



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 04:01 PM EST

PDB ID : 5ON6
Title : Crystal structure of haemanthamine bound to the 80S ribosome
Authors : Pellegrino, S.; Meyer, M.; Yusupova, G.; Yusupov, M.
Deposited on : 2017-08-03
Resolution : 3.10 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-20030736
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-20030736

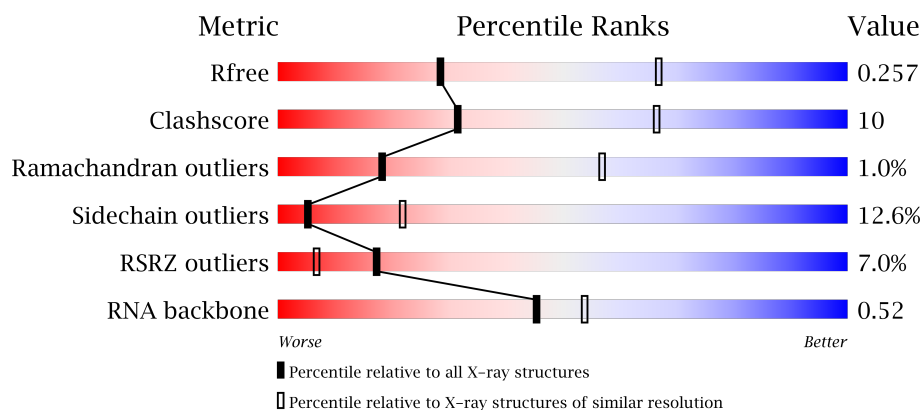
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

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	1	3396	<div> <div>3%</div> <div>56%</div> <div>29%</div> <div>7%</div> <div>7%</div> </div>
1	AR	3396	<div> <div>3%</div> <div>54%</div> <div>31%</div> <div>8%</div> <div>7%</div> </div>
2	3	121	<div> <div>66%</div> <div>30%</div> <div>.</div> </div>
2	AS	121	<div> <div>57%</div> <div>38%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	4	158	
3	AT	158	
4	CD	252	
4	j	252	
5	CE	386	
5	k	386	
6	CF	361	
6	l	361	
7	CG	296	
7	m	296	
8	CH	175	
8	n	175	
9	CI	222	
9	o	222	
10	CJ	233	
10	p	233	
11	CK	191	
11	q	191	
12	CL	220	
12	r	220	
13	CM	169	
13	s	169	
14	CN	193	
14	t	193	
15	CO	136	

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Mol	Chain	Length	Quality of chain
15	u	136	
16	CP	203	
16	v	203	
17	CQ	197	
17	w	197	
18	CR	183	
18	x	183	
19	CS	185	
19	y	185	
20	CT	188	
20	z	188	
21	0	172	
21	CU	172	
22	2	159	
22	CV	159	
23	5	100	
23	CW	100	
24	CX	136	
24	IR	136	
25	6	1800	
25	A	1800	
26	7	98	
26	CY	98	
27	8	121	
27	CZ	121	

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Mol	Chain	Length	Quality of chain
28	9	126	
28	DA	126	
29	AA	135	
29	DB	135	
30	AB	148	
30	DC	148	
31	AC	58	
31	DD	58	
32	AD	97	
32	DE	97	
33	AE	109	
33	DF	109	
34	AF	127	
34	DG	127	
35	AG	106	
35	DH	106	
36	AH	112	
36	DI	112	
37	AI	119	
37	DJ	119	
38	AJ	99	
38	DK	99	
39	AK	87	
39	DL	87	
40	AL	77	

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Mol	Chain	Length	Quality of chain
40	DM	77	
41	AM	50	
41	DN	50	
42	AN	52	
42	DO	52	
43	AO	25	
43	DP	25	
44	AP	105	
44	DQ	105	
45	AQ	91	
45	DR	91	
46	i	272	
47	m2	150	
48	sM	104	
49	p0	311	
50	B	206	
50	s0	206	
51	C	216	
51	s1	216	
52	D	217	
52	s2	217	
53	E	223	
53	s3	223	
54	F	260	
54	s4	260	

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Mol	Chain	Length	Quality of chain
55	G	206	
55	s5	206	
56	H	226	
56	s6	226	
57	I	186	
57	s7	186	
58	J	199	
58	s8	199	
59	K	185	
59	s9	185	
60	L	105	
60	c0	105	
61	M	155	
61	c1	155	
62	N	124	
62	c2	124	
63	O	150	
63	c3	150	
64	P	128	
64	c4	128	
65	Q	141	
65	c5	141	
66	R	142	
66	c6	142	
67	S	125	




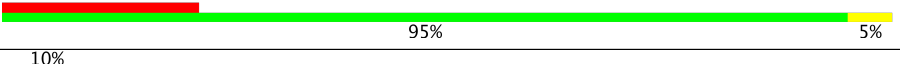
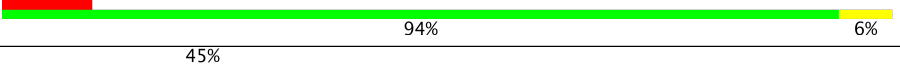

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Mol	Chain	Length	Quality of chain
67	c7	125	
68	T	145	
68	c8	145	
69	U	143	
69	c9	143	
70	V	110	
70	d0	110	
71	W	87	
71	d1	87	
72	X	129	
72	d2	129	
73	Y	144	
73	d3	144	
74	Z	134	
74	d4	134	
75	a	70	
75	d5	70	
76	b	97	
76	d6	97	
77	c	81	
77	d7	81	
78	d	63	
78	d8	63	
79	d9	53	
79	e	53	

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Mol	Chain	Length	Quality of chain
80	e0	62	
80	f	62	
81	g	71	
82	h	318	
82	sR	318	
83	e1	51	

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	OHX	1	3401	-	-	-	X
84	OHX	1	3402	-	-	-	X
84	OHX	1	3403	-	-	-	X
84	OHX	1	3404	-	-	-	X
84	OHX	1	3405	-	-	-	X
84	OHX	1	3406	-	-	-	X
84	OHX	1	3407	-	-	-	X
84	OHX	1	3408	-	-	-	X
84	OHX	1	3409	-	-	-	X
84	OHX	1	3410	-	-	-	X
84	OHX	1	3411	-	-	-	X
84	OHX	1	3412	-	-	-	X
84	OHX	1	3413	-	-	-	X
84	OHX	1	3414	-	-	-	X
84	OHX	1	3415	-	-	-	X
84	OHX	1	3416	-	-	-	X
84	OHX	1	3417	-	-	-	X
84	OHX	1	3418	-	-	-	X
84	OHX	1	3419	-	-	-	X
84	OHX	1	3420	-	-	-	X
84	OHX	1	3421	-	-	-	X
84	OHX	1	3422	-	-	-	X
84	OHX	1	3423	-	-	-	X
84	OHX	1	3425	-	-	-	X
84	OHX	1	3426	-	-	-	X
84	OHX	1	3427	-	-	-	X
84	OHX	1	3428	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	1	3431	-	-	-	X
84	OHX	1	3432	-	-	-	X
84	OHX	1	3433	-	-	-	X
84	OHX	1	3436	-	-	-	X
84	OHX	1	3437	-	-	-	X
84	OHX	1	3438	-	-	-	X
84	OHX	1	3442	-	-	-	X
84	OHX	1	3445	-	-	-	X
84	OHX	1	3449	-	-	-	X
84	OHX	1	3462	-	-	-	X
84	OHX	1	3473	-	-	X	-
84	OHX	1	3506	-	-	-	X
84	OHX	1	3507	-	-	-	X
84	OHX	1	3539	-	-	-	X
84	OHX	1	3541	-	-	-	X
84	OHX	1	3543	-	-	-	X
84	OHX	1	3551	-	-	-	X
84	OHX	1	3556	-	-	-	X
84	OHX	1	3572	-	-	-	X
84	OHX	1	3575	-	-	-	X
84	OHX	1	3577	-	-	-	X
84	OHX	1	3582	-	-	-	X
84	OHX	1	3584	-	-	-	X
84	OHX	1	3591	-	-	-	X
84	OHX	1	3592	-	-	-	X
84	OHX	1	3596	-	-	-	X
84	OHX	1	3599	-	-	-	X
84	OHX	1	3601	-	-	-	X
84	OHX	1	3604	-	-	-	X
84	OHX	1	3605	-	-	-	X
84	OHX	1	3606	-	-	-	X
84	OHX	1	3608	-	-	-	X
84	OHX	1	3609	-	-	-	X
84	OHX	1	3612	-	-	-	X
84	OHX	1	3613	-	-	-	X
84	OHX	1	3616	-	-	-	X
84	OHX	1	3620	-	-	-	X
84	OHX	1	3623	-	-	-	X
84	OHX	1	3626	-	-	-	X
84	OHX	1	3629	-	-	-	X
84	OHX	1	3631	-	-	-	X
84	OHX	1	3636	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	1	3638	-	-	-	X
84	OHX	1	3640	-	-	-	X
84	OHX	1	3641	-	-	-	X
84	OHX	1	3642	-	-	-	X
84	OHX	1	3643	-	-	-	X
84	OHX	1	3645	-	-	-	X
84	OHX	1	3646	-	-	-	X
84	OHX	1	3649	-	-	-	X
84	OHX	1	3650	-	-	-	X
84	OHX	1	3653	-	-	-	X
84	OHX	1	3655	-	-	-	X
84	OHX	1	3657	-	-	-	X
84	OHX	1	3659	-	-	-	X
84	OHX	1	3661	-	-	-	X
84	OHX	1	3662	-	-	-	X
84	OHX	1	3665	-	-	-	X
84	OHX	1	3666	-	-	-	X
84	OHX	1	3672	-	-	-	X
84	OHX	1	3673	-	-	-	X
84	OHX	1	3675	-	-	-	X
84	OHX	1	3676	-	-	-	X
84	OHX	1	3677	-	-	-	X
84	OHX	1	3679	-	-	-	X
84	OHX	1	3680	-	-	-	X
84	OHX	1	3683	-	-	-	X
84	OHX	1	3685	-	-	-	X
84	OHX	1	3687	-	-	-	X
84	OHX	1	3690	-	-	-	X
84	OHX	1	3692	-	-	-	X
84	OHX	1	3694	-	-	-	X
84	OHX	1	3695	-	-	-	X
84	OHX	1	3697	-	-	-	X
84	OHX	1	3699	-	-	-	X
84	OHX	1	3701	-	-	-	X
84	OHX	1	3703	-	-	-	X
84	OHX	1	3704	-	-	-	X
84	OHX	1	3705	-	-	-	X
84	OHX	1	3707	-	-	-	X
84	OHX	1	3708	-	-	-	X
84	OHX	1	3711	-	-	-	X
84	OHX	1	3717	-	-	-	X
84	OHX	1	3719	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	1	3720	-	-	X	-
84	OHX	1	3721	-	-	-	X
84	OHX	1	3723	-	-	-	X
84	OHX	2	201	-	-	-	X
84	OHX	3	208	-	-	-	X
84	OHX	4	201	-	-	-	X
84	OHX	4	202	-	-	-	X
84	OHX	4	208	-	-	-	X
84	OHX	4	209	-	-	-	X
84	OHX	4	210	-	-	-	X
84	OHX	4	212	-	-	-	X
84	OHX	4	213	-	-	-	X
84	OHX	4	214	-	-	-	X
84	OHX	4	215	-	-	-	X
84	OHX	4	216	-	-	-	X
84	OHX	6	1901	-	-	-	X
84	OHX	6	1902	-	-	-	X
84	OHX	6	1903	-	-	-	X
84	OHX	6	1904	-	-	-	X
84	OHX	6	1906	-	-	-	X
84	OHX	6	1907	-	-	-	X
84	OHX	6	1909	-	-	-	X
84	OHX	6	1910	-	-	-	X
84	OHX	6	1968	-	-	-	X
84	OHX	6	1971	-	-	-	X
84	OHX	6	1972	-	-	-	X
84	OHX	6	1975	-	-	X	-
84	OHX	6	1978	-	-	-	X
84	OHX	6	1979	-	-	-	X
84	OHX	6	1980	-	-	-	X
84	OHX	6	1986	-	-	-	X
84	OHX	6	1987	-	-	-	X
84	OHX	6	1989	-	-	-	X
84	OHX	6	1991	-	-	-	X
84	OHX	6	1992	-	-	-	X
84	OHX	6	1993	-	-	-	X
84	OHX	6	1994	-	-	-	X
84	OHX	6	2001	-	-	X	X
84	OHX	6	2005	-	-	-	X
84	OHX	6	2011	-	-	-	X
84	OHX	6	2013	-	-	-	X
84	OHX	6	2015	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	6	2019	-	-	-	X
84	OHX	6	2025	-	-	X	X
84	OHX	6	2027	-	-	-	X
84	OHX	6	2028	-	-	-	X
84	OHX	6	2029	-	-	-	X
84	OHX	6	2030	-	-	-	X
84	OHX	6	2031	-	-	-	X
84	OHX	6	2032	-	-	-	X
84	OHX	6	2033	-	-	-	X
84	OHX	6	2035	-	-	-	X
84	OHX	6	2038	-	-	-	X
84	OHX	6	2039	-	-	-	X
84	OHX	6	2041	-	-	-	X
84	OHX	6	2043	-	-	-	X
84	OHX	6	2044	-	-	-	X
84	OHX	6	2046	-	-	-	X
84	OHX	6	2050	-	-	-	X
84	OHX	6	2051	-	-	-	X
84	OHX	6	2052	-	-	-	X
84	OHX	A	1901	-	-	-	X
84	OHX	A	1902	-	-	-	X
84	OHX	A	1903	-	-	-	X
84	OHX	A	1905	-	-	-	X
84	OHX	A	1908	-	-	-	X
84	OHX	A	1909	-	-	X	-
84	OHX	A	1918	-	-	-	X
84	OHX	A	1940	-	-	-	X
84	OHX	A	1947	-	-	-	X
84	OHX	A	1953	-	-	-	X
84	OHX	A	1964	-	-	-	X
84	OHX	A	1970	-	-	-	X
84	OHX	A	1979	-	-	-	X
84	OHX	A	1980	-	-	-	X
84	OHX	A	1982	-	-	-	X
84	OHX	A	1985	-	-	-	X
84	OHX	A	1990	-	-	-	X
84	OHX	A	1994	-	-	-	X
84	OHX	A	1996	-	-	-	X
84	OHX	A	1997	-	-	-	X
84	OHX	A	2003	-	-	-	X
84	OHX	A	2006	-	-	-	X
84	OHX	A	2009	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	A	2012	-	-	-	X
84	OHX	A	2013	-	-	-	X
84	OHX	A	2014	-	-	-	X
84	OHX	A	2015	-	-	-	X
84	OHX	A	2017	-	-	-	X
84	OHX	A	2018	-	-	-	X
84	OHX	A	2021	-	-	-	X
84	OHX	A	2024	-	-	X	-
84	OHX	A	2026	-	-	-	X
84	OHX	A	2030	-	-	-	X
84	OHX	A	2031	-	-	-	X
84	OHX	A	2035	-	-	-	X
84	OHX	A	2040	-	-	-	X
84	OHX	AC	101	-	-	-	X
84	OHX	AH	201	-	-	-	X
84	OHX	AM	101	-	-	-	X
84	OHX	AR	3401	-	-	-	X
84	OHX	AR	3402	-	-	-	X
84	OHX	AR	3403	-	-	-	X
84	OHX	AR	3404	-	-	-	X
84	OHX	AR	3405	-	-	-	X
84	OHX	AR	3406	-	-	-	X
84	OHX	AR	3407	-	-	-	X
84	OHX	AR	3408	-	-	-	X
84	OHX	AR	3409	-	-	-	X
84	OHX	AR	3410	-	-	-	X
84	OHX	AR	3411	-	-	-	X
84	OHX	AR	3412	-	-	-	X
84	OHX	AR	3413	-	-	-	X
84	OHX	AR	3414	-	-	-	X
84	OHX	AR	3415	-	-	-	X
84	OHX	AR	3416	-	-	-	X
84	OHX	AR	3417	-	-	-	X
84	OHX	AR	3418	-	-	-	X
84	OHX	AR	3420	-	-	-	X
84	OHX	AR	3421	-	-	-	X
84	OHX	AR	3422	-	-	-	X
84	OHX	AR	3423	-	-	-	X
84	OHX	AR	3424	-	-	-	X
84	OHX	AR	3425	-	-	-	X
84	OHX	AR	3426	-	-	-	X
84	OHX	AR	3427	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	AR	3431	-	-	-	X
84	OHX	AR	3432	-	-	-	X
84	OHX	AR	3439	-	-	-	X
84	OHX	AR	3443	-	-	X	-
84	OHX	AR	3455	-	-	-	X
84	OHX	AR	3459	-	-	-	X
84	OHX	AR	3493	-	-	-	X
84	OHX	AR	3496	-	-	-	X
84	OHX	AR	3501	-	-	-	X
84	OHX	AR	3511	-	-	X	-
84	OHX	AR	3520	-	-	-	X
84	OHX	AR	3521	-	-	X	X
84	OHX	AR	3524	-	-	-	X
84	OHX	AR	3543	-	-	-	X
84	OHX	AR	3547	-	-	-	X
84	OHX	AR	3552	-	-	-	X
84	OHX	AR	3561	-	-	-	X
84	OHX	AR	3566	-	-	-	X
84	OHX	AR	3568	-	-	-	X
84	OHX	AR	3570	-	-	-	X
84	OHX	AR	3573	-	-	-	X
84	OHX	AR	3575	-	-	-	X
84	OHX	AR	3576	-	-	-	X
84	OHX	AR	3579	-	-	-	X
84	OHX	AR	3582	-	-	-	X
84	OHX	AR	3588	-	-	-	X
84	OHX	AR	3590	-	-	-	X
84	OHX	AR	3592	-	-	-	X
84	OHX	AR	3596	-	-	-	X
84	OHX	AR	3599	-	-	-	X
84	OHX	AR	3600	-	-	-	X
84	OHX	AR	3601	-	-	-	X
84	OHX	AR	3603	-	-	-	X
84	OHX	AR	3606	-	-	-	X
84	OHX	AR	3607	-	-	-	X
84	OHX	AR	3610	-	-	-	X
84	OHX	AR	3612	-	-	-	X
84	OHX	AR	3613	-	-	-	X
84	OHX	AR	3616	-	-	-	X
84	OHX	AR	3617	-	-	-	X
84	OHX	AR	3619	-	-	-	X
84	OHX	AR	3625	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	AR	3626	-	-	-	X
84	OHX	AR	3632	-	-	-	X
84	OHX	AR	3636	-	-	-	X
84	OHX	AR	3638	-	-	-	X
84	OHX	AR	3640	-	-	-	X
84	OHX	AR	3641	-	-	-	X
84	OHX	AR	3643	-	-	-	X
84	OHX	AR	3644	-	-	-	X
84	OHX	AR	3645	-	-	-	X
84	OHX	AR	3646	-	-	-	X
84	OHX	AR	3648	-	-	-	X
84	OHX	AR	3652	-	-	-	X
84	OHX	AR	3653	-	-	-	X
84	OHX	AR	3654	-	-	-	X
84	OHX	AR	3657	-	-	-	X
84	OHX	AR	3658	-	-	-	X
84	OHX	AR	3659	-	-	-	X
84	OHX	AR	3660	-	-	-	X
84	OHX	AR	3661	-	-	-	X
84	OHX	AR	3663	-	-	-	X
84	OHX	AR	3667	-	-	-	X
84	OHX	AR	3668	-	-	-	X
84	OHX	AR	3671	-	-	-	X
84	OHX	AR	3672	-	-	-	X
84	OHX	AR	3677	-	-	-	X
84	OHX	AR	3683	-	-	-	X
84	OHX	AR	3684	-	-	-	X
84	OHX	AR	3685	-	-	-	X
84	OHX	AR	3688	-	-	-	X
84	OHX	AR	3689	-	-	-	X
84	OHX	AR	3690	-	-	-	X
84	OHX	AR	3691	-	-	-	X
84	OHX	AR	3693	-	-	-	X
84	OHX	AR	3695	-	-	-	X
84	OHX	AR	3696	-	-	X	-
84	OHX	AR	3698	-	-	X	X
84	OHX	AR	3699	-	-	-	X
84	OHX	AR	3700	-	-	-	X
84	OHX	AR	3703	-	-	-	X
84	OHX	AR	3705	-	-	-	X
84	OHX	AR	3709	-	-	-	X
84	OHX	AR	3712	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	AR	3714	-	-	-	X
84	OHX	AR	3715	-	-	X	X
84	OHX	AR	3717	-	-	-	X
84	OHX	AR	3721	-	-	-	X
84	OHX	AR	3722	-	-	-	X
84	OHX	AR	3726	-	-	-	X
84	OHX	AR	3728	-	-	-	X
84	OHX	AR	3729	-	-	-	X
84	OHX	AR	3731	-	-	X	-
84	OHX	AR	3732	-	-	-	X
84	OHX	AR	3735	-	-	-	X
84	OHX	AR	3736	-	-	-	X
84	OHX	AR	3737	-	-	-	X
84	OHX	AR	3743	-	-	-	X
84	OHX	AS	203	-	-	X	-
84	OHX	AS	210	-	-	X	-
84	OHX	AS	211	-	-	-	X
84	OHX	AT	201	-	-	-	X
84	OHX	AT	202	-	-	-	X
84	OHX	AT	208	-	-	-	X
84	OHX	AT	214	-	-	-	X
84	OHX	CV	201	-	-	-	X
84	OHX	K	201	-	-	-	X
84	OHX	M	201	-	-	-	X
84	OHX	c1	201	-	-	-	X
84	OHX	c4	201	-	-	-	X
84	OHX	d9	101	-	-	-	X
84	OHX	e	101	-	-	-	X
84	OHX	l	401	-	-	-	X
84	OHX	x	201	-	-	-	X
84	OHX	x	202	-	-	-	X
84	OHX	y	201	-	-	-	X
85	MG	1	3725	-	-	-	X
85	MG	1	3730	-	-	-	X
85	MG	1	3731	-	-	-	X
85	MG	1	3732	-	-	-	X
85	MG	1	3734	-	-	-	X
85	MG	1	3738	-	-	-	X
85	MG	1	3739	-	-	-	X
85	MG	1	3740	-	-	-	X
85	MG	1	3741	-	-	-	X
85	MG	1	3746	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	1	3748	-	-	-	X
85	MG	1	3756	-	-	-	X
85	MG	1	3760	-	-	-	X
85	MG	1	3764	-	-	-	X
85	MG	1	3778	-	-	-	X
85	MG	1	3779	-	-	-	X
85	MG	1	3783	-	-	-	X
85	MG	1	3793	-	-	-	X
85	MG	1	3795	-	-	-	X
85	MG	1	3796	-	-	-	X
85	MG	1	3798	-	-	-	X
85	MG	1	3799	-	-	-	X
85	MG	1	3801	-	-	-	X
85	MG	1	3809	-	-	-	X
85	MG	1	3819	-	-	-	X
85	MG	1	3822	-	-	-	X
85	MG	1	3823	-	-	-	X
85	MG	1	3828	-	-	-	X
85	MG	1	3829	-	-	-	X
85	MG	1	3833	-	-	-	X
85	MG	1	3836	-	-	-	X
85	MG	1	3837	-	-	-	X
85	MG	1	3841	-	-	-	X
85	MG	1	3843	-	-	-	X
85	MG	1	3845	-	-	-	X
85	MG	1	3846	-	-	-	X
85	MG	1	3856	-	-	-	X
85	MG	1	3858	-	-	-	X
85	MG	1	3859	-	-	-	X
85	MG	1	3860	-	-	-	X
85	MG	1	3866	-	-	-	X
85	MG	1	3867	-	-	-	X
85	MG	1	3868	-	-	-	X
85	MG	1	3869	-	-	-	X
85	MG	1	3871	-	-	-	X
85	MG	1	3875	-	-	-	X
85	MG	1	3876	-	-	-	X
85	MG	1	3879	-	-	-	X
85	MG	1	3882	-	-	-	X
85	MG	1	3884	-	-	-	X
85	MG	1	3885	-	-	-	X
85	MG	1	3886	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	1	3887	-	-	-	X
85	MG	1	3889	-	-	-	X
85	MG	1	3890	-	-	-	X
85	MG	1	3891	-	-	-	X
85	MG	1	3892	-	-	-	X
85	MG	1	3894	-	-	-	X
85	MG	1	3899	-	-	-	X
85	MG	1	3900	-	-	-	X
85	MG	1	3901	-	-	-	X
85	MG	1	3902	-	-	-	X
85	MG	1	3904	-	-	-	X
85	MG	1	3905	-	-	-	X
85	MG	1	3909	-	-	-	X
85	MG	1	3911	-	-	-	X
85	MG	1	3912	-	-	-	X
85	MG	1	3914	-	-	-	X
85	MG	1	3916	-	-	-	X
85	MG	1	3917	-	-	-	X
85	MG	1	3924	-	-	-	X
85	MG	1	3939	-	-	-	X
85	MG	1	3946	-	-	-	X
85	MG	1	3959	-	-	-	X
85	MG	1	3962	-	-	-	X
85	MG	1	3978	-	-	-	X
85	MG	1	3990	-	-	-	X
85	MG	1	4027	-	-	-	X
85	MG	1	4031	-	-	-	X
85	MG	1	4048	-	-	-	X
85	MG	1	4052	-	-	-	X
85	MG	1	4064	-	-	-	X
85	MG	1	4066	-	-	-	X
85	MG	1	4078	-	-	-	X
85	MG	1	4083	-	-	-	X
85	MG	1	4084	-	-	-	X
85	MG	1	4096	-	-	-	X
85	MG	1	4100	-	-	-	X
85	MG	1	4125	-	-	-	X
85	MG	1	4126	-	-	-	X
85	MG	1	4127	-	-	-	X
85	MG	1	4135	-	-	-	X
85	MG	1	4142	-	-	-	X
85	MG	1	4167	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	1	4168	-	-	-	X
85	MG	1	4186	-	-	-	X
85	MG	1	4188	-	-	-	X
85	MG	1	4189	-	-	-	X
85	MG	1	4193	-	-	-	X
85	MG	1	4195	-	-	-	X
85	MG	1	4196	-	-	-	X
85	MG	1	4204	-	-	-	X
85	MG	1	4207	-	-	-	X
85	MG	1	4208	-	-	-	X
85	MG	1	4215	-	-	-	X
85	MG	1	4222	-	-	-	X
85	MG	4	221	-	-	-	X
85	MG	4	224	-	-	-	X
85	MG	4	225	-	-	-	X
85	MG	4	227	-	-	-	X
85	MG	6	2053	-	-	-	X
85	MG	6	2057	-	-	-	X
85	MG	6	2059	-	-	-	X
85	MG	6	2061	-	-	-	X
85	MG	6	2068	-	-	-	X
85	MG	6	2071	-	-	-	X
85	MG	6	2077	-	-	-	X
85	MG	6	2078	-	-	-	X
85	MG	6	2082	-	-	-	X
85	MG	6	2086	-	-	-	X
85	MG	6	2088	-	-	-	X
85	MG	6	2091	-	-	-	X
85	MG	6	2093	-	-	-	X
85	MG	6	2098	-	-	-	X
85	MG	6	2099	-	-	-	X
85	MG	6	2103	-	-	-	X
85	MG	6	2107	-	-	-	X
85	MG	6	2108	-	-	-	X
85	MG	6	2116	-	-	-	X
85	MG	6	2122	-	-	-	X
85	MG	6	2125	-	-	-	X
85	MG	6	2140	-	-	-	X
85	MG	6	2144	-	-	-	X
85	MG	6	2154	-	-	-	X
85	MG	6	2155	-	-	-	X
85	MG	6	2158	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	6	2161	-	-	-	X
85	MG	6	2197	-	-	-	X
85	MG	A	2047	-	-	-	X
85	MG	A	2052	-	-	-	X
85	MG	A	2053	-	-	-	X
85	MG	A	2055	-	-	-	X
85	MG	A	2056	-	-	-	X
85	MG	A	2057	-	-	-	X
85	MG	A	2061	-	-	-	X
85	MG	A	2062	-	-	-	X
85	MG	A	2064	-	-	-	X
85	MG	A	2066	-	-	-	X
85	MG	A	2072	-	-	-	X
85	MG	A	2077	-	-	-	X
85	MG	A	2078	-	-	-	X
85	MG	A	2079	-	-	-	X
85	MG	A	2080	-	-	-	X
85	MG	A	2088	-	-	-	X
85	MG	A	2095	-	-	-	X
85	MG	A	2100	-	-	-	X
85	MG	A	2101	-	-	-	X
85	MG	A	2105	-	-	-	X
85	MG	A	2108	-	-	-	X
85	MG	A	2109	-	-	-	X
85	MG	A	2115	-	-	-	X
85	MG	A	2119	-	-	-	X
85	MG	A	2126	-	-	-	X
85	MG	A	2129	-	-	-	X
85	MG	A	2131	-	-	-	X
85	MG	A	2138	-	-	-	X
85	MG	A	2147	-	-	-	X
85	MG	A	2153	-	-	-	X
85	MG	A	2155	-	-	-	X
85	MG	AB	203	-	-	-	X
85	MG	AB	206	-	-	-	X
85	MG	AF	202	-	-	-	X
85	MG	AK	103	-	-	-	X
85	MG	AR	3747	-	-	-	X
85	MG	AR	3750	-	-	-	X
85	MG	AR	3751	-	-	-	X
85	MG	AR	3753	-	-	-	X
85	MG	AR	3756	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	AR	3757	-	-	-	X
85	MG	AR	3763	-	-	-	X
85	MG	AR	3764	-	-	-	X
85	MG	AR	3767	-	-	-	X
85	MG	AR	3772	-	-	-	X
85	MG	AR	3786	-	-	-	X
85	MG	AR	3790	-	-	-	X
85	MG	AR	3794	-	-	-	X
85	MG	AR	3801	-	-	-	X
85	MG	AR	3804	-	-	-	X
85	MG	AR	3809	-	-	-	X
85	MG	AR	3810	-	-	-	X
85	MG	AR	3814	-	-	-	X
85	MG	AR	3816	-	-	-	X
85	MG	AR	3819	-	-	-	X
85	MG	AR	3825	-	-	-	X
85	MG	AR	3826	-	-	-	X
85	MG	AR	3833	-	-	-	X
85	MG	AR	3841	-	-	-	X
85	MG	AR	3844	-	-	-	X
85	MG	AR	3848	-	-	-	X
85	MG	AR	3850	-	-	-	X
85	MG	AR	3853	-	-	-	X
85	MG	AR	3857	-	-	-	X
85	MG	AR	3859	-	-	-	X
85	MG	AR	3860	-	-	-	X
85	MG	AR	3863	-	-	-	X
85	MG	AR	3864	-	-	-	X
85	MG	AR	3865	-	-	-	X
85	MG	AR	3871	-	-	-	X
85	MG	AR	3873	-	-	-	X
85	MG	AR	3874	-	-	-	X
85	MG	AR	3879	-	-	-	X
85	MG	AR	3888	-	-	-	X
85	MG	AR	3893	-	-	-	X
85	MG	AR	3895	-	-	-	X
85	MG	AR	3896	-	-	-	X
85	MG	AR	3897	-	-	-	X
85	MG	AR	3901	-	-	-	X
85	MG	AR	3904	-	-	-	X
85	MG	AR	3905	-	-	-	X
85	MG	AR	3906	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	AR	3909	-	-	-	X
85	MG	AR	3910	-	-	-	X
85	MG	AR	3912	-	-	-	X
85	MG	AR	3913	-	-	-	X
85	MG	AR	3914	-	-	-	X
85	MG	AR	3915	-	-	-	X
85	MG	AR	3918	-	-	-	X
85	MG	AR	3919	-	-	-	X
85	MG	AR	3926	-	-	-	X
85	MG	AR	3930	-	-	-	X
85	MG	AR	3933	-	-	-	X
85	MG	AR	3934	-	-	-	X
85	MG	AR	3936	-	-	-	X
85	MG	AR	3937	-	-	-	X
85	MG	AR	3938	-	-	-	X
85	MG	AR	3939	-	-	-	X
85	MG	AR	3940	-	-	-	X
85	MG	AR	3941	-	-	-	X
85	MG	AR	3942	-	-	-	X
85	MG	AR	3950	-	-	-	X
85	MG	AR	3961	-	-	-	X
85	MG	AR	3964	-	-	-	X
85	MG	AR	3966	-	-	-	X
85	MG	AR	3977	-	-	-	X
85	MG	AR	3978	-	-	-	X
85	MG	AR	3985	-	-	-	X
85	MG	AR	3987	-	-	-	X
85	MG	AR	3993	-	-	-	X
85	MG	AR	3994	-	-	-	X
85	MG	AR	4002	-	-	-	X
85	MG	AR	4007	-	-	-	X
85	MG	AR	4012	-	-	-	X
85	MG	AR	4019	-	-	-	X
85	MG	AR	4024	-	-	-	X
85	MG	AR	4034	-	-	-	X
85	MG	AR	4038	-	-	-	X
85	MG	AR	4041	-	-	-	X
85	MG	AR	4051	-	-	-	X
85	MG	AR	4075	-	-	-	X
85	MG	AR	4080	-	-	-	X
85	MG	AR	4082	-	-	-	X
85	MG	AR	4083	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	AR	4090	-	-	-	X
85	MG	AR	4091	-	-	-	X
85	MG	AR	4102	-	-	-	X
85	MG	AR	4111	-	-	-	X
85	MG	AR	4114	-	-	-	X
85	MG	AR	4138	-	-	-	X
85	MG	AR	4140	-	-	-	X
85	MG	AR	4141	-	-	-	X
85	MG	AR	4155	-	-	-	X
85	MG	AR	4161	-	-	-	X
85	MG	AR	4169	-	-	-	X
85	MG	AR	4179	-	-	-	X
85	MG	AR	4188	-	-	-	X
85	MG	AR	4189	-	-	-	X
85	MG	AR	4198	-	-	-	X
85	MG	AR	4202	-	-	-	X
85	MG	AR	4203	-	-	-	X
85	MG	AR	4206	-	-	-	X
85	MG	AR	4226	-	-	-	X
85	MG	AR	4227	-	-	-	X
85	MG	AR	4228	-	-	-	X
85	MG	AR	4230	-	-	-	X
85	MG	AR	4241	-	-	-	X
85	MG	AR	4247	-	-	-	X
85	MG	AR	4249	-	-	-	X
85	MG	AR	4252	-	-	-	X
85	MG	AT	218	-	-	-	X
85	MG	AT	221	-	-	-	X
85	MG	AT	230	-	-	-	X
85	MG	CD	301	-	-	-	X
85	MG	CD	302	-	-	-	X
85	MG	CE	404	-	-	-	X
85	MG	CE	405	-	-	-	X
85	MG	CE	407	-	-	-	X
85	MG	CI	301	-	-	-	X
85	MG	CP	502	-	-	-	X
85	MG	CQ	202	-	-	-	X
85	MG	CR	201	-	-	-	X
85	MG	CR	205	-	-	-	X
85	MG	CU	201	-	-	-	X
85	MG	CX	203	-	-	-	X
85	MG	DC	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	DH	203	-	-	-	X
85	MG	F	301	-	-	-	X
85	MG	b	101	-	-	-	X
85	MG	c1	202	-	-	-	X
85	MG	c8	202	-	-	-	X
85	MG	d3	202	-	-	-	X
85	MG	d6	102	-	-	-	X
85	MG	k	404	-	-	-	X
85	MG	l	404	-	-	-	X
85	MG	r	302	-	-	-	X
85	MG	s8	302	-	-	-	X
85	MG	sM	202	-	-	-	X
85	MG	v	302	-	-	-	X
85	MG	w	202	-	-	-	X
85	MG	x	204	-	-	-	X
85	MG	x	205	-	-	-	X
85	MG	x	208	-	-	-	X
85	MG	x	209	-	-	-	X
86	HN8	1	4223	-	-	-	X
86	HN8	AR	4263	-	-	-	X
87	GOL	A	2160	-	-	-	X
87	GOL	AR	4261	-	-	-	X
87	GOL	v	305	-	-	-	X
88	ZN	d7	101	-	-	-	X

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 410383 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
1	AR	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
2	AS	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
3	AT	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	j	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
4	CD	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	k	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
5	CE	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	l	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
6	CF	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	m	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
7	CG	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	n	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
8	CH	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	o	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
9	CI	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	p	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
10	CJ	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	q	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
11	CK	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	r	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
12	CL	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	s	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
13	CM	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	t	193	Total	C	N	O	0	0	0
			1543	962	315	266			
14	CN	193	Total	C	N	O	0	0	0
			1543	962	315	266			

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	u	136	Total	C	N	O	0	0	0
			1053	675	199	177			
15	CO	136	Total	C	N	O	0	0	0
			1053	675	199	177			

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	v	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
16	CP	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	w	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
17	CQ	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	x	183	Total	C	N	O	S	0	0	0
			1420	882	281	257				
18	CR	183	Total	C	N	O	S	0	0	0
			1420	882	281	257				

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	y	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
19	CS	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	z	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				
20	CT	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
21	CU	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	2	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
22	CV	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	5	100	Total	C	N	O	0	0	0
			796	516	131	149			
23	CW	100	Total	C	N	O	0	0	0
			796	516	131	149			

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	IR	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
24	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 25 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	6	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			
25	A	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

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

- Molecule 27 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	8	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
27	CZ	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	9	126	Total	C	N	O		0	0	0
			993	625	192	176				
28	DA	126	Total	C	N	O		0	0	0
			993	625	192	176				

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AA	135	Total	C	N	O		0	0	0
			1092	710	202	180				
29	DB	135	Total	C	N	O		0	0	0
			1092	710	202	180				

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AB	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
30	DC	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AC	58	Total	C	N	O		0	0	0
			462	289	100	73				
31	DD	58	Total	C	N	O		0	0	0
			462	289	100	73				

- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AD	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
32	DE	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AE	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
33	DF	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AF	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
34	DG	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AG	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
35	DH	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AH	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
36	DI	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AI	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
37	DJ	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AJ	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
38	DK	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	AK	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
39	DL	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	AL	77	Total	C	N	O	0	0	0
			612	391	115	106			
40	DM	77	Total	C	N	O	0	0	0
			612	391	115	106			

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AM	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
41	DN	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AN	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DO	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 43 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AO	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
43	DP	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AP	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
44	DQ	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 45 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	AQ	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
45	DR	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 46 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	i	159	Total	C	N	O	0	0	0
			1104	652	221	231			

- Molecule 47 is a protein called 60S ribosomal protein L12.

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

- Molecule 48 is a protein called Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	sM	104	Total	C	N	O			
			680	403	140	137	0	0	0

- Molecule 49 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 50 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 51 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 52 is a protein called 40S ribosomal protein S2.

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

- Molecule 53 is a protein called 40S ribosomal protein S3.

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

- Molecule 54 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 55 is a protein called 40S ribosomal protein S5.

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

- Molecule 56 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 57 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 58 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 59 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	K	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

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

- Molecule 60 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	L	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
60	c0	96	Total	C	N	O	S	0	0	0
			760	489	125	144	2			

- Molecule 61 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 62 is a protein called 40S ribosomal protein S12.

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

- Molecule 63 is a protein called 40S ribosomal protein S13.

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

- Molecule 64 is a protein called 40S ribosomal protein S14-B.

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

- Molecule 65 is a protein called 40S ribosomal protein S15.

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

- Molecule 66 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	R	141	Total	C	N	O	S	0	0	0
			1105	708	203	194				
66	c6	142	Total	C	N	O	S	0	0	0
			1111	711	204	196				

- Molecule 67 is a protein called 40S ribosomal protein S17-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S20.

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

- Molecule 71 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 75 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
75	a	70	Total	C	N	O	0	0	0
			563	360	104	99			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
75	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 76 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 77 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	c	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
77	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 78 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	d	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
78	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 79 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	e	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
79	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	f	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
80	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	g	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			

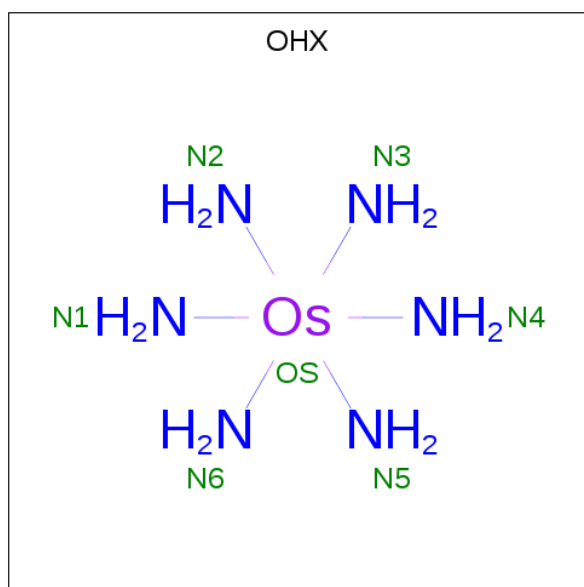
- Molecule 82 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	h	318	Total	C	N	O	S	0	0	0
			2441	1544	419	470	8			
82	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	e1	51	Total	C	N	O	S	0	0	0
			397	249	73	71	4			

- Molecule 84 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	4	1	Total	N	Os	0	0
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84	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	y	1	Total	N	Os	0	0
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84	2	1	Total	N	Os	0	0
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84	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	1	Total	N	Os	0	0
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84	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	1	Total	N	Os	0	0
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84	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	1	Total	N	Os	0	0
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84	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	1	Total	N	Os	0	0
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84	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	1	Total	N	Os	0	0
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84	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	1	Total	N	Os	0	0
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84	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	AC	1	Total 7	N 6	Os 1	0	0
84	AG	1	Total 7	N 6	Os 1	0	0
84	AH	1	Total 7	N 6	Os 1	0	0
84	AK	1	Total 7	N 6	Os 1	0	0
84	AM	1	Total 7	N 6	Os 1	0	0
84	AP	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
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84	AR	1	Total	N	Os	0	0
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			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
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84	AS	1	Total	N	Os	0	0
			7	6	1		
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84	AS	1	Total	N	Os	0	0
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84	AS	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AT	1	Total 7	N 6	Os 1	0	0
84	AT	1	Total 7	N 6	Os 1	0	0
84	AT	1	Total 7	N 6	Os 1	0	0
84	AT	1	Total 7	N 6	Os 1	0	0
84	AT	1	Total 7	N 6	Os 1	0	0
84	CE	1	Total 7	N 6	Os 1	0	0
84	CE	1	Total 7	N 6	Os 1	0	0
84	CF	1	Total 7	N 6	Os 1	0	0
84	CF	1	Total 7	N 6	Os 1	0	0
84	CG	1	Total 7	N 6	Os 1	0	0
84	CG	1	Total 7	N 6	Os 1	0	0
84	CK	1	Total 7	N 6	Os 1	0	0
84	CL	1	Total 7	N 6	Os 1	0	0
84	CM	1	Total 7	N 6	Os 1	0	0
84	CP	1	Total 7	N 6	Os 1	0	0
84	CV	1	Total 7	N 6	Os 1	0	0
84	CX	1	Total 7	N 6	Os 1	0	0
84	CX	1	Total 7	N 6	Os 1	0	0
84	DD	1	Total 7	N 6	Os 1	0	0
84	DH	1	Total 7	N 6	Os 1	0	0
84	DQ	1	Total 7	N 6	Os 1	0	0

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	J	1	Total	N	Os	0	0
			7	6	1		
84	K	1	Total	N	Os	0	0
			7	6	1		
84	M	1	Total	N	Os	0	0
			7	6	1		
84	O	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	Q	1	Total	N	Os	0	0
			7	6	1		
84	T	1	Total	N	Os	0	0
			7	6	1		
84	e	1	Total	N	Os	0	0
			7	6	1		
84	h	1	Total	N	Os	0	0
			7	6	1		
84	s8	1	Total	N	Os	0	0
			7	6	1		
84	c1	1	Total	N	Os	0	0
			7	6	1		
84	c3	1	Total	N	Os	0	0
			7	6	1		
84	c4	1	Total	N	Os	0	0
			7	6	1		
84	c5	1	Total	N	Os	0	0
			7	6	1		
84	c8	1	Total	N	Os	0	0
			7	6	1		
84	d9	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AP	1	Total	Mg	0	0
			1	1		
85	AK	1	Total	Mg	0	0
			1	1		
85	DQ	2	Total	Mg	0	0
			2	2		
85	AB	7	Total	Mg	0	0
			7	7		
85	c6	1	Total	Mg	0	0
			1	1		
85	6	146	Total	Mg	0	0
			146	146		
85	DO	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	sM	2	Total 2	Mg 2	0	0
85	d5	1	Total 1	Mg 1	0	0
85	t	3	Total 3	Mg 3	0	0
85	CD	2	Total 2	Mg 2	0	0
85	lR	1	Total 1	Mg 1	0	0
85	CR	5	Total 5	Mg 5	0	0
85	o	2	Total 2	Mg 2	0	0
85	DC	4	Total 4	Mg 4	0	0
85	AS	20	Total 20	Mg 20	0	0
85	DH	2	Total 2	Mg 2	0	0
85	c9	1	Total 1	Mg 1	0	0
85	k	3	Total 3	Mg 3	0	0
85	CO	1	Total 1	Mg 1	0	0
85	CU	1	Total 1	Mg 1	0	0
85	b	1	Total 1	Mg 1	0	0
85	DL	1	Total 1	Mg 1	0	0
85	V	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	w	2	Total 2	Mg 2	0	0
85	CK	1	Total 1	Mg 1	0	0
85	CQ	4	Total 4	Mg 4	0	0

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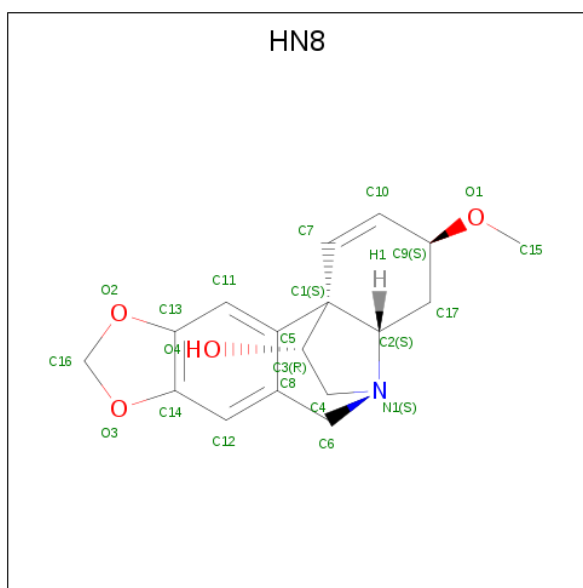
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	n	1	Total 1	Mg 1	0	0
85	x	7	Total 7	Mg 7	0	0
85	T	1	Total 1	Mg 1	0	0
85	AR	515	Total 515	Mg 515	0	0
85	d6	2	Total 2	Mg 2	0	0
85	s6	1	Total 1	Mg 1	0	0
85	s	1	Total 1	Mg 1	0	0
85	DI	2	Total 2	Mg 2	0	0
85	CG	2	Total 2	Mg 2	0	0
85	j	2	Total 2	Mg 2	0	0
85	1	498	Total 498	Mg 498	0	0
85	D	1	Total 1	Mg 1	0	0
85	CM	2	Total 2	Mg 2	0	0
85	d3	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	v	3	Total 3	Mg 3	0	0
85	CJ	1	Total 1	Mg 1	0	0
85	A	116	Total 116	Mg 116	0	0
85	CP	4	Total 4	Mg 4	0	0
85	4	25	Total 25	Mg 25	0	0
85	DA	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	U	1	Total 1	Mg 1	0	0
85	r	1	Total 1	Mg 1	0	0
85	CF	1	Total 1	Mg 1	0	0
85	CX	2	Total 2	Mg 2	0	0
85	AG	1	Total 1	Mg 1	0	0
85	DE	1	Total 1	Mg 1	0	0
85	AH	1	Total 1	Mg 1	0	0
85	F	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	CI	1	Total 1	Mg 1	0	0
85	d4	1	Total 1	Mg 1	0	0
85	H	1	Total 1	Mg 1	0	0
85	z	1	Total 1	Mg 1	0	0
85	AT	14	Total 14	Mg 14	0	0
85	CL	1	Total 1	Mg 1	0	0
85	s4	1	Total 1	Mg 1	0	0
85	CE	5	Total 5	Mg 5	0	0
85	Y	1	Total 1	Mg 1	0	0
85	l	3	Total 3	Mg 3	0	0
85	3	13	Total 13	Mg 13	0	0
85	AF	2	Total 2	Mg 2	0	0

- Molecule 86 is Haemanthamine (three-letter code: HN8) (formula: $C_{17}H_{19}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
86	1	1	Total	C	N	O	0	0
			22	17	1	4		
86	AR	1	Total	C	N	O	0	0
			22	17	1	4		

- Molecule 87 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	v	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total	C	O	0	0
			6	3	3		
87	AR	1	Total	C	O	0	0
			6	3	3		
87	AR	1	Total	C	O	0	0
			6	3	3		
87	A	1	Total	C	O	0	0
			6	3	3		

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

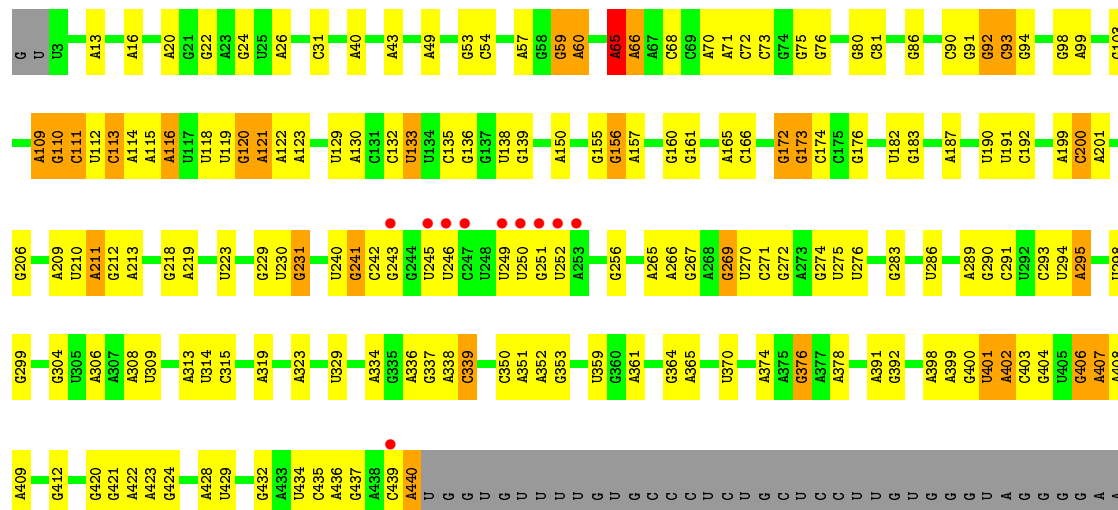
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	AP	1	Total	Zn	0	0
			1	1		
88	g	1	Total	Zn	0	0
			1	1		
88	AQ	1	Total	Zn	0	0
			1	1		
88	AK	1	Total	Zn	0	0
			1	1		
88	DQ	1	Total	Zn	0	0
			1	1		
88	e	1	Total	Zn	0	0
			1	1		
88	b	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		
88	c	1	Total	Zn	0	0
			1	1		
88	DL	1	Total	Zn	0	0
			1	1		
88	d9	1	Total	Zn	0	0
			1	1		
88	DR	1	Total	Zn	0	0
			1	1		
88	DO	1	Total	Zn	0	0
			1	1		
88	AN	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0	0
			1	1		

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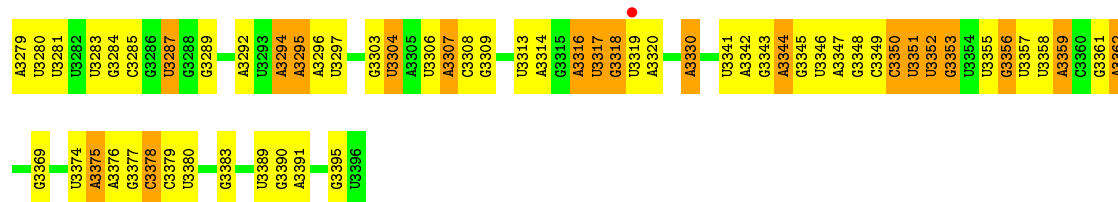
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	d6	1	Total	Zn	0	0
			1	1		





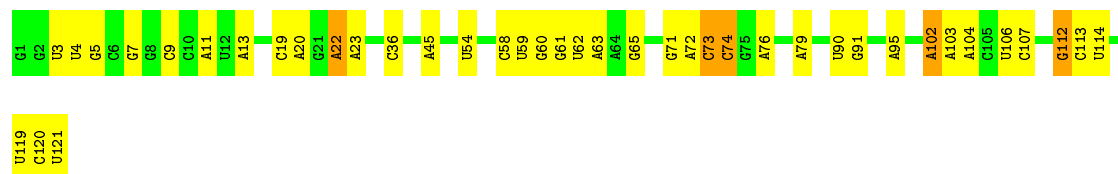
G1838	G1839	A1841	A1842	C1846	A1847	C1848	A1858	G1861	G1862	G1863	C1866	A1874	G1878	A1879	A1886	A1887	G1888	G1889	A1893	A1895	G1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	G1914	A1915	A1916	U1925	A1932	A1933	A1936	U1937	G1940	C1941	U1942	C1943	U1944	A1945																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
U1742	U1746	A1750	G1751	G1758	C1759	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1783	U1784	U1785	U1786	A1787	U1788	G1789	U1794	A1797	U1798	A1799	A1800	A1801	A1802	A1803	A1804	A1805	A1806	G1807	G1808	A1809	A1810	A1814	U1815	A1816	G1817	U1820	U1821	A1827	A1828	G1833	U1834	A1835																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
U1641	A1642	A1643	C1644	U1645	C1657	G1658	U1659	C1660	G1661	G1662	C1663	G1674	G1675	A1676	G1677	U1682	A1683	U1688	U1689	A1696	C1701	U1702	C1706	A1707	C1711	G1712	A1713	A1714	A1715	U1716	U1717	G1718	G1719	U1720	U1721	U1722	A1723	U1724	C1725	G1726	G1727	G1728	A1729	U1730	G1734	G1735	G1736	U1740	A1741																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
G1561	C1562	U1563	U1564	G1565	A1566	U1567	U1568	U1569	U1570	A1571	U1572	G1573	C1574	A1575	G1576	C1577	C1578	C1579	A1580	C1581	C1582	U1583	A1587	A1588	A1589	C1590	G1591	G1592	A1593	C1596	C1597	A1603	G1604	G1605	A1606	C1614	G1615	U1616	G1617	G1618	A1619	U1620	A1621	U1622	C1628	U1629	U1630	C1631	A1637	A1638	C1639	G1640																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
U1436	C1437	A1438	U1439	U1445	A1446	G1447	U1450	U1451	A1452	A1453	A1456	G1464	U1471	U1472	U1473	A1474	G1480	A1481	A1482	G1483	U1484	U1485	A1486	U1487	G1488	G1489	G1490	A1491	A1492	A1493	C1494	C1495	C1496	C1497	A1498	C1499	G1500	U1501	A1506	G1507	C1508	G1521	U1524	A1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
A1245	G1246	G1249	A1250	G1251	A1252	G1256	U1257	U1258	A1259	A1260	G1261	A1262	A1263	G1266	U1267	U1268	A1273	A1274	C1275	U1276	C1284	G1285	C1292	G1295	A1304	U1305	G1306	G1307	A1308	U1309	G1310	G1311	G1312	G1313	A1317	A1318	G1319	U1329	A1330	U1331	U1334	G1337	U1338	U1339	U1340	U1341	G1345																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
G1145	G1149	A1150	G1151	G1152	A1153	A1154	G1155	G1156	A1157	A1158	A1159	G1171	G1174	G1178	A1179	U1181	A1184	C1185	A1190	U1191	C1192	A1193	C1196	C1201	A1202	G1209	A1212	G1213	U1214	U1215	C1216	A1217	G1221	G1222	C1232	U1235	G1236	G1237	C1238	U1239	A1240	U1241	G1242	G1243	A1244																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U1039	A1040	U1041	C1042	C1043	A1047	A1048	C1049	G1052	G1053	A1054	A1055	G1066	G1072	C1076	A1080	U1081	U1082	A1093	U1094	U1095	U1096	G1097	C1100	G1101	A1102	A1103	A1104	U1108	U1109	U1110	U1111	G1116	G1117	U1128	A1129	G1130	G1131	G1132	A1133	G1134	G1135	A1136	G1139	G1140	C1141	G1142	U1143	U1144																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
U956	C957	C958	C959	U960	G964	U976	C977	G978	U979	A980	U981	C982	A983	U984	U985	U986	U990	G993	G994	U995	A996	A997	U998	G999	C1000	G1001	A1002	A1003	A1006	G1010	U1014	U1015	C1016	G1017	G1018	G1019	G1020	G1021	G1024	A1025	U1028	G1029	U942	U943	C944	C945	U946	G953	C954	U954	U955	C956	U957	U958	A959																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
U858	A959	U863	U864	C865	G865	U867	U868	A878	U879	U880	C881	G887	U888	G889	A890	U891	G894	A895	A896	U897	U898	U899	A904	U905	A906	G907	U908	G909	U910	G911	G912	A913	A914	A915	A916	U917	A921	U922	C923	G924	A925	A926	C927	A936	C937	C938	U939	G940	U941	U942	U943	C944	C945	U946	G953	C954	U954	U955	C956	U957	U958	A959																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
G644	C645	A649	C650	G651	U652	A653	C654	U655	A656	G657	U658	A659	U660	U661	C662	C663	U664	A665	C670	U673	A677	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	A691	A692	U693	A694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U141





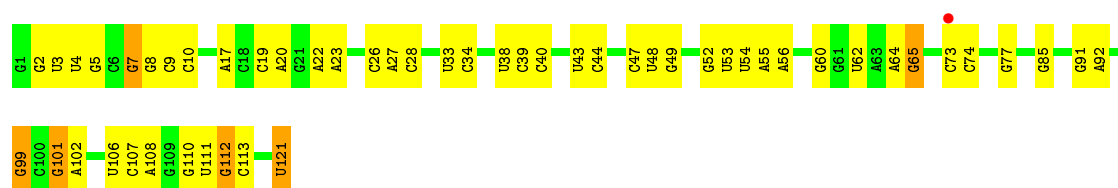
• Molecule 2: 5S ribosomal RNA

Chain 3: 66% 30% .



