85	0
87	OHX	1	4027	7/7	0.94	0.29	6.64	75,75,75,75	3
86	MG	5	3682	1/1	0.91	0.52	6.63	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	6	2146	7/7	0.91	0.48	6.62	48,48,48,48	4
86	MG	5	3506	1/1	0.94	0.39	6.59	38,38,38,38	0
87	OHX	1	4005	7/7	0.97	0.35	6.59	40,40,40,40	4
87	OHX	2	2095	7/7	0.97	0.34	6.56	75,75,75,75	5
86	MG	1	3572	1/1	0.86	0.70	6.54	57,57,57,57	0
87	OHX	5	4083	7/7	0.96	0.30	6.41	35,35,35,35	6
87	OHX	6	2110	7/7	0.92	0.32	6.38	112,112,112,112	6
87	OHX	6	2025	7/7	0.97	0.32	6.38	62,62,62,62	2
86	MG	5	3705	1/1	0.84	0.42	6.36	32,32,32,32	0
87	OHX	1	3820	7/7	0.97	0.38	6.29	47,47,47,47	4
86	MG	5	3717	1/1	0.96	0.52	6.24	26,26,26,26	1
86	MG	5	3491	1/1	0.94	0.46	6.24	30,30,30,30	0
87	OHX	3	211	7/7	0.96	0.33	6.24	64,64,64,64	3
87	OHX	5	4142	7/7	0.83	0.33	6.22	50,50,50,50	4
86	MG	2	1975	1/1	0.88	0.41	6.21	60,60,60,60	0
87	OHX	2	2011	7/7	0.90	0.32	6.18	83,83,83,83	3
86	MG	5	4175	1/1	0.95	0.40	6.18	36,36,36,36	0
87	OHX	5	3903	7/7	0.98	0.28	6.15	49,49,49,49	2
86	MG	8	206	1/1	0.75	0.44	6.12	43,43,43,43	0
86	MG	5	3729	1/1	0.82	0.50	6.11	41,41,41,41	0
87	OHX	7	218	7/7	0.98	0.29	6.10	67,67,67,67	3
87	OHX	1	3791	7/7	0.98	0.30	6.08	41,41,41,41	2
86	MG	5	3779	1/1	0.95	0.28	5.97	30,30,30,30	0
87	OHX	1	4010	7/7	0.95	0.27	5.96	44,44,44,44	5
87	OHX	5	4115	7/7	0.87	0.33	5.93	52,52,52,52	4
86	MG	1	3586	1/1	0.88	0.29	5.92	45,45,45,45	0
87	OHX	5	3984	7/7	0.96	0.19	5.92	55,55,55,55	2
87	OHX	2	2097	7/7	0.95	0.37	5.84	73,73,73,73	5
87	OHX	5	3875	7/7	0.96	0.32	5.82	43,43,43,43	3
87	OHX	1	3793	7/7	0.98	0.27	5.81	68,68,68,68	4
86	MG	1	3426	1/1	0.95	0.48	5.77	52,52,52,52	0
86	MG	5	3569	1/1	0.98	0.41	5.77	29,29,29,29	0
86	MG	1	4115	1/1	0.96	0.28	5.75	42,42,42,42	0
87	OHX	1	3915	7/7	0.85	0.40	5.73	66,66,66,66	4
87	OHX	1	3906	7/7	0.96	0.33	5.68	65,65,65,65	4
87	OHX	1	3807	7/7	0.97	0.33	5.68	73,73,73,73	2
86	MG	1	3618	1/1	0.88	0.37	5.63	39,39,39,39	0
87	OHX	1	3859	7/7	0.96	0.28	5.63	53,53,53,53	2
87	OHX	1	3846	7/7	0.98	0.22	5.60	119,119,119,119	3
87	OHX	5	3844	7/7	0.99	0.25	5.59	48,48,48,48	2
87	OHX	5	3845	7/7	0.98	0.28	5.54	37,37,37,37	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3406	1/1	0.86	0.28	5.51	44,44,44,44	0
86	MG	6	1952	1/1	0.95	0.66	5.48	53,53,53,53	0
87	OHX	5	4101	7/7	0.94	0.23	5.48	45,45,45,45	5
87	OHX	5	4007	7/7	0.94	0.30	5.47	66,66,66,66	3
87	OHX	1	3887	7/7	0.95	0.20	5.42	131,131,131,131	5
87	OHX	1	3876	7/7	0.98	0.30	5.36	41,41,41,41	2
87	OHX	6	2122	7/7	0.95	0.33	5.32	77,77,77,77	4
87	OHX	5	3942	7/7	0.97	0.29	5.32	44,44,44,44	2
86	MG	1	3476	1/1	0.90	0.29	5.31	43,43,43,43	0
86	MG	5	3530	1/1	0.98	0.24	5.31	55,55,55,55	0
87	OHX	1	3955	7/7	0.90	0.27	5.30	71,71,71,71	3
87	OHX	1	4095	7/7	0.91	0.25	5.29	55,55,55,55	5
86	MG	1	3511	1/1	0.97	0.51	5.20	36,36,36,36	0
86	MG	6	1910	1/1	0.90	0.30	5.16	91,91,91,91	0
86	MG	2	1926	1/1	0.95	0.31	5.14	76,76,76,76	0
86	MG	1	3589	1/1	0.98	0.31	5.14	40,40,40,40	0
86	MG	6	1974	1/1	0.45	0.36	5.11	94,94,94,94	0
87	OHX	2	2108	7/7	0.96	0.24	5.08	79,79,79,79	5
86	MG	1	3556	1/1	0.98	0.41	5.04	29,29,29,29	0
87	OHX	6	2043	7/7	0.95	0.32	5.03	90,90,90,90	5
87	OHX	8	222	7/7	0.92	0.27	5.00	75,75,75,75	5
87	OHX	5	4086	7/7	0.88	0.27	4.98	39,39,39,39	5
87	OHX	4	231	7/7	0.85	0.31	4.97	73,73,73,73	5
87	OHX	6	2126	7/7	0.95	0.31	4.94	53,53,53,53	3
86	MG	5	3471	1/1	0.94	0.37	4.92	39,39,39,39	0
87	OHX	6	2158	7/7	0.87	0.30	4.91	131,131,131,131	7
86	MG	m5	301	1/1	0.87	0.35	4.84	46,46,46,46	0
87	OHX	6	2020	7/7	0.97	0.22	4.82	100,100,100,100	4
87	OHX	5	3851	7/7	0.99	0.28	4.80	55,55,55,55	2
86	MG	5	3678	1/1	0.98	0.47	4.79	31,31,31,31	1
87	OHX	1	3815	7/7	0.98	0.24	4.76	85,85,85,85	3
86	MG	4	233	1/1	0.81	0.51	4.74	62,62,62,62	0
87	OHX	1	4072	7/7	0.94	0.30	4.72	47,47,47,47	3
86	MG	2	1981	1/1	0.96	0.48	4.69	79,79,79,79	0
86	MG	5	3638	1/1	0.96	0.29	4.69	36,36,36,36	0
86	MG	1	3563	1/1	0.93	0.29	4.69	41,41,41,41	0
87	OHX	4	224	7/7	0.96	0.25	4.69	44,44,44,44	3
86	MG	5	3456	1/1	0.94	0.30	4.68	38,38,38,38	0
86	MG	12	302	1/1	0.92	0.46	4.64	45,45,45,45	0
86	MG	5	3590	1/1	0.96	0.38	4.63	42,42,42,42	0
87	OHX	5	4027	7/7	0.96	0.24	4.54	72,72,72,72	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3778	7/7	0.99	0.27	4.54	64,64,64,64	1
87	OHX	1	3825	7/7	0.94	0.28	4.54	91,91,91,91	5
87	OHX	6	2107	7/7	0.93	0.27	4.52	81,81,81,81	5
87	OHX	1	3853	7/7	0.96	0.32	4.52	54,54,54,54	3
87	OHX	1	3849	7/7	0.94	0.27	4.51	48,48,48,48	5
87	OHX	5	3904	7/7	0.98	0.28	4.50	51,51,51,51	4
87	OHX	5	3965	7/7	0.96	0.23	4.50	50,50,50,50	4
86	MG	1	3429	1/1	0.93	0.29	4.45	36,36,36,36	0
87	OHX	1	3936	7/7	0.97	0.31	4.41	54,54,54,54	3
87	OHX	5	4052	7/7	0.94	0.21	4.39	65,65,65,65	5
86	MG	5	3591	1/1	0.93	0.46	4.37	35,35,35,35	0
87	OHX	5	3976	7/7	0.96	0.24	4.36	58,58,58,58	4
87	OHX	5	3914	7/7	0.97	0.27	4.31	39,39,39,39	4
87	OHX	2	2129	7/7	0.92	0.27	4.29	87,87,87,87	5
86	MG	2	1950	1/1	0.73	0.30	4.27	108,108,108,108	0
87	OHX	5	4012	7/7	0.90	0.20	4.25	119,119,119,119	4
87	OHX	1	3843	7/7	0.98	0.26	4.24	55,55,55,55	2
87	OHX	6	2073	7/7	0.96	0.33	4.22	69,69,69,69	5
87	OHX	1	4030	7/7	0.91	0.23	4.22	130,130,130,130	6
86	MG	6	1915	1/1	0.64	0.36	4.22	75,75,75,75	0
86	MG	6	1978	1/1	0.81	0.59	4.21	77,77,77,77	0
87	OHX	2	2148	7/7	0.92	0.29	4.21	69,69,69,69	6
87	OHX	2	2134	7/7	0.86	0.30	4.21	74,74,74,74	4
87	OHX	7	219	7/7	0.99	0.24	4.14	67,67,67,67	2
87	OHX	5	4049	7/7	0.92	0.32	4.13	45,45,45,45	3
86	MG	5	3796	1/1	0.96	0.28	4.12	39,39,39,39	0
87	OHX	2	1998	7/7	0.97	0.20	4.12	116,116,116,116	2
86	MG	2	1931	1/1	0.96	0.38	4.10	65,65,65,65	0
86	MG	1	3401	1/1	0.96	0.31	4.08	43,43,43,43	0
86	MG	6	1938	1/1	0.93	0.30	4.04	60,60,60,60	0
87	OHX	1	4066	7/7	0.89	0.27	4.03	63,63,63,63	6
87	OHX	6	2088	7/7	0.92	0.28	4.03	99,99,99,99	3
87	OHX	5	3916	7/7	0.94	0.34	4.02	49,49,49,49	3
87	OHX	1	3896	7/7	0.99	0.33	4.00	49,49,49,49	2
87	OHX	6	2089	7/7	0.96	0.24	3.99	56,56,56,56	4
87	OHX	6	2044	7/7	0.96	0.25	3.99	46,46,46,46	2
86	MG	1	3567	1/1	0.83	0.37	3.96	48,48,48,48	0
87	OHX	5	4124	7/7	0.90	0.35	3.96	48,48,48,48	5
86	MG	1	3479	1/1	0.98	0.29	3.94	45,45,45,45	0
87	OHX	5	3822	7/7	0.99	0.23	3.92	53,53,53,53	2
87	OHX	1	4071	7/7	0.95	0.31	3.90	42,42,42,42	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	4116	1/1	0.99	0.38	3.89	33,33,33,33	0
87	OHX	5	4048	7/7	0.95	0.24	3.88	37,37,37,37	3
86	MG	l3	402	1/1	0.97	0.53	3.86	39,39,39,39	1
87	OHX	6	2150	7/7	0.89	0.30	3.85	78,78,78,78	6
86	MG	5	3596	1/1	0.91	0.26	3.85	44,44,44,44	0
87	OHX	5	3855	7/7	0.98	0.26	3.83	65,65,65,65	3
87	OHX	5	4011	7/7	0.95	0.27	3.81	41,41,41,41	4
87	OHX	5	4010	7/7	0.90	0.26	3.79	120,120,120,120	3
87	OHX	2	2027	7/7	0.96	0.28	3.79	75,75,75,75	4
89	SPS	5	3402	23/23	0.95	0.35	3.77	35,38,52,54	23
87	OHX	1	3903	7/7	0.98	0.21	3.77	53,53,53,53	3
87	OHX	5	3881	7/7	0.97	0.20	3.72	89,89,89,89	3
87	OHX	1	3874	7/7	0.97	0.27	3.71	50,50,50,50	3
87	OHX	5	3909	7/7	0.97	0.27	3.68	57,57,57,57	3
87	OHX	5	3928	7/7	0.98	0.29	3.66	41,41,41,41	4
87	OHX	1	3993	7/7	0.95	0.21	3.66	94,94,94,94	7
87	OHX	5	3833	7/7	0.99	0.27	3.65	51,51,51,51	1
87	OHX	1	4024	7/7	0.91	0.29	3.64	42,42,42,42	3
87	OHX	6	2106	7/7	0.96	0.25	3.62	85,85,85,85	4
87	OHX	5	3843	7/7	1.00	0.23	3.62	62,62,62,62	2
87	OHX	5	3894	7/7	0.97	0.22	3.61	63,63,63,63	3
86	MG	1	3481	1/1	0.95	0.34	3.61	40,40,40,40	0
86	MG	2	1912	1/1	0.74	0.53	3.59	88,88,88,88	0
87	OHX	4	216	7/7	0.98	0.24	3.52	61,61,61,61	3
87	OHX	6	2041	7/7	0.98	0.26	3.52	56,56,56,56	4
87	OHX	1	4006	7/7	0.95	0.26	3.50	48,48,48,48	5
86	MG	6	1944	1/1	0.80	0.29	3.48	63,63,63,63	0
86	MG	1	3719	1/1	0.85	0.48	3.48	65,65,65,65	0
86	MG	5	3564	1/1	0.96	0.33	3.46	32,32,32,32	0
87	OHX	1	3947	7/7	0.96	0.28	3.45	80,80,80,80	3
87	OHX	6	2164	7/7	0.86	0.37	3.44	44,44,44,44	5
87	OHX	1	4048	7/7	0.88	0.23	3.42	116,116,116,116	5
87	OHX	2	2057	7/7	0.94	0.29	3.39	79,79,79,79	1
87	OHX	5	3839	7/7	0.99	0.24	3.39	65,65,65,65	2
87	OHX	5	3937	7/7	0.96	0.20	3.39	50,50,50,50	3
87	OHX	6	2065	7/7	0.94	0.17	3.39	138,138,138,138	5
86	MG	d6	102	1/1	0.81	0.60	3.37	68,68,68,68	0
87	OHX	5	3998	7/7	0.97	0.28	3.37	38,38,38,38	5
87	OHX	5	3865	7/7	0.97	0.26	3.37	60,60,60,60	3
87	OHX	1	3830	7/7	0.98	0.21	3.36	99,99,99,99	3
87	OHX	1	3923	7/7	0.98	0.24	3.35	40,40,40,40	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	1925	1/1	0.83	0.30	3.34	49,49,49,49	0
87	OHX	8	220	7/7	0.97	0.25	3.32	62,62,62,62	3
87	OHX	1	3966	7/7	0.92	0.28	3.31	35,35,35,35	3
87	OHX	6	2058	7/7	0.98	0.23	3.31	72,72,72,72	2
87	OHX	3	214	7/7	0.97	0.25	3.29	83,83,83,83	4
87	OHX	6	2092	7/7	0.97	0.27	3.28	69,69,69,69	4
87	OHX	M0	302	7/7	0.94	0.41	3.27	55,55,55,55	4
87	OHX	5	3893	7/7	0.98	0.25	3.26	50,50,50,50	2
87	OHX	8	214	7/7	0.98	0.27	3.24	60,60,60,60	3
86	MG	6	1951	1/1	0.90	0.57	3.22	43,43,43,43	0
87	OHX	5	3989	7/7	0.97	0.24	3.22	44,44,44,44	4
87	OHX	1	3898	7/7	0.96	0.21	3.21	89,89,89,89	5
87	OHX	2	1995	7/7	0.99	0.30	3.21	76,76,76,76	2
87	OHX	1	3911	7/7	0.97	0.22	3.20	61,61,61,61	3
86	MG	1	3403	1/1	0.91	0.27	3.18	42,42,42,42	0
87	OHX	1	4032	7/7	0.91	0.28	3.18	52,52,52,52	3
86	MG	5	3672	1/1	0.82	0.29	3.18	78,78,78,78	0
87	OHX	6	2128	7/7	0.97	0.36	3.17	53,53,53,53	4
87	OHX	1	3835	7/7	0.98	0.29	3.16	62,62,62,62	1
87	OHX	1	4003	7/7	0.96	0.19	3.14	63,63,63,63	3
87	OHX	5	4046	7/7	0.91	0.33	3.11	28,28,28,28	1
87	OHX	5	3935	7/7	0.94	0.22	3.10	49,49,49,49	3
87	OHX	1	3885	7/7	0.98	0.26	3.10	53,53,53,53	3
87	OHX	1	3962	7/7	0.97	0.34	3.08	59,59,59,59	2
86	MG	6	1929	1/1	0.96	0.30	3.08	49,49,49,49	0
87	OHX	5	3986	7/7	0.99	0.25	3.06	41,41,41,41	3
86	MG	5	3741	1/1	0.93	0.33	3.05	31,31,31,31	1
87	OHX	5	3900	7/7	0.99	0.26	3.04	43,43,43,43	3
87	OHX	3	219	7/7	0.77	0.25	3.03	82,82,82,82	5
87	OHX	2	2117	7/7	0.85	0.33	3.02	93,93,93,93	4
87	OHX	5	3877	7/7	0.99	0.21	3.02	73,73,73,73	3
86	MG	6	1906	1/1	0.93	0.35	3.00	76,76,76,76	0
86	MG	5	3462	1/1	0.90	0.27	3.00	39,39,39,39	0
87	OHX	5	3818	7/7	0.99	0.25	2.98	51,51,51,51	3
87	OHX	6	2137	7/7	0.89	0.21	2.93	95,95,95,95	4
86	MG	1	3739	1/1	0.81	0.36	2.93	72,72,72,72	0
86	MG	6	1968	1/1	0.97	0.26	2.91	48,48,48,48	0
87	OHX	1	3886	7/7	0.95	0.23	2.90	56,56,56,56	4
87	OHX	5	4024	7/7	0.97	0.28	2.88	50,50,50,50	2
87	OHX	7	224	7/7	0.90	0.24	2.84	54,54,54,54	5
87	OHX	2	2051	7/7	0.95	0.26	2.83	101,101,101,101	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4015	7/7	0.97	0.27	2.82	47,47,47,47	2
87	OHX	5	4117	7/7	0.97	0.26	2.82	49,49,49,49	4
87	OHX	1	3800	7/7	0.99	0.28	2.81	44,44,44,44	3
87	OHX	5	4082	7/7	0.93	0.29	2.81	53,53,53,53	3
87	OHX	5	3888	7/7	0.95	0.46	2.79	42,42,42,42	3
86	MG	5	3405	1/1	0.88	0.26	2.79	47,47,47,47	0
87	OHX	1	3976	7/7	0.96	0.30	2.78	41,41,41,41	4
87	OHX	5	3939	7/7	0.97	0.26	2.78	62,62,62,62	2
86	MG	n6	201	1/1	0.86	0.43	2.76	56,56,56,56	0
86	MG	1	3441	1/1	0.97	0.45	2.76	52,52,52,52	0
87	OHX	1	3841	7/7	0.97	0.20	2.76	70,70,70,70	3
87	OHX	5	3949	7/7	0.95	0.19	2.74	95,95,95,95	4
87	OHX	2	2056	7/7	0.98	0.25	2.74	99,99,99,99	4
86	MG	2	1962	1/1	0.94	0.36	2.73	88,88,88,88	0
86	MG	5	3409	1/1	0.83	0.29	2.72	29,29,29,29	0
87	OHX	5	4054	7/7	0.93	0.30	2.72	56,56,56,56	4
87	OHX	5	4120	7/7	0.92	0.25	2.72	68,68,68,68	7
87	OHX	6	2029	7/7	0.96	0.24	2.70	68,68,68,68	2
87	OHX	6	2032	7/7	0.98	0.20	2.66	117,117,117,117	2
87	OHX	1	4008	7/7	0.96	0.27	2.65	47,47,47,47	5
87	OHX	1	4016	7/7	0.93	0.34	2.65	56,56,56,56	3
87	OHX	6	2072	7/7	0.95	0.30	2.63	76,76,76,76	3
87	OHX	1	3784	7/7	0.99	0.26	2.62	73,73,73,73	2
87	OHX	5	4159	7/7	0.90	0.37	2.62	37,37,37,37	5
86	MG	6	2010	1/1	0.91	0.25	2.60	53,53,53,53	0
87	OHX	5	3943	7/7	0.98	0.23	2.60	42,42,42,42	3
87	OHX	19	201	7/7	0.92	0.31	2.60	61,61,61,61	2
87	OHX	2	2132	7/7	0.96	0.32	2.58	87,87,87,87	3
87	OHX	5	3910	7/7	0.98	0.22	2.58	44,44,44,44	4
87	OHX	5	4123	7/7	0.94	0.30	2.57	51,51,51,51	6
87	OHX	2	2037	7/7	0.97	0.27	2.57	73,73,73,73	4
87	OHX	1	3834	7/7	0.97	0.28	2.56	62,62,62,62	3
87	OHX	5	3966	7/7	0.97	0.24	2.56	49,49,49,49	5
86	MG	1	3661	1/1	0.78	0.26	2.55	51,51,51,51	0
87	OHX	1	3798	7/7	0.99	0.21	2.55	69,69,69,69	1
86	MG	5	3680	1/1	0.81	0.34	2.54	43,43,43,43	0
87	OHX	1	3884	7/7	0.97	0.20	2.52	74,74,74,74	4
