



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 02:43 AM EDT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

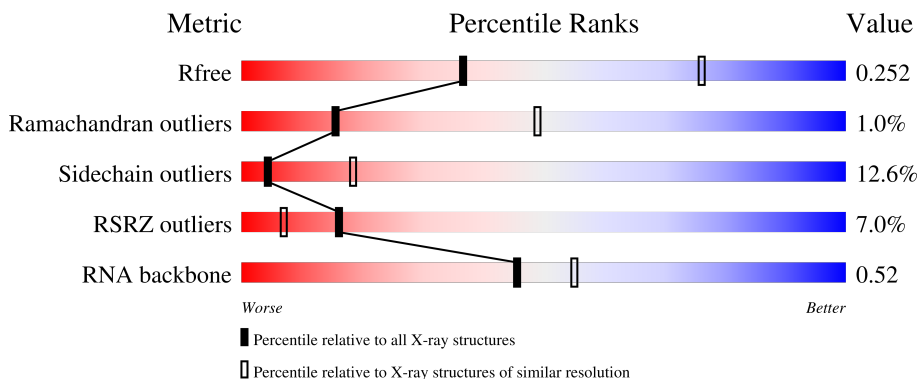
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1094 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	AR	3396	
2	3	121	
2	AS	121	
3	4	158	

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Mol	Chain	Length	Quality of chain
3	AT	158	4% 82% 18%
4	CD	252	% 90% 10%
4	j	252	89% 11%
5	CE	386	87% 13%
5	k	386	% 87% 13%
6	CF	361	90% 10%
6	l	361	89% 10%
7	CG	296	4% 86% 14%
7	m	296	6% 90% 10%
8	CH	175	2% 78% 11% 11%
8	n	175	% 81% 7% 11%
9	CI	222	% 89% 10%
9	o	222	2% 90% 9%
10	CJ	233	14% 92% 8%
10	p	233	6% 91% 9%
11	CK	191	2% 85% 15%
11	q	191	87% 13%
12	CL	220	6% 84% 12%
12	r	220	% 82% 14%
13	CM	169	% 85% 15%
13	s	169	2% 85% 14%
14	CN	193	8% 83% 15%
14	t	193	86% 13%
15	CO	136	% 88% 11%
15	u	136	2% 85% 15%

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Mol	Chain	Length	Quality of chain
16	CP	203	92% 8%
16	v	203	90% 10%
17	CQ	197	2% 90% 9%
17	w	197	88% 11%
18	CR	183	16% 87% 13%
18	x	183	11% 87% 12%
19	CS	185	87% 13%
19	y	185	89% 10%
20	CT	188	5% 89% 11%
20	z	188	4% 93% 7%
21	0	172	85% 14%
21	CU	172	85% 15%
22	2	159	86% 14%
22	CV	159	84% 16%
23	5	100	12% 93% 7%
23	CW	100	21% 89% 11%
24	CX	136	92% 8%
24	IR	136	3% 89% 11%
25	6	1800	6% 77% 22%
25	A	1800	7% 74% 24%
26	7	98	30% 95% 5%
26	CY	98	11% 88% 11%
27	8	121	89% 11%
27	CZ	121	3% 88% 12%
28	9	126	5% 89% 11%

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Mol	Chain	Length	Quality of chain
28	DA	126	6% 89% 11%
29	AA	135	35% 90% 8% ..
29	DB	135	12% 89% 10% .
30	AB	148	91% 8%
30	DC	148	% 88% 11% .
31	AC	58	88% 12%
31	DD	58	86% 12% .
32	AD	97	6% 89% 11%
32	DE	97	95% 5%
33	AE	109	2% 88% 12%
33	DF	109	3% 83% 17%
34	AF	127	2% 88% 12%
34	DG	127	2% 90% 10%
35	AG	106	% 92% 8%
35	DH	106	% 93% 6% .
36	AH	112	5% 90% 9% .
36	DI	112	% 91% 9%
37	AI	119	5% 89% 10% .
37	DJ	119	5% 83% 16% .
38	AJ	99	3% 85% 15%
38	DK	99	4% 90% 10%
39	AK	87	3% 92% 8%
39	DL	87	3% 87% 13%
40	AL	77	3% 87% 13%
40	DM	77	39% 91% 9%

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Mol	Chain	Length	Quality of chain
41	AM	50	86% 14%
41	DN	50	92% 8%
42	AN	52	10% 85% 15%
42	DO	52	2% 90% 10%
43	AO	25	88% 12%
43	DP	25	84% 16%
44	AP	105	9% 92% 8%
44	DQ	105	91% 9%
45	AQ	91	87% 13%
45	DR	91	91% 9%
46	i	272	7% 51% 7% 42%
47	m2	150	100%
48	sM	104	6% 92% 7%
49	p0	311	17% 41% 5% 54%
50	B	206	13% 88% 12%
50	s0	206	4% 86% 14%
51	C	216	36% 88% 11%
51	s1	216	6% 86% 13%
52	D	217	% 88% 12%
52	s2	217	% 84% 16%
53	E	223	9% 89% 10%
53	s3	223	12% 90% 9%
54	F	260	8% 90% 10%
54	s4	260	3% 91% 9%
55	G	206	11% 89% 10%

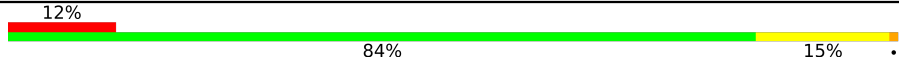

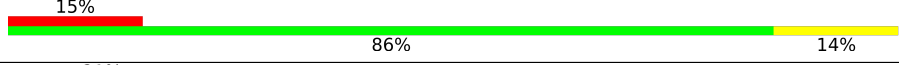
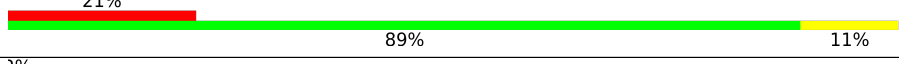
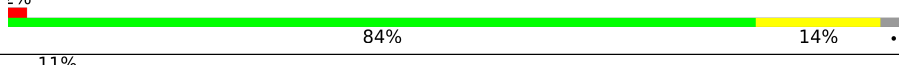
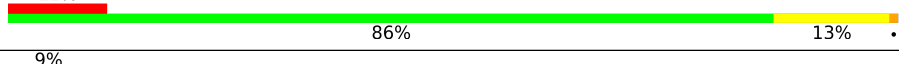
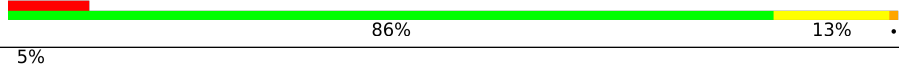

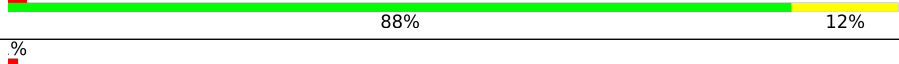
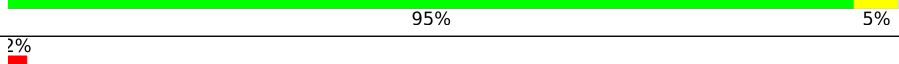


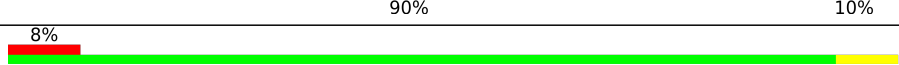
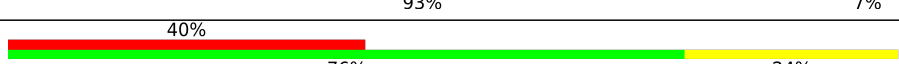
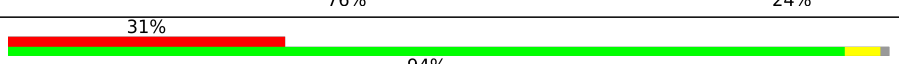
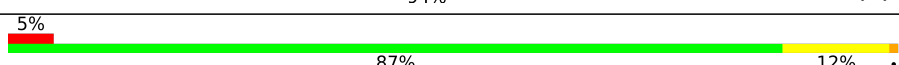
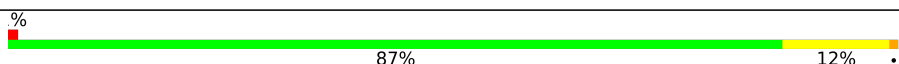
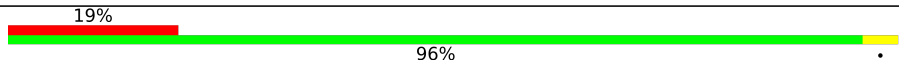
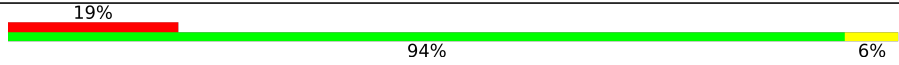


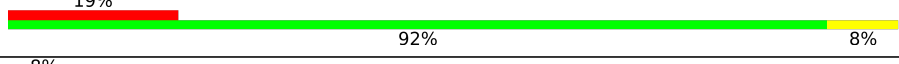
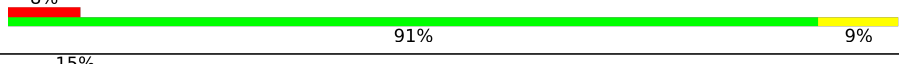


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Mol	Chain	Length	Quality of chain
55	s5	206	17% 91% 9%
56	H	226	17% 87% 13%
56	s6	226	12% 85% 11% .
57	I	186	16% 87% 12% ..
57	s7	186	17% 87% 12% .
58	J	199	5% 87% 6% . 6%
58	s8	199	7% 88% 6% . 6%
59	K	185	18% 86% 12% .
59	s9	185	8% 84% 16%
60	L	105	15% 82% 9% . 9%
60	c0	105	52% 78% 10% . 9%
61	M	155	10% 92% 8%
61	c1	155	5% 84% 10% . 6%
62	N	124	52% 81% 18% .
62	c2	124	70% 83% 15% .
63	O	150	6% 89% 10% .
63	c3	150	3% 86% 12% .
64	P	128	28% 90% 9% ..
64	c4	128	9% 89% 11%
65	Q	141	5% 79% 8% . 12%
65	c5	141	11% 82% 12% . .
66	R	142	18% 87% 12% ..
66	c6	142	11% 82% 18%
67	S	125	11% 84% 11% . .
67	c7	125	5% 82% 11% 6%

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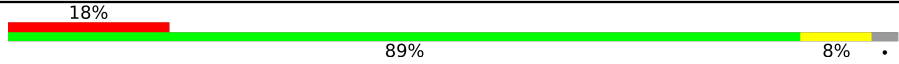
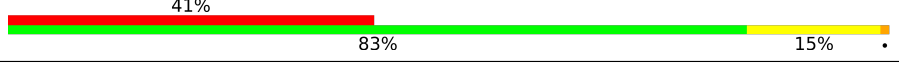
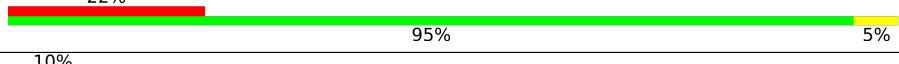
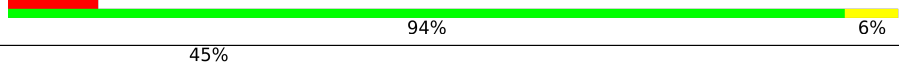

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Mol	Chain	Length	Quality of chain
68	T	145	
68	c8	145	
69	U	143	
69	c9	143	
70	V	110	
70	d0	110	
71	W	87	
71	d1	87	
72	X	129	
72	d2	129	
73	Y	144	
73	d3	144	
74	Z	134	
74	d4	134	
75	a	70	
75	d5	70	
76	b	97	
76	d6	97	
77	c	81	
77	d7	81	
78	d	63	
78	d8	63	
79	d9	53	
79	e	53	
80	e0	62	