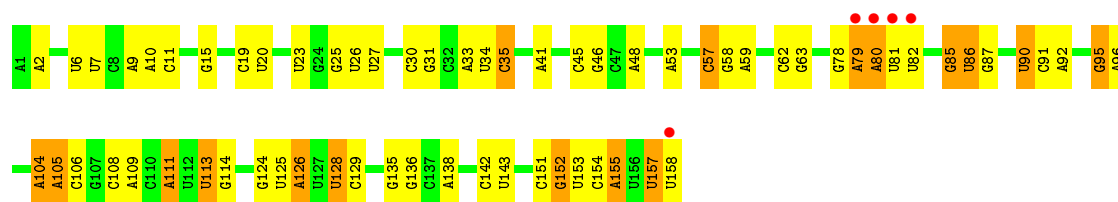
• Molecule 2: 5S ribosomal RNA

Chain AS: 57% 38% 5%



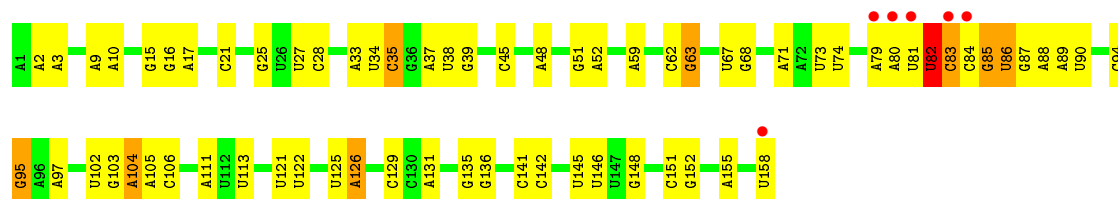
• Molecule 3: 5.8S ribosomal RNA

Chain 4: 3% 58% 31% 11%



• Molecule 3: 5.8S ribosomal RNA

Chain AT: 4% 57% 37% 5%

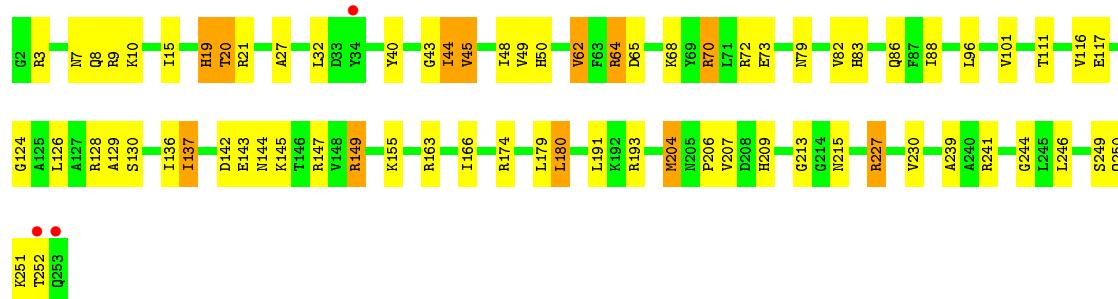
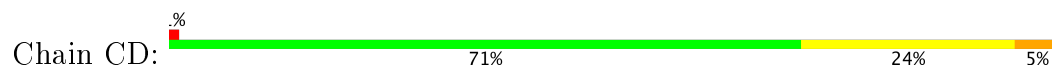


• Molecule 4: 60S ribosomal protein L2-A

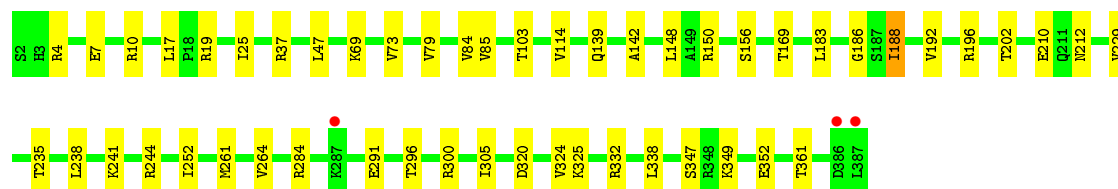
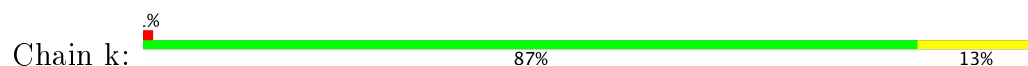
Chain j: 89% 11%



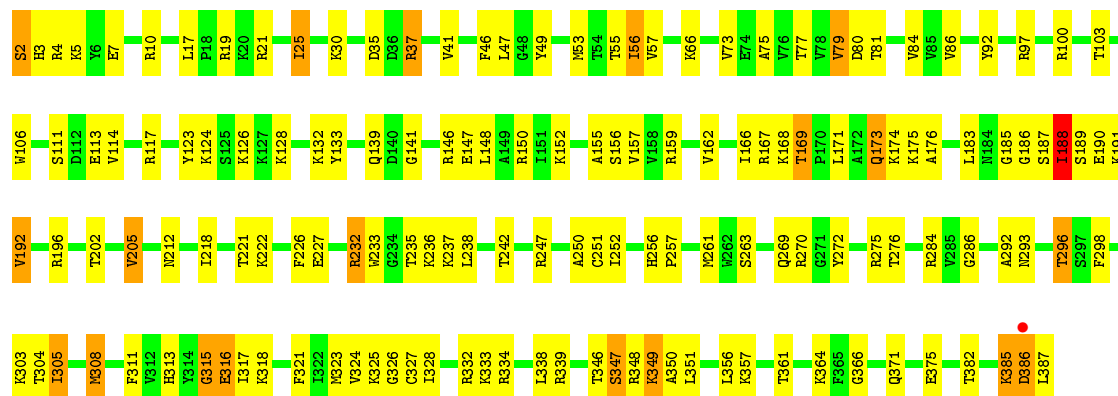
- Molecule 4: 60S ribosomal protein L2-A



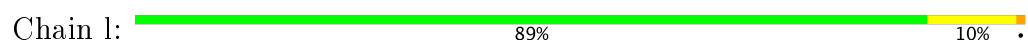
- Molecule 5: 60S ribosomal protein L3

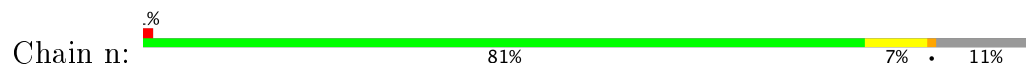


- Molecule 5: 60S ribosomal protein L3

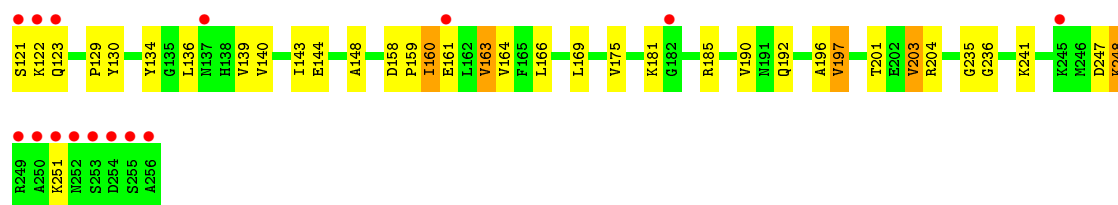


- Molecule 6: 60S ribosomal protein L4-A









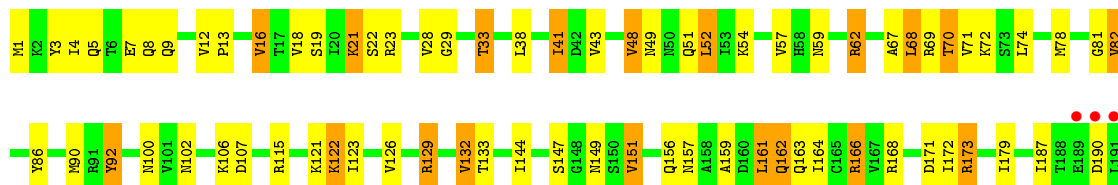
• Molecule 11: 60S ribosomal protein L9-A

Chain q: 87% 13%



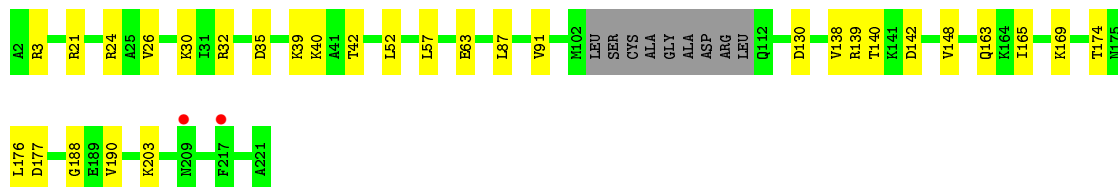
• Molecule 11: 60S ribosomal protein L9-A

Chain CK: 2% 62% 28% 10%



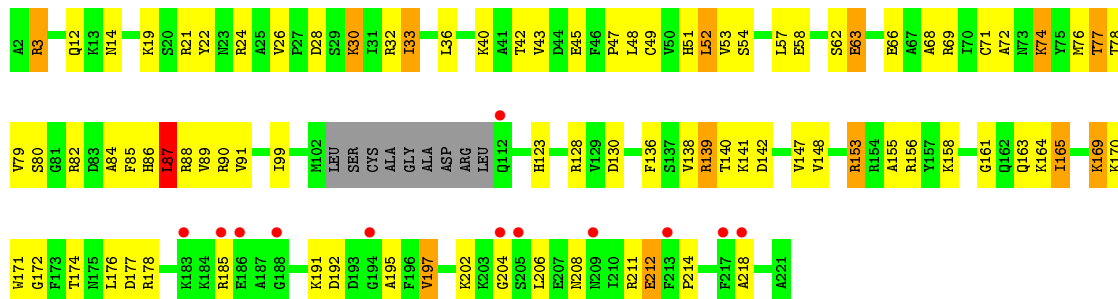
• Molecule 12: 60S ribosomal protein L10

Chain r: 82% 14%



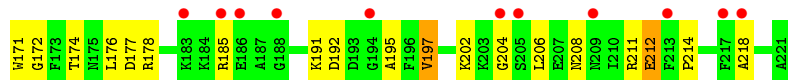
• Molecule 12: 60S ribosomal protein L10

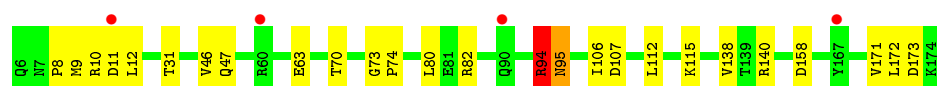
Chain CL: 5% 55% 34% 6%



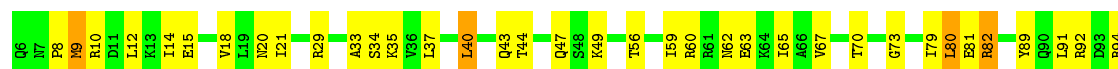
• Molecule 13: 60S ribosomal protein L11-B

Chain s: 2% 85% 14%

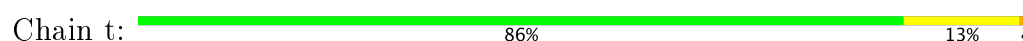




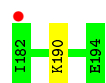
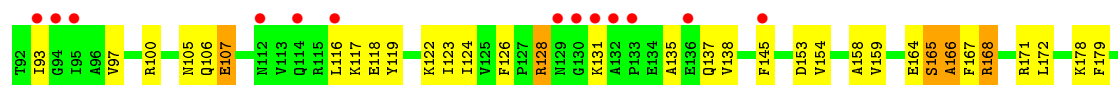
- Molecule 13: 60S ribosomal protein L11-B



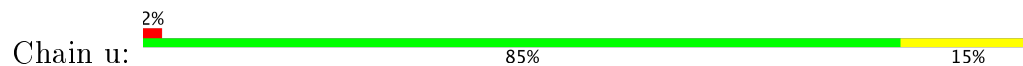
- Molecule 14: 60S ribosomal protein L13-A



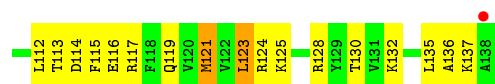
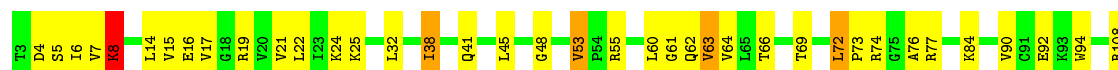
- Molecule 14: 60S ribosomal protein L13-A



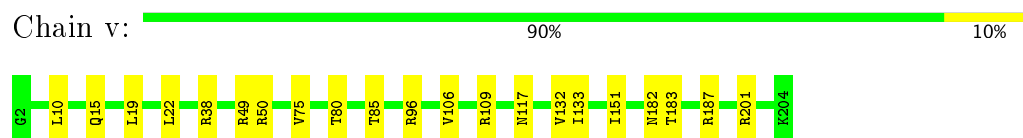
- Molecule 15: 60S ribosomal protein L14-A



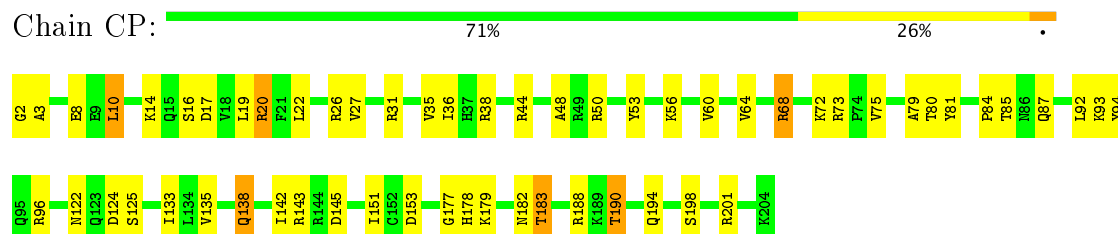
- Molecule 15: 60S ribosomal protein L14-A



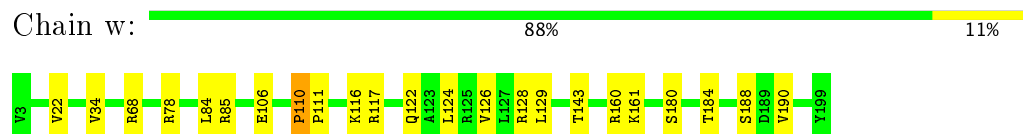
- Molecule 16: 60S ribosomal protein L15-A



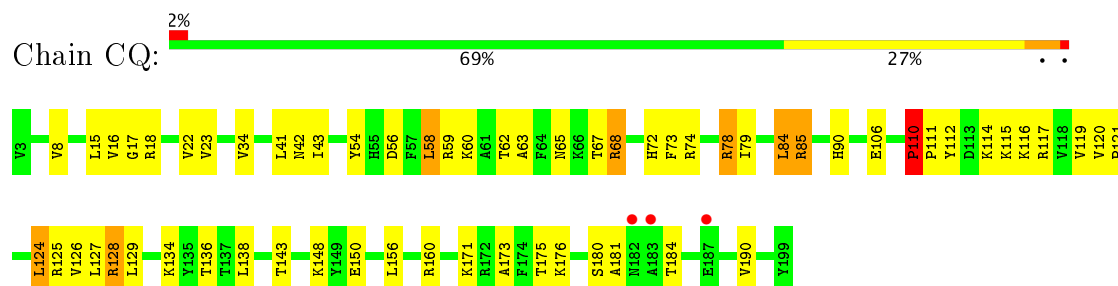
- Molecule 16: 60S ribosomal protein L15-A



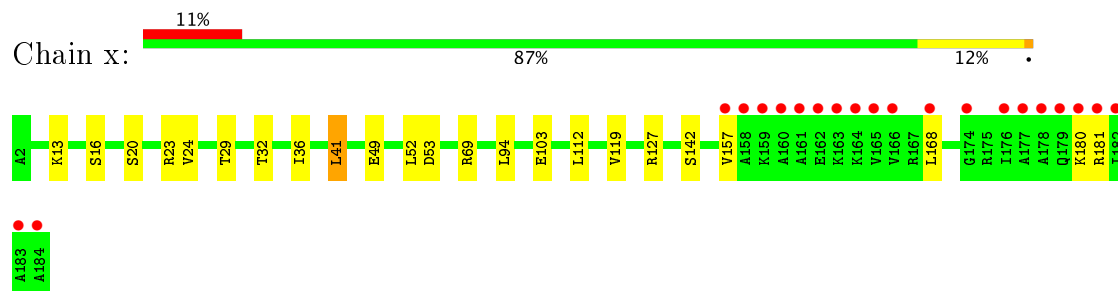
- Molecule 17: 60S ribosomal protein L16-A



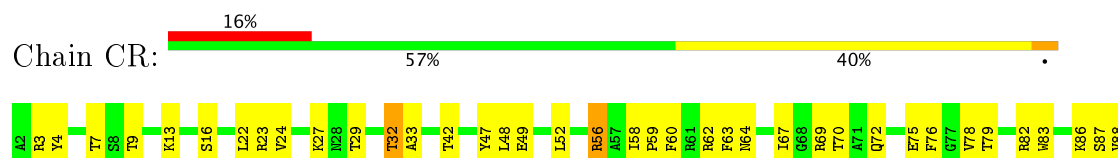
- Molecule 17: 60S ribosomal protein L16-A

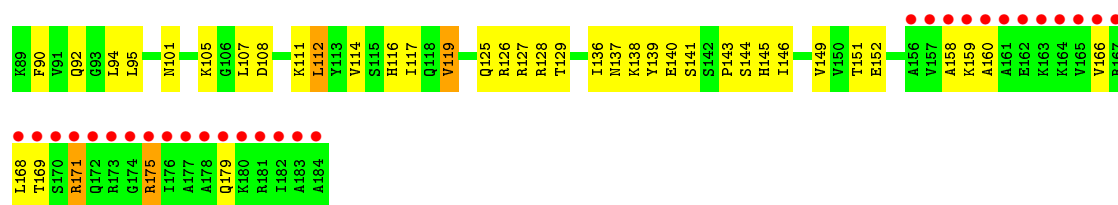


- Molecule 18: 60S ribosomal protein L17-A



- Molecule 18: 60S ribosomal protein L17-A





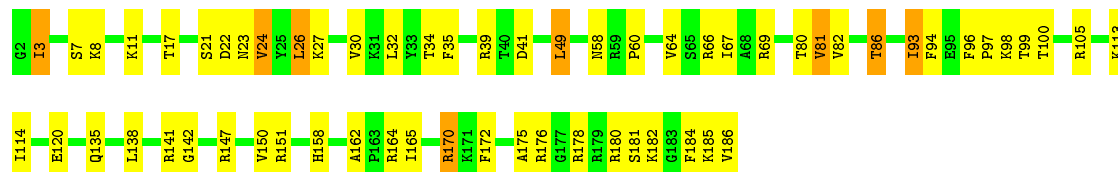
- Molecule 19: 60S ribosomal protein L18-A

Chain y: 89% 10% .



- Molecule 19: 60S ribosomal protein L18-A

Chain CS: 67% 29% .



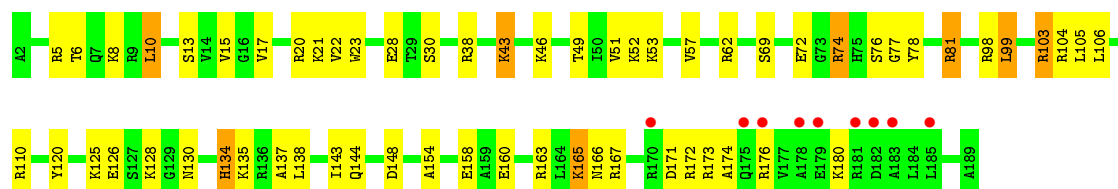
- Molecule 20: 60S ribosomal protein L19-A

Chain z: 4% 93% 7% .



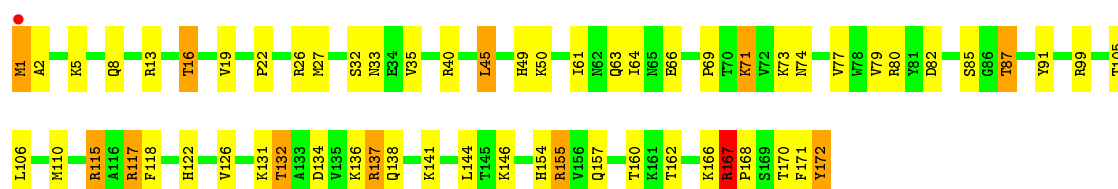
- Molecule 20: 60S ribosomal protein L19-A

Chain CT: 5% 68% 28% .

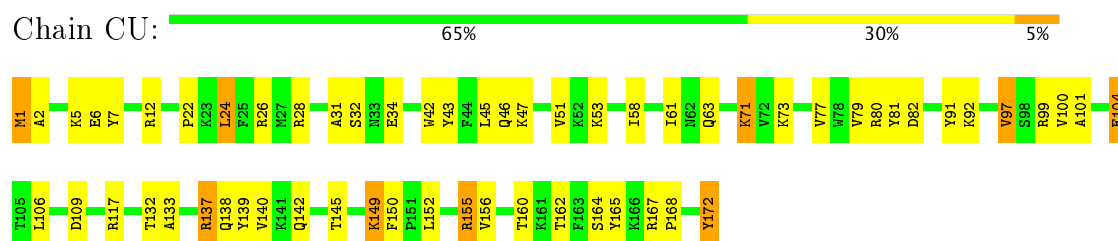


- Molecule 21: 60S ribosomal protein L20-A

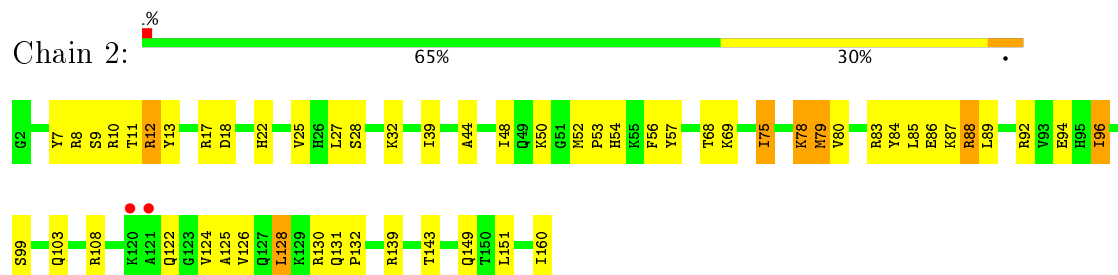
Chain 0: 65% 28% 6% .



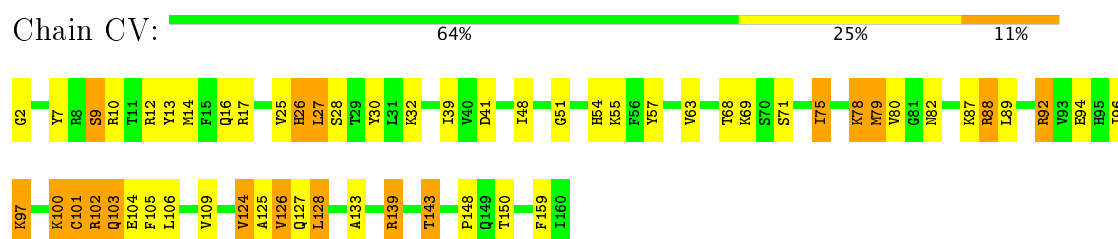
- Molecule 21: 60S ribosomal protein L20-A



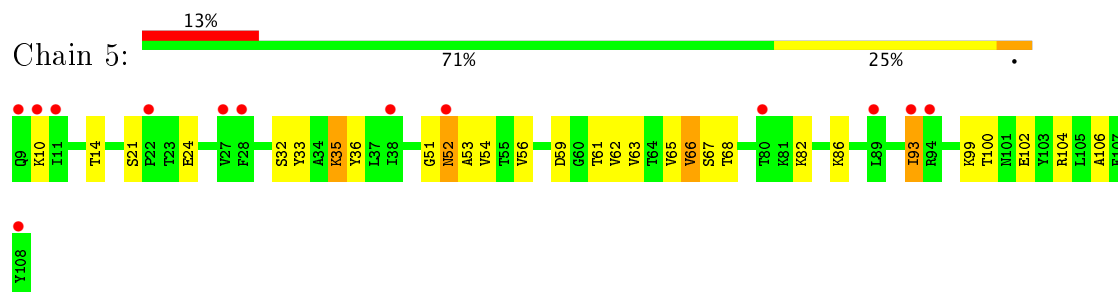
- Molecule 22: 60S ribosomal protein L21-A



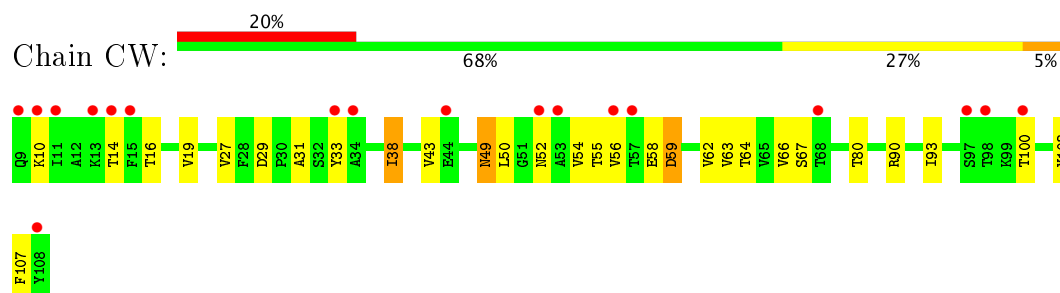
- Molecule 22: 60S ribosomal protein L21-A



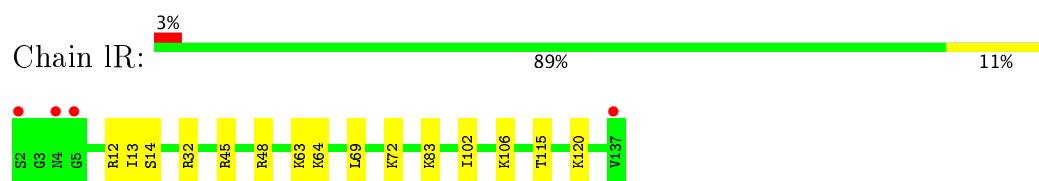
- Molecule 23: 60S ribosomal protein L22-A



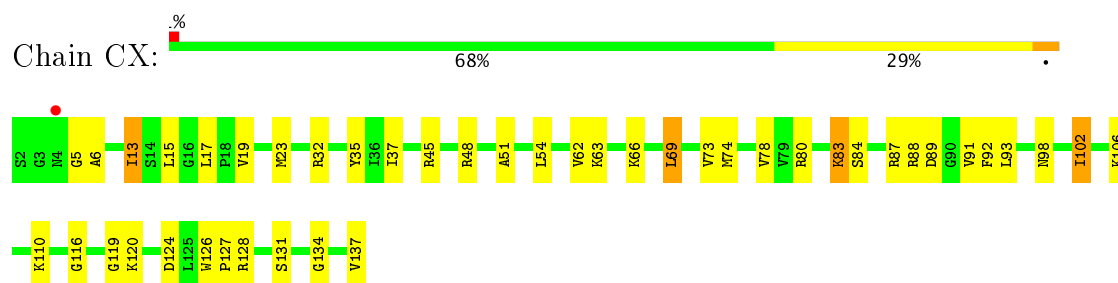
- Molecule 23: 60S ribosomal protein L22-A



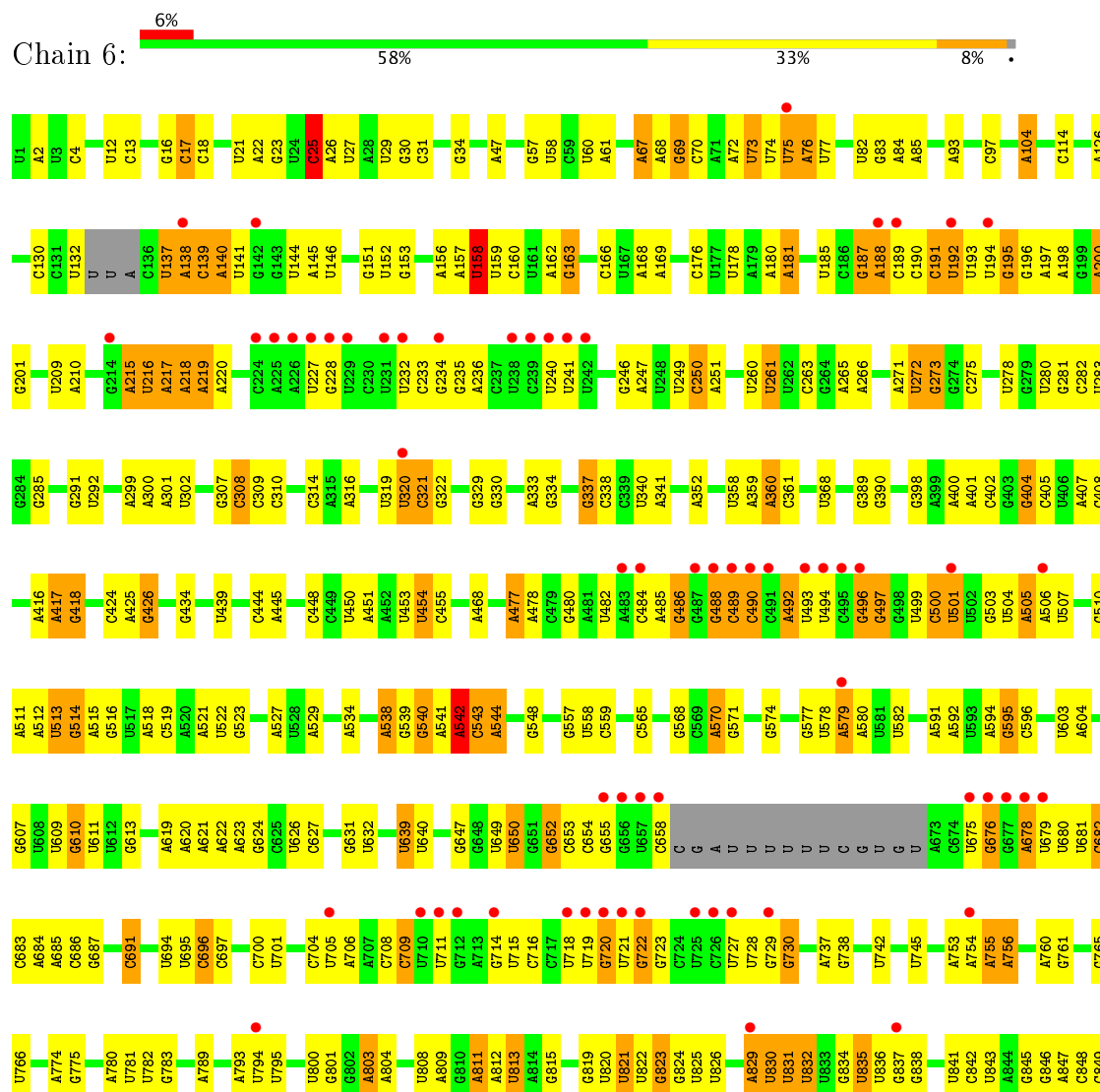
• Molecule 24: 60S ribosomal protein L23-A

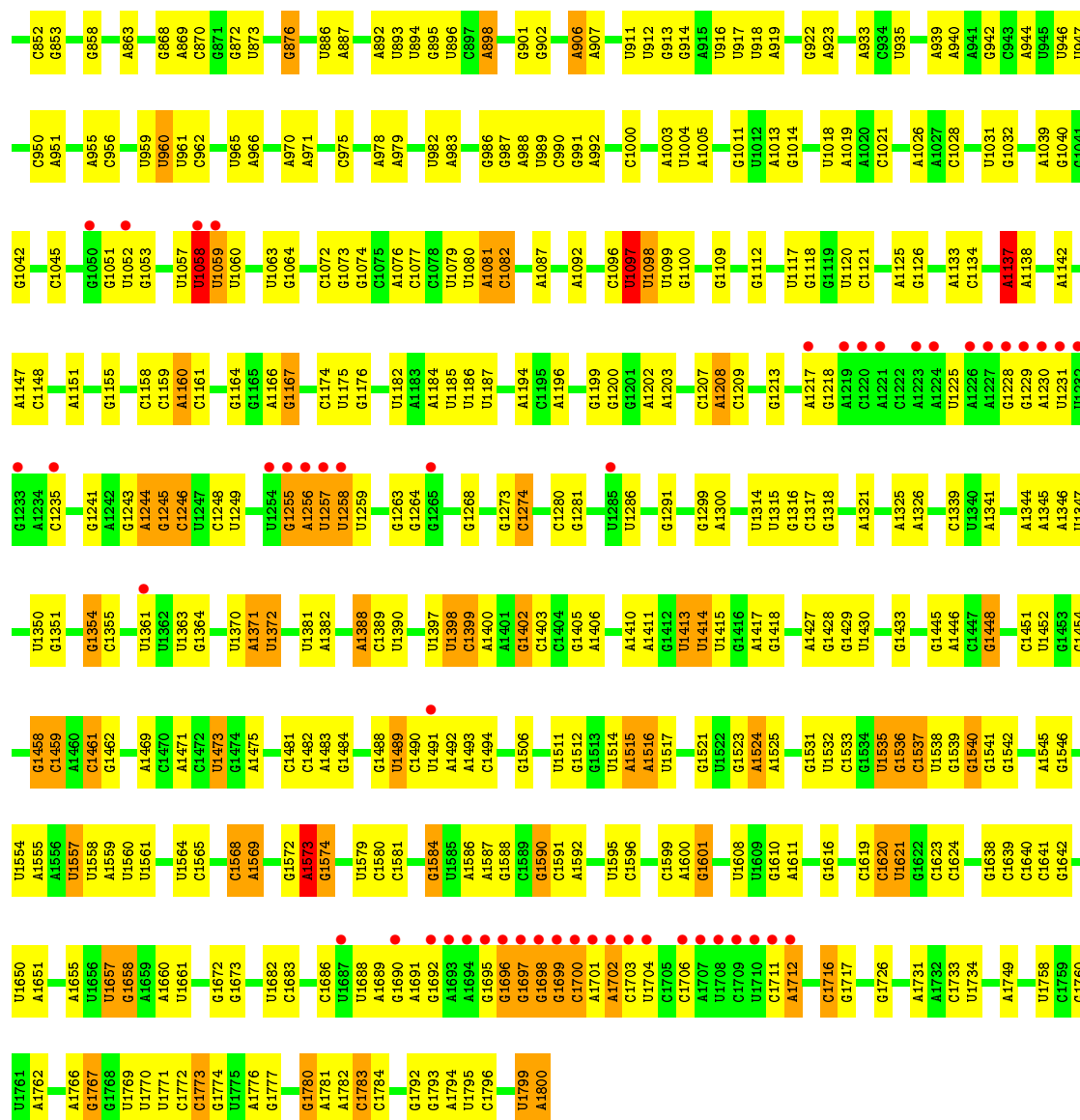


• Molecule 24: 60S ribosomal protein L23-A

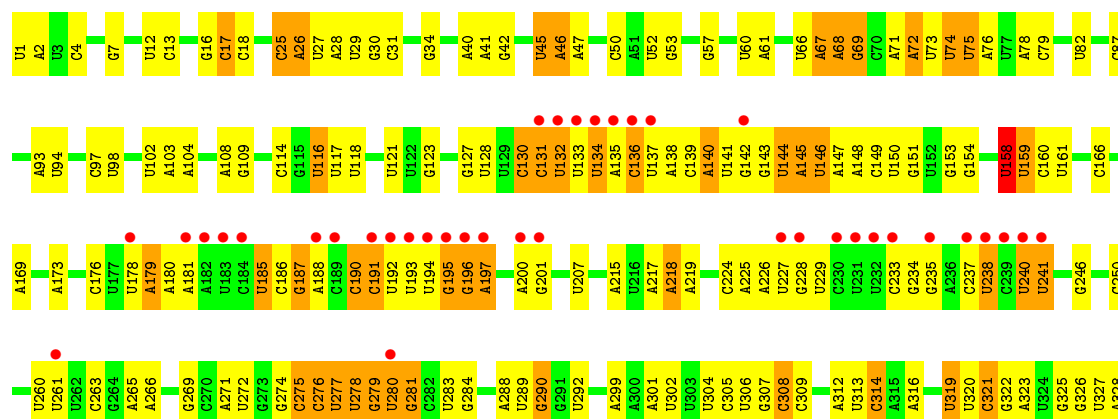


• Molecule 25: 18S ribosomal RNA

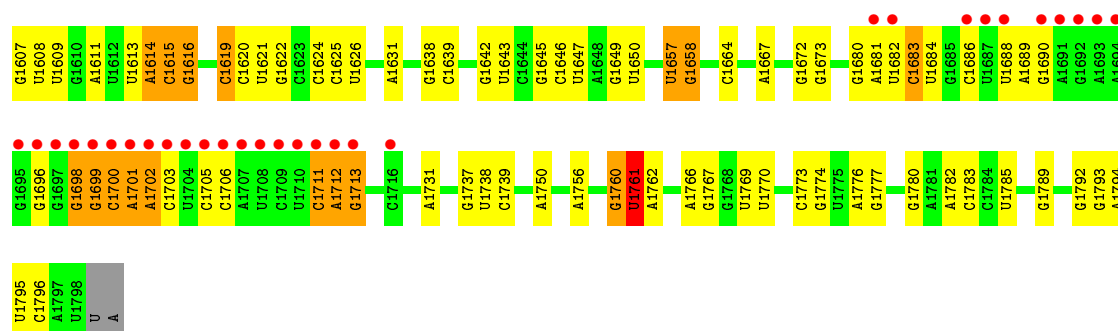




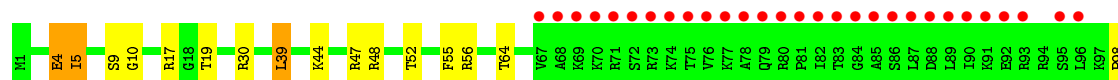
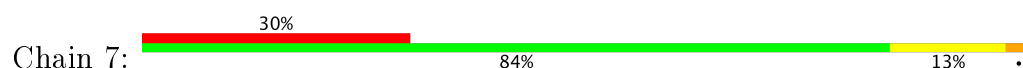
• Molecule 25: 18S ribosomal RNA



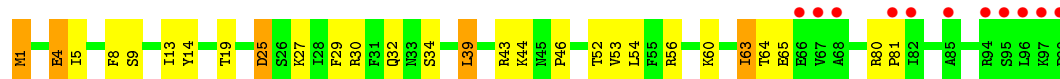
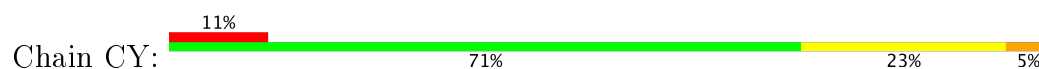
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C1456	C1359	U1257	C1173	U1080	U989	U888	U812	A734	U	U603	U507	A438	A331
G1457	A1360	U1258	C1174	A1081	G991	A892	A815	C735	G	A604	U508	U439	G337
C1458	U1361	U1261	U1175	C1082	A992	U893	G816	C736	A	A605	G510	C338	C338
C1459	U1362	U1262	U1176	G1083	A993	U894	A817	A737	U	A606	A511	C444	C339
A1460	U1363	U1263	C1177	A1087	G994	U895	C818	G738	C	G607	A512	A445	
C1461	C1365	G1267	G1178	A1088	A995	G895	G819	G739	U	U608	U513	A446	U350
G1462	U1366	G1268	U1179	A1089	U996	G896	G820	C741		A678	A515	U447	A450
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C1470	A1371	G1270	U1183	A1092	U1004	U910	U822	U743		U612	U517	A452	G356
A1471	C1368	U1271	A1184	A1093	A1005	U911	G823	U744		U613	A518	U453	
C1472	U1369	C1274	U1186	C1096	G1008	U912	U824	U745		U617	C519	U454	A359
U1473	U1370		U1188	U1097	U1012	U913	U825	U749		A684	A520	U455	A360
A1474	U1371	G1277	A1193	C1098	U1017	U914	U826	A753		A685	A521	G458	C361
C1475	U1372	G1278	A1194	U1099	U1018	U915	U827	A754		C827	U522	G459	
C1476	A1381	C1279	C1195	G1100	C1016	A916	U828	A755		A620	U523	A460	G372
A1481	A1382	G1280	C1196	G1101	U1017	U917	A829	A756		A621	A527	A461	U375
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G1504	U1414	G1324	G1228	A1146	G1042	C949	A856	C784		U484	U558	U484	G403
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C1518	U1438	A1345	U1244	A1161	A1063	U968	G868	G722		C658	A581	U496	A417
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A1600	G1521	U1349	U1248	G1165	C1068	U970	C870	U800		G	U583	U498	C424
G1601	U1522	U1350	U1249	A1166	C1069	A974	G871	G801		A	U584	U499	A425
U1603	A1524	G1351	U1250	A1167	G1073	U975	G872	G802		U	C583	U500	G426
U1604	C1447	U1251	G1074	U1168	U1074	U976	U873	A804		U	A591	U501	C427
A1526	U1448	U1251	G1074	U1168	C1075	U976	U873	U808		U	A592	U502	A428
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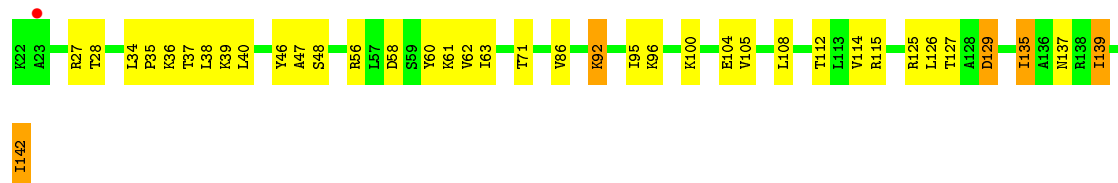
- Molecule 26: 60S ribosomal protein L24-A



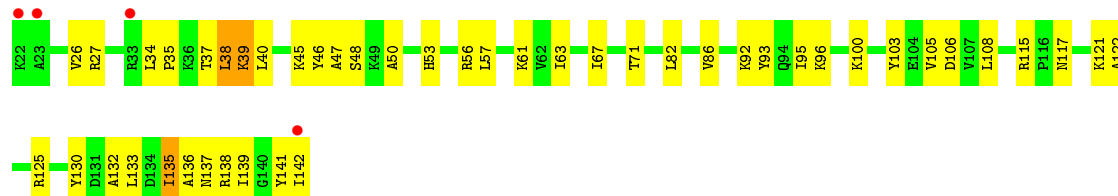
- Molecule 26: 60S ribosomal protein L24-A



- Molecule 27: 60S ribosomal protein L25

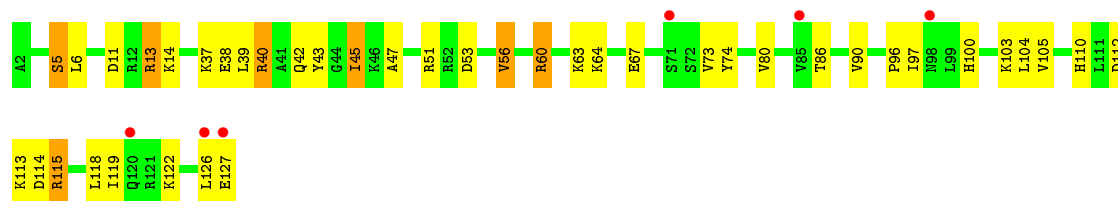


- Molecule 27: 60S ribosomal protein L25

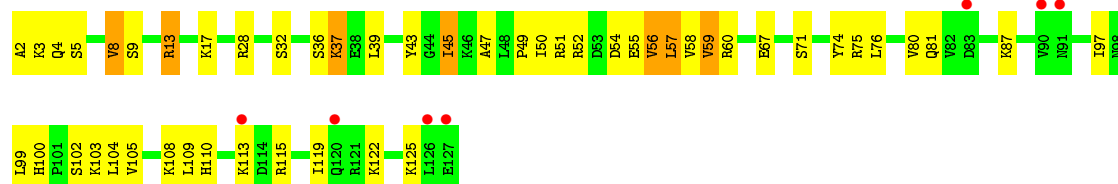


- Molecule 28: 60S ribosomal protein L26-A

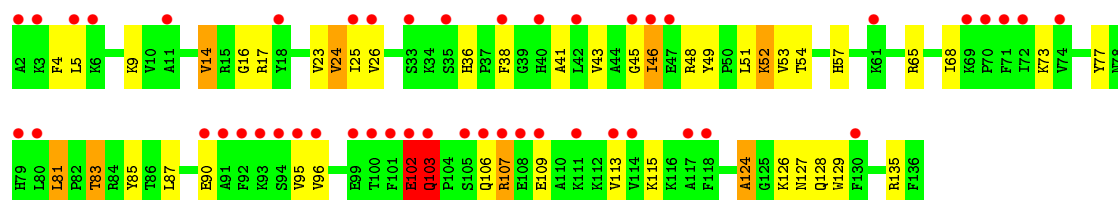




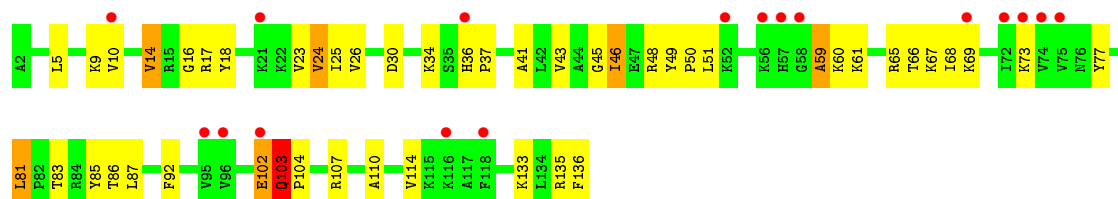
• Molecule 28: 60S ribosomal protein L26-A



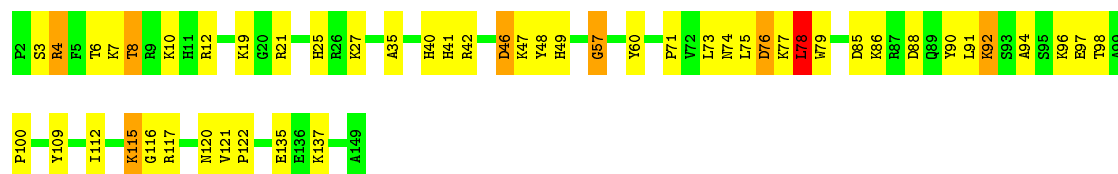
• Molecule 29: 60S ribosomal protein L27-A



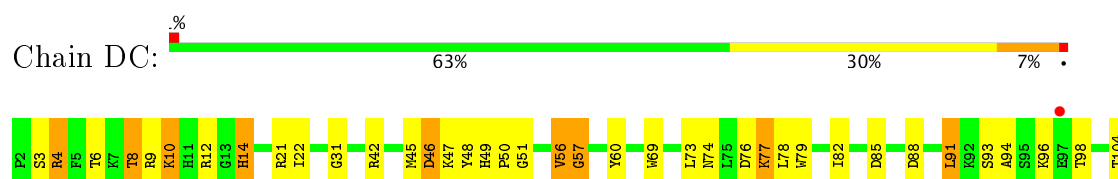
• Molecule 29: 60S ribosomal protein L27-A



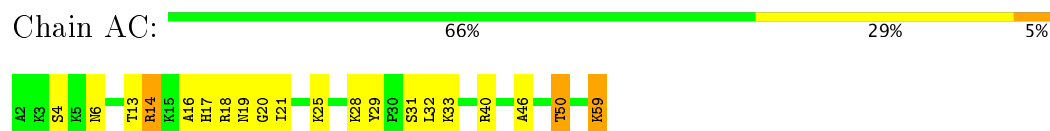
• Molecule 30: 60S ribosomal protein L28



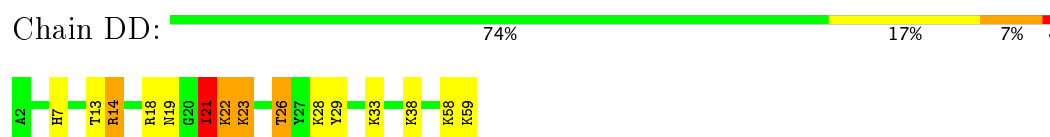
• Molecule 30: 60S ribosomal protein L28



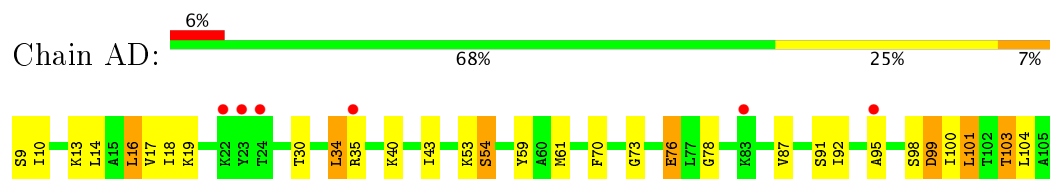
- Molecule 31: 60S ribosomal protein L29



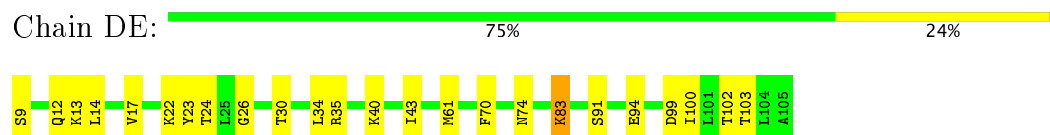
- Molecule 31: 60S ribosomal protein L29



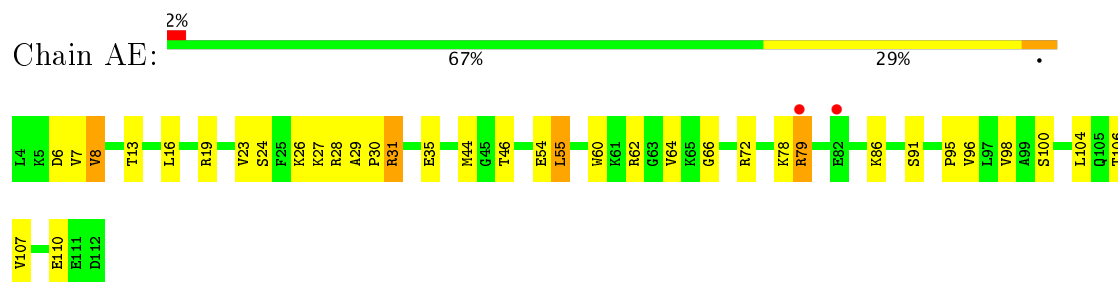
- Molecule 32: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L30



- Molecule 33: 60S ribosomal protein L31-A

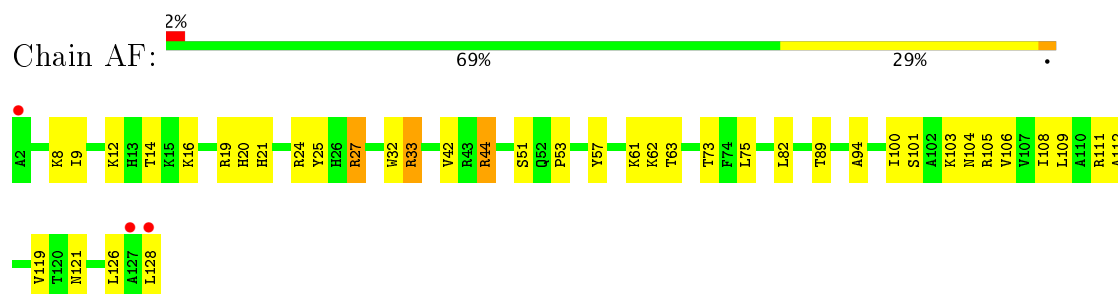


- Molecule 33: 60S ribosomal protein L31-A

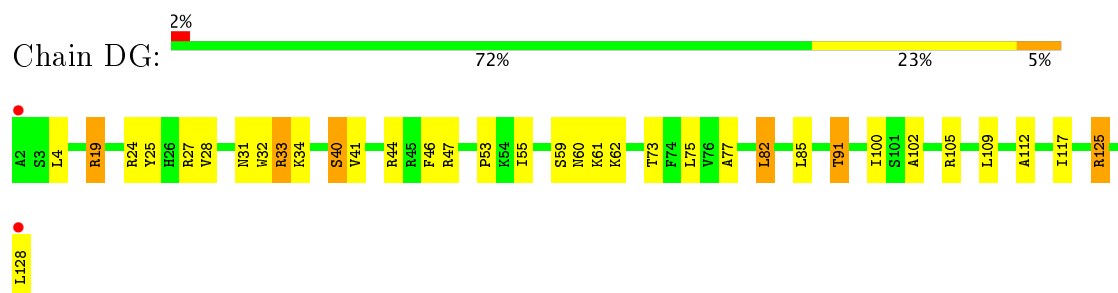




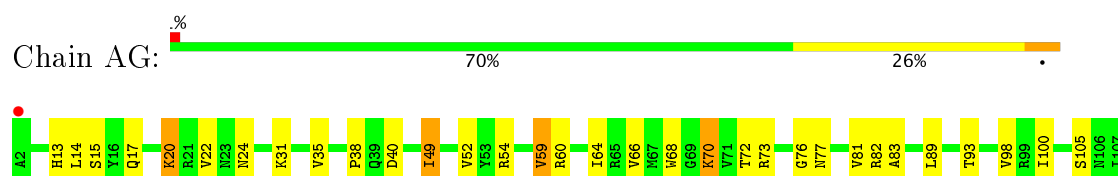
- Molecule 34: 60S ribosomal protein L32



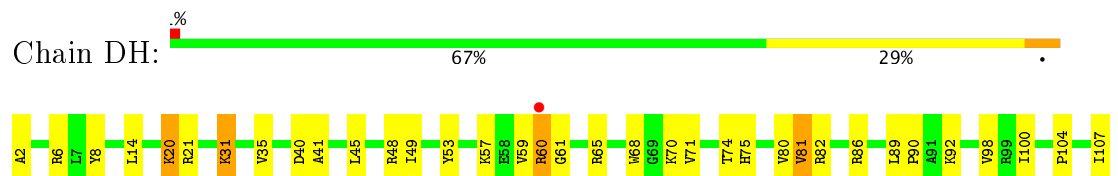
- Molecule 34: 60S ribosomal protein L32



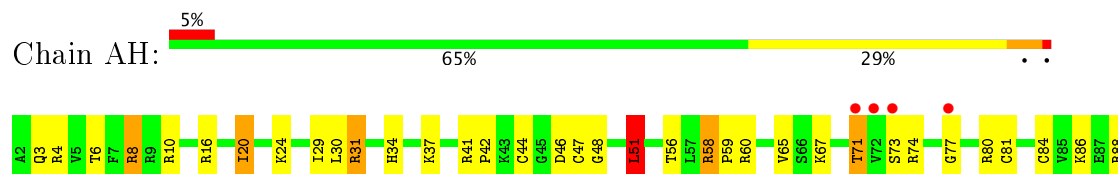
- Molecule 35: 60S ribosomal protein L33-A

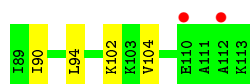


- Molecule 35: 60S ribosomal protein L33-A

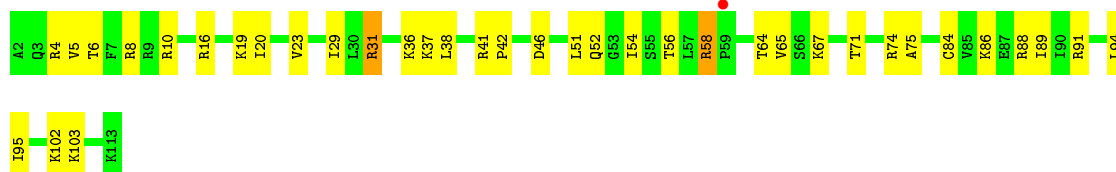


- Molecule 36: 60S ribosomal protein L34-A

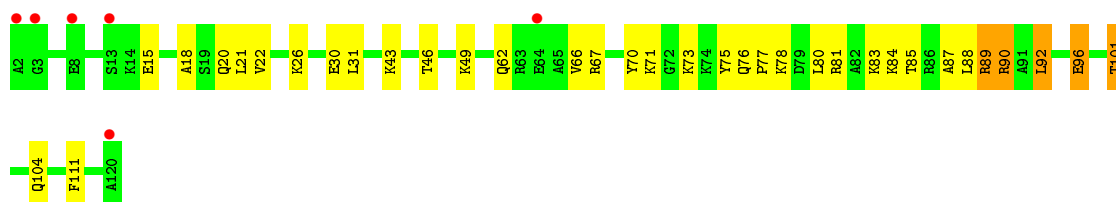
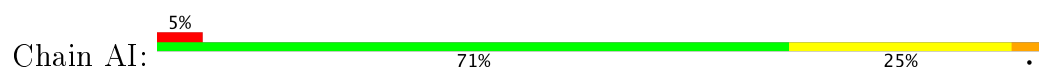




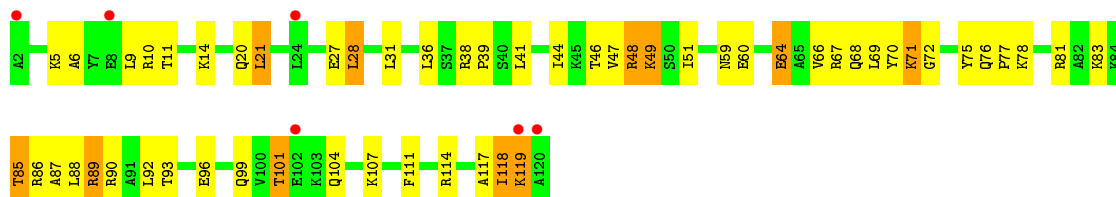
- Molecule 36: 60S ribosomal protein L34-A



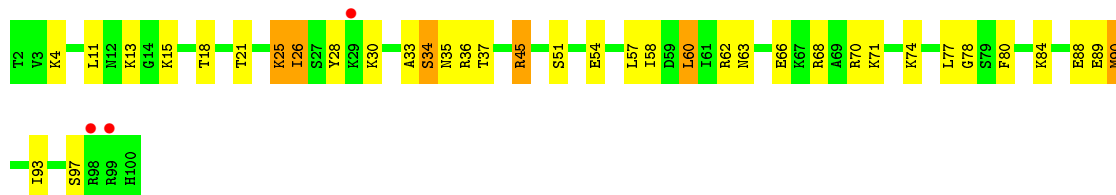
- Molecule 37: 60S ribosomal protein L35-A



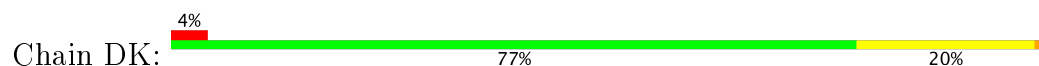
- Molecule 37: 60S ribosomal protein L35-A

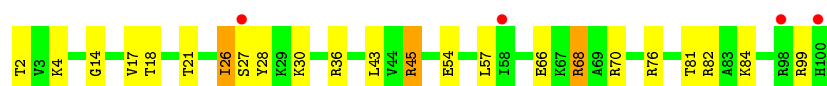


- Molecule 38: 60S ribosomal protein L36-A



- Molecule 38: 60S ribosomal protein L36-A

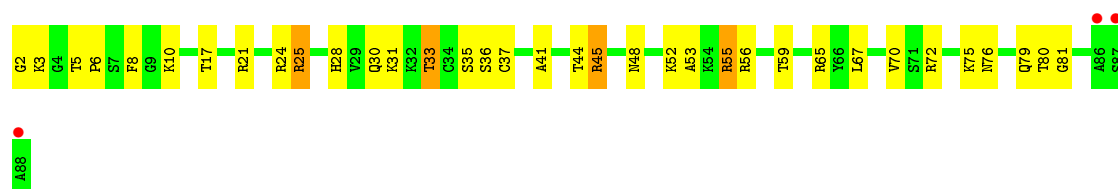




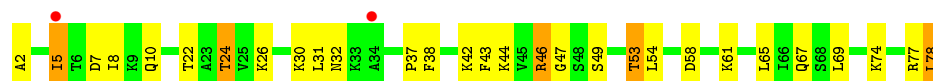
- Molecule 39: 60S ribosomal protein L37-A



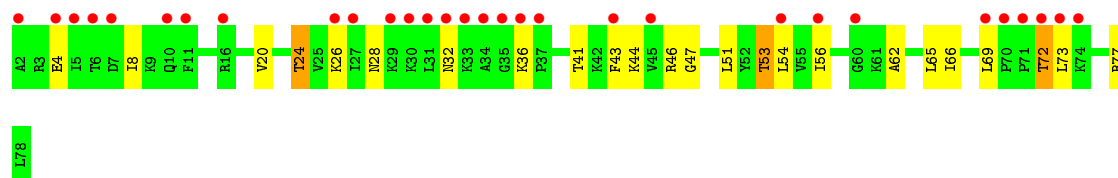
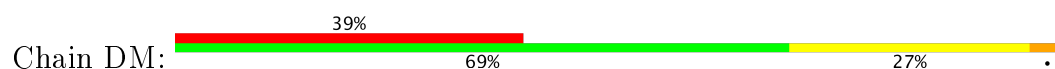
- Molecule 39: 60S ribosomal protein L37-A