87	OHX	5	3854	7/7	0.98	0.23	2.52	71,71,71,71	3
87	OHX	5	3873	7/7	0.97	0.23	2.50	62,62,62,62	3
87	OHX	5	4134	7/7	0.93	0.24	2.49	54,54,54,54	4
87	OHX	5	4093	7/7	0.96	0.29	2.49	36,36,36,36	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3808	7/7	0.98	0.24	2.49	74,74,74,74	3
86	MG	5	3800	1/1	0.87	0.36	2.48	44,44,44,44	0
87	OHX	2	2008	7/7	0.98	0.22	2.47	89,89,89,89	5
86	MG	5	3769	1/1	0.98	0.30	2.46	47,47,47,47	0
87	OHX	2	2032	7/7	0.97	0.23	2.46	102,102,102,102	6
87	OHX	2	2136	7/7	0.97	0.24	2.45	74,74,74,74	6
86	MG	1	3738	1/1	0.97	0.25	2.43	41,41,41,41	0
87	OHX	1	3822	7/7	0.99	0.22	2.43	50,50,50,50	4
86	MG	1	3668	1/1	0.98	0.24	2.41	38,38,38,38	1
87	OHX	o7	503	7/7	0.99	0.29	2.40	62,62,62,62	1
87	OHX	6	2178	7/7	0.68	0.28	2.38	145,145,145,145	6
86	MG	n8	201	1/1	0.93	0.32	2.37	37,37,37,37	0
86	MG	d2	201	1/1	0.98	0.31	2.36	59,59,59,59	0
87	OHX	5	4162	7/7	0.94	0.30	2.35	36,36,36,36	4
87	OHX	2	2047	7/7	0.95	0.23	2.34	80,80,80,80	4
87	OHX	1	3890	7/7	0.95	0.30	2.34	48,48,48,48	3
87	OHX	1	3888	7/7	0.98	0.27	2.33	71,71,71,71	3
86	MG	6	1975	1/1	0.95	0.21	2.31	90,90,90,90	0
86	MG	5	3785	1/1	0.98	0.27	2.29	35,35,35,35	0
86	MG	L2	302	1/1	0.97	0.30	2.29	41,41,41,41	0
87	OHX	5	3911	7/7	0.99	0.17	2.28	107,107,107,107	2
87	OHX	1	4084	7/7	0.94	0.25	2.26	42,42,42,42	5
87	OHX	N9	101	7/7	1.00	0.22	2.26	64,64,64,64	1
87	OHX	1	3938	7/7	0.97	0.24	2.26	53,53,53,53	3
86	MG	1	3578	1/1	0.94	0.30	2.24	60,60,60,60	0
87	OHX	O9	101	7/7	0.81	0.37	2.20	51,51,51,51	6
87	OHX	1	3782	7/7	0.99	0.23	2.16	71,71,71,71	4
86	MG	1	3737	1/1	0.76	0.42	2.14	63,63,63,63	0
87	OHX	5	3941	7/7	0.92	0.28	2.12	50,50,50,50	5
86	MG	5	3546	1/1	0.95	0.34	2.11	53,53,53,53	0
87	OHX	2	2091	7/7	0.97	0.27	2.11	89,89,89,89	5
86	MG	s8	302	1/1	0.83	0.45	2.10	49,49,49,49	0
87	OHX	5	3862	7/7	0.98	0.20	2.09	85,85,85,85	3
87	OHX	1	4107	7/7	0.89	0.17	2.09	91,91,91,91	6
86	MG	5	3606	1/1	0.95	0.26	2.09	36,36,36,36	0
87	OHX	1	4083	7/7	0.92	0.20	2.08	45,45,45,45	4
87	OHX	6	2045	7/7	0.97	0.23	2.07	91,91,91,91	5
87	OHX	5	3922	7/7	0.99	0.26	2.07	41,41,41,41	1
86	MG	2	1938	1/1	0.72	0.26	2.05	72,72,72,72	0
87	OHX	1	3786	7/7	0.99	0.20	2.04	94,94,94,94	3
87	OHX	5	3948	7/7	0.95	0.22	2.04	56,56,56,56	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3794	7/7	0.99	0.30	2.04	69,69,69,69	2
87	OHX	5	4038	7/7	0.97	0.21	2.03	72,72,72,72	4
87	OHX	2	2125	7/7	0.90	0.24	2.02	147,147,147,147	6
87	OHX	5	3964	7/7	0.97	0.20	2.00	49,49,49,49	4
87	OHX	5	3840	7/7	1.00	0.20	1.99	51,51,51,51	1
86	MG	1	3409	1/1	0.89	0.28	1.96	52,52,52,52	0
87	OHX	6	2014	7/7	0.99	0.25	1.96	76,76,76,76	3
87	OHX	6	2151	7/7	0.96	0.24	1.94	65,65,65,65	4
87	OHX	1	3868	7/7	0.99	0.19	1.94	53,53,53,53	4
87	OHX	1	3799	7/7	0.99	0.22	1.93	78,78,78,78	3
87	OHX	5	3968	7/7	0.96	0.20	1.91	105,105,105,105	5
87	OHX	8	219	7/7	0.98	0.23	1.88	44,44,44,44	3
87	OHX	1	3872	7/7	0.98	0.25	1.86	44,44,44,44	4
87	OHX	m8	201	7/7	0.95	0.29	1.85	47,47,47,47	3
86	MG	2	1966	1/1	0.90	0.24	1.84	74,74,74,74	0
87	OHX	1	3902	7/7	0.97	0.24	1.83	53,53,53,53	3
87	OHX	5	3972	7/7	0.99	0.25	1.82	39,39,39,39	4
87	OHX	1	3773	7/7	0.99	0.26	1.81	49,49,49,49	2
86	MG	2	1967	1/1	0.79	0.29	1.80	93,93,93,93	0
87	OHX	6	2019	7/7	0.99	0.24	1.79	79,79,79,79	2
87	OHX	1	3826	7/7	0.98	0.19	1.79	84,84,84,84	4
87	OHX	5	3878	7/7	0.98	0.26	1.79	59,59,59,59	3
87	OHX	5	3857	7/7	0.98	0.22	1.78	72,72,72,72	3
87	OHX	2	2079	7/7	0.98	0.34	1.78	82,82,82,82	3
87	OHX	1	4040	7/7	0.97	0.25	1.77	52,52,52,52	4
87	OHX	6	2119	7/7	0.96	0.25	1.76	60,60,60,60	3
87	OHX	6	2017	7/7	0.99	0.23	1.75	59,59,59,59	2
87	OHX	1	3840	7/7	0.98	0.19	1.74	85,85,85,85	3
87	OHX	6	2066	7/7	0.94	0.17	1.74	162,162,162,162	3
87	OHX	5	3898	7/7	0.98	0.21	1.73	49,49,49,49	3
87	OHX	5	3874	7/7	0.98	0.25	1.73	49,49,49,49	2
87	OHX	1	3996	7/7	0.95	0.24	1.72	64,64,64,64	5
87	OHX	5	4156	7/7	0.87	0.27	1.72	44,44,44,44	5
87	OHX	1	4092	7/7	0.92	0.26	1.72	47,47,47,47	3
87	OHX	2	2122	7/7	0.83	0.38	1.71	91,91,91,91	7
87	OHX	1	3787	7/7	0.97	0.22	1.69	72,72,72,72	3
87	OHX	6	2070	7/7	0.98	0.22	1.68	87,87,87,87	3
87	OHX	5	4055	7/7	0.97	0.21	1.67	40,40,40,40	6
87	OHX	6	2147	7/7	0.94	0.25	1.65	64,64,64,64	4
87	OHX	5	4018	7/7	0.96	0.17	1.63	76,76,76,76	6
87	OHX	6	2093	7/7	0.97	0.20	1.62	45,45,45,45	2
87	OHX	4	223	7/7	0.97	0.17	1.61	86,86,86,86	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2045	7/7	0.94	0.26	1.61	95,95,95,95	4
86	MG	1	3478	1/1	0.89	0.20	1.60	60,60,60,60	0
87	OHX	1	4018	7/7	0.93	0.24	1.59	69,69,69,69	3
86	MG	1	3474	1/1	0.86	0.32	1.58	48,48,48,48	0
87	OHX	2	2058	7/7	0.95	0.31	1.57	67,67,67,67	4
87	OHX	5	4065	7/7	0.96	0.26	1.55	38,38,38,38	4
86	MG	1	3592	1/1	0.85	0.21	1.53	61,61,61,61	0
87	OHX	5	3901	7/7	0.97	0.21	1.52	72,72,72,72	3
87	OHX	5	3831	7/7	0.99	0.23	1.52	56,56,56,56	2
86	MG	2	1942	1/1	0.88	0.26	1.51	69,69,69,69	0
87	OHX	M6	203	7/7	0.98	0.35	1.50	43,43,43,43	2
87	OHX	1	3767	7/7	0.99	0.19	1.49	77,77,77,77	2
87	OHX	5	3830	7/7	1.00	0.21	1.48	61,61,61,61	1
86	MG	1	3758	1/1	0.90	0.24	1.48	48,48,48,48	0
87	OHX	2	2012	7/7	0.98	0.23	1.46	87,87,87,87	3
87	OHX	6	2061	7/7	0.97	0.25	1.46	86,86,86,86	4
87	OHX	6	2172	7/7	0.90	0.39	1.42	69,69,69,69	3
87	OHX	4	217	7/7	0.98	0.25	1.42	55,55,55,55	2
87	OHX	5	4096	7/7	0.93	0.20	1.42	75,75,75,75	6
87	OHX	2	2036	7/7	0.89	0.18	1.42	145,145,145,145	5
87	OHX	5	3993	7/7	0.96	0.23	1.41	42,42,42,42	4
87	OHX	6	2149	7/7	0.88	0.28	1.40	95,95,95,95	6
87	OHX	1	3929	7/7	0.97	0.22	1.38	53,53,53,53	4
87	OHX	5	3944	7/7	0.96	0.27	1.36	46,46,46,46	3
86	MG	5	3422	1/1	0.69	0.23	1.36	43,43,43,43	0
87	OHX	m0	301	7/7	0.95	0.37	1.35	49,49,49,49	3
87	OHX	5	4103	7/7	0.93	0.42	1.33	68,68,68,68	6
86	MG	1	3693	1/1	0.88	0.20	1.32	49,49,49,49	0
87	OHX	2	2150	7/7	0.76	0.15	1.32	151,151,151,151	7
86	MG	1	3733	1/1	0.99	0.27	1.31	40,40,40,40	0
87	OHX	1	3827	7/7	0.99	0.26	1.31	45,45,45,45	4
87	OHX	1	3833	7/7	0.98	0.25	1.31	71,71,71,71	4
87	OHX	1	3958	7/7	0.95	0.28	1.30	45,45,45,45	4
87	OHX	5	4074	7/7	0.92	0.23	1.29	47,47,47,47	3
87	OHX	1	4085	7/7	0.91	0.19	1.26	61,61,61,61	6
87	OHX	1	3817	7/7	0.98	0.19	1.25	109,109,109,109	5
87	OHX	6	2112	7/7	0.97	0.28	1.25	66,66,66,66	4
87	OHX	5	3913	7/7	0.96	0.22	1.25	74,74,74,74	4
87	OHX	1	3821	7/7	0.96	0.28	1.24	66,66,66,66	5
87	OHX	5	4069	7/7	0.96	0.20	1.24	73,73,73,73	3
87	OHX	6	2108	7/7	0.96	0.16	1.23	109,109,109,109	6
87	OHX	5	3936	7/7	0.98	0.24	1.23	53,53,53,53	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3981	7/7	0.96	0.34	1.23	53,53,53,53	3
87	OHX	1	4029	7/7	0.86	0.28	1.22	82,82,82,82	3
86	MG	5	3418	1/1	0.94	0.22	1.21	36,36,36,36	0
87	OHX	1	3944	7/7	0.98	0.23	1.21	48,48,48,48	4
87	OHX	2	2074	7/7	0.92	0.26	1.18	85,85,85,85	3
87	OHX	5	4058	7/7	0.94	0.26	1.18	47,47,47,47	3
87	OHX	q2	502	7/7	0.98	0.25	1.17	47,47,47,47	2
86	MG	6	1973	1/1	0.91	0.32	1.17	51,51,51,51	0
87	OHX	5	4163	7/7	0.88	0.28	1.16	61,61,61,61	7
87	OHX	5	4017	7/7	0.98	0.27	1.15	48,48,48,48	4
87	OHX	6	2049	7/7	0.98	0.20	1.14	97,97,97,97	3
87	OHX	1	3889	7/7	0.98	0.23	1.13	48,48,48,48	2
87	OHX	8	211	7/7	0.99	0.24	1.13	57,57,57,57	3
87	OHX	6	2035	7/7	0.98	0.24	1.11	82,82,82,82	3
87	OHX	1	3766	7/7	0.99	0.23	1.11	61,61,61,61	2
87	OHX	2	2093	7/7	0.93	0.23	1.11	110,110,110,110	5
87	OHX	5	3826	7/7	0.99	0.20	1.11	80,80,80,80	1
87	OHX	5	3892	7/7	0.99	0.24	1.10	59,59,59,59	2
86	MG	1	3440	1/1	0.93	0.51	1.09	49,49,49,49	0
87	OHX	M0	303	7/7	0.82	0.27	1.07	101,101,101,101	6
87	OHX	1	3775	7/7	0.99	0.18	1.07	66,66,66,66	2
87	OHX	6	2116	7/7	0.98	0.24	1.06	61,61,61,61	2
87	OHX	2	2002	7/7	0.97	0.23	1.05	101,101,101,101	3
86	MG	1	3480	1/1	0.90	0.38	1.05	46,46,46,46	0
87	OHX	7	214	7/7	0.99	0.28	1.05	70,70,70,70	1
87	OHX	1	3892	7/7	0.96	0.23	1.02	65,65,65,65	3
87	OHX	1	4019	7/7	0.87	0.29	1.01	47,47,47,47	2
87	OHX	5	4137	7/7	0.96	0.25	1.01	44,44,44,44	5
87	OHX	2	2123	7/7	0.85	0.33	1.00	121,121,121,121	5
87	OHX	4	232	7/7	0.94	0.25	1.00	65,65,65,65	5
87	OHX	5	3832	7/7	1.00	0.21	0.99	59,59,59,59	2
87	OHX	4	218	7/7	0.98	0.25	0.97	60,60,60,60	4
87	OHX	6	2021	7/7	0.99	0.23	0.96	69,69,69,69	3
87	OHX	5	4037	7/7	0.96	0.17	0.96	106,106,106,106	4
87	OHX	1	3900	7/7	0.95	0.25	0.95	57,57,57,57	3
87	OHX	6	2091	7/7	0.97	0.25	0.94	83,83,83,83	3
87	OHX	M5	302	7/7	0.99	0.21	0.94	61,61,61,61	2
87	OHX	1	3763	7/7	0.99	0.24	0.94	58,58,58,58	2
87	OHX	1	3867	7/7	0.85	0.32	0.93	51,51,51,51	4
87	OHX	1	3831	7/7	0.98	0.21	0.91	48,48,48,48	3
87	OHX	1	3991	7/7	0.97	0.27	0.90	57,57,57,57	3
87	OHX	6	2028	7/7	0.99	0.20	0.88	63,63,63,63	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	4	215	7/7	0.99	0.20	0.87	59,59,59,59	3
87	OHX	5	4097	7/7	0.90	0.20	0.87	106,106,106,106	5
87	OHX	6	2078	7/7	0.96	0.23	0.86	60,60,60,60	5
87	OHX	5	3985	7/7	0.97	0.26	0.85	58,58,58,58	5
87	OHX	2	2024	7/7	0.97	0.25	0.85	100,100,100,100	6
86	MG	1	3676	1/1	0.94	0.25	0.84	52,52,52,52	0
86	MG	n8	202	1/1	0.89	0.31	0.83	50,50,50,50	0
87	OHX	2	2115	7/7	0.94	0.24	0.83	91,91,91,91	6
87	OHX	1	3928	7/7	0.87	0.28	0.80	49,49,49,49	3
87	OHX	6	2103	7/7	0.91	0.26	0.79	67,67,67,67	4
87	OHX	1	3880	7/7	0.98	0.22	0.78	47,47,47,47	5
87	OHX	2	2053	7/7	0.95	0.25	0.76	107,107,107,107	4
88	ZN	d7	101	1/1	0.88	0.41	0.76	147,147,147,147	0
87	OHX	5	3821	7/7	1.00	0.20	0.76	61,61,61,61	2
87	OHX	2	2147	7/7	0.91	0.21	0.75	116,116,116,116	6
87	OHX	5	4057	7/7	0.94	0.24	0.75	36,36,36,36	6
87	OHX	1	3829	7/7	0.97	0.23	0.75	59,59,59,59	2
86	MG	5	3548	1/1	0.85	0.32	0.74	43,43,43,43	0
87	OHX	3	215	7/7	0.96	0.15	0.72	90,90,90,90	3
87	OHX	1	4007	7/7	0.97	0.20	0.72	43,43,43,43	4
87	OHX	5	3816	7/7	0.99	0.19	0.71	53,53,53,53	4
87	OHX	1	4020	7/7	0.96	0.25	0.70	47,47,47,47	3
87	OHX	1	3948	7/7	0.98	0.21	0.70	37,37,37,37	2
87	OHX	1	3789	7/7	0.99	0.19	0.69	74,74,74,74	2
86	MG	5	3595	1/1	0.94	0.22	0.68	47,47,47,47	0
87	OHX	5	4056	7/7	0.94	0.24	0.67	50,50,50,50	2
87	OHX	8	213	7/7	0.98	0.21	0.64	62,62,62,62	4
86	MG	1	3615	1/1	0.85	0.30	0.63	68,68,68,68	0
87	OHX	5	4068	7/7	0.93	0.23	0.63	58,58,58,58	5
87	OHX	1	4059	7/7	0.96	0.29	0.63	72,72,72,72	4
87	OHX	2	2003	7/7	0.99	0.24	0.63	76,76,76,76	5
87	OHX	1	4080	7/7	0.91	0.25	0.63	57,57,57,57	4
87	OHX	5	3829	7/7	0.99	0.17	0.62	67,67,67,67	0
86	MG	c8	201	1/1	0.72	0.34	0.61	84,84,84,84	0
87	OHX	1	4100	7/7	0.93	0.27	0.59	38,38,38,38	3
87	OHX	m5	303	7/7	1.00	0.19	0.57	61,61,61,61	2
87	OHX	2	2077	7/7	0.91	0.23	0.55	108,108,108,108	7
87	OHX	5	3886	7/7	0.99	0.23	0.55	44,44,44,44	2
87	OHX	1	3845	7/7	0.97	0.15	0.55	123,123,123,123	3
87	OHX	2	2133	7/7	0.73	0.20	0.53	214,214,214,214	6
87	OHX	1	4022	7/7	0.93	0.22	0.51	71,71,71,71	6
87	OHX	5	3890	7/7	0.97	0.26	0.50	66,66,66,66	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3940	7/7	0.96	0.20	0.49	77,77,77,77	5
87	OHX	5	3925	7/7	0.88	0.27	0.48	60,60,60,60	4
87	OHX	6	2083	7/7	0.96	0.22	0.48	94,94,94,94	7
87	OHX	5	3879	7/7	0.99	0.20	0.48	47,47,47,47	3
87	OHX	6	2095	7/7	0.95	0.20	0.47	99,99,99,99	3
87	OHX	1	3847	7/7	0.99	0.18	0.47	56,56,56,56	3
87	OHX	1	3777	7/7	0.99	0.21	0.46	61,61,61,61	3
87	OHX	5	3887	7/7	0.98	0.21	0.46	43,43,43,43	3
87	OHX	6	2033	7/7	0.99	0.24	0.46	56,56,56,56	5
87	OHX	1	3774	7/7	0.99	0.17	0.45	71,71,71,71	3
86	MG	5	3539	1/1	0.92	0.31	0.44	62,62,62,62	0
86	MG	d3	201	1/1	0.94	0.37	0.43	50,50,50,50	0
87	OHX	2	1992	7/7	0.99	0.19	0.43	98,98,98,98	1
87	OHX	6	2018	7/7	0.99	0.19	0.42	90,90,90,90	2
87	OHX	1	4031	7/7	0.93	0.23	0.41	65,65,65,65	6
87	OHX	2	2144	7/7	0.90	0.49	0.41	103,103,103,103	6
87	OHX	2	2064	7/7	0.90	0.19	0.41	135,135,135,135	5
86	MG	SM	301	1/1	0.93	0.20	0.40	58,58,58,58	0
87	OHX	m7	203	7/7	0.92	0.37	0.39	47,47,47,47	5
87	OHX	1	3848	7/7	0.97	0.22	0.38	76,76,76,76	3
87	OHX	1	4076	7/7	0.89	0.26	0.36	45,45,45,45	5
87	OHX	d4	201	7/7	0.91	0.27	0.35	90,90,90,90	6
87	OHX	5	4014	7/7	0.95	0.23	0.34	36,36,36,36	4
87	OHX	2	1993	7/7	0.98	0.22	0.32	96,96,96,96	2
86	MG	6	1948	1/1	0.92	0.27	0.32	85,85,85,85	0
86	MG	3	207	1/1	0.91	0.35	0.31	66,66,66,66	0
87	OHX	5	4060	7/7	0.91	0.22	0.31	55,55,55,55	4
87	OHX	n3	202	7/7	0.97	0.19	0.31	60,60,60,60	3
86	MG	1	3601	1/1	0.90	0.21	0.30	72,72,72,72	0