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Mol	Chain	Length	Quality of chain
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	AR	3737	-	-	-	X
85	MG	1	3744	-	-	-	X
85	MG	1	3800	-	-	-	X
85	MG	1	3801	-	-	-	X
85	MG	1	3820	-	-	-	X
85	MG	1	3930	-	-	-	X
85	MG	1	3941	-	-	-	X
85	MG	1	3965	-	-	-	X
85	MG	1	3983	-	-	-	X
85	MG	1	4001	-	-	-	X
85	MG	1	4012	-	-	-	X
85	MG	1	4023	-	-	-	X
85	MG	1	4053	-	-	-	X
85	MG	1	4092	-	-	-	X
85	MG	1	4101	-	-	-	X
85	MG	1	4104	-	-	-	X
85	MG	1	4129	-	-	-	X
85	MG	1	4152	-	-	-	X
85	MG	1	4158	-	-	-	X
85	MG	1	4190	-	-	-	X
85	MG	4	221	-	-	-	X
85	MG	4	229	-	-	-	X
85	MG	4	235	-	-	-	X
85	MG	6	2076	-	-	-	X
85	MG	6	2083	-	-	-	X
85	MG	6	2092	-	-	-	X
85	MG	6	2133	-	-	-	X
85	MG	6	2154	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	6	2158	-	-	-	X
85	MG	6	2163	-	-	-	X
85	MG	6	2167	-	-	-	X
85	MG	6	2174	-	-	-	X
85	MG	6	2176	-	-	-	X
85	MG	6	2180	-	-	-	X
85	MG	6	2183	-	-	-	X
85	MG	6	2185	-	-	-	X
85	MG	6	2188	-	-	-	X
85	MG	6	2191	-	-	-	X
85	MG	6	2192	-	-	-	X
85	MG	6	2193	-	-	-	X
85	MG	6	2197	-	-	-	X
85	MG	A	2045	-	-	-	X
85	MG	A	2062	-	-	-	X
85	MG	A	2099	-	-	-	X
85	MG	A	2103	-	-	-	X
85	MG	A	2116	-	-	-	X
85	MG	A	2118	-	-	-	X
85	MG	A	2128	-	-	-	X
85	MG	A	2130	-	-	-	X
85	MG	A	2131	-	-	-	X
85	MG	A	2135	-	-	-	X
85	MG	A	2136	-	-	-	X
85	MG	A	2151	-	-	-	X
85	MG	A	2155	-	-	-	X
85	MG	AR	3803	-	-	-	X
85	MG	AR	3890	-	-	-	X
85	MG	AR	3971	-	-	-	X
85	MG	AR	3976	-	-	-	X
85	MG	AR	3998	-	-	-	X
85	MG	AR	4003	-	-	-	X
85	MG	AR	4005	-	-	-	X
85	MG	AR	4022	-	-	-	X
85	MG	AR	4024	-	-	-	X
85	MG	AR	4030	-	-	-	X
85	MG	AR	4034	-	-	-	X
85	MG	AR	4085	-	-	-	X
85	MG	AR	4097	-	-	-	X
85	MG	AR	4102	-	-	-	X
85	MG	AR	4110	-	-	-	X
85	MG	AR	4156	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
85	MG	AR	4174	-	-	-	X
85	MG	AR	4196	-	-	-	X
85	MG	AR	4255	-	-	-	X
85	MG	AS	228	-	-	-	X
85	MG	CD	302	-	-	-	X
85	MG	V	201	-	-	-	X
85	MG	b	101	-	-	-	X
85	MG	l	403	-	-	-	X
85	MG	x	206	-	-	-	X
87	GOL	6	2199	-	-	-	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
			Total	C	N	O	P			
1	1	3149	67355	30086	12142	21978	3149	0	0	0
1	AR	3149	67355	30086	12142	21978	3149	0	0	0

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O			
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
			Total	C	N	O	S			
15	u	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
15	CO	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O			
18	x	183	Total	C	N	O	0	0	0
			1420	882	281	257			
18	CR	183	Total	C	N	O	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
			Total	C	N	O	S			
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
			Total	C	N	O			
20	z	188	Total	C	N	O	0	0	0
			1521	935	326	260			
20	CT	188	Total	C	N	O	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	
			Total	C	N				O
48	sM	104	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
			Total	C	N	O	S			
49	p0	143	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
			Total	C	N	O	S			
50	B	206	1577	1014	278	283	2	0	0	0
50	s0	206	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
			Total	C	N	O	S			
51	C	214	1709	1084	310	311	4	0	0	0
51	s1	216	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
			Total	C	N	O	S			
52	D	217	1635	1047	289	297	2	0	0	0
52	s2	217	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
			Total	C	N	O	S			
53	E	223	1734	1101	313	314	6	0	0	0
53	s3	223	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
			Total	C	N	O	S			
59	s9	185	1494	943	289	261	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O			
66	R	141	Total	C	N	O	0	0	0
			1105	708	203	194			
66	c6	142	Total	C	N	O	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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
81	g	71	Total 566	C 362	N 106	O 94	S 4	0	0	0

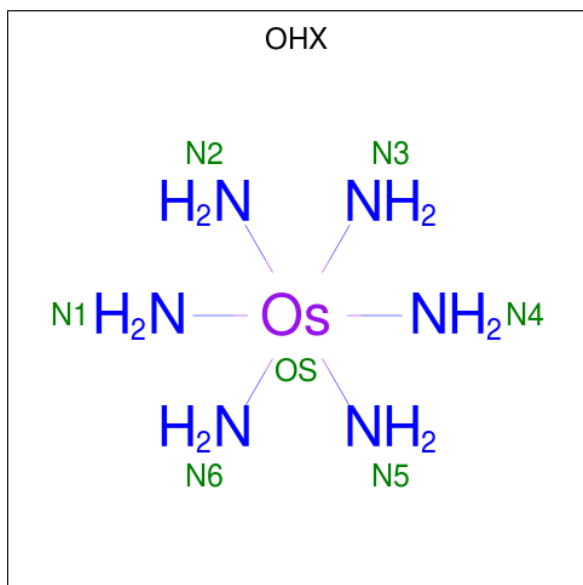
- Molecule 82 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

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

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

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

- Molecule 84 is osmium (III) hexammine (three-letter code: OHX) (formula: H<sub>12</sub>N<sub>6</sub>Os).



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	1	1		0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	k	1	7	6	1	0	0
84	l	1	7	6	1	0	0
84	r	1	7	6	1	0	0
84	v	1	7	6	1	0	0
84	x	1	7	6	1	0	0
84	x	1	7	6	1	0	0
84	y	1	7	6	1	0	0
84	z	1	7	6	1	0	0
84	2	1	7	6	1	0	0
84	6	1	7	6	1	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
			<b>Total</b>	<b>N</b>	<b>Os</b>		
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	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	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	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	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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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	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	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	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	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	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

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

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

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

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

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

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
			Total	N	Os		
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	1	498	Total 498	Mg 498	0	0
85	3	13	Total 13	Mg 13	0	0
85	4	25	Total 25	Mg 25	0	0
85	j	2	Total 2	Mg 2	0	0
85	k	3	Total 3	Mg 3	0	0
85	l	3	Total 3	Mg 3	0	0
85	n	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	o	2	Total Mg 2 2	0	0
85	r	1	Total Mg 1 1	0	0
85	s	1	Total Mg 1 1	0	0
85	t	3	Total Mg 3 3	0	0
85	v	3	Total Mg 3 3	0	0
85	w	2	Total Mg 2 2	0	0
85	x	7	Total Mg 7 7	0	0
85	z	1	Total Mg 1 1	0	0
85	lR	1	Total Mg 1 1	0	0
85	6	146	Total Mg 146 146	0	0
85	AB	7	Total Mg 7 7	0	0
85	AF	2	Total Mg 2 2	0	0
85	AG	1	Total Mg 1 1	0	0
85	AH	1	Total Mg 1 1	0	0
85	AK	1	Total Mg 1 1	0	0
85	AP	1	Total Mg 1 1	0	0
85	AR	515	Total Mg 515 515	0	0
85	AS	20	Total Mg 20 20	0	0
85	AT	14	Total Mg 14 14	0	0
85	CD	2	Total Mg 2 2	0	0
85	CE	5	Total Mg 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	CF	1	Total 1	Mg 1	0	0
85	CG	2	Total 2	Mg 2	0	0
85	CI	1	Total 1	Mg 1	0	0
85	CJ	1	Total 1	Mg 1	0	0
85	CK	1	Total 1	Mg 1	0	0
85	CL	1	Total 1	Mg 1	0	0
85	CM	2	Total 2	Mg 2	0	0
85	CO	1	Total 1	Mg 1	0	0
85	CP	4	Total 4	Mg 4	0	0
85	CQ	4	Total 4	Mg 4	0	0
85	CR	5	Total 5	Mg 5	0	0
85	CU	1	Total 1	Mg 1	0	0
85	CX	2	Total 2	Mg 2	0	0
85	DA	2	Total 2	Mg 2	0	0
85	DC	4	Total 4	Mg 4	0	0
85	DE	1	Total 1	Mg 1	0	0
85	DH	2	Total 2	Mg 2	0	0
85	DI	2	Total 2	Mg 2	0	0
85	DL	1	Total 1	Mg 1	0	0
85	DO	1	Total 1	Mg 1	0	0
85	DQ	2	Total 2	Mg 2	0	0

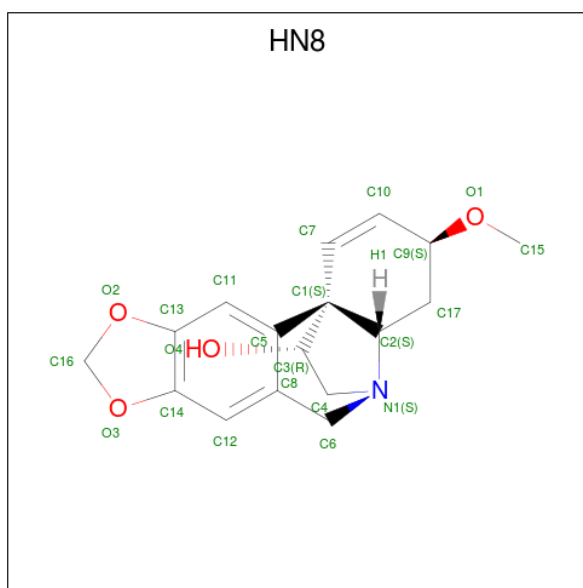
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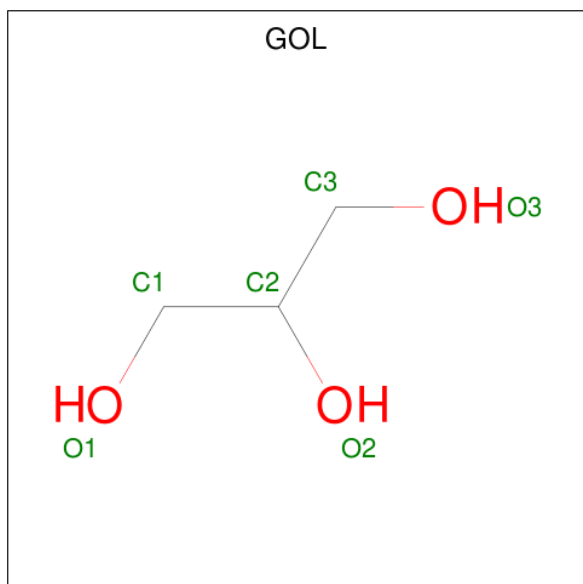
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	sM	2	Total 2	Mg 2	0	0
85	A	116	Total 116	Mg 116	0	0
85	D	1	Total 1	Mg 1	0	0
85	F	1	Total 1	Mg 1	0	0
85	H	1	Total 1	Mg 1	0	0
85	T	1	Total 1	Mg 1	0	0
85	U	1	Total 1	Mg 1	0	0
85	V	1	Total 1	Mg 1	0	0
85	Y	1	Total 1	Mg 1	0	0
85	b	1	Total 1	Mg 1	0	0
85	s4	1	Total 1	Mg 1	0	0
85	s6	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	c1	1	Total 1	Mg 1	0	0
85	c6	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	d4	1	Total 1	Mg 1	0	0
85	d5	1	Total 1	Mg 1	0	0
85	d6	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	AK	1	Total	Zn	0	0
			1	1		
88	AN	1	Total	Zn	0	0
			1	1		
88	AP	1	Total	Zn	0	0
			1	1		
88	AQ	1	Total	Zn	0	0
			1	1		
88	DL	1	Total	Zn	0	0
			1	1		
88	DO	1	Total	Zn	0	0
			1	1		
88	DQ	1	Total	Zn	0	0
			1	1		
88	DR	1	Total	Zn	0	0
			1	1		
88	b	1	Total	Zn	0	0
			1	1		
88	c	1	Total	Zn	0	0
			1	1		
88	e	1	Total	Zn	0	0
			1	1		
88	g	1	Total	Zn	0	0
			1	1		
88	d6	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0	0
			1	1		
88	d9	1	Total	Zn	0	0
			1	1		