- Molecule 40: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L38



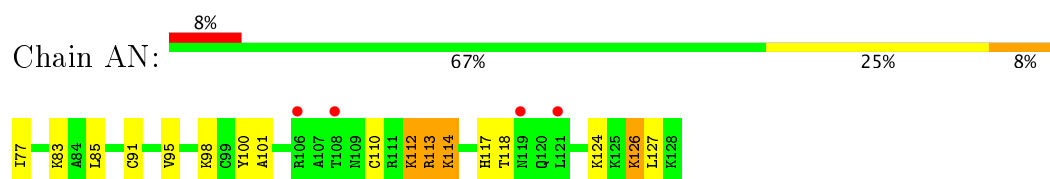
- Molecule 41: 60S ribosomal protein L39



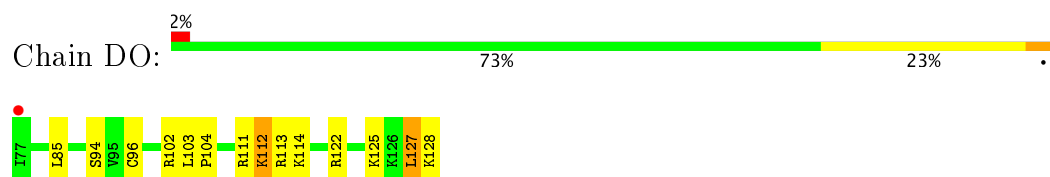
- Molecule 41: 60S ribosomal protein L39



- Molecule 42: Ubiquitin-60S ribosomal protein L40



- Molecule 42: Ubiquitin-60S ribosomal protein L40



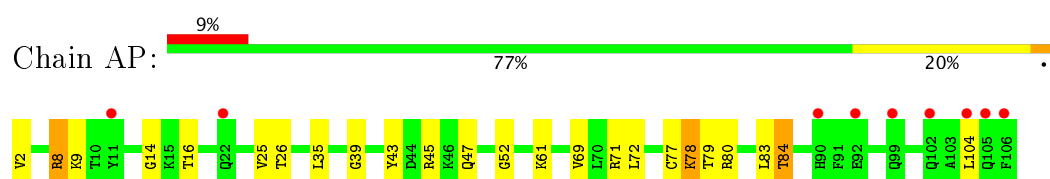
- Molecule 43: 60S ribosomal protein L41-B



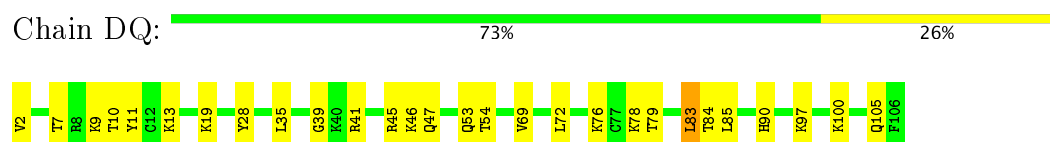
- Molecule 43: 60S ribosomal protein L41-B



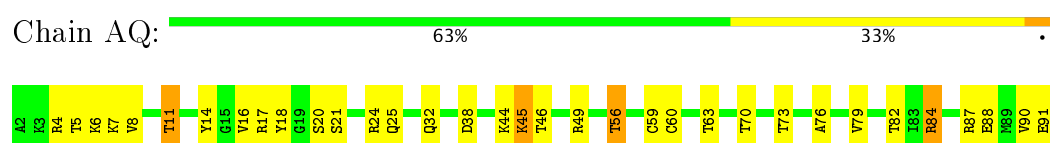
- Molecule 44: 60S ribosomal protein L42-A



- Molecule 44: 60S ribosomal protein L42-A



- Molecule 45: 60S ribosomal protein L43-A



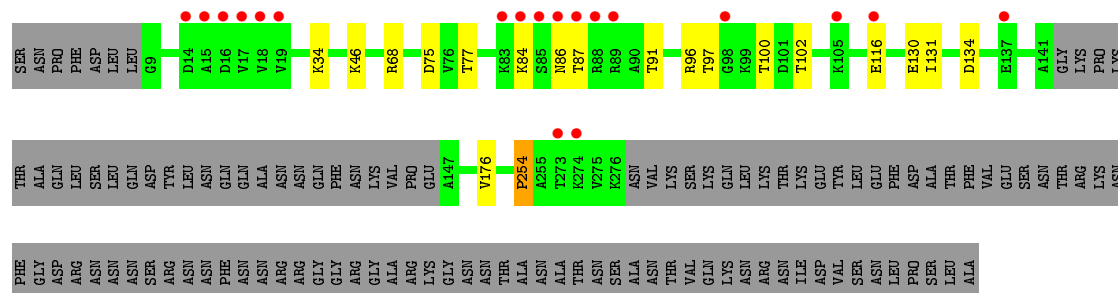
- Molecule 45: 60S ribosomal protein L43-A

Chain DR: 

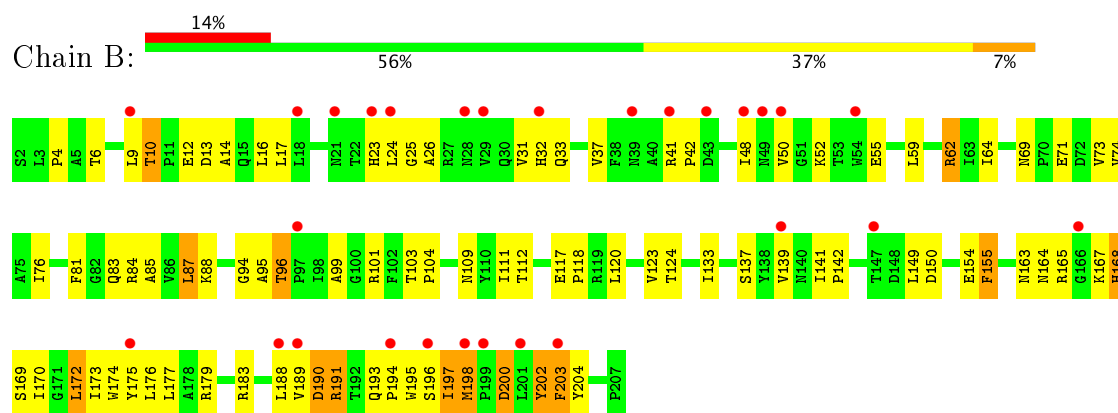


- Molecule 46: Suppressor protein STM1

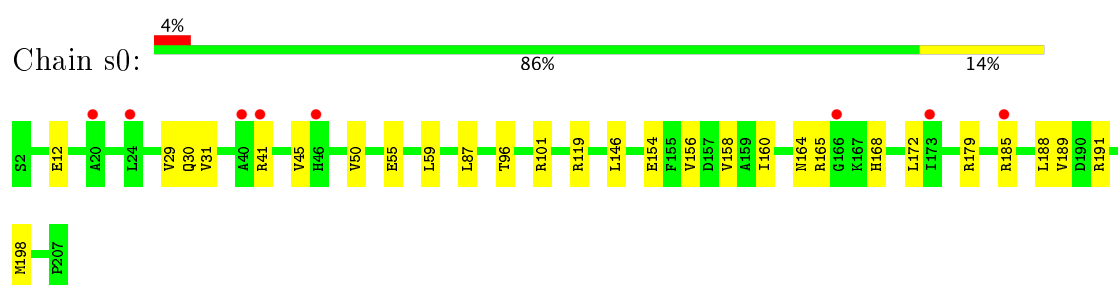
Chain i: 



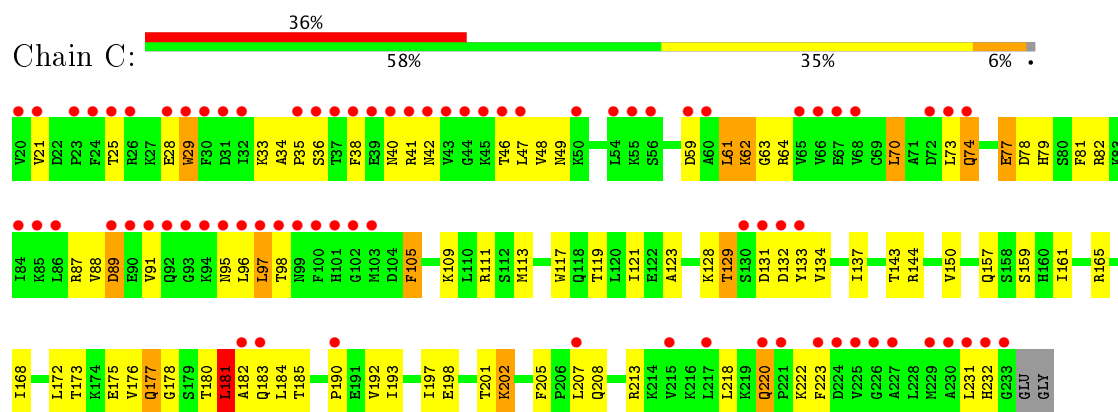
- Molecule 50: 40S ribosomal protein S0-A



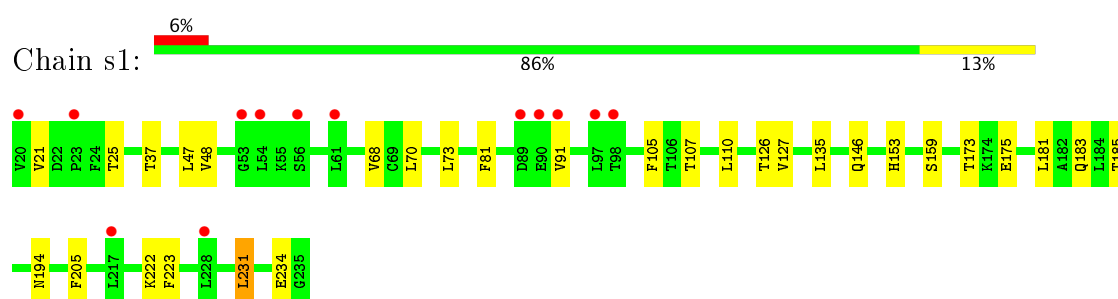
- Molecule 50: 40S ribosomal protein S0-A



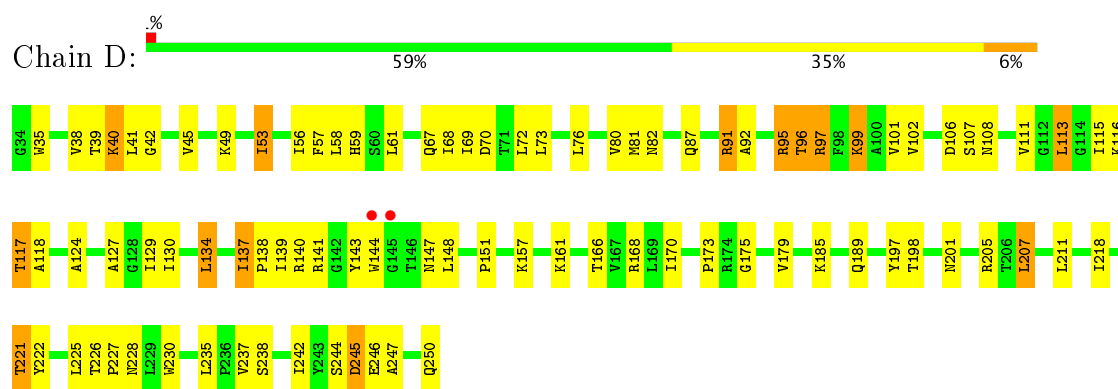
- Molecule 51: 40S ribosomal protein S1-A



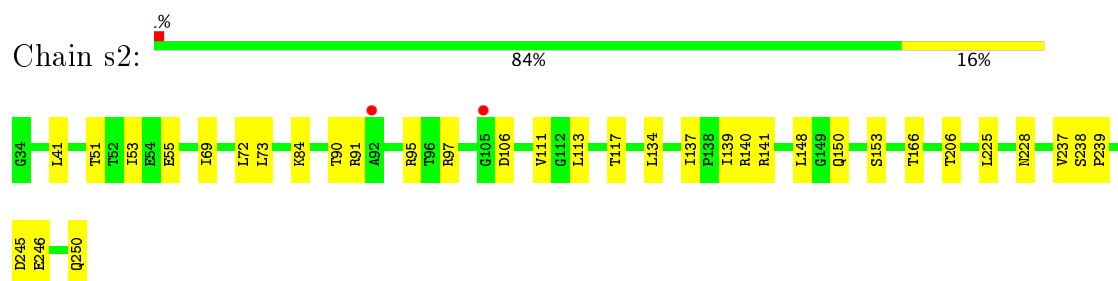
- Molecule 51: 40S ribosomal protein S1-A



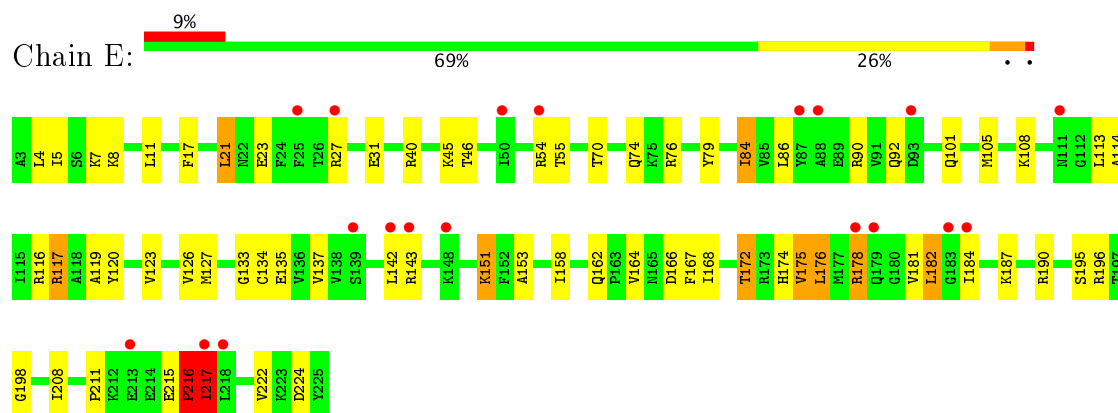
- Molecule 52: 40S ribosomal protein S2



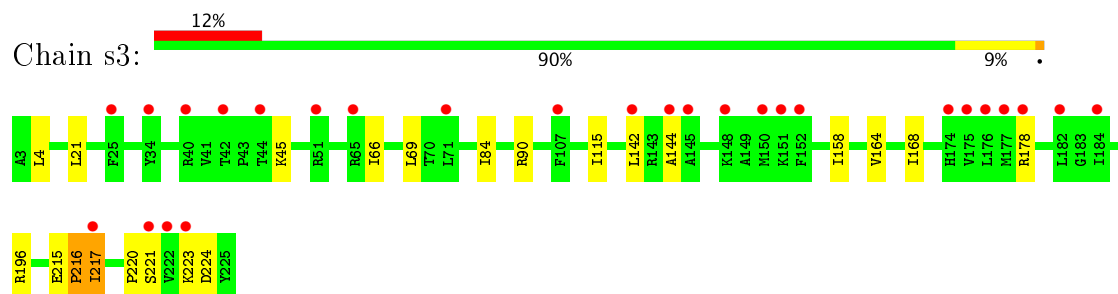
• Molecule 52: 40S ribosomal protein S2



• Molecule 53: 40S ribosomal protein S3

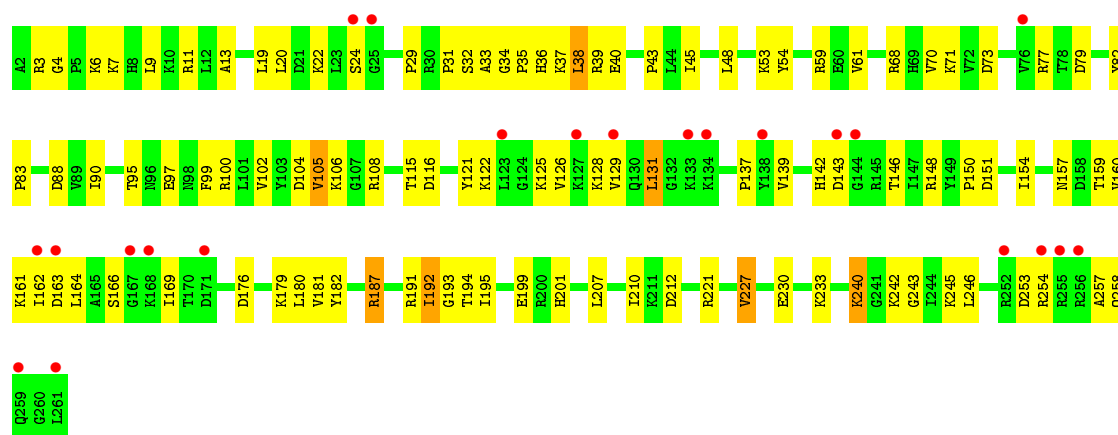


• Molecule 53: 40S ribosomal protein S3



• Molecule 54: 40S ribosomal protein S4-A

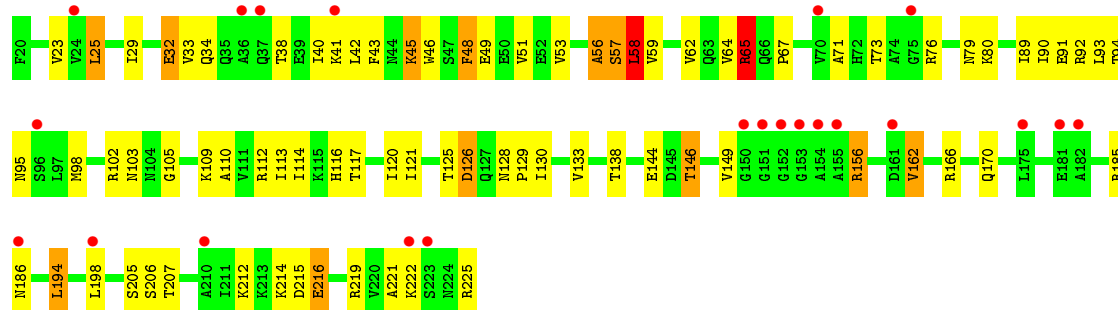




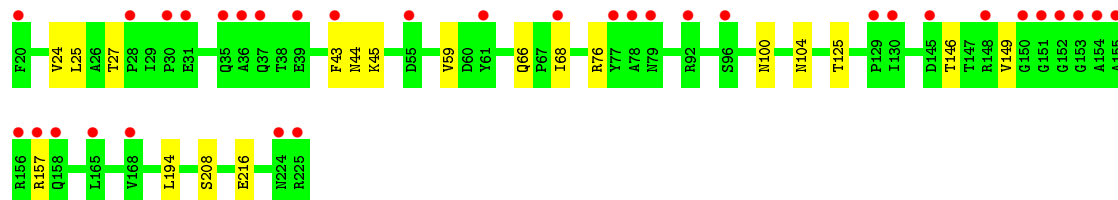
• Molecule 54: 40S ribosomal protein S4-A



• Molecule 55: 40S ribosomal protein S5

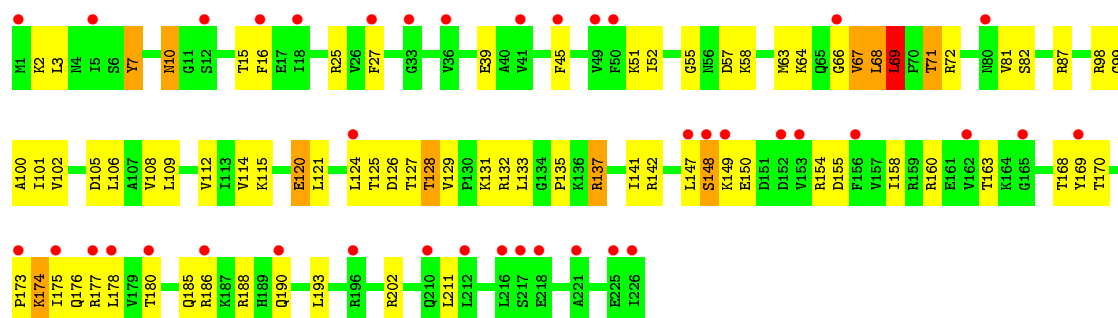


• Molecule 55: 40S ribosomal protein S5

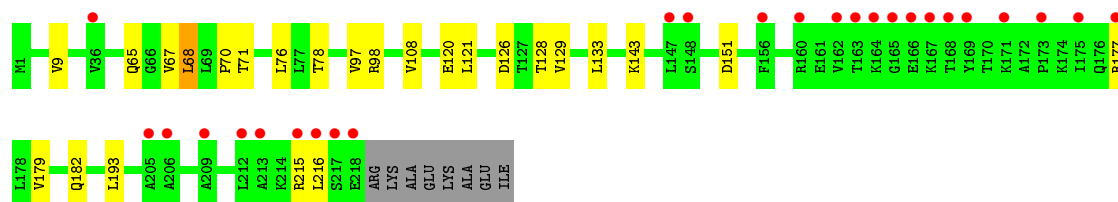
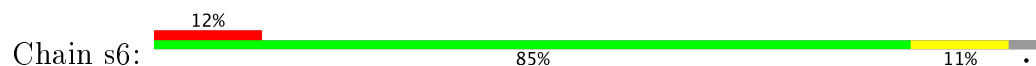


• Molecule 56: 40S ribosomal protein S6-A

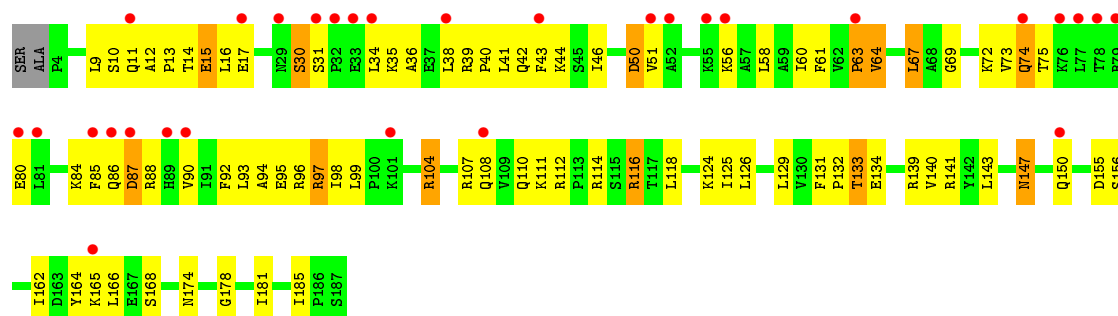




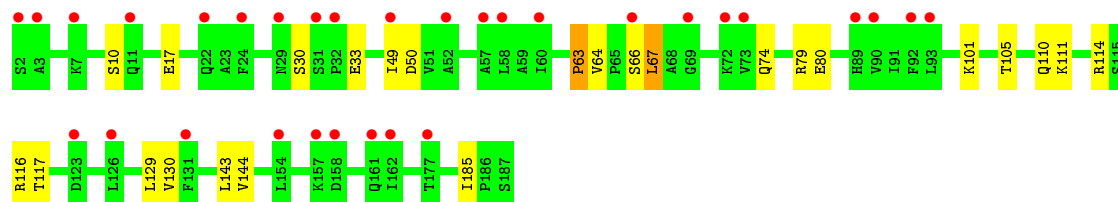
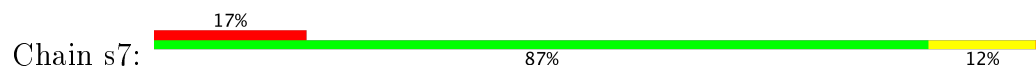
- Molecule 56: 40S ribosomal protein S6-A



- Molecule 57: 40S ribosomal protein S7-A

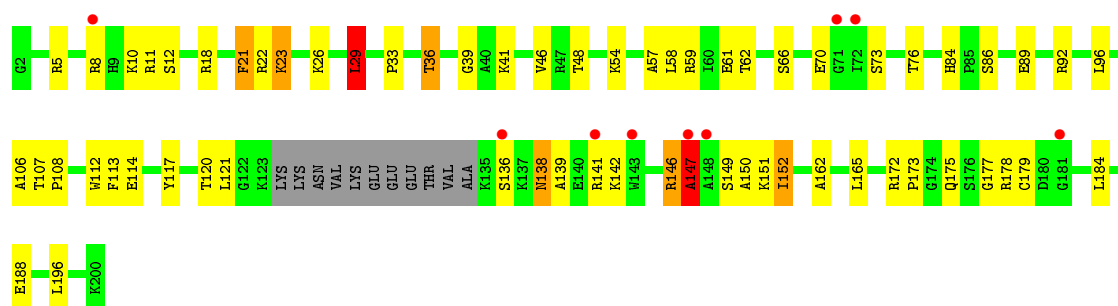


- Molecule 57: 40S ribosomal protein S7-A

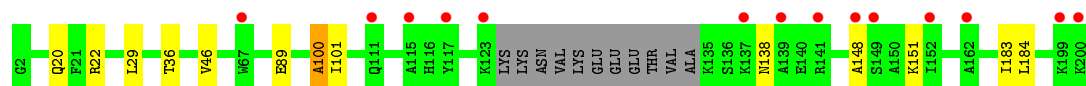
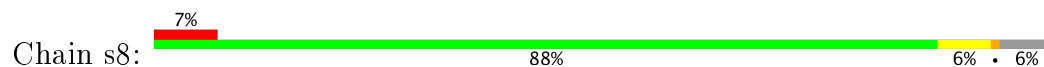


- Molecule 58: 40S ribosomal protein S8-A

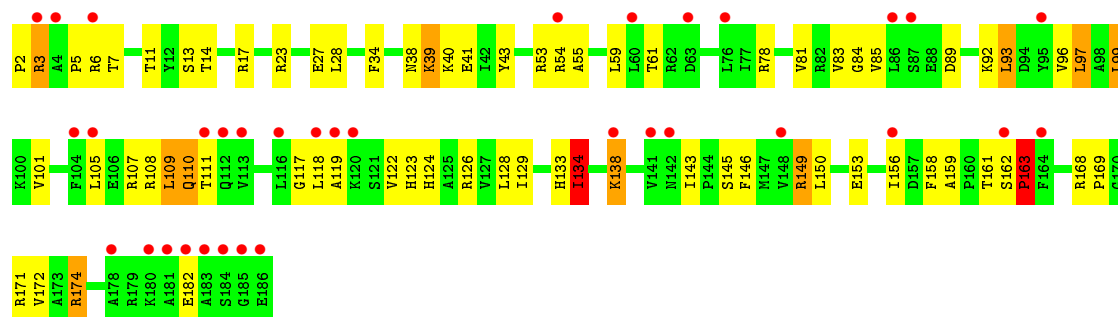




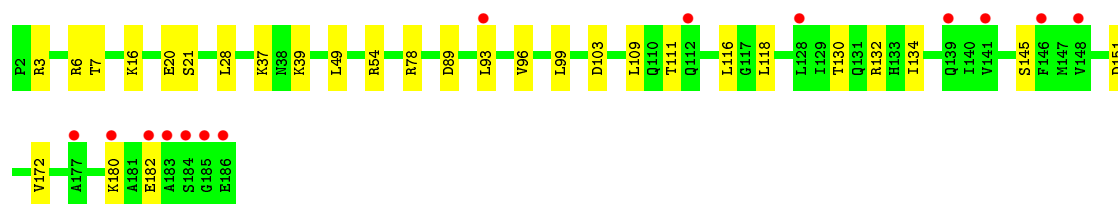
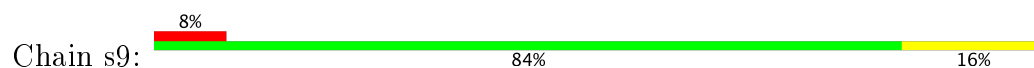
• Molecule 58: 40S ribosomal protein S8-A



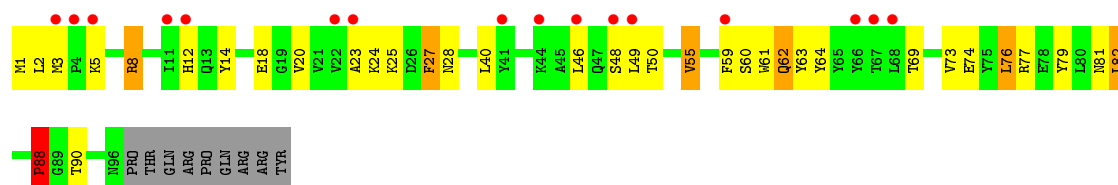
• Molecule 59: 40S ribosomal protein S9-A



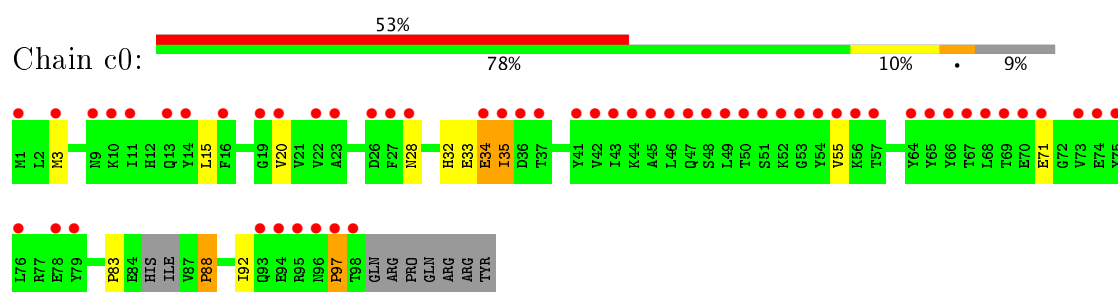
• Molecule 59: 40S ribosomal protein S9-A



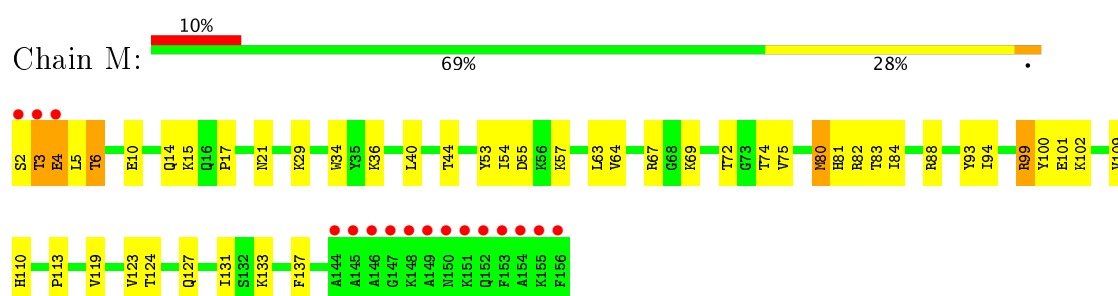
• Molecule 60: 40S ribosomal protein S10-A



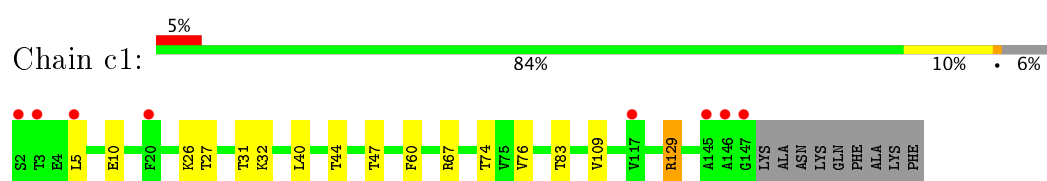
- Molecule 60: 40S ribosomal protein S10-A



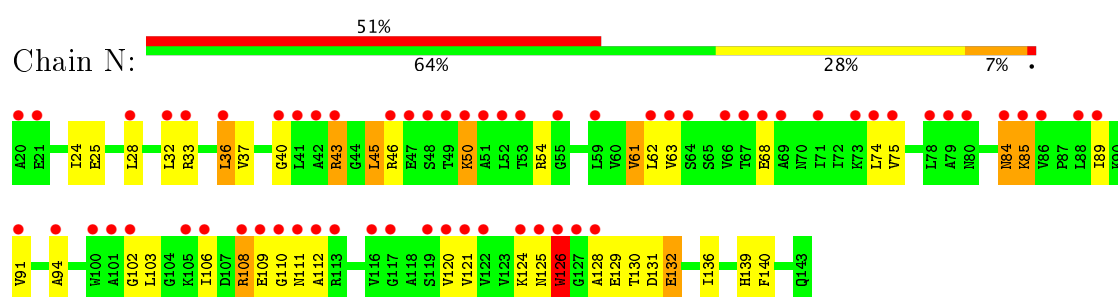
- Molecule 61: 40S ribosomal protein S11-A



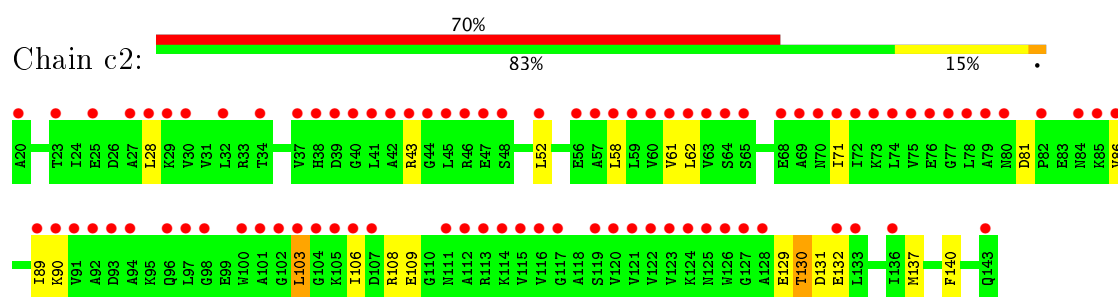
- Molecule 61: 40S ribosomal protein S11-A



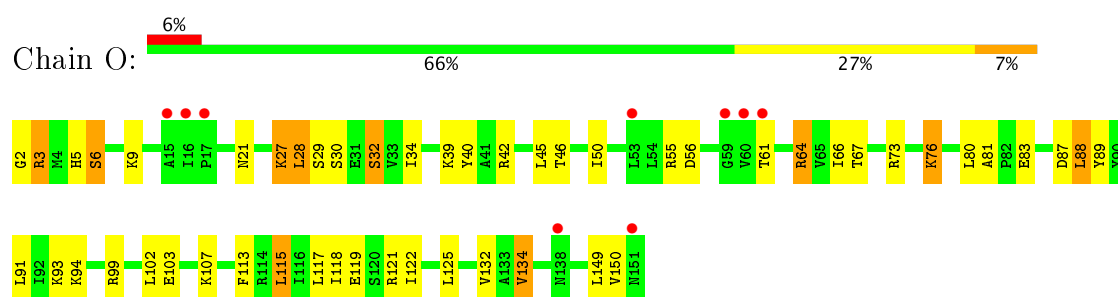
- Molecule 62: 40S ribosomal protein S12



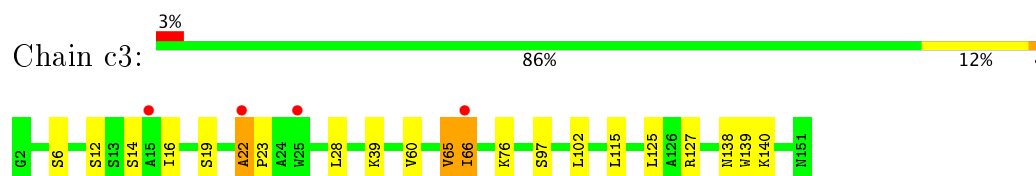
- Molecule 62: 40S ribosomal protein S12



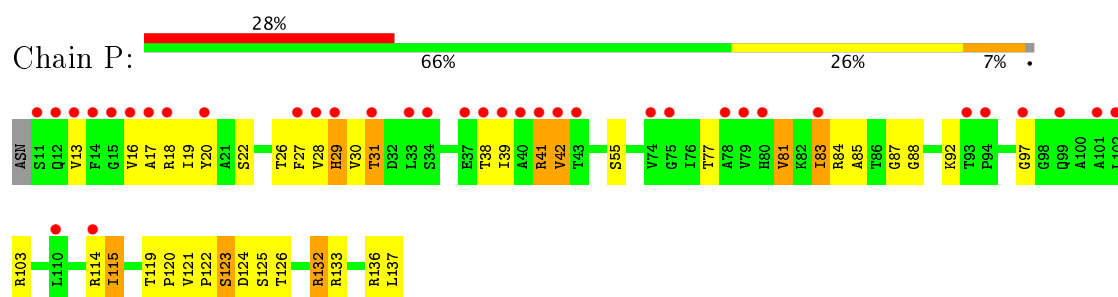
- Molecule 63: 40S ribosomal protein S13



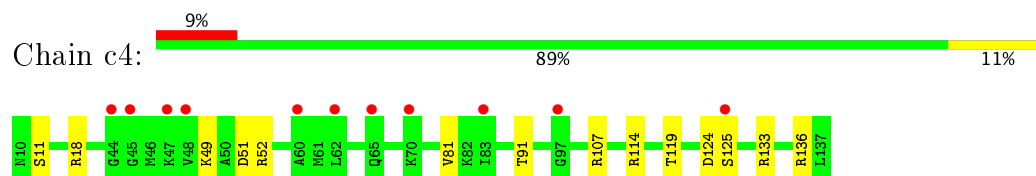
- Molecule 63: 40S ribosomal protein S13



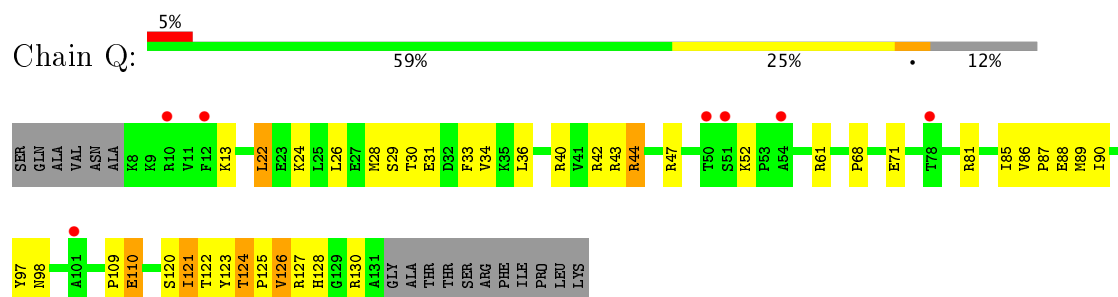
- Molecule 64: 40S ribosomal protein S14-B



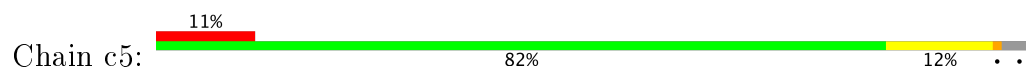
- Molecule 64: 40S ribosomal protein S14-B

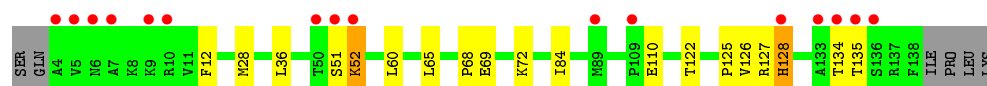


- Molecule 65: 40S ribosomal protein S15

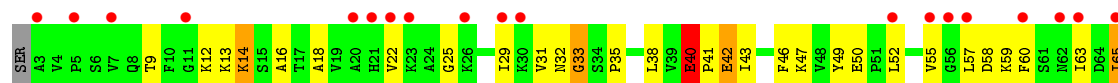


- Molecule 65: 40S ribosomal protein S15

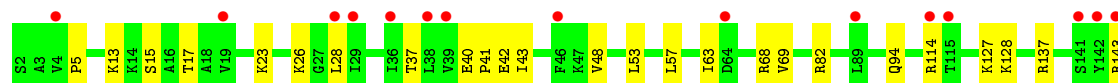
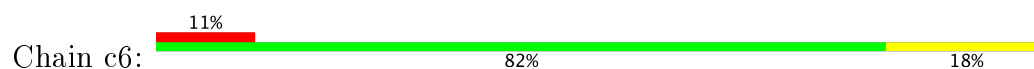




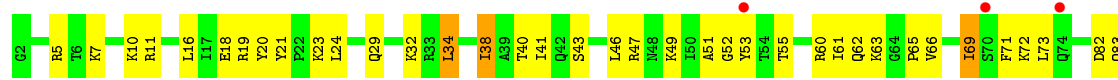
- Molecule 66: 40S ribosomal protein S16-A



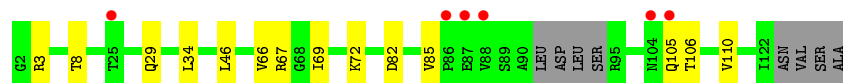
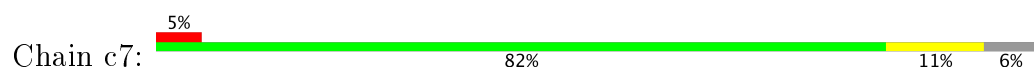
- Molecule 66: 40S ribosomal protein S16-A



- Molecule 67: 40S ribosomal protein S17-A



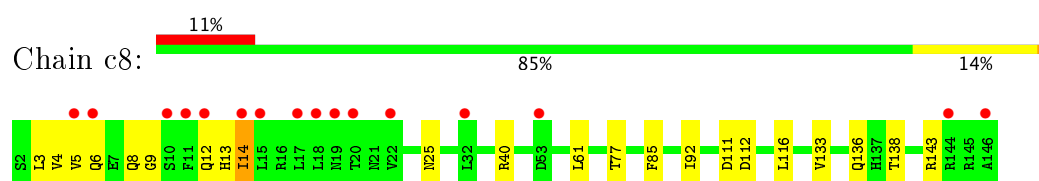
- Molecule 67: 40S ribosomal protein S17-A



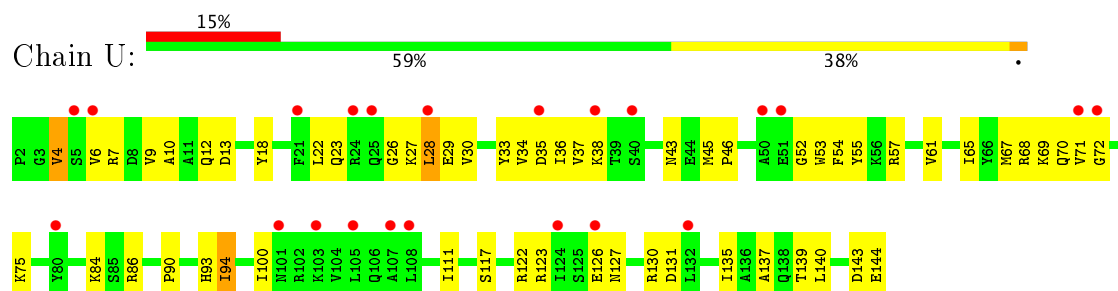
- Molecule 68: 40S ribosomal protein S18-A



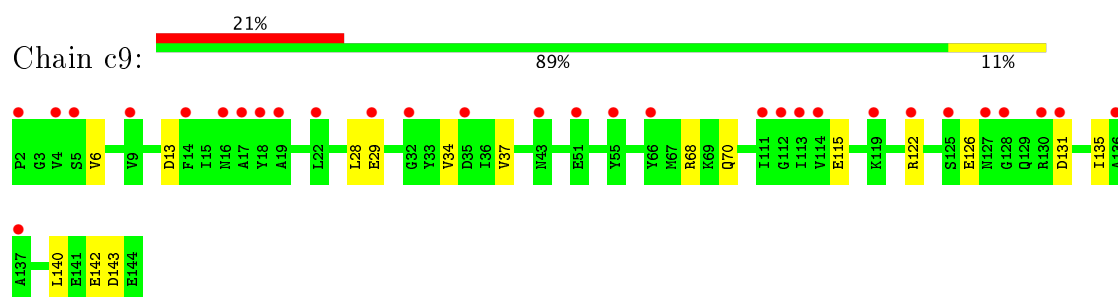
- Molecule 68: 40S ribosomal protein S18-A



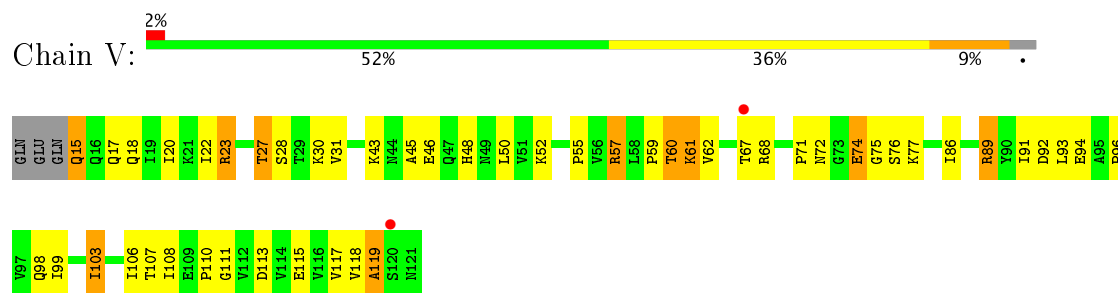
- Molecule 69: 40S ribosomal protein S19-A



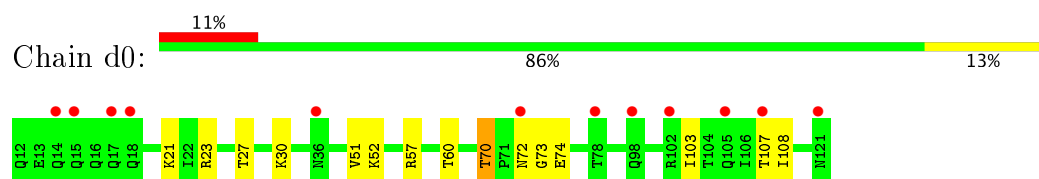
- Molecule 69: 40S ribosomal protein S19-A



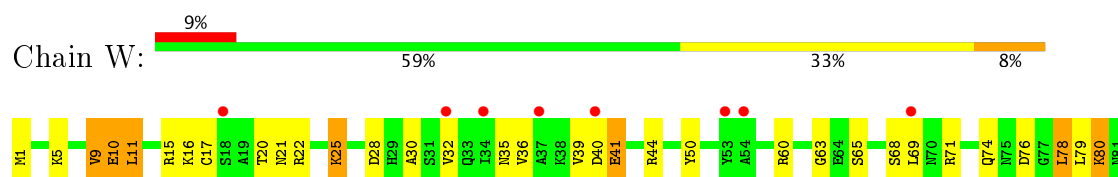
- Molecule 70: 40S ribosomal protein S20



- Molecule 70: 40S ribosomal protein S20

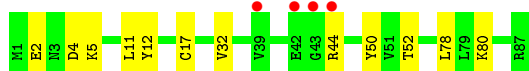
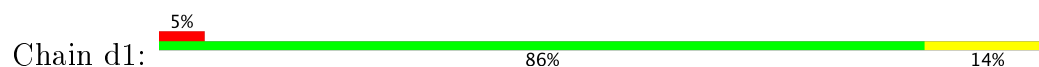


- Molecule 71: 40S ribosomal protein S21-A





- Molecule 71: 40S ribosomal protein S21-A



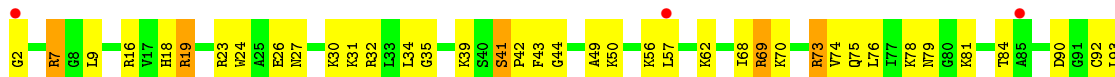
- Molecule 72: 40S ribosomal protein S22-A



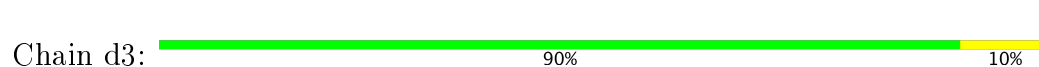
- Molecule 72: 40S ribosomal protein S22-A



- Molecule 73: 40S ribosomal protein S23-A

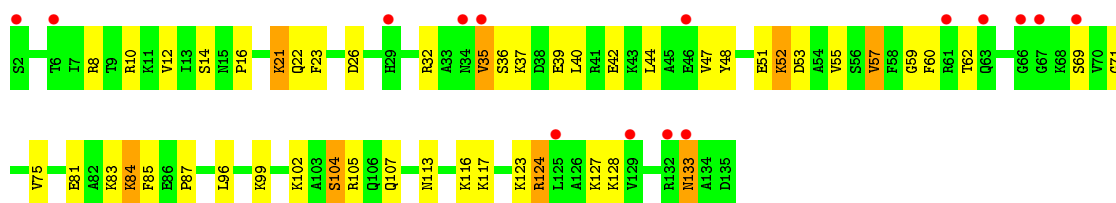


- Molecule 73: 40S ribosomal protein S23-A



- Molecule 74: 40S ribosomal protein S24-A

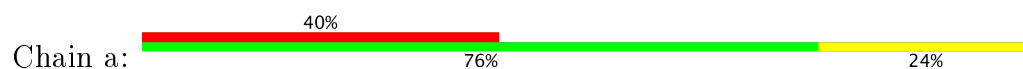




- Molecule 74: 40S ribosomal protein S24-A



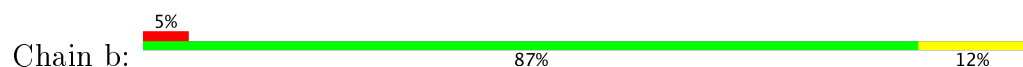
- Molecule 75: 40S ribosomal protein S25-A



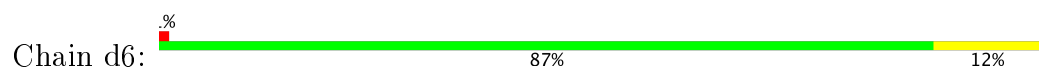
- Molecule 75: 40S ribosomal protein S25-A



- Molecule 76: 40S ribosomal protein S26-B



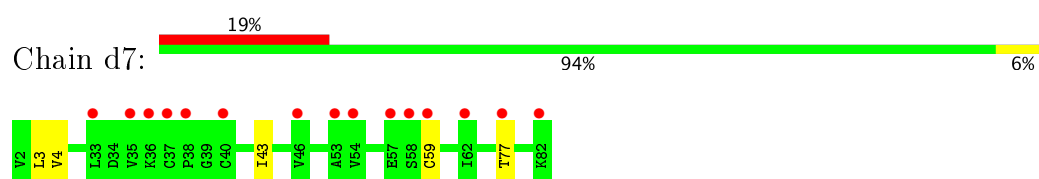
- Molecule 76: 40S ribosomal protein S26-B



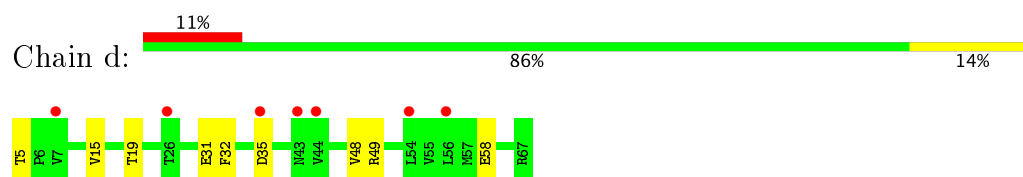
- Molecule 77: 40S ribosomal protein S27-A



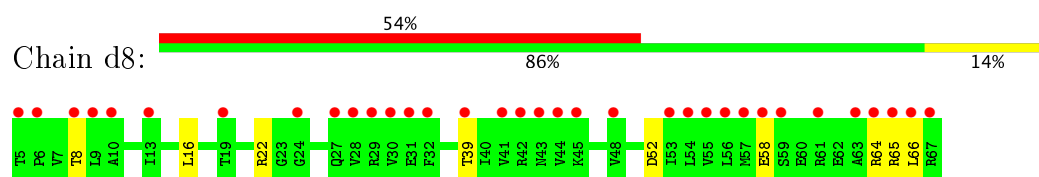
- Molecule 77: 40S ribosomal protein S27-A



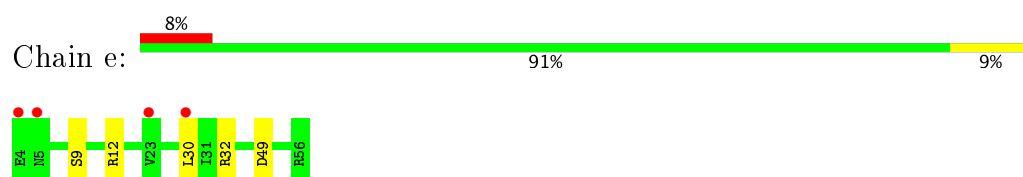
- Molecule 78: 40S ribosomal protein S28-A



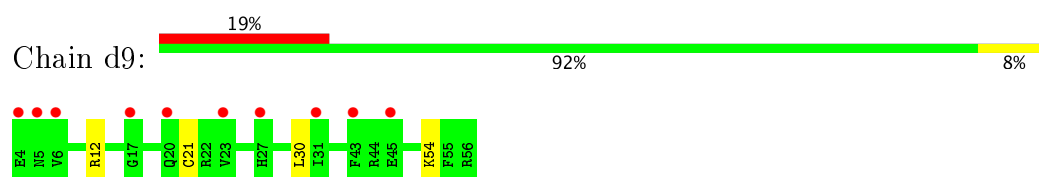
- Molecule 78: 40S ribosomal protein S28-A



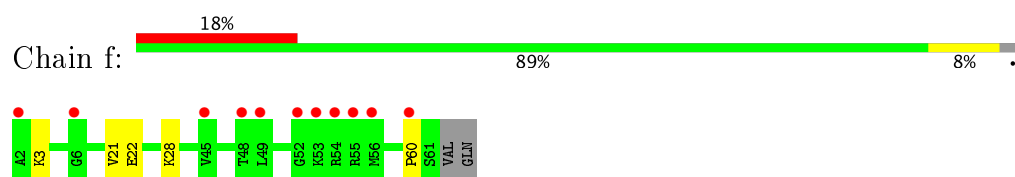
- Molecule 79: 40S ribosomal protein S29-A



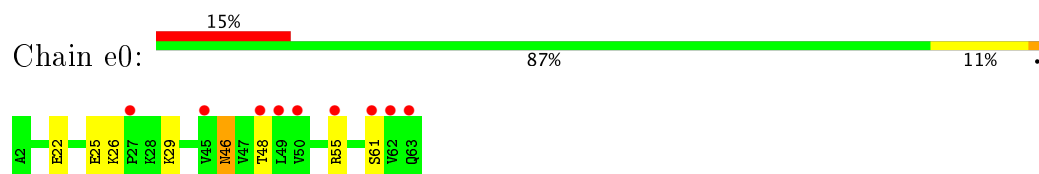
- Molecule 79: 40S ribosomal protein S29-A



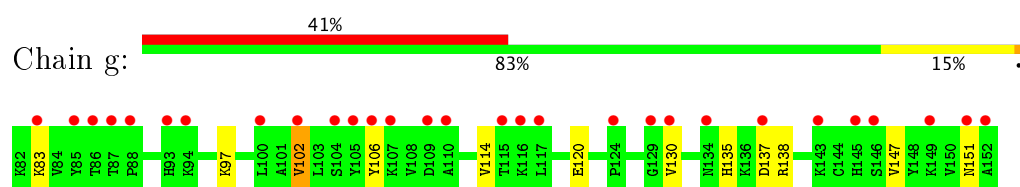
- Molecule 80: 40S ribosomal protein S30-A



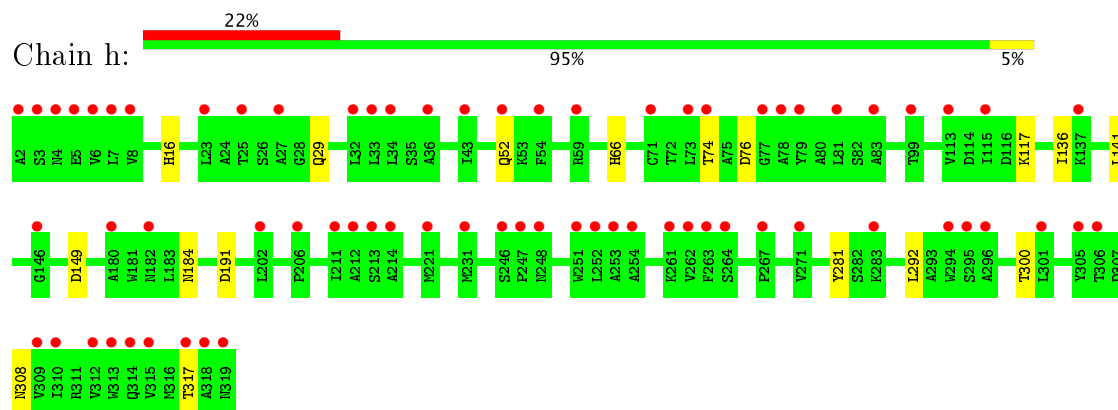
- Molecule 80: 40S ribosomal protein S30-A



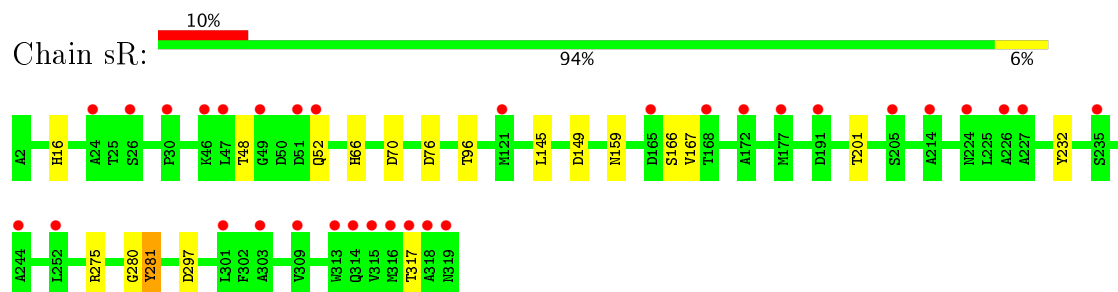
- Molecule 81: Ubiquitin-40S ribosomal protein S31



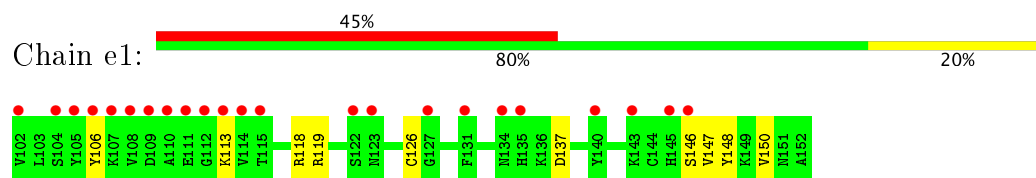
- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 83: Ubiquitin-40S ribosomal protein S31



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	303.13Å 286.50Å 435.66Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	99.84 – 3.10 99.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (99.84-3.10) 99.5 (99.94-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.13Å)	Xtriage
Refinement program	PHENIX dev_2450	Depositor
R, R_{free}	0.222 , 0.252 0.228 , 0.257	Depositor DCC
R_{free} test set	26196 reflections (2.03%)	DCC
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	410383	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: GOL, ZN, OHX, MG, HN8