87	OHX	1	3901	7/7	0.99	0.18	0.29	62,62,62,62	4
87	OHX	1	3780	7/7	0.99	0.25	0.29	75,75,75,75	1
87	OHX	2	2061	7/7	0.98	0.22	0.29	88,88,88,88	5
87	OHX	o7	502	7/7	0.93	0.26	0.29	83,83,83,83	4
87	OHX	1	4044	7/7	0.87	0.25	0.27	108,108,108,108	4
87	OHX	M8	201	7/7	0.94	0.23	0.25	47,47,47,47	3
87	OHX	5	3819	7/7	1.00	0.19	0.23	52,52,52,52	3
87	OHX	5	3927	7/7	0.96	0.14	0.21	146,146,146,146	3
87	OHX	5	4000	7/7	0.96	0.21	0.21	41,41,41,41	4
87	OHX	2	2059	7/7	0.94	0.23	0.21	101,101,101,101	4
87	OHX	1	3914	7/7	0.94	0.23	0.20	79,79,79,79	3
87	OHX	2	2075	7/7	0.96	0.21	0.20	80,80,80,80	6
87	OHX	4	228	7/7	0.98	0.18	0.19	60,60,60,60	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	3920	7/7	0.98	0.21	0.19	57,57,57,57	2
87	OHX	5	4040	7/7	0.96	0.20	0.19	73,73,73,73	4
87	OHX	6	2057	7/7	0.96	0.22	0.19	58,58,58,58	2
87	OHX	c5	202	7/7	0.90	0.45	0.19	109,109,109,109	6
87	OHX	5	3979	7/7	0.98	0.20	0.18	55,55,55,55	3
87	OHX	2	2072	7/7	0.86	0.20	0.18	187,187,187,187	7
87	OHX	1	3762	7/7	1.00	0.19	0.18	55,55,55,55	3
87	OHX	1	4109	7/7	0.94	0.20	0.17	48,48,48,48	4
87	OHX	5	3953	7/7	0.99	0.19	0.17	49,49,49,49	2
86	MG	6	2005	1/1	0.99	0.42	0.16	88,88,88,88	0
87	OHX	1	3861	7/7	0.99	0.20	0.15	60,60,60,60	3
87	OHX	5	3823	7/7	1.00	0.20	0.15	62,62,62,62	2
87	OHX	5	3959	7/7	0.98	0.21	0.15	44,44,44,44	3
86	MG	5	3554	1/1	0.86	0.24	0.15	54,54,54,54	0
87	OHX	6	2056	7/7	0.98	0.18	0.14	73,73,73,73	3
87	OHX	6	2012	7/7	1.00	0.21	0.14	70,70,70,70	3
87	OHX	Q2	503	7/7	0.99	0.20	0.14	46,46,46,46	2
87	OHX	5	4073	7/7	0.96	0.17	0.14	77,77,77,77	6
87	OHX	1	3790	7/7	0.99	0.22	0.13	48,48,48,48	3
86	MG	1	3571	1/1	0.98	0.27	0.13	53,53,53,53	0
87	OHX	3	209	7/7	0.99	0.21	0.12	76,76,76,76	4
87	OHX	2	2021	7/7	0.97	0.19	0.12	99,99,99,99	5
87	OHX	5	3884	7/7	0.98	0.16	0.10	78,78,78,78	3
86	MG	2	1954	1/1	0.94	0.26	0.10	105,105,105,105	0
87	OHX	5	3945	7/7	0.98	0.18	0.09	109,109,109,109	4
87	OHX	7	217	7/7	0.99	0.20	0.07	40,40,40,40	1
86	MG	6	1936	1/1	0.95	0.33	0.06	76,76,76,76	0
87	OHX	5	3880	7/7	0.98	0.19	0.06	96,96,96,96	2
87	OHX	1	3842	7/7	0.98	0.21	0.06	80,80,80,80	3
87	OHX	6	2144	7/7	0.96	0.21	0.04	85,85,85,85	7
87	OHX	1	3771	7/7	0.99	0.20	0.04	59,59,59,59	2
87	OHX	6	2123	7/7	0.93	0.21	0.04	70,70,70,70	4
87	OHX	5	4020	7/7	0.98	0.22	0.04	36,36,36,36	2
87	OHX	2	2094	7/7	0.97	0.23	0.03	87,87,87,87	5
87	OHX	1	3770	7/7	0.99	0.18	0.02	61,61,61,61	2
87	OHX	2	2112	7/7	0.88	0.19	0.02	121,121,121,121	6
86	MG	2	1934	1/1	0.96	0.24	0.02	80,80,80,80	0
86	MG	1	3549	1/1	0.99	0.22	0.00	59,59,59,59	0
87	OHX	2	2009	7/7	0.98	0.18	-0.01	89,89,89,89	4
87	OHX	1	3806	7/7	0.99	0.23	-0.01	52,52,52,52	2
87	OHX	4	221	7/7	0.95	0.19	-0.02	61,61,61,61	3
87	OHX	1	3878	7/7	0.98	0.19	-0.02	58,58,58,58	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	3926	7/7	0.98	0.18	-0.02	64,64,64,64	5
87	OHX	5	4119	7/7	0.97	0.21	-0.03	64,64,64,64	5
87	OHX	1	3832	7/7	0.97	0.19	-0.04	80,80,80,80	3
87	OHX	5	3825	7/7	1.00	0.20	-0.05	46,46,46,46	1
87	OHX	2	1999	7/7	0.96	0.16	-0.05	113,113,113,113	2
87	OHX	6	2181	7/7	0.90	0.19	-0.05	117,117,117,117	7
87	OHX	5	3896	7/7	0.99	0.20	-0.05	46,46,46,46	5
87	OHX	5	3952	7/7	0.99	0.20	-0.06	45,45,45,45	3
87	OHX	2	2046	7/7	0.96	0.22	-0.06	83,83,83,83	7
87	OHX	5	4001	7/7	0.97	0.20	-0.06	70,70,70,70	4
87	OHX	1	3779	7/7	1.00	0.19	-0.07	49,49,49,49	4
87	OHX	1	3860	7/7	0.99	0.21	-0.08	38,38,38,38	2
87	OHX	6	2175	7/7	0.89	0.18	-0.08	100,100,100,100	6
87	OHX	s8	303	7/7	0.93	0.23	-0.09	105,105,105,105	3
87	OHX	1	3934	7/7	0.97	0.19	-0.09	54,54,54,54	3
87	OHX	5	3824	7/7	0.99	0.18	-0.10	58,58,58,58	1
87	OHX	5	3841	7/7	0.99	0.19	-0.10	38,38,38,38	3
87	OHX	6	2138	7/7	0.93	0.26	-0.11	120,120,120,120	7
87	OHX	1	4054	7/7	0.95	0.22	-0.11	77,77,77,77	6
87	OHX	6	2135	7/7	0.87	0.29	-0.12	94,94,94,94	7
87	OHX	2	2007	7/7	0.96	0.20	-0.12	94,94,94,94	5
87	OHX	2	2067	7/7	0.97	0.17	-0.12	132,132,132,132	4
87	OHX	1	3813	7/7	0.98	0.25	-0.12	52,52,52,52	2
86	MG	2	1953	1/1	0.62	0.22	-0.13	89,89,89,89	0
87	OHX	5	3885	7/7	0.99	0.18	-0.13	79,79,79,79	3
87	OHX	1	3776	7/7	0.99	0.20	-0.14	55,55,55,55	1
87	OHX	5	4021	7/7	0.98	0.23	-0.15	37,37,37,37	1
86	MG	1	3651	1/1	0.97	0.23	-0.17	49,49,49,49	0
87	OHX	5	3834	7/7	0.99	0.19	-0.19	54,54,54,54	1
86	MG	L2	301	1/1	0.93	0.24	-0.21	37,37,37,37	0
87	OHX	C8	201	7/7	0.97	0.20	-0.21	111,111,111,111	4
86	MG	1	3669	1/1	0.92	0.15	-0.21	59,59,59,59	0
87	OHX	1	3990	7/7	0.95	0.15	-0.22	92,92,92,92	6
87	OHX	6	2145	7/7	0.92	0.21	-0.22	92,92,92,92	4
87	OHX	5	4043	7/7	0.96	0.22	-0.22	51,51,51,51	3
87	OHX	5	3967	7/7	0.99	0.20	-0.23	47,47,47,47	4
87	OHX	3	216	7/7	0.97	0.20	-0.24	49,49,49,49	5
87	OHX	6	2169	7/7	0.90	0.19	-0.24	89,89,89,89	4
87	OHX	S1	301	7/7	0.96	0.17	-0.24	121,121,121,121	2
86	MG	1	3595	1/1	0.91	0.30	-0.24	78,78,78,78	0
87	OHX	5	3863	7/7	0.99	0.16	-0.24	88,88,88,88	3
87	OHX	1	3765	7/7	0.99	0.17	-0.25	65,65,65,65	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3912	7/7	0.94	0.19	-0.25	126,126,126,126	4
87	OHX	s1	301	7/7	0.98	0.19	-0.25	95,95,95,95	2
87	OHX	1	3907	7/7	0.96	0.23	-0.25	71,71,71,71	3
87	OHX	5	3848	7/7	0.99	0.17	-0.26	100,100,100,100	3
87	OHX	6	2159	7/7	0.92	0.22	-0.27	93,93,93,93	5
87	OHX	M5	303	7/7	0.98	0.22	-0.27	72,72,72,72	4
87	OHX	6	2034	7/7	0.99	0.18	-0.28	66,66,66,66	5
87	OHX	1	4101	7/7	0.89	0.25	-0.28	66,66,66,66	4
87	OHX	5	4147	7/7	0.90	0.19	-0.28	100,100,100,100	6
87	OHX	1	3812	7/7	0.98	0.15	-0.29	88,88,88,88	3
87	OHX	2	2062	7/7	0.95	0.20	-0.29	109,109,109,109	6
87	OHX	1	3969	7/7	0.98	0.17	-0.30	65,65,65,65	4
87	OHX	5	3954	7/7	0.96	0.13	-0.30	149,149,149,149	4
87	OHX	5	4064	7/7	0.99	0.21	-0.30	39,39,39,39	3
87	OHX	2	1991	7/7	0.99	0.18	-0.31	88,88,88,88	0
87	OHX	2	2035	7/7	0.89	0.22	-0.31	116,116,116,116	5
87	OHX	2	2073	7/7	0.97	0.20	-0.31	63,63,63,63	6
87	OHX	1	3951	7/7	0.97	0.15	-0.32	159,159,159,159	7
87	OHX	d9	102	7/7	0.95	0.31	-0.32	106,106,106,106	6
87	OHX	1	3974	7/7	0.93	0.25	-0.32	63,63,63,63	5
86	MG	6	1949	1/1	0.95	0.23	-0.33	77,77,77,77	0
87	OHX	1	3769	7/7	0.99	0.20	-0.33	64,64,64,64	2
87	OHX	2	2030	7/7	0.97	0.18	-0.34	98,98,98,98	5
87	OHX	6	2059	7/7	0.98	0.19	-0.34	61,61,61,61	3
88	ZN	o7	501	1/1	0.99	0.18	-0.34	45,45,45,45	0
87	OHX	s9	201	7/7	0.94	0.26	-0.37	71,71,71,71	5
87	OHX	5	4050	7/7	0.93	0.20	-0.38	64,64,64,64	6
87	OHX	1	3783	7/7	0.99	0.17	-0.38	83,83,83,83	2
86	MG	o4	201	1/1	0.92	0.28	-0.39	53,53,53,53	0
87	OHX	2	2124	7/7	0.84	0.18	-0.39	128,128,128,128	6
87	OHX	6	2031	7/7	0.98	0.18	-0.40	80,80,80,80	4
87	OHX	1	4051	7/7	0.97	0.21	-0.41	58,58,58,58	3
87	OHX	5	4081	7/7	0.90	0.14	-0.41	92,92,92,92	3
87	OHX	s1	302	7/7	0.89	0.22	-0.42	99,99,99,99	6
87	OHX	6	2030	7/7	0.99	0.20	-0.42	57,57,57,57	2
87	OHX	6	2121	7/7	0.91	0.27	-0.43	86,86,86,86	5
87	OHX	5	4111	7/7	0.94	0.20	-0.44	51,51,51,51	6
87	OHX	1	4047	7/7	0.92	0.15	-0.44	101,101,101,101	5
87	OHX	S9	201	7/7	0.95	0.25	-0.45	94,94,94,94	6
87	OHX	1	3839	7/7	0.99	0.19	-0.47	64,64,64,64	3
87	OHX	1	3931	7/7	0.98	0.21	-0.48	43,43,43,43	4
87	OHX	1	4082	7/7	0.92	0.20	-0.48	63,63,63,63	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3932	7/7	0.97	0.20	-0.49	57,57,57,57	5
87	OHX	1	3863	7/7	0.99	0.20	-0.49	42,42,42,42	3
87	OHX	2	2031	7/7	0.98	0.18	-0.50	81,81,81,81	4
87	OHX	1	3764	7/7	1.00	0.18	-0.51	65,65,65,65	2
87	OHX	5	4143	7/7	0.90	0.24	-0.51	65,65,65,65	5
87	OHX	1	3792	7/7	0.98	0.21	-0.51	74,74,74,74	3
87	OHX	5	3987	7/7	0.92	0.21	-0.51	64,64,64,64	5
87	OHX	2	2101	7/7	0.91	0.18	-0.51	110,110,110,110	5
87	OHX	5	3820	7/7	0.99	0.18	-0.52	64,64,64,64	2
87	OHX	6	2084	7/7	0.95	0.22	-0.53	104,104,104,104	5
87	OHX	6	2027	7/7	0.99	0.18	-0.53	76,76,76,76	2
87	OHX	2	2065	7/7	0.92	0.20	-0.53	106,106,106,106	5
87	OHX	5	3856	7/7	0.99	0.19	-0.54	54,54,54,54	1
87	OHX	1	4061	7/7	0.90	0.21	-0.54	72,72,72,72	4
87	OHX	L3	404	7/7	0.81	0.27	-0.55	84,84,84,84	6
87	OHX	1	3866	7/7	0.97	0.20	-0.55	69,69,69,69	3
87	OHX	8	223	7/7	0.96	0.14	-0.55	95,95,95,95	7
86	MG	2	1969	1/1	0.56	0.26	-0.56	108,108,108,108	0
86	MG	5	3423	1/1	0.89	0.23	-0.56	56,56,56,56	0
87	OHX	m0	302	7/7	0.95	0.23	-0.57	96,96,96,96	5
87	OHX	6	2040	7/7	0.99	0.15	-0.57	123,123,123,123	5
87	OHX	5	4127	7/7	0.92	0.22	-0.57	47,47,47,47	4
87	OHX	2	2105	7/7	0.87	0.24	-0.59	87,87,87,87	3
87	OHX	5	3870	7/7	0.96	0.23	-0.59	72,72,72,72	2
87	OHX	8	228	7/7	0.89	0.19	-0.59	101,101,101,101	6
87	OHX	2	2034	7/7	0.95	0.17	-0.59	119,119,119,119	4
87	OHX	1	3952	7/7	0.92	0.16	-0.60	140,140,140,140	5
86	MG	1	3631	1/1	0.97	0.22	-0.60	42,42,42,42	0
87	OHX	2	2084	7/7	0.96	0.18	-0.61	95,95,95,95	5
87	OHX	1	4081	7/7	0.93	0.22	-0.61	43,43,43,43	5
87	OHX	O4	202	7/7	0.92	0.25	-0.62	82,82,82,82	5
87	OHX	5	3846	7/7	0.99	0.20	-0.64	48,48,48,48	1
87	OHX	1	3978	7/7	0.96	0.16	-0.64	77,77,77,77	3
87	OHX	6	2142	7/7	0.94	0.31	-0.66	95,95,95,95	7
87	OHX	5	4026	7/7	0.97	0.18	-0.67	49,49,49,49	3
87	OHX	5	4148	7/7	0.85	0.15	-0.67	145,145,145,145	7
86	MG	M0	301	1/1	0.93	0.21	-0.67	50,50,50,50	0
87	OHX	O3	202	7/7	0.98	0.22	-0.69	52,52,52,52	4
87	OHX	2	2066	7/7	0.97	0.13	-0.69	160,160,160,160	7
87	OHX	4	226	7/7	0.97	0.15	-0.69	103,103,103,103	6
86	MG	2	1914	1/1	0.93	0.24	-0.70	83,83,83,83	0
87	OHX	O7	103	7/7	0.97	0.18	-0.71	78,78,78,78	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2127	7/7	0.93	0.17	-0.71	128,128,128,128	7
87	OHX	1	3761	7/7	1.00	0.19	-0.72	57,57,57,57	1
87	OHX	L5	301	7/7	0.96	0.18	-0.72	88,88,88,88	6
87	OHX	S6	301	7/7	0.86	0.15	-0.72	117,117,117,117	7
87	OHX	1	4011	7/7	0.95	0.20	-0.73	62,62,62,62	3
87	OHX	6	2022	7/7	0.99	0.19	-0.73	67,67,67,67	2
86	MG	1	3421	1/1	0.93	0.21	-0.74	58,58,58,58	0
87	OHX	6	2067	7/7	0.98	0.11	-0.75	154,154,154,154	3
87	OHX	1	3802	7/7	0.99	0.18	-0.75	60,60,60,60	2
87	OHX	1	3926	7/7	0.98	0.18	-0.76	57,57,57,57	4
87	OHX	5	3869	7/7	0.98	0.19	-0.76	76,76,76,76	5
87	OHX	6	2023	7/7	0.99	0.19	-0.76	80,80,80,80	3
87	OHX	1	3988	7/7	0.95	0.17	-0.77	87,87,87,87	5
87	OHX	5	4113	7/7	0.96	0.18	-0.78	55,55,55,55	4
87	OHX	5	3917	7/7	0.98	0.19	-0.80	36,36,36,36	2
87	OHX	1	3935	7/7	0.97	0.15	-0.80	71,71,71,71	2
87	OHX	6	2170	7/7	0.96	0.14	-0.81	83,83,83,83	7
89	SPS	B	101	23/23	0.97	0.21	-0.81	39,42,55,58	0
87	OHX	6	2055	7/7	0.99	0.13	-0.81	113,113,113,113	4
87	OHX	6	2141	7/7	0.86	0.19	-0.82	151,151,151,151	7
87	OHX	1	3785	7/7	0.99	0.20	-0.82	59,59,59,59	2
87	OHX	1	4001	7/7	0.97	0.16	-0.82	61,61,61,61	4
87	OHX	2	2014	7/7	0.98	0.10	-0.82	130,130,130,130	7
86	MG	6	1922	1/1	0.97	0.18	-0.83	55,55,55,55	0
87	OHX	5	4029	7/7	0.97	0.14	-0.83	70,70,70,70	5
87	OHX	6	2134	7/7	0.94	0.13	-0.85	163,163,163,163	7
87	OHX	2	2068	7/7	0.93	0.20	-0.85	103,103,103,103	7
87	OHX	6	2099	7/7	0.96	0.19	-0.86	81,81,81,81	5
87	OHX	6	2090	7/7	0.96	0.20	-0.86	91,91,91,91	7
87	OHX	8	212	7/7	0.99	0.17	-0.87	57,57,57,57	2
86	MG	1	3543	1/1	0.82	0.15	-0.87	58,58,58,58	0
87	OHX	5	3938	7/7	0.97	0.16	-0.87	92,92,92,92	2
87	OHX	1	4049	7/7	0.97	0.15	-0.87	61,61,61,61	5
87	OHX	5	3842	7/7	0.98	0.20	-0.88	64,64,64,64	1
87	OHX	6	2094	7/7	0.98	0.18	-0.89	109,109,109,109	6
86	MG	sM	301	1/1	0.76	0.21	-0.90	53,53,53,53	0
87	OHX	1	4033	7/7	0.94	0.18	-0.91	66,66,66,66	5
87	OHX	5	3906	7/7	0.98	0.18	-0.92	63,63,63,63	3
87	OHX	2	2000	7/7	0.98	0.20	-0.93	105,105,105,105	3
87	OHX	2	2100	7/7	0.97	0.13	-0.93	83,83,83,83	4
87	OHX	5	3907	7/7	0.99	0.19	-0.93	45,45,45,45	4
87	OHX	5	3932	7/7	0.98	0.14	-0.94	94,94,94,94	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	6	2104	7/7	0.94	0.17	-0.94	91,91,91,91	5
87	OHX	15	303	7/7	0.95	0.19	-0.94	90,90,90,90	6
87	OHX	6	2050	7/7	0.97	0.18	-0.95	87,87,87,87	5
87	OHX	5	3996	7/7	0.96	0.16	-0.95	62,62,62,62	5
86	MG	M6	201	1/1	0.94	0.17	-0.95	34,34,34,34	0
87	OHX	5	3991	7/7	0.97	0.17	-0.97	80,80,80,80	5
87	OHX	2	2139	7/7	0.92	0.18	-0.98	114,114,114,114	6
88	ZN	q3	501	1/1	1.00	0.15	-0.98	62,62,62,62	0
87	OHX	1	3964	7/7	0.94	0.17	-0.99	71,71,71,71	4
87	OHX	2	2088	7/7	0.95	0.18	-0.99	91,91,91,91	6
87	OHX	2	2048	7/7	0.98	0.13	-1.01	141,141,141,141	5
87	OHX	2	2004	7/7	0.96	0.12	-1.01	135,135,135,135	5
87	OHX	2	2096	7/7	0.94	0.17	-1.01	108,108,108,108	6