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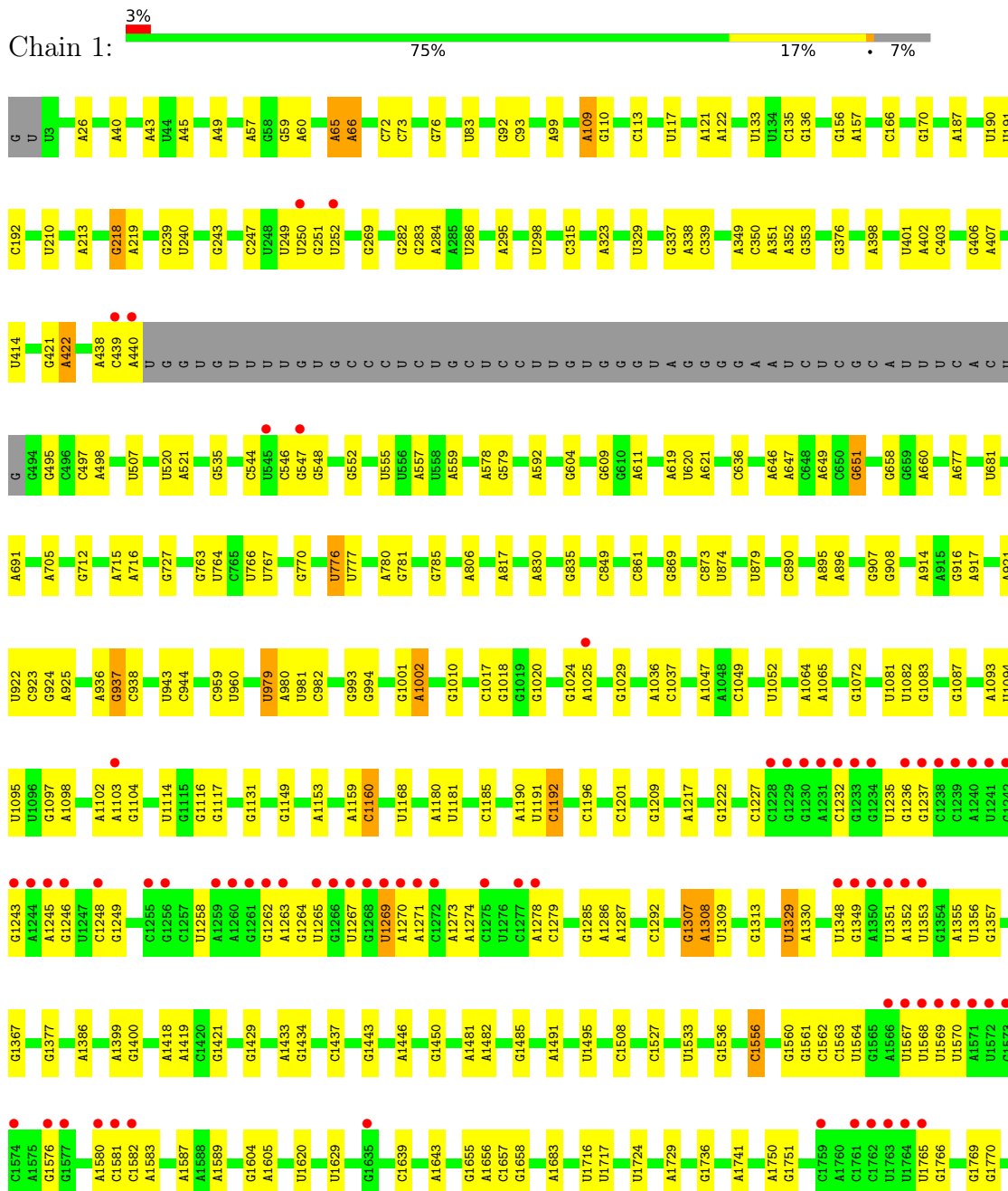
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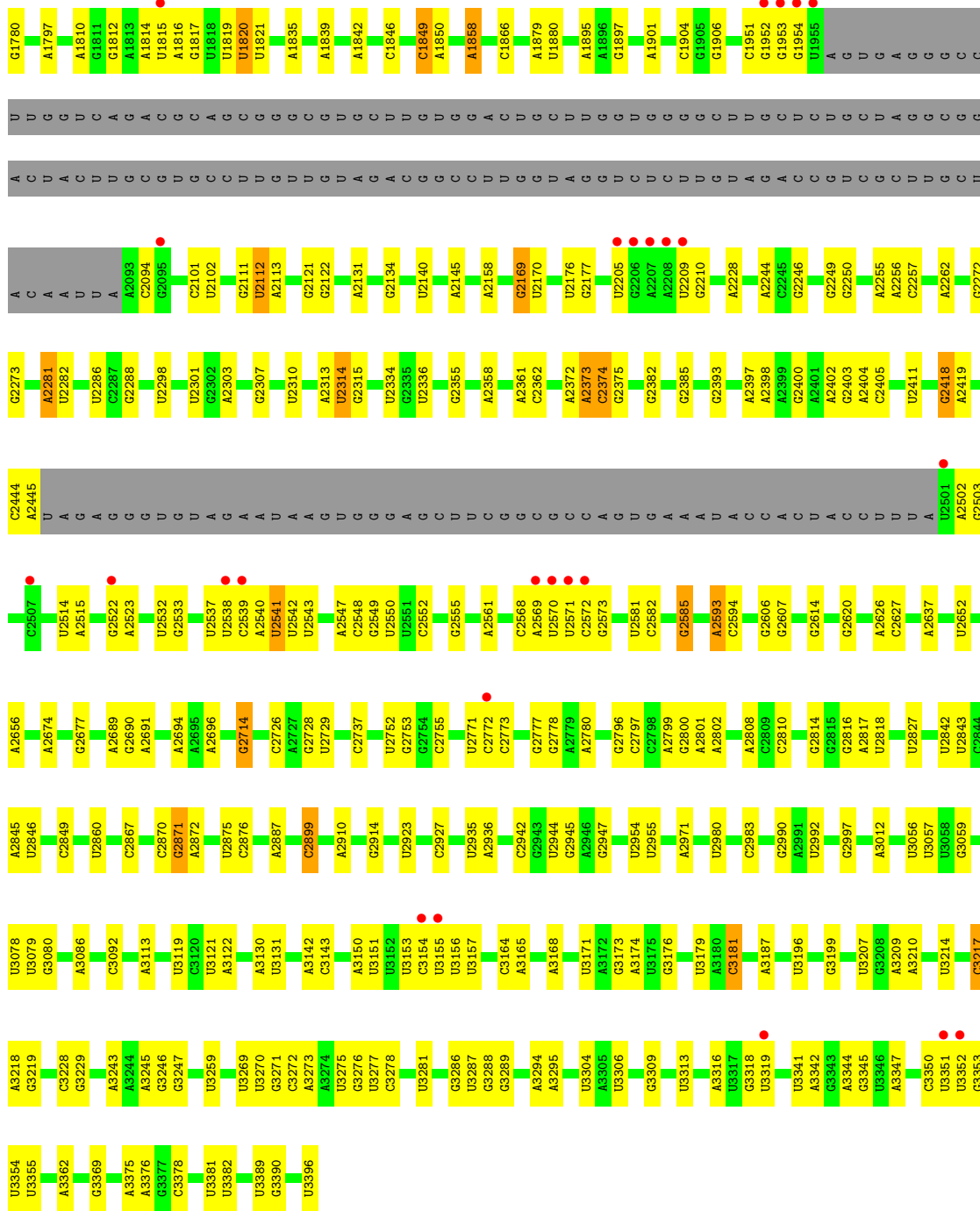
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
88	e1	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots [i](#)

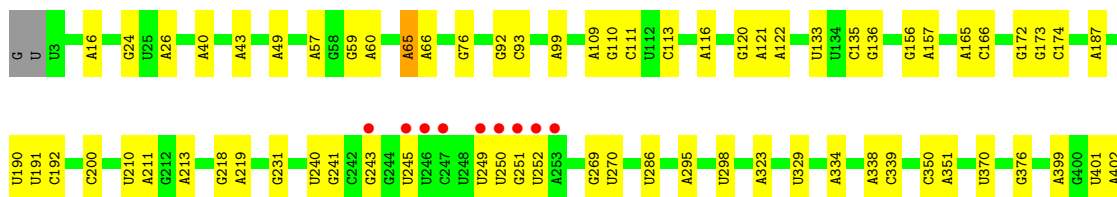
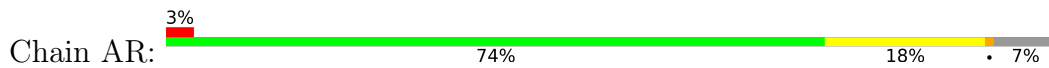
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