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	1	0.60	1/75394 (0.0%)	1.02	117/117545 (0.1%)
1	AR	0.61	0/75394	1.03	127/117545 (0.1%)
2	3	0.51	0/2883	0.88	0/4491
2	AS	0.57	0/2883	0.97	1/4491 (0.0%)
3	4	0.57	0/3746	0.97	0/5832
3	AT	0.50	0/3746	0.90	2/5832 (0.0%)
4	CD	0.36	0/1948	0.55	0/2617
4	j	0.39	0/1948	0.60	0/2617
5	CE	0.44	1/3146 (0.0%)	0.61	0/4228
5	k	0.39	0/3146	0.58	0/4228
6	CF	0.40	1/2800 (0.0%)	0.62	2/3790 (0.1%)
6	l	0.41	0/2800	0.62	2/3790 (0.1%)
7	CG	0.40	0/2425	0.55	0/3271
7	m	0.34	0/2425	0.53	0/3271
8	CH	0.41	0/1260	0.56	0/1694
8	n	0.39	0/1260	0.53	0/1694
9	CI	0.44	0/1821	0.61	1/2451 (0.0%)
9	o	0.43	0/1821	0.60	1/2451 (0.0%)
10	CJ	0.32	0/1836	0.48	0/2481
10	p	0.32	0/1836	0.49	0/2481
11	CK	0.40	0/1539	0.57	0/2073
11	q	0.39	0/1539	0.56	0/2073
12	CL	0.42	0/1741	0.57	1/2335 (0.0%)
12	r	0.42	0/1741	0.57	1/2335 (0.0%)
13	CM	0.41	1/1374 (0.1%)	0.60	1/1842 (0.1%)
13	s	0.33	0/1374	0.56	0/1842
14	CN	0.39	1/1568 (0.1%)	0.58	1/2106 (0.0%)
14	t	0.42	1/1568 (0.1%)	0.57	0/2106
15	CO	0.40	0/1068	0.59	1/1438 (0.1%)
15	u	0.40	0/1068	0.55	0/1438
16	CP	0.35	0/1757	0.53	0/2354
16	v	0.39	0/1757	0.58	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CQ	0.51	0/1585	0.61	2/2128 (0.1%)
17	w	0.46	0/1585	0.59	0/2128
18	CR	0.45	0/1443	0.61	0/1944
18	x	0.42	0/1443	0.61	1/1944 (0.1%)
19	CS	0.41	0/1465	0.58	0/1965
19	y	0.40	0/1465	0.60	1/1965 (0.1%)
20	CT	0.34	0/1538	0.49	0/2050
20	z	0.32	0/1538	0.47	0/2050
21	0	0.40	0/1481	0.58	0/1990
21	CU	0.44	0/1481	0.59	0/1990
22	2	0.40	0/1300	0.57	0/1743
22	CV	0.46	0/1300	0.58	0/1743
23	5	0.30	0/812	0.47	0/1099
23	CW	0.35	0/812	0.51	0/1099
24	CX	0.46	0/1018	0.59	0/1369
24	lR	0.41	0/1018	0.58	0/1369
25	6	0.43	0/42490	0.88	37/66207 (0.1%)
25	A	0.39	0/42443	0.87	34/66134 (0.1%)
26	7	0.35	0/712	0.50	0/958
26	CY	0.38	0/712	0.54	0/958
27	8	0.35	0/979	0.55	0/1321
27	CZ	0.35	0/979	0.52	0/1321
28	9	0.37	0/1004	0.58	0/1341
28	DA	0.38	0/1004	0.55	0/1341
29	AA	0.36	0/1118	0.50	0/1497
29	DB	0.47	1/1118 (0.1%)	0.48	0/1497
30	AB	0.43	0/1204	0.64	0/1612
30	DC	0.39	0/1204	0.62	0/1612
31	AC	0.34	0/473	0.54	0/629
31	DD	0.39	0/473	0.57	0/629
32	AD	0.30	0/751	0.48	0/1008
32	DE	0.30	0/751	0.47	0/1008
33	AE	0.39	0/890	0.54	0/1196
33	DF	0.37	0/890	0.55	0/1196
34	AF	0.42	0/1041	0.59	0/1394
34	DG	0.42	0/1041	0.57	0/1394
35	AG	0.47	0/868	0.57	0/1168
35	DH	0.46	0/868	0.62	0/1168
36	AH	0.36	0/890	0.57	1/1189 (0.1%)
36	DI	0.35	0/890	0.54	0/1189
37	AI	0.37	0/978	0.53	0/1301
37	DJ	0.35	0/978	0.52	1/1301 (0.1%)
38	AJ	0.33	0/778	0.52	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DK	0.32	0/778	0.51	0/1034
39	AK	0.39	0/696	0.60	0/923
39	DL	0.39	0/696	0.58	0/923
40	AL	0.34	0/618	0.50	0/826
40	DM	0.32	0/618	0.49	0/826
41	AM	0.40	0/443	0.59	0/588
41	DN	0.36	0/443	0.59	0/588
42	AN	0.44	0/423	0.56	0/562
42	DO	0.43	0/423	0.60	0/562
43	AO	0.36	0/234	0.62	0/300
43	DP	0.39	0/234	0.51	0/300
44	AP	0.41	0/860	0.59	0/1136
44	DQ	0.41	0/860	0.59	0/1136
45	AQ	0.40	0/701	0.56	0/934
45	DR	0.39	0/701	0.58	0/934
46	i	0.31	0/1113	0.54	1/1502 (0.1%)
48	sM	0.34	0/480	0.58	0/642
49	p0	0.30	0/1091	0.53	2/1472 (0.1%)
50	B	0.29	0/1617	0.51	0/2215
50	s0	0.36	1/1623 (0.1%)	0.49	0/2222
51	C	0.27	0/1735	0.54	0/2335
51	s1	0.30	0/1748	0.55	1/2352 (0.0%)
52	D	0.30	0/1665	0.50	0/2263
52	s2	0.31	0/1665	0.52	0/2263
53	E	0.30	0/1759	0.51	0/2368
53	s3	0.28	0/1759	0.50	0/2368
54	F	0.31	0/2109	0.53	0/2839
54	s4	0.36	1/2109 (0.0%)	0.52	0/2839
55	G	0.27	0/1629	0.50	0/2202
55	s5	0.29	0/1629	0.47	0/2202
56	H	0.32	0/1823	0.51	1/2439 (0.0%)
56	s6	0.32	0/1779	0.53	0/2379
57	I	0.30	0/1506	0.52	0/2028
57	s7	0.30	0/1516	0.51	0/2043
58	J	0.31	0/1514	0.57	1/2021 (0.0%)
58	s8	0.33	0/1514	0.53	0/2021
59	K	0.29	0/1519	0.49	0/2035
59	s9	0.30	0/1519	0.49	0/2035
60	L	0.29	0/789	0.57	1/1067 (0.1%)
60	c0	0.27	0/775	0.62	3/1045 (0.3%)
61	M	0.33	0/1239	0.52	0/1673
61	c1	0.34	0/1194	0.52	0/1610
62	N	0.30	0/898	0.62	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
62	c2	0.35	1/898 (0.1%)	0.62	1/1220 (0.1%)
63	O	0.31	0/1215	0.49	0/1638
63	c3	0.32	0/1215	0.53	0/1638
64	P	0.28	0/901	0.54	0/1217
64	c4	0.32	0/960	0.55	0/1290
65	Q	0.31	0/998	0.49	0/1341
65	c5	0.29	0/1060	0.60	0/1426
66	R	0.29	0/1125	0.55	0/1510
66	c6	0.29	0/1131	0.54	0/1518
67	S	0.29	0/935	0.52	0/1254
67	c7	0.28	0/914	0.48	0/1224
68	T	0.29	0/1211	0.50	0/1628
68	c8	0.29	0/1211	0.50	0/1628
69	U	0.29	0/1130	0.46	0/1517
69	c9	0.29	0/1130	0.46	0/1517
70	V	0.27	0/865	0.51	0/1169
70	d0	0.29	0/892	0.52	0/1205
71	W	0.31	0/693	0.50	0/935
71	d1	0.30	0/693	0.51	0/935
72	X	0.30	0/1038	0.55	0/1395
72	d2	0.31	0/1038	0.52	0/1395
73	Y	0.33	0/1139	0.55	0/1518
73	d3	0.35	0/1139	0.54	0/1518
74	Z	0.31	0/1087	0.49	0/1449
74	d4	0.32	0/1087	0.54	0/1449
75	a	0.29	0/571	0.53	0/768
75	d5	0.27	0/566	0.46	0/761
76	b	0.34	0/782	0.61	0/1047
76	d6	0.33	0/782	0.60	0/1047
77	c	0.27	0/620	0.54	0/838
77	d7	0.28	0/620	0.54	0/838
78	d	0.43	1/499 (0.2%)	0.53	0/670
78	d8	0.28	0/499	0.62	0/670
79	d9	0.33	0/452	0.51	0/600
79	e	0.30	0/452	0.50	0/600
80	e0	0.32	0/499	0.49	0/665
80	f	0.29	0/483	0.48	0/643
81	g	0.29	0/577	0.58	0/770
82	h	0.26	0/2494	0.49	0/3393
82	sR	0.27	0/2495	0.50	0/3395
83	e1	0.27	0/404	0.56	0/542
All	All	0.47	11/429967 (0.0%)	0.83	346/631328 (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
5	CE	0	3
5	k	0	2
6	l	0	2
7	CG	0	3
7	m	0	1
9	CI	0	2
9	o	0	2
10	CJ	0	2
10	p	0	1
11	CK	0	1
11	q	0	1
12	CL	0	1
13	CM	0	2
13	s	0	2
14	CN	0	1
14	t	0	2
15	CO	0	1
15	u	0	1
16	CP	0	1
17	CQ	0	1
17	w	0	1
18	x	0	1
19	CS	0	1
21	CU	0	2
26	CY	0	1
29	AA	0	2
30	DC	0	2
31	AC	0	1
31	DD	0	1
37	AI	0	1
37	DJ	0	1
50	B	0	1
51	s1	0	1
53	E	0	2
53	s3	0	2
55	G	0	3
55	s5	0	1
56	H	0	2
57	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
57	s7	0	2
58	J	0	2
58	s8	0	2
59	K	0	1
60	c0	0	1
61	M	0	1
62	N	0	1
62	c2	0	2
63	c3	0	2
64	P	0	1
64	c4	0	2
65	Q	0	1
65	c5	0	2
66	R	0	2
66	c6	0	4
67	S	0	1
67	c7	0	2
68	T	0	3
68	c8	0	1
70	d0	0	1
74	d4	0	1
75	a	0	2
76	b	0	2
80	e0	0	1
81	g	0	1
82	sR	0	1
83	e1	0	1
All	All	0	103

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	DB	36	HIS	C-N	11.46	1.56	1.34
54	s4	82	TYR	C-N	-8.48	1.18	1.34
14	t	132	ALA	C-N	8.06	1.49	1.34
50	s0	160	ILE	C-N	-7.98	1.19	1.34
78	d	5	THR	C-N	7.62	1.48	1.34

The worst 5 of 346 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3278	C	N1-C2-O2	10.14	124.98	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	1	2373	A	O5'-P-OP1	-9.82	96.86	105.70
1	1	1308	A	C8-N9-C4	-8.98	102.21	105.80
1	AR	2846	U	N3-C2-O2	-8.79	116.05	122.20
1	AR	2714	G	N3-C4-C5	8.71	132.95	128.60

There are no chirality outliers.

5 of 103 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	k	186	GLY	Peptide
5	k	349	LYS	Peptide
6	l	291	ASN	Peptide
6	l	338	LYS	Peptide
7	m	258	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	67355	0	33847	658	0
1	AR	67355	0	33845	844	0
2	3	2579	0	1304	20	0
2	AS	2579	0	1304	42	0
3	4	3353	0	1695	38	0
3	AT	3353	0	1695	45	0
4	CD	1914	0	1981	45	0
4	j	1914	0	1981	0	0
5	CE	3075	0	3141	105	0
5	k	3075	0	3142	0	0
6	CF	2748	0	2859	80	0
6	l	2748	0	2859	0	0
7	CG	2375	0	2325	73	0
7	m	2375	0	2325	0	0
8	CH	1239	0	1326	27	0
8	n	1239	0	1326	0	0
9	CI	1784	0	1862	45	0
9	o	1784	0	1862	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	CJ	1804	0	1877	45	0
10	p	1804	0	1877	0	0
11	CK	1518	0	1587	55	0
11	q	1518	0	1587	0	0
12	CL	1705	0	1736	54	0
12	r	1705	0	1736	0	0
13	CM	1353	0	1383	36	0
13	s	1353	0	1383	0	0
14	CN	1543	0	1608	57	0
14	t	1543	0	1608	0	0
15	CO	1053	0	1149	39	0
15	u	1053	0	1149	0	0
16	CP	1720	0	1779	41	0
16	v	1720	0	1779	0	0
17	CQ	1555	0	1659	49	0
17	w	1555	0	1659	0	0
18	CR	1420	0	1437	51	0
18	x	1420	0	1437	0	0
19	CS	1441	0	1543	38	0
19	y	1441	0	1543	0	0
20	CT	1521	0	1617	36	0
20	z	1521	0	1617	0	0
21	0	1445	0	1487	36	0
21	CU	1445	0	1487	37	0
22	2	1276	0	1323	32	0
22	CV	1276	0	1323	47	0
23	5	796	0	812	14	0
23	CW	796	0	812	17	0
24	CX	1003	0	1048	27	0
24	lR	1003	0	1048	0	0
25	6	37990	0	19115	356	0
25	A	37948	0	19094	563	0
26	7	699	0	640	10	0
26	CY	699	0	640	13	0
27	8	964	0	1025	23	0
27	CZ	964	0	1025	26	0
28	9	993	0	1081	25	0
28	DA	993	0	1081	30	0
29	AA	1092	0	1155	36	0
29	DB	1092	0	1155	35	0
30	AB	1173	0	1215	42	0
30	DC	1173	0	1215	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	AC	462	0	491	16	0
31	DD	462	0	491	13	0
32	AD	743	0	797	20	0
32	DE	743	0	797	15	0
33	AE	876	0	912	23	0
33	DF	876	0	912	23	0
34	AF	1020	0	1090	23	0
34	DG	1020	0	1090	24	0
35	AG	850	0	880	18	0
35	DH	850	0	880	23	0
36	AH	880	0	945	26	0
36	DI	880	0	945	26	0
37	AI	969	0	1078	23	0
37	DJ	969	0	1078	37	0
38	AJ	771	0	849	27	0
38	DK	771	0	849	13	0
39	AK	681	0	683	22	0
39	DL	681	0	683	27	0
40	AL	612	0	682	16	0
40	DM	612	0	682	14	0
41	AM	436	0	475	18	0
41	DN	436	0	475	14	0
42	AN	417	0	455	11	0
42	DO	417	0	455	8	0
43	AO	233	0	284	9	0
43	DP	233	0	284	11	0
44	AP	847	0	914	14	0
44	DQ	847	0	915	16	0
45	AQ	694	0	734	21	0
45	DR	694	0	734	19	0
46	i	1104	0	1002	0	0
47	m2	750	0	172	0	0
48	sM	680	0	540	0	0
49	p0	1076	0	1076	0	0
50	B	1577	0	1567	58	0
50	s0	1583	0	1578	0	0
51	C	1709	0	1784	64	0
51	s1	1722	0	1793	0	0
52	D	1635	0	1723	62	0
52	s2	1635	0	1723	0	0
53	E	1734	0	1817	46	0
53	s3	1734	0	1817	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	F	2068	0	2154	69	0
54	s4	2068	0	2154	0	0
55	G	1609	0	1675	55	0
55	s5	1609	0	1675	0	0
56	H	1799	0	1878	56	0
56	s6	1755	0	1846	0	0
57	I	1481	0	1572	63	0
57	s7	1491	0	1578	0	0
58	J	1489	0	1525	48	0
58	s8	1489	0	1525	0	0
59	K	1494	0	1573	49	0
59	s9	1494	0	1573	0	0
60	L	772	0	727	27	0
60	c0	760	0	696	0	0
61	M	1213	0	1257	33	0
61	c1	1168	0	1233	0	0
62	N	890	0	887	25	0
62	c2	890	0	887	0	0
63	O	1192	0	1255	26	0
63	c3	1192	0	1255	0	0
64	P	891	0	883	33	0
64	c4	949	0	985	0	0
65	Q	977	0	1002	27	0
65	c5	1039	0	1050	0	0
66	R	1105	0	1166	40	0
66	c6	1111	0	1171	0	0
67	S	926	0	930	34	0
67	c7	906	0	909	0	0
68	T	1192	0	1222	30	0
68	c8	1192	0	1222	0	0
69	U	1112	0	1124	32	0
69	c9	1112	0	1124	0	0
70	V	855	0	917	40	0
70	d0	882	0	939	0	0
71	W	684	0	672	21	0
71	d1	684	0	672	0	0
72	X	1021	0	1060	36	0
72	d2	1021	0	1060	0	0
73	Y	1121	0	1196	37	0
73	d3	1121	0	1196	0	0
74	Z	1073	0	1132	39	0
74	d4	1073	0	1132	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	a	563	0	603	0	0
75	d5	558	0	598	0	0
76	b	769	0	814	0	0
76	d6	769	0	814	0	0
77	c	610	0	633	0	0
77	d7	610	0	633	0	0
78	d	497	0	535	0	0
78	d8	497	0	535	0	0
79	d9	442	0	429	0	0
79	e	442	0	428	0	0
80	e0	491	0	542	0	0
80	f	475	0	525	0	0
81	g	566	0	602	0	0
82	h	2441	0	2397	0	0
82	sR	2442	0	2392	0	0
83	e1	397	0	396	0	0
84	1	2262	0	0	17	0
84	2	7	0	0	0	0
84	3	63	0	0	0	0
84	4	112	0	0	0	0
84	6	1064	0	0	10	0
84	A	1001	0	0	10	0
84	AC	7	0	0	0	0
84	AG	7	0	0	0	0
84	AH	7	0	0	0	0
84	AK	7	0	0	0	0
84	AM	7	0	0	0	0
84	AP	7	0	0	0	0
84	AR	2415	0	0	36	0
84	AS	77	0	0	5	0
84	AT	119	0	0	2	0
84	CE	14	0	0	0	0
84	CF	14	0	0	0	0
84	CG	14	0	0	1	0
84	CK	7	0	0	0	0
84	CL	7	0	0	0	0
84	CM	7	0	0	0	0
84	CP	7	0	0	0	0
84	CV	7	0	0	0	0
84	CX	14	0	0	1	0
84	DD	7	0	0	0	0
84	DH	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	DQ	7	0	0	0	0
84	J	7	0	0	0	0
84	K	7	0	0	0	0
84	M	7	0	0	0	0
84	O	7	0	0	0	0
84	Q	7	0	0	0	0
84	T	7	0	0	0	0
84	c1	7	0	0	0	0
84	c3	7	0	0	0	0
84	c4	7	0	0	0	0
84	c5	7	0	0	0	0
84	c8	7	0	0	0	0
84	d9	7	0	0	0	0
84	e	7	0	0	0	0
84	h	7	0	0	0	0
84	k	7	0	0	0	0
84	l	7	0	0	0	0
84	r	7	0	0	0	0
84	s8	7	0	0	0	0
84	sR	7	0	0	0	0
84	v	7	0	0	0	0
84	x	14	0	0	0	0
84	y	7	0	0	0	0
84	z	7	0	0	0	0
85	1	498	0	0	0	0
85	3	13	0	0	0	0
85	4	25	0	0	0	0
85	6	146	0	0	0	0
85	A	116	0	0	0	0
85	AB	7	0	0	0	0
85	AF	2	0	0	0	0
85	AG	1	0	0	0	0
85	AH	1	0	0	0	0
85	AK	1	0	0	0	0
85	AP	1	0	0	0	0
85	AR	515	0	0	0	0
85	AS	20	0	0	0	0
85	AT	14	0	0	0	0
85	CD	2	0	0	0	0
85	CE	5	0	0	0	0
85	CF	1	0	0	0	0
85	CG	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	CI	1	0	0	0	0
85	CJ	1	0	0	0	0
85	CK	1	0	0	0	0
85	CL	1	0	0	0	0
85	CM	2	0	0	0	0
85	CO	1	0	0	0	0
85	CP	4	0	0	0	0
85	CQ	4	0	0	0	0
85	CR	5	0	0	0	0
85	CU	1	0	0	0	0
85	CX	2	0	0	0	0
85	D	1	0	0	0	0
85	DA	2	0	0	0	0
85	DC	4	0	0	0	0
85	DE	1	0	0	0	0
85	DH	2	0	0	0	0
85	DI	2	0	0	0	0
85	DL	1	0	0	0	0
85	DO	1	0	0	0	0
85	DQ	2	0	0	0	0
85	F	1	0	0	0	0
85	H	1	0	0	0	0
85	T	1	0	0	0	0
85	U	1	0	0	0	0
85	V	1	0	0	0	0
85	Y	1	0	0	0	0
85	b	1	0	0	0	0
85	c1	1	0	0	0	0
85	c6	1	0	0	0	0
85	c8	1	0	0	0	0
85	c9	1	0	0	0	0
85	d3	2	0	0	0	0
85	d4	1	0	0	0	0
85	d5	1	0	0	0	0
85	d6	2	0	0	0	0
85	j	2	0	0	0	0
85	k	3	0	0	0	0
85	l	3	0	0	0	0
85	lR	1	0	0	0	0
85	n	1	0	0	0	0
85	o	2	0	0	0	0
85	r	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	s	1	0	0	0	0
85	s4	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	1	0	0	0	0
85	sM	2	0	0	0	0
85	t	3	0	0	0	0
85	v	3	0	0	0	0
85	w	2	0	0	0	0
85	x	7	0	0	0	0
85	z	1	0	0	0	0
86	1	22	0	0	0	0
86	AR	22	0	0	0	0
87	6	6	0	8	0	0
87	A	6	0	8	0	0
87	AR	12	0	14	3	0
87	v	6	0	8	0	0
88	AK	1	0	0	0	0
88	AN	1	0	0	0	0
88	AP	1	0	0	0	0
88	AQ	1	0	0	0	0
88	DL	1	0	0	0	0
88	DO	1	0	0	0	0
88	DQ	1	0	0	0	0
88	DR	1	0	0	0	0
88	b	1	0	0	0	0
88	c	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	e	1	0	0	0	0
88	e1	1	0	0	0	0
88	g	1	0	0	0	0
All	All	410383	0	296944	4796	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 10.

The worst 5 of 4796 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)
1:1:1481:A:O2'	1:1:1858:A:N3	1.96	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:Q:68:PRO:HG2	65:Q:71:GLU:HB3	1.51	0.93
5:CE:296:THR:HG22	5:CE:298:PHE:H	1.35	0.91
1:AR:2108:C:H1'	1:AR:3344:A:H8	1.37	0.90
1:1:1230:G:H1	1:1:1279:C:H42	1.19	0.90

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	
4	CD	250/252 (99%)	226 (90%)	23 (9%)	1 (0%)	38	75
4	j	250/252 (99%)	230 (92%)	19 (8%)	1 (0%)	38	75
5	CE	384/386 (100%)	349 (91%)	31 (8%)	4 (1%)	18	57
5	k	384/386 (100%)	348 (91%)	33 (9%)	3 (1%)	22	62
6	CF	359/361 (99%)	326 (91%)	33 (9%)	0	100	100
6	l	359/361 (99%)	320 (89%)	37 (10%)	2 (1%)	28	67
7	CG	294/296 (99%)	254 (86%)	38 (13%)	2 (1%)	25	64
7	m	294/296 (99%)	263 (90%)	30 (10%)	1 (0%)	44	79
8	CH	152/175 (87%)	139 (91%)	12 (8%)	1 (1%)	25	64
8	n	152/175 (87%)	145 (95%)	6 (4%)	1 (1%)	25	64
9	CI	220/222 (99%)	199 (90%)	16 (7%)	5 (2%)	7	33
9	o	220/222 (99%)	204 (93%)	13 (6%)	3 (1%)	13	47
10	CJ	231/233 (99%)	201 (87%)	28 (12%)	2 (1%)	20	60
10	p	231/233 (99%)	207 (90%)	24 (10%)	0	100	100
11	CK	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
11	q	189/191 (99%)	168 (89%)	21 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	CL	207/220 (94%)	188 (91%)	19 (9%)	0	100	100
12	r	207/220 (94%)	189 (91%)	17 (8%)	1 (0%)	32	71
13	CM	167/169 (99%)	145 (87%)	19 (11%)	3 (2%)	10	40
13	s	167/169 (99%)	137 (82%)	23 (14%)	7 (4%)	3	19
14	CN	191/193 (99%)	168 (88%)	17 (9%)	6 (3%)	5	26
14	t	191/193 (99%)	171 (90%)	13 (7%)	7 (4%)	4	22
15	CO	134/136 (98%)	122 (91%)	11 (8%)	1 (1%)	25	64
15	u	134/136 (98%)	120 (90%)	13 (10%)	1 (1%)	25	64
16	CP	201/203 (99%)	188 (94%)	13 (6%)	0	100	100
16	v	201/203 (99%)	177 (88%)	23 (11%)	1 (0%)	32	71
17	CQ	195/197 (99%)	185 (95%)	8 (4%)	2 (1%)	18	57
17	w	195/197 (99%)	187 (96%)	6 (3%)	2 (1%)	18	57
18	CR	181/183 (99%)	161 (89%)	17 (9%)	3 (2%)	11	42
18	x	181/183 (99%)	164 (91%)	17 (9%)	0	100	100
19	CS	183/185 (99%)	166 (91%)	16 (9%)	1 (0%)	32	71
19	y	183/185 (99%)	167 (91%)	16 (9%)	0	100	100
20	CT	186/188 (99%)	171 (92%)	15 (8%)	0	100	100
20	z	186/188 (99%)	175 (94%)	11 (6%)	0	100	100
21	0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	28	67
21	CU	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
22	2	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	14	48
22	CV	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	28	67
23	5	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
23	CW	98/100 (98%)	81 (83%)	16 (16%)	1 (1%)	18	57
24	CX	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
24	IR	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
26	7	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
26	CY	96/98 (98%)	79 (82%)	15 (16%)	2 (2%)	8	36
27	8	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
27	CZ	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
28	9	124/126 (98%)	113 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	DA	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
29	AA	133/135 (98%)	115 (86%)	15 (11%)	3 (2%)	7	33
29	DB	133/135 (98%)	119 (90%)	10 (8%)	4 (3%)	5	27
30	AB	146/148 (99%)	125 (86%)	19 (13%)	2 (1%)	13	47
30	DC	146/148 (99%)	123 (84%)	21 (14%)	2 (1%)	13	47
31	AC	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
31	DD	56/58 (97%)	50 (89%)	5 (9%)	1 (2%)	10	40
32	AD	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
32	DE	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
33	AE	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	20	60
33	DF	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	20	60
34	AF	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
34	DG	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
35	AG	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
35	DH	104/106 (98%)	99 (95%)	4 (4%)	1 (1%)	18	57
36	AH	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
36	DI	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
37	AI	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	20	60
37	DJ	117/119 (98%)	109 (93%)	7 (6%)	1 (1%)	20	60
38	AJ	97/99 (98%)	83 (86%)	11 (11%)	3 (3%)	5	26
38	DK	97/99 (98%)	84 (87%)	13 (13%)	0	100	100
39	AK	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
39	DL	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
40	AL	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
40	DM	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
41	AM	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
41	DN	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
42	AN	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
42	DO	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
43	AO	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
43	DP	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	AP	103/105 (98%)	84 (82%)	19 (18%)	0	100	100
44	DQ	103/105 (98%)	88 (85%)	15 (15%)	0	100	100
45	AQ	89/91 (98%)	79 (89%)	10 (11%)	0	100	100
45	DR	89/91 (98%)	82 (92%)	7 (8%)	0	100	100
46	i	155/272 (57%)	121 (78%)	30 (19%)	4 (3%)	6	31
48	sM	61/104 (59%)	45 (74%)	14 (23%)	2 (3%)	4	25
49	p0	139/311 (45%)	131 (94%)	8 (6%)	0	100	100
50	B	204/206 (99%)	157 (77%)	40 (20%)	7 (3%)	4	24
50	s0	204/206 (99%)	172 (84%)	30 (15%)	2 (1%)	18	57
51	C	212/216 (98%)	167 (79%)	43 (20%)	2 (1%)	20	60
51	s1	214/216 (99%)	190 (89%)	23 (11%)	1 (0%)	32	71
52	D	215/217 (99%)	189 (88%)	25 (12%)	1 (0%)	32	71
52	s2	215/217 (99%)	190 (88%)	23 (11%)	2 (1%)	20	60
53	E	221/223 (99%)	200 (90%)	19 (9%)	2 (1%)	20	60
53	s3	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	10	40
54	F	258/260 (99%)	233 (90%)	25 (10%)	0	100	100
54	s4	258/260 (99%)	229 (89%)	28 (11%)	1 (0%)	38	75
55	G	204/206 (99%)	166 (81%)	36 (18%)	2 (1%)	18	57
55	s5	204/206 (99%)	168 (82%)	36 (18%)	0	100	100
56	H	224/226 (99%)	202 (90%)	19 (8%)	3 (1%)	14	48
56	s6	216/226 (96%)	199 (92%)	15 (7%)	2 (1%)	20	60
57	I	182/186 (98%)	154 (85%)	25 (14%)	3 (2%)	11	43
57	s7	184/186 (99%)	158 (86%)	21 (11%)	5 (3%)	6	30
58	J	184/199 (92%)	159 (86%)	21 (11%)	4 (2%)	8	35
58	s8	184/199 (92%)	159 (86%)	23 (12%)	2 (1%)	17	54
59	K	183/185 (99%)	160 (87%)	21 (12%)	2 (1%)	17	54
59	s9	183/185 (99%)	161 (88%)	22 (12%)	0	100	100
60	L	94/105 (90%)	70 (74%)	23 (24%)	1 (1%)	17	54
60	c0	92/105 (88%)	61 (66%)	25 (27%)	6 (6%)	1	9
61	M	153/155 (99%)	137 (90%)	14 (9%)	2 (1%)	14	48
61	c1	144/155 (93%)	128 (89%)	15 (10%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	N	122/124 (98%)	81 (66%)	33 (27%)	8 (7%)	1	9
62	c2	122/124 (98%)	81 (66%)	37 (30%)	4 (3%)	4	25
63	O	148/150 (99%)	137 (93%)	9 (6%)	2 (1%)	13	47
63	c3	148/150 (99%)	128 (86%)	14 (10%)	6 (4%)	3	19
64	P	125/128 (98%)	103 (82%)	21 (17%)	1 (1%)	22	62
64	c4	126/128 (98%)	110 (87%)	16 (13%)	0	100	100
65	Q	122/141 (86%)	100 (82%)	19 (16%)	3 (2%)	6	31
65	c5	133/141 (94%)	99 (74%)	27 (20%)	7 (5%)	2	14
66	R	139/142 (98%)	122 (88%)	16 (12%)	1 (1%)	25	64
66	c6	140/142 (99%)	124 (89%)	15 (11%)	1 (1%)	25	64
67	S	116/125 (93%)	93 (80%)	22 (19%)	1 (1%)	20	60
67	c7	113/125 (90%)	91 (80%)	21 (19%)	1 (1%)	20	60
68	T	143/145 (99%)	126 (88%)	16 (11%)	1 (1%)	25	64
68	c8	143/145 (99%)	121 (85%)	19 (13%)	3 (2%)	8	36
69	U	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
69	c9	141/143 (99%)	130 (92%)	11 (8%)	0	100	100
70	V	105/110 (96%)	89 (85%)	15 (14%)	1 (1%)	18	57
70	d0	108/110 (98%)	92 (85%)	14 (13%)	2 (2%)	9	39
71	W	85/87 (98%)	62 (73%)	22 (26%)	1 (1%)	15	51
71	d1	85/87 (98%)	77 (91%)	7 (8%)	1 (1%)	15	51
72	X	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	22	62
72	d2	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
73	Y	142/144 (99%)	115 (81%)	24 (17%)	3 (2%)	8	36
73	d3	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
74	Z	132/134 (98%)	120 (91%)	10 (8%)	2 (2%)	12	45
74	d4	132/134 (98%)	114 (86%)	16 (12%)	2 (2%)	12	45
75	a	68/70 (97%)	51 (75%)	14 (21%)	3 (4%)	3	18
75	d5	67/70 (96%)	56 (84%)	11 (16%)	0	100	100
76	b	95/97 (98%)	66 (70%)	24 (25%)	5 (5%)	2	14
76	d6	95/97 (98%)	73 (77%)	20 (21%)	2 (2%)	8	36
77	c	79/81 (98%)	65 (82%)	14 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	d7	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
78	d	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
78	d8	61/63 (97%)	47 (77%)	14 (23%)	0	100	100
79	d9	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
79	e	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
80	e0	60/62 (97%)	52 (87%)	8 (13%)	0	100	100
80	f	58/62 (94%)	47 (81%)	10 (17%)	1 (2%)	11	42
81	g	69/71 (97%)	38 (55%)	31 (45%)	0	100	100
82	h	316/318 (99%)	277 (88%)	39 (12%)	0	100	100
82	sR	316/318 (99%)	285 (90%)	30 (10%)	1 (0%)	44	79
83	e1	49/51 (96%)	30 (61%)	18 (37%)	1 (2%)	9	37
All	All	22260/23067 (96%)	19629 (88%)	2417 (11%)	214 (1%)	18	57

5 of 214 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	l	339	LEU
13	s	74	PRO
13	s	95	ASN
13	s	172	LEU
14	t	47	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	193/194 (100%)	169 (88%)	24 (12%)	5	23
4	j	193/194 (100%)	166 (86%)	27 (14%)	4	18
5	CE	319/322 (99%)	272 (85%)	47 (15%)	3	16
5	k	321/322 (100%)	274 (85%)	47 (15%)	3	16
6	CF	288/288 (100%)	256 (89%)	32 (11%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	l	288/288 (100%)	249 (86%)	39 (14%)	4	19
7	CG	244/244 (100%)	207 (85%)	37 (15%)	3	14
7	m	244/244 (100%)	216 (88%)	28 (12%)	6	27
8	CH	134/152 (88%)	116 (87%)	18 (13%)	4	19
8	n	134/152 (88%)	120 (90%)	14 (10%)	8	31
9	CI	186/186 (100%)	167 (90%)	19 (10%)	8	32
9	o	186/186 (100%)	165 (89%)	21 (11%)	7	28
10	CJ	187/191 (98%)	172 (92%)	15 (8%)	14	47
10	p	187/191 (98%)	167 (89%)	20 (11%)	8	30
11	CK	171/171 (100%)	143 (84%)	28 (16%)	2	12
11	q	171/171 (100%)	148 (86%)	23 (14%)	4	19
12	CL	177/186 (95%)	151 (85%)	26 (15%)	3	16
12	r	177/186 (95%)	149 (84%)	28 (16%)	3	13
13	CM	147/147 (100%)	125 (85%)	22 (15%)	3	15
13	s	147/147 (100%)	127 (86%)	20 (14%)	4	19
14	CN	154/154 (100%)	128 (83%)	26 (17%)	2	11
14	t	154/154 (100%)	136 (88%)	18 (12%)	6	26
15	CO	107/107 (100%)	93 (87%)	14 (13%)	5	20
15	u	107/107 (100%)	89 (83%)	18 (17%)	2	11
16	CP	175/175 (100%)	160 (91%)	15 (9%)	12	44
16	v	175/175 (100%)	155 (89%)	20 (11%)	7	27
17	CQ	160/160 (100%)	144 (90%)	16 (10%)	9	33
17	w	160/160 (100%)	139 (87%)	21 (13%)	5	20
18	CR	140/145 (97%)	120 (86%)	20 (14%)	4	17
18	x	140/145 (97%)	118 (84%)	22 (16%)	3	13
19	CS	150/150 (100%)	128 (85%)	22 (15%)	3	16
19	y	150/150 (100%)	130 (87%)	20 (13%)	4	20
20	CT	153/153 (100%)	132 (86%)	21 (14%)	4	19
20	z	153/153 (100%)	140 (92%)	13 (8%)	12	44
21	0	156/156 (100%)	131 (84%)	25 (16%)	3	12
21	CU	156/156 (100%)	133 (85%)	23 (15%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	2	136/136 (100%)	116 (85%)	20 (15%)	3	16
22	CV	136/136 (100%)	112 (82%)	24 (18%)	2	10
23	5	87/87 (100%)	80 (92%)	7 (8%)	14	47
23	CW	87/87 (100%)	77 (88%)	10 (12%)	6	27
24	CX	104/104 (100%)	93 (89%)	11 (11%)	8	30
24	IR	104/104 (100%)	89 (86%)	15 (14%)	4	16
26	7	57/86 (66%)	52 (91%)	5 (9%)	12	42
26	CY	57/86 (66%)	47 (82%)	10 (18%)	2	10
27	8	104/105 (99%)	91 (88%)	13 (12%)	5	22
27	CZ	104/105 (99%)	90 (86%)	14 (14%)	4	19
28	9	109/109 (100%)	95 (87%)	14 (13%)	5	21
28	DA	109/109 (100%)	95 (87%)	14 (13%)	5	21
29	AA	115/115 (100%)	104 (90%)	11 (10%)	10	36
29	DB	115/115 (100%)	104 (90%)	11 (10%)	10	36
30	AB	118/118 (100%)	106 (90%)	12 (10%)	8	32
30	DC	118/118 (100%)	103 (87%)	15 (13%)	5	21
31	AC	46/46 (100%)	40 (87%)	6 (13%)	5	21
31	DD	46/46 (100%)	39 (85%)	7 (15%)	3	14
32	AD	81/81 (100%)	70 (86%)	11 (14%)	4	19
32	DE	81/81 (100%)	76 (94%)	5 (6%)	21	57
33	AE	92/96 (96%)	80 (87%)	12 (13%)	5	21
33	DF	92/96 (96%)	75 (82%)	17 (18%)	2	8
34	AF	109/109 (100%)	94 (86%)	15 (14%)	4	19
34	DG	109/109 (100%)	96 (88%)	13 (12%)	6	25
35	AG	90/90 (100%)	81 (90%)	9 (10%)	9	33
35	DH	90/90 (100%)	83 (92%)	7 (8%)	15	48
36	AH	95/95 (100%)	84 (88%)	11 (12%)	6	26
36	DI	95/95 (100%)	85 (90%)	10 (10%)	8	31
37	AI	104/104 (100%)	92 (88%)	12 (12%)	6	27
37	DJ	104/104 (100%)	86 (83%)	18 (17%)	2	10
38	AJ	81/81 (100%)	69 (85%)	12 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DK	81/81 (100%)	71 (88%)	10 (12%)	5	23
39	AK	70/70 (100%)	63 (90%)	7 (10%)	9	33
39	DL	70/70 (100%)	59 (84%)	11 (16%)	3	13
40	AL	68/68 (100%)	58 (85%)	10 (15%)	3	16
40	DM	68/68 (100%)	61 (90%)	7 (10%)	8	32
41	AM	45/45 (100%)	38 (84%)	7 (16%)	3	13
41	DN	45/45 (100%)	41 (91%)	4 (9%)	11	41
42	AN	47/47 (100%)	39 (83%)	8 (17%)	2	11
42	DO	47/47 (100%)	42 (89%)	5 (11%)	8	30
43	AO	23/23 (100%)	20 (87%)	3 (13%)	5	21
43	DP	23/23 (100%)	19 (83%)	4 (17%)	2	10
44	AP	90/90 (100%)	82 (91%)	8 (9%)	11	41
44	DQ	90/90 (100%)	81 (90%)	9 (10%)	9	33
45	AQ	71/71 (100%)	59 (83%)	12 (17%)	2	11
45	DR	71/71 (100%)	63 (89%)	8 (11%)	7	28
46	i	97/227 (43%)	82 (84%)	15 (16%)	3	14
48	sM	54/54 (100%)	47 (87%)	7 (13%)	5	21
49	p0	105/253 (42%)	91 (87%)	14 (13%)	4	20
50	B	164/173 (95%)	146 (89%)	18 (11%)	7	30
50	s0	165/173 (95%)	140 (85%)	25 (15%)	3	14
51	C	191/192 (100%)	167 (87%)	24 (13%)	5	22
51	s1	192/192 (100%)	164 (85%)	28 (15%)	3	16
52	D	176/176 (100%)	151 (86%)	25 (14%)	4	17
52	s2	176/176 (100%)	144 (82%)	32 (18%)	2	9
53	E	182/182 (100%)	159 (87%)	23 (13%)	5	22
53	s3	182/182 (100%)	164 (90%)	18 (10%)	9	34
54	F	221/221 (100%)	196 (89%)	25 (11%)	7	28
54	s4	221/221 (100%)	200 (90%)	21 (10%)	10	37
55	G	173/173 (100%)	153 (88%)	20 (12%)	6	26
55	s5	173/173 (100%)	155 (90%)	18 (10%)	8	31
56	H	188/193 (97%)	163 (87%)	25 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	s6	187/193 (97%)	163 (87%)	24 (13%)	5	21
57	I	165/166 (99%)	146 (88%)	19 (12%)	6	27
57	s7	165/166 (99%)	145 (88%)	20 (12%)	6	24
58	J	150/160 (94%)	139 (93%)	11 (7%)	16	50
58	s8	150/160 (94%)	140 (93%)	10 (7%)	19	54
59	K	158/158 (100%)	134 (85%)	24 (15%)	3	14
59	s9	158/158 (100%)	129 (82%)	29 (18%)	2	9
60	L	77/98 (79%)	68 (88%)	9 (12%)	6	26
60	c0	73/98 (74%)	65 (89%)	8 (11%)	7	30
61	M	129/136 (95%)	120 (93%)	9 (7%)	18	52
61	c1	129/136 (95%)	113 (88%)	16 (12%)	5	23
62	N	88/100 (88%)	73 (83%)	15 (17%)	2	11
62	c2	88/100 (88%)	73 (83%)	15 (17%)	2	11
63	O	127/127 (100%)	110 (87%)	17 (13%)	4	19
63	c3	127/127 (100%)	111 (87%)	16 (13%)	5	22
64	P	81/97 (84%)	70 (86%)	11 (14%)	4	19
64	c4	97/97 (100%)	85 (88%)	12 (12%)	5	23
65	Q	101/117 (86%)	92 (91%)	9 (9%)	11	41
65	c5	103/117 (88%)	91 (88%)	12 (12%)	6	26
66	R	117/118 (99%)	101 (86%)	16 (14%)	4	19
66	c6	118/118 (100%)	98 (83%)	20 (17%)	2	11
67	S	94/113 (83%)	80 (85%)	14 (15%)	3	15
67	c7	92/113 (81%)	81 (88%)	11 (12%)	6	24
68	T	128/128 (100%)	108 (84%)	20 (16%)	3	13
68	c8	128/128 (100%)	109 (85%)	19 (15%)	3	15
69	U	115/115 (100%)	95 (83%)	20 (17%)	2	10
69	c9	115/115 (100%)	99 (86%)	16 (14%)	4	18
70	V	100/103 (97%)	86 (86%)	14 (14%)	4	18
70	d0	103/103 (100%)	90 (87%)	13 (13%)	5	22
71	W	74/74 (100%)	62 (84%)	12 (16%)	3	12
71	d1	74/74 (100%)	63 (85%)	11 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	X	110/110 (100%)	95 (86%)	15 (14%)	4	19
72	d2	110/110 (100%)	103 (94%)	7 (6%)	20	56
73	Y	119/119 (100%)	102 (86%)	17 (14%)	4	17
73	d3	119/119 (100%)	104 (87%)	15 (13%)	5	22
74	Z	112/112 (100%)	101 (90%)	11 (10%)	9	35
74	d4	112/112 (100%)	105 (94%)	7 (6%)	21	56
75	a	61/61 (100%)	49 (80%)	12 (20%)	1	6
75	d5	61/61 (100%)	58 (95%)	3 (5%)	29	66
76	b	83/83 (100%)	76 (92%)	7 (8%)	13	44
76	d6	83/83 (100%)	71 (86%)	12 (14%)	4	16
77	c	70/70 (100%)	67 (96%)	3 (4%)	33	70
77	d7	70/70 (100%)	65 (93%)	5 (7%)	17	52
78	d	56/56 (100%)	48 (86%)	8 (14%)	4	17
78	d8	56/56 (100%)	47 (84%)	9 (16%)	3	12
79	d9	47/47 (100%)	43 (92%)	4 (8%)	12	44
79	e	47/47 (100%)	42 (89%)	5 (11%)	8	30
80	e0	53/53 (100%)	45 (85%)	8 (15%)	3	15
80	f	51/53 (96%)	47 (92%)	4 (8%)	15	48
81	g	62/62 (100%)	50 (81%)	12 (19%)	1	7
82	h	260/261 (100%)	243 (94%)	17 (6%)	20	55
82	sR	260/261 (100%)	242 (93%)	18 (7%)	18	53
83	e1	43/43 (100%)	35 (81%)	8 (19%)	2	8
All	All	18684/19337 (97%)	16334 (87%)	2350 (13%)	5	22

5 of 2350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	CT	22	VAL
40	DM	69	LEU
66	c6	43	ILE
21	CU	132	THR
29	DB	66	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
40	DM	32	ASN
57	I	74	GLN
57	s7	71	HIS
51	C	177	GLN
12	r	163	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3396 (92%)	559 (17%)	46 (1%)
1	AR	3145/3396 (92%)	562 (17%)	58 (1%)
2	3	120/121 (99%)	13 (10%)	0
2	AS	120/121 (99%)	14 (11%)	1 (0%)
25	6	1780/1800 (98%)	376 (21%)	32 (1%)
25	A	1778/1800 (98%)	419 (23%)	45 (2%)
3	4	157/158 (99%)	34 (21%)	2 (1%)
3	AT	157/158 (99%)	29 (18%)	2 (1%)
All	All	10402/10950 (94%)	2006 (19%)	186 (1%)

5 of 2006 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	26	A
1	1	40	A
1	1	43	A
1	1	45	A
1	1	49	A

5 of 186 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AR	715	A
1	AR	1589	A
25	A	1207	C
1	AR	873	C
1	AR	1238	C

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2548 ligands modelled in this entry, 1 is modelled with single atom and 1477 are monoatomic - leaving 1070 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	$\# Z > 2$
84	OHX	1	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3426	-	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
84	OHX	1	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3469	-	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
84	OHX	1	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3512	-	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
84	OHX	1	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3539	84	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3555	-	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
84	OHX	1	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3598	-	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
84	OHX	1	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3641	-	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
84	OHX	1	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3684	-	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
84	OHX	1	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3696	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3697	84	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3713	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3715	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3716	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3719	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3721	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3723	1	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3724	-	0,6,6	0.00	-	0,15,15	0.00	-
86	HN8	1	4223	-	26,26,26	0.27	0	36,41,41	1.04	2 (5%)
84	OHX	2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	202	-	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
84	OHX	3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	205	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	206	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	207	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	208	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	209	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	203	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	204	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	205	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	206	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	207	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	208	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	209	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	210	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	211	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	212	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	213	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	214	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	215	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	216	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1920	-	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
84	OHX	6	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1963	-	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
84	OHX	6	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2006	-	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
84	OHX	6	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	GOL	6	2199	-	5,5,5	0.09	0	5,5,5	0.36	0
84	OHX	A	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1939	-	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
84	OHX	A	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1982	-	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
84	OHX	A	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2025	-	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
84	OHX	A	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	GOL	A	2160	-	5,5,5	0.11	0	5,5,5	0.32	0
84	OHX	AC	101	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AG	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AH	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AK	102	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AM	101	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AP	502	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3418	-	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
84	OHX	AR	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3461	-	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
84	OHX	AR	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3477	84	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3489	87	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3504	-	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
84	OHX	AR	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3547	-	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
84	OHX	AR	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3590	-	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
84	OHX	AR	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3633	-	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
84	OHX	AR	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3676	-	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
84	OHX	AR	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3696	84	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3697	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3713	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3715	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3716	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3719	-	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
84	OHX	AR	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3721	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3722	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3723	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3724	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3725	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3726	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3727	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3728	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3729	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3730	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3731	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3732	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3733	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3734	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3735	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3736	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3737	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3738	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3739	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3740	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3741	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3742	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3743	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3744	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3745	-	0,6,6	0.00	-	0,15,15	0.00	-
87	GOL	AR	4261	1	5,5,5	0.16	0	5,5,5	0.31	0
87	GOL	AR	4262	84	5,5,5	0.28	0	5,5,5	0.54	0
86	HN8	AR	4263	-	26,26,26	0.28	0	36,41,41	1.69	4 (11%)
84	OHX	AS	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	203	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	204	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	205	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	206	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	207	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	208	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	209	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	210	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	211	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	203	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AT	204	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	205	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	206	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	207	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	208	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	209	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	210	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	211	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	212	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	213	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	214	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	215	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	216	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	217	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CE	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CE	402	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CF	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CF	402	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CG	301	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CG	302	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CK	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CL	301	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CM	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CP	501	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CV	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CX	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CX	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	DD	101	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	DH	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	DQ	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	J	301	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	K	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	M	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	O	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	Q	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	T	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	c1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	c4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	c8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	d9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	e	101	-	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
84	OHX	h	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	k	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	l	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	r	301	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	s8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	v	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	GOL	v	305	-	5,5,5	0.14	0	5,5,5	0.55	0
84	OHX	x	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	x	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	y	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	z	201	-	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
84	OHX	1	3401	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3402	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3403	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3404	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3405	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3406	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3407	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3408	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3409	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3410	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3411	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3412	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3413	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3414	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3415	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3416	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3417	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3418	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3419	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3420	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3421	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3422	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3423	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3424	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3425	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3426	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3427	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3428	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3429	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3430	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3431	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3432	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3433	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3434	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3435	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3436	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3437	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3438	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3439	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3440	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3441	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3442	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3443	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3444	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3445	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3446	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3447	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3448	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3449	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3450	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3451	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3452	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3453	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3454	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3455	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3456	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3457	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3458	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3459	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3460	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3461	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3462	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3463	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3464	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3465	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3466	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3467	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3468	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3469	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3470	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3471	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3472	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3473	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3474	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3475	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3476	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3477	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3478	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3479	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3480	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3481	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3482	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3483	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3484	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3485	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3486	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3487	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3488	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3489	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3490	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3491	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3492	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3493	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3494	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3495	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3496	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3497	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3498	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3499	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3500	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3501	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3502	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3503	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3504	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3505	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3506	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3507	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3508	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3509	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3510	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3511	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3512	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3513	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3514	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3515	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3516	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3517	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3518	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3519	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3520	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3521	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3522	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3523	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3524	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3525	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3526	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3527	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3528	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3529	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3530	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3531	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3532	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3533	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3534	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3535	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3536	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3537	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3538	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3539	84	-	0/0/0/0	0/0/0/0
84	OHX	1	3540	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3541	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3542	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3543	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3544	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3545	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3546	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3547	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3548	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3549	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3550	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3551	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3552	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3553	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3554	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3555	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3556	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3557	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3558	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3559	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3560	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3561	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3562	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3563	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3564	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3565	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3566	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3567	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3568	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3569	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3570	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3571	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3572	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3573	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3574	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3575	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3576	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3577	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3578	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3579	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3580	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3581	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3582	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3583	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3584	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3585	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3586	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3587	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3588	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3589	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3590	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3591	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3592	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3593	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3594	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3595	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3596	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3597	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3598	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3599	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3600	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3601	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3602	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3603	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3604	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3605	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3606	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3607	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3608	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3609	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3610	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3611	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3612	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3613	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3614	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3615	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3616	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3617	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3618	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3619	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3620	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3621	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3622	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3623	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3624	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3625	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3626	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3627	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3628	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3629	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3630	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3631	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3632	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3633	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3634	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3635	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3636	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3637	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3638	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3639	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3640	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3641	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3642	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3643	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3644	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3645	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3646	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3647	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3648	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3649	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3650	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3651	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3652	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3653	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3654	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3655	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3656	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3657	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3658	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3659	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3660	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3661	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3662	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3663	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3664	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3665	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3666	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3667	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3668	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3669	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3670	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3671	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3672	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3673	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3674	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3675	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3676	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3677	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3678	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3679	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3680	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3681	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3682	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3683	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3684	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3685	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3686	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3687	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3688	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3689	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3690	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3691	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3692	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3693	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3694	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3695	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3696	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3697	84	-	0/0/0/0	0/0/0/0
84	OHX	1	3698	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3699	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3700	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3701	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3702	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3703	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3704	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3705	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3706	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3707	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3708	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3709	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3710	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3711	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3712	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3713	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3714	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3715	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3716	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3717	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3718	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3719	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3720	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3721	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3723	1	-	0/0/0/0	0/0/0/0
84	OHX	1	3724	-	-	0/0/0/0	0/0/0/0
86	HN8	1	4223	-	-	0/2/48/48	0/3/5/5
84	OHX	2	201	-	-	0/0/0/0	0/0/0/0
84	OHX	3	201	-	-	0/0/0/0	0/0/0/0
84	OHX	3	202	-	-	0/0/0/0	0/0/0/0
84	OHX	3	203	-	-	0/0/0/0	0/0/0/0
84	OHX	3	204	-	-	0/0/0/0	0/0/0/0
84	OHX	3	205	-	-	0/0/0/0	0/0/0/0
84	OHX	3	206	-	-	0/0/0/0	0/0/0/0
84	OHX	3	207	-	-	0/0/0/0	0/0/0/0
84	OHX	3	208	-	-	0/0/0/0	0/0/0/0
84	OHX	3	209	-	-	0/0/0/0	0/0/0/0
84	OHX	4	201	-	-	0/0/0/0	0/0/0/0
84	OHX	4	202	-	-	0/0/0/0	0/0/0/0
84	OHX	4	203	-	-	0/0/0/0	0/0/0/0
84	OHX	4	204	-	-	0/0/0/0	0/0/0/0
84	OHX	4	205	-	-	0/0/0/0	0/0/0/0
84	OHX	4	206	-	-	0/0/0/0	0/0/0/0
84	OHX	4	207	-	-	0/0/0/0	0/0/0/0
84	OHX	4	208	-	-	0/0/0/0	0/0/0/0
84	OHX	4	209	-	-	0/0/0/0	0/0/0/0
84	OHX	4	210	-	-	0/0/0/0	0/0/0/0
84	OHX	4	211	-	-	0/0/0/0	0/0/0/0
84	OHX	4	212	-	-	0/0/0/0	0/0/0/0
84	OHX	4	213	-	-	0/0/0/0	0/0/0/0
84	OHX	4	214	-	-	0/0/0/0	0/0/0/0
84	OHX	4	215	-	-	0/0/0/0	0/0/0/0
84	OHX	4	216	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1901	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1902	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1903	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1904	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1905	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1906	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1907	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1908	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1909	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1910	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	6	1911	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1912	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1913	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1914	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1915	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1916	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1917	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1918	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1919	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1920	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1921	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1922	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1923	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1924	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1925	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1926	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1927	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1928	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1929	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1930	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1931	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1932	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1933	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1934	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1935	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1936	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1937	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1938	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1939	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1940	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1941	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1942	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1943	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1944	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1945	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1946	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1947	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1948	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1949	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1950	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1951	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1952	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	6	1953	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1954	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1955	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1956	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1957	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1958	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1959	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1960	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1961	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1962	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1963	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1964	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1965	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1966	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1967	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1968	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1969	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1970	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1971	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1972	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1973	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1974	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1975	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1976	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1977	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1978	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1979	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1980	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1981	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1982	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1983	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1984	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1985	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1986	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1987	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1988	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1989	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1990	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1991	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1992	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1993	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1994	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	6	1995	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1996	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1997	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1998	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1999	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2000	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2001	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2002	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2003	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2004	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2005	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2006	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2007	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2008	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2009	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2010	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2011	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2012	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2013	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2014	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2015	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2016	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2017	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2018	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2019	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2020	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2021	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2022	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2023	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2024	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2025	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2026	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2027	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2028	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2029	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2030	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2031	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2032	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2033	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2034	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2035	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2036	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	6	2037	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2038	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2039	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2040	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2041	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2042	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2043	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
87	GOL	6	2199	-	-	0/4/4/4	0/0/0/0
84	OHX	A	1901	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1902	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1903	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1904	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1905	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1906	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1907	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1908	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1909	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1910	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1911	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1912	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1913	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1914	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1915	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1916	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1917	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1918	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1919	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1920	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1921	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1922	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1923	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1924	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1925	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	A	1926	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1927	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1928	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1929	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1930	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1931	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1932	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1933	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1934	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1935	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1936	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1937	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1938	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1939	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1940	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1941	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1942	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1943	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1944	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1945	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1946	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1947	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1948	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1949	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1950	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1951	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1952	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1953	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1954	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1955	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1956	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1957	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1958	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1959	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1960	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1961	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1962	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1963	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1964	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1965	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1966	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1967	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	A	1968	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1969	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1970	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1971	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1972	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1973	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1974	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1975	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1976	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1977	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1978	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1979	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1980	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1981	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1982	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1983	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1984	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1985	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1986	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1987	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1988	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1989	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1990	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1991	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1992	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1993	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1994	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1995	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1996	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1997	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1998	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1999	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2000	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2001	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2002	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2003	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2004	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2005	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2006	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2007	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2008	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2009	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	A	2010	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2011	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2012	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2013	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2014	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2015	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2016	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2017	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2018	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2019	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2020	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2021	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2022	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2023	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2024	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2025	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2026	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2027	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2028	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2029	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2030	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2031	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2032	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2033	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2034	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2035	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2036	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2037	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2038	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2039	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2040	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2041	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2042	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2043	-	-	0/0/0/0	0/0/0/0
87	GOL	A	2160	-	-	0/4/4/4	0/0/0/0
84	OHX	AC	101	-	-	0/0/0/0	0/0/0/0
84	OHX	AG	201	-	-	0/0/0/0	0/0/0/0
84	OHX	AH	201	-	-	0/0/0/0	0/0/0/0
84	OHX	AK	102	-	-	0/0/0/0	0/0/0/0
84	OHX	AM	101	-	-	0/0/0/0	0/0/0/0
84	OHX	AP	502	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3401	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3402	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3403	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3404	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3405	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3406	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3407	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3408	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3409	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3410	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3411	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3412	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3413	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3414	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3415	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3416	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3417	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3418	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3419	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3420	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3421	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3422	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3423	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3424	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3425	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3426	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3427	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3428	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3429	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3430	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3431	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3432	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3433	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3434	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3435	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3436	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3437	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3438	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3439	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3440	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3441	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3442	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3443	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3444	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3445	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3446	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3447	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3448	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3449	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3450	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3451	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3452	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3453	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3454	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3455	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3456	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3457	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3458	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3459	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3460	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3461	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3462	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3463	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3464	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3465	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3466	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3467	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3468	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3469	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3470	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3471	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3472	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3473	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3474	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3475	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3476	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3477	84	-	0/0/0/0	0/0/0/0
84	OHX	AR	3478	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3479	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3480	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3481	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3482	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3483	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3484	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3485	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3486	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3487	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3488	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3489	87	-	0/0/0/0	0/0/0/0
84	OHX	AR	3490	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3491	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3492	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3493	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3494	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3495	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3496	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3497	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3498	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3499	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3500	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3501	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3502	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3503	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3504	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3505	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3506	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3507	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3508	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3509	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3510	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3511	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3512	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3513	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3514	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3515	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3516	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3517	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3518	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3519	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3520	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3521	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3522	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3523	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3524	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3525	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3526	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3527	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3528	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3529	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3530	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3531	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3532	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3533	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3534	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3535	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3536	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3537	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3538	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3539	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3540	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3541	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3542	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3543	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3544	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3545	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3546	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3547	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3548	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3549	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3550	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3551	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3552	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3553	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3554	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3555	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3556	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3557	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3558	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3559	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3560	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3561	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3562	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3563	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3564	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3565	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3566	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3567	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3568	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3569	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3570	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3571	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3572	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3573	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3574	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3575	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3576	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3577	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3578	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3579	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3580	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3581	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3582	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3583	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3584	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3585	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3586	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3587	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3588	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3589	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3590	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3591	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3592	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3593	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3594	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3595	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3596	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3597	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3598	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3599	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3600	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3601	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3602	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3603	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3604	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3605	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3606	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3607	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3608	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3609	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3610	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3611	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3612	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3613	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3614	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3615	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3616	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3617	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3618	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3619	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3620	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3621	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3622	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3623	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3624	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3625	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3626	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3627	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3628	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3629	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3630	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3631	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3632	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3633	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3634	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3635	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3636	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3637	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3638	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3639	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3640	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3641	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3642	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3643	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3644	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3645	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3646	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3647	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3648	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3649	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3650	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3651	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3652	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3653	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3654	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3655	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3656	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3657	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3658	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3659	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3660	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3661	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3662	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3663	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3664	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3665	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3666	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3667	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3668	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3669	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3670	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3671	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3672	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3673	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3674	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3675	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3676	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3677	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3678	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3679	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3680	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3681	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3682	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3683	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3684	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3685	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3686	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3687	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3688	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3689	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3690	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3691	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3692	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3693	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3694	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3695	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3696	84	-	0/0/0/0	0/0/0/0
84	OHX	AR	3697	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3698	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3699	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3700	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3701	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3702	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3703	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3704	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3705	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3706	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3707	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3708	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3709	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3710	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3711	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3712	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3713	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3714	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3715	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3716	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3717	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3718	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3719	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3720	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3721	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3722	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3723	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3724	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3725	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3726	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3727	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3728	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3729	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3730	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3731	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3732	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3733	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3734	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3735	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3736	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3737	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3738	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3739	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3740	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3741	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3742	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3743	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3744	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3745	-	-	0/0/0/0	0/0/0/0
87	GOL	AR	4261	1	-	0/4/4/4	0/0/0/0
87	GOL	AR	4262	84	-	0/4/4/4	0/0/0/0
86	HN8	AR	4263	-	-	0/2/48/48	0/3/5/5
84	OHX	AS	201	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	202	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	203	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	204	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	205	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	206	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	207	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	208	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	209	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	210	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	211	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	201	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	202	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	203	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	204	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	205	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	206	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	207	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	208	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	209	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	210	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	211	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	212	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	213	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	214	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	215	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	216	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	217	-	-	0/0/0/0	0/0/0/0
84	OHX	CE	401	-	-	0/0/0/0	0/0/0/0
84	OHX	CE	402	-	-	0/0/0/0	0/0/0/0
84	OHX	CF	401	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	CF	402	-	-	0/0/0/0	0/0/0/0
84	OHX	CG	301	-	-	0/0/0/0	0/0/0/0
84	OHX	CG	302	-	-	0/0/0/0	0/0/0/0
84	OHX	CK	201	-	-	0/0/0/0	0/0/0/0
84	OHX	CL	301	-	-	0/0/0/0	0/0/0/0
84	OHX	CM	201	-	-	0/0/0/0	0/0/0/0
84	OHX	CP	501	-	-	0/0/0/0	0/0/0/0
84	OHX	CV	201	-	-	0/0/0/0	0/0/0/0
84	OHX	CX	201	-	-	0/0/0/0	0/0/0/0
84	OHX	CX	202	-	-	0/0/0/0	0/0/0/0
84	OHX	DD	101	-	-	0/0/0/0	0/0/0/0
84	OHX	DH	201	-	-	0/0/0/0	0/0/0/0
84	OHX	DQ	201	-	-	0/0/0/0	0/0/0/0
84	OHX	J	301	-	-	0/0/0/0	0/0/0/0
84	OHX	K	201	-	-	0/0/0/0	0/0/0/0
84	OHX	M	201	-	-	0/0/0/0	0/0/0/0
84	OHX	O	201	-	-	0/0/0/0	0/0/0/0
84	OHX	Q	201	-	-	0/0/0/0	0/0/0/0
84	OHX	T	201	-	-	0/0/0/0	0/0/0/0
84	OHX	c1	201	-	-	0/0/0/0	0/0/0/0
84	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
84	OHX	c4	201	-	-	0/0/0/0	0/0/0/0
84	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
84	OHX	c8	201	-	-	0/0/0/0	0/0/0/0
84	OHX	d9	101	-	-	0/0/0/0	0/0/0/0
84	OHX	e	101	-	-	0/0/0/0	0/0/0/0
84	OHX	h	401	-	-	0/0/0/0	0/0/0/0
84	OHX	k	401	-	-	0/0/0/0	0/0/0/0
84	OHX	l	401	-	-	0/0/0/0	0/0/0/0
84	OHX	r	301	-	-	0/0/0/0	0/0/0/0
84	OHX	s8	301	-	-	0/0/0/0	0/0/0/0
84	OHX	sR	401	-	-	0/0/0/0	0/0/0/0
84	OHX	v	301	-	-	0/0/0/0	0/0/0/0
87	GOL	v	305	-	-	0/4/4/4	0/0/0/0
84	OHX	x	201	-	-	0/0/0/0	0/0/0/0
84	OHX	x	202	-	-	0/0/0/0	0/0/0/0
84	OHX	y	201	-	-	0/0/0/0	0/0/0/0
84	OHX	z	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	AR	4263	HN8	C5-C1-C2	-5.98	102.67	106.80
86	AR	4263	HN8	C5-C1-C3	-5.14	100.15	105.94
86	1	4223	HN8	O1-C9-C17	-2.42	102.25	109.31
86	AR	4263	HN8	C3-C1-C2	2.84	107.05	102.25
86	1	4223	HN8	C5-C1-C7	3.85	116.17	114.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