87	OHX	1	3925	7/7	0.95	0.19	-1.02	96,96,96,96	5
87	OHX	1	3973	7/7	0.96	0.17	-1.03	63,63,63,63	5
87	OHX	1	3943	7/7	0.98	0.12	-1.04	97,97,97,97	6
87	OHX	1	3824	7/7	0.99	0.17	-1.04	68,68,68,68	3
87	OHX	1	3854	7/7	0.99	0.17	-1.05	43,43,43,43	4
87	OHX	1	3977	7/7	0.97	0.15	-1.07	72,72,72,72	7
87	OHX	5	4139	7/7	0.94	0.15	-1.08	88,88,88,88	7
88	ZN	O7	101	1/1	0.99	0.16	-1.08	47,47,47,47	0
87	OHX	5	3905	7/7	0.99	0.18	-1.08	60,60,60,60	4
87	OHX	5	4003	7/7	0.98	0.15	-1.12	55,55,55,55	2
87	OHX	5	3872	7/7	0.98	0.17	-1.13	58,58,58,58	4
87	OHX	o6	201	7/7	0.92	0.23	-1.13	68,68,68,68	4
87	OHX	1	3844	7/7	0.98	0.13	-1.14	98,98,98,98	5
87	OHX	1	3908	7/7	0.94	0.17	-1.14	91,91,91,91	3
86	MG	5	3771	1/1	0.93	0.17	-1.15	37,37,37,37	0
87	OHX	6	2053	7/7	0.97	0.17	-1.16	92,92,92,92	5
87	OHX	D9	102	7/7	0.95	0.14	-1.17	97,97,97,97	6
87	OHX	5	4108	7/7	0.96	0.18	-1.17	53,53,53,53	5
87	OHX	1	3809	7/7	0.98	0.18	-1.18	80,80,80,80	2
87	OHX	5	4109	7/7	0.93	0.13	-1.18	133,133,133,133	5
87	OHX	2	2052	7/7	0.97	0.15	-1.18	90,90,90,90	5
87	OHX	5	3827	7/7	0.99	0.19	-1.18	50,50,50,50	3
87	OHX	1	3797	7/7	1.00	0.18	-1.18	54,54,54,54	2
87	OHX	2	2085	7/7	0.96	0.17	-1.19	103,103,103,103	4
86	MG	2	1944	1/1	0.96	0.11	-1.21	102,102,102,102	0
87	OHX	1	4053	7/7	0.95	0.19	-1.22	43,43,43,43	3
87	OHX	2	2026	7/7	0.95	0.21	-1.23	103,103,103,103	4
87	OHX	5	4145	7/7	0.95	0.20	-1.23	71,71,71,71	5
87	OHX	5	3997	7/7	0.98	0.18	-1.24	43,43,43,43	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	1931	1/1	0.83	0.15	-1.24	92,92,92,92	0
87	OHX	2	2113	7/7	0.93	0.12	-1.25	152,152,152,152	7
87	OHX	6	2115	7/7	0.96	0.17	-1.25	58,58,58,58	2
87	OHX	6	2013	7/7	0.99	0.18	-1.26	87,87,87,87	2
86	MG	1	3616	1/1	0.95	0.10	-1.26	58,58,58,58	0
86	MG	2	1983	1/1	0.97	0.17	-1.27	84,84,84,84	0
87	OHX	1	3982	7/7	0.97	0.20	-1.27	47,47,47,47	5
87	OHX	5	4102	7/7	0.96	0.19	-1.27	40,40,40,40	5
87	OHX	6	2068	7/7	0.98	0.13	-1.27	103,103,103,103	4
87	OHX	5	3850	7/7	0.99	0.17	-1.27	55,55,55,55	4
87	OHX	2	2082	7/7	0.97	0.16	-1.28	90,90,90,90	5
87	OHX	l3	404	7/7	0.93	0.15	-1.29	72,72,72,72	4
87	OHX	1	3967	7/7	0.94	0.16	-1.29	82,82,82,82	3
87	OHX	5	3836	7/7	1.00	0.17	-1.29	71,71,71,71	0
87	OHX	1	3891	7/7	0.91	0.17	-1.30	103,103,103,103	5
87	OHX	5	4009	7/7	0.96	0.17	-1.30	72,72,72,72	5
87	OHX	5	3852	7/7	0.99	0.17	-1.32	56,56,56,56	3
87	OHX	2	2063	7/7	0.96	0.09	-1.33	153,153,153,153	7
87	OHX	6	2130	7/7	0.88	0.16	-1.35	153,153,153,153	7
88	ZN	E1	501	1/1	0.97	0.05	-1.37	145,145,145,145	0
87	OHX	5	3853	7/7	0.99	0.14	-1.37	78,78,78,78	2
87	OHX	2	2099	7/7	0.91	0.11	-1.40	185,185,185,185	7
87	OHX	2	2089	7/7	0.95	0.13	-1.40	116,116,116,116	7
87	OHX	1	3877	7/7	0.98	0.12	-1.42	95,95,95,95	2
87	OHX	1	3781	7/7	0.99	0.18	-1.42	76,76,76,76	2
87	OHX	1	3950	7/7	0.97	0.17	-1.44	41,41,41,41	4
86	MG	6	1960	1/1	0.73	0.11	-1.45	65,65,65,65	0
87	OHX	2	2078	7/7	0.97	0.13	-1.45	115,115,115,115	7
87	OHX	1	3917	7/7	0.98	0.18	-1.47	54,54,54,54	4
87	OHX	5	4013	7/7	0.97	0.19	-1.47	48,48,48,48	3
86	MG	6	1903	1/1	0.93	0.13	-1.48	88,88,88,88	0
88	ZN	d9	101	1/1	0.99	0.10	-1.49	91,91,91,91	0
88	ZN	q0	500	1/1	0.99	0.13	-1.49	42,42,42,42	0
87	OHX	sR	401	7/7	0.95	0.14	-1.49	129,129,129,129	6
86	MG	5	3608	1/1	0.95	0.17	-1.52	35,35,35,35	0
88	ZN	Q2	501	1/1	0.98	0.06	-1.52	77,77,77,77	0
87	OHX	2	2013	7/7	0.98	0.14	-1.55	94,94,94,94	4
88	ZN	q2	501	1/1	0.97	0.07	-1.56	71,71,71,71	0
87	OHX	5	4135	7/7	0.86	0.14	-1.58	180,180,180,180	7
86	MG	5	3732	1/1	0.95	0.12	-1.61	50,50,50,50	0
86	MG	6	2185	1/1	0.87	0.18	-1.62	83,83,83,83	0
87	OHX	2	2040	7/7	0.98	0.14	-1.63	89,89,89,89	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2029	7/7	0.97	0.13	-1.63	98,98,98,98	5
87	OHX	5	3999	7/7	0.99	0.16	-1.67	45,45,45,45	2
87	OHX	2	2005	7/7	0.97	0.16	-1.68	99,99,99,99	3
86	MG	O4	201	1/1	0.85	0.13	-1.70	77,77,77,77	0
87	OHX	l3	403	7/7	0.99	0.14	-1.71	50,50,50,50	3
87	OHX	2	2006	7/7	0.98	0.13	-1.71	93,93,93,93	3
87	OHX	C5	201	7/7	0.96	0.10	-1.72	122,122,122,122	7
87	OHX	5	3897	7/7	0.99	0.15	-1.73	58,58,58,58	4
87	OHX	2	2028	7/7	0.99	0.12	-1.73	108,108,108,108	5
87	OHX	1	4086	7/7	0.95	0.19	-1.75	65,65,65,65	4
87	OHX	5	3929	7/7	0.98	0.17	-1.77	55,55,55,55	2
86	MG	2	1980	1/1	0.96	0.11	-1.78	104,104,104,104	0
88	ZN	Q0	500	1/1	0.98	0.11	-1.79	54,54,54,54	0
87	OHX	SR	401	7/7	0.96	0.11	-1.80	144,144,144,144	6
87	OHX	1	3803	7/7	0.99	0.17	-1.81	73,73,73,73	3
87	OHX	1	3937	7/7	0.95	0.10	-1.81	110,110,110,110	6
87	OHX	5	4084	7/7	0.95	0.11	-1.82	143,143,143,143	7
87	OHX	6	2109	7/7	0.98	0.12	-1.84	99,99,99,99	6
86	MG	5	3478	1/1	0.95	0.11	-1.84	70,70,70,70	0
87	OHX	5	4100	7/7	0.97	0.17	-1.85	69,69,69,69	3
87	OHX	6	2038	7/7	0.99	0.17	-1.85	61,61,61,61	5
87	OHX	S8	301	7/7	0.94	0.12	-1.86	115,115,115,115	7
86	MG	6	2184	1/1	0.99	0.12	-1.87	91,91,91,91	0
87	OHX	2	2114	7/7	0.90	0.17	-1.90	103,103,103,103	4
87	OHX	6	2101	7/7	0.98	0.18	-1.91	62,62,62,62	2
87	OHX	m5	305	7/7	0.99	0.14	-1.95	76,76,76,76	3
87	OHX	4	220	7/7	0.97	0.17	-1.95	84,84,84,84	3
87	OHX	L3	403	7/7	0.97	0.15	-1.95	72,72,72,72	5
87	OHX	6	2039	7/7	0.95	0.12	-1.96	126,126,126,126	5
87	OHX	1	3788	7/7	0.99	0.20	-1.96	58,58,58,58	4
87	OHX	5	3951	7/7	0.96	0.12	-1.99	100,100,100,100	2
87	OHX	1	3942	7/7	0.96	0.12	-2.00	94,94,94,94	4
86	MG	5	3523	1/1	0.95	0.13	-2.04	48,48,48,48	0
87	OHX	2	2020	7/7	0.96	0.13	-2.04	117,117,117,117	3
88	ZN	D9	101	1/1	0.99	0.06	-2.05	89,89,89,89	0
87	OHX	o3	202	7/7	0.98	0.17	-2.10	52,52,52,52	3
87	OHX	2	2080	7/7	0.97	0.14	-2.10	91,91,91,91	4
88	ZN	Q3	501	1/1	0.99	0.09	-2.11	78,78,78,78	0
86	MG	s4	601	1/1	0.86	0.13	-2.17	66,66,66,66	0
87	OHX	2	2071	7/7	0.98	0.18	-2.17	72,72,72,72	6
86	MG	5	3500	1/1	0.98	0.17	-2.20	42,42,42,42	0
87	OHX	6	2074	7/7	0.97	0.15	-2.22	70,70,70,70	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2055	7/7	0.96	0.16	-2.25	63,63,63,63	5
87	OHX	1	3823	7/7	0.99	0.11	-2.25	111,111,111,111	4
87	OHX	5	4107	7/7	0.95	0.18	-2.26	66,66,66,66	3
88	ZN	e1	501	1/1	0.94	0.04	-2.26	173,173,173,173	0
87	OHX	6	2063	7/7	0.98	0.08	-2.26	147,147,147,147	6
87	OHX	c5	201	7/7	0.90	0.15	-2.28	129,129,129,129	6
87	OHX	5	3828	7/7	0.99	0.21	-2.28	44,44,44,44	5
86	MG	2	1941	1/1	0.92	0.09	-2.31	100,100,100,100	0
87	OHX	2	1994	7/7	0.99	0.14	-2.32	97,97,97,97	2
87	OHX	1	4056	7/7	0.96	0.14	-2.33	85,85,85,85	5
87	OHX	2	2038	7/7	0.98	0.10	-2.33	119,119,119,119	6
87	OHX	6	2082	7/7	0.97	0.14	-2.34	99,99,99,99	5
87	OHX	2	2001	7/7	0.99	0.13	-2.35	120,120,120,120	2
87	OHX	5	4087	7/7	0.98	0.17	-2.37	39,39,39,39	4
87	OHX	2	2110	7/7	0.95	0.14	-2.37	112,112,112,112	5
90	PRO	B	102	7/8	0.94	0.19	-2.38	41,41,51,51	0
87	OHX	5	4067	7/7	0.99	0.14	-2.40	49,49,49,49	3
87	OHX	14	402	7/7	0.97	0.19	-2.45	69,69,69,69	5
86	MG	5	3702	1/1	0.98	0.09	-2.48	58,58,58,58	0
87	OHX	5	3838	7/7	1.00	0.16	-2.53	64,64,64,64	2
87	OHX	5	3866	7/7	0.99	0.10	-2.57	126,126,126,126	2
86	MG	5	3463	1/1	0.72	0.15	-2.63	125,125,125,125	0
87	OHX	2	1997	7/7	0.99	0.11	-2.65	107,107,107,107	5
87	OHX	6	2105	7/7	0.95	0.17	-2.73	81,81,81,81	4
86	MG	5	3630	1/1	0.88	0.20	-2.74	52,52,52,52	0
87	OHX	L4	401	7/7	0.96	0.14	-2.76	67,67,67,67	7
86	MG	5	3758	1/1	0.89	0.11	-2.77	46,46,46,46	0
87	OHX	6	2069	7/7	0.97	0.17	-2.77	73,73,73,73	4
88	ZN	d6	101	1/1	0.98	0.05	-2.82	84,84,84,84	0
87	OHX	1	3895	7/7	0.97	0.16	-2.83	57,57,57,57	4
87	OHX	5	3817	7/7	0.99	0.17	-2.85	57,57,57,57	0
87	OHX	6	2100	7/7	0.99	0.14	-2.88	71,71,71,71	3
86	MG	1	3633	1/1	0.88	0.15	-2.88	59,59,59,59	0
87	OHX	2	2070	7/7	0.96	0.11	-3.01	108,108,108,108	5
86	MG	2	1946	1/1	0.87	0.08	-3.02	108,108,108,108	0
86	MG	1	3484	1/1	0.98	0.12	-3.05	52,52,52,52	0
87	OHX	2	2016	7/7	0.98	0.14	-3.18	96,96,96,96	4
87	OHX	6	2026	7/7	0.99	0.19	-3.22	66,66,66,66	1
86	MG	6	1908	1/1	0.93	0.13	-3.25	109,109,109,109	0
87	OHX	1	3933	7/7	0.97	0.14	-3.26	91,91,91,91	4
87	OHX	1	3894	7/7	0.98	0.09	-3.50	132,132,132,132	7
86	MG	2	1976	1/1	0.88	0.09	-3.81	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3999	7/7	0.93	0.06	-3.90	215,215,215,215	2
87	OHX	1	3941	7/7	0.97	0.16	-4.00	51,51,51,51	3
86	MG	6	2003	1/1	0.97	0.10	-4.11	96,96,96,96	0
88	ZN	D6	500	1/1	0.98	0.07	-4.56	103,103,103,103	0
87	OHX	l5	302	7/7	0.92	0.12	-4.67	105,105,105,105	4
90	PRO	C	101	7/8	0.95	0.17	-4.70	35,35,45,45	0
86	MG	6	1977	1/1	0.97	0.10	-4.81	57,57,57,57	0
87	OHX	5	3963	7/7	0.97	0.09	-5.25	107,107,107,107	2
87	OHX	6	2015	7/7	0.99	0.14	-5.92	78,78,78,78	3
86	MG	1	3683	1/1	0.94	0.15	-8.18	39,39,39,39	1
86	MG	5	3580	1/1	0.96	0.59	-	24,24,24,24	0
86	MG	1	3579	1/1	0.98	0.69	-	35,35,35,35	0
86	MG	1	3427	1/1	0.97	0.85	-	42,42,42,42	0
86	MG	5	3798	1/1	0.97	0.42	-	42,42,42,42	0
86	MG	6	1992	1/1	0.80	0.33	-	61,61,61,61	0
86	MG	6	1997	1/1	0.95	0.48	-	53,53,53,53	0
87	OHX	c8	202	7/7	0.95	0.23	-	99,99,99,99	5
86	MG	5	3787	1/1	0.89	0.31	-	68,68,68,68	0
87	OHX	1	4028	7/7	0.94	0.19	-	58,58,58,58	3
86	MG	1	3598	1/1	0.92	0.34	-	39,39,39,39	0
86	MG	1	3584	1/1	0.95	0.75	-	33,33,33,33	0
87	OHX	1	4108	7/7	0.87	0.23	-	59,59,59,59	5
86	MG	2	1902	1/1	0.83	0.98	-	49,49,49,49	0
87	OHX	1	3864	7/7	0.98	0.35	-	104,104,104,104	3
87	OHX	1	3927	7/7	0.94	0.33	-	51,51,51,51	3
86	MG	5	3764	1/1	0.94	0.14	-	39,39,39,39	0
86	MG	2	1971	1/1	0.95	0.19	-	81,81,81,81	0
86	MG	5	3442	1/1	0.98	0.61	-	44,44,44,44	0
87	OHX	2	2126	7/7	0.94	0.52	-	64,64,64,64	4
87	OHX	5	4034	7/7	0.97	0.29	-	40,40,40,40	3
86	MG	1	3674	1/1	0.86	0.36	-	68,68,68,68	0
86	MG	1	3423	1/1	0.75	0.47	-	46,46,46,46	0
86	MG	M7	204	1/1	0.92	0.46	-	46,46,46,46	0
87	OHX	2	2086	7/7	0.93	0.25	-	112,112,112,112	5
87	OHX	6	2152	7/7	0.88	0.14	-	107,107,107,107	5
86	MG	1	3558	1/1	0.89	0.52	-	35,35,35,35	0
86	MG	1	3698	1/1	0.96	0.25	-	42,42,42,42	0
86	MG	1	3714	1/1	0.70	0.70	-	46,46,46,46	0
87	OHX	5	4131	7/7	0.89	0.47	-	45,45,45,45	4
86	MG	5	3697	1/1	0.75	0.62	-	42,42,42,42	0
86	MG	1	3521	1/1	0.97	0.66	-	43,43,43,43	0
86	MG	5	3509	1/1	0.93	0.66	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2002	1/1	0.90	0.32	-	66,66,66,66	0
86	MG	1	3449	1/1	0.78	0.40	-	57,57,57,57	0
87	OHX	6	2052	7/7	0.98	0.17	-	67,67,67,67	3
86	MG	1	3749	1/1	0.94	0.55	-	17,17,17,17	0
87	OHX	1	3979	7/7	0.93	0.09	-	197,197,197,197	5
86	MG	5	3777	1/1	0.79	0.31	-	115,115,115,115	0
86	MG	1	3700	1/1	0.75	0.33	-	51,51,51,51	0
87	OHX	5	4094	7/7	0.81	0.39	-	41,41,41,41	2
87	OHX	2	2049	7/7	0.87	0.28	-	100,100,100,100	4
86	MG	5	3666	1/1	0.90	0.46	-	86,86,86,86	0
86	MG	1	3499	1/1	0.98	0.54	-	37,37,37,37	0
86	MG	6	1954	1/1	0.80	0.63	-	64,64,64,64	0
86	MG	5	3600	1/1	0.98	0.71	-	26,26,26,26	0
87	OHX	1	3837	7/7	0.99	0.21	-	60,60,60,60	2
86	MG	5	3515	1/1	0.94	0.57	-	21,21,21,21	0
86	MG	m5	302	1/1	0.92	0.27	-	67,67,67,67	0
86	MG	1	3405	1/1	0.93	0.55	-	132,132,132,132	0
86	MG	1	3605	1/1	0.89	0.30	-	44,44,44,44	0
87	OHX	5	3978	7/7	0.98	0.32	-	67,67,67,67	3
87	OHX	2	2146	7/7	0.93	0.18	-	87,87,87,87	7
86	MG	2	1958	1/1	0.64	0.54	-	104,104,104,104	0
86	MG	1	3750	1/1	0.84	0.82	-	48,48,48,48	0
86	MG	1	3652	1/1	0.89	0.32	-	48,48,48,48	0
87	OHX	5	4032	7/7	0.94	0.15	-	98,98,98,98	7
87	OHX	5	4151	7/7	0.94	0.29	-	76,76,76,76	5
87	OHX	5	4149	7/7	0.92	0.21	-	62,62,62,62	5
86	MG	D3	201	1/1	0.69	0.40	-	54,54,54,54	0
87	OHX	6	2179	7/7	0.89	0.24	-	61,61,61,61	7
87	OHX	6	2165	7/7	0.93	0.31	-	74,74,74,74	6
86	MG	5	3685	1/1	0.78	0.34	-	92,92,92,92	0
86	MG	1	3483	1/1	0.81	0.81	-	54,54,54,54	0
86	MG	1	3637	1/1	0.89	0.67	-	46,46,46,46	0
87	OHX	5	3883	7/7	0.98	0.18	-	63,63,63,63	3
86	MG	1	3682	1/1	0.86	0.30	-	36,36,36,36	0
86	MG	5	3628	1/1	0.90	0.29	-	35,35,35,35	0
86	MG	5	3797	1/1	0.93	0.39	-	42,42,42,42	0
86	MG	5	3815	1/1	0.56	0.44	-	39,39,39,39	0
87	OHX	1	4091	7/7	0.94	0.32	-	42,42,42,42	4
86	MG	5	3477	1/1	0.95	0.83	-	21,21,21,21	0
86	MG	5	3434	1/1	0.93	0.32	-	33,33,33,33	0
86	MG	5	3650	1/1	0.78	0.41	-	42,42,42,42	0
86	MG	M7	203	1/1	0.87	0.40	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3516	1/1	0.93	0.40	-	28,28,28,28	0
86	MG	s8	301	1/1	0.89	0.40	-	52,52,52,52	0
86	MG	5	3806	1/1	0.74	0.27	-	54,54,54,54	0
86	MG	5	3427	1/1	0.95	0.51	-	45,45,45,45	0