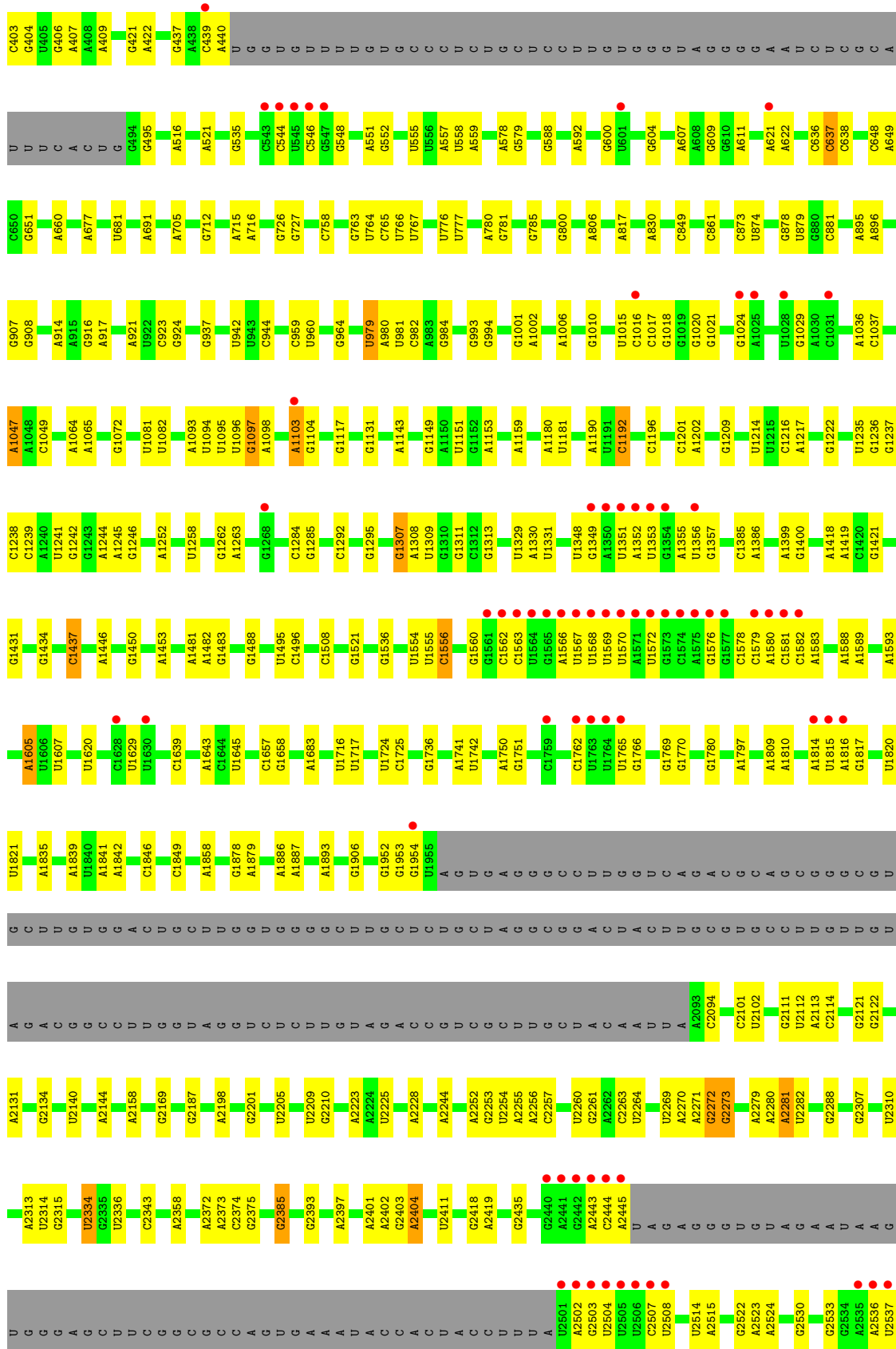
- Molecule 1: 25S ribosomal RNA

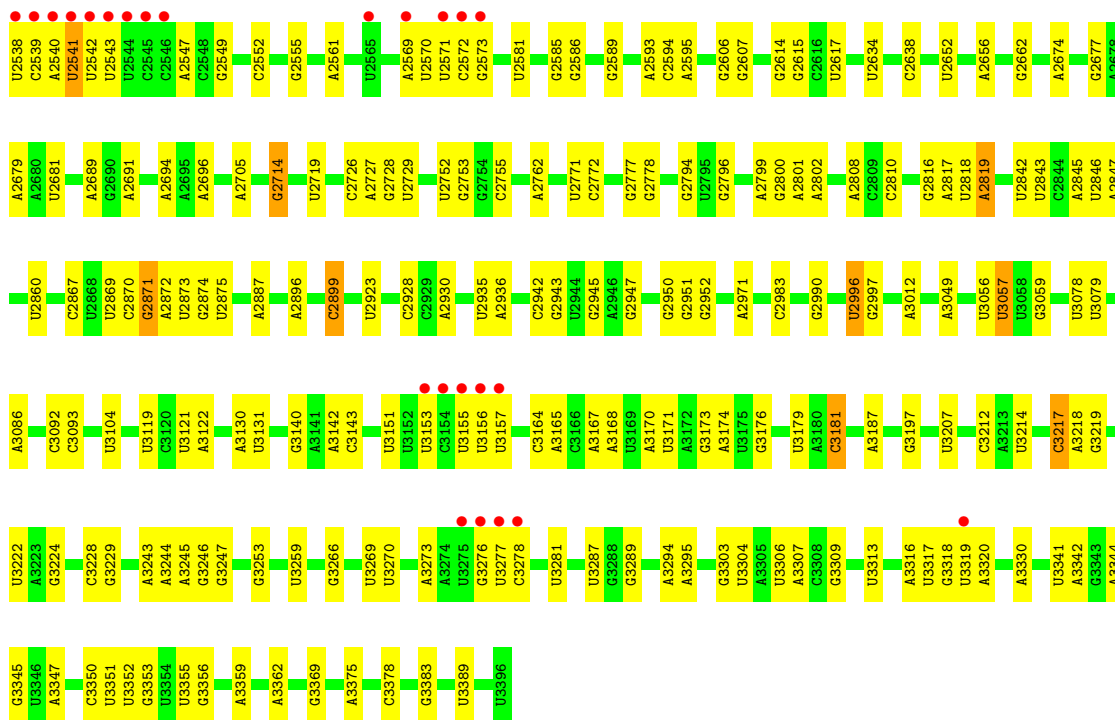




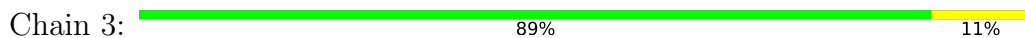
● Molecule 1: 25S ribosomal RNA



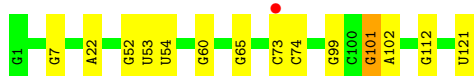
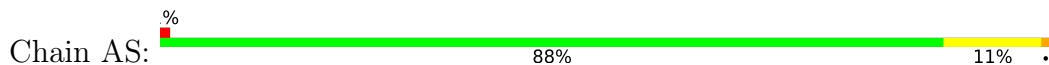




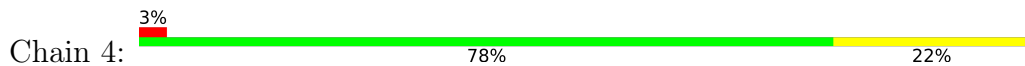
● Molecule 2: 5S ribosomal RNA



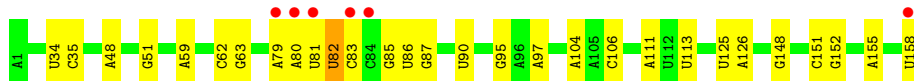
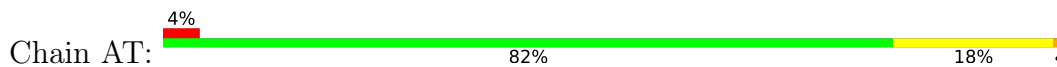
● Molecule 2: 5S ribosomal RNA



● Molecule 3: 5.8S ribosomal RNA




● Molecule 3: 5.8S ribosomal RNA





- Molecule 4: 60S ribosomal protein L2-A

Chain j:  89% 11%

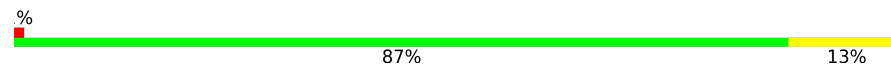


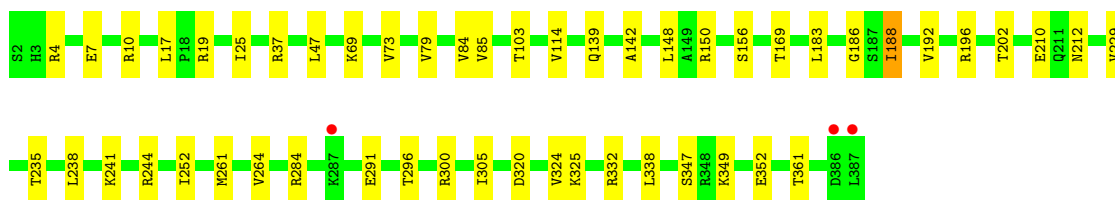
- Molecule 4: 60S ribosomal protein L2-A

Chain CD:  90% 10%




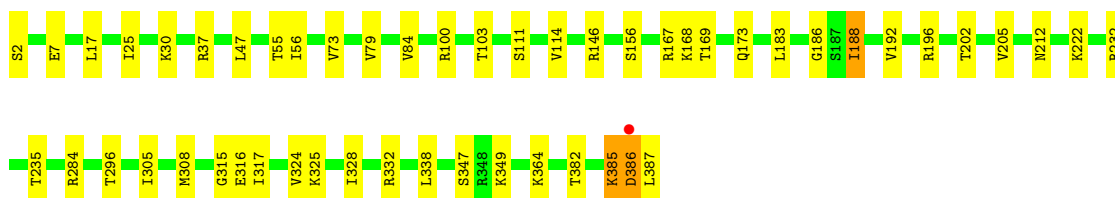
- Molecule 5: 60S ribosomal protein L3

Chain k:  87% 13%




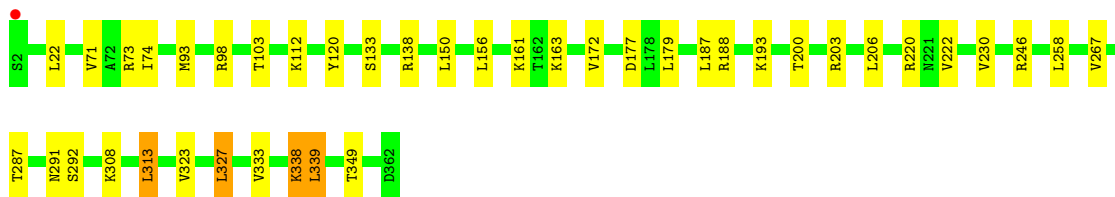
- Molecule 5: 60S ribosomal protein L3

Chain CE:  87% 13%



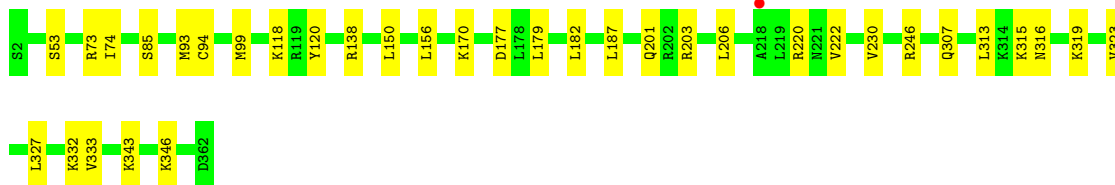
- Molecule 6: 60S ribosomal protein L4-A

Chain l:  89% 10%

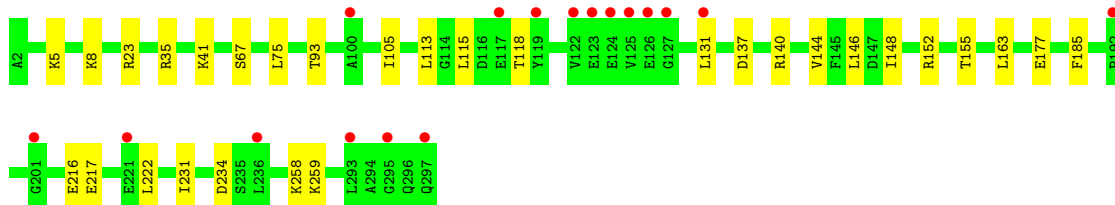
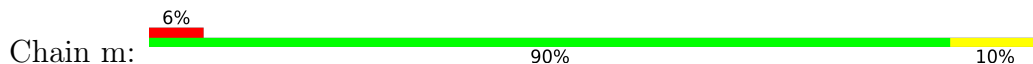