57 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3473	OHX	6	0
84	1	3493	OHX	2	0
84	1	3506	OHX	1	0
84	1	3510	OHX	1	0
84	1	3539	OHX	2	0
84	1	3559	OHX	1	0
84	1	3575	OHX	1	0
84	1	3604	OHX	1	0
84	1	3661	OHX	1	0
84	1	3666	OHX	1	0
84	1	3682	OHX	1	0
84	1	3683	OHX	1	0
84	1	3697	OHX	2	0
84	1	3704	OHX	1	0
84	1	3720	OHX	6	0
84	6	1915	OHX	3	0
84	6	1975	OHX	4	0
84	6	2001	OHX	4	0
84	6	2013	OHX	1	0
84	6	2025	OHX	4	0
84	A	1909	OHX	6	0
84	A	1914	OHX	1	0
84	A	1968	OHX	3	0
84	A	2009	OHX	3	0
84	A	2024	OHX	6	0
84	AR	3413	OHX	1	0
84	AR	3443	OHX	6	0
84	AR	3477	OHX	2	0
84	AR	3501	OHX	2	0
84	AR	3502	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3511	OHX	4	0
84	AR	3521	OHX	4	0
84	AR	3534	OHX	2	0
84	AR	3554	OHX	1	0
84	AR	3566	OHX	2	0
84	AR	3590	OHX	2	0
84	AR	3591	OHX	1	0
84	AR	3627	OHX	1	0
84	AR	3642	OHX	2	0
84	AR	3645	OHX	1	0
84	AR	3671	OHX	1	0
84	AR	3687	OHX	2	0
84	AR	3689	OHX	1	0
84	AR	3693	OHX	1	0
84	AR	3696	OHX	4	0
84	AR	3698	OHX	4	0
84	AR	3715	OHX	4	0
84	AR	3731	OHX	6	0
84	AR	3743	OHX	2	0
87	AR	4261	GOL	1	0
87	AR	4262	GOL	2	0
84	AS	203	OHX	5	0
84	AS	210	OHX	5	0
84	AT	203	OHX	2	0
84	AT	212	OHX	2	0
84	CG	302	OHX	1	0
84	CX	202	OHX	1	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
48	sM	2
50	s0	1
47	m2	1
25	A	1

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Mol	Chain	Number of breaks
54	s4	1
5	CE	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	85:SER	C	119:UNK	N	44.14
1	sM	139:UNK	C	155:UNK	N	37.59
1	A	1716:C	O3'	1717:G	P	4.52
1	m2	23:UNK	C	28:UNK	N	3.62
1	CE	168:LYS	C	169:THR	N	1.19

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1	3149/3396 (92%)	0.21	98 (3%)	49	26	26, 47, 129, 223	0
1	AR	3149/3396 (92%)	0.30	103 (3%)	47	24	27, 49, 123, 225	0
2	3	121/121 (100%)	-0.11	0	100	100	35, 63, 75, 82	0
2	AS	121/121 (100%)	-0.04	1 (0%)	86	71	34, 52, 66, 73	0
3	4	158/158 (100%)	0.21	5 (3%)	48	25	34, 51, 91, 138	0
3	AT	158/158 (100%)	0.24	6 (3%)	41	20	34, 60, 99, 128	0
4	CD	252/252 (100%)	0.04	3 (1%)	79	61	33, 52, 74, 82	0
4	j	252/252 (100%)	0.04	1 (0%)	92	84	31, 46, 64, 77	0
5	CE	386/386 (100%)	-0.18	1 (0%)	93	86	25, 41, 55, 95	0
5	k	386/386 (100%)	-0.02	3 (0%)	86	71	25, 48, 62, 80	0
6	CF	361/361 (100%)	-0.11	1 (0%)	93	86	31, 47, 65, 88	0
6	l	361/361 (100%)	-0.12	1 (0%)	93	86	27, 44, 62, 71	0
7	CG	296/296 (100%)	0.15	13 (4%)	35	17	39, 57, 83, 104	0
7	m	296/296 (100%)	0.48	17 (5%)	24	11	46, 69, 89, 115	0
8	CH	156/175 (89%)	0.07	3 (1%)	67	46	37, 46, 68, 84	0
8	n	156/175 (89%)	0.04	1 (0%)	89	77	36, 43, 66, 86	0
9	CI	222/222 (100%)	-0.13	3 (1%)	75	57	27, 35, 78, 133	0
9	o	222/222 (100%)	-0.16	4 (1%)	69	47	29, 38, 73, 123	0
10	CJ	233/233 (100%)	0.79	32 (13%)	3	1	70, 82, 123, 144	0
10	p	233/233 (100%)	0.49	13 (5%)	25	11	56, 70, 105, 116	0
11	CK	191/191 (100%)	-0.16	3 (1%)	72	51	35, 45, 66, 82	0
11	q	191/191 (100%)	-0.24	0	100	100	42, 53, 66, 86	0
12	CL	211/220 (95%)	0.45	12 (5%)	24	11	39, 59, 80, 93	0
12	r	211/220 (95%)	-0.04	2 (0%)	84	69	33, 46, 81, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CM	169/169 (100%)	-0.18	1 (0%) 89 77	40, 61, 75, 83	0
13	s	169/169 (100%)	0.09	4 (2%) 59 37	55, 77, 90, 96	0
14	CN	193/193 (100%)	0.54	15 (7%) 14 5	41, 62, 101, 119	0
14	t	193/193 (100%)	-0.05	0 100 100	33, 53, 95, 125	0
15	CO	136/136 (100%)	-0.35	1 (0%) 87 75	34, 40, 63, 71	0
15	u	136/136 (100%)	-0.29	3 (2%) 62 41	37, 43, 60, 68	0
16	CP	203/203 (100%)	-0.12	0 100 100	38, 55, 67, 71	0
16	v	203/203 (100%)	-0.17	0 100 100	33, 44, 57, 64	0
17	CQ	197/197 (100%)	-0.20	3 (1%) 74 54	25, 30, 60, 66	0
17	w	197/197 (100%)	-0.27	0 100 100	28, 34, 55, 60	0
18	CR	183/183 (100%)	1.33	29 (15%) 2 1	31, 39, 137, 167	0
18	x	183/183 (100%)	0.53	21 (11%) 5 2	32, 40, 105, 140	0
19	CS	185/185 (100%)	-0.16	0 100 100	32, 45, 56, 60	0
19	y	185/185 (100%)	-0.14	0 100 100	33, 43, 63, 87	0
20	CT	188/188 (100%)	0.12	9 (4%) 31 14	48, 63, 158, 169	0
20	z	188/188 (100%)	0.16	7 (3%) 42 21	48, 64, 150, 167	0
21	0	172/172 (100%)	-0.19	1 (0%) 89 77	35, 41, 55, 65	0
21	CU	172/172 (100%)	-0.35	0 100 100	30, 37, 50, 57	0
22	2	159/159 (100%)	-0.07	2 (1%) 77 59	34, 45, 87, 97	0
22	CV	159/159 (100%)	-0.21	0 100 100	31, 41, 74, 84	0
23	5	100/100 (100%)	0.81	13 (13%) 4 2	79, 93, 105, 123	0
23	CW	100/100 (100%)	1.12	20 (20%) 1 0	77, 87, 98, 119	0
24	CX	136/136 (100%)	0.14	1 (0%) 87 75	29, 38, 57, 59	0
24	IR	136/136 (100%)	0.04	4 (2%) 52 28	31, 43, 56, 62	0
25	6	1783/1800 (99%)	0.43	114 (6%) 20 7	41, 78, 169, 233	0
25	A	1781/1800 (98%)	0.51	125 (7%) 17 7	49, 87, 186, 250	0
26	7	98/98 (100%)	1.75	29 (29%) 1 0	43, 59, 150, 157	0
26	CY	98/98 (100%)	0.41	11 (11%) 6 2	38, 53, 145, 177	0
27	8	121/121 (100%)	-0.03	1 (0%) 86 71	44, 57, 77, 117	0
27	CZ	121/121 (100%)	0.05	4 (3%) 47 24	48, 64, 85, 100	0
28	9	126/126 (100%)	0.67	6 (4%) 31 14	40, 55, 64, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DA	126/126 (100%)	0.69	7 (5%) 25 11	40, 57, 73, 82	0
29	AA	135/135 (100%)	1.73	47 (34%) 0 0	69, 83, 94, 104	0
29	DB	135/135 (100%)	0.89	17 (12%) 4 2	81, 95, 110, 120	0
30	AB	148/148 (100%)	-0.08	0 100 100	27, 46, 73, 86	0
30	DC	148/148 (100%)	0.02	1 (0%) 87 75	30, 51, 71, 77	0
31	AC	58/58 (100%)	-0.07	0 100 100	32, 52, 102, 122	0
31	DD	58/58 (100%)	-0.06	0 100 100	38, 51, 80, 89	0
32	AD	97/97 (100%)	0.38	6 (6%) 21 8	67, 77, 99, 110	0
32	DE	97/97 (100%)	-0.29	0 100 100	71, 83, 105, 109	0
33	AE	109/109 (100%)	0.20	2 (1%) 69 47	42, 56, 95, 106	0
33	DF	109/109 (100%)	0.19	3 (2%) 53 29	41, 52, 92, 111	0
34	AF	127/127 (100%)	0.01	3 (2%) 59 37	25, 40, 52, 69	0
34	DG	127/127 (100%)	0.06	2 (1%) 72 51	24, 43, 55, 77	0
35	AG	106/106 (100%)	-0.15	1 (0%) 84 69	31, 36, 61, 72	0
35	DH	106/106 (100%)	-0.13	1 (0%) 84 69	28, 35, 64, 87	0
36	AH	112/112 (100%)	0.26	6 (5%) 26 12	43, 63, 104, 114	0
36	DI	112/112 (100%)	0.29	1 (0%) 84 69	46, 68, 113, 125	0
37	AI	119/119 (100%)	0.28	6 (5%) 30 13	46, 61, 70, 77	0
37	DJ	119/119 (100%)	0.27	6 (5%) 30 13	51, 67, 81, 88	0
38	AJ	99/99 (100%)	0.24	3 (3%) 51 27	52, 61, 93, 113	0
38	DK	99/99 (100%)	0.26	4 (4%) 39 19	59, 70, 92, 110	0
39	AK	87/87 (100%)	0.10	3 (3%) 46 23	32, 36, 63, 86	0
39	DL	87/87 (100%)	0.24	3 (3%) 46 23	36, 42, 77, 113	0
40	AL	77/77 (100%)	0.19	2 (2%) 56 33	67, 79, 101, 108	0
40	DM	77/77 (100%)	1.93	30 (38%) 0 0	76, 88, 107, 115	0
41	AM	50/50 (100%)	-0.07	0 100 100	42, 45, 52, 62	0
41	DN	50/50 (100%)	-0.04	0 100 100	45, 49, 59, 70	0
42	AN	52/52 (100%)	0.61	4 (7%) 14 5	37, 43, 61, 69	0
42	DO	52/52 (100%)	0.02	1 (1%) 67 46	32, 35, 48, 62	0
43	AO	25/25 (100%)	-0.14	0 100 100	52, 54, 59, 59	0
43	DP	25/25 (100%)	-0.20	0 100 100	43, 46, 59, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AP	105/105 (100%)	0.66	9 (8%) 11 4	34, 50, 74, 103	0
44	DQ	105/105 (100%)	0.25	0 100 100	37, 50, 65, 97	0
45	AQ	91/91 (100%)	-0.22	0 100 100	40, 50, 67, 80	0
45	DR	91/91 (100%)	-0.24	0 100 100	39, 53, 69, 79	0
46	i	159/272 (58%)	0.57	19 (11%) 5 2	70, 90, 143, 148	0
47	m2	0/150	-	-	-	-
48	sM	63/104 (60%)	0.77	6 (9%) 9 3	62, 91, 108, 114	0
49	p0	143/311 (45%)	1.60	53 (37%) 0 0	89, 108, 172, 179	0
50	B	206/206 (100%)	0.86	28 (13%) 3 1	93, 110, 125, 146	0
50	s0	206/206 (100%)	0.32	8 (3%) 40 19	77, 97, 115, 120	0
51	C	214/216 (99%)	1.63	77 (35%) 0 0	93, 121, 142, 150	0
51	s1	216/216 (100%)	0.53	13 (6%) 23 9	68, 83, 110, 129	0
52	D	217/217 (100%)	0.03	2 (0%) 84 69	68, 87, 108, 125	0
52	s2	217/217 (100%)	0.07	2 (0%) 84 69	57, 76, 92, 106	0
53	E	223/223 (100%)	0.64	19 (8%) 11 4	74, 91, 118, 137	0
53	s3	223/223 (100%)	0.70	27 (12%) 5 2	75, 103, 134, 148	0
54	F	260/260 (100%)	0.62	22 (8%) 11 4	63, 87, 97, 121	0
54	s4	260/260 (100%)	0.16	7 (2%) 55 30	53, 84, 98, 128	0
55	G	206/206 (100%)	0.77	22 (10%) 7 2	92, 112, 131, 141	0
55	s5	206/206 (100%)	0.95	34 (16%) 2 1	74, 95, 114, 122	0
56	H	226/226 (100%)	0.87	40 (17%) 2 1	61, 94, 116, 143	0
56	s6	218/226 (96%)	0.63	26 (11%) 5 2	52, 83, 111, 124	0
57	I	184/186 (98%)	1.03	30 (16%) 2 1	87, 119, 148, 156	0
57	s7	186/186 (100%)	0.99	31 (16%) 2 1	77, 112, 147, 152	0
58	J	188/199 (94%)	0.29	9 (4%) 31 14	53, 70, 111, 126	0
58	s8	188/199 (94%)	0.57	14 (7%) 15 5	49, 73, 124, 140	0
59	K	185/185 (100%)	1.07	34 (18%) 1 1	77, 95, 129, 158	0
59	s9	185/185 (100%)	0.68	14 (7%) 15 5	67, 85, 116, 151	0
60	L	96/105 (91%)	1.12	16 (16%) 2 1	81, 102, 129, 139	0
60	c0	96/105 (91%)	2.34	56 (58%) 0 0	96, 126, 139, 147	0
61	M	155/155 (100%)	0.83	16 (10%) 7 2	56, 70, 126, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
61	c1	146/155 (94%)	0.46	8 (5%) 26 11	55, 70, 104, 131	0
62	N	124/124 (100%)	1.99	63 (50%) 0 0	133, 140, 152, 160	0
62	c2	124/124 (100%)	3.01	87 (70%) 0 0	161, 169, 184, 190	0
63	O	150/150 (100%)	0.41	9 (6%) 23 9	64, 85, 100, 104	0
63	c3	150/150 (100%)	0.16	4 (2%) 55 30	59, 78, 96, 111	0
64	P	127/128 (99%)	1.41	36 (28%) 1 0	66, 119, 135, 138	0
64	c4	128/128 (100%)	0.64	11 (8%) 11 4	57, 81, 91, 94	0
65	Q	124/141 (87%)	0.49	7 (5%) 25 11	75, 89, 126, 146	0
65	c5	135/141 (95%)	0.80	16 (11%) 5 2	82, 97, 119, 131	0
66	R	141/142 (99%)	1.05	26 (18%) 1 1	81, 107, 115, 120	0
66	c6	142/142 (100%)	0.70	15 (10%) 7 2	67, 91, 106, 127	0
67	S	120/125 (96%)	0.56	13 (10%) 6 2	90, 109, 134, 138	0
67	c7	117/125 (93%)	0.13	6 (5%) 29 13	78, 97, 122, 130	0
68	T	145/145 (100%)	0.79	17 (11%) 5 2	71, 99, 129, 140	0
68	c8	145/145 (100%)	0.70	16 (11%) 6 2	79, 91, 116, 127	0
69	U	143/143 (100%)	0.99	22 (15%) 2 1	84, 102, 119, 133	0
69	c9	143/143 (100%)	1.11	30 (20%) 1 0	71, 86, 106, 119	0
70	V	107/110 (97%)	0.14	2 (1%) 67 46	73, 109, 141, 145	0
70	d0	110/110 (100%)	0.46	12 (10%) 6 2	70, 111, 154, 172	0
71	W	87/87 (100%)	0.61	8 (9%) 10 3	90, 96, 115, 124	0
71	d1	87/87 (100%)	0.14	4 (4%) 33 15	75, 83, 110, 121	0
72	X	129/129 (100%)	0.15	2 (1%) 72 51	68, 81, 88, 101	0
72	d2	129/129 (100%)	0.06	1 (0%) 86 71	57, 70, 81, 97	0
73	Y	144/144 (100%)	0.22	3 (2%) 64 43	57, 62, 73, 88	0
73	d3	144/144 (100%)	-0.07	0 100 100	46, 52, 66, 78	0
74	Z	134/134 (100%)	0.47	15 (11%) 6 2	69, 97, 114, 125	0
74	d4	134/134 (100%)	0.23	11 (8%) 12 5	62, 88, 103, 122	0
75	a	70/70 (100%)	2.04	28 (40%) 0 0	111, 123, 138, 139	0
75	d5	69/70 (98%)	1.43	22 (31%) 0 0	93, 113, 124, 127	0
76	b	97/97 (100%)	0.43	5 (5%) 28 12	67, 83, 135, 138	0
76	d6	97/97 (100%)	0.13	1 (1%) 82 67	51, 63, 95, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
77	c	81/81 (100%)	1.04	15 (18%)	1	1	82, 95, 127, 134	0
77	d7	81/81 (100%)	1.14	15 (18%)	1	1	72, 87, 126, 132	0
78	d	63/63 (100%)	0.97	7 (11%)	6	2	104, 121, 132, 134	0
78	d8	63/63 (100%)	1.96	34 (53%)	0	0	91, 107, 121, 125	0
79	d9	53/53 (100%)	1.19	10 (18%)	1	1	71, 82, 120, 128	0
79	e	53/53 (100%)	0.68	4 (7%)	15	5	75, 80, 96, 104	0
80	e0	62/62 (100%)	0.97	9 (14%)	3	1	59, 83, 113, 125	0
80	f	60/62 (96%)	1.14	11 (18%)	1	1	63, 92, 131, 134	0
81	g	71/71 (100%)	1.74	29 (40%)	0	0	105, 124, 144, 150	0
82	h	318/318 (100%)	1.11	70 (22%)	1	0	97, 115, 135, 147	0
82	sR	318/318 (100%)	0.61	32 (10%)	8	2	99, 121, 140, 157	0
83	e1	51/51 (100%)	2.31	23 (45%)	0	0	145, 157, 165, 167	0
All	All	33004/34167 (96%)	0.38	2302 (6%)	17	7	24, 66, 132, 250	0