86	MG	1	3455	1/1	0.97	0.52	-	29,29,29,29	0
87	OHX	1	4002	7/7	0.96	0.35	-	65,65,65,65	7
87	OHX	5	4028	7/7	0.97	0.13	-	76,76,76,76	4
87	OHX	5	4128	7/7	0.95	0.31	-	37,37,37,37	3
86	MG	6	1909	1/1	0.90	0.30	-	53,53,53,53	0
86	MG	2	1929	1/1	0.83	0.36	-	83,83,83,83	0
86	MG	6	1994	1/1	0.94	0.73	-	49,49,49,49	0
86	MG	7	205	1/1	0.97	0.53	-	26,26,26,26	0
86	MG	5	3562	1/1	0.88	0.50	-	44,44,44,44	0
86	MG	5	3470	1/1	0.94	0.25	-	51,51,51,51	0
87	OHX	1	3918	7/7	0.98	0.14	-	91,91,91,91	5
87	OHX	5	4044	7/7	0.96	0.42	-	48,48,48,48	2
87	OHX	1	3805	7/7	0.99	0.16	-	93,93,93,93	4
86	MG	5	3668	1/1	0.85	0.20	-	36,36,36,36	1
86	MG	o3	201	1/1	0.69	0.36	-	51,51,51,51	0
86	MG	5	3454	1/1	0.97	0.58	-	31,31,31,31	0
86	MG	1	3657	1/1	0.85	0.66	-	49,49,49,49	0
87	OHX	1	3873	7/7	0.98	0.22	-	53,53,53,53	5
86	MG	5	3401	1/1	0.84	0.08	-	54,54,54,54	0
86	MG	6	1995	1/1	0.89	0.51	-	47,47,47,47	0
87	OHX	4	229	7/7	0.95	0.21	-	45,45,45,45	3
86	MG	5	3479	1/1	0.91	0.10	-	47,47,47,47	0
87	OHX	5	4146	7/7	0.84	0.26	-	89,89,89,89	7
86	MG	1	3436	1/1	0.93	0.98	-	39,39,39,39	0
86	MG	1	3528	1/1	0.92	0.52	-	47,47,47,47	0
87	OHX	5	4039	7/7	0.92	0.33	-	149,149,149,149	6
87	OHX	5	3934	7/7	0.99	0.18	-	45,45,45,45	1
87	OHX	5	4059	7/7	0.95	0.37	-	45,45,45,45	5
86	MG	1	3673	1/1	0.83	0.58	-	39,39,39,39	0
87	OHX	5	4157	7/7	0.87	0.40	-	35,35,35,35	3
87	OHX	1	3984	7/7	0.96	0.10	-	127,127,127,127	7
87	OHX	6	2177	7/7	0.89	0.14	-	141,141,141,141	7
86	MG	2	1928	1/1	0.97	0.30	-	71,71,71,71	0
86	MG	1	3428	1/1	0.84	0.34	-	52,52,52,52	0
87	OHX	1	3956	7/7	0.97	0.15	-	57,57,57,57	5
87	OHX	5	4161	7/7	0.77	0.37	-	100,100,100,100	7
86	MG	1	3701	1/1	0.86	0.28	-	52,52,52,52	0
86	MG	1	3702	1/1	0.83	0.52	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3574	1/1	0.92	0.95	-	30,30,30,30	0
86	MG	5	3726	1/1	0.86	0.58	-	44,44,44,44	0
86	MG	1	3623	1/1	0.90	0.20	-	57,57,57,57	0
86	MG	5	3701	1/1	0.83	0.32	-	54,54,54,54	0
86	MG	2	1913	1/1	0.94	0.28	-	79,79,79,79	0
86	MG	5	3414	1/1	0.94	0.27	-	44,44,44,44	0
87	OHX	5	4090	7/7	0.89	0.35	-	45,45,45,45	2
86	MG	1	3663	1/1	0.78	1.03	-	44,44,44,44	0
87	OHX	6	2160	7/7	0.97	0.18	-	69,69,69,69	5
87	OHX	5	4035	7/7	0.95	0.29	-	38,38,38,38	5
87	OHX	5	3994	7/7	0.95	0.24	-	88,88,88,88	5
86	MG	5	3693	1/1	0.81	0.31	-	55,55,55,55	0
86	MG	1	3412	1/1	0.97	0.27	-	68,68,68,68	0
86	MG	5	3607	1/1	0.90	0.47	-	50,50,50,50	0
87	OHX	1	4079	7/7	0.86	0.24	-	108,108,108,108	6
86	MG	5	3646	1/1	0.85	0.25	-	55,55,55,55	0
87	OHX	8	216	7/7	0.95	0.23	-	78,78,78,78	5
87	OHX	2	2041	7/7	0.97	0.09	-	141,141,141,141	6
87	OHX	8	210	7/7	1.00	0.18	-	64,64,64,64	1
86	MG	6	1969	1/1	0.97	0.44	-	55,55,55,55	0
87	OHX	5	4031	7/7	0.95	0.20	-	71,71,71,71	4
86	MG	5	3532	1/1	0.96	0.71	-	28,28,28,28	0
86	MG	1	3614	1/1	0.90	0.55	-	54,54,54,54	0
86	MG	5	3716	1/1	0.96	0.67	-	16,16,16,16	0
87	OHX	5	4170	7/7	0.89	0.19	-	90,90,90,90	5
87	OHX	2	2090	7/7	0.98	0.23	-	94,94,94,94	6
86	MG	3	203	1/1	0.79	0.77	-	42,42,42,42	0
87	OHX	2	2042	7/7	0.98	0.21	-	68,68,68,68	5
86	MG	1	3704	1/1	0.91	0.38	-	59,59,59,59	0
86	MG	1	3662	1/1	0.68	0.79	-	101,101,101,101	0
86	MG	5	3552	1/1	0.91	0.54	-	26,26,26,26	0
86	MG	1	3671	1/1	0.94	0.49	-	47,47,47,47	0
87	OHX	5	4150	7/7	0.93	0.24	-	53,53,53,53	4
86	MG	1	3624	1/1	0.94	0.35	-	33,33,33,33	0
86	MG	5	3805	1/1	0.96	0.61	-	37,37,37,37	0
86	MG	2	1957	1/1	0.77	0.55	-	99,99,99,99	0
87	OHX	6	2124	7/7	0.96	0.11	-	103,103,103,103	6
86	MG	m7	202	1/1	0.95	0.36	-	34,34,34,34	0
86	MG	5	3655	1/1	0.95	0.60	-	41,41,41,41	0
86	MG	5	3464	1/1	0.92	0.80	-	44,44,44,44	0
87	OHX	2	2069	7/7	0.95	0.19	-	115,115,115,115	4
86	MG	1	3457	1/1	0.85	0.65	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3590	1/1	0.99	0.30	-	43,43,43,43	0
87	OHX	2	2098	7/7	0.95	0.24	-	111,111,111,111	6
86	MG	5	3429	1/1	0.94	0.36	-	36,36,36,36	0
87	OHX	1	4103	7/7	0.92	0.25	-	53,53,53,53	5
86	MG	5	3699	1/1	0.89	0.30	-	43,43,43,43	0
86	MG	5	3574	1/1	0.91	0.53	-	36,36,36,36	0
86	MG	2	1916	1/1	0.81	0.71	-	63,63,63,63	0
86	MG	5	3804	1/1	0.96	0.26	-	37,37,37,37	0
87	OHX	5	4114	7/7	0.92	0.20	-	63,63,63,63	6
86	MG	1	3740	1/1	0.98	0.26	-	62,62,62,62	0
87	OHX	6	2174	7/7	0.92	0.31	-	92,92,92,92	6
86	MG	1	3613	1/1	0.89	0.81	-	58,58,58,58	0
86	MG	5	3404	1/1	0.81	0.73	-	49,49,49,49	0
87	OHX	6	2079	7/7	0.98	0.26	-	51,51,51,51	3
87	OHX	C3	201	7/7	0.93	0.27	-	100,100,100,100	5
86	MG	5	3715	1/1	0.97	0.33	-	34,34,34,34	0
86	MG	5	3484	1/1	0.87	0.50	-	38,38,38,38	0
86	MG	1	3620	1/1	0.92	0.36	-	32,32,32,32	0
87	OHX	5	4125	7/7	0.92	0.21	-	98,98,98,98	3
86	MG	5	3669	1/1	0.82	0.41	-	35,35,35,35	0
86	MG	1	3729	1/1	0.77	0.40	-	69,69,69,69	0
87	OHX	2	2087	7/7	0.96	0.14	-	89,89,89,89	5
86	MG	1	3568	1/1	0.88	0.46	-	36,36,36,36	0
87	OHX	5	3969	7/7	0.95	0.21	-	80,80,80,80	3
86	MG	5	3486	1/1	0.82	0.67	-	37,37,37,37	0
87	OHX	5	3908	7/7	0.97	0.19	-	77,77,77,77	4
87	OHX	1	3870	7/7	0.95	0.28	-	67,67,67,67	3
86	MG	m3	201	1/1	0.86	0.51	-	40,40,40,40	0
86	MG	n0	201	1/1	0.85	0.34	-	41,41,41,41	0
87	OHX	1	3836	7/7	0.98	0.17	-	98,98,98,98	3
87	OHX	1	4104	7/7	0.86	0.24	-	73,73,73,73	6
86	MG	1	3608	1/1	0.71	0.44	-	46,46,46,46	0
86	MG	5	3722	1/1	0.78	0.40	-	52,52,52,52	0
87	OHX	1	4098	7/7	0.82	0.34	-	61,61,61,61	5
86	MG	5	3639	1/1	0.83	0.16	-	50,50,50,50	0
86	MG	4	202	1/1	0.54	0.67	-	57,57,57,57	0
86	MG	5	3667	1/1	0.87	0.44	-	33,33,33,33	0
86	MG	5	3640	1/1	0.81	1.16	-	55,55,55,55	0
86	MG	6	1945	1/1	0.95	0.55	-	51,51,51,51	0
87	OHX	5	4130	7/7	0.92	0.19	-	64,64,64,64	5
86	MG	1	3500	1/1	0.96	0.84	-	30,30,30,30	0
86	MG	1	3619	1/1	0.92	0.43	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3748	1/1	0.89	0.44	-	67,67,67,67	0
86	MG	1	3536	1/1	0.95	0.58	-	29,29,29,29	0
86	MG	N6	201	1/1	0.81	0.47	-	70,70,70,70	0
86	MG	5	3604	1/1	0.96	0.47	-	33,33,33,33	0
87	OHX	14	403	7/7	0.97	0.14	-	51,51,51,51	7
86	MG	5	3748	1/1	0.97	0.57	-	30,30,30,30	0
86	MG	1	3504	1/1	0.95	0.65	-	42,42,42,42	0
86	MG	5	3728	1/1	0.92	0.19	-	47,47,47,47	0
86	MG	1	3462	1/1	0.92	0.73	-	44,44,44,44	0
86	MG	5	3749	1/1	0.79	0.41	-	37,37,37,37	0
87	OHX	1	3818	7/7	0.99	0.26	-	62,62,62,62	2
86	MG	2	1979	1/1	0.86	0.44	-	70,70,70,70	0
86	MG	6	1956	1/1	0.98	0.38	-	44,44,44,44	0
87	OHX	1	3922	7/7	0.98	0.21	-	82,82,82,82	3
87	OHX	5	4015	7/7	0.95	0.19	-	62,62,62,62	7
87	OHX	5	4166	7/7	0.96	0.29	-	38,38,38,38	3
86	MG	5	3504	1/1	0.94	0.85	-	25,25,25,25	0
86	MG	1	3706	1/1	0.98	0.23	-	38,38,38,38	0
87	OHX	5	4095	7/7	0.97	0.12	-	119,119,119,119	7
86	MG	1	3688	1/1	0.93	0.74	-	39,39,39,39	0
87	OHX	5	3891	7/7	0.98	0.31	-	63,63,63,63	3
87	OHX	2	2023	7/7	0.97	0.11	-	106,106,106,106	4
87	OHX	6	2133	7/7	0.91	0.35	-	125,125,125,125	6
87	OHX	8	227	7/7	0.88	0.46	-	73,73,73,73	5
86	MG	1	3439	1/1	0.96	0.31	-	60,60,60,60	0
86	MG	1	3736	1/1	0.95	0.11	-	50,50,50,50	0
86	MG	1	4117	1/1	0.95	0.98	-	47,47,47,47	0
87	OHX	5	4110	7/7	0.95	0.21	-	74,74,74,74	7
86	MG	1	3726	1/1	0.85	0.27	-	64,64,64,64	0
87	OHX	1	3953	7/7	0.97	0.27	-	58,58,58,58	2
87	OHX	2	2143	7/7	0.87	0.34	-	84,84,84,84	5
86	MG	1	3596	1/1	0.90	0.37	-	46,46,46,46	0
86	MG	2	1919	1/1	0.87	0.33	-	62,62,62,62	0
86	MG	1	3553	1/1	0.96	0.53	-	24,24,24,24	0
87	OHX	5	4116	7/7	0.94	0.35	-	40,40,40,40	5
86	MG	5	3614	1/1	0.86	0.51	-	35,35,35,35	0
86	MG	5	3458	1/1	0.97	0.49	-	34,34,34,34	0
86	MG	6	1972	1/1	0.53	0.34	-	81,81,81,81	0
86	MG	5	3417	1/1	0.76	0.51	-	36,36,36,36	0
86	MG	5	3766	1/1	0.85	0.32	-	43,43,43,43	0
87	OHX	1	3994	7/7	0.97	0.20	-	54,54,54,54	5
87	OHX	5	3864	7/7	0.98	0.18	-	86,86,86,86	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	4	203	1/1	0.86	0.63	-	64,64,64,64	0
87	OHX	5	4061	7/7	0.80	0.46	-	56,56,56,56	3
86	MG	5	3518	1/1	0.98	0.79	-	35,35,35,35	0
86	MG	1	3404	1/1	0.94	0.57	-	57,57,57,57	0
87	OHX	1	4070	7/7	0.88	0.18	-	111,111,111,111	6
86	MG	1	3537	1/1	0.93	0.45	-	57,57,57,57	0
86	MG	1	3508	1/1	0.87	0.59	-	38,38,38,38	0
87	OHX	4	219	7/7	0.97	0.17	-	81,81,81,81	2
86	MG	5	3559	1/1	0.99	0.70	-	27,27,27,27	0
86	MG	6	1991	1/1	0.96	0.15	-	77,77,77,77	0
86	MG	2	1963	1/1	0.79	0.17	-	83,83,83,83	0
86	MG	5	3747	1/1	0.91	0.07	-	124,124,124,124	0
86	MG	5	3778	1/1	0.96	0.63	-	35,35,35,35	0
86	MG	5	3467	1/1	0.76	0.43	-	47,47,47,47	0
86	MG	1	3632	1/1	0.93	0.67	-	47,47,47,47	0
87	OHX	4	222	7/7	0.96	0.20	-	61,61,61,61	3
86	MG	5	3529	1/1	0.96	0.50	-	31,31,31,31	0
86	MG	5	3535	1/1	0.97	0.81	-	29,29,29,29	0
86	MG	6	1942	1/1	0.93	0.41	-	43,43,43,43	0
87	OHX	3	217	7/7	0.91	0.36	-	78,78,78,78	4
87	OHX	5	4071	7/7	0.96	0.34	-	40,40,40,40	4
86	MG	1	3626	1/1	0.89	0.47	-	46,46,46,46	0
87	OHX	1	3965	7/7	0.94	0.32	-	56,56,56,56	3
86	MG	1	3678	1/1	0.92	0.41	-	53,53,53,53	0
86	MG	5	3610	1/1	0.95	0.46	-	38,38,38,38	0
86	MG	1	3602	1/1	0.93	0.33	-	58,58,58,58	0
86	MG	1	3646	1/1	0.92	0.29	-	39,39,39,39	0
86	MG	1	3519	1/1	0.95	0.87	-	49,49,49,49	0
86	MG	1	3744	1/1	0.95	0.34	-	44,44,44,44	0
86	MG	5	3664	1/1	0.94	0.25	-	43,43,43,43	0
87	OHX	1	4094	7/7	0.89	0.20	-	77,77,77,77	4
86	MG	5	3793	1/1	0.91	0.19	-	45,45,45,45	0
86	MG	5	3411	1/1	0.80	0.24	-	47,47,47,47	0
87	OHX	1	4097	7/7	0.93	0.20	-	42,42,42,42	6
87	OHX	1	4099	7/7	0.87	0.35	-	53,53,53,53	3
86	MG	6	1959	1/1	0.94	0.35	-	98,98,98,98	0
86	MG	5	3619	1/1	0.89	0.67	-	39,39,39,39	0
87	OHX	5	4089	7/7	0.95	0.26	-	51,51,51,51	4
86	MG	5	3631	1/1	0.85	0.72	-	36,36,36,36	0
86	MG	1	3718	1/1	0.93	0.62	-	52,52,52,52	0
86	MG	1	3747	1/1	0.75	0.34	-	48,48,48,48	0
87	OHX	5	4140	7/7	0.89	0.41	-	49,49,49,49	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3710	1/1	0.84	0.24	-	46,46,46,46	0
87	OHX	5	3961	7/7	0.96	0.25	-	47,47,47,47	4
86	MG	5	3468	1/1	0.78	0.47	-	38,38,38,38	1
86	MG	5	3538	1/1	0.97	0.52	-	33,33,33,33	0
87	OHX	1	4023	7/7	0.95	0.38	-	73,73,73,73	3
86	MG	5	3707	1/1	0.90	0.15	-	50,50,50,50	0
86	MG	1	3647	1/1	0.94	0.47	-	64,64,64,64	0
87	OHX	2	2131	7/7	0.93	0.12	-	109,109,109,109	5
86	MG	2	1961	1/1	0.95	0.53	-	86,86,86,86	0
86	MG	5	3743	1/1	0.85	0.45	-	57,57,57,57	0
87	OHX	8	230	7/7	0.93	0.28	-	62,62,62,62	5
86	MG	1	3475	1/1	0.87	0.51	-	44,44,44,44	0
87	OHX	5	3859	7/7	0.98	0.20	-	88,88,88,88	3
86	MG	5	3723	1/1	0.95	0.35	-	35,35,35,35	0
86	MG	1	3534	1/1	0.85	0.25	-	69,69,69,69	0
87	OHX	1	4060	7/7	0.98	0.27	-	65,65,65,65	4
86	MG	5	3439	1/1	0.93	0.38	-	36,36,36,36	0
86	MG	5	3802	1/1	0.87	0.36	-	35,35,35,35	0
87	OHX	8	215	7/7	0.98	0.20	-	85,85,85,85	3
86	MG	5	3453	1/1	0.90	0.49	-	59,59,59,59	0
86	MG	5	3629	1/1	0.84	0.37	-	56,56,56,56	0
86	MG	1	3649	1/1	0.92	0.43	-	37,37,37,37	0
87	OHX	6	2154	7/7	0.94	0.30	-	49,49,49,49	3
87	OHX	6	2016	7/7	0.98	0.22	-	83,83,83,83	4
87	OHX	5	4075	7/7	0.94	0.20	-	43,43,43,43	3
87	OHX	2	2135	7/7	0.67	0.15	-	188,188,188,188	6
86	MG	5	3689	1/1	0.76	0.64	-	75,75,75,75	0
87	OHX	1	3945	7/7	0.94	0.28	-	57,57,57,57	5
86	MG	1	3658	1/1	0.86	0.54	-	42,42,42,42	0
86	MG	5	3780	1/1	0.89	0.52	-	43,43,43,43	0
86	MG	5	4173	1/1	0.97	0.41	-	33,33,33,33	0
86	MG	5	3481	1/1	0.95	0.72	-	37,37,37,37	0
87	OHX	5	3882	7/7	0.99	0.25	-	53,53,53,53	1
86	MG	5	3437	1/1	0.89	0.60	-	39,39,39,39	0
87	OHX	2	2033	7/7	0.98	0.26	-	78,78,78,78	3
86	MG	2	1960	1/1	0.74	0.27	-	76,76,76,76	0
86	MG	1	3577	1/1	0.87	0.67	-	39,39,39,39	0
87	OHX	4	225	7/7	0.95	0.19	-	106,106,106,106	5
86	MG	6	1912	1/1	0.94	0.71	-	39,39,39,39	0
86	MG	5	3670	1/1	0.94	0.35	-	84,84,84,84	0
87	OHX	5	3981	7/7	0.95	0.20	-	58,58,58,58	3
87	OHX	2	2107	7/7	0.89	0.50	-	66,66,66,66	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3684	1/1	0.96	0.29	-	52,52,52,52	0
86	MG	1	3526	1/1	0.92	0.51	-	45,45,45,45	0
86	MG	2	1978	1/1	0.59	0.32	-	74,74,74,74	0
86	MG	5	3763	1/1	0.97	0.32	-	43,43,43,43	0
86	MG	1	3435	1/1	0.98	0.90	-	25,25,25,25	0
87	OHX	2	2015	7/7	0.99	0.13	-	90,90,90,90	4
86	MG	6	1965	1/1	0.80	0.38	-	48,48,48,48	0
87	OHX	2	2043	7/7	0.92	0.25	-	100,100,100,100	4
86	MG	1	3514	1/1	0.97	0.43	-	35,35,35,35	0
87	OHX	5	4141	7/7	0.90	0.29	-	58,58,58,58	4
86	MG	5	3431	1/1	0.87	0.30	-	32,32,32,32	0
86	MG	1	3434	1/1	0.87	0.54	-	62,62,62,62	0
86	MG	1	3759	1/1	0.92	0.29	-	48,48,48,48	0
86	MG	5	3740	1/1	0.67	0.50	-	66,66,66,66	0
87	OHX	5	4154	7/7	0.93	0.14	-	97,97,97,97	7