- Molecule 6: 60S ribosomal protein L4-A

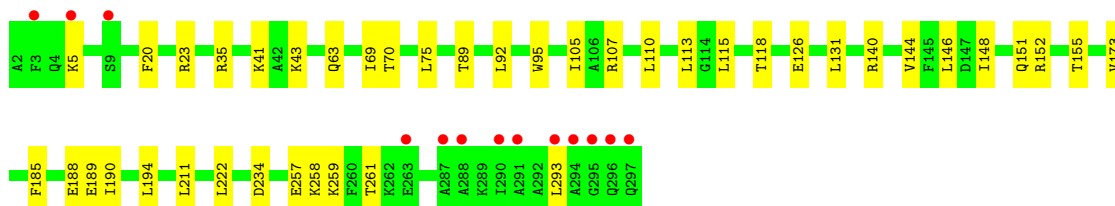
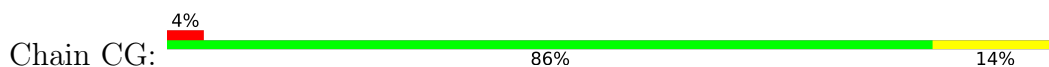
Chain CF:  90% 10%



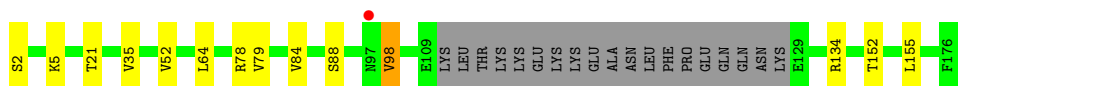
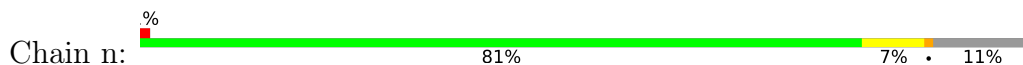
• Molecule 7: 60S ribosomal protein L5



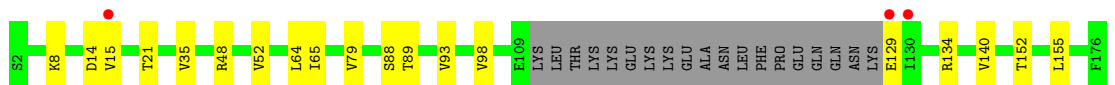
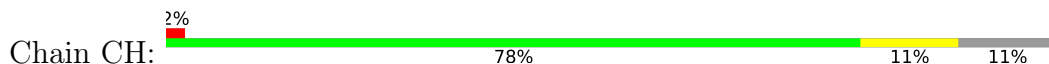
• Molecule 7: 60S ribosomal protein L5



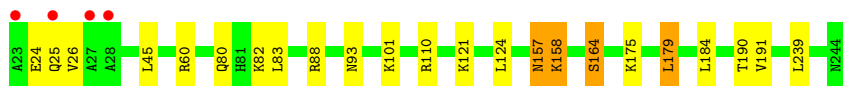
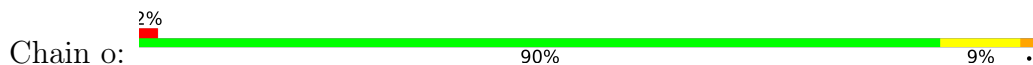
• Molecule 8: 60S ribosomal protein L6-A



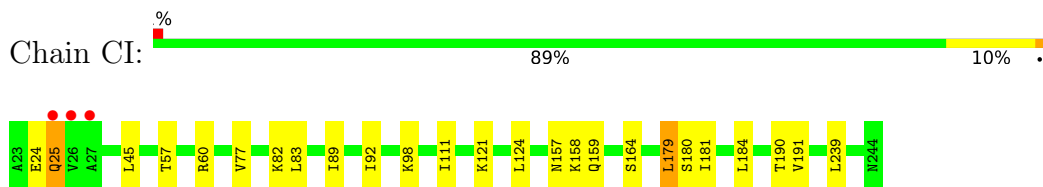
• Molecule 8: 60S ribosomal protein L6-A



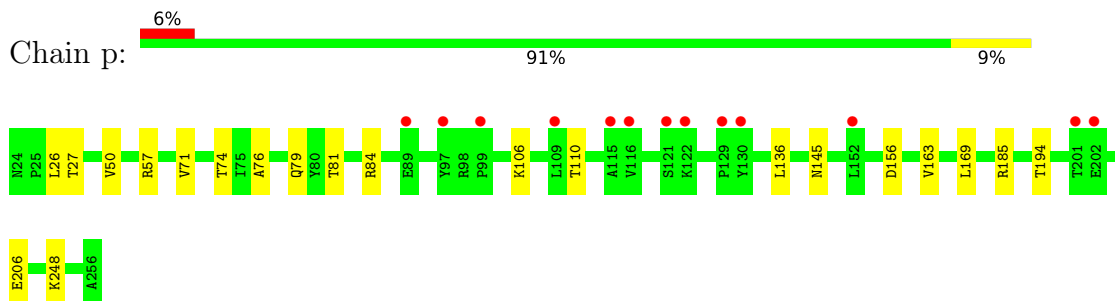
• Molecule 9: 60S ribosomal protein L7-A



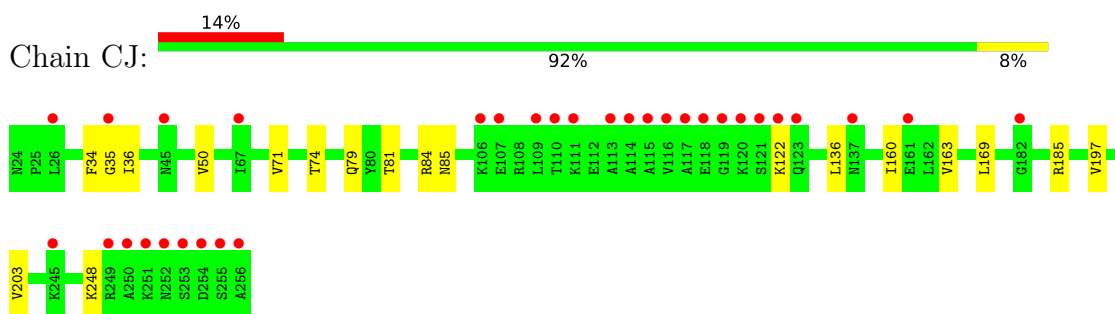
- Molecule 9: 60S ribosomal protein L7-A



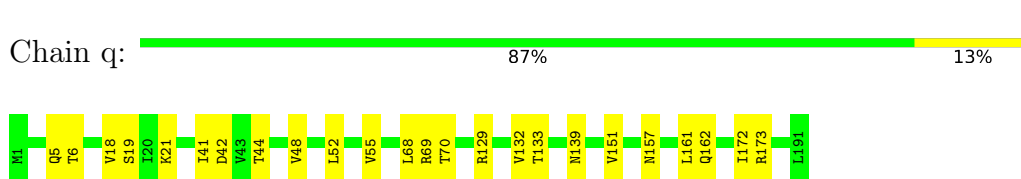
- Molecule 10: 60S ribosomal protein L8-A



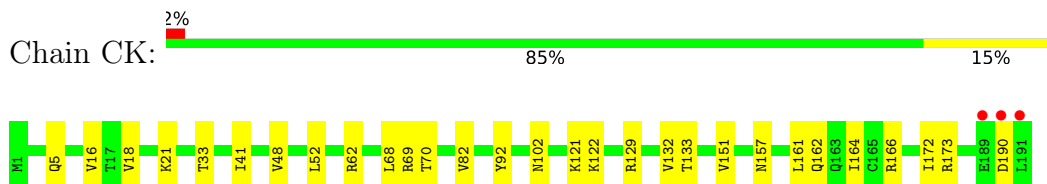
- Molecule 10: 60S ribosomal protein L8-A



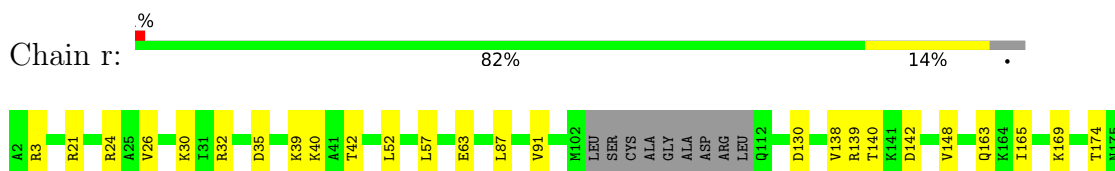
- Molecule 11: 60S ribosomal protein L9-A

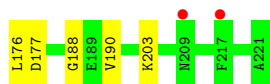


- Molecule 11: 60S ribosomal protein L9-A

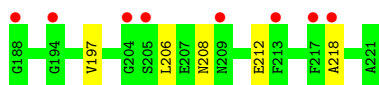
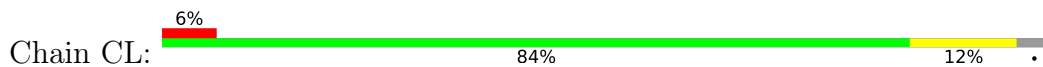


- Molecule 12: 60S ribosomal protein L10

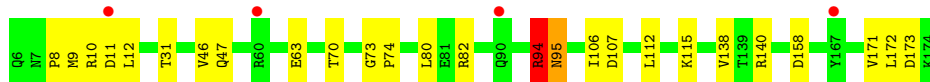
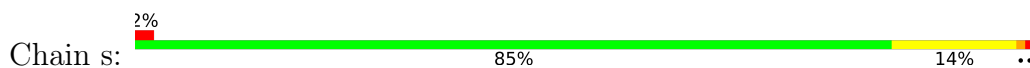




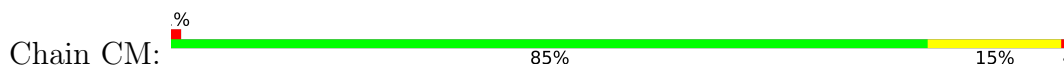
- Molecule 12: 60S ribosomal protein L10



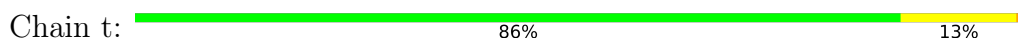
- Molecule 13: 60S ribosomal protein L11-B



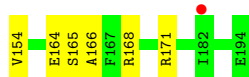
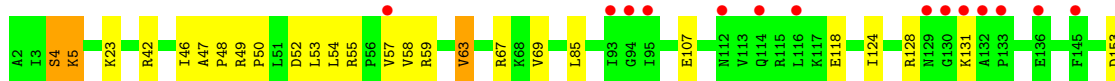
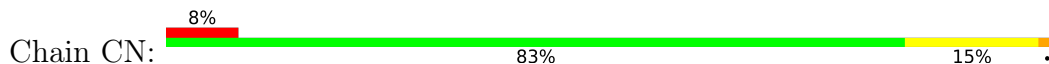
- Molecule 13: 60S ribosomal protein L11-B



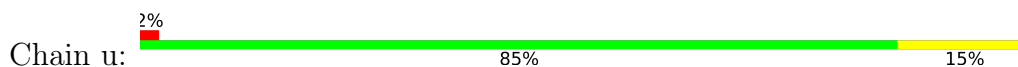
- Molecule 14: 60S ribosomal protein L13-A



- Molecule 14: 60S ribosomal protein L13-A

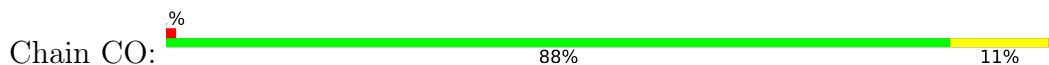


- Molecule 15: 60S ribosomal protein L14-A

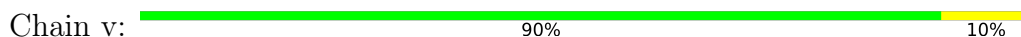




- Molecule 15: 60S ribosomal protein L14-A



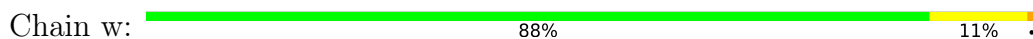
- Molecule 16: 60S ribosomal protein L15-A