The worst 5 of 2302 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	CR	161	ALA	24.0
18	CR	162	GLU	20.3
26	7	76	VAL	17.9
18	CR	160	ALA	16.2
26	7	75	THR	15.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
85	MG	1	4126	1/1	0.94	0.97	65.65	33,33,33,33	0
85	MG	AR	4189	1/1	0.92	1.14	55.57	32,32,32,32	0
85	MG	1	4031	1/1	0.99	0.55	52.89	21,21,21,21	0
85	MG	6	2108	1/1	0.94	0.56	50.10	50,50,50,50	0
85	MG	AR	3809	1/1	0.94	0.65	48.65	37,37,37,37	0
85	MG	CE	405	1/1	0.95	0.89	48.12	26,26,26,26	0
85	MG	1	3833	1/1	0.92	0.70	44.59	24,24,24,24	0
85	MG	x	205	1/1	0.90	0.66	44.53	33,33,33,33	0
85	MG	A	2078	1/1	0.93	0.68	44.04	54,54,54,54	0
85	MG	AR	3919	1/1	0.96	0.43	39.71	34,34,34,34	0
85	MG	AR	3893	1/1	0.94	0.95	36.88	50,50,50,50	0
85	MG	AR	4102	1/1	0.57	0.97	36.12	30,30,30,30	0
85	MG	AR	3905	1/1	0.93	0.48	34.66	29,29,29,29	0
85	MG	1	3904	1/1	0.98	0.53	34.58	25,25,25,25	0
84	OHX	1	3655	7/7	0.93	0.37	33.37	138,138,138,139	0
85	MG	1	4048	1/1	0.95	0.83	33.02	33,33,33,33	0
85	MG	1	3856	1/1	0.96	0.68	32.97	24,24,24,24	0
85	MG	AT	221	1/1	0.82	0.76	31.91	52,52,52,52	0
85	MG	1	4168	1/1	0.96	0.45	31.18	20,20,20,20	0
85	MG	1	3887	1/1	0.97	0.83	30.98	42,42,42,42	0
85	MG	A	2079	1/1	0.97	0.64	29.07	58,58,58,58	0
85	MG	1	3905	1/1	0.92	0.47	28.94	38,38,38,38	0
85	MG	x	209	1/1	0.87	0.66	28.59	39,39,39,39	0
85	MG	A	2126	1/1	0.92	0.68	28.24	64,64,64,64	0
85	MG	A	2047	1/1	0.84	0.65	28.18	55,55,55,55	0
85	MG	AR	3888	1/1	0.94	0.67	27.41	24,24,24,24	0
85	MG	1	3764	1/1	0.92	0.57	27.14	41,41,41,41	0
85	MG	1	3912	1/1	0.93	0.59	27.00	22,22,22,22	0
85	MG	AR	4230	1/1	0.92	0.55	26.87	18,18,18,18	0
85	MG	AR	4188	1/1	0.84	1.11	26.60	31,31,31,31	0
85	MG	AR	3961	1/1	0.92	0.53	26.48	43,43,43,43	0
85	MG	AR	3912	1/1	0.94	0.54	26.34	23,23,23,23	0
84	OHX	1	3642	7/7	0.90	0.45	26.30	135,135,136,136	0
84	OHX	6	2038	7/7	0.93	0.41	26.26	148,148,148,148	0
85	MG	1	3911	1/1	0.99	0.65	25.89	21,21,21,21	0
85	MG	6	2077	1/1	0.92	0.54	25.02	39,39,39,39	0
85	MG	AR	3937	1/1	0.95	0.67	24.81	27,27,27,27	0
85	MG	1	3885	1/1	0.98	0.49	24.78	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	3933	1/1	0.96	0.47	24.77	24,24,24,24	0
85	MG	AR	3941	1/1	0.96	0.46	24.54	36,36,36,36	0
84	OHX	AR	3717	7/7	0.84	0.42	24.38	144,144,144,144	0
85	MG	AR	3871	1/1	0.96	0.40	24.21	28,28,28,28	0
85	MG	6	2098	1/1	0.98	0.53	23.94	68,68,68,68	0
85	MG	1	3890	1/1	0.94	0.47	23.87	34,34,34,34	0
85	MG	1	3914	1/1	0.95	0.50	23.81	19,19,19,19	0
85	MG	1	3756	1/1	0.93	0.42	23.71	32,32,32,32	0
85	MG	AR	3879	1/1	0.94	0.64	23.56	22,22,22,22	0
84	OHX	AR	3726	7/7	0.88	0.42	23.26	118,118,118,118	0
85	MG	1	3909	1/1	0.97	0.57	23.15	25,25,25,25	0
85	MG	AR	3874	1/1	0.96	0.60	22.97	27,27,27,27	0
85	MG	AR	3993	1/1	0.94	0.35	22.96	28,28,28,28	0
84	OHX	A	1953	7/7	0.94	0.41	22.79	146,147,147,147	0
85	MG	1	4195	1/1	0.94	0.46	22.70	29,29,29,29	0
85	MG	A	2053	1/1	0.86	0.72	22.46	57,57,57,57	0
84	OHX	AR	3579	7/7	0.95	0.34	22.03	130,130,130,130	0
85	MG	A	2077	1/1	0.97	0.59	21.99	48,48,48,48	0
84	OHX	AR	3690	7/7	0.88	0.47	21.95	117,118,118,118	0
84	OHX	AR	3648	7/7	0.96	0.55	21.88	130,131,131,131	0
85	MG	AR	4051	1/1	0.88	0.38	21.87	40,40,40,40	0
85	MG	AR	4155	1/1	0.81	0.45	21.63	34,34,34,34	0
85	MG	1	4222	1/1	0.96	0.65	21.62	13,13,13,13	0
85	MG	1	4215	1/1	0.98	0.62	21.48	27,27,27,27	0
85	MG	CE	407	1/1	0.81	0.59	21.42	41,41,41,41	0
85	MG	1	4186	1/1	0.95	0.52	21.28	25,25,25,25	0
85	MG	1	3796	1/1	0.95	0.54	21.03	18,18,18,18	0
85	MG	AR	3940	1/1	0.99	0.49	20.96	21,21,21,21	0
85	MG	AR	3767	1/1	0.94	0.58	20.74	35,35,35,35	0
85	MG	1	3731	1/1	0.85	0.49	20.68	36,36,36,36	0
84	OHX	1	3596	7/7	0.91	0.49	20.67	143,144,144,144	0
85	MG	6	2158	1/1	0.46	0.75	20.63	74,74,74,74	0
85	MG	A	2055	1/1	0.93	0.47	20.45	71,71,71,71	0
85	MG	A	2066	1/1	0.96	0.59	20.38	79,79,79,79	0
85	MG	1	3859	1/1	0.95	0.44	20.02	28,28,28,28	0
85	MG	AR	3906	1/1	0.97	0.36	19.83	33,33,33,33	0
85	MG	AR	3804	1/1	0.92	0.45	19.83	27,27,27,27	0
85	MG	4	221	1/1	0.63	0.54	19.68	51,51,51,51	0
84	OHX	AR	3641	7/7	0.93	0.48	19.59	133,133,133,133	0
85	MG	1	4125	1/1	0.87	0.38	19.56	23,23,23,23	0
85	MG	AR	3930	1/1	0.97	0.62	19.52	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3860	1/1	0.94	0.47	19.39	36,36,36,36	0
85	MG	1	3875	1/1	0.98	0.46	19.37	23,23,23,23	0
85	MG	1	3891	1/1	0.98	0.60	19.22	17,17,17,17	0
85	MG	AR	3977	1/1	0.92	0.42	19.20	41,41,41,41	0
85	MG	1	3783	1/1	0.98	0.46	19.12	18,18,18,18	0
85	MG	1	3889	1/1	0.98	0.54	19.11	23,23,23,23	0
85	MG	AR	4080	1/1	0.87	0.51	19.07	32,32,32,32	0
85	MG	AR	3763	1/1	0.98	0.59	18.79	17,17,17,17	0
85	MG	AR	3915	1/1	0.95	0.61	18.74	28,28,28,28	0
85	MG	AR	4002	1/1	0.93	0.50	18.59	28,28,28,28	0
85	MG	A	2153	1/1	0.94	0.58	18.55	51,51,51,51	0
85	MG	6	2161	1/1	0.86	0.49	18.39	58,58,58,58	0
84	OHX	AR	3592	7/7	0.95	0.34	18.27	114,114,114,114	0
85	MG	AR	3914	1/1	0.90	0.43	18.02	32,32,32,32	0
85	MG	1	3843	1/1	0.83	0.41	17.92	24,24,24,24	0
84	OHX	6	2033	7/7	0.92	0.40	17.86	150,151,151,152	0
85	MG	1	4204	1/1	0.97	0.51	17.83	34,34,34,34	0
84	OHX	1	3640	7/7	0.96	0.35	17.73	124,124,124,125	0
85	MG	1	3828	1/1	0.93	0.55	17.66	30,30,30,30	0
85	MG	1	3732	1/1	0.91	0.44	17.66	26,26,26,26	0
85	MG	1	3962	1/1	0.90	0.41	17.55	39,39,39,39	0
85	MG	1	4196	1/1	0.98	0.42	17.34	30,30,30,30	0
84	OHX	1	3719	7/7	0.90	0.52	17.29	120,120,121,121	0
84	OHX	1	3717	7/7	0.81	0.54	17.26	144,144,144,145	0
85	MG	AR	3859	1/1	0.94	0.49	17.24	29,29,29,29	0
85	MG	1	3801	1/1	0.77	0.54	17.09	37,37,37,37	0
85	MG	4	224	1/1	0.95	0.40	17.09	33,33,33,33	0
85	MG	AR	4247	1/1	0.95	0.46	17.09	22,22,22,22	0
85	MG	k	404	1/1	0.95	0.67	17.04	32,32,32,32	0
85	MG	1	3799	1/1	0.85	0.41	16.98	37,37,37,37	0
84	OHX	A	2012	7/7	0.92	0.37	16.83	139,140,140,140	0
84	OHX	1	3711	7/7	0.93	0.59	16.82	119,120,120,120	0
85	MG	1	4208	1/1	0.95	0.32	16.78	37,37,37,37	0
85	MG	AR	3860	1/1	0.98	0.51	16.70	23,23,23,23	0
85	MG	CR	201	1/1	0.94	0.65	16.63	29,29,29,29	0
84	OHX	A	2026	7/7	0.90	0.40	16.59	123,123,124,124	0
85	MG	AR	4024	1/1	0.74	0.79	16.56	53,53,53,53	0
84	OHX	AR	3652	7/7	0.87	0.43	16.33	112,112,113,113	0
85	MG	6	2107	1/1	0.95	0.55	16.32	43,43,43,43	0
84	OHX	A	2035	7/7	0.91	0.48	16.27	130,131,131,131	0
84	OHX	AR	3660	7/7	0.94	0.43	16.07	123,123,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2140	1/1	0.82	0.40	16.06	69,69,69,69	0
85	MG	AR	4249	1/1	0.96	0.44	15.98	24,24,24,24	0
85	MG	AR	3896	1/1	0.91	0.55	15.96	36,36,36,36	0
85	MG	AR	3909	1/1	0.99	0.57	15.96	25,25,25,25	0
85	MG	AR	3904	1/1	0.95	0.52	15.89	21,21,21,21	0
85	MG	AR	3985	1/1	0.97	0.49	15.81	35,35,35,35	0
85	MG	6	2078	1/1	0.90	0.45	15.79	42,42,42,42	0
85	MG	1	3858	1/1	0.99	0.37	15.77	25,25,25,25	0
85	MG	1	3869	1/1	0.90	0.49	15.63	34,34,34,34	0
85	MG	A	2105	1/1	0.93	0.43	15.57	94,94,94,94	0
84	OHX	1	3695	7/7	0.91	0.61	15.46	154,154,155,155	0
85	MG	AR	3913	1/1	0.87	0.43	15.31	26,26,26,26	0
84	OHX	AR	3657	7/7	0.92	0.38	15.30	114,114,115,115	0
85	MG	AR	3942	1/1	0.95	0.56	14.97	31,31,31,31	0
85	MG	1	3845	1/1	0.87	0.40	14.88	18,18,18,18	0
85	MG	6	2071	1/1	0.97	0.49	14.88	45,45,45,45	0
85	MG	AT	230	1/1	0.98	0.42	14.78	39,39,39,39	0
84	OHX	AR	3729	7/7	0.89	0.46	14.65	120,120,120,121	0
85	MG	1	3822	1/1	0.97	0.49	14.64	18,18,18,18	0
85	MG	1	3902	1/1	0.95	0.50	14.59	35,35,35,35	0
85	MG	AR	4082	1/1	0.94	0.34	14.52	24,24,24,24	0
85	MG	AR	4241	1/1	0.99	0.39	14.46	17,17,17,17	0
85	MG	6	2053	1/1	0.97	0.57	14.34	41,41,41,41	0
85	MG	6	2057	1/1	0.97	0.56	14.26	51,51,51,51	0
85	MG	AR	3747	1/1	0.92	0.30	14.23	23,23,23,23	0
85	MG	AR	3857	1/1	0.95	0.53	14.19	20,20,20,20	0
85	MG	AR	3918	1/1	0.95	0.48	14.16	27,27,27,27	0
84	OHX	1	3641	7/7	0.94	0.35	14.13	141,141,141,141	0
85	MG	AR	4198	1/1	0.80	0.59	14.07	51,51,51,51	0
85	MG	6	2068	1/1	0.83	0.46	14.06	61,61,61,61	0
85	MG	AR	3926	1/1	0.96	0.37	13.99	33,33,33,33	0
85	MG	AR	4140	1/1	0.85	0.49	13.85	44,44,44,44	0
85	MG	AR	3772	1/1	0.96	0.52	13.85	37,37,37,37	0
85	MG	1	3819	1/1	0.83	0.40	13.70	27,27,27,27	0
85	MG	6	2197	1/1	0.78	0.57	13.64	56,56,56,56	0
85	MG	AR	3938	1/1	0.97	0.39	13.54	34,34,34,34	0
85	MG	AR	3786	1/1	0.97	0.48	13.53	25,25,25,25	0
85	MG	AR	3756	1/1	0.82	0.35	13.47	36,36,36,36	0
85	MG	AK	103	1/1	0.96	0.44	13.43	36,36,36,36	0
85	MG	AR	3810	1/1	0.97	0.51	13.25	27,27,27,27	0
85	MG	1	3829	1/1	0.94	0.53	13.15	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	A	2062	1/1	0.72	0.71	13.11	65,65,65,65	0
84	OHX	AR	3409	7/7	0.99	0.34	13.07	120,120,120,121	0
85	MG	A	2138	1/1	0.96	0.46	13.06	66,66,66,66	0
84	OHX	AT	201	7/7	0.99	0.33	13.06	109,109,110,110	0
84	OHX	AR	3691	7/7	0.94	0.40	12.93	116,116,116,117	0
84	OHX	6	2046	7/7	0.86	0.36	12.91	151,152,152,152	0
85	MG	A	2119	1/1	0.96	0.35	12.84	57,57,57,57	0
85	MG	1	4193	1/1	0.87	0.37	12.80	23,23,23,23	0
85	MG	1	4189	1/1	0.93	0.36	12.78	27,27,27,27	0
85	MG	AR	4227	1/1	0.94	0.33	12.71	22,22,22,22	0
85	MG	1	4027	1/1	0.81	0.39	12.69	35,35,35,35	0
85	MG	1	3841	1/1	0.95	0.59	12.69	29,29,29,29	0
85	MG	1	3779	1/1	0.83	0.48	12.65	55,55,55,55	0
85	MG	1	3746	1/1	0.91	0.41	12.64	26,26,26,26	0
85	MG	AR	4090	1/1	0.83	0.49	12.58	57,57,57,57	0
85	MG	AR	4091	1/1	0.96	0.31	12.50	35,35,35,35	0
85	MG	AR	4252	1/1	0.90	0.37	12.43	50,50,50,50	0
84	OHX	1	3672	7/7	0.92	0.41	12.40	147,147,147,148	0
84	OHX	AR	3732	7/7	0.92	0.52	12.39	146,146,147,147	0
85	MG	1	3886	1/1	0.88	0.41	12.36	21,21,21,21	0
84	OHX	AR	3632	7/7	0.96	0.35	12.25	117,117,118,118	0
85	MG	AR	3863	1/1	0.98	0.57	12.24	21,21,21,21	0
85	MG	1	3868	1/1	0.93	0.42	12.24	29,29,29,29	0
85	MG	AR	4034	1/1	0.73	0.45	12.20	60,60,60,60	0
85	MG	AR	4138	1/1	0.95	0.48	12.16	28,28,28,28	0
85	MG	AB	203	1/1	0.91	0.34	12.15	32,32,32,32	0
85	MG	6	2082	1/1	0.90	0.48	12.13	54,54,54,54	0
84	OHX	AR	3685	7/7	0.94	0.33	12.01	120,121,121,121	0
85	MG	1	3894	1/1	0.95	0.48	11.87	22,22,22,22	0
84	OHX	1	3692	7/7	0.92	0.29	11.87	113,113,113,113	0
84	OHX	1	3661	7/7	0.93	0.32	11.83	119,120,120,120	0
84	OHX	A	1970	7/7	0.91	0.35	11.80	132,132,133,133	0
85	MG	AR	3966	1/1	0.93	0.45	11.80	38,38,38,38	0
85	MG	A	2080	1/1	0.88	0.39	11.79	65,65,65,65	0
84	OHX	1	3723	7/7	0.89	0.35	11.71	113,113,113,113	0
84	OHX	1	3694	7/7	0.93	0.41	11.68	116,116,117,117	0
84	OHX	A	2013	7/7	0.94	0.34	11.65	132,133,133,133	0
85	MG	AR	3901	1/1	0.95	0.45	11.63	29,29,29,29	0
84	OHX	AR	3728	7/7	0.85	0.41	11.63	151,152,152,152	0
85	MG	AR	3873	1/1	0.85	0.46	11.57	31,31,31,31	0
84	OHX	AR	3677	7/7	0.91	0.38	11.48	110,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3882	1/1	0.99	0.45	11.38	32,32,32,32	0
84	OHX	6	2039	7/7	0.90	0.62	11.38	132,133,133,134	0
85	MG	A	2057	1/1	0.92	0.46	11.35	70,70,70,70	0
85	MG	AR	4141	1/1	0.78	0.36	11.32	37,37,37,37	0
85	MG	A	2109	1/1	0.86	0.41	11.27	60,60,60,60	0
84	OHX	AR	3626	7/7	0.96	0.30	11.05	122,123,123,123	0
84	OHX	AR	3735	7/7	0.94	0.30	11.04	129,129,129,129	0
85	MG	1	3795	1/1	0.94	0.29	11.03	26,26,26,26	0
85	MG	A	2052	1/1	0.93	0.42	11.00	53,53,53,53	0
84	OHX	AR	3417	7/7	0.98	0.26	10.93	111,112,112,112	0
85	MG	AR	3757	1/1	0.93	0.41	10.81	31,31,31,31	0
85	MG	1	3879	1/1	0.95	0.38	10.81	45,45,45,45	0
84	OHX	1	3403	7/7	0.98	0.30	10.74	113,113,113,114	0
84	OHX	x	201	7/7	0.90	0.39	10.74	110,110,110,110	0
84	OHX	AR	3401	7/7	0.98	0.39	10.73	121,121,121,122	0
84	OHX	1	3707	7/7	0.90	0.40	10.72	125,125,126,126	0
84	OHX	AR	3601	7/7	0.95	0.42	10.63	127,127,128,128	0
84	OHX	AR	3402	7/7	0.99	0.39	10.59	113,113,113,113	0
85	MG	AR	3750	1/1	0.90	0.41	10.57	27,27,27,27	0
84	OHX	1	3708	7/7	0.87	0.39	10.55	134,134,134,134	0
84	OHX	6	1901	7/7	0.99	0.34	10.52	119,120,120,120	0
84	OHX	AR	3645	7/7	0.98	0.34	10.47	118,118,118,118	0
84	OHX	AR	3413	7/7	0.99	0.26	10.43	107,107,107,107	0
84	OHX	1	3408	7/7	0.99	0.32	10.36	112,112,112,113	0
85	MG	AR	4226	1/1	0.92	0.41	10.35	24,24,24,24	0
85	MG	AR	3801	1/1	0.94	0.38	10.35	32,32,32,32	0
85	MG	1	4096	1/1	0.96	0.41	10.31	27,27,27,27	0
85	MG	AR	4075	1/1	0.83	0.31	10.29	36,36,36,36	0
84	OHX	AR	3693	7/7	0.96	0.41	10.27	131,131,131,131	0
85	MG	AR	4161	1/1	0.74	0.27	10.26	39,39,39,39	0
84	OHX	1	3409	7/7	0.99	0.30	10.19	116,116,117,117	0
84	OHX	AR	3410	7/7	0.99	0.31	10.09	109,109,109,110	0
85	MG	AR	3850	1/1	0.97	0.28	10.05	24,24,24,24	0
84	OHX	1	3677	7/7	0.96	0.33	10.02	116,116,117,117	0
85	MG	1	3836	1/1	0.97	0.39	9.93	36,36,36,36	0
85	MG	AR	3950	1/1	0.65	0.27	9.89	47,47,47,47	0
85	MG	1	3760	1/1	0.97	0.36	9.85	27,27,27,27	0
84	OHX	1	3401	7/7	0.99	0.38	9.84	114,114,115,115	0
84	OHX	1	3402	7/7	0.99	0.35	9.73	114,115,115,115	0
85	MG	CU	201	1/1	0.87	0.40	9.71	38,38,38,38	0
84	OHX	AR	3411	7/7	0.98	0.30	9.70	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3700	7/7	0.95	0.47	9.58	135,135,135,135	0
84	OHX	1	3705	7/7	0.94	0.38	9.50	131,131,132,132	0
85	MG	1	4142	1/1	0.98	0.26	9.48	38,38,38,38	0
84	OHX	4	201	7/7	0.98	0.35	9.42	108,108,108,108	0
85	MG	CD	302	1/1	0.73	0.49	9.41	36,36,36,36	0
85	MG	1	3866	1/1	0.82	0.39	9.34	34,34,34,34	0
85	MG	AR	4019	1/1	0.84	0.27	9.33	45,45,45,45	0
84	OHX	4	213	7/7	0.91	0.31	9.32	117,117,117,117	0
85	MG	A	2072	1/1	0.93	0.39	9.21	66,66,66,66	0
85	MG	6	2059	1/1	0.86	0.43	9.14	70,70,70,70	0
85	MG	d6	102	1/1	0.97	0.50	9.09	38,38,38,38	0
84	OHX	6	1980	7/7	0.96	0.34	9.09	116,116,116,116	0
85	MG	AR	4202	1/1	0.95	0.56	9.06	29,29,29,29	0
84	OHX	6	1979	7/7	0.94	0.46	9.06	135,135,136,136	0
84	OHX	A	1990	7/7	0.97	0.27	8.96	135,135,136,136	0
85	MG	1	3899	1/1	0.91	0.35	8.93	39,39,39,39	0
85	MG	AR	3790	1/1	0.96	0.34	8.92	22,22,22,22	0
84	OHX	1	3592	7/7	0.96	0.33	8.88	117,117,117,117	0
85	MG	AR	3865	1/1	0.95	0.41	8.74	24,24,24,24	0
85	MG	AR	3751	1/1	0.82	0.36	8.72	36,36,36,36	0
85	MG	CD	301	1/1	0.90	0.37	8.71	34,34,34,34	0
84	OHX	A	1903	7/7	0.98	0.35	8.68	149,149,150,150	0
85	MG	AR	3936	1/1	0.96	0.52	8.68	20,20,20,20	0
85	MG	A	2131	1/1	0.74	0.43	8.62	64,64,64,64	0
84	OHX	1	3699	7/7	0.97	0.40	8.62	130,131,131,131	0
85	MG	1	3871	1/1	0.92	0.47	8.61	30,30,30,30	0
84	OHX	1	3680	7/7	0.96	0.32	8.58	122,122,122,122	0
85	MG	6	2155	1/1	0.94	0.86	8.54	58,58,58,58	0
85	MG	A	2061	1/1	0.92	0.50	8.53	59,59,59,59	0
85	MG	AR	3994	1/1	0.83	0.32	8.50	25,25,25,25	0
85	MG	AR	4041	1/1	0.93	0.36	8.49	34,34,34,34	0
85	MG	1	3939	1/1	0.88	0.29	8.46	39,39,39,39	0
85	MG	4	225	1/1	0.92	0.32	8.43	25,25,25,25	0
84	OHX	A	2021	7/7	0.91	0.43	8.43	133,133,134,134	0
84	OHX	4	214	7/7	0.94	0.46	8.40	140,140,140,140	0
84	OHX	AM	101	7/7	0.90	0.43	8.37	121,121,121,121	0
84	OHX	AR	3640	7/7	0.87	0.32	8.32	126,126,126,126	0
84	OHX	A	1982	7/7	0.97	0.30	8.30	121,122,122,122	0
84	OHX	AR	3610	7/7	0.95	0.38	8.29	137,138,138,138	0
85	MG	CX	203	1/1	0.97	0.39	8.22	19,19,19,19	0
85	MG	1	3876	1/1	0.96	0.40	8.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3978	1/1	0.94	0.35	8.13	46,46,46,46	0
84	OHX	AR	3658	7/7	0.95	0.35	8.09	122,123,123,123	0
85	MG	1	3730	1/1	0.94	0.34	8.03	36,36,36,36	0
84	OHX	AR	3407	7/7	0.98	0.34	8.01	113,113,113,113	0
84	OHX	6	1902	7/7	0.99	0.34	7.89	136,136,137,137	0
85	MG	1	3725	1/1	0.99	0.38	7.83	34,34,34,34	0
84	OHX	AR	3684	7/7	0.96	0.52	7.80	124,125,125,125	0
85	MG	1	3892	1/1	0.87	0.41	7.78	23,23,23,23	0
85	MG	6	2099	1/1	0.82	0.39	7.77	51,51,51,51	0
85	MG	AR	3897	1/1	0.91	0.44	7.76	51,51,51,51	0
84	OHX	1	3631	7/7	0.94	0.31	7.74	116,116,117,117	0
85	MG	6	2091	1/1	0.92	0.41	7.74	61,61,61,61	0
84	OHX	4	210	7/7	0.95	0.26	7.71	108,108,108,108	0
84	OHX	1	3645	7/7	0.97	0.34	7.68	125,126,126,126	0
85	MG	6	2061	1/1	0.96	0.32	7.67	100,100,100,100	0
85	MG	1	3901	1/1	0.91	0.49	7.67	39,39,39,39	0
84	OHX	1	3657	7/7	0.95	0.28	7.66	123,123,124,124	0
84	OHX	1	3407	7/7	0.98	0.31	7.65	106,106,107,107	0
85	MG	1	3793	1/1	0.90	0.30	7.61	37,37,37,37	0
84	OHX	1	3575	7/7	0.95	0.27	7.58	116,117,117,117	0
84	OHX	1	3539	7/7	0.95	0.28	7.53	119,119,119,119	0
84	OHX	AR	3683	7/7	0.97	0.36	7.49	126,127,127,127	0
84	OHX	AR	3406	7/7	0.98	0.34	7.49	112,112,113,113	0
84	OHX	AR	3654	7/7	0.94	0.50	7.43	137,137,138,138	0
85	MG	AR	4228	1/1	0.95	0.37	7.34	27,27,27,27	0
84	OHX	AR	3415	7/7	0.98	0.35	7.30	109,109,110,110	0
84	OHX	1	3665	7/7	0.92	0.36	7.29	129,129,129,129	0
84	OHX	AR	3403	7/7	0.99	0.28	7.24	110,110,110,110	0
85	MG	1	3846	1/1	0.95	0.28	7.17	39,39,39,39	0
84	OHX	A	2014	7/7	0.94	0.35	7.17	127,128,128,128	0
85	MG	A	2155	1/1	0.61	0.46	7.16	75,75,75,75	0
84	OHX	1	3604	7/7	0.95	0.34	7.16	116,116,117,117	0
84	OHX	1	3601	7/7	0.96	0.30	7.13	112,112,112,112	0
85	MG	AR	3819	1/1	0.98	0.36	7.08	37,37,37,37	0
85	MG	AR	4111	1/1	0.95	0.35	7.04	37,37,37,37	0
84	OHX	AR	3590	7/7	0.94	0.37	7.03	113,113,113,113	0
85	MG	A	2108	1/1	0.97	0.62	6.98	57,57,57,57	0
85	MG	AR	3826	1/1	0.95	0.32	6.84	23,23,23,23	0
85	MG	AR	3753	1/1	0.90	0.33	6.84	26,26,26,26	0
84	OHX	1	3412	7/7	0.99	0.30	6.81	114,114,115,115	0
85	MG	A	2064	1/1	0.95	0.34	6.80	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	A	1980	7/7	0.96	0.26	6.76	137,137,138,138	0
84	OHX	6	2019	7/7	0.94	0.30	6.71	140,140,141,141	0
85	MG	1	4188	1/1	0.96	0.37	6.71	28,28,28,28	0
84	OHX	1	3421	7/7	0.99	0.29	6.71	115,115,116,116	0
85	MG	A	2101	1/1	0.85	0.38	6.69	64,64,64,64	0
85	MG	AT	218	1/1	0.69	0.34	6.69	30,30,30,30	0
85	MG	1	3823	1/1	0.65	0.27	6.68	41,41,41,41	0
84	OHX	AR	3644	7/7	0.92	0.31	6.68	126,127,127,127	0
84	OHX	6	1903	7/7	0.99	0.29	6.66	117,118,118,118	0
84	OHX	4	202	7/7	0.99	0.32	6.64	112,112,112,113	0
84	OHX	4	208	7/7	0.97	0.36	6.63	106,106,106,106	0
84	OHX	6	1987	7/7	0.93	0.28	6.58	137,137,138,138	0
85	MG	1	3837	1/1	0.93	0.33	6.57	26,26,26,26	0
85	MG	AR	3844	1/1	0.96	0.40	6.56	27,27,27,27	0
85	MG	A	2088	1/1	0.87	0.53	6.53	59,59,59,59	0
85	MG	AR	3978	1/1	0.94	0.36	6.52	49,49,49,49	0
84	OHX	AR	3625	7/7	0.97	0.36	6.52	134,134,134,134	0
84	OHX	6	2031	7/7	0.94	0.31	6.48	125,126,126,126	0
84	OHX	AR	3714	7/7	0.95	0.33	6.48	132,132,133,133	0
84	OHX	1	3591	7/7	0.94	0.28	6.47	109,109,109,109	0
84	OHX	6	1972	7/7	0.95	0.42	6.46	142,143,143,144	0
84	OHX	1	3666	7/7	0.92	0.42	6.45	117,118,118,118	0
84	OHX	1	3673	7/7	0.91	0.56	6.44	133,133,133,133	0
85	MG	x	204	1/1	0.92	0.35	6.44	28,28,28,28	0
84	OHX	A	1994	7/7	0.96	0.28	6.40	142,143,144,144	0
84	OHX	AR	3600	7/7	0.94	0.33	6.39	119,119,119,119	0
85	MG	AR	4083	1/1	0.89	0.28	6.36	31,31,31,31	0
84	OHX	A	1901	7/7	0.98	0.29	6.36	127,127,127,128	0
85	MG	1	3867	1/1	0.95	0.43	6.32	35,35,35,35	0
85	MG	1	3740	1/1	0.92	0.36	6.32	30,30,30,30	0
84	OHX	1	3659	7/7	0.91	0.32	6.27	140,140,140,141	0
85	MG	AR	4206	1/1	0.81	0.28	6.23	33,33,33,33	0
85	MG	1	4084	1/1	0.88	0.27	6.19	32,32,32,32	0
84	OHX	AR	3521	7/7	0.96	0.28	6.18	117,118,118,118	0
84	OHX	1	3685	7/7	0.96	0.40	6.14	121,121,121,121	0
84	OHX	AR	3408	7/7	0.99	0.33	6.14	107,107,107,107	0
84	OHX	6	2011	7/7	0.96	0.43	6.10	146,146,147,147	0
85	MG	1	3990	1/1	0.92	0.30	6.10	24,24,24,24	0
84	OHX	AR	3715	7/7	0.96	0.29	6.09	118,118,119,119	0
84	OHX	1	3410	7/7	0.98	0.32	6.08	112,112,112,112	0
84	OHX	6	2001	7/7	0.90	0.28	6.07	119,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	1	3683	7/7	0.96	0.33	6.05	118,118,118,118	0
84	OHX	1	3679	7/7	0.94	0.30	6.00	131,131,132,132	0
84	OHX	AR	3689	7/7	0.94	0.34	5.96	118,118,119,119	0
84	OHX	AR	3414	7/7	0.98	0.30	5.95	113,113,114,114	0
85	MG	x	208	1/1	0.88	0.33	5.92	46,46,46,46	0
84	OHX	1	3582	7/7	0.96	0.29	5.92	121,121,121,121	0
84	OHX	AR	3638	7/7	0.95	0.42	5.89	119,119,119,119	0
85	MG	AR	3841	1/1	0.84	0.29	5.85	54,54,54,54	0
87	GOL	A	2160	6/6	0.82	0.35	5.85	60,60,60,60	0
85	MG	1	4078	1/1	0.98	0.29	5.84	24,24,24,24	0
84	OHX	1	3406	7/7	0.99	0.33	5.80	108,108,108,108	0
85	MG	s8	302	1/1	0.97	0.33	5.80	51,51,51,51	0
84	OHX	A	1985	7/7	0.89	0.31	5.79	140,140,141,141	0
84	OHX	AR	3699	7/7	0.96	0.36	5.78	117,117,117,117	0
85	MG	6	2122	1/1	0.86	0.48	5.76	61,61,61,61	0
84	OHX	1	3415	7/7	0.98	0.32	5.75	123,124,124,124	0
84	OHX	1	3462	7/7	0.94	0.21	5.74	119,120,120,120	0
84	OHX	6	2041	7/7	0.90	0.34	5.73	143,144,145,145	0
84	OHX	6	2030	7/7	0.92	0.29	5.73	118,118,118,119	0
85	MG	6	2103	1/1	0.88	0.33	5.72	69,69,69,69	0
84	OHX	1	3431	7/7	0.96	0.30	5.72	114,114,114,114	0
84	OHX	1	3662	7/7	0.95	0.31	5.71	116,116,116,116	0
85	MG	A	2056	1/1	0.91	0.34	5.66	65,65,65,65	0
84	OHX	AR	3613	7/7	0.96	0.29	5.65	112,112,112,112	0
84	OHX	6	2005	7/7	0.92	0.42	5.57	126,126,127,127	0
84	OHX	A	2006	7/7	0.92	0.31	5.57	149,150,150,150	0
84	OHX	A	2017	7/7	0.92	0.31	5.56	158,159,160,160	0
84	OHX	AR	3703	7/7	0.95	0.51	5.54	136,136,136,136	0
84	OHX	6	1910	7/7	0.98	0.26	5.48	119,120,120,120	0
85	MG	1	4127	1/1	0.80	0.26	5.47	45,45,45,45	0
84	OHX	1	3697	7/7	0.98	0.25	5.46	119,119,120,120	0
85	MG	CQ	202	1/1	0.94	0.33	5.45	32,32,32,32	0
84	OHX	AR	3404	7/7	0.99	0.33	5.44	112,112,112,112	0
84	OHX	AR	3688	7/7	0.95	0.29	5.39	136,136,137,137	0
84	OHX	A	1996	7/7	0.93	0.32	5.38	139,140,140,141	0
84	OHX	1	3420	7/7	0.98	0.29	5.38	118,118,118,118	0
84	OHX	AT	202	7/7	0.98	0.30	5.36	106,106,106,106	0
85	MG	4	227	1/1	0.91	0.40	5.35	52,52,52,52	0
84	OHX	1	3608	7/7	0.97	0.25	5.35	118,119,119,119	0
85	MG	v	302	1/1	0.97	0.33	5.34	36,36,36,36	0
84	OHX	AT	208	7/7	0.97	0.31	5.30	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	AS	211	7/7	0.91	0.29	5.30	141,141,142,142	0
85	MG	6	2125	1/1	0.93	0.32	5.27	75,75,75,75	0
84	OHX	A	1902	7/7	0.99	0.26	5.27	122,122,123,123	0
84	OHX	AR	3619	7/7	0.96	0.35	5.27	122,123,123,124	0
84	OHX	AR	3552	7/7	0.94	0.28	5.25	114,114,114,114	0
84	OHX	AR	3612	7/7	0.96	0.34	5.22	111,111,111,111	0
85	MG	1	4135	1/1	0.86	0.48	5.20	51,51,51,51	0
85	MG	AF	202	1/1	0.78	0.27	5.19	28,28,28,28	0
84	OHX	1	3620	7/7	0.89	0.35	5.18	118,118,118,118	0
85	MG	1	3809	1/1	0.95	0.27	5.17	39,39,39,39	0
84	OHX	A	2031	7/7	0.95	0.35	5.16	159,160,161,161	0
84	OHX	6	2028	7/7	0.94	0.40	5.16	123,124,124,124	0
84	OHX	AR	3661	7/7	0.97	0.46	5.14	112,112,112,113	0
85	MG	1	4066	1/1	0.94	0.27	5.14	20,20,20,20	0
84	OHX	1	3418	7/7	0.99	0.27	5.10	114,115,115,115	0
85	MG	CP	502	1/1	0.84	0.42	5.05	45,45,45,45	0
85	MG	6	2154	1/1	0.71	0.41	5.02	54,54,54,54	0
85	MG	1	3946	1/1	0.93	0.28	5.00	34,34,34,34	0
84	OHX	1	3643	7/7	0.92	0.39	4.99	114,114,114,114	0
84	OHX	1	3442	7/7	0.97	0.24	4.99	120,121,121,121	0
85	MG	1	3748	1/1	0.99	0.34	4.98	44,44,44,44	0
84	OHX	1	3626	7/7	0.90	0.36	4.98	124,124,124,124	0
85	MG	AR	3764	1/1	0.89	0.34	4.92	33,33,33,33	0
84	OHX	6	2050	7/7	0.92	0.47	4.91	159,159,160,160	0
84	OHX	1	3433	7/7	0.99	0.26	4.89	118,119,119,119	0
84	OHX	6	1906	7/7	0.99	0.29	4.87	122,123,123,124	0
85	MG	b	101	1/1	0.77	0.45	4.87	65,65,65,65	0
84	OHX	1	3506	7/7	0.97	0.29	4.85	109,109,110,110	0
84	OHX	A	2003	7/7	0.96	0.32	4.83	129,130,130,130	0
84	OHX	1	3419	7/7	0.99	0.26	4.82	107,107,107,107	0
85	MG	6	2093	1/1	0.96	0.33	4.80	47,47,47,47	0
86	HN8	AR	4263	22/22	0.95	0.26	4.76	27,27,27,27	22
85	MG	l	404	1/1	0.95	0.34	4.76	35,35,35,35	0
85	MG	AR	3987	1/1	0.97	0.30	4.75	31,31,31,31	0
84	OHX	AR	3524	7/7	0.94	0.29	4.75	118,119,119,119	0
85	MG	AR	4012	1/1	0.95	0.35	4.75	30,30,30,30	0
84	OHX	AR	3737	7/7	0.71	0.46	4.73	158,158,158,159	0
84	OHX	4	212	7/7	0.97	0.28	4.71	128,128,128,128	0
84	OHX	AR	3418	7/7	0.99	0.30	4.71	116,116,117,117	0
84	OHX	1	3650	7/7	0.94	0.27	4.70	128,128,128,128	0
85	MG	AR	4169	1/1	0.81	0.29	4.70	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	1	3609	7/7	0.93	0.40	4.68	119,120,120,120	0
85	MG	1	3884	1/1	0.91	0.34	4.66	29,29,29,29	0
85	MG	1	3738	1/1	0.94	0.35	4.64	28,28,28,28	0
84	OHX	A	2030	7/7	0.90	0.47	4.60	142,143,143,144	0
85	MG	AR	3934	1/1	0.91	0.31	4.59	32,32,32,32	0
85	MG	AR	3833	1/1	0.69	0.30	4.58	49,49,49,49	0
84	OHX	6	1986	7/7	0.93	0.32	4.57	147,148,148,148	0
84	OHX	AR	3426	7/7	0.99	0.27	4.57	111,112,112,112	0
85	MG	1	3778	1/1	0.87	0.46	4.56	49,49,49,49	0
84	OHX	6	1968	7/7	0.97	0.26	4.55	122,122,123,123	0
84	OHX	AR	3412	7/7	0.98	0.28	4.55	109,109,109,109	0
85	MG	AR	4114	1/1	0.94	0.28	4.54	40,40,40,40	0
84	OHX	6	1992	7/7	0.93	0.23	4.52	137,137,138,138	0
84	OHX	AR	3698	7/7	0.94	0.41	4.51	123,123,123,124	0
85	MG	AR	3910	1/1	0.99	0.32	4.49	23,23,23,23	0
85	MG	A	2115	1/1	0.92	0.38	4.48	83,83,83,83	0
85	MG	CR	205	1/1	0.89	0.40	4.46	31,31,31,31	0
85	MG	AR	3895	1/1	0.96	0.28	4.43	43,43,43,43	0
85	MG	1	4207	1/1	0.95	0.28	4.43	36,36,36,36	0
84	OHX	AR	3695	7/7	0.91	0.30	4.41	122,122,123,123	0
84	OHX	AR	3576	7/7	0.97	0.31	4.41	128,128,129,129	0
84	OHX	6	2015	7/7	0.95	0.35	4.36	135,135,136,136	0
84	OHX	A	2009	7/7	0.96	0.38	4.34	126,126,127,127	0
84	OHX	6	2052	7/7	0.90	0.33	4.32	143,144,144,144	0
85	MG	1	4064	1/1	0.85	0.30	4.32	58,58,58,58	0
85	MG	CE	404	1/1	0.88	0.29	4.32	27,27,27,27	0
85	MG	AR	3964	1/1	0.79	0.29	4.32	35,35,35,35	0
84	OHX	AR	3520	7/7	0.97	0.31	4.27	112,112,113,113	0
84	OHX	1	3436	7/7	0.99	0.28	4.26	115,115,115,115	0
84	OHX	AR	3582	7/7	0.98	0.28	4.22	114,114,114,114	0
84	OHX	AR	3607	7/7	0.94	0.30	4.20	113,113,113,113	0
84	OHX	AR	3575	7/7	0.95	0.28	4.17	119,120,120,120	0
84	OHX	1	3432	7/7	0.98	0.27	4.17	117,117,117,117	0
84	OHX	AR	3709	7/7	0.92	0.28	4.08	110,111,111,111	0
84	OHX	AR	3712	7/7	0.94	0.27	4.07	109,109,109,109	0
84	OHX	A	1964	7/7	0.95	0.28	4.07	122,122,123,123	0
84	OHX	1	3690	7/7	0.92	0.41	4.05	122,123,123,123	0
84	OHX	AR	3646	7/7	0.90	0.37	4.03	108,108,108,108	0
85	MG	A	2129	1/1	0.87	0.30	4.02	57,57,57,57	0
84	OHX	AR	3421	7/7	0.99	0.25	4.02	113,113,113,113	0
85	MG	6	2144	1/1	0.89	0.38	4.02	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
84	OHX	AR	3643	7/7	0.97	0.30	4.02	120,121,121,121	0
84	OHX	AR	3663	7/7	0.93	0.29	3.97	147,148,148,148	0
84	OHX	AH	201	7/7	0.95	0.44	3.96	129,129,129,130	0
84	OHX	6	1989	7/7	0.93	0.43	3.96	143,144,144,145	0
84	OHX	1	3427	7/7	0.99	0.26	3.95	112,113,113,113	0
84	OHX	AR	3743	7/7	0.96	0.33	3.93	109,109,109,109	0
84	OHX	AR	3606	7/7	0.93	0.31	3.92	113,113,114,114	0
84	OHX	1	3676	7/7	0.91	0.29	3.92	149,150,150,150	0
84	OHX	6	1978	7/7	0.96	0.29	3.91	117,117,117,118	0
85	MG	CI	301	1/1	0.94	0.26	3.91	33,33,33,33	0
84	OHX	AR	3493	7/7	0.97	0.25	3.90	114,114,114,114	0
84	OHX	A	1918	7/7	0.93	0.23	3.90	128,129,129,129	0
84	OHX	AR	3596	7/7	0.93	0.24	3.85	121,121,122,122	0
84	OHX	6	1991	7/7	0.98	0.29	3.84	133,134,134,135	0
84	OHX	1	3413	7/7	0.99	0.32	3.81	112,113,113,113	0
84	OHX	1	3425	7/7	0.97	0.25	3.79	108,109,109,109	0
85	MG	1	3734	1/1	0.93	0.34	3.78	43,43,43,43	0
84	OHX	1	3577	7/7	0.96	0.31	3.77	118,118,119,119	0
87	GOL	AR	4261	6/6	0.78	0.34	3.75	48,48,48,48	0
85	MG	AR	3864	1/1	0.92	0.29	3.73	40,40,40,40	0
84	OHX	AR	3422	7/7	0.99	0.27	3.72	112,112,112,112	0
85	MG	6	2088	1/1	0.76	0.35	3.72	82,82,82,82	0
85	MG	AR	3939	1/1	0.96	0.31	3.71	31,31,31,31	0
85	MG	A	2100	1/1	0.92	0.44	3.71	92,92,92,92	0
85	MG	DH	203	1/1	0.95	0.29	3.70	31,31,31,31	0
84	OHX	AR	3588	7/7	0.96	0.27	3.69	112,112,112,113	0
84	OHX	1	3426	7/7	0.99	0.28	3.67	120,120,120,120	0
84	OHX	1	3721	7/7	0.89	0.35	3.67	127,127,127,128	0
84	OHX	6	1909	7/7	0.97	0.26	3.66	137,138,138,139	0
84	OHX	AR	3672	7/7	0.98	0.29	3.66	109,110,110,110	0
84	OHX	K	201	7/7	0.93	0.51	3.64	137,137,138,138	0
84	OHX	AR	3573	7/7	0.98	0.21	3.63	123,123,123,123	0
84	OHX	6	2029	7/7	0.96	0.41	3.63	152,153,153,154	0
84	OHX	A	1997	7/7	0.96	0.28	3.61	139,140,140,140	0
84	OHX	1	3445	7/7	0.96	0.26	3.61	111,112,112,112	0
84	OHX	1	3416	7/7	0.99	0.24	3.60	109,109,109,109	0
84	OHX	3	208	7/7	0.97	0.30	3.59	116,116,116,116	0
84	OHX	x	202	7/7	0.93	0.36	3.58	144,144,145,145	0
84	OHX	1	3649	7/7	0.95	0.35	3.57	113,113,113,113	0
84	OHX	1	3703	7/7	0.96	0.46	3.57	131,131,132,132	0
84	OHX	A	1905	7/7	0.99	0.29	3.56	128,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	3848	1/1	0.97	0.28	3.56	31,31,31,31	0
84	OHX	A	1947	7/7	0.96	0.27	3.53	129,129,130,130	0
84	OHX	1	3584	7/7	0.96	0.24	3.52	114,114,114,114	0
84	OHX	AC	101	7/7	0.98	0.30	3.51	114,115,115,115	0
84	OHX	1	3605	7/7	0.94	0.33	3.50	129,130,130,130	0
84	OHX	M	201	7/7	0.97	0.38	3.47	137,137,138,138	0
84	OHX	2	201	7/7	0.99	0.31	3.46	119,119,120,120	0
84	OHX	A	2040	7/7	0.93	0.37	3.46	162,162,162,162	0
84	OHX	AR	3424	7/7	0.99	0.27	3.46	112,112,113,113	0
84	OHX	CV	201	7/7	0.99	0.31	3.45	117,117,117,117	0
84	OHX	1	3653	7/7	0.90	0.29	3.42	133,133,133,133	0
85	MG	c1	202	1/1	0.93	0.41	3.41	67,67,67,67	0
84	OHX	AR	3653	7/7	0.97	0.30	3.41	120,120,121,121	0
85	MG	6	2086	1/1	0.69	0.25	3.40	82,82,82,82	0
84	OHX	6	2043	7/7	0.93	0.30	3.40	145,145,146,146	0
84	OHX	AR	3420	7/7	0.99	0.29	3.39	113,114,114,114	0
84	OHX	1	3556	7/7	0.93	0.27	3.37	117,117,117,117	0
84	OHX	AR	3405	7/7	0.99	0.34	3.37	119,119,120,120	0
84	OHX	e	101	7/7	0.96	0.41	3.36	143,144,145,145	0
84	OHX	AR	3459	7/7	0.97	0.26	3.34	114,114,115,115	0
84	OHX	1	3414	7/7	0.99	0.27	3.34	109,109,109,109	0
85	MG	AR	4007	1/1	0.96	0.28	3.33	29,29,29,29	0
84	OHX	6	1993	7/7	0.94	0.28	3.32	134,135,135,135	0
84	OHX	1	3687	7/7	0.88	0.42	3.32	149,149,150,150	0
86	HN8	1	4223	22/22	0.95	0.24	3.25	32,32,32,32	0
85	MG	DC	202	1/1	0.86	0.30	3.25	48,48,48,48	0
84	OHX	1	3437	7/7	0.99	0.24	3.25	116,117,117,117	0
84	OHX	1	3551	7/7	0.97	0.27	3.23	118,118,119,119	0
84	OHX	1	3646	7/7	0.97	0.25	3.22	117,118,118,118	0
84	OHX	AR	3416	7/7	0.99	0.29	3.22	114,114,115,115	0
85	MG	AB	206	1/1	0.94	0.27	3.22	26,26,26,26	0
85	MG	AR	3825	1/1	0.94	0.27	3.21	33,33,33,33	0
85	MG	6	2116	1/1	0.93	0.21	3.20	62,62,62,62	0
85	MG	1	4083	1/1	0.94	0.29	3.17	41,41,41,41	0
84	OHX	1	3543	7/7	0.96	0.22	3.17	119,119,120,120	0
84	OHX	6	1907	7/7	0.97	0.32	3.15	135,136,136,137	0
84	OHX	1	3599	7/7	0.95	0.43	3.14	115,116,116,116	0
85	MG	d3	202	1/1	0.95	0.33	3.14	47,47,47,47	0
84	OHX	1	3422	7/7	0.99	0.26	3.12	116,116,117,117	0
84	OHX	AR	3721	7/7	0.92	0.38	3.12	139,139,140,140	0
84	OHX	AR	3722	7/7	0.88	0.31	3.12	140,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	6	2035	7/7	0.93	0.36	3.12	142,142,143,143	0
84	OHX	1	401	7/7	0.92	0.41	3.11	143,143,144,144	0
84	OHX	AR	3423	7/7	0.99	0.28	3.10	110,111,111,111	0
84	OHX	4	209	7/7	0.97	0.23	3.09	113,113,113,113	0
84	OHX	AR	3636	7/7	0.93	0.48	3.08	133,133,134,134	0
84	OHX	AR	3547	7/7	0.97	0.28	3.06	116,116,116,117	0
84	OHX	6	1994	7/7	0.96	0.25	3.04	170,170,170,170	0
85	MG	AR	3814	1/1	0.86	0.31	3.03	105,105,105,105	0
84	OHX	AR	3705	7/7	0.85	0.36	3.03	141,142,142,142	0
84	OHX	1	3623	7/7	0.96	0.22	3.01	114,114,115,115	0
84	OHX	1	3411	7/7	0.99	0.29	3.01	111,112,112,112	0
85	MG	1	3900	1/1	0.97	0.34	3.01	42,42,42,42	0
84	OHX	1	3638	7/7	0.97	0.33	3.00	122,123,123,123	0
84	OHX	AR	3427	7/7	0.95	0.29	2.99	110,110,111,111	0
84	OHX	1	3612	7/7	0.95	0.31	2.99	122,122,122,122	0
84	OHX	AR	3501	7/7	0.97	0.32	2.97	113,113,114,114	0
84	OHX	AR	3431	7/7	0.99	0.24	2.96	109,109,110,110	0
84	OHX	1	3629	7/7	0.94	0.22	2.94	148,148,148,149	0
84	OHX	1	3572	7/7	0.97	0.27	2.94	118,119,119,119	0
84	OHX	AR	3568	7/7	0.95	0.25	2.91	117,117,117,117	0
84	OHX	AR	3566	7/7	0.97	0.24	2.90	115,115,115,116	0
84	OHX	AR	3616	7/7	0.97	0.34	2.90	109,110,110,110	0
84	OHX	AR	3617	7/7	0.96	0.28	2.89	123,123,123,123	0
85	MG	1	3959	1/1	0.85	0.27	2.88	66,66,66,66	0
85	MG	AR	4179	1/1	0.97	0.27	2.85	43,43,43,43	0
84	OHX	1	3438	7/7	0.97	0.25	2.84	117,117,117,117	0
84	OHX	4	216	7/7	0.93	0.26	2.83	126,126,126,126	0
84	OHX	1	3507	7/7	0.96	0.23	2.82	113,113,114,114	0
85	MG	1	4052	1/1	0.96	0.29	2.81	21,21,21,21	0
84	OHX	6	1971	7/7	0.94	0.24	2.81	136,136,136,137	0
84	OHX	1	3428	7/7	0.99	0.28	2.80	126,126,127,127	0
84	OHX	1	3701	7/7	0.91	0.31	2.80	139,139,140,140	0
84	OHX	A	1940	7/7	0.97	0.29	2.80	137,138,138,139	0
84	OHX	AT	214	7/7	0.95	0.34	2.80	131,131,131,132	0
85	MG	1	3739	1/1	0.83	0.32	2.78	51,51,51,51	0
84	OHX	6	2032	7/7	0.93	0.50	2.76	131,131,132,132	0
84	OHX	6	2025	7/7	0.94	0.39	2.70	120,120,121,121	0
84	OHX	A	1979	7/7	0.97	0.22	2.70	142,143,144,144	0
85	MG	AR	3853	1/1	0.95	0.26	2.69	43,43,43,43	0
85	MG	A	2147	1/1	0.93	0.27	2.69	79,79,79,79	0
84	OHX	6	2027	7/7	0.95	0.47	2.68	146,147,147,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	A	1908	7/7	0.98	0.24	2.68	141,142,143,143	0
84	OHX	1	3423	7/7	0.99	0.26	2.67	120,120,121,121	0
85	MG	F	301	1/1	0.92	0.33	2.65	64,64,64,64	0
84	OHX	4	215	7/7	0.91	0.28	2.65	137,138,138,138	0
84	OHX	6	2044	7/7	0.96	0.35	2.65	140,141,141,141	0
85	MG	AR	4038	1/1	0.92	0.23	2.64	35,35,35,35	0
84	OHX	AR	3496	7/7	0.97	0.24	2.61	112,113,113,113	0
84	OHX	1	3417	7/7	0.98	0.31	2.59	116,117,117,117	0
84	OHX	1	3405	7/7	0.99	0.37	2.59	124,125,125,125	0
85	MG	AR	3794	1/1	0.82	0.25	2.59	34,34,34,34	0
84	OHX	1	3606	7/7	0.95	0.39	2.59	138,138,138,138	0
87	GOL	v	305	6/6	0.86	0.26	2.55	38,38,38,38	0
84	OHX	AR	3603	7/7	0.95	0.24	2.55	107,107,107,107	0
84	OHX	AR	3736	7/7	0.93	0.28	2.53	132,132,132,133	0
84	OHX	6	2013	7/7	0.93	0.33	2.53	121,122,122,122	0
84	OHX	AR	3439	7/7	0.98	0.25	2.52	119,120,120,120	0
85	MG	1	3916	1/1	0.96	0.29	2.51	26,26,26,26	0
85	MG	sM	202	1/1	0.94	0.55	2.49	42,42,42,42	0
84	OHX	AR	3543	7/7	0.96	0.24	2.49	123,123,123,123	0
85	MG	1	3798	1/1	0.98	0.23	2.47	32,32,32,32	0
84	OHX	AR	3667	7/7	0.94	0.38	2.47	146,147,147,147	0
85	MG	1	3917	1/1	0.91	0.26	2.46	30,30,30,30	0
84	OHX	AR	3671	7/7	0.96	0.28	2.46	113,113,113,113	0
85	MG	1	3741	1/1	0.95	0.25	2.45	37,37,37,37	0
84	OHX	1	3541	7/7	0.96	0.25	2.44	119,119,120,120	0
85	MG	A	2095	1/1	0.85	0.25	2.42	96,96,96,96	0
84	OHX	AR	3668	7/7	0.92	0.37	2.42	131,132,132,132	0
84	OHX	1	3675	7/7	0.94	0.30	2.41	140,141,141,141	0
85	MG	w	202	1/1	0.91	0.31	2.41	31,31,31,31	0
84	OHX	6	2051	7/7	0.89	0.29	2.39	172,172,172,173	0
85	MG	1	4100	1/1	0.91	0.27	2.38	53,53,53,53	0
84	OHX	y	201	7/7	0.94	0.32	2.36	128,129,129,129	0
84	OHX	AR	3599	7/7	0.92	0.24	2.35	136,136,136,136	0
84	OHX	AR	3432	7/7	0.97	0.27	2.34	117,117,117,118	0
85	MG	AR	3816	1/1	0.83	0.24	2.33	39,39,39,39	0
85	MG	AR	4203	1/1	0.94	0.24	2.32	29,29,29,29	0
84	OHX	1	3449	7/7	0.97	0.23	2.32	117,117,118,118	0
84	OHX	1	3404	7/7	0.98	0.35	2.29	120,120,121,121	0
85	MG	1	3924	1/1	0.95	0.37	2.29	60,60,60,60	0
84	OHX	1	3616	7/7	0.95	0.31	2.24	146,146,147,147	0
85	MG	c8	202	1/1	0.91	0.33	2.23	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3570	7/7	0.96	0.25	2.23	120,121,121,121	0
84	OHX	1	3636	7/7	0.93	0.33	2.22	126,126,126,126	0
85	MG	1	4167	1/1	0.94	0.23	2.20	23,23,23,23	0
84	OHX	AR	3425	7/7	0.98	0.23	2.20	105,106,106,106	0
84	OHX	A	2018	7/7	0.94	0.34	2.18	155,155,156,156	0
84	OHX	6	1904	7/7	0.99	0.27	2.12	124,124,124,125	0
84	OHX	AR	3455	7/7	0.97	0.22	2.10	111,112,112,112	0
85	MG	r	302	1/1	0.89	0.22	2.09	37,37,37,37	0
84	OHX	c4	201	7/7	0.89	0.53	2.06	152,152,153,153	0
84	OHX	AR	3561	7/7	0.97	0.24	2.04	110,110,110,111	0
84	OHX	1	3704	7/7	0.93	0.32	2.04	116,117,117,117	0
84	OHX	1	3670	7/7	0.96	0.24	1.98	111,111,111,111	0
84	OHX	AR	3704	7/7	0.93	0.38	1.95	133,133,133,133	0
84	OHX	1	3563	7/7	0.93	0.24	1.95	114,114,115,115	0
85	MG	6	2129	1/1	0.91	0.39	1.94	62,62,62,62	0
85	MG	j	302	1/1	0.81	0.25	1.93	35,35,35,35	0
85	MG	1	3873	1/1	0.89	0.23	1.91	48,48,48,48	0
85	MG	AR	3858	1/1	0.98	0.32	1.91	36,36,36,36	0
85	MG	1	4034	1/1	0.98	0.25	1.91	42,42,42,42	0
84	OHX	6	2002	7/7	0.91	0.27	1.90	132,133,133,134	0
85	MG	6	2131	1/1	0.98	0.24	1.89	44,44,44,44	0
85	MG	AR	3956	1/1	0.90	0.22	1.88	29,29,29,29	0
84	OHX	6	2022	7/7	0.93	0.29	1.88	153,154,154,155	0
85	MG	1	3942	1/1	0.92	0.26	1.85	32,32,32,32	0
84	OHX	AR	3611	7/7	0.94	0.23	1.84	126,126,126,126	0
84	OHX	AR	3553	7/7	0.96	0.29	1.80	113,113,113,113	0
84	OHX	AT	215	7/7	0.94	0.20	1.80	137,138,138,138	0
84	OHX	AR	3583	7/7	0.95	0.22	1.78	113,114,114,114	0
85	MG	A	2084	1/1	0.77	0.22	1.78	72,72,72,72	0
85	MG	CM	203	1/1	0.95	0.21	1.77	55,55,55,55	0
84	OHX	A	1909	7/7	0.95	0.24	1.76	151,151,152,153	0
84	OHX	6	1985	7/7	0.96	0.33	1.75	130,130,131,131	0
84	OHX	AR	3621	7/7	0.96	0.35	1.74	135,135,136,136	0
85	MG	A	2149	1/1	0.89	0.25	1.74	60,60,60,60	0
84	OHX	A	1973	7/7	0.95	0.28	1.73	167,168,169,169	0
85	MG	6	2128	1/1	0.95	0.23	1.72	47,47,47,47	0
85	MG	1	3830	1/1	0.90	0.22	1.71	44,44,44,44	0
84	OHX	AR	3438	7/7	0.99	0.22	1.71	108,108,108,108	0
84	OHX	d9	101	7/7	0.92	0.48	1.66	153,153,154,154	0
84	OHX	1	3652	7/7	0.92	0.33	1.65	110,110,110,110	0
84	OHX	AR	3587	7/7	0.95	0.24	1.64	126,126,126,126	0
84	OHX	AR	3562	7/7	0.96	0.24	1.63	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3585	7/7	0.97	0.20	1.62	117,117,117,117	0
84	OHX	1	3630	7/7	0.98	0.33	1.62	113,113,114,114	0
84	OHX	1	3554	7/7	0.95	0.24	1.61	129,129,130,130	0
84	OHX	1	3613	7/7	0.97	0.47	1.59	120,120,121,121	0
84	OHX	1	3424	7/7	0.99	0.23	1.58	115,115,115,115	0
85	MG	1	4163	1/1	0.84	0.24	1.58	44,44,44,44	0
84	OHX	A	2024	7/7	0.95	0.24	1.58	151,152,153,153	0
84	OHX	1	3444	7/7	0.98	0.23	1.56	116,116,117,117	0
85	MG	6	2145	1/1	0.85	0.20	1.56	59,59,59,59	0
85	MG	AR	3752	1/1	0.83	0.21	1.53	37,37,37,37	0
84	OHX	6	1927	7/7	0.97	0.22	1.51	124,124,125,125	0
84	OHX	1	3621	7/7	0.95	0.23	1.50	125,126,126,126	0
85	MG	1	4095	1/1	0.96	0.20	1.48	61,61,61,61	0
84	OHX	AR	3730	7/7	0.91	0.33	1.48	176,176,176,176	0
84	OHX	AR	3620	7/7	0.97	0.33	1.45	143,144,144,144	0
84	OHX	AR	3435	7/7	0.98	0.22	1.43	112,113,113,113	0
84	OHX	1	3585	7/7	0.97	0.23	1.43	115,115,116,116	0
84	OHX	c1	201	7/7	0.96	0.41	1.43	147,148,148,149	0
84	OHX	1	3681	7/7	0.95	0.32	1.41	127,127,127,128	0
85	MG	DI	202	1/1	0.79	0.36	1.38	56,56,56,56	0
84	OHX	6	2004	7/7	0.91	0.40	1.38	157,157,158,158	0
84	OHX	CE	402	7/7	0.93	0.38	1.37	138,139,139,139	0
84	OHX	6	2021	7/7	0.90	0.25	1.36	181,181,182,182	0
85	MG	AR	4212	1/1	0.95	0.27	1.31	31,31,31,31	0
84	OHX	1	3524	7/7	0.98	0.21	1.28	116,117,117,117	0
84	OHX	3	207	7/7	0.96	0.20	1.28	137,138,138,138	0
85	MG	AR	4069	1/1	0.89	0.23	1.27	26,26,26,26	0
84	OHX	AR	3701	7/7	0.93	0.29	1.27	128,128,128,128	0
85	MG	AR	4176	1/1	0.91	0.23	1.26	33,33,33,33	0
84	OHX	1	3451	7/7	0.96	0.22	1.25	111,111,111,111	0
84	OHX	CX	202	7/7	0.96	0.27	1.24	117,118,118,118	0
84	OHX	1	3523	7/7	0.98	0.19	1.24	119,119,120,120	0
84	OHX	1	3688	7/7	0.92	0.25	1.23	129,130,130,130	0
84	OHX	6	1932	7/7	0.93	0.23	1.22	132,132,133,133	0
84	OHX	AR	3659	7/7	0.94	0.54	1.22	136,136,137,137	0
84	OHX	1	3574	7/7	0.97	0.28	1.21	116,116,117,117	0
84	OHX	AR	3687	7/7	0.96	0.37	1.19	121,121,122,122	0
84	OHX	AR	3591	7/7	0.97	0.25	1.18	112,112,112,112	0
84	OHX	A	2029	7/7	0.90	0.20	1.16	184,184,184,184	0
84	OHX	AR	3442	7/7	0.97	0.22	1.15	112,112,112,112	0
84	OHX	1	3589	7/7	0.96	0.23	1.14	113,113,113,113	0
85	MG	AR	4175	1/1	0.88	0.25	1.13	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	A	2004	7/7	0.97	0.22	1.12	139,139,140,140	0
84	OHX	1	3568	7/7	0.97	0.28	1.11	115,116,116,116	0
85	MG	AB	207	1/1	0.84	0.24	1.11	34,34,34,34	0
84	OHX	AR	3436	7/7	0.98	0.24	1.09	109,109,109,109	0
84	OHX	AR	3428	7/7	0.99	0.21	1.05	115,115,115,116	0
85	MG	z	202	1/1	0.98	0.28	1.03	59,59,59,59	0
84	OHX	1	3519	7/7	0.96	0.22	1.03	116,116,116,116	0
84	OHX	1	3525	7/7	0.95	0.21	0.98	114,114,114,115	0
84	OHX	AR	3593	7/7	0.94	0.23	0.96	113,114,114,114	0
84	OHX	A	1986	7/7	0.95	0.28	0.95	168,169,170,170	0
84	OHX	AR	3515	7/7	0.98	0.22	0.94	113,113,114,114	0
84	OHX	6	2012	7/7	0.95	0.21	0.93	136,136,137,137	0
84	OHX	DD	101	7/7	0.98	0.29	0.93	113,114,114,114	0
84	OHX	AR	3441	7/7	0.96	0.18	0.93	116,117,117,117	0
84	OHX	1	3617	7/7	0.96	0.23	0.92	122,122,122,122	0
84	OHX	AS	210	7/7	0.92	0.24	0.92	115,115,116,116	0
84	OHX	AR	3536	7/7	0.96	0.22	0.92	123,124,124,124	0
84	OHX	6	2037	7/7	0.93	0.40	0.88	137,137,138,138	0
84	OHX	AR	3655	7/7	0.94	0.24	0.88	129,129,130,130	0
84	OHX	A	1983	7/7	0.96	0.24	0.84	142,142,143,143	0
84	OHX	AR	3618	7/7	0.95	0.21	0.82	113,113,114,114	0
84	OHX	A	1977	7/7	0.95	0.25	0.82	153,154,154,155	0
85	MG	1	3932	1/1	0.89	0.19	0.82	55,55,55,55	0
84	OHX	AR	3707	7/7	0.88	0.25	0.82	129,129,130,130	0
84	OHX	AR	3565	7/7	0.95	0.20	0.81	113,113,113,113	0
84	OHX	1	3458	7/7	0.96	0.20	0.81	116,116,116,117	0
85	MG	1	4114	1/1	0.97	0.23	0.80	52,52,52,52	0
84	OHX	CF	401	7/7	0.89	0.31	0.80	146,146,147,147	0
84	OHX	1	3467	7/7	0.98	0.17	0.78	123,123,124,124	0
84	OHX	AR	3440	7/7	0.99	0.18	0.77	125,125,125,126	0
84	OHX	1	3429	7/7	0.99	0.22	0.76	110,110,110,110	0
84	OHX	A	1999	7/7	0.96	0.24	0.74	146,146,147,147	0
84	OHX	A	1921	7/7	0.97	0.22	0.74	142,143,144,144	0
84	OHX	1	3537	7/7	0.95	0.24	0.73	115,115,115,116	0
84	OHX	6	1908	7/7	0.99	0.25	0.72	120,120,121,121	0
84	OHX	6	1981	7/7	0.98	0.29	0.72	139,140,140,140	0
84	OHX	AR	3662	7/7	0.96	0.22	0.71	111,111,112,112	0
84	OHX	AR	3545	7/7	0.96	0.24	0.71	108,108,108,108	0
84	OHX	6	1913	7/7	0.98	0.26	0.68	133,134,135,135	0
85	MG	6	2171	1/1	0.88	0.25	0.68	56,56,56,56	0
85	MG	AR	3769	1/1	0.93	0.26	0.68	59,59,59,59	0
85	MG	AR	4027	1/1	0.92	0.23	0.67	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	A	1976	7/7	0.96	0.18	0.67	123,124,124,124	0
84	OHX	A	1962	7/7	0.98	0.21	0.66	132,133,133,134	0
84	OHX	A	2002	7/7	0.95	0.31	0.66	147,148,149,149	0
84	OHX	1	3498	7/7	0.94	0.21	0.65	115,116,116,116	0
84	OHX	6	1962	7/7	0.94	0.30	0.64	136,137,137,137	0
84	OHX	6	1911	7/7	0.97	0.24	0.63	134,135,135,135	0
85	MG	1	4134	1/1	0.99	0.20	0.62	63,63,63,63	0
85	MG	AR	4048	1/1	0.97	0.23	0.62	34,34,34,34	0
84	OHX	AR	3528	7/7	0.94	0.21	0.61	108,108,108,108	0
84	OHX	1	3440	7/7	0.98	0.22	0.61	110,110,111,111	0
85	MG	6	2135	1/1	0.95	0.24	0.61	49,49,49,49	0
85	MG	AR	3982	1/1	0.86	0.24	0.60	53,53,53,53	0
88	ZN	d7	101	1/1	0.79	0.47	0.60	143,143,143,143	0
85	MG	1	3805	1/1	0.85	0.20	0.58	29,29,29,29	0
85	MG	1	4164	1/1	0.99	0.22	0.57	58,58,58,58	0
84	OHX	1	3536	7/7	0.97	0.22	0.55	109,109,109,109	0
84	OHX	A	2043	7/7	0.90	0.19	0.55	155,156,156,157	0
84	OHX	AG	201	7/7	0.97	0.21	0.55	114,115,115,115	0
85	MG	1	4071	1/1	0.95	0.20	0.54	40,40,40,40	0
84	OHX	A	2028	7/7	0.94	0.34	0.54	157,157,158,158	0
88	ZN	c	101	1/1	0.93	0.34	0.54	145,145,145,145	0
85	MG	DA	201	1/1	0.87	0.28	0.53	48,48,48,48	0
84	OHX	6	1977	7/7	0.92	0.25	0.52	150,151,151,152	0
85	MG	A	2092	1/1	0.86	0.27	0.52	91,91,91,91	0
84	OHX	A	2038	7/7	0.91	0.34	0.51	146,147,147,147	0
84	OHX	1	3455	7/7	0.96	0.16	0.51	127,127,127,128	0
84	OHX	AR	3466	7/7	0.96	0.18	0.51	120,120,121,121	0
85	MG	AR	3946	1/1	0.90	0.30	0.50	59,59,59,59	0
84	OHX	AR	3742	7/7	0.93	0.25	0.50	128,129,129,129	0
84	OHX	1	3660	7/7	0.94	0.28	0.50	153,153,154,154	0
84	OHX	A	2016	7/7	0.96	0.28	0.49	142,143,143,144	0