86	MG	1	3727	1/1	0.90	0.35	-	48,48,48,48	0
86	MG	5	3757	1/1	0.94	0.32	-	36,36,36,36	0
86	MG	5	3452	1/1	0.89	0.98	-	33,33,33,33	0
86	MG	1	3606	1/1	0.97	0.21	-	43,43,43,43	0
86	MG	2	1990	1/1	0.95	0.53	-	49,49,49,49	0
87	OHX	6	2143	7/7	0.91	0.38	-	51,51,51,51	3
87	OHX	8	217	7/7	0.91	0.36	-	63,63,63,63	4
86	MG	5	3756	1/1	0.56	0.17	-	73,73,73,73	0
86	MG	5	3557	1/1	0.91	0.56	-	31,31,31,31	0
86	MG	1	3565	1/1	0.89	0.50	-	40,40,40,40	0
86	MG	1	3635	1/1	0.93	0.25	-	88,88,88,88	0
86	MG	1	3629	1/1	0.81	0.98	-	33,33,33,33	0
87	OHX	6	2183	7/7	0.73	0.61	-	76,76,76,76	5
86	MG	5	3657	1/1	0.91	0.34	-	27,27,27,27	0
86	MG	1	3461	1/1	0.83	0.41	-	57,57,57,57	0
87	OHX	6	2048	7/7	0.98	0.19	-	65,65,65,65	4
87	OHX	1	3975	7/7	0.84	0.25	-	88,88,88,88	3
86	MG	6	1982	1/1	0.77	1.00	-	53,53,53,53	0
86	MG	5	3609	1/1	0.85	0.19	-	49,49,49,49	0
86	MG	5	3558	1/1	0.98	0.58	-	22,22,22,22	0
86	MG	1	3610	1/1	0.94	0.65	-	45,45,45,45	0
86	MG	6	1986	1/1	0.68	0.96	-	93,93,93,93	0
86	MG	1	3640	1/1	0.96	0.47	-	62,62,62,62	0
86	MG	6	1967	1/1	0.85	0.35	-	76,76,76,76	0
87	OHX	1	3850	7/7	0.98	0.28	-	47,47,47,47	3
87	OHX	6	2096	7/7	0.97	0.14	-	94,94,94,94	5
87	OHX	1	4102	7/7	0.88	0.26	-	65,65,65,65	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3679	1/1	0.71	0.30	-	59,59,59,59	0
86	MG	5	3704	1/1	0.94	0.14	-	66,66,66,66	0
86	MG	5	3461	1/1	0.39	0.22	-	109,109,109,109	0
86	MG	1	3494	1/1	0.95	0.42	-	42,42,42,42	0
86	MG	2	1908	1/1	0.81	0.30	-	90,90,90,90	0
87	OHX	5	3971	7/7	0.96	0.19	-	89,89,89,89	1
86	MG	2	1923	1/1	0.84	0.88	-	45,45,45,45	0
87	OHX	6	2046	7/7	0.98	0.35	-	60,60,60,60	2
86	MG	1	3425	1/1	0.99	0.90	-	27,27,27,27	0
86	MG	2	1904	1/1	0.67	0.42	-	90,90,90,90	0
87	OHX	1	4096	7/7	0.90	0.21	-	80,80,80,80	4
86	MG	1	3518	1/1	0.95	0.66	-	31,31,31,31	0
87	OHX	2	2076	7/7	0.92	0.23	-	87,87,87,87	5
86	MG	5	3605	1/1	0.96	0.16	-	39,39,39,39	1
86	MG	5	3408	1/1	0.82	0.53	-	45,45,45,45	0
87	OHX	1	3995	7/7	0.93	0.56	-	50,50,50,50	2
87	OHX	6	2139	7/7	0.97	0.18	-	86,86,86,86	3
87	OHX	1	4009	7/7	0.86	0.22	-	131,131,131,131	7
87	OHX	5	4006	7/7	0.98	0.23	-	40,40,40,40	3
87	OHX	5	3958	7/7	0.99	0.17	-	61,61,61,61	4
86	MG	5	3579	1/1	0.90	0.64	-	38,38,38,38	0
86	MG	5	3620	1/1	0.85	0.47	-	36,36,36,36	0
86	MG	1	3564	1/1	0.97	0.41	-	30,30,30,30	0
86	MG	L3	401	1/1	0.98	0.30	-	41,41,41,41	0
86	MG	1	3722	1/1	0.96	0.23	-	43,43,43,43	0
86	MG	4	204	1/1	0.70	0.61	-	58,58,58,58	0
86	MG	2	1987	1/1	0.36	0.29	-	104,104,104,104	0
87	OHX	6	2087	7/7	0.92	0.26	-	109,109,109,109	6
86	MG	1	3544	1/1	0.85	0.53	-	55,55,55,55	0
86	MG	6	1979	1/1	0.85	0.33	-	101,101,101,101	0
86	MG	5	3549	1/1	0.96	0.84	-	44,44,44,44	0
86	MG	7	209	1/1	0.96	0.13	-	54,54,54,54	0
86	MG	6	2004	1/1	0.54	0.80	-	74,74,74,74	0
86	MG	6	1905	1/1	0.91	0.35	-	51,51,51,51	0
87	OHX	6	2075	7/7	0.98	0.25	-	76,76,76,76	3
86	MG	5	3782	1/1	0.90	0.29	-	38,38,38,38	0
86	MG	5	3634	1/1	0.85	0.17	-	50,50,50,50	0
86	MG	5	3627	1/1	0.88	0.49	-	92,92,92,92	0
86	MG	6	1970	1/1	0.81	1.02	-	64,64,64,64	0
86	MG	1	3741	1/1	0.91	0.42	-	46,46,46,46	0
86	MG	5	3688	1/1	0.91	0.43	-	40,40,40,40	0
86	MG	5	3473	1/1	0.95	0.31	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	4121	7/7	0.87	0.29	-	52,52,52,52	3
86	MG	2	1973	1/1	0.67	0.38	-	80,80,80,80	0
86	MG	5	3755	1/1	0.90	0.56	-	42,42,42,42	0
86	MG	5	3624	1/1	0.79	0.41	-	51,51,51,51	0
86	MG	5	3480	1/1	0.69	0.21	-	76,76,76,76	0
86	MG	5	3445	1/1	0.66	0.48	-	64,64,64,64	0
86	MG	5	3524	1/1	0.97	0.69	-	31,31,31,31	0
87	OHX	5	4062	7/7	0.95	0.30	-	39,39,39,39	3
86	MG	1	3650	1/1	0.89	0.25	-	47,47,47,47	0
86	MG	1	3634	1/1	0.77	0.65	-	41,41,41,41	0
86	MG	5	3496	1/1	0.97	0.46	-	36,36,36,36	0
87	OHX	3	218	7/7	0.94	0.30	-	54,54,54,54	5
86	MG	2	1982	1/1	0.97	0.74	-	46,46,46,46	0
86	MG	5	3784	1/1	0.91	0.26	-	57,57,57,57	0
87	OHX	1	3869	7/7	0.98	0.20	-	92,92,92,92	3
87	OHX	1	3893	7/7	0.94	0.17	-	155,155,155,155	6
86	MG	6	1985	1/1	0.71	0.44	-	55,55,55,55	0
87	OHX	5	3950	7/7	0.96	0.43	-	67,67,67,67	5
86	MG	1	3672	1/1	0.88	0.44	-	76,76,76,76	0
86	MG	5	3583	1/1	0.96	0.44	-	27,27,27,27	0
86	MG	5	3714	1/1	0.73	0.29	-	62,62,62,62	0
86	MG	7	208	1/1	0.88	0.26	-	45,45,45,45	0
86	MG	1	3593	1/1	0.98	0.24	-	50,50,50,50	0
86	MG	5	3618	1/1	0.97	0.32	-	47,47,47,47	0
86	MG	5	3611	1/1	0.91	0.32	-	40,40,40,40	0
86	MG	1	3486	1/1	0.99	0.61	-	39,39,39,39	0
86	MG	1	3703	1/1	0.93	0.43	-	40,40,40,40	0
86	MG	5	3443	1/1	0.72	0.43	-	34,34,34,34	0
86	MG	2	1970	1/1	0.88	0.56	-	65,65,65,65	0
86	MG	7	206	1/1	0.98	0.39	-	34,34,34,34	0
87	OHX	1	3998	7/7	0.97	0.26	-	107,107,107,107	4
86	MG	1	3452	1/1	0.85	0.74	-	55,55,55,55	0
86	MG	1	3492	1/1	0.91	0.62	-	32,32,32,32	0
86	MG	7	210	1/1	0.84	0.28	-	43,43,43,43	0
87	OHX	1	3972	7/7	0.97	0.21	-	55,55,55,55	4
87	OHX	1	4013	7/7	0.93	0.34	-	54,54,54,54	3
87	OHX	5	3876	7/7	0.99	0.17	-	62,62,62,62	3
86	MG	7	212	1/1	0.87	0.81	-	51,51,51,51	0
86	MG	5	3613	1/1	0.95	0.65	-	41,41,41,41	0
86	MG	2	1948	1/1	0.86	0.56	-	72,72,72,72	0
87	OHX	2	2116	7/7	0.93	0.18	-	127,127,127,127	7
87	OHX	5	3975	7/7	0.96	0.16	-	115,115,115,115	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3510	1/1	0.94	0.36	-	39,39,39,39	0
87	OHX	6	2166	7/7	0.93	0.30	-	66,66,66,66	4
87	OHX	5	3919	7/7	0.98	0.21	-	36,36,36,36	2
86	MG	1	3547	1/1	0.95	0.94	-	32,32,32,32	0
86	MG	5	3696	1/1	0.81	0.18	-	61,61,61,61	0
87	OHX	2	2092	7/7	0.91	0.41	-	73,73,73,73	5
86	MG	1	3644	1/1	0.91	0.31	-	52,52,52,52	0
87	OHX	2	2060	7/7	0.96	0.30	-	89,89,89,89	6
87	OHX	6	2062	7/7	0.97	0.13	-	117,117,117,117	4
86	MG	1	3451	1/1	0.97	0.46	-	53,53,53,53	0
86	MG	2	1927	1/1	0.60	0.21	-	85,85,85,85	0
87	OHX	5	3895	7/7	0.98	0.27	-	42,42,42,42	4
86	MG	5	3663	1/1	0.87	0.31	-	62,62,62,62	0
86	MG	1	3445	1/1	0.94	0.79	-	57,57,57,57	0
87	OHX	1	3852	7/7	0.98	0.25	-	70,70,70,70	3
87	OHX	1	3768	7/7	1.00	0.23	-	52,52,52,52	2
87	OHX	n9	101	7/7	0.99	0.20	-	62,62,62,62	2
87	OHX	1	4039	7/7	0.87	0.09	-	278,278,278,278	6
87	OHX	2	2142	7/7	0.82	0.16	-	132,132,132,132	7
87	OHX	5	4152	7/7	0.78	0.49	-	35,35,35,35	4
87	OHX	4	227	7/7	0.88	0.55	-	51,51,51,51	4
86	MG	1	3535	1/1	0.83	0.51	-	39,39,39,39	0
86	MG	6	1939	1/1	0.94	0.33	-	34,34,34,34	0
86	MG	5	3791	1/1	0.87	0.34	-	55,55,55,55	0
86	MG	5	3731	1/1	0.96	0.32	-	30,30,30,30	0
87	OHX	6	2077	7/7	0.94	0.24	-	98,98,98,98	5
87	OHX	1	3997	7/7	0.95	0.24	-	55,55,55,55	5
87	OHX	1	3804	7/7	0.99	0.19	-	62,62,62,62	1
87	OHX	1	4073	7/7	0.83	0.46	-	71,71,71,71	5
86	MG	1	3417	1/1	0.89	0.38	-	78,78,78,78	0
86	MG	5	3661	1/1	0.89	0.63	-	42,42,42,42	0
86	MG	2	1935	1/1	0.98	0.27	-	70,70,70,70	0
86	MG	5	3665	1/1	0.96	0.40	-	54,54,54,54	0
86	MG	1	3680	1/1	0.90	0.69	-	45,45,45,45	0
86	MG	2	1956	1/1	0.92	0.87	-	70,70,70,70	0
86	MG	8	205	1/1	0.97	0.30	-	47,47,47,47	0
86	MG	1	3645	1/1	0.91	0.27	-	51,51,51,51	0
86	MG	1	3566	1/1	0.88	0.30	-	47,47,47,47	0
86	MG	7	201	1/1	0.91	0.54	-	41,41,41,41	0
87	OHX	6	2054	7/7	0.98	0.12	-	87,87,87,87	3
87	OHX	5	4047	7/7	0.86	0.23	-	69,69,69,69	3
87	OHX	1	3959	7/7	0.98	0.23	-	112,112,112,112	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3671	1/1	0.72	0.57	-	62,62,62,62	0
86	MG	5	3692	1/1	0.90	0.40	-	38,38,38,38	0
86	MG	5	3441	1/1	0.93	0.28	-	32,32,32,32	0
87	OHX	6	2071	7/7	0.92	0.40	-	58,58,58,58	4
87	OHX	5	4133	7/7	0.93	0.10	-	157,157,157,157	7
87	OHX	5	3921	7/7	0.95	0.14	-	119,119,119,119	6
86	MG	5	3753	1/1	0.91	0.47	-	51,51,51,51	0
86	MG	6	1926	1/1	0.92	0.20	-	65,65,65,65	0
87	OHX	6	2111	7/7	0.94	0.24	-	73,73,73,73	5
87	OHX	2	2149	7/7	0.70	0.28	-	137,137,137,137	6
86	MG	3	205	1/1	0.90	0.52	-	68,68,68,68	0
86	MG	6	1935	1/1	0.85	0.87	-	44,44,44,44	0
86	MG	1	3660	1/1	0.89	0.15	-	82,82,82,82	0
86	MG	5	3812	1/1	0.84	0.61	-	31,31,31,31	0
86	MG	5	3653	1/1	0.97	0.55	-	31,31,31,31	0
87	OHX	5	3860	7/7	0.99	0.20	-	46,46,46,46	3
87	OHX	1	3881	7/7	0.98	0.17	-	86,86,86,86	4
86	MG	5	3466	1/1	0.90	0.44	-	47,47,47,47	0
87	OHX	6	2114	7/7	0.91	0.24	-	66,66,66,66	3
86	MG	1	3713	1/1	0.87	1.07	-	40,40,40,40	0
87	OHX	6	2081	7/7	0.97	0.21	-	74,74,74,74	6
86	MG	L6	201	1/1	0.81	0.19	-	57,57,57,57	0
86	MG	5	3435	1/1	0.83	0.43	-	44,44,44,44	0
86	MG	1	3447	1/1	0.97	0.50	-	51,51,51,51	0
86	MG	5	3648	1/1	0.75	0.65	-	47,47,47,47	0
87	OHX	1	4012	7/7	0.95	0.26	-	64,64,64,64	1
86	MG	1	3430	1/1	0.93	0.17	-	57,57,57,57	0
87	OHX	1	3904	7/7	0.94	0.45	-	59,59,59,59	3
86	MG	5	3788	1/1	0.90	0.24	-	49,49,49,49	0
86	MG	5	3712	1/1	0.88	0.38	-	38,38,38,38	0
87	OHX	1	3857	7/7	0.98	0.27	-	54,54,54,54	4
86	MG	M6	202	1/1	0.79	0.29	-	40,40,40,40	0
87	OHX	2	2111	7/7	0.90	0.28	-	112,112,112,112	5
87	OHX	2	2039	7/7	0.98	0.17	-	103,103,103,103	7
86	MG	5	3641	1/1	0.94	0.44	-	39,39,39,39	0
87	OHX	1	3924	7/7	0.89	0.26	-	71,71,71,71	4
86	MG	1	3491	1/1	0.79	0.62	-	51,51,51,51	0
87	OHX	2	2018	7/7	0.98	0.16	-	74,74,74,74	5
87	OHX	1	3957	7/7	0.97	0.24	-	49,49,49,49	5
86	MG	5	3575	1/1	0.96	0.48	-	28,28,28,28	0
86	MG	5	3573	1/1	0.89	0.29	-	37,37,37,37	0
87	OHX	5	4112	7/7	0.96	0.28	-	52,52,52,52	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3679	1/1	0.46	0.42	-	70,70,70,70	0
86	MG	6	1953	1/1	0.84	0.42	-	63,63,63,63	0
86	MG	17	2201	1/1	0.91	0.27	-	46,46,46,46	0
87	OHX	5	4167	7/7	0.93	0.26	-	64,64,64,64	5
86	MG	5	3649	1/1	0.86	0.59	-	29,29,29,29	0
86	MG	M9	201	1/1	0.81	0.31	-	75,75,75,75	0
86	MG	2	1940	1/1	0.87	0.68	-	80,80,80,80	0
86	MG	5	3568	1/1	0.92	0.60	-	38,38,38,38	0
86	MG	4	209	1/1	0.98	0.46	-	63,63,63,63	0
86	MG	4	208	1/1	0.94	0.41	-	51,51,51,51	0
87	OHX	6	2157	7/7	0.91	0.23	-	90,90,90,90	7
86	MG	5	3676	1/1	0.95	0.35	-	29,29,29,29	0
86	MG	5	3450	1/1	0.86	0.48	-	40,40,40,40	0
86	MG	7	204	1/1	0.94	0.69	-	44,44,44,44	0
86	MG	5	3459	1/1	0.70	0.51	-	36,36,36,36	0
86	MG	1	3542	1/1	0.94	0.43	-	50,50,50,50	0
86	MG	5	3542	1/1	0.76	0.54	-	41,41,41,41	0
86	MG	1	3569	1/1	0.96	0.72	-	39,39,39,39	0
86	MG	N8	201	1/1	0.91	0.32	-	30,30,30,30	0
87	OHX	5	4080	7/7	0.94	0.42	-	35,35,35,35	3
86	MG	1	3581	1/1	0.97	0.81	-	29,29,29,29	0
86	MG	7	202	1/1	0.94	0.78	-	19,19,19,19	0
87	OHX	1	4046	7/7	0.93	0.36	-	50,50,50,50	2
87	OHX	1	4090	7/7	0.87	0.32	-	47,47,47,47	4
87	OHX	2	2152	7/7	0.87	0.31	-	122,122,122,122	6
86	MG	8	202	1/1	0.80	0.36	-	57,57,57,57	0
86	MG	1	3690	1/1	0.87	0.49	-	63,63,63,63	0
87	OHX	2	2118	7/7	0.94	0.15	-	143,143,143,143	7
86	MG	5	3684	1/1	0.71	0.92	-	48,48,48,48	0
87	OHX	1	4057	7/7	0.95	0.10	-	109,109,109,109	5
86	MG	2	1925	1/1	0.87	0.26	-	67,67,67,67	0
87	OHX	5	3889	7/7	0.97	0.20	-	69,69,69,69	3
86	MG	8	201	1/1	0.95	0.29	-	42,42,42,42	0
86	MG	1	3550	1/1	0.97	0.70	-	33,33,33,33	0
87	OHX	6	2168	7/7	0.86	0.26	-	76,76,76,76	3
87	OHX	1	3865	7/7	0.99	0.13	-	75,75,75,75	2
86	MG	5	3727	1/1	0.88	0.42	-	44,44,44,44	0
86	MG	6	1940	1/1	0.95	0.52	-	36,36,36,36	0
87	OHX	1	4045	7/7	0.95	0.31	-	54,54,54,54	1
86	MG	M7	201	1/1	0.69	0.58	-	71,71,71,71	0
86	MG	6	1962	1/1	0.95	0.15	-	93,93,93,93	0
86	MG	2	1988	1/1	0.95	0.13	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	3849	7/7	0.98	0.26	-	51,51,51,51	2
86	MG	1	3416	1/1	0.91	1.00	-	43,43,43,43	0
87	OHX	1	4026	7/7	0.90	0.37	-	52,52,52,52	5
87	OHX	5	3982	7/7	0.95	0.36	-	46,46,46,46	3
86	MG	1	3548	1/1	0.98	0.66	-	30,30,30,30	0
87	OHX	5	3930	7/7	0.99	0.26	-	54,54,54,54	4
87	OHX	5	4005	7/7	0.93	0.48	-	109,109,109,109	5
86	MG	2	1930	1/1	0.74	0.39	-	72,72,72,72	0
87	OHX	m5	304	7/7	0.98	0.28	-	54,54,54,54	3
86	MG	1	3463	1/1	0.86	0.34	-	39,39,39,39	0
86	MG	1	3541	1/1	0.96	0.65	-	28,28,28,28	0
86	MG	5	3598	1/1	0.74	0.57	-	39,39,39,39	0
86	MG	5	3647	1/1	0.95	0.32	-	37,37,37,37	0
87	OHX	5	3980	7/7	0.98	0.23	-	69,69,69,69	3
86	MG	2	1939	1/1	0.56	0.55	-	130,130,130,130	0
86	MG	6	1988	1/1	0.86	0.30	-	80,80,80,80	0
87	OHX	5	4165	7/7	0.78	0.54	-	49,49,49,49	4
86	MG	2	1974	1/1	0.67	0.38	-	83,83,83,83	0
86	MG	5	3636	1/1	0.67	0.57	-	36,36,36,36	0
86	MG	1	3410	1/1	0.82	0.57	-	39,39,39,39	0
86	MG	1	3442	1/1	0.90	0.18	-	52,52,52,52	0
86	MG	1	3724	1/1	0.97	0.37	-	55,55,55,55	0
87	OHX	7	215	7/7	0.98	0.20	-	60,60,60,60	5
86	MG	5	3673	1/1	0.58	0.23	-	65,65,65,65	0
87	OHX	5	3858	7/7	0.99	0.24	-	55,55,55,55	1