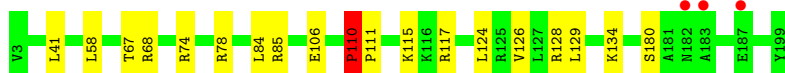
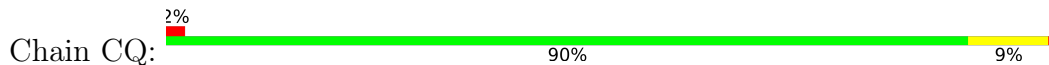
- Molecule 16: 60S ribosomal protein L15-A



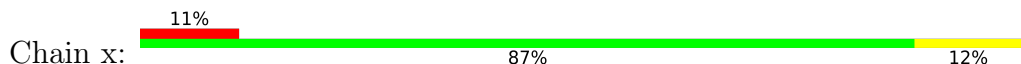
- Molecule 17: 60S ribosomal protein L16-A



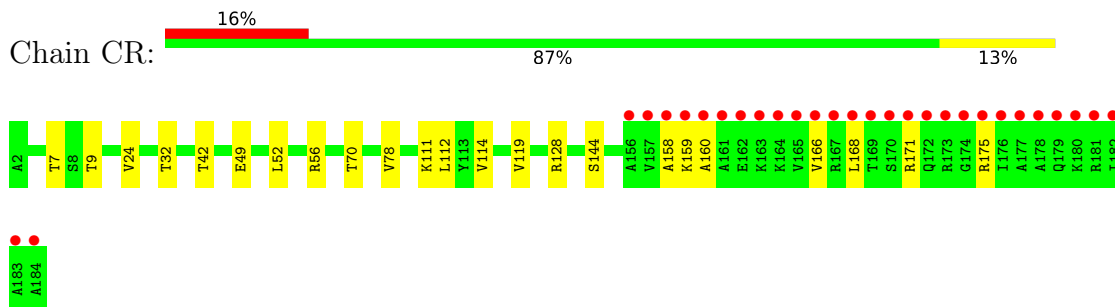
- Molecule 17: 60S ribosomal protein L16-A



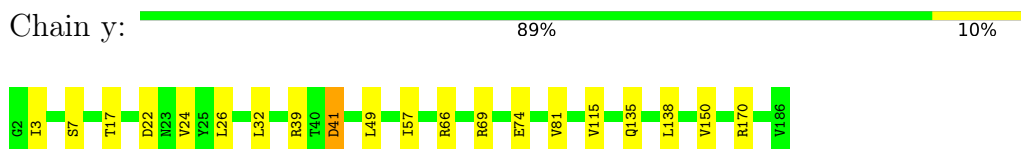
- Molecule 18: 60S ribosomal protein L17-A



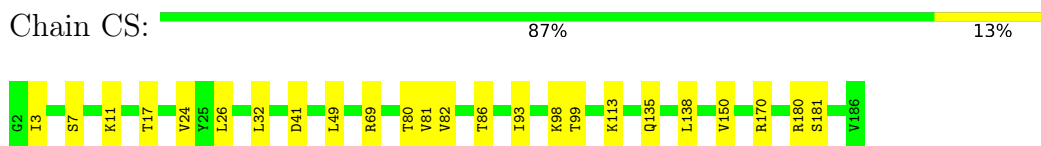
- Molecule 18: 60S ribosomal protein L17-A



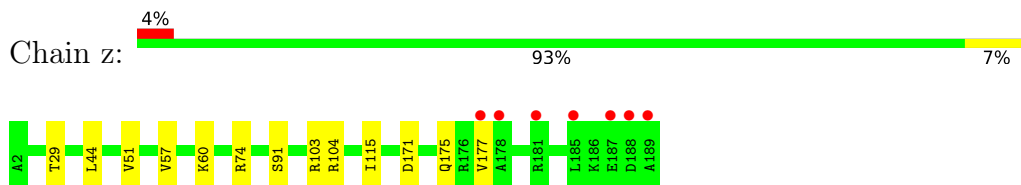
- Molecule 19: 60S ribosomal protein L18-A



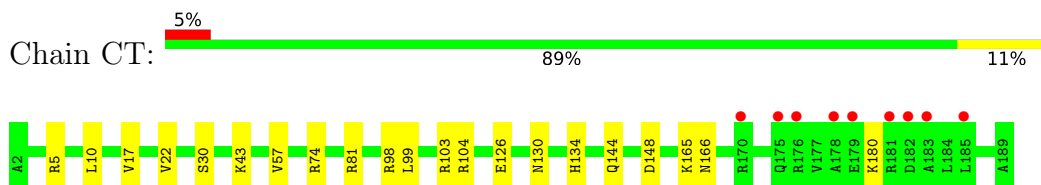
- Molecule 19: 60S ribosomal protein L18-A



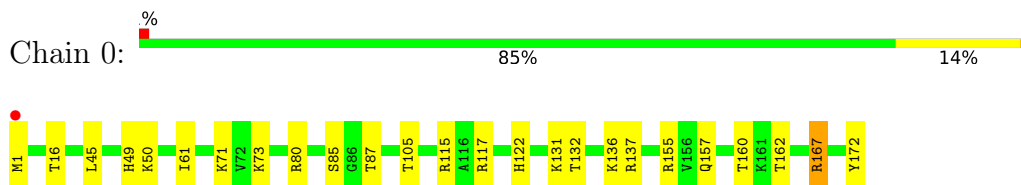
- Molecule 20: 60S ribosomal protein L19-A




- Molecule 20: 60S ribosomal protein L19-A



- Molecule 21: 60S ribosomal protein L20-A




- Molecule 21: 60S ribosomal protein L20-A

Chain CU:  85% 15%




- Molecule 22: 60S ribosomal protein L21-A

Chain 2:  86% 14%




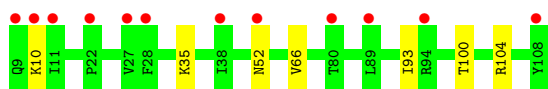
- Molecule 22: 60S ribosomal protein L21-A

Chain CV:  84% 16%

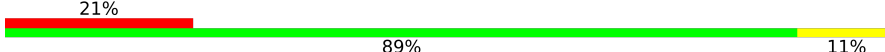


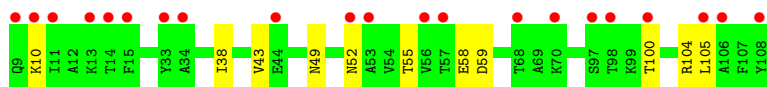
- Molecule 23: 60S ribosomal protein L22-A