85	MG	AB	204	1/1	0.90	0.29	0.49	52,52,52,52	0
85	MG	AR	3817	1/1	0.72	0.24	0.47	112,112,112,112	0
84	OHX	AR	3511	7/7	0.95	0.26	0.46	108,108,108,108	0
84	OHX	1	3489	7/7	0.96	0.21	0.45	113,113,114,114	0
84	OHX	A	1957	7/7	0.98	0.23	0.45	133,134,134,134	0
84	OHX	1	3499	7/7	0.98	0.23	0.43	111,111,111,111	0
84	OHX	1	3517	7/7	0.95	0.26	0.43	119,119,120,120	0
84	OHX	1	3469	7/7	0.95	0.21	0.42	117,117,118,118	0
85	MG	A	2086	1/1	0.91	0.24	0.42	66,66,66,66	0
84	OHX	A	2015	7/7	0.89	0.40	0.41	169,170,171,172	0
84	OHX	1	3587	7/7	0.98	0.23	0.41	133,133,133,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	1	3468	7/7	0.98	0.20	0.40	116,117,117,117	0
84	OHX	6	2034	7/7	0.96	0.19	0.40	155,155,155,155	0
84	OHX	k	401	7/7	0.96	0.27	0.39	118,118,118,118	0
84	OHX	AR	3623	7/7	0.96	0.29	0.38	138,139,139,139	0
85	MG	1	3789	1/1	0.91	0.17	0.36	42,42,42,42	0
84	OHX	AR	3555	7/7	0.96	0.21	0.35	115,115,115,115	0
85	MG	6	2087	1/1	0.86	0.30	0.33	56,56,56,56	0
84	OHX	AR	3531	7/7	0.94	0.19	0.32	115,115,115,115	0
85	MG	CP	505	1/1	0.96	0.28	0.32	71,71,71,71	0
84	OHX	6	1996	7/7	0.96	0.20	0.31	154,154,155,155	0
85	MG	AR	3775	1/1	0.97	0.23	0.30	22,22,22,22	0
84	OHX	A	1935	7/7	0.95	0.23	0.27	140,140,141,141	0
84	OHX	A	1904	7/7	0.99	0.23	0.27	133,134,134,134	0
85	MG	1	3811	1/1	0.78	0.30	0.27	44,44,44,44	0
84	OHX	A	1998	7/7	0.97	0.25	0.24	158,159,160,160	0
84	OHX	6	1916	7/7	0.98	0.21	0.23	119,120,120,120	0
84	OHX	AR	3437	7/7	0.98	0.23	0.23	108,108,108,108	0
84	OHX	1	3724	7/7	0.86	0.22	0.22	113,113,113,113	0
84	OHX	1	3581	7/7	0.95	0.22	0.22	112,113,113,113	0
85	MG	AS	222	1/1	0.98	0.21	0.20	44,44,44,44	0
85	MG	6	2184	1/1	0.98	0.22	0.19	83,83,83,83	0
84	OHX	A	2033	7/7	0.94	0.25	0.18	146,146,147,147	0
85	MG	1	3757	1/1	0.96	0.19	0.16	38,38,38,38	0
84	OHX	AR	3450	7/7	0.98	0.16	0.16	127,127,127,128	0
85	MG	1	3974	1/1	0.92	0.22	0.16	28,28,28,28	0
84	OHX	1	3607	7/7	0.97	0.17	0.16	122,122,122,122	0
84	OHX	1	3471	7/7	0.96	0.21	0.15	112,112,113,113	0
84	OHX	1	3492	7/7	0.97	0.19	0.14	117,118,118,118	0
84	OHX	6	1919	7/7	0.94	0.21	0.13	121,121,122,122	0
85	MG	A	2144	1/1	0.96	0.39	0.13	69,69,69,69	0
84	OHX	AR	3731	7/7	0.96	0.19	0.13	117,117,117,117	0
84	OHX	AT	213	7/7	0.91	0.25	0.12	137,137,137,137	0
84	OHX	AS	201	7/7	0.98	0.24	0.12	119,119,119,120	0
85	MG	6	2142	1/1	0.91	0.24	0.12	83,83,83,83	0
84	OHX	A	1910	7/7	0.97	0.23	0.10	138,139,139,140	0
84	OHX	1	3593	7/7	0.96	0.15	0.10	166,167,167,167	0
84	OHX	A	1958	7/7	0.95	0.22	0.10	173,173,173,173	0
84	OHX	3	206	7/7	0.94	0.20	0.08	127,127,128,128	0
84	OHX	AR	3460	7/7	0.95	0.20	0.05	112,112,112,112	0
85	MG	1	4103	1/1	0.96	0.27	0.05	60,60,60,60	0
84	OHX	CK	201	7/7	0.96	0.21	0.05	118,118,119,119	0
84	OHX	AR	3433	7/7	0.98	0.21	0.05	110,110,110,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3512	7/7	0.96	0.18	0.02	118,118,119,119	0
84	OHX	1	3578	7/7	0.97	0.19	-0.00	107,107,107,107	0
84	OHX	1	3583	7/7	0.95	0.16	0.00	131,132,132,132	0
85	MG	s4	301	1/1	0.90	0.23	-0.01	59,59,59,59	0
84	OHX	1	3485	7/7	0.93	0.16	-0.01	120,121,121,121	0
84	OHX	AR	3580	7/7	0.96	0.20	-0.03	117,118,118,118	0
85	MG	s6	301	1/1	0.87	0.29	-0.07	77,77,77,77	0
85	MG	6	2056	1/1	0.92	0.22	-0.07	77,77,77,77	0
84	OHX	A	1911	7/7	0.97	0.22	-0.07	139,140,141,141	0
85	MG	AR	4095	1/1	0.96	0.22	-0.07	25,25,25,25	0
84	OHX	AR	3557	7/7	0.96	0.16	-0.08	123,123,124,124	0
85	MG	A	2054	1/1	0.75	0.23	-0.09	66,66,66,66	0
85	MG	3	219	1/1	0.96	0.20	-0.09	56,56,56,56	0
84	OHX	AR	3541	7/7	0.96	0.19	-0.10	125,125,125,125	0
84	OHX	1	3565	7/7	0.96	0.25	-0.12	131,131,131,131	0
84	OHX	6	1999	7/7	0.94	0.26	-0.12	138,139,139,140	0
84	OHX	A	1978	7/7	0.96	0.26	-0.12	143,144,144,145	0
84	OHX	6	1998	7/7	0.96	0.33	-0.14	146,146,147,147	0
84	OHX	1	3671	7/7	0.95	0.24	-0.15	149,150,150,150	0
85	MG	AR	3891	1/1	0.89	0.27	-0.16	69,69,69,69	0
85	MG	6	2063	1/1	0.97	0.20	-0.16	82,82,82,82	0
85	MG	o	302	1/1	0.92	0.21	-0.16	39,39,39,39	0
85	MG	CK	202	1/1	0.96	0.20	-0.17	44,44,44,44	0
84	OHX	AT	212	7/7	0.94	0.30	-0.17	128,128,128,128	0
84	OHX	6	1990	7/7	0.96	0.29	-0.17	129,130,130,130	0
84	OHX	AT	210	7/7	0.96	0.20	-0.19	119,119,120,120	0
84	OHX	6	2047	7/7	0.94	0.32	-0.21	161,162,162,162	0
84	OHX	A	1971	7/7	0.85	0.23	-0.22	149,150,151,151	0
84	OHX	A	1946	7/7	0.86	0.22	-0.24	165,166,166,167	0
84	OHX	1	3441	7/7	0.98	0.20	-0.25	116,116,116,117	0
84	OHX	1	3482	7/7	0.98	0.18	-0.26	117,117,117,117	0
84	OHX	AR	3563	7/7	0.94	0.17	-0.27	122,122,123,123	0
84	OHX	AR	3681	7/7	0.94	0.23	-0.29	140,140,140,141	0
84	OHX	AR	3723	7/7	0.93	0.29	-0.31	146,146,147,147	0
84	OHX	6	1925	7/7	0.97	0.20	-0.32	122,122,122,123	0
84	OHX	1	3481	7/7	0.95	0.19	-0.32	116,117,117,117	0
84	OHX	AR	3505	7/7	0.98	0.20	-0.32	114,114,115,115	0
84	OHX	6	1995	7/7	0.96	0.24	-0.34	133,134,134,135	0
88	ZN	DR	501	1/1	0.99	0.15	-0.34	59,59,59,59	0
84	OHX	A	1914	7/7	0.98	0.23	-0.35	126,127,127,127	0
84	OHX	AR	3484	7/7	0.97	0.19	-0.36	114,114,114,114	0
85	MG	CX	204	1/1	0.91	0.21	-0.37	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	6	1960	7/7	0.87	0.22	-0.38	118,118,118,118	0
85	MG	1	3807	1/1	0.80	0.18	-0.38	41,41,41,41	0
84	OHX	1	3579	7/7	0.96	0.17	-0.38	119,120,120,120	0
84	OHX	A	2042	7/7	0.90	0.21	-0.39	172,173,173,174	0
84	OHX	A	1913	7/7	0.97	0.20	-0.39	126,126,127,127	0
84	OHX	A	1963	7/7	0.94	0.18	-0.39	150,151,152,152	0
85	MG	AR	3953	1/1	0.97	0.19	-0.40	34,34,34,34	0
84	OHX	AR	3574	7/7	0.97	0.17	-0.42	112,113,113,113	0
84	OHX	6	1930	7/7	0.98	0.21	-0.42	121,121,122,122	0
84	OHX	AR	3458	7/7	0.97	0.19	-0.43	114,114,114,115	0
85	MG	6	2104	1/1	0.96	0.20	-0.43	70,70,70,70	0
84	OHX	AR	3448	7/7	0.98	0.17	-0.43	115,115,115,115	0
85	MG	o	301	1/1	0.93	0.19	-0.44	34,34,34,34	0
84	OHX	A	1942	7/7	0.98	0.19	-0.45	133,133,134,134	0
84	OHX	1	3558	7/7	0.97	0.17	-0.45	134,134,135,135	0
84	OHX	Q	201	7/7	0.94	0.26	-0.45	165,165,165,165	0
84	OHX	A	2001	7/7	0.96	0.20	-0.45	136,137,137,138	0
85	MG	1	3839	1/1	0.95	0.20	-0.47	27,27,27,27	0
84	OHX	3	204	7/7	0.97	0.15	-0.48	124,125,125,125	0
84	OHX	s8	301	7/7	0.91	0.32	-0.49	167,167,168,168	0
84	OHX	CL	301	7/7	0.95	0.21	-0.50	121,122,122,122	0
84	OHX	AR	3457	7/7	0.98	0.18	-0.50	108,108,108,109	0
84	OHX	1	3446	7/7	0.97	0.19	-0.52	116,116,116,116	0
84	OHX	AR	3514	7/7	0.96	0.19	-0.52	112,112,112,113	0
85	MG	A	2089	1/1	0.85	0.19	-0.52	90,90,90,90	0
84	OHX	1	3447	7/7	0.98	0.20	-0.52	113,113,113,113	0
84	OHX	1	3461	7/7	0.98	0.18	-0.53	110,110,111,111	0
85	MG	1	4016	1/1	0.93	0.18	-0.54	39,39,39,39	0
84	OHX	AR	3486	7/7	0.98	0.19	-0.55	111,111,111,111	0
84	OHX	A	1954	7/7	0.97	0.17	-0.55	135,136,136,136	0
84	OHX	1	3603	7/7	0.97	0.17	-0.55	123,123,124,124	0
84	OHX	6	2018	7/7	0.88	0.23	-0.57	189,189,189,189	0
84	OHX	6	1912	7/7	0.99	0.18	-0.58	122,122,123,123	0
84	OHX	A	1919	7/7	0.98	0.17	-0.59	121,122,122,122	0
84	OHX	AR	3738	7/7	0.90	0.15	-0.59	141,142,142,142	0
85	MG	CO	201	1/1	0.96	0.19	-0.59	44,44,44,44	0
84	OHX	sR	401	7/7	0.98	0.22	-0.60	161,161,162,162	0
84	OHX	AR	3477	7/7	0.98	0.20	-0.61	112,112,113,113	0
85	MG	1	3769	1/1	0.95	0.19	-0.62	45,45,45,45	0
85	MG	AR	3749	1/1	0.82	0.19	-0.62	42,42,42,42	0
84	OHX	A	1987	7/7	0.97	0.15	-0.62	128,128,129,129	0
84	OHX	CP	501	7/7	0.98	0.20	-0.63	126,126,126,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	CG	302	7/7	0.92	0.38	-0.64	147,147,147,148	0
84	OHX	6	1950	7/7	0.93	0.21	-0.67	135,135,136,136	0
84	OHX	6	1973	7/7	0.95	0.22	-0.67	137,138,138,138	0
84	OHX	AR	3462	7/7	0.99	0.16	-0.67	116,116,116,116	0
85	MG	AR	4158	1/1	0.93	0.20	-0.67	29,29,29,29	0
84	OHX	AR	3451	7/7	0.98	0.20	-0.67	114,114,114,114	0
85	MG	1	3897	1/1	0.88	0.21	-0.67	46,46,46,46	0
84	OHX	r	301	7/7	0.94	0.20	-0.68	115,115,115,115	0
84	OHX	CG	301	7/7	0.94	0.16	-0.69	142,143,143,144	0
85	MG	1	3918	1/1	0.97	0.19	-0.71	31,31,31,31	0
84	OHX	A	1952	7/7	0.98	0.20	-0.71	128,129,129,129	0
84	OHX	1	3566	7/7	0.97	0.18	-0.71	113,113,114,114	0
84	OHX	AR	3692	7/7	0.90	0.32	-0.72	170,171,171,171	0
84	OHX	AR	3474	7/7	0.95	0.19	-0.72	114,114,114,115	0
84	OHX	1	3473	7/7	0.96	0.15	-0.73	114,115,115,115	0
84	OHX	6	2000	7/7	0.96	0.17	-0.75	130,130,131,131	0
84	OHX	AR	3508	7/7	0.98	0.21	-0.77	109,109,109,109	0
84	OHX	6	2008	7/7	0.91	0.18	-0.78	136,136,136,136	0
84	OHX	A	1992	7/7	0.97	0.21	-0.78	140,141,142,142	0
84	OHX	AS	207	7/7	0.98	0.16	-0.79	122,122,122,123	0
84	OHX	T	201	7/7	0.96	0.19	-0.79	145,146,146,147	0
84	OHX	AR	3473	7/7	0.97	0.11	-0.79	111,111,112,112	0
84	OHX	6	1982	7/7	0.96	0.17	-0.80	147,147,148,148	0
84	OHX	1	3491	7/7	0.98	0.18	-0.80	120,120,121,121	0
84	OHX	AR	3537	7/7	0.95	0.15	-0.81	131,132,132,132	0
84	OHX	1	3534	7/7	0.97	0.19	-0.81	113,113,113,113	0
84	OHX	6	1976	7/7	0.96	0.13	-0.82	146,147,147,148	0
84	OHX	1	3500	7/7	0.96	0.16	-0.84	119,120,120,120	0
85	MG	j	301	1/1	0.93	0.21	-0.84	29,29,29,29	0
84	OHX	v	301	7/7	0.97	0.20	-0.85	113,113,114,114	0
84	OHX	A	1945	7/7	0.97	0.18	-0.85	143,144,144,145	0
85	MG	AR	3768	1/1	0.94	0.18	-0.87	39,39,39,39	0
84	OHX	A	1916	7/7	0.98	0.18	-0.87	136,137,137,138	0
84	OHX	J	301	7/7	0.97	0.25	-0.88	157,157,158,158	0
84	OHX	1	3542	7/7	0.97	0.17	-0.88	119,119,120,120	0
84	OHX	1	3637	7/7	0.96	0.15	-0.88	140,140,140,141	0
84	OHX	A	1932	7/7	0.97	0.18	-0.88	141,142,142,143	0
84	OHX	1	3502	7/7	0.97	0.18	-0.88	114,114,114,114	0
84	OHX	1	3573	7/7	0.97	0.18	-0.88	131,131,132,132	0
84	OHX	6	1923	7/7	0.98	0.17	-0.89	121,121,122,122	0
84	OHX	6	2009	7/7	0.95	0.17	-0.90	126,127,127,128	0
84	OHX	1	3454	7/7	0.98	0.19	-0.90	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	A	1915	7/7	0.95	0.21	-0.92	142,143,143,144	0
88	ZN	d9	102	1/1	0.97	0.13	-0.93	83,83,83,83	0
84	OHX	AR	3605	7/7	0.95	0.16	-0.93	128,128,128,129	0
85	MG	CJ	301	1/1	0.82	0.22	-0.93	78,78,78,78	0
84	OHX	6	1914	7/7	0.99	0.20	-0.94	133,133,134,134	0
85	MG	1	4149	1/1	0.98	0.18	-0.94	54,54,54,54	0
84	OHX	6	1983	7/7	0.97	0.18	-0.96	128,129,129,129	0
84	OHX	6	1942	7/7	0.98	0.16	-0.96	135,135,136,136	0
85	MG	AR	3780	1/1	0.81	0.17	-0.96	88,88,88,88	0
85	MG	CR	203	1/1	0.86	0.15	-0.97	95,95,95,95	0
84	OHX	A	2019	7/7	0.92	0.29	-0.97	176,176,176,176	0
84	OHX	1	3470	7/7	0.98	0.18	-0.97	115,115,115,115	0
84	OHX	6	2020	7/7	0.95	0.18	-0.97	135,136,136,137	0
85	MG	DI	201	1/1	0.89	0.22	-0.98	68,68,68,68	0
85	MG	AR	3762	1/1	0.97	0.17	-0.99	24,24,24,24	0
84	OHX	AR	3482	7/7	0.98	0.18	-0.99	111,112,112,112	0
88	ZN	AQ	501	1/1	1.00	0.13	-0.99	56,56,56,56	0
84	OHX	AK	102	7/7	0.95	0.18	-0.99	105,105,105,105	0
84	OHX	1	3588	7/7	0.95	0.19	-0.99	128,128,128,128	0
84	OHX	A	1907	7/7	0.99	0.19	-1.00	133,134,134,134	0
84	OHX	1	3501	7/7	0.90	0.17	-1.01	126,126,127,127	0
84	OHX	CE	401	7/7	0.98	0.17	-1.01	114,114,115,115	0
88	ZN	d6	103	1/1	1.00	0.13	-1.01	53,53,53,53	0
84	OHX	AR	3630	7/7	0.97	0.13	-1.02	124,125,125,125	0
84	OHX	6	1940	7/7	0.94	0.13	-1.02	149,150,151,151	0
84	OHX	AR	3494	7/7	0.97	0.15	-1.02	124,125,125,125	0
84	OHX	AT	203	7/7	0.97	0.14	-1.03	117,117,117,117	0
85	MG	AR	3955	1/1	0.66	0.17	-1.05	34,34,34,34	0
84	OHX	1	3516	7/7	0.98	0.12	-1.06	116,117,117,117	0
84	OHX	c5	201	7/7	0.92	0.19	-1.07	161,161,161,161	0
84	OHX	A	1920	7/7	0.99	0.14	-1.08	128,128,129,129	0
84	OHX	1	3634	7/7	0.95	0.17	-1.08	132,132,132,133	0
84	OHX	h	401	7/7	0.97	0.15	-1.08	175,176,177,177	0
84	OHX	1	3544	7/7	0.95	0.16	-1.08	116,117,117,117	0
84	OHX	AR	3478	7/7	0.97	0.17	-1.09	110,110,110,111	0
84	OHX	1	3576	7/7	0.97	0.14	-1.10	131,131,132,132	0
84	OHX	A	1912	7/7	0.98	0.19	-1.11	137,137,138,138	0
84	OHX	1	3430	7/7	0.98	0.19	-1.12	110,110,110,110	0
85	MG	AR	4178	1/1	0.92	0.19	-1.12	24,24,24,24	0
85	MG	1	3933	1/1	0.88	0.11	-1.14	49,49,49,49	0
84	OHX	AT	206	7/7	0.97	0.11	-1.15	123,124,124,124	0
84	OHX	CX	201	7/7	0.98	0.17	-1.15	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	DA	202	1/1	0.92	0.20	-1.15	45,45,45,45	0
85	MG	AR	3760	1/1	0.81	0.14	-1.16	53,53,53,53	0
84	OHX	6	1922	7/7	0.98	0.18	-1.16	121,122,122,122	0
85	MG	CE	406	1/1	0.94	0.19	-1.20	25,25,25,25	0
84	OHX	A	1966	7/7	0.93	0.19	-1.21	131,131,132,132	0
84	OHX	AS	206	7/7	0.97	0.13	-1.21	124,124,125,125	0
84	OHX	AP	502	7/7	0.97	0.17	-1.22	112,113,113,113	0
84	OHX	AR	3602	7/7	0.89	0.18	-1.23	143,143,144,144	0
84	OHX	1	3450	7/7	0.99	0.17	-1.24	121,122,122,123	0
84	OHX	A	1972	7/7	0.98	0.22	-1.25	148,148,148,148	0
88	ZN	DO	201	1/1	0.99	0.15	-1.26	32,32,32,32	0
85	MG	H	301	1/1	0.91	0.10	-1.26	83,83,83,83	0
84	OHX	1	3571	7/7	0.97	0.18	-1.27	111,111,112,112	0
84	OHX	6	1915	7/7	0.99	0.17	-1.27	119,119,120,120	0
84	OHX	AR	3470	7/7	0.98	0.17	-1.27	115,116,116,116	0
84	OHX	6	1963	7/7	0.98	0.15	-1.29	125,125,126,126	0
84	OHX	4	207	7/7	0.98	0.12	-1.29	118,119,119,119	0
84	OHX	A	1937	7/7	0.97	0.16	-1.29	153,154,155,155	0
84	OHX	1	3548	7/7	0.97	0.11	-1.31	134,134,134,134	0
84	OHX	AR	3465	7/7	0.98	0.17	-1.32	118,118,118,118	0
84	OHX	AR	3598	7/7	0.96	0.18	-1.32	117,118,118,118	0
84	OHX	1	3488	7/7	0.92	0.17	-1.33	109,109,109,110	0
84	OHX	1	3495	7/7	0.97	0.14	-1.35	114,115,115,115	0
84	OHX	6	1924	7/7	0.98	0.15	-1.36	134,135,135,135	0
85	MG	AR	3882	1/1	0.89	0.14	-1.36	47,47,47,47	0
84	OHX	AR	3487	7/7	0.98	0.13	-1.37	107,107,107,107	0
84	OHX	1	3479	7/7	0.98	0.17	-1.37	108,109,109,109	0
84	OHX	AR	3523	7/7	0.98	0.14	-1.38	107,108,108,108	0
84	OHX	AR	3469	7/7	0.97	0.14	-1.40	121,122,122,122	0
88	ZN	b	102	1/1	0.99	0.16	-1.44	71,71,71,71	0
84	OHX	AR	3533	7/7	0.97	0.18	-1.45	111,111,111,111	0
84	OHX	AR	3517	7/7	0.88	0.16	-1.47	145,146,146,146	0
84	OHX	A	1931	7/7	0.97	0.10	-1.48	139,140,140,140	0
84	OHX	AR	3551	7/7	0.96	0.14	-1.48	129,129,130,130	0
84	OHX	AR	3558	7/7	0.97	0.16	-1.48	137,137,137,137	0
84	OHX	A	2010	7/7	0.98	0.14	-1.49	157,158,158,159	0
84	OHX	AR	3584	7/7	0.97	0.13	-1.49	131,131,131,132	0
85	MG	AR	4135	1/1	0.89	0.18	-1.50	62,62,62,62	0
84	OHX	1	3527	7/7	0.96	0.12	-1.51	135,135,136,136	0
84	OHX	A	1917	7/7	0.97	0.17	-1.52	130,131,131,131	0
84	OHX	AR	3449	7/7	0.99	0.14	-1.54	116,117,117,117	0
85	MG	1	3777	1/1	0.89	0.17	-1.55	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3454	7/7	0.98	0.17	-1.56	112,112,113,113	0
84	OHX	4	204	7/7	0.97	0.15	-1.56	108,108,108,108	0
84	OHX	AR	3504	7/7	0.97	0.18	-1.57	110,110,110,110	0
84	OHX	1	3547	7/7	0.96	0.11	-1.57	120,121,121,121	0
84	OHX	6	1918	7/7	0.98	0.17	-1.59	116,117,117,117	0
85	MG	AR	4167	1/1	0.93	0.25	-1.61	71,71,71,71	0
84	OHX	1	3505	7/7	0.98	0.18	-1.62	116,116,117,117	0
84	OHX	6	1959	7/7	0.97	0.17	-1.64	137,138,138,139	0
85	MG	sM	201	1/1	0.93	0.12	-1.64	41,41,41,41	0
84	OHX	AS	203	7/7	0.98	0.16	-1.65	116,116,116,116	0
88	ZN	g	501	1/1	0.96	0.06	-1.65	119,119,119,119	0
84	OHX	A	1933	7/7	0.96	0.13	-1.67	122,122,122,123	0
88	ZN	AN	500	1/1	1.00	0.13	-1.68	38,38,38,38	0
84	OHX	AR	3492	7/7	0.97	0.15	-1.68	116,116,117,117	0
84	OHX	1	3590	7/7	0.98	0.12	-1.68	137,138,138,138	0
84	OHX	AR	3444	7/7	0.98	0.15	-1.70	112,112,112,112	0
84	OHX	AT	209	7/7	0.97	0.11	-1.70	121,121,122,122	0
84	OHX	AR	3577	7/7	0.95	0.09	-1.73	156,157,158,158	0
84	OHX	AR	3452	7/7	0.98	0.18	-1.74	121,121,122,122	0
84	OHX	6	1952	7/7	0.96	0.14	-1.75	148,148,148,148	0
84	OHX	1	3460	7/7	0.98	0.16	-1.76	118,118,118,119	0
84	OHX	AR	3696	7/7	0.97	0.18	-1.77	112,113,113,113	0
84	OHX	AR	3538	7/7	0.95	0.16	-1.79	123,123,124,124	0
84	OHX	6	1947	7/7	0.96	0.14	-1.79	121,122,122,122	0
84	OHX	1	3531	7/7	0.96	0.19	-1.80	114,114,114,114	0
84	OHX	DQ	201	7/7	0.98	0.15	-1.81	111,111,111,111	0
84	OHX	AR	3443	7/7	0.98	0.14	-1.83	116,116,117,117	0
84	OHX	4	205	7/7	0.97	0.17	-1.84	106,106,106,106	0
84	OHX	AR	3594	7/7	0.97	0.20	-1.85	114,114,115,115	0
85	MG	AH	202	1/1	0.90	0.15	-1.86	58,58,58,58	0
85	MG	1	4140	1/1	0.46	0.30	-1.88	187,187,187,187	0
84	OHX	6	1967	7/7	0.97	0.16	-1.88	126,127,127,127	0
84	OHX	AR	3581	7/7	0.96	0.18	-1.91	109,109,109,109	0
84	OHX	1	3529	7/7	0.97	0.17	-1.91	115,115,115,116	0
84	OHX	AR	3532	7/7	0.95	0.14	-1.92	135,136,136,137	0
84	OHX	AR	3527	7/7	0.93	0.20	-1.93	112,112,112,112	0
85	MG	1	4021	1/1	0.91	0.15	-1.94	44,44,44,44	0
84	OHX	6	1961	7/7	0.93	0.19	-1.94	128,129,129,130	0
85	MG	AR	4066	1/1	0.95	0.14	-1.96	56,56,56,56	0
84	OHX	A	2008	7/7	0.97	0.16	-1.97	132,132,133,133	0
84	OHX	AR	3530	7/7	0.96	0.17	-1.97	112,113,113,113	0
84	OHX	AR	3669	7/7	0.96	0.17	-1.98	175,176,176,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	ZN	AK	101	1/1	1.00	0.15	-2.00	34,34,34,34	0
84	OHX	AR	3429	7/7	0.99	0.19	-2.01	112,112,112,112	0
84	OHX	6	1964	7/7	0.97	0.12	-2.01	123,123,124,124	0
84	OHX	A	1967	7/7	0.98	0.12	-2.02	119,119,120,120	0
84	OHX	AR	3480	7/7	0.97	0.12	-2.02	113,114,114,114	0
84	OHX	1	3715	7/7	0.95	0.09	-2.03	166,166,167,167	0
84	OHX	AR	3499	7/7	0.95	0.15	-2.04	125,126,126,126	0
85	MG	T	202	1/1	0.86	0.09	-2.04	97,97,97,97	0
85	MG	1	4218	1/1	0.92	0.14	-2.04	32,32,32,32	0
84	OHX	6	1946	7/7	0.96	0.17	-2.05	127,128,128,129	0
84	OHX	A	1975	7/7	0.96	0.10	-2.06	156,158,158,158	0
84	OHX	1	3522	7/7	0.98	0.13	-2.06	120,121,121,121	0
84	OHX	AR	3485	7/7	0.98	0.15	-2.08	114,114,115,115	0
84	OHX	AR	3472	7/7	0.95	0.16	-2.08	111,111,111,112	0
84	OHX	6	1988	7/7	0.96	0.14	-2.11	133,133,133,134	0
85	MG	1	3950	1/1	0.94	0.14	-2.12	38,38,38,38	0
84	OHX	6	1929	7/7	0.94	0.11	-2.13	157,158,159,159	0
84	OHX	A	1925	7/7	0.99	0.11	-2.13	136,137,137,137	0
88	ZN	e1	501	1/1	0.96	0.06	-2.13	153,153,153,153	0
85	MG	AR	3875	1/1	0.94	0.16	-2.14	45,45,45,45	0
84	OHX	1	3466	7/7	0.97	0.16	-2.14	114,115,115,115	0
85	MG	1	3977	1/1	0.95	0.14	-2.15	48,48,48,48	0
84	OHX	6	1953	7/7	0.97	0.12	-2.17	132,133,133,134	0
84	OHX	1	3530	7/7	0.98	0.13	-2.18	138,138,139,139	0
84	OHX	4	203	7/7	0.97	0.15	-2.19	106,107,107,107	0
84	OHX	AS	208	7/7	0.97	0.10	-2.20	138,139,139,139	0
84	OHX	1	3552	7/7	0.93	0.10	-2.20	150,150,151,151	0
84	OHX	6	1966	7/7	0.95	0.15	-2.22	133,133,134,134	0
88	ZN	e	102	1/1	0.99	0.09	-2.23	79,79,79,79	0
84	OHX	A	1950	7/7	0.98	0.13	-2.23	127,128,128,128	0
84	OHX	AR	3525	7/7	0.98	0.06	-2.23	119,119,120,120	0
84	OHX	6	1945	7/7	0.98	0.17	-2.24	126,127,127,128	0
84	OHX	1	3493	7/7	0.98	0.17	-2.26	115,116,116,116	0
84	OHX	6	1938	7/7	0.97	0.13	-2.30	130,131,131,131	0
85	MG	6	2137	1/1	0.93	0.12	-2.30	82,82,82,82	0
84	OHX	AR	3489	7/7	0.98	0.15	-2.32	114,114,114,114	0
84	OHX	A	1955	7/7	0.96	0.13	-2.37	145,146,147,147	0
84	OHX	AR	3483	7/7	0.97	0.17	-2.39	111,111,111,111	0
84	OHX	AR	3550	7/7	0.98	0.14	-2.40	107,107,107,107	0
88	ZN	DQ	202	1/1	0.99	0.03	-2.44	63,63,63,63	0
84	OHX	6	1939	7/7	0.97	0.10	-2.45	131,132,132,133	0
84	OHX	AR	3673	7/7	0.95	0.19	-2.45	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	6	1920	7/7	0.98	0.14	-2.46	133,133,134,134	0
84	OHX	1	3453	7/7	0.98	0.14	-2.47	120,120,120,120	0
84	OHX	1	3480	7/7	0.97	0.14	-2.49	119,119,119,120	0
84	OHX	6	1933	7/7	0.97	0.13	-2.50	116,116,117,117	0
84	OHX	AR	3589	7/7	0.98	0.13	-2.51	109,110,110,110	0
84	OHX	AR	3481	7/7	0.98	0.20	-2.52	106,106,107,107	0
85	MG	1	4166	1/1	0.94	0.16	-2.52	47,47,47,47	0
84	OHX	6	1958	7/7	0.98	0.15	-2.54	126,127,127,127	0
84	OHX	A	1974	7/7	0.94	0.14	-2.55	167,167,168,168	0
84	OHX	DH	201	7/7	0.98	0.13	-2.56	113,113,113,113	0
85	MG	AR	4192	1/1	0.92	0.19	-2.57	29,29,29,29	0
84	OHX	6	1917	7/7	0.99	0.16	-2.58	131,131,132,132	0
84	OHX	A	1965	7/7	0.97	0.16	-2.61	134,135,135,136	0
84	OHX	AR	3539	7/7	0.97	0.14	-2.62	127,128,128,128	0
84	OHX	1	3557	7/7	0.98	0.16	-2.65	117,118,118,118	0
84	OHX	AR	3500	7/7	0.98	0.11	-2.66	115,115,115,115	0
88	ZN	DL	101	1/1	0.99	0.20	-2.69	41,41,41,41	0
84	OHX	AR	3507	7/7	0.98	0.08	-2.70	123,123,123,123	0
84	OHX	6	1921	7/7	0.96	0.17	-2.72	141,141,142,143	0
84	OHX	6	1955	7/7	0.97	0.13	-2.75	179,179,179,179	0
85	MG	c9	201	1/1	0.82	0.10	-2.75	79,79,79,79	0
84	OHX	AT	207	7/7	0.97	0.15	-2.78	117,117,117,117	0
84	OHX	1	3546	7/7	0.97	0.17	-2.78	127,127,127,127	0
84	OHX	1	3459	7/7	0.98	0.19	-2.78	108,108,108,108	0
85	MG	6	2150	1/1	0.89	0.13	-2.81	77,77,77,77	0
84	OHX	1	3533	7/7	0.98	0.13	-2.82	149,149,150,150	0
84	OHX	A	1922	7/7	0.98	0.11	-2.84	123,124,124,124	0
84	OHX	AR	3497	7/7	0.98	0.09	-2.88	124,125,125,126	0
85	MG	6	2182	1/1	0.98	0.14	-2.88	83,83,83,83	0
84	OHX	AR	3554	7/7	0.97	0.15	-2.89	112,112,112,112	0
84	OHX	AR	3463	7/7	0.97	0.17	-2.91	110,110,111,111	0
84	OHX	6	1937	7/7	0.98	0.11	-2.92	119,120,120,120	0
84	OHX	AT	204	7/7	0.98	0.11	-2.92	105,105,105,106	0
84	OHX	AR	3464	7/7	0.98	0.17	-2.93	106,106,106,106	0
84	OHX	AR	3498	7/7	0.98	0.15	-2.98	123,123,123,124	0
85	MG	AR	3945	1/1	0.82	0.15	-3.02	40,40,40,40	0
84	OHX	6	1957	7/7	0.97	0.14	-3.02	129,130,130,131	0
84	OHX	AT	205	7/7	0.97	0.15	-3.03	108,108,108,108	0
85	MG	1	3815	1/1	0.97	0.15	-3.04	40,40,40,40	0
84	OHX	1	3510	7/7	0.96	0.16	-3.04	111,111,111,111	0
84	OHX	1	3484	7/7	0.98	0.10	-3.08	125,126,126,126	0
84	OHX	A	1944	7/7	0.96	0.12	-3.11	138,139,139,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	DC	204	1/1	0.94	0.14	-3.11	35,35,35,35	0
84	OHX	A	1927	7/7	0.97	0.14	-3.14	138,138,139,139	0
84	OHX	6	1951	7/7	0.98	0.14	-3.18	134,134,135,135	0
84	OHX	1	3560	7/7	0.98	0.12	-3.22	111,112,112,112	0
84	OHX	1	3463	7/7	0.97	0.13	-3.24	121,121,122,122	0
84	OHX	1	3487	7/7	0.95	0.17	-3.24	115,115,116,116	0
85	MG	1	4029	1/1	0.89	0.11	-3.24	47,47,47,47	0
84	OHX	A	1923	7/7	0.98	0.13	-3.32	124,125,125,125	0
84	OHX	6	1954	7/7	0.95	0.09	-3.32	178,178,178,178	0
84	OHX	6	1934	7/7	0.97	0.13	-3.33	139,139,140,140	0
84	OHX	6	1956	7/7	0.95	0.12	-3.34	174,174,175,175	0
84	OHX	A	1961	7/7	0.98	0.11	-3.35	149,150,151,151	0
84	OHX	1	3464	7/7	0.99	0.20	-3.36	109,109,109,109	0
84	OHX	AR	3544	7/7	0.95	0.16	-3.42	109,109,110,110	0
84	OHX	6	1941	7/7	0.96	0.13	-3.47	120,120,121,121	0
85	MG	1	4047	1/1	0.98	0.12	-3.48	57,57,57,57	0
84	OHX	AR	3502	7/7	0.98	0.17	-3.65	113,114,114,114	0
84	OHX	1	3475	7/7	0.98	0.14	-3.67	117,117,118,118	0
84	OHX	1	3528	7/7	0.97	0.12	-3.72	119,120,120,120	0
84	OHX	6	1928	7/7	0.98	0.08	-3.74	126,126,127,127	0
84	OHX	AR	3491	7/7	0.97	0.13	-3.74	108,108,109,109	0
84	OHX	AR	3522	7/7	0.96	0.13	-3.80	114,114,115,115	0
84	OHX	A	1939	7/7	0.97	0.11	-3.82	140,141,141,142	0
84	OHX	AR	3609	7/7	0.98	0.16	-3.83	107,107,107,107	0
84	OHX	1	3555	7/7	0.98	0.17	-3.85	111,111,112,112	0
84	OHX	6	1926	7/7	0.98	0.12	-3.88	120,121,121,121	0
84	OHX	AR	3430	7/7	0.98	0.14	-3.92	107,107,107,107	0
84	OHX	A	1926	7/7	0.97	0.08	-3.93	127,127,127,128	0
84	OHX	6	1944	7/7	0.98	0.10	-3.95	143,143,144,144	0
84	OHX	1	3486	7/7	0.98	0.14	-3.96	116,117,117,117	0
84	OHX	1	3538	7/7	0.97	0.09	-4.07	125,125,125,126	0
88	ZN	AP	501	1/1	0.99	0.04	-4.17	61,61,61,61	0
84	OHX	AR	3560	7/7	0.97	0.19	-4.22	135,135,136,136	0
85	MG	1	3810	1/1	0.98	0.12	-4.24	32,32,32,32	0
84	OHX	1	3476	7/7	0.97	0.14	-4.26	111,111,111,112	0
84	OHX	1	3477	7/7	0.98	0.12	-4.34	109,109,109,109	0
84	OHX	1	3535	7/7	0.98	0.17	-4.37	111,111,111,112	0
84	OHX	AR	3476	7/7	0.98	0.17	-4.37	109,109,109,109	0
84	OHX	A	1948	7/7	0.97	0.13	-4.49	139,140,140,140	0
84	OHX	A	1949	7/7	0.98	0.08	-4.49	148,149,149,149	0
84	OHX	AR	3488	7/7	0.98	0.09	-4.52	118,118,119,119	0
84	OHX	6	1948	7/7	0.98	0.13	-4.53	127,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	AS	204	7/7	0.98	0.15	-4.68	113,113,113,113	0
84	OHX	1	3682	7/7	0.97	0.14	-4.69	110,110,111,111	0
85	MG	1	3921	1/1	0.93	0.12	-4.78	57,57,57,57	0
84	OHX	A	1924	7/7	0.99	0.09	-4.79	132,132,133,133	0
85	MG	1	3925	1/1	0.82	0.13	-4.84	46,46,46,46	0
84	OHX	3	202	7/7	0.97	0.12	-4.85	115,116,116,116	0
84	OHX	AR	3535	7/7	0.97	0.13	-4.87	114,115,115,115	0
84	OHX	1	3513	7/7	0.98	0.11	-4.88	113,113,114,114	0
84	OHX	AR	3479	7/7	0.97	0.15	-4.88	110,110,110,110	0
84	OHX	1	3497	7/7	0.96	0.11	-4.89	125,125,126,126	0
84	OHX	AR	3461	7/7	0.98	0.14	-4.90	110,111,111,111	0
84	OHX	A	1984	7/7	0.98	0.10	-4.97	130,130,131,131	0
84	OHX	A	1928	7/7	0.97	0.13	-5.00	125,126,126,126	0
84	OHX	1	3511	7/7	0.98	0.14	-5.02	109,109,109,109	0
84	OHX	1	3518	7/7	0.96	0.15	-5.06	109,110,110,110	0
84	OHX	1	3483	7/7	0.96	0.12	-5.08	113,113,113,113	0
84	OHX	AR	3490	7/7	0.98	0.12	-5.10	112,112,112,113	0
84	OHX	1	3618	7/7	0.93	0.19	-5.15	190,190,190,190	0
84	OHX	AR	3744	7/7	0.98	0.17	-5.18	109,110,110,110	0
84	OHX	1	3678	7/7	0.97	0.15	-5.31	117,117,118,118	0
84	OHX	AR	3471	7/7	0.98	0.13	-5.46	109,109,109,109	0
84	OHX	AR	3467	7/7	0.97	0.13	-5.48	108,109,109,109	0
84	OHX	6	2003	7/7	0.97	0.13	-5.64	126,126,127,127	0
84	OHX	AR	3519	7/7	0.97	0.15	-5.66	108,109,109,109	0
84	OHX	AR	3529	7/7	0.98	0.12	-5.70	108,109,109,109	0
84	OHX	A	1941	7/7	0.97	0.12	-5.74	136,137,137,137	0
84	OHX	1	3532	7/7	0.98	0.07	-5.88	159,159,159,159	0
84	OHX	AR	3495	7/7	0.95	0.17	-5.93	113,113,114,114	0
84	OHX	AR	3513	7/7	0.97	0.09	-6.19	150,151,151,151	0
84	OHX	3	203	7/7	0.97	0.11	-6.21	118,118,118,119	0
84	OHX	A	1956	7/7	0.97	0.14	-6.47	133,133,134,134	0
84	OHX	AS	205	7/7	0.98	0.11	-6.74	113,113,114,114	0
84	OHX	A	1938	7/7	0.98	0.14	-6.82	126,127,127,127	0
85	MG	1	3920	1/1	0.91	0.10	-8.18	41,41,41,41	0
84	OHX	1	3472	7/7	0.98	0.17	-8.24	110,111,111,111	0
84	OHX	AR	3509	7/7	0.99	0.10	-8.36	106,106,106,106	0
84	OHX	1	3515	7/7	0.98	0.10	-8.47	110,110,110,110	0
85	MG	AR	4089	1/1	0.83	0.10	-9.56	62,62,62,62	0
84	OHX	AR	3578	7/7	0.99	0.14	-10.49	109,109,110,110	0
85	MG	AR	4164	1/1	0.86	0.22	-	41,41,41,41	0
85	MG	6	2159	1/1	0.94	0.08	-	82,82,82,82	0
84	OHX	AR	3597	7/7	0.93	0.30	-	150,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3936	1/1	0.86	0.54	-	61,61,61,61	0
85	MG	1	3751	1/1	0.79	0.35	-	40,40,40,40	0
84	OHX	1	3714	7/7	0.86	0.51	-	146,147,147,148	0
85	MG	1	4105	1/1	0.96	0.49	-	26,26,26,26	0
85	MG	AR	3861	1/1	0.88	0.37	-	30,30,30,30	0
85	MG	A	2151	1/1	0.69	0.69	-	52,52,52,52	0
84	OHX	1	3663	7/7	0.94	0.19	-	111,111,111,111	0
84	OHX	6	1975	7/7	0.89	0.42	-	120,120,120,120	0
85	MG	6	2179	1/1	0.95	0.36	-	43,43,43,43	0
85	MG	A	2099	1/1	0.69	0.69	-	71,71,71,71	0
85	MG	A	2044	1/1	0.93	0.80	-	50,50,50,50	0
84	OHX	1	3569	7/7	0.97	0.28	-	111,111,111,111	0
85	MG	AR	3951	1/1	0.96	0.53	-	29,29,29,29	0
85	MG	1	4011	1/1	0.91	0.37	-	44,44,44,44	0
85	MG	6	2133	1/1	0.70	0.66	-	61,61,61,61	0
85	MG	1	3954	1/1	0.81	0.15	-	46,46,46,46	0
85	MG	6	2194	1/1	0.62	0.15	-	108,108,108,108	0
85	MG	CF	403	1/1	0.87	0.40	-	34,34,34,34	0
85	MG	1	4036	1/1	0.89	0.42	-	70,70,70,70	0
87	GOL	6	2199	6/6	0.79	0.44	-	49,49,49,49	0
84	OHX	AR	3665	7/7	0.91	0.39	-	133,133,133,133	0
85	MG	1	4015	1/1	0.90	0.37	-	67,67,67,67	0
85	MG	6	2070	1/1	0.83	0.38	-	73,73,73,73	0
84	OHX	1	3478	7/7	0.99	0.14	-	125,125,125,126	0
85	MG	AR	4100	1/1	0.91	0.28	-	57,57,57,57	0
85	MG	AR	4185	1/1	0.93	0.37	-	38,38,38,38	0
85	MG	AB	201	1/1	0.91	0.28	-	34,34,34,34	0
85	MG	AR	3813	1/1	0.94	0.16	-	55,55,55,55	0
85	MG	1	3808	1/1	0.94	0.47	-	43,43,43,43	0
85	MG	AR	4124	1/1	0.86	0.18	-	39,39,39,39	0
85	MG	k	402	1/1	0.91	0.37	-	37,37,37,37	0
84	OHX	AR	3642	7/7	0.97	0.24	-	122,122,122,122	0
85	MG	AR	4190	1/1	0.98	0.19	-	30,30,30,30	0
85	MG	AR	4043	1/1	0.89	0.38	-	37,37,37,37	0
85	MG	A	2142	1/1	0.85	0.12	-	80,80,80,80	0
85	MG	AR	3995	1/1	0.75	0.34	-	65,65,65,65	0
85	MG	1	4041	1/1	0.93	0.16	-	45,45,45,45	0
85	MG	1	3781	1/1	0.96	0.39	-	33,33,33,33	0
85	MG	1	3784	1/1	0.97	0.46	-	26,26,26,26	0
85	MG	6	2089	1/1	0.95	0.44	-	44,44,44,44	0
85	MG	4	218	1/1	0.95	0.60	-	49,49,49,49	0
85	MG	6	2177	1/1	0.96	0.19	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	3829	1/1	0.86	0.66	-	66,66,66,66	0
85	MG	6	2139	1/1	0.90	0.22	-	45,45,45,45	0
85	MG	AR	3766	1/1	0.96	0.14	-	96,96,96,96	0
85	MG	1	3788	1/1	0.95	0.53	-	45,45,45,45	0
85	MG	1	3792	1/1	0.96	0.52	-	37,37,37,37	0
84	OHX	1	3545	7/7	0.95	0.21	-	120,120,120,120	0
84	OHX	1	3435	7/7	0.96	0.27	-	114,114,114,114	0
85	MG	AR	3822	1/1	0.95	0.32	-	46,46,46,46	0
85	MG	1	3934	1/1	0.88	0.44	-	54,54,54,54	0
85	MG	AR	4014	1/1	0.82	0.39	-	57,57,57,57	0
85	MG	1	4090	1/1	0.94	0.21	-	42,42,42,42	0
85	MG	AR	3886	1/1	0.95	0.70	-	30,30,30,30	0
84	OHX	AR	3706	7/7	0.93	0.34	-	155,155,155,156	0
85	MG	1	4150	1/1	0.58	0.26	-	49,49,49,49	0
85	MG	1	4156	1/1	0.90	0.19	-	44,44,44,44	0
85	MG	6	2168	1/1	0.61	0.31	-	132,132,132,132	0
85	MG	1	4089	1/1	0.92	0.21	-	42,42,42,42	0
84	OHX	AR	3637	7/7	0.95	0.40	-	129,129,129,129	0
85	MG	AR	4070	1/1	0.90	0.19	-	50,50,50,50	0
84	OHX	AR	3548	7/7	0.96	0.16	-	121,121,122,122	0
85	MG	A	2065	1/1	0.90	0.73	-	57,57,57,57	0
85	MG	AR	3827	1/1	0.75	0.34	-	58,58,58,58	0
84	OHX	AR	3542	7/7	0.97	0.11	-	152,152,152,153	0
85	MG	4	234	1/1	0.83	0.43	-	44,44,44,44	0
84	OHX	1	3700	7/7	0.90	0.37	-	148,148,149,149	0
85	MG	AR	4086	1/1	0.84	0.40	-	42,42,42,42	0
85	MG	1	3893	1/1	0.98	0.26	-	26,26,26,26	0
85	MG	1	4221	1/1	0.96	0.52	-	35,35,35,35	0
84	OHX	1	3686	7/7	0.93	0.58	-	156,156,157,157	0
84	OHX	AR	3711	7/7	0.93	0.37	-	144,144,145,145	0
85	MG	A	2063	1/1	0.95	0.50	-	51,51,51,51	0
84	OHX	1	3456	7/7	0.98	0.16	-	111,111,111,111	0
85	MG	AR	4103	1/1	0.85	0.19	-	47,47,47,47	0
84	OHX	CM	201	7/7	0.94	0.34	-	150,150,151,151	0
85	MG	1	3767	1/1	0.87	0.12	-	60,60,60,60	0
85	MG	AR	3970	1/1	0.97	0.23	-	50,50,50,50	0
84	OHX	A	2034	7/7	0.83	0.20	-	231,232,232,232	0
85	MG	1	3971	1/1	0.87	0.46	-	35,35,35,35	0
85	MG	AR	4112	1/1	0.96	0.15	-	54,54,54,54	0
85	MG	A	2123	1/1	0.93	0.50	-	55,55,55,55	0
85	MG	AR	4025	1/1	0.85	0.25	-	31,31,31,31	0
85	MG	6	2138	1/1	0.83	0.30	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	4005	1/1	0.78	0.62	-	40,40,40,40	0
85	MG	AR	3770	1/1	0.91	0.44	-	32,32,32,32	0
85	MG	AR	4044	1/1	0.84	0.56	-	60,60,60,60	0
85	MG	6	2081	1/1	0.77	0.25	-	55,55,55,55	0
85	MG	1	3935	1/1	0.98	0.23	-	47,47,47,47	0
84	OHX	A	2037	7/7	0.92	0.44	-	153,154,154,155	0
85	MG	A	2127	1/1	0.83	0.29	-	83,83,83,83	0
84	OHX	A	1936	7/7	0.96	0.17	-	126,127,127,128	0
85	MG	AR	3948	1/1	0.90	0.54	-	40,40,40,40	0
85	MG	x	203	1/1	0.82	0.39	-	63,63,63,63	0
84	OHX	A	2011	7/7	0.92	0.23	-	149,149,150,150	0
84	OHX	A	2025	7/7	0.87	0.48	-	173,173,173,173	0
85	MG	1	4012	1/1	0.78	0.44	-	50,50,50,50	0
85	MG	A	2094	1/1	0.83	0.38	-	110,110,110,110	0
85	MG	6	2075	1/1	0.96	0.14	-	76,76,76,76	0
85	MG	6	2096	1/1	0.94	0.57	-	68,68,68,68	0
85	MG	AR	3973	1/1	0.83	0.23	-	40,40,40,40	0
85	MG	v	303	1/1	0.83	0.24	-	44,44,44,44	0
85	MG	A	2118	1/1	0.75	0.92	-	80,80,80,80	0
85	MG	AR	4218	1/1	0.93	0.27	-	54,54,54,54	0
85	MG	A	2157	1/1	0.92	0.79	-	75,75,75,75	0
85	MG	AR	4046	1/1	0.84	0.26	-	46,46,46,46	0
85	MG	6	2110	1/1	0.85	0.54	-	54,54,54,54	0
84	OHX	A	1995	7/7	0.95	0.17	-	151,152,152,152	0
84	OHX	1	3684	7/7	0.96	0.41	-	141,141,141,141	0
85	MG	A	2075	1/1	0.86	0.43	-	74,74,74,74	0
85	MG	6	2198	1/1	0.90	0.56	-	49,49,49,49	0
85	MG	AR	4106	1/1	0.98	0.07	-	46,46,46,46	0
85	MG	A	2113	1/1	0.90	0.48	-	73,73,73,73	0
85	MG	6	2064	1/1	0.83	0.68	-	53,53,53,53	0
85	MG	AR	4209	1/1	0.92	0.41	-	74,74,74,74	0
85	MG	1	3999	1/1	0.89	0.33	-	41,41,41,41	0
85	MG	AR	3797	1/1	0.97	0.27	-	31,31,31,31	0
85	MG	1	3844	1/1	0.98	0.41	-	28,28,28,28	0
85	MG	AR	4020	1/1	0.87	0.23	-	41,41,41,41	0
85	MG	AR	3849	1/1	0.97	0.45	-	35,35,35,35	0
85	MG	AT	227	1/1	0.86	0.88	-	79,79,79,79	0
85	MG	A	2085	1/1	0.70	0.40	-	63,63,63,63	0
85	MG	3	212	1/1	0.88	0.44	-	62,62,62,62	0
85	MG	CR	204	1/1	0.86	0.21	-	46,46,46,46	0
85	MG	1	3949	1/1	0.92	0.47	-	44,44,44,44	0
85	MG	AR	4159	1/1	0.86	0.38	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	4115	1/1	0.97	0.33	-	46,46,46,46	0
84	OHX	AR	3639	7/7	0.91	0.22	-	138,139,139,139	0
84	OHX	1	3526	7/7	0.96	0.29	-	114,115,115,115	0
85	MG	AR	3823	1/1	0.92	0.51	-	39,39,39,39	0
85	MG	1	4023	1/1	0.79	0.48	-	57,57,57,57	0
85	MG	6	2163	1/1	0.77	0.42	-	48,48,48,48	0
84	OHX	1	3452	7/7	0.98	0.16	-	109,109,109,109	0
85	MG	AR	4253	1/1	0.84	0.17	-	41,41,41,41	0
85	MG	A	2114	1/1	0.81	0.39	-	76,76,76,76	0
84	OHX	AR	3628	7/7	0.96	0.32	-	147,148,148,148	0
85	MG	1	4025	1/1	0.94	0.48	-	32,32,32,32	0
84	OHX	A	1969	7/7	0.95	0.34	-	144,144,145,145	0
85	MG	1	3854	1/1	0.96	0.62	-	34,34,34,34	0
85	MG	1	4123	1/1	0.94	0.22	-	51,51,51,51	0
85	MG	AR	4081	1/1	0.98	0.24	-	55,55,55,55	0
85	MG	CG	304	1/1	0.81	0.25	-	56,56,56,56	0
84	OHX	A	1959	7/7	0.94	0.20	-	137,138,139,139	0
85	MG	1	4118	1/1	0.83	0.34	-	43,43,43,43	0
85	MG	1	3771	1/1	0.90	0.42	-	33,33,33,33	0
84	OHX	1	3494	7/7	0.97	0.13	-	119,119,120,120	0
85	MG	AR	3989	1/1	0.95	0.23	-	44,44,44,44	0
85	MG	A	2141	1/1	0.99	0.31	-	101,101,101,101	0
84	OHX	1	3651	7/7	0.92	0.26	-	130,130,131,131	0
85	MG	AS	213	1/1	0.90	0.45	-	26,26,26,26	0
85	MG	A	2087	1/1	0.88	0.49	-	78,78,78,78	0
85	MG	A	2104	1/1	0.93	0.15	-	137,137,137,137	0
85	MG	1	4119	1/1	0.82	0.28	-	35,35,35,35	0
85	MG	1	4180	1/1	0.98	0.35	-	45,45,45,45	0
85	MG	A	2097	1/1	0.94	0.57	-	53,53,53,53	0
85	MG	A	2106	1/1	0.90	0.49	-	58,58,58,58	0
85	MG	1	4202	1/1	0.84	0.56	-	19,19,19,19	0
85	MG	6	2193	1/1	0.79	0.45	-	55,55,55,55	0
85	MG	1	3992	1/1	0.91	0.24	-	40,40,40,40	0
85	MG	A	2048	1/1	0.83	0.33	-	52,52,52,52	0
84	OHX	AR	3503	7/7	0.95	0.17	-	120,120,121,121	0
85	MG	AB	205	1/1	0.91	0.22	-	40,40,40,40	0
85	MG	1	3820	1/1	0.68	0.60	-	65,65,65,65	0
85	MG	1	4191	1/1	0.97	0.44	-	29,29,29,29	0
85	MG	3	217	1/1	0.91	0.36	-	40,40,40,40	0
85	MG	AR	3838	1/1	0.88	0.37	-	27,27,27,27	0
85	MG	4	238	1/1	0.79	0.26	-	35,35,35,35	0
84	OHX	AR	3702	7/7	0.94	0.40	-	139,139,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	3996	1/1	0.92	0.33	-	56,56,56,56	0
84	OHX	A	1989	7/7	0.96	0.36	-	154,155,155,155	0
85	MG	AR	3781	1/1	0.98	0.25	-	23,23,23,23	0
85	MG	1	3872	1/1	0.95	0.59	-	32,32,32,32	0
85	MG	DH	202	1/1	0.96	0.26	-	40,40,40,40	0
84	OHX	1	3716	7/7	0.91	0.45	-	138,138,139,139	0
85	MG	6	2065	1/1	0.93	0.58	-	40,40,40,40	0
84	OHX	1	3540	7/7	0.94	0.18	-	111,111,111,111	0
85	MG	AR	4110	1/1	0.80	0.50	-	46,46,46,46	0
84	OHX	6	1970	7/7	0.98	0.26	-	126,126,127,127	0
85	MG	A	2103	1/1	0.69	0.55	-	73,73,73,73	0
85	MG	AT	228	1/1	0.82	0.37	-	47,47,47,47	0
85	MG	1	4094	1/1	0.96	0.15	-	78,78,78,78	0
85	MG	AR	4130	1/1	0.88	0.15	-	31,31,31,31	0
85	MG	AR	4036	1/1	0.94	0.27	-	41,41,41,41	0
85	MG	AR	3921	1/1	0.77	0.31	-	38,38,38,38	0
85	MG	1	3787	1/1	0.88	0.46	-	46,46,46,46	0
85	MG	AR	4132	1/1	0.97	0.15	-	49,49,49,49	0
84	OHX	1	3696	7/7	0.90	0.39	-	146,146,147,147	0
85	MG	AR	4162	1/1	0.94	0.60	-	56,56,56,56	0
85	MG	AR	4207	1/1	0.87	0.50	-	48,48,48,48	0
85	MG	AR	4125	1/1	0.64	0.28	-	82,82,82,82	0
85	MG	1	4216	1/1	0.96	0.39	-	23,23,23,23	0
84	OHX	AR	3447	7/7	0.97	0.25	-	112,112,112,112	0
84	OHX	AR	3569	7/7	0.97	0.29	-	137,137,137,138	0
84	OHX	AR	3633	7/7	0.96	0.28	-	124,125,125,125	0
85	MG	AR	3962	1/1	0.93	0.19	-	93,93,93,93	0
85	MG	1	3994	1/1	0.79	0.27	-	47,47,47,47	0
85	MG	AR	4033	1/1	0.90	0.26	-	40,40,40,40	0
84	OHX	A	1988	7/7	0.97	0.23	-	139,140,141,141	0
84	OHX	AR	3675	7/7	0.93	0.33	-	138,139,139,139	0
85	MG	1	4179	1/1	0.95	0.23	-	38,38,38,38	0
85	MG	AR	4177	1/1	0.91	0.30	-	32,32,32,32	0
85	MG	1	3896	1/1	0.93	0.30	-	36,36,36,36	0
85	MG	1	4006	1/1	0.84	0.58	-	47,47,47,47	0
85	MG	A	2091	1/1	0.80	0.43	-	71,71,71,71	0
84	OHX	6	2040	7/7	0.87	0.29	-	184,184,185,185	0
85	MG	1	4130	1/1	0.89	0.27	-	45,45,45,45	0
85	MG	AR	3968	1/1	0.78	0.32	-	30,30,30,30	0
85	MG	AR	4181	1/1	0.72	0.24	-	50,50,50,50	0
85	MG	1	4141	1/1	0.95	0.38	-	64,64,64,64	0
85	MG	1	3785	1/1	0.88	0.45	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2157	1/1	0.78	0.28	-	56,56,56,56	0
85	MG	6	2109	1/1	0.91	0.42	-	56,56,56,56	0
85	MG	1	3780	1/1	0.97	0.33	-	17,17,17,17	0
85	MG	d4	201	1/1	0.87	0.38	-	53,53,53,53	0
85	MG	A	2102	1/1	0.90	0.49	-	58,58,58,58	0
85	MG	V	201	1/1	0.77	0.50	-	70,70,70,70	0
84	OHX	1	3710	7/7	0.90	0.33	-	136,137,137,137	0
85	MG	6	2196	1/1	0.91	0.76	-	48,48,48,48	0
85	MG	1	3938	1/1	0.92	0.21	-	34,34,34,34	0
84	OHX	AS	209	7/7	0.93	0.31	-	140,140,140,140	0
85	MG	1	3888	1/1	0.98	0.40	-	29,29,29,29	0
84	OHX	6	1905	7/7	0.97	0.34	-	132,133,133,134	0
85	MG	1	4185	1/1	0.97	0.50	-	27,27,27,27	0
85	MG	AR	4153	1/1	0.89	0.19	-	88,88,88,88	0
84	OHX	1	3632	7/7	0.94	0.34	-	156,156,156,156	0
85	MG	6	2060	1/1	0.92	0.34	-	47,47,47,47	0
85	MG	6	2118	1/1	0.84	0.15	-	93,93,93,93	0
85	MG	AR	3965	1/1	0.93	0.25	-	50,50,50,50	0
85	MG	AR	4235	1/1	0.97	0.37	-	26,26,26,26	0
84	OHX	1	3713	7/7	0.93	0.26	-	138,138,138,139	0
85	MG	3	221	1/1	0.89	0.46	-	34,34,34,34	0
84	OHX	1	3549	7/7	0.97	0.15	-	120,120,120,120	0
85	MG	6	2170	1/1	0.98	0.17	-	64,64,64,64	0
85	MG	1	3804	1/1	0.93	0.50	-	35,35,35,35	0
85	MG	6	2188	1/1	0.76	0.54	-	66,66,66,66	0
84	OHX	AR	3720	7/7	0.89	0.33	-	152,152,152,152	0
85	MG	t	202	1/1	0.68	0.26	-	101,101,101,101	0
85	MG	AR	3999	1/1	0.88	0.30	-	44,44,44,44	0
85	MG	A	2143	1/1	0.92	0.38	-	106,106,106,106	0
85	MG	1	4058	1/1	0.92	0.31	-	51,51,51,51	0
85	MG	A	2120	1/1	0.95	0.22	-	85,85,85,85	0
84	OHX	6	1943	7/7	0.97	0.09	-	124,124,125,125	0
85	MG	A	2076	1/1	0.93	0.35	-	51,51,51,51	0
85	MG	AR	3796	1/1	0.91	0.41	-	64,64,64,64	0
85	MG	1	4060	1/1	0.82	0.36	-	44,44,44,44	0
85	MG	1	4077	1/1	0.85	0.27	-	33,33,33,33	0
84	OHX	AR	3627	7/7	0.96	0.32	-	127,128,128,128	0
85	MG	6	2187	1/1	0.96	0.18	-	82,82,82,82	0
84	OHX	AR	3664	7/7	0.83	0.43	-	180,180,181,181	0
84	OHX	1	3615	7/7	0.94	0.37	-	133,133,133,134	0
85	MG	1	4139	1/1	0.94	0.28	-	31,31,31,31	0
85	MG	AR	4061	1/1	0.92	0.53	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	4201	1/1	0.94	0.49	-	28,28,28,28	0
85	MG	AR	4042	1/1	0.90	0.12	-	57,57,57,57	0
85	MG	6	2105	1/1	0.86	0.48	-	64,64,64,64	0
85	MG	1	3842	1/1	0.96	0.55	-	25,25,25,25	0
85	MG	6	2183	1/1	0.79	0.58	-	71,71,71,71	0
85	MG	CR	202	1/1	0.84	0.28	-	29,29,29,29	0
84	OHX	AR	3631	7/7	0.90	0.18	-	175,176,177,177	0
85	MG	AR	4154	1/1	0.89	0.31	-	39,39,39,39	0
85	MG	6	2101	1/1	0.96	0.51	-	53,53,53,53	0
84	OHX	1	3614	7/7	0.93	0.27	-	133,133,133,134	0
85	MG	k	403	1/1	0.94	0.20	-	30,30,30,30	0
85	MG	AR	3828	1/1	0.96	0.61	-	60,60,60,60	0
84	OHX	6	2014	7/7	0.95	0.34	-	129,129,129,130	0
85	MG	1	3744	1/1	0.77	0.42	-	83,83,83,83	0
85	MG	AR	4107	1/1	0.94	0.13	-	78,78,78,78	0
85	MG	AR	3969	1/1	0.94	0.13	-	60,60,60,60	0
85	MG	3	222	1/1	0.93	0.38	-	52,52,52,52	0
85	MG	AR	3975	1/1	0.83	0.27	-	31,31,31,31	0
85	MG	1	4110	1/1	0.88	0.24	-	30,30,30,30	0
85	MG	1	3776	1/1	0.96	0.49	-	43,43,43,43	0
85	MG	1	4155	1/1	0.77	0.23	-	53,53,53,53	0
85	MG	AS	224	1/1	0.88	0.24	-	55,55,55,55	0
85	MG	1	4172	1/1	0.96	0.40	-	67,67,67,67	0
85	MG	1	4214	1/1	0.92	0.39	-	43,43,43,43	0
85	MG	1	4128	1/1	0.87	0.45	-	51,51,51,51	0
85	MG	AR	4133	1/1	0.96	0.27	-	25,25,25,25	0
85	MG	1	3735	1/1	0.94	0.35	-	24,24,24,24	0
85	MG	1	4175	1/1	0.96	0.45	-	39,39,39,39	0
85	MG	6	2124	1/1	0.73	0.28	-	66,66,66,66	0
85	MG	6	2085	1/1	0.90	0.47	-	75,75,75,75	0
84	OHX	1	3658	7/7	0.97	0.34	-	142,143,143,143	0
85	MG	4	231	1/1	0.90	0.23	-	58,58,58,58	0
85	MG	1	4112	1/1	0.97	0.43	-	32,32,32,32	0
85	MG	1	3947	1/1	0.92	0.21	-	26,26,26,26	0
85	MG	AR	4128	1/1	0.81	0.21	-	55,55,55,55	0
85	MG	1	3733	1/1	0.95	0.49	-	26,26,26,26	0
85	MG	AR	3947	1/1	0.87	0.50	-	44,44,44,44	0
85	MG	1	3985	1/1	0.82	0.60	-	50,50,50,50	0
85	MG	1	4033	1/1	0.88	0.21	-	58,58,58,58	0
84	OHX	A	1960	7/7	0.95	0.18	-	151,151,151,152	0
85	MG	1	4092	1/1	0.78	0.64	-	54,54,54,54	0
85	MG	AR	3890	1/1	0.60	0.42	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3656	7/7	0.97	0.31	-	134,134,134,134	0
84	OHX	AR	3635	7/7	0.93	0.22	-	137,138,138,138	0
85	MG	1	4049	1/1	0.94	0.25	-	32,32,32,32	0
85	MG	AR	3795	1/1	0.96	0.66	-	49,49,49,49	0
85	MG	1	4121	1/1	0.98	0.10	-	64,64,64,64	0
85	MG	1	4190	1/1	0.73	0.56	-	25,25,25,25	0
85	MG	AR	3856	1/1	0.95	0.71	-	27,27,27,27	0
85	MG	1	3919	1/1	0.95	0.27	-	33,33,33,33	0
84	OHX	1	3567	7/7	0.95	0.24	-	128,129,129,129	0
85	MG	AR	4233	1/1	0.92	0.33	-	31,31,31,31	0
85	MG	AR	3881	1/1	0.95	0.29	-	30,30,30,30	0
85	MG	DE	201	1/1	0.81	0.28	-	72,72,72,72	0
85	MG	AR	4210	1/1	0.88	0.71	-	54,54,54,54	0
85	MG	AR	4186	1/1	0.89	0.21	-	33,33,33,33	0
85	MG	1	4020	1/1	0.90	0.38	-	34,34,34,34	0
84	OHX	AR	3719	7/7	0.84	0.42	-	133,133,133,133	0
85	MG	AR	3907	1/1	0.88	0.63	-	25,25,25,25	0
85	MG	1	4081	1/1	0.74	0.39	-	29,29,29,29	0
85	MG	1	4183	1/1	0.86	0.17	-	44,44,44,44	0
85	MG	AG	202	1/1	0.91	0.20	-	43,43,43,43	0
85	MG	AR	4234	1/1	0.84	0.45	-	32,32,32,32	0
85	MG	1	3755	1/1	0.92	0.42	-	36,36,36,36	0
85	MG	6	2175	1/1	0.99	0.10	-	118,118,118,118	0
85	MG	AR	3812	1/1	0.83	0.42	-	32,32,32,32	0
84	OHX	AR	3718	7/7	0.91	0.46	-	166,167,167,167	0
85	MG	AS	229	1/1	0.96	0.24	-	46,46,46,46	0
85	MG	AT	222	1/1	0.75	0.35	-	43,43,43,43	0
85	MG	6	2121	1/1	0.92	0.28	-	41,41,41,41	0
85	MG	A	2098	1/1	0.81	0.48	-	65,65,65,65	0
84	OHX	1	3669	7/7	0.94	0.39	-	131,131,131,131	0
85	MG	AR	3986	1/1	0.80	0.21	-	56,56,56,56	0
85	MG	AR	4148	1/1	0.89	0.28	-	43,43,43,43	0
84	OHX	6	1931	7/7	0.98	0.10	-	115,116,116,116	0
85	MG	A	2073	1/1	0.95	0.57	-	50,50,50,50	0
84	OHX	1	3633	7/7	0.97	0.30	-	134,134,135,135	0
85	MG	AR	3765	1/1	0.90	0.39	-	71,71,71,71	0
85	MG	AR	4216	1/1	0.91	0.20	-	44,44,44,44	0
85	MG	4	230	1/1	0.93	0.34	-	35,35,35,35	0
85	MG	1	3728	1/1	0.92	0.61	-	52,52,52,52	0
85	MG	1	4220	1/1	0.94	0.57	-	35,35,35,35	0
85	MG	1	4187	1/1	0.78	0.35	-	43,43,43,43	0
85	MG	A	2051	1/1	0.90	0.47	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	A	2130	1/1	0.46	0.62	-	74,74,74,74	0
85	MG	1	3803	1/1	0.88	0.42	-	41,41,41,41	0
85	MG	AT	231	1/1	0.80	0.83	-	52,52,52,52	0
85	MG	1	3937	1/1	0.93	0.12	-	68,68,68,68	0
85	MG	AR	4031	1/1	0.92	0.20	-	39,39,39,39	0
85	MG	AR	3831	1/1	0.94	0.23	-	44,44,44,44	0
84	OHX	AR	3740	7/7	0.93	0.25	-	161,161,161,162	0
85	MG	AS	216	1/1	0.96	0.50	-	23,23,23,23	0
85	MG	AR	3867	1/1	0.95	0.55	-	18,18,18,18	0
84	OHX	1	3706	7/7	0.95	0.30	-	136,137,137,138	0
85	MG	1	4067	1/1	0.98	0.09	-	40,40,40,40	0
85	MG	AR	3824	1/1	0.91	0.13	-	77,77,77,77	0
85	MG	1	4070	1/1	0.85	0.20	-	68,68,68,68	0
85	MG	6	2115	1/1	0.86	0.41	-	85,85,85,85	0
85	MG	1	3745	1/1	0.99	0.67	-	31,31,31,31	0
85	MG	AR	4165	1/1	0.92	0.21	-	43,43,43,43	0
85	MG	AP	503	1/1	0.96	0.28	-	27,27,27,27	0
85	MG	AR	3832	1/1	0.91	0.53	-	30,30,30,30	0
85	MG	1	3928	1/1	0.89	0.27	-	34,34,34,34	0
85	MG	AS	231	1/1	0.97	0.19	-	56,56,56,56	0
85	MG	1	3863	1/1	0.82	0.21	-	55,55,55,55	0
85	MG	1	4122	1/1	0.97	0.25	-	78,78,78,78	0
85	MG	AR	3894	1/1	0.86	0.53	-	45,45,45,45	0
85	MG	A	2137	1/1	0.96	0.49	-	58,58,58,58	0
85	MG	1	4124	1/1	0.69	0.22	-	48,48,48,48	0