86	MG	5	3801	1/1	0.84	0.76	-	44,44,44,44	0
86	MG	1	3456	1/1	0.99	0.41	-	32,32,32,32	0
86	MG	6	1927	1/1	0.91	0.34	-	63,63,63,63	0
86	MG	1	3712	1/1	0.94	0.53	-	44,44,44,44	0
87	OHX	5	4155	7/7	0.93	0.20	-	49,49,49,49	6
86	MG	L7	303	1/1	0.91	0.23	-	50,50,50,50	0
86	MG	1	3709	1/1	0.91	0.21	-	48,48,48,48	0
86	MG	5	3662	1/1	0.83	0.26	-	48,48,48,48	0
86	MG	6	1993	1/1	0.74	0.31	-	66,66,66,66	0
87	OHX	5	4171	7/7	0.87	0.65	-	45,45,45,45	3
87	OHX	5	3861	7/7	0.98	0.25	-	47,47,47,47	2
86	MG	6	1957	1/1	0.95	0.11	-	94,94,94,94	0
87	OHX	M9	202	7/7	0.86	0.20	-	77,77,77,77	3
87	OHX	1	3882	7/7	0.99	0.21	-	64,64,64,64	3
86	MG	1	3529	1/1	0.89	0.54	-	34,34,34,34	0
86	MG	5	3742	1/1	0.96	0.46	-	32,32,32,32	0
86	MG	5	3754	1/1	0.86	0.96	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2000	1/1	0.94	0.89	-	48,48,48,48	0
86	MG	1	3460	1/1	0.89	0.32	-	49,49,49,49	0
87	OHX	6	2148	7/7	0.95	0.30	-	54,54,54,54	3
86	MG	2	1985	1/1	0.58	0.53	-	86,86,86,86	0
86	MG	5	3659	1/1	0.97	0.62	-	46,46,46,46	0
87	OHX	5	4079	7/7	0.94	0.27	-	55,55,55,55	3
86	MG	6	1937	1/1	0.57	0.89	-	98,98,98,98	0
87	OHX	5	3973	7/7	0.95	0.30	-	53,53,53,53	4
86	MG	5	3547	1/1	0.88	0.59	-	25,25,25,25	0
87	OHX	2	2025	7/7	0.97	0.21	-	79,79,79,79	5
87	OHX	c3	201	7/7	0.93	0.26	-	84,84,84,84	4
87	OHX	1	3855	7/7	0.97	0.30	-	87,87,87,87	3
86	MG	5	3415	1/1	0.94	0.64	-	31,31,31,31	0
86	MG	5	3733	1/1	0.84	0.27	-	45,45,45,45	0
86	MG	1	3446	1/1	0.95	0.44	-	41,41,41,41	0
86	MG	5	3446	1/1	0.98	0.40	-	31,31,31,31	0
87	OHX	6	2118	7/7	0.91	0.35	-	89,89,89,89	5
86	MG	2	1903	1/1	0.89	0.66	-	43,43,43,43	0
86	MG	1	3695	1/1	0.65	0.40	-	58,58,58,58	0
86	MG	1	3599	1/1	0.92	0.49	-	32,32,32,32	0
86	MG	5	3578	1/1	0.94	0.40	-	17,17,17,17	0
87	OHX	2	2081	7/7	0.95	0.20	-	120,120,120,120	6
87	OHX	1	3814	7/7	0.98	0.22	-	76,76,76,76	3
87	OHX	5	4118	7/7	0.90	0.35	-	52,52,52,52	3
86	MG	2	1901	1/1	0.82	0.25	-	87,87,87,87	0
86	MG	1	3525	1/1	0.93	0.69	-	35,35,35,35	0
87	OHX	1	3910	7/7	0.95	0.17	-	81,81,81,81	4
86	MG	1	3746	1/1	0.83	0.46	-	43,43,43,43	0
86	MG	1	4114	1/1	0.95	0.34	-	41,41,41,41	0
86	MG	1	3612	1/1	0.78	0.31	-	55,55,55,55	0
86	MG	5	3444	1/1	0.92	0.45	-	38,38,38,38	0
86	MG	5	3751	1/1	0.94	0.33	-	40,40,40,40	0
86	MG	5	3768	1/1	0.82	0.90	-	50,50,50,50	0
87	OHX	2	2130	7/7	0.87	0.32	-	84,84,84,84	4
87	OHX	5	3902	7/7	0.99	0.33	-	91,91,91,91	2
86	MG	5	3474	1/1	0.96	0.58	-	51,51,51,51	0
86	MG	4	205	1/1	0.82	0.74	-	44,44,44,44	0
86	MG	5	3533	1/1	0.97	0.54	-	25,25,25,25	0
86	MG	5	3759	1/1	0.86	0.22	-	53,53,53,53	0
86	MG	1	3677	1/1	0.84	0.34	-	46,46,46,46	0
86	MG	5	3721	1/1	0.95	0.69	-	41,41,41,41	0
87	OHX	5	4153	7/7	0.90	0.21	-	111,111,111,111	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3493	1/1	0.93	0.71	-	42,42,42,42	0
87	OHX	5	4092	7/7	0.96	0.18	-	55,55,55,55	6
86	MG	5	3799	1/1	0.96	0.28	-	70,70,70,70	0
86	MG	1	3745	1/1	0.79	0.48	-	53,53,53,53	0
87	OHX	5	4085	7/7	0.81	0.47	-	70,70,70,70	4
87	OHX	1	4106	7/7	0.85	0.20	-	72,72,72,72	4
87	OHX	2	2050	7/7	0.93	0.21	-	129,129,129,129	6
87	OHX	M7	205	7/7	0.93	0.19	-	57,57,57,57	5
86	MG	4	213	1/1	0.79	0.50	-	41,41,41,41	0
87	OHX	L3	402	7/7	0.98	0.19	-	59,59,59,59	4
86	MG	O3	201	1/1	0.93	0.56	-	37,37,37,37	0
87	OHX	6	2163	7/7	0.83	0.38	-	61,61,61,61	4
87	OHX	5	3990	7/7	0.94	0.47	-	37,37,37,37	3
86	MG	5	3494	1/1	0.93	0.38	-	33,33,33,33	0
87	OHX	1	3819	7/7	0.98	0.29	-	81,81,81,81	3
87	OHX	1	4088	7/7	0.93	0.21	-	92,92,92,92	7
87	OHX	1	3862	7/7	0.96	0.18	-	83,83,83,83	3
87	OHX	1	4089	7/7	0.80	0.38	-	55,55,55,55	6
87	OHX	1	4093	7/7	0.89	0.49	-	64,64,64,64	4
86	MG	5	3807	1/1	0.95	0.23	-	36,36,36,36	0
86	MG	1	3721	1/1	0.93	0.47	-	43,43,43,43	0
87	OHX	O1	201	7/7	0.96	0.20	-	93,93,93,93	3
87	OHX	5	3988	7/7	0.94	0.22	-	158,158,158,158	5
86	MG	5	3483	1/1	0.96	0.65	-	28,28,28,28	0
86	MG	5	3713	1/1	0.78	0.41	-	36,36,36,36	0
86	MG	5	3809	1/1	0.94	0.36	-	50,50,50,50	0
86	MG	1	3622	1/1	0.89	0.64	-	44,44,44,44	0
86	MG	5	3703	1/1	0.97	0.69	-	2,2,2,2	0
86	MG	4	212	1/1	0.93	0.41	-	64,64,64,64	0
86	MG	1	3711	1/1	0.82	0.34	-	54,54,54,54	0
86	MG	6	1916	1/1	0.97	0.62	-	66,66,66,66	0
87	OHX	5	3983	7/7	0.97	0.30	-	56,56,56,56	4
86	MG	5	3612	1/1	0.69	0.54	-	42,42,42,42	0
87	OHX	1	3851	7/7	0.99	0.22	-	46,46,46,46	3
86	MG	5	3625	1/1	0.88	0.39	-	42,42,42,42	0
87	OHX	2	2140	7/7	0.93	0.29	-	85,85,85,85	5
87	OHX	6	2076	7/7	0.98	0.17	-	52,52,52,52	5
86	MG	6	2011	1/1	0.81	0.74	-	48,48,48,48	0
87	OHX	6	2132	7/7	0.95	0.24	-	94,94,94,94	6
86	MG	1	3424	1/1	0.94	0.44	-	59,59,59,59	0
87	OHX	2	2104	7/7	0.79	0.21	-	119,119,119,119	5
86	MG	5	3587	1/1	0.96	0.70	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4037	7/7	0.93	0.35	-	84,84,84,84	7
86	MG	6	1950	1/1	0.90	0.36	-	66,66,66,66	0
86	MG	1	3666	1/1	0.88	0.49	-	65,65,65,65	0
87	OHX	1	4035	7/7	0.96	0.15	-	65,65,65,65	4
86	MG	6	1964	1/1	0.92	0.25	-	82,82,82,82	0
87	OHX	2	2145	7/7	0.87	0.22	-	103,103,103,103	4
86	MG	5	3734	1/1	0.96	0.22	-	37,37,37,37	0
86	MG	5	3433	1/1	0.99	0.51	-	33,33,33,33	0
87	OHX	2	2102	7/7	0.95	0.18	-	118,118,118,118	5
86	MG	1	3617	1/1	0.78	0.56	-	41,41,41,41	0
87	OHX	2	2103	7/7	0.92	0.38	-	118,118,118,118	4
87	OHX	1	3961	7/7	0.96	0.33	-	45,45,45,45	5
87	OHX	5	4122	7/7	0.86	0.40	-	76,76,76,76	5
86	MG	5	3602	1/1	0.87	0.27	-	50,50,50,50	0
86	MG	6	1998	1/1	0.91	0.69	-	42,42,42,42	0
86	MG	2	1965	1/1	0.55	0.86	-	76,76,76,76	0
86	MG	1	3753	1/1	0.91	0.79	-	107,107,107,107	0
87	OHX	N8	202	7/7	0.90	0.37	-	90,90,90,90	7
86	MG	2	1936	1/1	0.73	0.16	-	83,83,83,83	0
87	OHX	m4	201	7/7	0.96	0.70	-	108,108,108,108	7
87	OHX	6	2176	7/7	0.91	0.27	-	62,62,62,62	7
86	MG	1	3402	1/1	0.99	0.70	-	36,36,36,36	0
86	MG	5	3520	1/1	0.90	0.49	-	44,44,44,44	0
87	OHX	5	3835	7/7	0.99	0.19	-	65,65,65,65	3
86	MG	5	3642	1/1	0.88	0.68	-	64,64,64,64	0
86	MG	6	1921	1/1	0.92	0.45	-	66,66,66,66	0
86	MG	1	3411	1/1	0.94	0.55	-	43,43,43,43	0
86	MG	5	3660	1/1	0.85	0.36	-	64,64,64,64	0
87	OHX	6	2117	7/7	0.96	0.21	-	65,65,65,65	3
86	MG	1	3752	1/1	0.84	0.19	-	64,64,64,64	0
86	MG	1	3512	1/1	0.91	0.70	-	31,31,31,31	0
86	MG	1	3655	1/1	0.96	0.84	-	44,44,44,44	0
86	MG	6	1996	1/1	0.60	0.63	-	70,70,70,70	0
86	MG	6	2008	1/1	0.76	0.96	-	61,61,61,61	0
86	MG	1	3551	1/1	0.86	0.54	-	38,38,38,38	0
86	MG	5	3687	1/1	0.95	0.18	-	47,47,47,47	0
86	MG	5	3738	1/1	0.95	0.42	-	109,109,109,109	0
86	MG	1	3468	1/1	0.94	0.75	-	39,39,39,39	0
86	MG	2	1943	1/1	0.36	0.40	-	115,115,115,115	0
87	OHX	1	4063	7/7	0.89	0.13	-	159,159,159,159	7
87	OHX	5	3970	7/7	0.92	0.29	-	41,41,41,41	7
86	MG	5	3739	1/1	0.94	0.33	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4077	7/7	0.90	0.23	-	62,62,62,62	4
87	OHX	6	2080	7/7	0.92	0.41	-	82,82,82,82	1
86	MG	7	213	1/1	0.96	0.19	-	49,49,49,49	0
86	MG	6	1983	1/1	0.88	0.89	-	57,57,57,57	0
86	MG	5	3792	1/1	0.94	0.68	-	37,37,37,37	0
87	OHX	1	3816	7/7	0.98	0.28	-	62,62,62,62	5
86	MG	1	3594	1/1	0.94	0.41	-	48,48,48,48	0
86	MG	5	3571	1/1	0.91	0.44	-	21,21,21,21	0
86	MG	5	3551	1/1	0.76	0.53	-	52,52,52,52	0
87	OHX	3	213	7/7	0.95	0.19	-	82,82,82,82	5
87	OHX	6	2024	7/7	0.99	0.15	-	99,99,99,99	3
86	MG	2	1906	1/1	0.83	0.38	-	68,68,68,68	0
87	OHX	5	4002	7/7	0.97	0.19	-	54,54,54,54	3
86	MG	1	3522	1/1	0.96	0.53	-	31,31,31,31	0
86	MG	1	3686	1/1	0.93	0.69	-	35,35,35,35	0
87	OHX	1	4041	7/7	0.93	0.23	-	46,46,46,46	4
87	OHX	2	2137	7/7	0.89	0.18	-	219,219,219,219	7
86	MG	1	3459	1/1	0.79	0.70	-	60,60,60,60	0
87	OHX	1	4036	7/7	0.94	0.15	-	83,83,83,83	6
87	OHX	1	3828	7/7	0.98	0.27	-	63,63,63,63	2
86	MG	1	3432	1/1	0.95	0.36	-	49,49,49,49	0
87	OHX	6	2113	7/7	0.97	0.27	-	67,67,67,67	3
86	MG	3	208	1/1	0.84	0.82	-	42,42,42,42	0
86	MG	5	3637	1/1	0.55	0.43	-	50,50,50,50	0
86	MG	1	3667	1/1	0.90	0.48	-	58,58,58,58	0
86	MG	5	3492	1/1	0.94	0.71	-	42,42,42,42	0
87	OHX	2	2109	7/7	0.84	0.29	-	105,105,105,105	6
87	OHX	2	2019	7/7	0.97	0.22	-	81,81,81,81	3
87	OHX	1	3916	7/7	0.96	0.42	-	54,54,54,54	4
86	MG	5	3410	1/1	0.86	0.51	-	44,44,44,44	0
86	MG	5	3488	1/1	0.91	0.56	-	39,39,39,39	0
86	MG	1	3654	1/1	0.94	0.43	-	39,39,39,39	0
86	MG	5	3425	1/1	0.74	0.47	-	45,45,45,45	0
87	OHX	5	4036	7/7	0.94	0.18	-	93,93,93,93	5
86	MG	5	3511	1/1	0.97	0.60	-	28,28,28,28	0
87	OHX	1	3905	7/7	0.97	0.22	-	57,57,57,57	1
86	MG	4	211	1/1	0.82	0.36	-	60,60,60,60	0
86	MG	2	1968	1/1	0.96	0.14	-	101,101,101,101	0
86	MG	5	3789	1/1	0.78	0.33	-	69,69,69,69	0
87	OHX	5	4022	7/7	0.97	0.24	-	39,39,39,39	2
86	MG	Q2	502	1/1	0.90	0.12	-	63,63,63,63	0
87	OHX	5	4136	7/7	0.90	0.42	-	50,50,50,50	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3525	1/1	0.97	0.47	-	29,29,29,29	0
86	MG	5	3406	1/1	0.93	0.59	-	35,35,35,35	0
86	MG	2	1955	1/1	0.86	0.96	-	62,62,62,62	0
87	OHX	5	3933	7/7	0.98	0.22	-	38,38,38,38	2
87	OHX	1	3960	7/7	0.95	0.20	-	42,42,42,42	4
87	OHX	1	4017	7/7	0.94	0.31	-	46,46,46,46	2
86	MG	5	3750	1/1	0.94	0.73	-	53,53,53,53	0
86	MG	8	208	1/1	0.79	0.67	-	55,55,55,55	0
86	MG	1	3630	1/1	0.88	0.38	-	76,76,76,76	0
86	MG	6	1955	1/1	0.88	0.42	-	60,60,60,60	0
87	OHX	5	3992	7/7	0.94	0.31	-	38,38,38,38	4
86	MG	1	3453	1/1	0.99	0.81	-	39,39,39,39	0
87	OHX	1	3909	7/7	0.98	0.37	-	73,73,73,73	4
87	OHX	2	2054	7/7	0.93	0.26	-	103,103,103,103	5
86	MG	5	3534	1/1	0.91	0.51	-	36,36,36,36	0
86	MG	6	1932	1/1	0.67	0.48	-	72,72,72,72	0
86	MG	6	1902	1/1	0.91	0.90	-	40,40,40,40	0
86	MG	1	3754	1/1	0.70	0.46	-	71,71,71,71	0
86	MG	2	1907	1/1	0.89	0.55	-	62,62,62,62	0
87	OHX	5	4144	7/7	0.96	0.22	-	70,70,70,70	7
87	OHX	5	4070	7/7	0.96	0.23	-	45,45,45,45	3
86	MG	1	3656	1/1	0.84	0.60	-	46,46,46,46	0
86	MG	5	3510	1/1	0.94	0.26	-	43,43,43,43	0
87	OHX	5	4066	7/7	0.95	0.36	-	34,34,34,34	4
87	OHX	5	3957	7/7	0.98	0.28	-	42,42,42,42	2
86	MG	6	1980	1/1	0.38	0.27	-	76,76,76,76	0
86	MG	S2	301	1/1	0.89	0.80	-	62,62,62,62	0
86	MG	1	3734	1/1	0.96	0.59	-	35,35,35,35	1
86	MG	1	3730	1/1	0.94	0.14	-	36,36,36,36	0
86	MG	1	3552	1/1	0.97	0.74	-	37,37,37,37	0
86	MG	5	3645	1/1	0.84	0.53	-	56,56,56,56	0
87	OHX	6	2036	7/7	0.98	0.21	-	58,58,58,58	3
86	MG	5	3623	1/1	0.96	0.38	-	31,31,31,31	0
86	MG	1	3716	1/1	0.96	0.33	-	65,65,65,65	0
86	MG	5	3762	1/1	0.83	0.65	-	38,38,38,38	0
86	MG	1	3420	1/1	0.82	0.41	-	45,45,45,45	0
86	MG	5	3438	1/1	0.90	0.46	-	30,30,30,30	0
86	MG	1	3699	1/1	0.94	0.29	-	49,49,49,49	0
86	MG	1	3755	1/1	0.84	0.35	-	45,45,45,45	0
87	OHX	6	2047	7/7	0.98	0.20	-	67,67,67,67	5
86	MG	1	3760	1/1	0.80	0.14	-	62,62,62,62	0
86	MG	1	3443	1/1	0.85	0.55	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3458	1/1	0.88	0.64	-	51,51,51,51	0
86	MG	l3	401	1/1	0.92	0.50	-	27,27,27,27	0
87	OHX	8	229	7/7	0.82	0.36	-	68,68,68,68	3
86	MG	5	3752	1/1	0.97	0.64	-	30,30,30,30	0
87	OHX	7	223	7/7	0.93	0.35	-	54,54,54,54	4
88	ZN	D7	101	1/1	0.69	0.39	-	161,161,161,161	0
87	OHX	1	4065	7/7	0.91	0.36	-	59,59,59,59	5
87	OHX	5	3918	7/7	0.95	0.29	-	73,73,73,73	3
87	OHX	5	4041	7/7	0.97	0.29	-	43,43,43,43	3
86	MG	7	211	1/1	0.89	0.48	-	57,57,57,57	0
86	MG	5	3658	1/1	0.86	0.37	-	39,39,39,39	0
86	MG	5	3652	1/1	0.97	0.29	-	47,47,47,47	0
86	MG	5	3795	1/1	0.97	0.45	-	42,42,42,42	0
86	MG	5	3475	1/1	0.98	0.30	-	42,42,42,42	0
86	MG	l5	301	1/1	0.93	0.15	-	63,63,63,63	0
87	OHX	2	2044	7/7	0.94	0.19	-	98,98,98,98	6
86	MG	5	3576	1/1	0.81	0.45	-	31,31,31,31	0
86	MG	1	3438	1/1	0.98	0.34	-	33,33,33,33	0
86	MG	5	3808	1/1	0.86	0.42	-	42,42,42,42	0
86	MG	1	3611	1/1	0.93	0.27	-	41,41,41,41	0
86	MG	8	209	1/1	0.92	0.19	-	48,48,48,48	0
86	MG	1	3503	1/1	0.93	0.54	-	37,37,37,37	0
86	MG	5	3449	1/1	0.89	0.81	-	45,45,45,45	0
86	MG	1	3708	1/1	0.72	0.51	-	42,42,42,42	0
87	OHX	6	2173	7/7	0.87	0.27	-	64,64,64,64	5
87	OHX	6	2156	7/7	0.93	0.09	-	150,150,150,150	5
87	OHX	5	4104	7/7	0.90	0.28	-	84,84,84,84	4
86	MG	6	1930	1/1	0.96	0.72	-	45,45,45,45	0
87	OHX	1	4014	7/7	0.92	0.26	-	60,60,60,60	3
87	OHX	5	4004	7/7	0.95	0.20	-	82,82,82,82	3
86	MG	5	3675	1/1	0.87	0.27	-	51,51,51,51	0
86	MG	6	1914	1/1	0.82	0.77	-	62,62,62,62	0
86	MG	5	3482	1/1	0.72	0.86	-	52,52,52,52	0
86	MG	6	1928	1/1	0.90	0.38	-	57,57,57,57	0
86	MG	5	3681	1/1	0.86	0.45	-	45,45,45,45	0
87	OHX	1	4050	7/7	0.88	0.27	-	58,58,58,58	5
87	OHX	1	3772	7/7	0.99	0.20	-	67,67,67,67	2