Chain 5:  93% 7% 12%




- Molecule 23: 60S ribosomal protein L22-A

Chain CW:  89% 11% 21%



- Molecule 24: 60S ribosomal protein L23-A

Chain IR:  89% 11% 3%

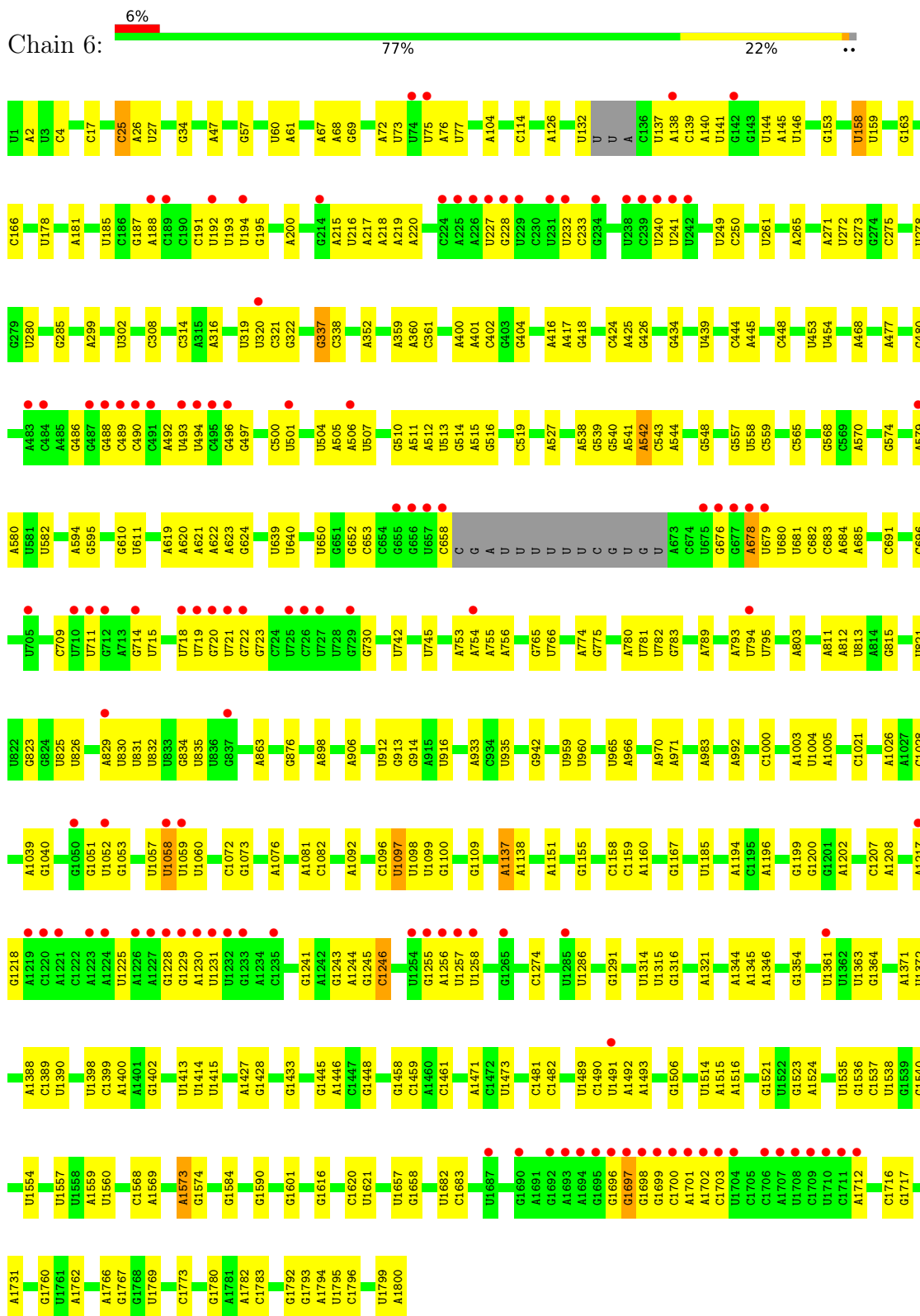


- Molecule 24: 60S ribosomal protein L23-A

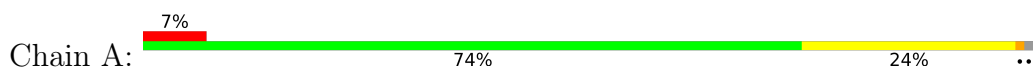
Chain CX:  92% 8%



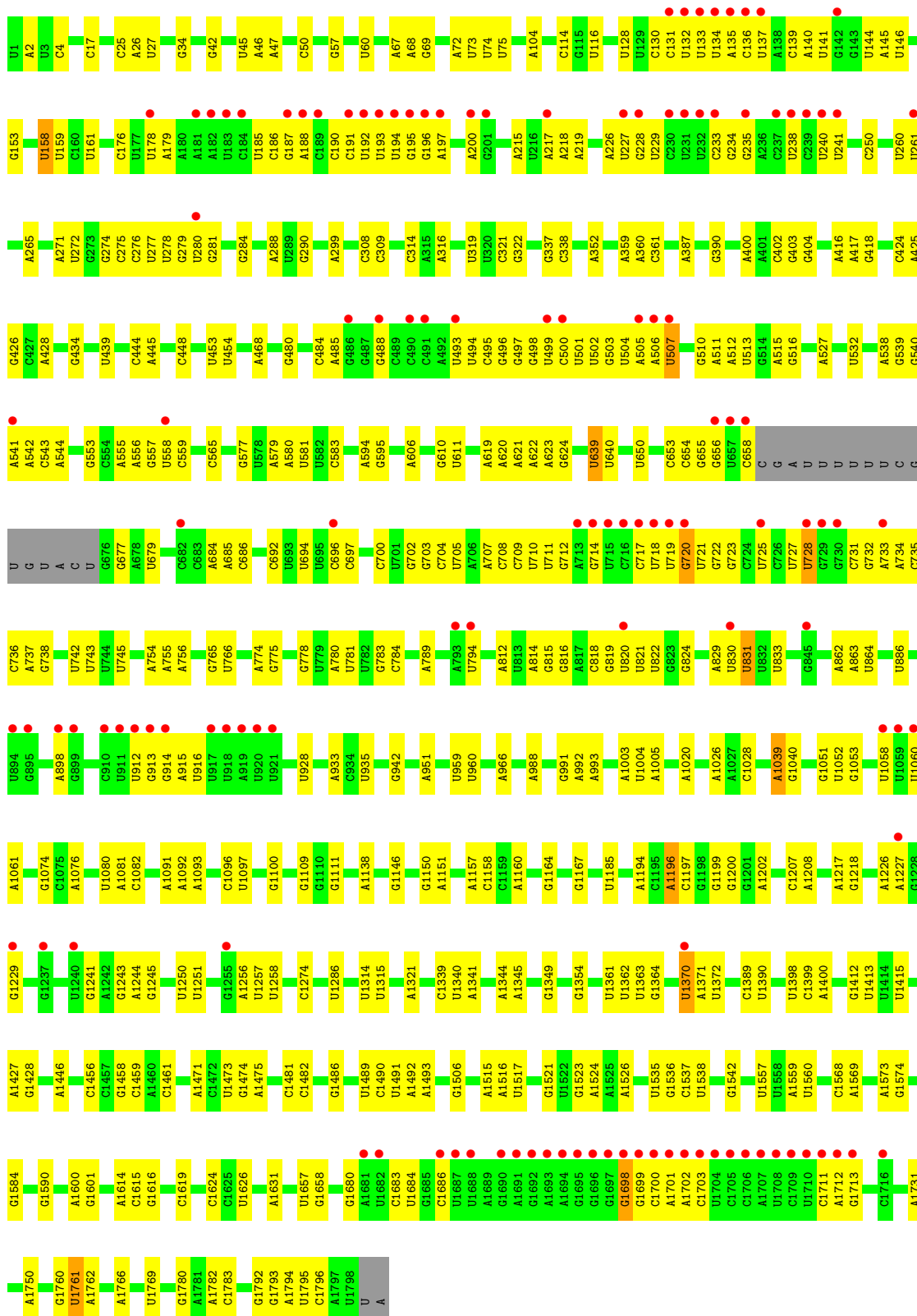
- Molecule 25: 18S ribosomal RNA



• Molecule 25: 18S ribosomal RNA

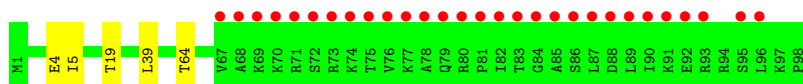




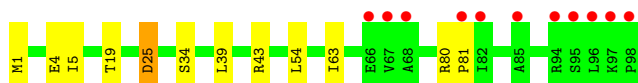
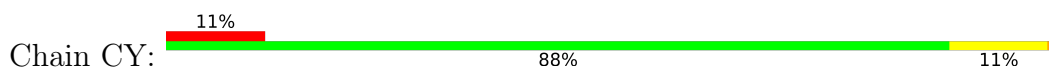


• Molecule 26: 60S ribosomal protein L24-A

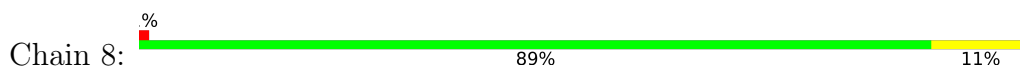




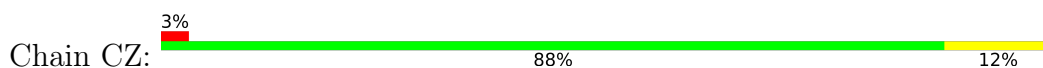
- Molecule 26: 60S ribosomal protein L24-A



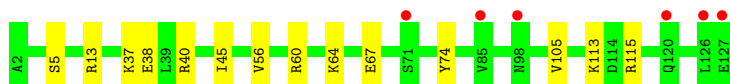
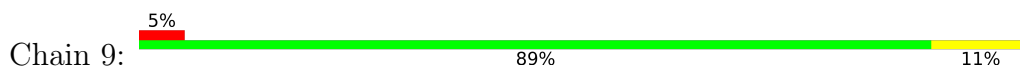
- Molecule 27: 60S ribosomal protein L25



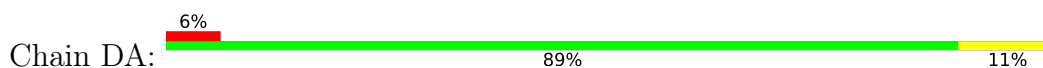
- Molecule 27: 60S ribosomal protein L25



- Molecule 28: 60S ribosomal protein L26-A

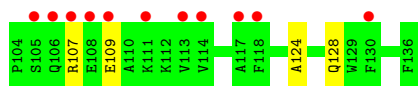


- Molecule 28: 60S ribosomal protein L26-A

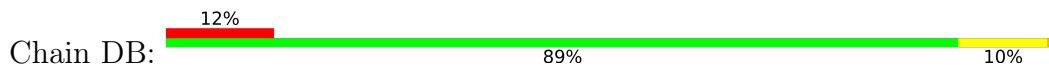


- Molecule 29: 60S ribosomal protein L27-A

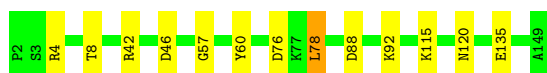




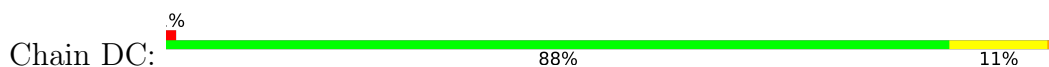
- Molecule 29: 60S ribosomal protein L27-A



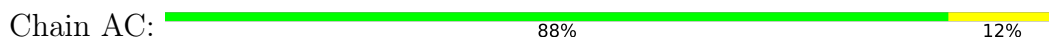
- Molecule 30: 60S ribosomal protein L28



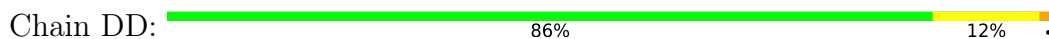
- Molecule 30: 60S ribosomal protein L28



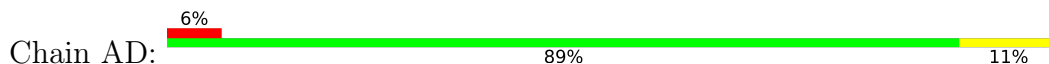
- Molecule 31: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L29



- Molecule 32: 60S ribosomal protein L30

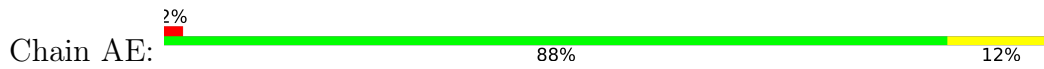


- Molecule 32: 60S ribosomal protein L30

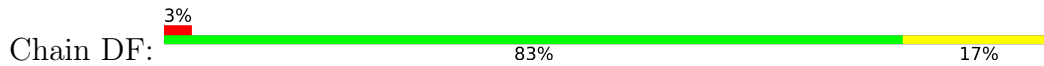




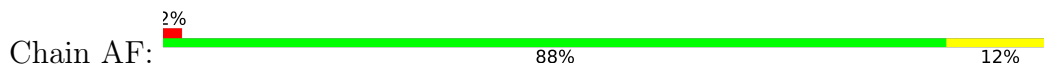
- Molecule 33: 60S ribosomal protein L31-A



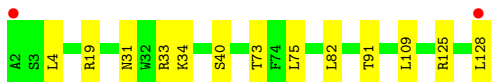
- Molecule 33: 60S ribosomal protein L31-A



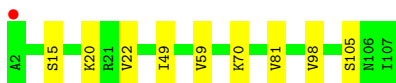
- Molecule 34: 60S ribosomal protein L32



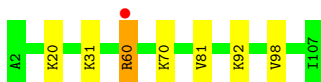
- Molecule 34: 60S ribosomal protein L32



- Molecule 35: 60S ribosomal protein L33-A



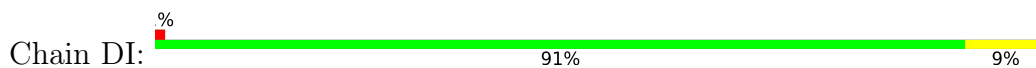
- Molecule 35: 60S ribosomal protein L33-A



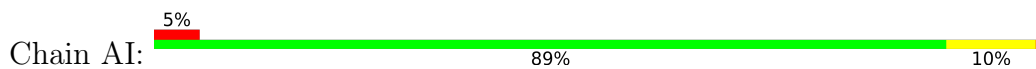
- Molecule 36: 60S ribosomal protein L34-A



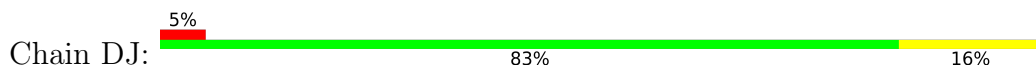
- Molecule 36: 60S ribosomal protein L34-A



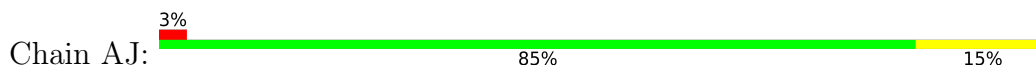
- Molecule 37: 60S ribosomal protein L35-A



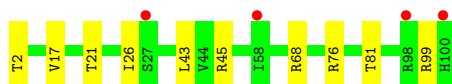
- Molecule 37: 60S ribosomal protein L35-A



- Molecule 38: 60S ribosomal protein L36-A



- Molecule 38: 60S ribosomal protein L36-A



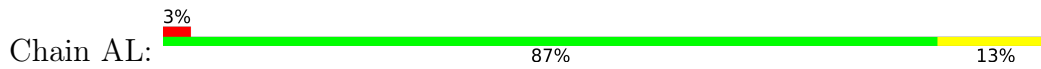
- Molecule 39: 60S ribosomal protein L37-A



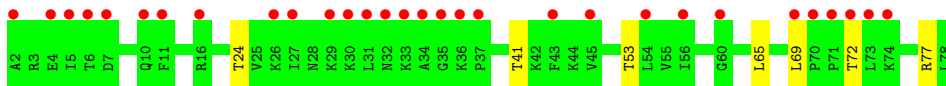
- Molecule 39: 60S ribosomal protein L37-A



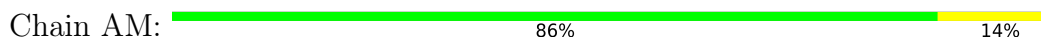
- Molecule 40: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L38