85	MG	4	240	1/1	0.89	0.57	-	32,32,32,32	0
85	MG	CE	403	1/1	0.82	0.32	-	22,22,22,22	0
85	MG	AR	3974	1/1	0.97	0.42	-	81,81,81,81	0
85	MG	AR	4223	1/1	0.80	0.30	-	61,61,61,61	0
85	MG	AR	4224	1/1	0.82	0.49	-	47,47,47,47	0
85	MG	1	3775	1/1	0.96	0.29	-	32,32,32,32	0
85	MG	1	4160	1/1	0.84	0.32	-	34,34,34,34	0
85	MG	1	3861	1/1	0.91	0.24	-	34,34,34,34	0
85	MG	6	2080	1/1	0.90	0.64	-	69,69,69,69	0
84	OHX	AR	3745	7/7	0.91	0.35	-	128,128,128,128	0
84	OHX	1	3644	7/7	0.90	0.25	-	166,167,167,167	0
85	MG	AR	3988	1/1	0.85	0.81	-	50,50,50,50	0
85	MG	AR	3748	1/1	0.93	0.38	-	44,44,44,44	0
85	MG	1	3825	1/1	0.99	0.41	-	31,31,31,31	0
85	MG	1	4042	1/1	0.85	0.41	-	48,48,48,48	0
84	OHX	1	3702	7/7	0.86	0.22	-	219,219,219,219	0
85	MG	1	4205	1/1	0.97	0.24	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	6	2016	7/7	0.94	0.25	-	120,120,121,121	0
85	MG	AR	4134	1/1	0.90	0.27	-	44,44,44,44	0
85	MG	AR	4187	1/1	0.86	0.43	-	36,36,36,36	0
84	OHX	1	3448	7/7	0.98	0.21	-	117,117,117,117	0
85	MG	AR	3872	1/1	0.94	0.34	-	43,43,43,43	0
84	OHX	1	3611	7/7	0.96	0.21	-	119,119,119,120	0
85	MG	6	2114	1/1	0.96	0.47	-	46,46,46,46	0
85	MG	1	3752	1/1	0.86	0.43	-	57,57,57,57	0
85	MG	1	4152	1/1	0.59	0.80	-	111,111,111,111	0
85	MG	1	4169	1/1	0.94	0.27	-	30,30,30,30	0
85	MG	AR	4000	1/1	0.96	0.44	-	25,25,25,25	0
84	OHX	6	2048	7/7	0.91	0.35	-	173,174,174,174	0
85	MG	6	2186	1/1	0.82	0.31	-	107,107,107,107	0
85	MG	AR	4113	1/1	0.84	0.57	-	37,37,37,37	0
85	MG	AR	4196	1/1	0.55	0.43	-	43,43,43,43	0
85	MG	1	4145	1/1	0.84	0.33	-	42,42,42,42	0
85	MG	1	3923	1/1	0.94	0.39	-	51,51,51,51	0
85	MG	s	300	1/1	0.72	0.27	-	70,70,70,70	0
85	MG	1	4091	1/1	0.84	0.32	-	47,47,47,47	0
85	MG	1	3984	1/1	0.85	0.27	-	70,70,70,70	0
85	MG	A	2050	1/1	0.85	0.39	-	67,67,67,67	0
84	OHX	A	2000	7/7	0.95	0.24	-	140,141,141,141	0
85	MG	1	4129	1/1	0.74	0.43	-	33,33,33,33	0
85	MG	6	2192	1/1	0.74	0.67	-	74,74,74,74	0
85	MG	AR	4237	1/1	0.95	0.20	-	39,39,39,39	0
85	MG	AR	3787	1/1	0.95	0.69	-	31,31,31,31	0
84	OHX	6	1935	7/7	0.97	0.14	-	121,121,121,122	0
85	MG	6	2195	1/1	0.86	0.65	-	35,35,35,35	0
85	MG	AR	4191	1/1	0.99	0.17	-	58,58,58,58	0
85	MG	AR	3774	1/1	0.98	0.15	-	30,30,30,30	0
85	MG	6	2117	1/1	0.75	0.28	-	65,65,65,65	0
84	OHX	1	3635	7/7	0.97	0.28	-	122,122,123,123	0
85	MG	AR	4120	1/1	0.86	0.27	-	31,31,31,31	0
85	MG	1	3851	1/1	0.90	0.36	-	34,34,34,34	0
85	MG	AR	3778	1/1	0.91	0.26	-	42,42,42,42	0
84	OHX	1	3628	7/7	0.96	0.26	-	144,145,145,145	0
85	MG	AR	4254	1/1	0.61	0.38	-	56,56,56,56	0
84	OHX	1	3648	7/7	0.94	0.25	-	119,120,120,120	0
85	MG	CM	202	1/1	0.76	0.15	-	62,62,62,62	0
85	MG	1	4211	1/1	0.87	0.63	-	42,42,42,42	0
85	MG	AR	4022	1/1	0.75	0.44	-	30,30,30,30	0
85	MG	AR	3883	1/1	0.94	0.54	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3940	1/1	0.85	0.37	-	43,43,43,43	0
85	MG	A	2049	1/1	0.94	0.50	-	54,54,54,54	0
85	MG	1	3743	1/1	0.96	0.28	-	79,79,79,79	0
85	MG	1	4148	1/1	0.76	0.18	-	53,53,53,53	0
85	MG	1	3812	1/1	0.96	0.64	-	64,64,64,64	0
85	MG	4	241	1/1	0.94	0.58	-	45,45,45,45	0
85	MG	6	2100	1/1	0.92	0.51	-	36,36,36,36	0
85	MG	AR	3845	1/1	0.87	0.41	-	23,23,23,23	0
84	OHX	AR	3564	7/7	0.94	0.14	-	155,155,155,155	0
85	MG	AR	3835	1/1	0.92	0.41	-	45,45,45,45	0
85	MG	1	3877	1/1	0.92	0.72	-	36,36,36,36	0
85	MG	1	3998	1/1	0.82	0.34	-	36,36,36,36	0
84	OHX	1	3709	7/7	0.86	0.35	-	157,158,158,158	0
84	OHX	3	209	7/7	0.90	0.28	-	152,152,152,152	0
85	MG	1	3883	1/1	0.97	0.41	-	22,22,22,22	0
85	MG	3	216	1/1	0.86	0.40	-	58,58,58,58	0
85	MG	1	4111	1/1	0.85	0.55	-	44,44,44,44	0
85	MG	1	3929	1/1	0.91	0.30	-	34,34,34,34	0
84	OHX	AR	3741	7/7	0.87	0.38	-	207,208,208,208	0
85	MG	A	2128	1/1	0.73	0.50	-	78,78,78,78	0
85	MG	AR	4076	1/1	0.83	0.32	-	48,48,48,48	0
85	MG	x	206	1/1	0.78	0.58	-	35,35,35,35	0
85	MG	1	3957	1/1	0.94	0.39	-	37,37,37,37	0
85	MG	6	2160	1/1	0.62	0.38	-	85,85,85,85	0
85	MG	6	2169	1/1	0.87	0.63	-	49,49,49,49	0
85	MG	1	3970	1/1	0.92	0.30	-	31,31,31,31	0
85	MG	AR	4088	1/1	0.95	0.40	-	25,25,25,25	0
85	MG	1	3951	1/1	0.45	0.33	-	69,69,69,69	0
85	MG	1	3881	1/1	0.89	0.55	-	31,31,31,31	0
84	OHX	1	3712	7/7	0.89	0.34	-	133,133,133,133	0
85	MG	1	3948	1/1	0.55	0.23	-	73,73,73,73	0
85	MG	AR	4127	1/1	0.86	0.16	-	77,77,77,77	0
84	OHX	AR	3614	7/7	0.96	0.20	-	114,114,114,114	0
85	MG	1	3853	1/1	0.84	0.55	-	48,48,48,48	0
85	MG	6	2164	1/1	0.87	0.35	-	53,53,53,53	0
84	OHX	AR	3733	7/7	0.89	0.33	-	187,188,188,188	0
84	OHX	AR	3647	7/7	0.92	0.30	-	126,126,127,127	0
85	MG	AR	4003	1/1	0.72	0.44	-	45,45,45,45	0
85	MG	AR	4222	1/1	0.73	0.39	-	58,58,58,58	0
85	MG	l	402	1/1	0.92	0.33	-	57,57,57,57	0
85	MG	1	4165	1/1	0.82	0.40	-	24,24,24,24	0
85	MG	AR	4056	1/1	0.82	0.38	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	6	2152	1/1	0.82	0.43	-	62,62,62,62	0
85	MG	AR	3808	1/1	0.92	0.34	-	28,28,28,28	0
85	MG	AR	4011	1/1	0.73	0.39	-	58,58,58,58	0
85	MG	1	3747	1/1	0.94	0.34	-	37,37,37,37	0
85	MG	1	3964	1/1	0.93	0.46	-	68,68,68,68	0
85	MG	AR	4251	1/1	0.88	0.41	-	59,59,59,59	0
85	MG	1	3758	1/1	0.88	0.50	-	32,32,32,32	0
84	OHX	6	2023	7/7	0.92	0.38	-	161,161,162,162	0
84	OHX	1	3512	7/7	0.98	0.17	-	110,110,110,110	0
84	OHX	CF	402	7/7	0.92	0.34	-	145,146,146,146	0
85	MG	AR	4018	1/1	0.92	0.21	-	36,36,36,36	0
85	MG	1	4117	1/1	0.90	0.31	-	41,41,41,41	0
85	MG	A	2096	1/1	0.94	0.41	-	62,62,62,62	0
84	OHX	A	1993	7/7	0.91	0.38	-	151,151,152,152	0
84	OHX	AR	3595	7/7	0.95	0.31	-	131,131,131,132	0
85	MG	6	2146	1/1	0.81	1.00	-	80,80,80,80	0
84	OHX	A	2022	7/7	0.94	0.36	-	167,167,167,167	0
85	MG	AR	4084	1/1	0.90	0.22	-	34,34,34,34	0
85	MG	AR	3862	1/1	0.85	0.21	-	56,56,56,56	0
85	MG	AR	4260	1/1	0.98	0.52	-	6,6,6,6	0
84	OHX	1	3693	7/7	0.96	0.27	-	118,118,118,118	0
85	MG	AR	3922	1/1	0.91	0.49	-	31,31,31,31	0
85	MG	1	3855	1/1	0.82	0.31	-	44,44,44,44	0
85	MG	AR	3811	1/1	0.82	0.20	-	50,50,50,50	0
85	MG	1	3832	1/1	0.86	0.41	-	26,26,26,26	0
85	MG	AR	4147	1/1	0.91	0.23	-	31,31,31,31	0
85	MG	6	2090	1/1	0.86	0.31	-	49,49,49,49	0
85	MG	AT	224	1/1	0.73	0.22	-	68,68,68,68	0
84	OHX	1	3625	7/7	0.97	0.22	-	135,135,135,135	0
85	MG	AR	3791	1/1	0.94	0.26	-	34,34,34,34	0
85	MG	6	2074	1/1	0.78	0.37	-	62,62,62,62	0
85	MG	AR	3928	1/1	0.93	0.46	-	39,39,39,39	0
85	MG	1	4057	1/1	0.94	0.23	-	26,26,26,26	0
84	OHX	1	3647	7/7	0.97	0.23	-	118,118,118,118	0
85	MG	1	4035	1/1	0.91	0.60	-	47,47,47,47	0
84	OHX	1	3562	7/7	0.97	0.14	-	121,121,121,121	0
84	OHX	AR	3694	7/7	0.92	0.33	-	146,147,147,147	0
85	MG	1	4206	1/1	0.94	0.30	-	30,30,30,30	0
84	OHX	AR	3567	7/7	0.96	0.15	-	121,121,121,121	0
84	OHX	AR	3518	7/7	0.98	0.10	-	118,119,119,119	0
85	MG	1	3922	1/1	0.94	0.45	-	45,45,45,45	0
85	MG	AR	4049	1/1	0.72	0.19	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	4072	1/1	0.97	0.18	-	46,46,46,46	0
85	MG	A	2059	1/1	0.95	0.61	-	53,53,53,53	0
85	MG	1	3726	1/1	0.89	0.84	-	54,54,54,54	0
85	MG	AR	4229	1/1	0.97	0.70	-	34,34,34,34	0
85	MG	6	2141	1/1	0.87	0.32	-	52,52,52,52	0
85	MG	1	3895	1/1	0.97	0.42	-	28,28,28,28	0
84	OHX	6	2045	7/7	0.83	0.34	-	141,141,142,142	0
85	MG	6	2095	1/1	0.92	0.43	-	41,41,41,41	0
85	MG	1	4099	1/1	0.92	0.23	-	44,44,44,44	0
85	MG	AR	4259	1/1	0.95	0.49	-	16,16,16,16	0
85	MG	AR	4166	1/1	0.90	0.16	-	38,38,38,38	0
84	OHX	1	3639	7/7	0.94	0.32	-	132,132,132,132	0
84	OHX	6	1936	7/7	0.97	0.15	-	116,116,117,117	0
85	MG	A	2071	1/1	0.94	0.33	-	64,64,64,64	0
85	MG	1	3763	1/1	0.94	0.66	-	29,29,29,29	0
85	MG	A	2152	1/1	0.81	0.70	-	43,43,43,43	0
84	OHX	3	201	7/7	0.98	0.19	-	121,121,121,122	0
85	MG	AR	4023	1/1	0.88	0.23	-	31,31,31,31	0
85	MG	6	2113	1/1	0.94	0.23	-	77,77,77,77	0
85	MG	A	2124	1/1	0.61	0.30	-	68,68,68,68	0
85	MG	1	4019	1/1	0.97	0.24	-	42,42,42,42	0
85	MG	AR	4129	1/1	0.95	0.36	-	26,26,26,26	0
84	OHX	A	2007	7/7	0.87	0.26	-	200,200,201,201	0
85	MG	AR	4047	1/1	0.88	0.14	-	54,54,54,54	0
85	MG	1	4002	1/1	0.92	0.55	-	37,37,37,37	0
85	MG	A	2133	1/1	0.88	0.20	-	72,72,72,72	0
85	MG	AR	3990	1/1	0.95	0.08	-	39,39,39,39	0
85	MG	AR	3836	1/1	0.82	0.45	-	48,48,48,48	0
85	MG	AR	3923	1/1	0.94	0.66	-	38,38,38,38	0
85	MG	AR	4231	1/1	0.91	0.35	-	32,32,32,32	0
85	MG	4	220	1/1	0.85	0.34	-	64,64,64,64	0
85	MG	1	4055	1/1	0.90	0.17	-	33,33,33,33	0
85	MG	A	2135	1/1	0.74	0.56	-	55,55,55,55	0
85	MG	1	3966	1/1	0.81	0.18	-	69,69,69,69	0
85	MG	AS	215	1/1	0.88	0.36	-	58,58,58,58	0
85	MG	AR	4201	1/1	0.93	0.26	-	35,35,35,35	0
85	MG	1	4069	1/1	0.96	0.43	-	46,46,46,46	0
85	MG	1	3772	1/1	0.61	0.20	-	35,35,35,35	0
85	MG	1	3996	1/1	0.87	0.44	-	64,64,64,64	0
85	MG	1	4014	1/1	0.80	0.37	-	57,57,57,57	0
85	MG	1	3813	1/1	0.48	0.37	-	61,61,61,61	0
85	MG	1	4107	1/1	0.92	0.16	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	4	217	1/1	0.93	0.56	-	52,52,52,52	0
85	MG	AR	3916	1/1	0.96	0.58	-	19,19,19,19	0
85	MG	AS	226	1/1	0.85	0.21	-	67,67,67,67	0
85	MG	AR	4163	1/1	0.89	0.23	-	62,62,62,62	0
85	MG	1	3816	1/1	0.75	0.34	-	44,44,44,44	0
85	MG	AR	4060	1/1	0.81	0.27	-	70,70,70,70	0
84	OHX	A	1968	7/7	0.97	0.34	-	125,125,126,126	0
84	OHX	1	3503	7/7	0.97	0.10	-	127,128,128,129	0
85	MG	1	4054	1/1	0.92	0.21	-	56,56,56,56	0
84	OHX	6	2036	7/7	0.93	0.39	-	135,135,136,136	0
85	MG	A	2083	1/1	0.81	0.18	-	68,68,68,68	0
85	MG	1	3759	1/1	0.86	0.12	-	41,41,41,41	0
85	MG	1	3850	1/1	0.92	0.48	-	31,31,31,31	0
84	OHX	AR	3679	7/7	0.96	0.25	-	153,153,153,154	0
85	MG	1	3980	1/1	0.96	0.27	-	73,73,73,73	0
85	MG	CP	503	1/1	0.97	0.41	-	38,38,38,38	0
85	MG	A	2146	1/1	0.72	0.16	-	120,120,120,120	0
85	MG	A	2110	1/1	0.87	0.67	-	116,116,116,116	0
84	OHX	4	211	7/7	0.96	0.14	-	138,139,139,140	0
85	MG	AR	4236	1/1	0.91	0.42	-	23,23,23,23	0
85	MG	1	3963	1/1	0.81	0.24	-	45,45,45,45	0
85	MG	1	4053	1/1	0.49	0.41	-	74,74,74,74	0
85	MG	A	2122	1/1	0.90	0.17	-	86,86,86,86	0
85	MG	6	2058	1/1	0.97	0.43	-	45,45,45,45	0
85	MG	4	229	1/1	0.56	0.41	-	54,54,54,54	0
85	MG	AR	4123	1/1	0.78	0.36	-	57,57,57,57	0
84	OHX	6	2042	7/7	0.94	0.34	-	151,151,151,151	0
84	OHX	AR	3650	7/7	0.93	0.44	-	118,118,118,118	0
84	OHX	6	2010	7/7	0.94	0.33	-	154,155,155,155	0
84	OHX	1	3602	7/7	0.97	0.23	-	128,128,128,129	0
85	MG	1	4098	1/1	0.83	0.27	-	47,47,47,47	0
84	OHX	A	1934	7/7	0.97	0.12	-	132,132,133,133	0
85	MG	1	4050	1/1	0.83	0.36	-	31,31,31,31	0
85	MG	A	2060	1/1	0.93	0.62	-	55,55,55,55	0
85	MG	6	2055	1/1	0.96	0.73	-	49,49,49,49	0
85	MG	AR	3944	1/1	0.83	0.17	-	38,38,38,38	0
84	OHX	AR	3676	7/7	0.96	0.29	-	122,122,123,123	0
85	MG	AR	3830	1/1	0.98	0.46	-	42,42,42,42	0
85	MG	6	2181	1/1	0.99	0.11	-	95,95,95,95	0
84	OHX	4	206	7/7	0.96	0.16	-	116,116,116,116	0
85	MG	1	3903	1/1	0.99	0.67	-	21,21,21,21	0
85	MG	1	3831	1/1	0.94	0.47	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3961	1/1	0.87	0.19	-	40,40,40,40	0
85	MG	A	2067	1/1	0.91	0.81	-	64,64,64,64	0
85	MG	1	3908	1/1	0.87	0.50	-	62,62,62,62	0
85	MG	1	3818	1/1	0.90	0.43	-	39,39,39,39	0
85	MG	6	2054	1/1	0.94	0.39	-	49,49,49,49	0
85	MG	4	235	1/1	0.76	0.50	-	70,70,70,70	0
85	MG	1	4030	1/1	0.91	0.72	-	72,72,72,72	0
84	OHX	1	3595	7/7	0.96	0.11	-	140,140,140,140	0
85	MG	AR	3967	1/1	0.89	0.55	-	42,42,42,42	0
85	MG	AR	4004	1/1	0.94	0.16	-	32,32,32,32	0
85	MG	6	2123	1/1	0.89	0.24	-	69,69,69,69	0
84	OHX	6	1965	7/7	0.97	0.24	-	116,117,117,117	0
85	MG	1	4079	1/1	0.92	0.21	-	97,97,97,97	0
85	MG	1	3907	1/1	0.95	0.33	-	40,40,40,40	0
84	OHX	AT	216	7/7	0.95	0.40	-	132,132,132,132	0
85	MG	6	2147	1/1	0.95	0.12	-	57,57,57,57	0
85	MG	AR	4087	1/1	0.76	0.36	-	63,63,63,63	0
85	MG	1	4194	1/1	0.94	0.50	-	22,22,22,22	0
84	OHX	AR	3419	7/7	0.99	0.27	-	122,122,123,123	0
85	MG	6	2176	1/1	0.32	0.67	-	93,93,93,93	0
85	MG	AR	4180	1/1	0.91	0.39	-	48,48,48,48	0
84	OHX	AR	3674	7/7	0.93	0.46	-	130,130,130,131	0
85	MG	1	4176	1/1	0.96	0.62	-	34,34,34,34	0
84	OHX	c3	201	7/7	0.91	0.24	-	155,156,156,157	0
85	MG	1	3817	1/1	0.98	0.26	-	23,23,23,23	0
85	MG	AR	4142	1/1	0.85	0.31	-	46,46,46,46	0
84	OHX	1	3439	7/7	0.98	0.19	-	109,109,109,109	0
84	OHX	AR	3510	7/7	0.98	0.13	-	117,118,118,118	0
84	OHX	AR	3540	7/7	0.97	0.16	-	108,108,108,108	0
85	MG	AR	3792	1/1	0.92	0.51	-	43,43,43,43	0
85	MG	AR	4215	1/1	0.75	0.28	-	70,70,70,70	0
85	MG	1	4022	1/1	0.91	0.59	-	53,53,53,53	0
85	MG	1	4161	1/1	0.73	0.25	-	69,69,69,69	0
84	OHX	A	2023	7/7	0.91	0.26	-	144,145,145,145	0
85	MG	1	3981	1/1	0.86	0.49	-	50,50,50,50	0
85	MG	6	2180	1/1	0.61	0.60	-	64,64,64,64	0
85	MG	1	4080	1/1	0.89	0.22	-	35,35,35,35	0
85	MG	AS	225	1/1	0.74	0.35	-	58,58,58,58	0
85	MG	AR	3788	1/1	0.93	0.50	-	28,28,28,28	0
85	MG	CQ	203	1/1	0.95	0.15	-	34,34,34,34	0
85	MG	1	4146	1/1	0.92	0.17	-	48,48,48,48	0
85	MG	AR	3798	1/1	0.93	0.33	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	6	2026	7/7	0.95	0.26	-	146,146,147,147	0
85	MG	1	4028	1/1	0.90	0.16	-	46,46,46,46	0
85	MG	AR	4072	1/1	0.91	0.25	-	70,70,70,70	0
85	MG	6	2174	1/1	0.70	0.44	-	58,58,58,58	0
84	OHX	AR	3546	7/7	0.96	0.21	-	123,124,124,124	0
85	MG	AR	3911	1/1	0.83	0.42	-	40,40,40,40	0
85	MG	AR	4017	1/1	0.85	0.31	-	95,95,95,95	0
85	MG	AR	3931	1/1	0.96	0.29	-	17,17,17,17	0
85	MG	AR	4093	1/1	0.85	0.37	-	46,46,46,46	0
85	MG	A	2090	1/1	0.93	0.20	-	57,57,57,57	0
85	MG	1	3736	1/1	0.97	0.60	-	31,31,31,31	0
85	MG	AR	3984	1/1	0.82	0.65	-	50,50,50,50	0
85	MG	1	3862	1/1	0.93	0.46	-	52,52,52,52	0
85	MG	3	210	1/1	0.92	0.39	-	59,59,59,59	0
85	MG	lR	201	1/1	0.96	0.36	-	26,26,26,26	0
85	MG	1	3824	1/1	0.95	0.39	-	25,25,25,25	0
84	OHX	1	3664	7/7	0.93	0.35	-	124,124,124,124	0
85	MG	AR	4032	1/1	0.84	0.37	-	48,48,48,48	0
85	MG	AT	226	1/1	0.84	0.30	-	63,63,63,63	0
84	OHX	1	3622	7/7	0.96	0.27	-	153,154,154,154	0
85	MG	1	3857	1/1	0.76	0.25	-	56,56,56,56	0
85	MG	1	4153	1/1	0.93	0.18	-	39,39,39,39	0
85	MG	AR	3866	1/1	0.99	0.23	-	34,34,34,34	0
85	MG	1	4005	1/1	0.89	0.35	-	36,36,36,36	0
85	MG	AR	4173	1/1	0.83	0.31	-	53,53,53,53	0
85	MG	AS	219	1/1	0.77	0.24	-	58,58,58,58	0
85	MG	4	239	1/1	0.96	0.70	-	43,43,43,43	0
85	MG	1	3910	1/1	0.98	0.58	-	19,19,19,19	0
85	MG	1	3753	1/1	0.94	0.54	-	35,35,35,35	0
85	MG	AR	4116	1/1	0.82	0.30	-	99,99,99,99	0
84	OHX	AR	3608	7/7	0.94	0.34	-	131,131,132,132	0
85	MG	6	2079	1/1	0.87	0.24	-	45,45,45,45	0
85	MG	1	4097	1/1	0.99	0.22	-	70,70,70,70	0
85	MG	AR	4170	1/1	0.70	0.27	-	32,32,32,32	0
85	MG	AR	4006	1/1	0.94	0.55	-	47,47,47,47	0
85	MG	d6	101	1/1	0.91	0.33	-	49,49,49,49	0
84	OHX	1	3514	7/7	0.94	0.18	-	112,112,112,112	0
84	OHX	A	2020	7/7	0.93	0.23	-	147,148,148,148	0
85	MG	1	4217	1/1	0.93	0.92	-	58,58,58,58	0
85	MG	CG	303	1/1	0.93	0.13	-	62,62,62,62	0
85	MG	AR	3852	1/1	0.87	0.24	-	37,37,37,37	0
85	MG	AR	3960	1/1	0.84	0.21	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	4160	1/1	0.77	0.26	-	78,78,78,78	0
85	MG	AR	3899	1/1	0.89	0.60	-	45,45,45,45	0
85	MG	1	4182	1/1	0.97	0.30	-	25,25,25,25	0
84	OHX	A	1943	7/7	0.97	0.21	-	133,133,134,134	0
84	OHX	6	1969	7/7	0.94	0.15	-	127,127,128,128	0
85	MG	1	3972	1/1	0.83	0.85	-	45,45,45,45	0
85	MG	6	2106	1/1	0.92	0.39	-	50,50,50,50	0
85	MG	3	213	1/1	0.96	0.45	-	48,48,48,48	0
85	MG	6	2072	1/1	0.82	0.70	-	40,40,40,40	0
85	MG	1	4046	1/1	0.78	0.34	-	37,37,37,37	0
85	MG	AR	4037	1/1	0.71	0.34	-	70,70,70,70	0
85	MG	AR	4245	1/1	0.83	0.22	-	26,26,26,26	0
85	MG	AR	4194	1/1	0.80	0.27	-	53,53,53,53	0
85	MG	1	3834	1/1	0.92	0.51	-	22,22,22,22	0
84	OHX	AR	3734	7/7	0.86	0.54	-	148,148,148,149	0
85	MG	AR	3892	1/1	0.91	0.48	-	31,31,31,31	0
85	MG	1	4004	1/1	0.64	0.26	-	44,44,44,44	0
84	OHX	6	2007	7/7	0.92	0.28	-	145,146,146,146	0
85	MG	DC	201	1/1	0.89	0.45	-	30,30,30,30	0
85	MG	1	4026	1/1	0.92	0.40	-	65,65,65,65	0
85	MG	1	3774	1/1	0.95	0.54	-	43,43,43,43	0
85	MG	AR	3870	1/1	0.98	0.70	-	33,33,33,33	0
84	OHX	1	3600	7/7	0.98	0.15	-	150,150,150,150	0
85	MG	DC	203	1/1	0.73	0.30	-	47,47,47,47	0
85	MG	1	4008	1/1	0.92	0.29	-	37,37,37,37	0
85	MG	6	2119	1/1	0.98	0.47	-	74,74,74,74	0
85	MG	6	2069	1/1	0.94	0.35	-	65,65,65,65	0
85	MG	1	4045	1/1	0.82	0.34	-	39,39,39,39	0
85	MG	AR	3782	1/1	0.74	0.35	-	36,36,36,36	0
85	MG	1	3768	1/1	0.94	0.41	-	36,36,36,36	0
85	MG	AR	4097	1/1	0.79	0.58	-	40,40,40,40	0
85	MG	AR	3971	1/1	0.78	0.42	-	57,57,57,57	0
85	MG	3	214	1/1	0.92	0.52	-	34,34,34,34	0
84	OHX	A	2032	7/7	0.94	0.20	-	154,154,155,155	0
85	MG	AS	212	1/1	0.95	0.33	-	41,41,41,41	0
85	MG	A	2132	1/1	0.90	0.26	-	98,98,98,98	0
84	OHX	3	205	7/7	0.91	0.21	-	127,128,128,128	0
85	MG	1	4197	1/1	0.96	0.34	-	32,32,32,32	0
85	MG	AR	4137	1/1	0.91	0.48	-	79,79,79,79	0
84	OHX	1	3691	7/7	0.77	0.31	-	201,201,201,201	0
84	OHX	AR	3678	7/7	0.93	0.42	-	137,137,137,138	0
85	MG	AS	228	1/1	0.56	0.43	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	3958	1/1	0.85	0.56	-	38,38,38,38	0
85	MG	AR	4145	1/1	0.86	0.20	-	70,70,70,70	0
85	MG	1	4120	1/1	0.96	0.40	-	27,27,27,27	0
85	MG	AR	4213	1/1	0.94	0.14	-	53,53,53,53	0
84	OHX	AR	3713	7/7	0.94	0.24	-	178,178,179,179	0
85	MG	1	4143	1/1	0.96	0.21	-	29,29,29,29	0
85	MG	AR	4068	1/1	0.91	0.12	-	99,99,99,99	0
85	MG	1	3826	1/1	0.93	0.25	-	33,33,33,33	0
84	OHX	AR	3680	7/7	0.95	0.41	-	141,141,142,142	0
85	MG	A	2045	1/1	0.75	0.79	-	58,58,58,58	0
85	MG	6	2092	1/1	0.79	0.57	-	93,93,93,93	0
85	MG	A	2139	1/1	0.70	0.36	-	64,64,64,64	0
85	MG	1	3956	1/1	0.89	0.54	-	34,34,34,34	0
85	MG	AR	3943	1/1	0.89	0.10	-	41,41,41,41	0
85	MG	AR	3761	1/1	0.81	0.33	-	31,31,31,31	0
85	MG	t	201	1/1	0.90	0.17	-	51,51,51,51	0
85	MG	AR	4101	1/1	0.82	0.25	-	48,48,48,48	0
85	MG	1	3749	1/1	0.95	0.26	-	24,24,24,24	0
85	MG	1	3750	1/1	0.79	0.18	-	55,55,55,55	0
85	MG	AR	3880	1/1	0.95	0.47	-	42,42,42,42	0
85	MG	AR	3957	1/1	0.86	0.13	-	55,55,55,55	0
85	MG	AR	4217	1/1	0.96	0.60	-	80,80,80,80	0
85	MG	U	201	1/1	0.86	0.42	-	76,76,76,76	0
84	OHX	AR	3670	7/7	0.93	0.19	-	143,143,144,144	0
85	MG	DL	102	1/1	0.88	0.50	-	39,39,39,39	0
85	MG	AR	3903	1/1	0.82	0.69	-	39,39,39,39	0
85	MG	AR	3773	1/1	0.90	0.29	-	41,41,41,41	0
85	MG	A	2082	1/1	0.94	0.23	-	61,61,61,61	0
85	MG	1	4043	1/1	0.97	0.32	-	27,27,27,27	0
84	OHX	1	3720	7/7	0.91	0.28	-	128,128,129,129	0
85	MG	c6	201	1/1	0.82	0.22	-	89,89,89,89	0
84	OHX	1	3559	7/7	0.95	0.17	-	143,143,143,144	0
85	MG	AR	3799	1/1	0.99	0.36	-	22,22,22,22	0
85	MG	AR	4121	1/1	0.96	0.30	-	27,27,27,27	0
85	MG	A	2112	1/1	0.70	0.37	-	86,86,86,86	0
85	MG	d3	201	1/1	0.94	0.25	-	49,49,49,49	0
85	MG	4	226	1/1	0.96	0.59	-	42,42,42,42	0
85	MG	1	3849	1/1	0.91	0.44	-	23,23,23,23	0
85	MG	6	2062	1/1	0.95	0.42	-	51,51,51,51	0
84	OHX	6	2006	7/7	0.89	0.29	-	151,151,152,152	0
84	OHX	AR	3682	7/7	0.96	0.52	-	144,144,144,145	0
85	MG	1	3742	1/1	0.94	0.47	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	3834	1/1	0.89	0.47	-	33,33,33,33	0
85	MG	1	3865	1/1	0.91	0.32	-	45,45,45,45	0
85	MG	1	4144	1/1	0.95	0.16	-	53,53,53,53	0
85	MG	1	4177	1/1	0.96	0.44	-	27,27,27,27	0
85	MG	AR	4150	1/1	0.88	0.17	-	44,44,44,44	0
85	MG	1	4138	1/1	0.87	0.28	-	33,33,33,33	0
85	MG	AR	4193	1/1	0.93	0.32	-	38,38,38,38	0
85	MG	1	3993	1/1	0.83	0.62	-	42,42,42,42	0
85	MG	CQ	201	1/1	0.93	0.38	-	34,34,34,34	0
85	MG	3	215	1/1	0.96	0.57	-	31,31,31,31	0
85	MG	1	4101	1/1	0.72	0.51	-	38,38,38,38	0
85	MG	6	2151	1/1	0.96	0.15	-	60,60,60,60	0
85	MG	1	3852	1/1	0.80	0.33	-	38,38,38,38	0
84	OHX	A	1929	7/7	0.98	0.15	-	123,123,124,124	0
85	MG	A	2070	1/1	0.88	0.53	-	79,79,79,79	0
85	MG	6	2126	1/1	0.95	0.29	-	53,53,53,53	0
84	OHX	AR	3453	7/7	0.98	0.10	-	106,106,107,107	0
84	OHX	AT	217	7/7	0.93	0.37	-	128,128,128,128	0
85	MG	1	4009	1/1	0.86	0.66	-	42,42,42,42	0
84	OHX	AS	202	7/7	0.98	0.22	-	124,124,125,125	0
85	MG	AR	4039	1/1	0.82	0.38	-	56,56,56,56	0
84	OHX	1	3667	7/7	0.95	0.30	-	127,127,128,128	0
84	OHX	1	3668	7/7	0.81	0.45	-	124,124,124,124	0
84	OHX	A	2039	7/7	0.91	0.41	-	166,167,168,168	0
85	MG	1	3945	1/1	0.88	0.29	-	57,57,57,57	0
85	MG	1	3770	1/1	0.94	0.25	-	29,29,29,29	0
85	MG	AR	3908	1/1	0.97	0.53	-	25,25,25,25	0
85	MG	AR	4030	1/1	0.72	0.57	-	59,59,59,59	0
85	MG	1	4056	1/1	0.74	0.30	-	51,51,51,51	0
85	MG	1	3986	1/1	0.94	0.26	-	42,42,42,42	0
85	MG	v	304	1/1	0.86	0.62	-	52,52,52,52	0
85	MG	AS	221	1/1	0.95	0.16	-	60,60,60,60	0
85	MG	1	4162	1/1	0.88	0.25	-	40,40,40,40	0
85	MG	AR	3789	1/1	0.91	0.39	-	36,36,36,36	0
85	MG	1	4044	1/1	0.80	0.32	-	47,47,47,47	0
85	MG	AR	4058	1/1	0.93	0.53	-	61,61,61,61	0
85	MG	1	4116	1/1	0.90	0.52	-	44,44,44,44	0
85	MG	A	2134	1/1	0.87	0.35	-	70,70,70,70	0
85	MG	1	3821	1/1	0.92	0.52	-	66,66,66,66	0
84	OHX	AR	3445	7/7	0.97	0.18	-	107,107,107,107	0
85	MG	1	3766	1/1	0.90	0.16	-	73,73,73,73	0
85	MG	1	4173	1/1	0.95	0.54	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3786	1/1	0.87	0.20	-	40,40,40,40	0
85	MG	AR	4094	1/1	0.83	0.31	-	43,43,43,43	0
85	MG	1	3835	1/1	0.98	0.47	-	30,30,30,30	0
85	MG	A	2068	1/1	0.84	0.56	-	84,84,84,84	0
85	MG	1	3983	1/1	0.74	0.52	-	55,55,55,55	0
85	MG	3	211	1/1	0.89	0.35	-	38,38,38,38	0
85	MG	AR	4104	1/1	0.57	0.39	-	66,66,66,66	0
84	OHX	A	2005	7/7	0.96	0.32	-	131,132,132,132	0
85	MG	Y	201	1/1	0.70	0.20	-	61,61,61,61	0
85	MG	1	4068	1/1	0.93	0.46	-	42,42,42,42	0
85	MG	AR	3800	1/1	0.93	0.65	-	33,33,33,33	0
84	OHX	1	3627	7/7	0.92	0.28	-	141,142,142,143	0
85	MG	AT	219	1/1	0.98	0.35	-	36,36,36,36	0
85	MG	AR	4242	1/1	0.93	0.46	-	35,35,35,35	0
85	MG	AS	227	1/1	0.92	0.32	-	45,45,45,45	0
85	MG	1	4192	1/1	0.97	0.67	-	21,21,21,21	0
85	MG	1	3754	1/1	0.85	0.52	-	37,37,37,37	0
85	MG	1	3840	1/1	0.81	0.31	-	78,78,78,78	0
85	MG	6	2165	1/1	0.91	0.35	-	51,51,51,51	0
85	MG	AR	4063	1/1	0.79	0.12	-	54,54,54,54	0
85	MG	AR	4099	1/1	0.89	0.16	-	41,41,41,41	0
84	OHX	AR	3634	7/7	0.94	0.26	-	112,112,113,113	0
85	MG	6	2083	1/1	0.75	0.45	-	63,63,63,63	0
85	MG	AR	3805	1/1	0.93	0.44	-	36,36,36,36	0
85	MG	4	232	1/1	0.80	0.28	-	37,37,37,37	0
85	MG	1	3791	1/1	0.94	0.60	-	54,54,54,54	0
85	MG	AR	4021	1/1	0.84	0.17	-	82,82,82,82	0
85	MG	AR	4098	1/1	0.90	0.20	-	46,46,46,46	0
85	MG	AT	225	1/1	0.86	0.90	-	53,53,53,53	0
85	MG	1	3988	1/1	0.73	0.37	-	34,34,34,34	0
85	MG	AR	4146	1/1	0.86	0.19	-	34,34,34,34	0
85	MG	6	2156	1/1	0.95	0.16	-	101,101,101,101	0
85	MG	AR	4171	1/1	0.77	0.17	-	88,88,88,88	0
85	MG	1	4132	1/1	0.98	0.12	-	86,86,86,86	0
85	MG	AR	3932	1/1	0.97	0.28	-	63,63,63,63	0
84	OHX	AR	3629	7/7	0.96	0.14	-	141,141,141,142	0
84	OHX	AR	3710	7/7	0.94	0.34	-	137,137,137,138	0
85	MG	1	3960	1/1	0.89	0.21	-	33,33,33,33	0
85	MG	AR	3842	1/1	0.87	0.16	-	47,47,47,47	0
85	MG	6	2073	1/1	0.95	0.52	-	48,48,48,48	0
85	MG	3	218	1/1	0.97	0.22	-	54,54,54,54	0
85	MG	AB	202	1/1	0.86	0.31	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	A	1981	7/7	0.92	0.16	-	194,195,195,195	0
84	OHX	1	3465	7/7	0.98	0.18	-	117,117,117,117	0
85	MG	6	2185	1/1	0.61	0.46	-	89,89,89,89	0
84	OHX	AR	3615	7/7	0.94	0.36	-	132,133,133,133	0
85	MG	6	2136	1/1	0.97	0.23	-	52,52,52,52	0
85	MG	AR	3902	1/1	0.92	0.57	-	42,42,42,42	0
85	MG	1	3797	1/1	0.85	0.18	-	79,79,79,79	0
85	MG	AR	3976	1/1	0.77	0.44	-	81,81,81,81	0
85	MG	AR	4257	1/1	0.76	0.32	-	51,51,51,51	0
85	MG	AR	3851	1/1	0.87	0.29	-	38,38,38,38	0
85	MG	A	2046	1/1	0.71	0.29	-	67,67,67,67	0
85	MG	1	4073	1/1	0.89	0.39	-	40,40,40,40	0
85	MG	AR	3779	1/1	0.80	0.38	-	73,73,73,73	0
85	MG	1	4059	1/1	0.97	0.42	-	51,51,51,51	0
85	MG	AR	4105	1/1	0.95	0.14	-	42,42,42,42	0
84	OHX	AR	3475	7/7	0.98	0.14	-	116,116,116,116	0
84	OHX	AR	3556	7/7	0.96	0.21	-	109,109,109,109	0
85	MG	1	3965	1/1	0.51	0.57	-	94,94,94,94	0
85	MG	6	2149	1/1	0.89	0.32	-	46,46,46,46	0
85	MG	A	2107	1/1	0.82	0.31	-	80,80,80,80	0
85	MG	1	3727	1/1	0.94	0.28	-	37,37,37,37	0
85	MG	4	223	1/1	0.94	0.59	-	27,27,27,27	0
85	MG	1	3827	1/1	0.98	0.73	-	32,32,32,32	0
85	MG	1	3955	1/1	0.82	0.43	-	51,51,51,51	0
85	MG	AR	3746	1/1	0.95	0.26	-	58,58,58,58	0
85	MG	AR	4184	1/1	0.91	0.16	-	69,69,69,69	0
85	MG	1	4032	1/1	0.96	0.31	-	42,42,42,42	0
85	MG	AR	4258	1/1	0.96	0.54	-	34,34,34,34	0
85	MG	6	2189	1/1	0.76	0.34	-	63,63,63,63	0
85	MG	1	3967	1/1	0.85	0.20	-	38,38,38,38	0
85	MG	1	3915	1/1	0.89	0.13	-	36,36,36,36	0
85	MG	1	4062	1/1	0.93	0.16	-	45,45,45,45	0
85	MG	AR	4151	1/1	0.95	0.11	-	148,148,148,148	0
85	MG	6	2127	1/1	0.91	0.47	-	54,54,54,54	0
85	MG	1	4087	1/1	0.78	0.23	-	59,59,59,59	0
85	MG	1	4171	1/1	0.95	0.23	-	85,85,85,85	0
85	MG	AR	4156	1/1	0.77	1.08	-	72,72,72,72	0
84	OHX	1	3490	7/7	0.99	0.17	-	113,113,113,113	0
85	MG	A	2117	1/1	0.71	0.19	-	71,71,71,71	0
84	OHX	1	3457	7/7	0.98	0.18	-	126,127,127,128	0
84	OHX	AR	3686	7/7	0.83	0.38	-	156,156,156,157	0
85	MG	1	3995	1/1	0.89	0.30	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3526	7/7	0.96	0.18	-	117,117,117,118	0
85	MG	A	2159	1/1	0.84	0.93	-	64,64,64,64	0
85	MG	d5	201	1/1	0.89	0.09	-	71,71,71,71	0
85	MG	AS	218	1/1	0.90	0.30	-	33,33,33,33	0
85	MG	AR	4256	1/1	0.91	0.43	-	49,49,49,49	0
85	MG	1	3973	1/1	0.93	0.47	-	37,37,37,37	0
85	MG	AR	3839	1/1	0.93	0.43	-	33,33,33,33	0
84	OHX	1	3718	7/7	0.90	0.39	-	149,149,149,149	0
85	MG	AR	4168	1/1	1.00	0.19	-	65,65,65,65	0
85	MG	AR	4108	1/1	0.94	0.19	-	36,36,36,36	0
85	MG	AR	4172	1/1	0.99	0.12	-	65,65,65,65	0
85	MG	AR	4200	1/1	0.81	0.25	-	48,48,48,48	0
85	MG	l	403	1/1	0.71	0.47	-	37,37,37,37	0
85	MG	AR	4071	1/1	0.86	0.27	-	39,39,39,39	0
85	MG	1	4147	1/1	0.90	0.21	-	48,48,48,48	0
85	MG	AR	4053	1/1	0.97	0.40	-	30,30,30,30	0
85	MG	AR	3959	1/1	0.94	0.28	-	32,32,32,32	0
85	MG	A	2136	1/1	0.75	0.70	-	74,74,74,74	0
85	MG	6	2084	1/1	0.96	0.22	-	48,48,48,48	0
85	MG	AR	4085	1/1	0.77	0.46	-	35,35,35,35	0
85	MG	AR	3887	1/1	0.99	0.46	-	21,21,21,21	0
84	OHX	AR	3446	7/7	0.99	0.17	-	112,113,113,113	0
85	MG	AR	4040	1/1	0.90	0.26	-	43,43,43,43	0
84	OHX	1	3580	7/7	0.97	0.34	-	115,116,116,116	0
85	MG	6	2153	1/1	0.95	0.27	-	97,97,97,97	0
85	MG	AR	3952	1/1	0.96	0.36	-	28,28,28,28	0
85	MG	A	2069	1/1	0.84	0.49	-	58,58,58,58	0
85	MG	AR	3846	1/1	0.96	0.56	-	33,33,33,33	0
85	MG	AR	3889	1/1	0.91	0.36	-	35,35,35,35	0
85	MG	1	4131	1/1	0.74	0.32	-	48,48,48,48	0
85	MG	AR	4204	1/1	0.93	0.30	-	38,38,38,38	0
85	MG	AR	4045	1/1	0.84	0.30	-	55,55,55,55	0
85	MG	AR	4026	1/1	0.91	0.33	-	60,60,60,60	0
85	MG	1	4108	1/1	0.87	0.21	-	42,42,42,42	0
85	MG	AR	4035	1/1	0.84	0.38	-	43,43,43,43	0
84	OHX	AR	3651	7/7	0.94	0.31	-	150,151,151,151	0
85	MG	6	2112	1/1	0.93	0.53	-	46,46,46,46	0
85	MG	1	3806	1/1	0.97	0.46	-	51,51,51,51	0
85	MG	1	3794	1/1	0.94	0.53	-	34,34,34,34	0
85	MG	1	4000	1/1	0.87	0.23	-	43,43,43,43	0
84	OHX	6	2049	7/7	0.93	0.33	-	170,171,171,171	0
85	MG	AR	3954	1/1	0.86	0.30	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	3777	1/1	0.89	0.31	-	37,37,37,37	0
84	OHX	1	3561	7/7	0.97	0.26	-	124,124,125,125	0
84	OHX	6	1949	7/7	0.96	0.11	-	135,136,136,136	0
85	MG	AR	4009	1/1	0.90	0.34	-	37,37,37,37	0
84	OHX	1	3521	7/7	0.98	0.14	-	116,117,117,117	0
84	OHX	1	3619	7/7	0.94	0.22	-	127,127,127,127	0
85	MG	AR	3949	1/1	0.94	0.19	-	32,32,32,32	0
85	MG	A	2121	1/1	0.51	0.31	-	62,62,62,62	0
85	MG	AR	4096	1/1	0.85	0.32	-	54,54,54,54	0
85	MG	AR	4208	1/1	0.98	0.21	-	57,57,57,57	0
85	MG	AR	4079	1/1	0.96	0.31	-	34,34,34,34	0
85	MG	1	4109	1/1	0.91	0.14	-	66,66,66,66	0
84	OHX	AR	3666	7/7	0.94	0.27	-	130,131,131,131	0
85	MG	6	2173	1/1	0.84	0.73	-	48,48,48,48	0
85	MG	A	2148	1/1	0.95	0.37	-	64,64,64,64	0
85	MG	1	4010	1/1	0.94	0.46	-	30,30,30,30	0
85	MG	AR	3784	1/1	0.94	0.24	-	51,51,51,51	0
84	OHX	AR	3622	7/7	0.94	0.24	-	130,131,131,131	0
85	MG	1	3930	1/1	0.69	0.57	-	40,40,40,40	0
84	OHX	AR	3434	7/7	0.99	0.22	-	111,111,111,111	0
85	MG	AR	3980	1/1	0.92	0.86	-	40,40,40,40	0
85	MG	4	222	1/1	0.88	0.28	-	33,33,33,33	0
85	MG	AR	4064	1/1	0.90	0.24	-	38,38,38,38	0
85	MG	1	4037	1/1	0.91	0.30	-	30,30,30,30	0
84	OHX	AR	3708	7/7	0.93	0.26	-	138,138,139,139	0
85	MG	6	2076	1/1	0.78	0.58	-	105,105,105,105	0
85	MG	AR	3963	1/1	0.94	0.20	-	49,49,49,49	0
85	MG	1	3989	1/1	0.60	0.26	-	55,55,55,55	0
85	MG	AR	4074	1/1	0.68	0.23	-	77,77,77,77	0
85	MG	1	4013	1/1	0.82	0.33	-	52,52,52,52	0
85	MG	AR	4182	1/1	0.81	0.37	-	79,79,79,79	0
84	OHX	1	3553	7/7	0.96	0.29	-	121,122,122,122	0
84	OHX	1	3674	7/7	0.95	0.28	-	136,136,137,137	0
85	MG	AR	3972	1/1	0.95	0.53	-	39,39,39,39	0
85	MG	AR	3981	1/1	0.94	0.14	-	33,33,33,33	0
85	MG	A	2140	1/1	0.82	0.82	-	82,82,82,82	0
84	OHX	1	3586	7/7	0.96	0.23	-	121,122,122,122	0
84	OHX	AR	3604	7/7	0.90	0.19	-	158,159,159,159	0
85	MG	AT	220	1/1	0.92	0.47	-	53,53,53,53	0
87	GOL	AR	4262	6/6	0.80	0.34	-	48,48,48,48	0
85	MG	AR	4205	1/1	0.91	0.24	-	59,59,59,59	0
85	MG	6	2148	1/1	0.95	0.43	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	4024	1/1	0.95	0.21	-	61,61,61,61	0
85	MG	AR	4243	1/1	0.93	0.59	-	30,30,30,30	0
85	MG	t	203	1/1	0.92	0.42	-	29,29,29,29	0
85	MG	AR	3806	1/1	0.97	0.29	-	57,57,57,57	0
85	MG	1	4181	1/1	0.94	0.35	-	23,23,23,23	0
85	MG	AR	4067	1/1	0.89	0.34	-	34,34,34,34	0
85	MG	AR	3802	1/1	0.95	0.12	-	40,40,40,40	0
85	MG	1	3737	1/1	0.90	0.93	-	57,57,57,57	0
85	MG	AR	3758	1/1	0.93	0.30	-	37,37,37,37	0
85	MG	AR	3869	1/1	0.97	0.40	-	31,31,31,31	0
84	OHX	AR	3559	7/7	0.97	0.31	-	121,121,121,121	0
84	OHX	1	3594	7/7	0.94	0.20	-	131,131,132,132	0
85	MG	1	4209	1/1	0.90	0.66	-	48,48,48,48	0
85	MG	1	3802	1/1	0.92	0.18	-	86,86,86,86	0
85	MG	1	4038	1/1	0.86	0.72	-	41,41,41,41	0
84	OHX	1	3570	7/7	0.98	0.09	-	144,144,145,145	0
85	MG	1	4065	1/1	0.84	0.31	-	48,48,48,48	0
85	MG	1	3800	1/1	0.79	0.61	-	45,45,45,45	0
85	MG	AR	3793	1/1	0.95	0.31	-	29,29,29,29	0
85	MG	AR	3754	1/1	0.93	0.31	-	40,40,40,40	0
85	MG	1	4040	1/1	0.80	0.30	-	74,74,74,74	0
85	MG	CL	302	1/1	0.87	0.36	-	68,68,68,68	0
85	MG	1	4178	1/1	0.93	0.40	-	28,28,28,28	0
85	MG	1	4085	1/1	0.91	0.39	-	51,51,51,51	0
85	MG	AR	3776	1/1	0.76	0.33	-	76,76,76,76	0
85	MG	1	3906	1/1	0.93	0.36	-	42,42,42,42	0
85	MG	AT	223	1/1	0.93	0.79	-	45,45,45,45	0
85	MG	AR	3840	1/1	0.86	0.31	-	47,47,47,47	0
85	MG	AR	3803	1/1	0.78	0.51	-	35,35,35,35	0
85	MG	1	3782	1/1	0.91	0.45	-	58,58,58,58	0
85	MG	AR	3920	1/1	0.93	0.50	-	27,27,27,27	0
84	OHX	1	3689	7/7	0.94	0.52	-	140,140,141,141	0
85	MG	AR	4052	1/1	0.99	0.12	-	86,86,86,86	0
85	MG	AR	3898	1/1	0.97	0.62	-	28,28,28,28	0
85	MG	AR	3900	1/1	0.94	0.81	-	37,37,37,37	0
84	OHX	c8	201	7/7	0.97	0.20	-	146,147,147,148	0
85	MG	AR	3843	1/1	0.93	0.35	-	30,30,30,30	0
85	MG	1	3814	1/1	0.72	0.22	-	77,77,77,77	0
85	MG	AR	4246	1/1	0.87	0.41	-	22,22,22,22	0
84	OHX	z	201	7/7	0.87	0.39	-	155,156,157,157	0
84	OHX	6	1974	7/7	0.97	0.15	-	121,121,122,122	0
85	MG	6	2191	1/1	0.65	0.44	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	AR	4055	1/1	0.92	0.17	-	40,40,40,40	0
85	MG	A	2156	1/1	0.86	0.62	-	45,45,45,45	0
85	MG	AR	4054	1/1	0.98	0.14	-	55,55,55,55	0
85	MG	1	4151	1/1	0.74	0.28	-	41,41,41,41	0
85	MG	1	4154	1/1	0.87	0.21	-	46,46,46,46	0
84	OHX	AR	3468	7/7	0.98	0.16	-	124,124,125,125	0
85	MG	w	201	1/1	0.95	0.42	-	37,37,37,37	0
84	OHX	AR	3724	7/7	0.95	0.27	-	130,130,131,131	0
85	MG	1	4174	1/1	0.91	0.83	-	55,55,55,55	0
84	OHX	1	3474	7/7	0.98	0.16	-	122,122,123,123	0
84	OHX	AR	3739	7/7	0.93	0.51	-	148,149,149,150	0
85	MG	6	2167	1/1	0.80	0.50	-	53,53,53,53	0
85	MG	AR	3929	1/1	0.91	0.37	-	25,25,25,25	0
85	MG	AR	4062	1/1	0.95	0.17	-	42,42,42,42	0
85	MG	AR	3877	1/1	0.95	0.34	-	22,22,22,22	0
85	MG	6	2134	1/1	0.89	0.22	-	80,80,80,80	0
85	MG	4	237	1/1	0.89	0.20	-	38,38,38,38	0
84	OHX	A	1930	7/7	0.97	0.10	-	122,122,123,123	0
85	MG	AR	3925	1/1	0.93	0.41	-	34,34,34,34	0
84	OHX	AR	3727	7/7	0.91	0.23	-	187,188,188,188	0
85	MG	AR	4092	1/1	0.86	0.31	-	47,47,47,47	0
85	MG	AR	4028	1/1	0.89	0.19	-	41,41,41,41	0
85	MG	AR	4136	1/1	0.91	0.27	-	36,36,36,36	0
85	MG	AR	4255	1/1	0.66	0.64	-	57,57,57,57	0
85	MG	1	4051	1/1	0.97	0.23	-	44,44,44,44	0
85	MG	1	4093	1/1	0.76	0.37	-	57,57,57,57	0
85	MG	1	4133	1/1	0.98	0.09	-	51,51,51,51	0
85	MG	AR	4225	1/1	0.77	0.35	-	34,34,34,34	0
85	MG	AR	3983	1/1	0.99	0.12	-	33,33,33,33	0
85	MG	AR	4122	1/1	0.60	0.25	-	68,68,68,68	0
85	MG	AR	4010	1/1	0.94	0.30	-	30,30,30,30	0
85	MG	AR	4078	1/1	0.93	0.52	-	60,60,60,60	0
85	MG	1	4115	1/1	0.88	0.23	-	36,36,36,36	0
84	OHX	1	3624	7/7	0.96	0.20	-	136,136,136,137	0
85	MG	AR	4073	1/1	0.89	0.39	-	40,40,40,40	0
85	MG	1	4076	1/1	0.99	0.24	-	64,64,64,64	0
85	MG	AR	3991	1/1	0.86	0.14	-	98,98,98,98	0
85	MG	AR	4152	1/1	0.93	0.22	-	38,38,38,38	0
84	OHX	1	3434	7/7	0.98	0.25	-	126,127,127,127	0
85	MG	AR	3935	1/1	0.86	0.62	-	49,49,49,49	0
84	OHX	A	1906	7/7	0.99	0.23	-	142,143,143,143	0
85	MG	AR	4057	1/1	0.93	0.39	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3997	1/1	0.82	0.17	-	54,54,54,54	0
85	MG	1	3790	1/1	0.76	0.12	-	43,43,43,43	0
85	MG	AR	3785	1/1	0.92	0.47	-	57,57,57,57	0
85	MG	6	2102	1/1	0.94	0.46	-	45,45,45,45	0
85	MG	1	4136	1/1	0.93	0.27	-	40,40,40,40	0
85	MG	A	2150	1/1	0.57	0.16	-	86,86,86,86	0
85	MG	1	3987	1/1	0.81	0.68	-	65,65,65,65	0
85	MG	1	3913	1/1	0.91	0.59	-	28,28,28,28	0
85	MG	1	4063	1/1	0.98	0.09	-	38,38,38,38	0
85	MG	AR	4139	1/1	0.91	0.35	-	46,46,46,46	0
85	MG	AR	3878	1/1	0.99	0.36	-	31,31,31,31	0
85	MG	1	4088	1/1	0.81	0.25	-	44,44,44,44	0
85	MG	1	3975	1/1	0.93	0.33	-	42,42,42,42	0
84	OHX	1	3509	7/7	0.96	0.14	-	119,120,120,120	0
85	MG	6	2143	1/1	0.91	0.31	-	75,75,75,75	0
85	MG	AR	3783	1/1	0.75	0.32	-	44,44,44,44	0
85	MG	1	4184	1/1	0.89	0.26	-	36,36,36,36	0
85	MG	AR	4109	1/1	0.93	0.16	-	39,39,39,39	0
85	MG	AR	3884	1/1	0.98	0.45	-	22,22,22,22	0
85	MG	AR	4077	1/1	0.93	0.32	-	40,40,40,40	0
84	OHX	AR	3716	7/7	0.92	0.37	-	143,143,143,143	0
85	MG	AR	4244	1/1	0.77	0.40	-	45,45,45,45	0
85	MG	6	2190	1/1	0.89	0.48	-	66,66,66,66	0
85	MG	1	4137	1/1	0.88	0.17	-	55,55,55,55	0
85	MG	1	3927	1/1	0.88	0.24	-	42,42,42,42	0
85	MG	1	3952	1/1	0.69	0.24	-	77,77,77,77	0
85	MG	AR	4157	1/1	0.86	0.28	-	75,75,75,75	0
85	MG	1	4170	1/1	0.81	0.49	-	41,41,41,41	0
85	MG	1	4039	1/1	0.92	0.48	-	40,40,40,40	0
85	MG	1	3878	1/1	0.97	0.58	-	24,24,24,24	0
85	MG	1	4159	1/1	0.80	0.40	-	43,43,43,43	0
84	OHX	A	1951	7/7	0.97	0.24	-	145,145,146,146	0
85	MG	AR	4029	1/1	0.86	0.22	-	42,42,42,42	0
85	MG	1	4075	1/1	0.95	0.43	-	41,41,41,41	0
84	OHX	1	3598	7/7	0.97	0.27	-	127,127,127,127	0
85	MG	1	4061	1/1	0.71	0.31	-	54,54,54,54	0
85	MG	AR	4174	1/1	0.69	0.42	-	39,39,39,39	0
85	MG	1	3969	1/1	0.92	0.21	-	41,41,41,41	0
85	MG	1	3953	1/1	0.86	0.20	-	46,46,46,46	0
85	MG	1	3979	1/1	0.91	0.31	-	39,39,39,39	0
85	MG	AR	4240	1/1	0.83	0.55	-	70,70,70,70	0
85	MG	AR	4118	1/1	0.86	0.41	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	1	3508	7/7	0.98	0.10	-	113,114,114,114	0
85	MG	AR	4001	1/1	0.94	0.22	-	38,38,38,38	0
84	OHX	AR	3549	7/7	0.97	0.20	-	116,117,117,117	0
85	MG	1	3880	1/1	0.94	0.59	-	31,31,31,31	0
85	MG	1	4074	1/1	0.80	0.24	-	37,37,37,37	0
85	MG	AR	3771	1/1	0.91	0.36	-	42,42,42,42	0
84	OHX	A	1991	7/7	0.94	0.24	-	157,157,158,158	0
85	MG	AR	3847	1/1	0.93	0.16	-	38,38,38,38	0
85	MG	AR	4199	1/1	0.95	0.36	-	45,45,45,45	0
85	MG	1	4082	1/1	0.85	0.30	-	35,35,35,35	0
85	MG	AR	4149	1/1	0.88	0.38	-	66,66,66,66	0
85	MG	A	2116	1/1	0.79	0.61	-	67,67,67,67	0
85	MG	1	4213	1/1	0.91	0.64	-	50,50,50,50	0
85	MG	AR	3820	1/1	0.92	0.26	-	43,43,43,43	0
84	OHX	1	3656	7/7	0.90	0.50	-	143,143,143,144	0
85	MG	AR	4059	1/1	0.89	0.20	-	47,47,47,47	0
85	MG	AR	4214	1/1	0.73	0.24	-	55,55,55,55	0
85	MG	AR	4008	1/1	0.94	0.25	-	26,26,26,26	0
85	MG	AR	3927	1/1	0.92	0.45	-	35,35,35,35	0
85	MG	A	2111	1/1	0.94	0.26	-	90,90,90,90	0
85	MG	1	4018	1/1	0.93	0.33	-	38,38,38,38	0
85	MG	AR	4238	1/1	0.85	0.39	-	36,36,36,36	0
84	OHX	A	2041	7/7	0.88	0.46	-	139,139,140,140	0
84	OHX	1	3597	7/7	0.96	0.39	-	117,117,118,118	0
85	MG	AR	4232	1/1	0.83	0.43	-	28,28,28,28	0
85	MG	AR	4248	1/1	0.86	0.94	-	45,45,45,45	0
85	MG	1	4157	1/1	0.97	0.49	-	60,60,60,60	0
85	MG	1	3848	1/1	0.92	0.41	-	60,60,60,60	0
85	MG	AR	4013	1/1	0.60	0.29	-	65,65,65,65	0
85	MG	1	3761	1/1	0.83	0.30	-	41,41,41,41	0
85	MG	A	2081	1/1	0.84	0.31	-	66,66,66,66	0
84	OHX	AR	3456	7/7	0.97	0.19	-	117,117,117,117	0
85	MG	AR	3992	1/1	0.92	0.64	-	67,67,67,67	0
85	MG	AR	4050	1/1	0.89	0.31	-	91,91,91,91	0
85	MG	1	3944	1/1	0.87	0.48	-	32,32,32,32	0
84	OHX	AT	211	7/7	0.96	0.11	-	137,138,138,138	0
84	OHX	AR	3649	7/7	0.93	0.50	-	144,144,144,144	0
85	MG	3	220	1/1	0.88	0.17	-	68,68,68,68	0
85	MG	6	2162	1/1	0.77	0.27	-	60,60,60,60	0
85	MG	AR	3868	1/1	0.88	0.47	-	25,25,25,25	0
85	MG	1	3729	1/1	0.93	0.32	-	90,90,90,90	0
85	MG	AR	4126	1/1	0.88	0.69	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	A	2154	1/1	0.97	0.93	-	45,45,45,45	0
84	OHX	1	3443	7/7	0.98	0.19	-	119,120,120,120	0
85	MG	x	207	1/1	0.89	0.30	-	33,33,33,33	0
85	MG	n	201	1/1	0.87	0.26	-	43,43,43,43	0
85	MG	CP	504	1/1	0.95	0.23	-	46,46,46,46	0
85	MG	6	2111	1/1	0.83	0.42	-	61,61,61,61	0
84	OHX	1	3654	7/7	0.96	0.14	-	136,136,136,137	0
85	MG	1	4104	1/1	0.60	0.45	-	53,53,53,53	0
85	MG	AR	4211	1/1	0.93	0.14	-	73,73,73,73	0
85	MG	AR	3755	1/1	0.90	0.19	-	56,56,56,56	0
84	OHX	AR	3624	7/7	0.95	0.33	-	150,150,151,151	0
85	MG	AR	4239	1/1	0.82	0.42	-	39,39,39,39	0
85	MG	1	3991	1/1	0.98	0.17	-	66,66,66,66	0
84	OHX	1	3564	7/7	0.97	0.24	-	126,126,127,127	0
85	MG	1	4102	1/1	0.90	0.37	-	57,57,57,57	0
85	MG	4	236	1/1	0.79	0.19	-	50,50,50,50	0
84	OHX	6	1997	7/7	0.95	0.36	-	132,132,133,133	0
85	MG	1	3898	1/1	0.90	0.46	-	33,33,33,33	0
85	MG	1	3765	1/1	0.90	0.49	-	21,21,21,21	0
85	MG	1	3976	1/1	0.78	0.14	-	61,61,61,61	0
85	MG	A	2074	1/1	0.96	0.41	-	55,55,55,55	0
85	MG	1	3773	1/1	0.93	0.21	-	38,38,38,38	0
85	MG	A	2145	1/1	0.99	0.21	-	92,92,92,92	0
85	MG	AR	3979	1/1	0.91	0.57	-	41,41,41,41	0
85	MG	AR	3876	1/1	0.98	0.55	-	27,27,27,27	0
85	MG	1	3864	1/1	0.92	0.25	-	38,38,38,38	0
85	MG	AR	4197	1/1	0.90	0.27	-	35,35,35,35	0
84	OHX	6	2017	7/7	0.96	0.29	-	135,135,136,136	0
84	OHX	AR	3571	7/7	0.93	0.18	-	125,125,125,125	0
85	MG	6	2172	1/1	0.96	0.26	-	38,38,38,38	0
85	MG	A	2125	1/1	0.89	0.85	-	56,56,56,56	0
84	OHX	AR	3586	7/7	0.96	0.24	-	119,119,120,120	0
85	MG	1	4113	1/1	0.88	0.26	-	57,57,57,57	0
85	MG	1	4017	1/1	0.93	0.21	-	101,101,101,101	0
84	OHX	A	2036	7/7	0.88	0.15	-	252,253,253,253	0
85	MG	6	2166	1/1	0.90	0.48	-	53,53,53,53	0
85	MG	AR	4065	1/1	0.95	0.25	-	31,31,31,31	0
85	MG	AS	220	1/1	0.64	0.37	-	68,68,68,68	0
85	MG	AR	4219	1/1	0.68	0.17	-	67,67,67,67	0
85	MG	AR	4221	1/1	0.83	0.28	-	35,35,35,35	0
84	OHX	1	3722	1/7	0.92	0.12	-	136,136,136,136	0
85	MG	DQ	203	1/1	0.86	0.22	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	DQ	204	1/1	0.91	0.35	-	32,32,32,32	0
85	MG	1	4203	1/1	0.81	0.24	-	31,31,31,31	0
85	MG	1	3870	1/1	0.83	0.28	-	47,47,47,47	0
85	MG	AR	4183	1/1	0.85	0.23	-	55,55,55,55	0
85	MG	AR	4016	1/1	0.93	0.36	-	33,33,33,33	0
85	MG	1	3838	1/1	0.96	0.57	-	33,33,33,33	0
85	MG	A	2093	1/1	0.88	0.13	-	100,100,100,100	0
85	MG	1	4001	1/1	0.79	0.45	-	47,47,47,47	0
85	MG	1	4086	1/1	0.93	0.29	-	32,32,32,32	0
85	MG	1	3926	1/1	0.86	0.16	-	37,37,37,37	0
85	MG	6	2067	1/1	0.93	0.30	-	45,45,45,45	0
85	MG	AR	4195	1/1	0.99	0.18	-	63,63,63,63	0
85	MG	1	3931	1/1	0.84	0.53	-	32,32,32,32	0
84	OHX	1	3504	7/7	0.97	0.18	-	127,127,127,128	0
85	MG	AR	3924	1/1	0.92	0.49	-	27,27,27,27	0
85	MG	AR	3855	1/1	0.95	0.43	-	33,33,33,33	0
85	MG	AS	217	1/1	0.81	0.47	-	44,44,44,44	0
85	MG	AR	3998	1/1	0.80	0.45	-	40,40,40,40	0
85	MG	6	2132	1/1	0.92	0.35	-	42,42,42,42	0
85	MG	6	2178	1/1	0.83	0.36	-	57,57,57,57	0
85	MG	AR	3759	1/1	0.85	0.62	-	34,34,34,34	0
85	MG	1	3968	1/1	0.96	0.47	-	29,29,29,29	0
85	MG	1	3958	1/1	0.49	0.38	-	44,44,44,44	0
85	MG	AR	3807	1/1	0.90	0.38	-	25,25,25,25	0
85	MG	1	4199	1/1	0.96	0.59	-	24,24,24,24	0
85	MG	AR	4119	1/1	0.71	0.39	-	91,91,91,91	0
84	OHX	1	3610	7/7	0.94	0.23	-	130,130,131,131	0
84	OHX	AR	3697	7/7	0.96	0.25	-	114,115,115,115	0
85	MG	1	3762	1/1	0.90	0.56	-	30,30,30,30	0
84	OHX	AR	3725	7/7	0.93	0.20	-	165,165,165,165	0
85	MG	6	2120	1/1	0.87	0.42	-	69,69,69,69	0
85	MG	AR	4250	1/1	0.87	0.80	-	59,59,59,59	0
85	MG	AR	3997	1/1	0.94	0.12	-	44,44,44,44	0
85	MG	6	2130	1/1	0.80	0.31	-	66,66,66,66	0
85	MG	6	2094	1/1	0.93	0.22	-	37,37,37,37	0
85	MG	1	4212	1/1	0.94	0.42	-	39,39,39,39	0
84	OHX	AR	3516	7/7	0.97	0.15	-	112,112,112,112	0
85	MG	AT	229	1/1	0.89	0.42	-	55,55,55,55	0
85	MG	AR	4131	1/1	0.98	0.09	-	39,39,39,39	0
84	OHX	AR	3572	7/7	0.98	0.28	-	118,119,119,119	0
84	OHX	AR	3534	7/7	0.96	0.16	-	109,109,109,109	0
84	OHX	AR	3506	7/7	0.92	0.21	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	OHX	1	3698	7/7	0.92	0.30	-	162,163,163,163	0
85	MG	AR	4220	1/1	0.78	0.39	-	44,44,44,44	0
84	OHX	A	2027	7/7	0.95	0.33	-	159,160,161,161	0
85	MG	1	4003	1/1	0.84	0.35	-	79,79,79,79	0
84	OHX	6	2024	7/7	0.93	0.35	-	151,152,152,153	0
84	OHX	O	201	7/7	0.96	0.28	-	158,159,159,160	0
85	MG	AF	201	1/1	0.93	0.30	-	41,41,41,41	0
84	OHX	6	1984	7/7	0.95	0.26	-	150,150,151,151	0
85	MG	6	2066	1/1	0.86	0.35	-	74,74,74,74	0
85	MG	1	4219	1/1	0.89	0.26	-	98,98,98,98	0
85	MG	AS	230	1/1	0.94	0.42	-	36,36,36,36	0
84	OHX	1	3496	7/7	0.98	0.16	-	115,115,115,115	0
85	MG	AR	3854	1/1	0.94	0.40	-	48,48,48,48	0
85	MG	CQ	204	1/1	0.85	0.41	-	30,30,30,30	0
85	MG	DO	202	1/1	0.93	0.26	-	42,42,42,42	0
85	MG	4	219	1/1	0.95	0.68	-	42,42,42,42	0
84	OHX	1	3550	7/7	0.95	0.18	-	115,115,115,116	0
85	MG	6	2097	1/1	0.94	0.42	-	46,46,46,46	0
85	MG	4	233	1/1	0.71	0.20	-	48,48,48,48	0
85	MG	1	3847	1/1	0.91	0.54	-	28,28,28,28	0
85	MG	A	2158	1/1	0.93	0.34	-	67,67,67,67	0
85	MG	1	4200	1/1	0.97	0.49	-	22,22,22,22	0
85	MG	1	4210	1/1	0.87	0.30	-	24,24,24,24	0
85	MG	1	3941	1/1	0.78	0.41	-	78,78,78,78	0
85	MG	1	3982	1/1	0.89	0.37	-	32,32,32,32	0
85	MG	D	301	1/1	0.89	0.58	-	58,58,58,58	0
85	MG	AR	3837	1/1	0.97	0.59	-	19,19,19,19	0
85	MG	AR	4117	1/1	0.74	0.31	-	64,64,64,64	0
85	MG	1	4106	1/1	0.95	0.34	-	67,67,67,67	0
85	MG	4	228	1/1	0.89	0.26	-	54,54,54,54	0
85	MG	AR	3917	1/1	0.94	0.50	-	42,42,42,42	0
85	MG	AR	3821	1/1	0.90	0.21	-	42,42,42,42	0
85	MG	AR	4015	1/1	0.93	0.16	-	45,45,45,45	0
85	MG	AR	3815	1/1	0.91	0.24	-	32,32,32,32	0
85	MG	AR	4143	1/1	0.93	0.26	-	34,34,34,34	0
85	MG	A	2058	1/1	0.97	0.67	-	46,46,46,46	0
85	MG	AS	223	1/1	0.88	0.28	-	41,41,41,41	0
84	OHX	1	3520	7/7	0.96	0.18	-	123,123,124,124	0
85	MG	1	4007	1/1	0.86	0.42	-	29,29,29,29	0
85	MG	AR	4144	1/1	0.93	0.33	-	41,41,41,41	0
85	MG	AS	214	1/1	0.92	0.30	-	52,52,52,52	0
85	MG	AR	3818	1/1	0.98	0.79	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	4198	1/1	0.90	0.60	-	43,43,43,43	0
85	MG	1	4158	1/1	0.75	0.45	-	47,47,47,47	0
85	MG	AR	3885	1/1	0.97	0.37	-	33,33,33,33	0
85	MG	1	3943	1/1	0.92	0.54	-	37,37,37,37	0
85	MG	1	3874	1/1	0.85	0.55	-	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.