86	MG	3	201	1/1	0.95	0.21	-	80,80,80,80	0
87	OHX	m9	201	7/7	0.92	0.22	-	61,61,61,61	6
87	OHX	1	4055	7/7	0.94	0.27	-	81,81,81,81	5
86	MG	5	3528	1/1	0.93	0.59	-	45,45,45,45	0
87	OHX	1	3987	7/7	0.96	0.22	-	73,73,73,73	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3710	1/1	0.94	0.47	-	32,32,32,32	0
86	MG	5	3531	1/1	0.93	0.66	-	35,35,35,35	0
86	MG	1	3639	1/1	0.77	0.70	-	56,56,56,56	0
87	OHX	4	230	7/7	0.95	0.19	-	75,75,75,75	5
86	MG	6	1961	1/1	0.75	0.16	-	95,95,95,95	0
86	MG	2	1977	1/1	0.91	0.99	-	72,72,72,72	0
86	MG	5	3786	1/1	0.92	0.27	-	33,33,33,33	0
86	MG	5	3698	1/1	0.95	0.32	-	39,39,39,39	0
87	OHX	5	3977	7/7	0.95	0.19	-	69,69,69,69	4
86	MG	5	3536	1/1	0.97	0.65	-	26,26,26,26	0
86	MG	5	3765	1/1	0.95	0.41	-	27,27,27,27	0
87	OHX	1	3796	7/7	0.98	0.27	-	57,57,57,57	4
86	MG	5	3691	1/1	0.93	0.32	-	38,38,38,38	0
86	MG	5	3770	1/1	0.86	0.42	-	36,36,36,36	0
87	OHX	m6	201	7/7	0.99	0.27	-	36,36,36,36	3
87	OHX	6	2182	7/7	0.91	0.34	-	113,113,113,113	7
86	MG	2	1952	1/1	0.92	0.45	-	64,64,64,64	0
86	MG	5	3622	1/1	0.83	0.46	-	42,42,42,42	0
87	OHX	5	3837	7/7	1.00	0.16	-	58,58,58,58	2
86	MG	4	206	1/1	0.92	0.25	-	41,41,41,41	0
86	MG	6	1924	1/1	0.92	0.53	-	48,48,48,48	0
86	MG	1	3641	1/1	0.87	0.47	-	49,49,49,49	0
86	MG	1	3470	1/1	0.95	0.61	-	46,46,46,46	0
86	MG	5	3803	1/1	0.85	0.28	-	49,49,49,49	0
86	MG	6	1958	1/1	0.99	0.62	-	44,44,44,44	0
86	MG	5	3567	1/1	0.97	0.63	-	22,22,22,22	0
86	MG	1	3444	1/1	0.87	0.50	-	35,35,35,35	0
86	MG	8	207	1/1	0.83	0.49	-	51,51,51,51	0
87	OHX	1	3930	7/7	0.96	0.35	-	118,118,118,118	2
86	MG	1	3728	1/1	0.94	0.61	-	47,47,47,47	0
87	OHX	1	4034	7/7	0.97	0.31	-	75,75,75,75	3
86	MG	5	3469	1/1	0.91	0.18	-	56,56,56,56	0
86	MG	1	3717	1/1	0.90	0.57	-	59,59,59,59	0
86	MG	1	3665	1/1	0.78	0.70	-	48,48,48,48	0
86	MG	5	3711	1/1	0.82	0.32	-	67,67,67,67	0
86	MG	5	3730	1/1	0.93	0.45	-	55,55,55,55	0
86	MG	2	1917	1/1	0.90	0.54	-	54,54,54,54	0
87	OHX	5	3847	7/7	0.99	0.21	-	54,54,54,54	1
86	MG	5	3708	1/1	0.86	0.67	-	51,51,51,51	0
86	MG	5	3736	1/1	0.94	0.77	-	40,40,40,40	0
87	OHX	5	4016	7/7	0.89	0.39	-	36,36,36,36	2
86	MG	5	3460	1/1	0.89	0.28	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3707	1/1	0.84	0.56	-	48,48,48,48	0
86	MG	1	3697	1/1	0.91	0.31	-	42,42,42,42	0
87	OHX	1	4087	7/7	0.95	0.26	-	44,44,44,44	6
86	MG	14	401	1/1	0.77	0.49	-	42,42,42,42	0
86	MG	6	1941	1/1	0.92	0.52	-	57,57,57,57	0
86	MG	6	2001	1/1	0.89	0.42	-	48,48,48,48	0
86	MG	5	3761	1/1	0.89	0.65	-	38,38,38,38	0
86	MG	1	3473	1/1	0.89	0.30	-	56,56,56,56	0
86	MG	5	3626	1/1	0.88	0.24	-	47,47,47,47	0
86	MG	2	1984	1/1	0.96	0.37	-	67,67,67,67	0
86	MG	5	3694	1/1	0.89	0.58	-	54,54,54,54	0
87	OHX	8	221	7/7	0.95	0.15	-	100,100,100,100	5
87	OHX	1	4068	7/7	0.92	0.27	-	39,39,39,39	3
86	MG	5	3540	1/1	0.98	0.53	-	41,41,41,41	0
87	OHX	6	2086	7/7	0.92	0.27	-	70,70,70,70	5
87	OHX	5	3955	7/7	0.98	0.21	-	40,40,40,40	2
86	MG	f	1001	1/1	0.92	0.32	-	53,53,53,53	0
86	MG	4	201	1/1	0.92	0.21	-	44,44,44,44	0
86	MG	1	3505	1/1	0.83	0.80	-	38,38,38,38	0
86	MG	1	3751	1/1	0.87	0.89	-	67,67,67,67	0
87	OHX	1	4111	7/7	0.91	0.15	-	104,104,104,104	7
86	MG	1	3607	1/1	0.85	0.55	-	85,85,85,85	0
87	OHX	1	4078	7/7	0.88	0.11	-	167,167,167,167	7
86	MG	1	3489	1/1	0.83	0.74	-	67,67,67,67	0
86	MG	1	3533	1/1	0.84	0.77	-	49,49,49,49	0
87	OHX	6	2060	7/7	0.95	0.20	-	96,96,96,96	1
86	MG	1	3431	1/1	0.96	0.39	-	47,47,47,47	0
86	MG	1	3694	1/1	0.94	0.20	-	46,46,46,46	0
86	MG	4	214	1/1	0.81	0.85	-	55,55,55,55	0
86	MG	6	1989	1/1	0.88	0.32	-	57,57,57,57	0
86	MG	1	3603	1/1	0.87	0.27	-	63,63,63,63	0
86	MG	1	3621	1/1	0.93	0.38	-	52,52,52,52	0
86	MG	5	3690	1/1	0.87	0.69	-	38,38,38,38	0
86	MG	5	3772	1/1	0.77	0.72	-	52,52,52,52	0
86	MG	1	3675	1/1	0.81	0.35	-	49,49,49,49	0
86	MG	5	3810	1/1	0.98	0.16	-	30,30,30,30	0
87	OHX	6	2042	7/7	0.99	0.28	-	62,62,62,62	3
86	MG	5	3615	1/1	0.89	0.22	-	42,42,42,42	0
87	OHX	1	4075	7/7	0.91	0.23	-	75,75,75,75	5
87	OHX	6	2098	7/7	0.96	0.22	-	87,87,87,87	5
86	MG	5	3760	1/1	0.96	0.19	-	38,38,38,38	0
86	MG	2	1951	1/1	0.85	0.37	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	1984	1/1	0.44	0.35	-	109,109,109,109	0
87	OHX	1	3913	7/7	0.96	0.21	-	54,54,54,54	3
86	MG	1	3604	1/1	0.88	0.66	-	39,39,39,39	0
86	MG	3	202	1/1	0.81	0.44	-	56,56,56,56	0
87	OHX	1	3980	7/7	0.94	0.32	-	51,51,51,51	1
86	MG	6	1999	1/1	0.94	0.72	-	36,36,36,36	0
86	MG	q3	502	1/1	0.96	0.52	-	48,48,48,48	0
87	OHX	s4	602	7/7	0.95	0.19	-	76,76,76,76	3
86	MG	1	3628	1/1	0.94	0.64	-	41,41,41,41	0
86	MG	1	3600	1/1	0.47	0.35	-	60,60,60,60	0
87	OHX	1	4069	7/7	0.86	0.34	-	58,58,58,58	5
86	MG	5	3633	1/1	0.88	0.41	-	36,36,36,36	0
87	OHX	1	3811	7/7	0.98	0.30	-	79,79,79,79	2
87	OHX	8	226	7/7	0.97	0.19	-	59,59,59,59	3
86	MG	6	1934	1/1	0.97	0.34	-	43,43,43,43	0
87	OHX	5	4168	7/7	0.86	0.27	-	81,81,81,81	7
87	OHX	1	3810	7/7	0.98	0.28	-	62,62,62,62	3
87	OHX	6	2064	7/7	0.96	0.21	-	98,98,98,98	5
86	MG	1	4113	1/1	0.93	0.16	-	64,64,64,64	0
86	MG	5	3487	1/1	0.86	0.35	-	44,44,44,44	0
86	MG	5	3476	1/1	0.98	0.43	-	27,27,27,27	0
86	MG	5	3695	1/1	0.81	0.55	-	45,45,45,45	0
87	OHX	6	2167	7/7	0.91	0.21	-	73,73,73,73	7
87	OHX	1	3986	7/7	0.94	0.21	-	76,76,76,76	3
86	MG	5	3485	1/1	0.90	0.35	-	51,51,51,51	0
86	MG	2	1924	1/1	0.94	0.53	-	100,100,100,100	0
86	MG	1	3591	1/1	0.75	0.29	-	53,53,53,53	0
87	OHX	2	1996	7/7	0.97	0.26	-	101,101,101,101	5
86	MG	2	1933	1/1	0.89	0.44	-	70,70,70,70	0
86	MG	2	1905	1/1	0.92	0.94	-	63,63,63,63	0
86	MG	2	1915	1/1	0.95	0.74	-	57,57,57,57	0
86	MG	1	3659	1/1	0.93	0.84	-	78,78,78,78	0
86	MG	6	1911	1/1	0.92	0.51	-	49,49,49,49	0
87	OHX	6	2171	7/7	0.91	0.37	-	53,53,53,53	7
86	MG	2	1918	1/1	0.98	0.36	-	68,68,68,68	0
87	OHX	6	2120	7/7	0.92	0.21	-	70,70,70,70	3
86	MG	1	3408	1/1	0.92	0.46	-	25,25,25,25	0
86	MG	6	2007	1/1	0.85	0.97	-	51,51,51,51	0
87	OHX	5	4091	7/7	0.95	0.45	-	33,33,33,33	2
87	OHX	5	4105	7/7	0.93	0.30	-	32,32,32,32	4
86	MG	5	3781	1/1	0.86	0.21	-	48,48,48,48	0
87	OHX	5	3867	7/7	0.98	0.24	-	74,74,74,74	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3526	1/1	0.97	0.43	-	32,32,32,32	0
86	MG	6	1919	1/1	0.82	1.06	-	64,64,64,64	0
87	OHX	m1	201	7/7	0.80	0.35	-	78,78,78,78	3
86	MG	5	3514	1/1	0.88	0.34	-	42,42,42,42	0
86	MG	1	3625	1/1	0.98	0.41	-	41,41,41,41	0
86	MG	5	3447	1/1	0.68	0.45	-	36,36,36,36	0
86	MG	6	1913	1/1	0.90	0.27	-	79,79,79,79	0
86	MG	1	3689	1/1	0.96	0.31	-	44,44,44,44	0
86	MG	2	1921	1/1	0.81	0.73	-	63,63,63,63	0
86	MG	1	3597	1/1	0.96	0.38	-	47,47,47,47	0
87	OHX	1	3801	7/7	0.99	0.18	-	71,71,71,71	3
87	OHX	1	4110	7/7	0.92	0.25	-	55,55,55,55	5
86	MG	5	3706	1/1	0.91	0.39	-	64,64,64,64	0
87	OHX	5	3871	7/7	0.97	0.27	-	82,82,82,82	3
86	MG	1	3485	1/1	0.92	0.28	-	58,58,58,58	0
86	MG	1	3418	1/1	0.92	0.69	-	47,47,47,47	0
86	MG	5	3448	1/1	0.87	0.43	-	32,32,32,32	0
86	MG	5	3632	1/1	0.98	0.42	-	34,34,34,34	0
86	MG	5	3489	1/1	0.95	0.33	-	40,40,40,40	0
86	MG	1	3520	1/1	0.89	0.49	-	35,35,35,35	0
87	OHX	6	2180	7/7	0.95	0.15	-	97,97,97,97	6
87	OHX	1	4052	7/7	0.94	0.36	-	58,58,58,58	4
87	OHX	6	2125	7/7	0.92	0.33	-	52,52,52,52	5
86	MG	M5	301	1/1	0.94	0.77	-	47,47,47,47	0
87	OHX	5	4129	7/7	0.86	0.16	-	171,171,171,171	7
86	MG	5	3814	1/1	0.85	0.75	-	44,44,44,44	0
86	MG	4	210	1/1	0.91	0.32	-	54,54,54,54	0
86	MG	5	3746	1/1	0.94	0.70	-	51,51,51,51	0
86	MG	2	1964	1/1	0.83	0.33	-	92,92,92,92	0
86	MG	L7	301	1/1	0.92	0.28	-	38,38,38,38	0
87	OHX	2	2083	7/7	0.95	0.47	-	87,87,87,87	2
86	MG	5	3776	1/1	0.81	0.42	-	41,41,41,41	0
87	OHX	5	4030	7/7	0.94	0.23	-	85,85,85,85	4
86	MG	1	3720	1/1	0.95	0.52	-	48,48,48,48	0
86	MG	1	3725	1/1	0.91	0.29	-	38,38,38,38	0
86	MG	1	3502	1/1	0.97	0.90	-	30,30,30,30	0
87	OHX	5	4063	7/7	0.97	0.31	-	52,52,52,52	3
86	MG	5	3709	1/1	0.94	0.38	-	55,55,55,55	0
86	MG	5	3790	1/1	0.89	0.20	-	46,46,46,46	0
86	MG	5	3773	1/1	0.82	0.69	-	55,55,55,55	0
86	MG	5	3603	1/1	0.88	0.37	-	33,33,33,33	0
87	OHX	1	4042	7/7	0.94	0.18	-	70,70,70,70	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3513	1/1	0.96	0.30	-	34,34,34,34	0
87	OHX	6	2037	7/7	0.98	0.23	-	101,101,101,101	3
86	MG	3	206	1/1	0.88	0.19	-	65,65,65,65	0
87	OHX	1	3921	7/7	0.98	0.13	-	82,82,82,82	3
87	OHX	5	4023	7/7	0.94	0.23	-	66,66,66,66	5
86	MG	5	3498	1/1	0.90	0.41	-	42,42,42,42	0
86	MG	1	3691	1/1	0.89	0.23	-	64,64,64,64	0
86	MG	1	3636	1/1	0.87	0.78	-	53,53,53,53	0
86	MG	2	1972	1/1	0.89	0.51	-	57,57,57,57	0
86	MG	q1	101	1/1	0.96	0.28	-	50,50,50,50	0
87	OHX	1	3949	7/7	0.92	0.46	-	111,111,111,111	7
86	MG	5	3424	1/1	0.95	0.26	-	41,41,41,41	0
87	OHX	5	4160	7/7	0.88	0.26	-	123,123,123,123	7
87	OHX	6	2085	7/7	0.99	0.32	-	76,76,76,76	2
87	OHX	1	3970	7/7	0.96	0.14	-	68,68,68,68	1
86	MG	6	1963	1/1	0.90	0.46	-	80,80,80,80	0
86	MG	1	3731	1/1	0.94	0.47	-	57,57,57,57	0
86	MG	1	3471	1/1	0.85	0.52	-	45,45,45,45	0
87	OHX	6	2136	7/7	0.91	0.33	-	62,62,62,62	4
87	OHX	5	4138	7/7	0.86	0.17	-	108,108,108,108	5
87	OHX	5	4098	7/7	0.93	0.23	-	73,73,73,73	5
87	OHX	1	3946	7/7	0.96	0.21	-	69,69,69,69	3
87	OHX	1	4067	7/7	0.87	0.29	-	107,107,107,107	7
87	OHX	5	4051	7/7	0.98	0.16	-	67,67,67,67	5
86	MG	6	1971	1/1	0.85	0.46	-	90,90,90,90	0
86	MG	1	3638	1/1	0.81	0.98	-	48,48,48,48	0
86	MG	2	1959	1/1	0.72	0.29	-	87,87,87,87	0
86	MG	1	3648	1/1	0.88	0.42	-	42,42,42,42	0
86	MG	5	3718	1/1	0.91	0.29	-	63,63,63,63	1
86	MG	1	3450	1/1	0.93	0.42	-	31,31,31,31	0
87	OHX	2	2128	7/7	0.95	0.11	-	115,115,115,115	7
86	MG	5	3503	1/1	0.97	0.53	-	28,28,28,28	0
87	OHX	1	3989	7/7	0.96	0.20	-	94,94,94,94	5
86	MG	5	3572	1/1	0.77	0.26	-	48,48,48,48	0
86	MG	5	3725	1/1	0.82	0.62	-	46,46,46,46	0
87	OHX	5	4078	7/7	0.94	0.26	-	54,54,54,54	5
86	MG	5	3724	1/1	0.96	0.26	-	51,51,51,51	0
86	MG	1	3692	1/1	0.71	0.55	-	61,61,61,61	0
86	MG	5	3499	1/1	0.81	0.46	-	40,40,40,40	0
87	OHX	1	3919	7/7	0.95	0.12	-	106,106,106,106	3
87	OHX	5	4045	7/7	0.92	0.18	-	53,53,53,53	5
86	MG	5	3683	1/1	0.90	0.28	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3858	7/7	0.97	0.15	-	98,98,98,98	4
86	MG	5	3430	1/1	0.93	0.40	-	41,41,41,41	0
86	MG	2	1949	1/1	0.79	1.01	-	86,86,86,86	0
86	MG	5	3775	1/1	0.97	0.13	-	75,75,75,75	0
86	MG	5	3502	1/1	0.74	0.50	-	57,57,57,57	0
87	OHX	5	3924	7/7	0.99	0.20	-	56,56,56,56	3
86	MG	6	2009	1/1	0.84	0.68	-	64,64,64,64	0
87	OHX	6	2140	7/7	0.92	0.27	-	74,74,74,74	6
86	MG	17	2200	1/1	0.58	0.31	-	50,50,50,50	0
87	OHX	2	2017	7/7	0.97	0.37	-	74,74,74,74	4
87	OHX	1	3795	7/7	0.98	0.16	-	85,85,85,85	2
86	MG	6	1947	1/1	0.90	0.46	-	50,50,50,50	0
87	OHX	2	2138	7/7	0.90	0.27	-	67,67,67,67	5
87	OHX	1	3954	7/7	0.97	0.22	-	122,122,122,122	3
87	OHX	6	2129	7/7	0.98	0.34	-	58,58,58,58	5
86	MG	6	1917	1/1	0.84	0.44	-	64,64,64,64	0
86	MG	2	1947	1/1	0.96	0.21	-	76,76,76,76	0
87	OHX	5	3946	7/7	0.98	0.26	-	45,45,45,45	3
86	MG	5	3432	1/1	0.94	0.33	-	37,37,37,37	0
87	OHX	5	3960	7/7	0.98	0.14	-	74,74,74,74	1
87	OHX	1	4025	7/7	0.96	0.21	-	56,56,56,56	3
86	MG	5	3621	1/1	0.89	0.36	-	62,62,62,62	0
86	MG	6	1987	1/1	0.90	0.51	-	77,77,77,77	0
86	MG	5	3813	1/1	0.88	1.03	-	42,42,42,42	0
86	MG	8	204	1/1	0.93	0.32	-	43,43,43,43	0
87	OHX	1	4021	7/7	0.91	0.41	-	58,58,58,58	3
86	MG	1	3643	1/1	0.88	0.83	-	38,38,38,38	0
86	MG	5	3635	1/1	0.95	0.55	-	43,43,43,43	0
86	MG	1	3685	1/1	0.85	0.30	-	43,43,43,43	0
86	MG	1	3723	1/1	0.76	0.55	-	67,67,67,67	0
86	MG	5	3700	1/1	0.95	0.37	-	38,38,38,38	0
86	MG	6	1920	1/1	0.89	0.43	-	46,46,46,46	0
86	MG	1	3515	1/1	0.94	0.40	-	28,28,28,28	0
86	MG	5	3745	1/1	0.71	0.46	-	76,76,76,76	0
86	MG	1	3532	1/1	0.92	0.32	-	42,42,42,42	0
86	MG	5	3811	1/1	0.96	0.39	-	32,32,32,32	0
86	MG	6	1976	1/1	0.95	0.19	-	32,32,32,32	0
86	MG	6	1946	1/1	0.89	0.69	-	53,53,53,53	0
86	MG	5	3490	1/1	0.82	0.69	-	41,41,41,41	0
86	MG	2	1945	1/1	0.80	0.23	-	107,107,107,107	0
86	MG	6	1907	1/1	0.87	0.42	-	51,51,51,51	0
86	MG	2	1986	1/1	0.40	0.40	-	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	7	207	1/1	0.76	0.44	-	55,55,55,55	0
86	MG	5	3616	1/1	0.95	0.83	-	35,35,35,35	0
86	MG	1	3487	1/1	0.87	0.41	-	49,49,49,49	0
86	MG	o2	201	1/1	0.92	0.61	-	35,35,35,35	1

6.5 Other polymers [i](#)

There are no such residues in this entry.