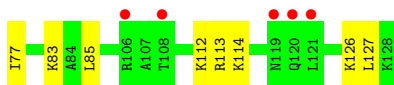
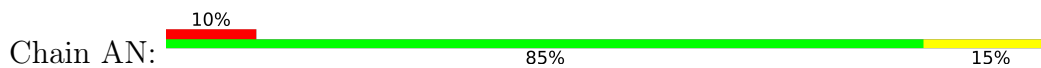
- Molecule 41: 60S ribosomal protein L39



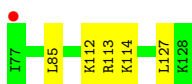
- Molecule 41: 60S ribosomal protein L39



- Molecule 42: Ubiquitin-60S ribosomal protein L40

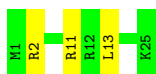


- Molecule 42: Ubiquitin-60S ribosomal protein L40




- Molecule 43: 60S ribosomal protein L41-B

Chain AO:  88% 12%



- Molecule 43: 60S ribosomal protein L41-B

Chain DP:  84% 16%



- Molecule 44: 60S ribosomal protein L42-A

Chain AP:  9% 92% 8%




- Molecule 44: 60S ribosomal protein L42-A

Chain DQ:  91% 9%



- Molecule 45: 60S ribosomal protein L43-A

Chain AQ:  87% 13%



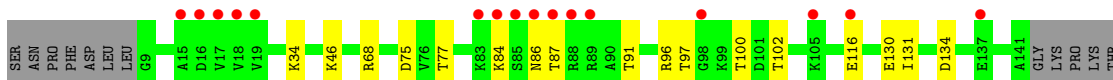
- Molecule 45: 60S ribosomal protein L43-A

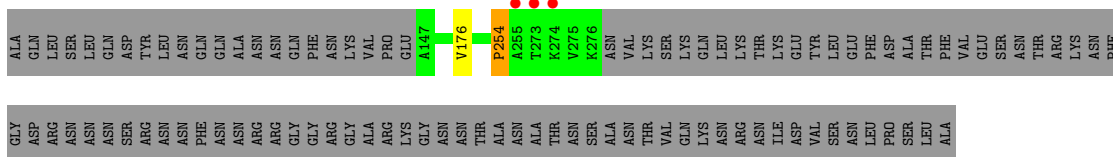
Chain DR:  91% 9%



- Molecule 46: Suppressor protein STM1

Chain i:  7% 51% 7% 42%





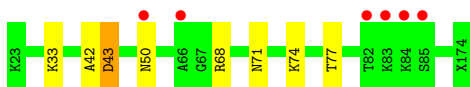
- Molecule 47: 60S ribosomal protein L12

Chain m2: 100%

There are no outlier residues recorded for this chain.

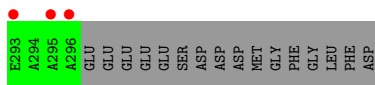
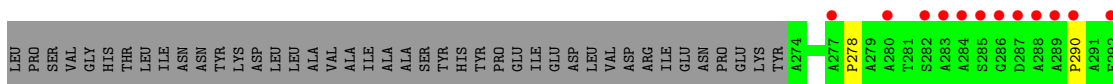
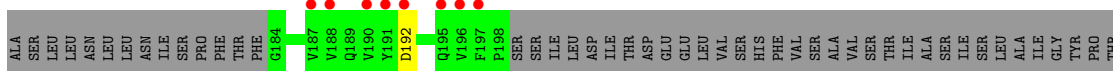
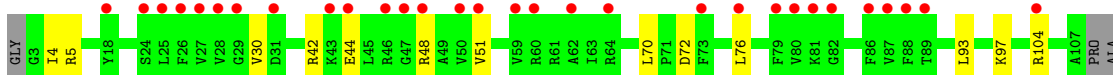
- Molecule 48: Suppressor protein STM1, Suppressor protein STM1

Chain sM: 6% 92% 7%



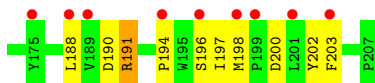
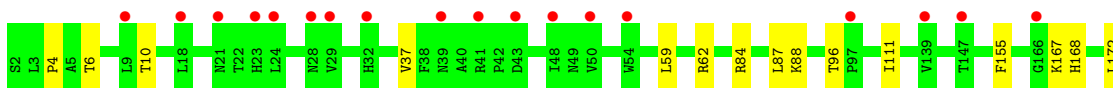
- Molecule 49: 60S acidic ribosomal protein P0

Chain p0: 17% 41% 5% 54%



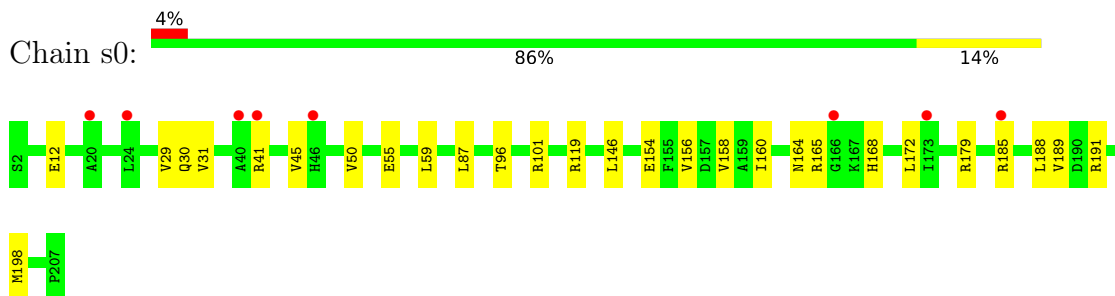
- Molecule 50: 40S ribosomal protein S0-A

Chain B: 13% 88% 12%

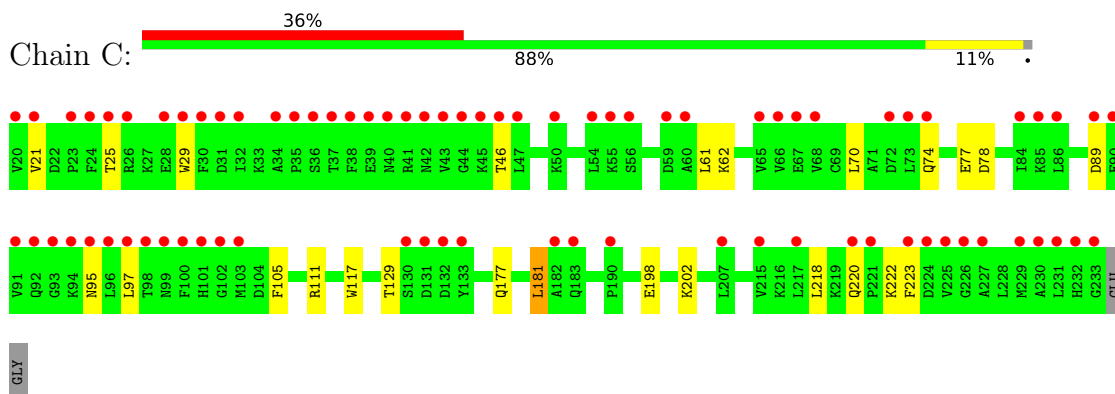




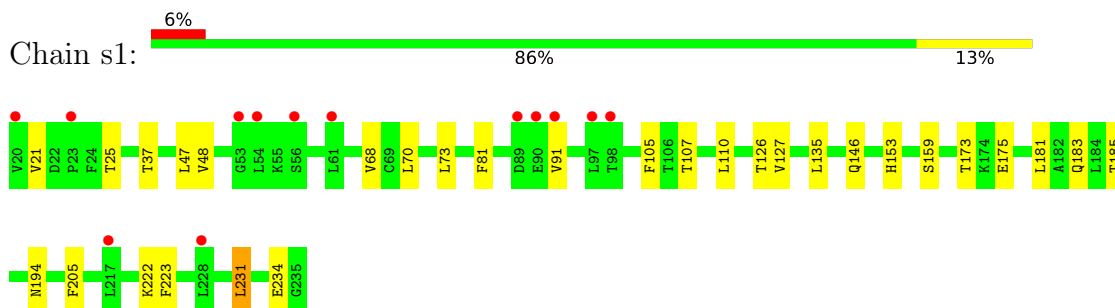
- Molecule 50: 40S ribosomal protein S0-A



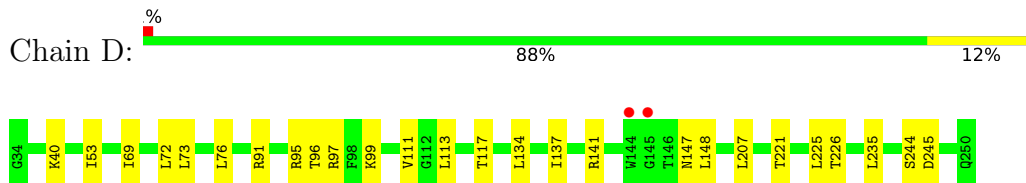
- Molecule 51: 40S ribosomal protein S1-A



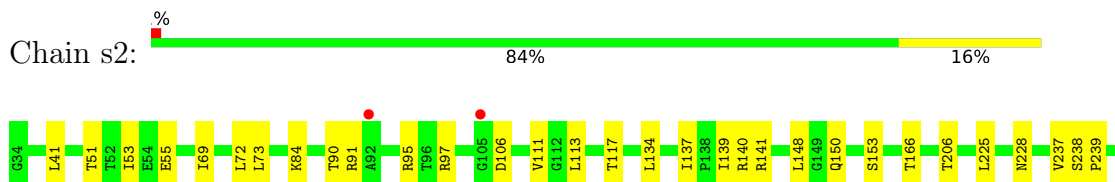
- Molecule 51: 40S ribosomal protein S1-A



- Molecule 52: 40S ribosomal protein S2

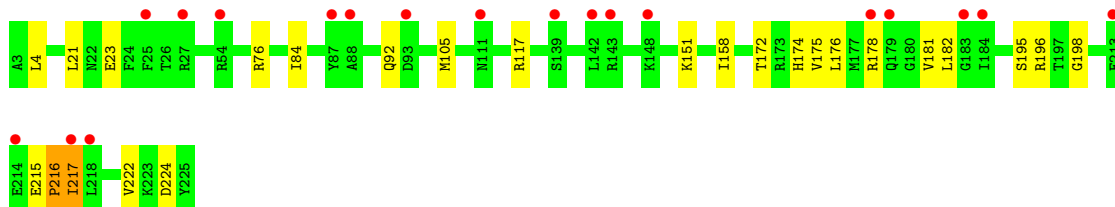
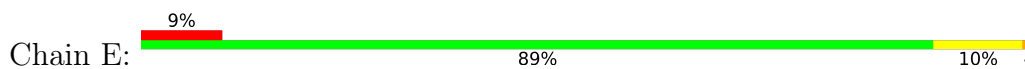


- Molecule 52: 40S ribosomal protein S2

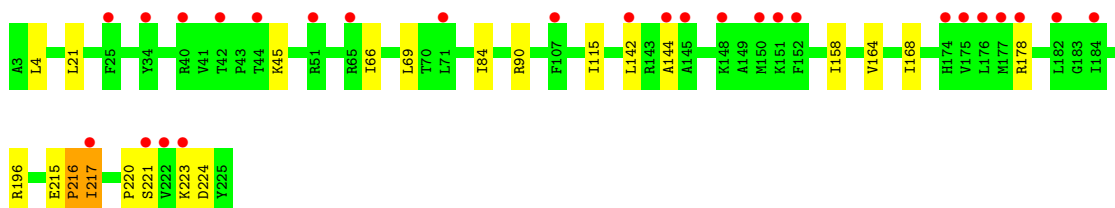
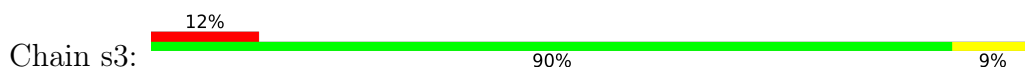




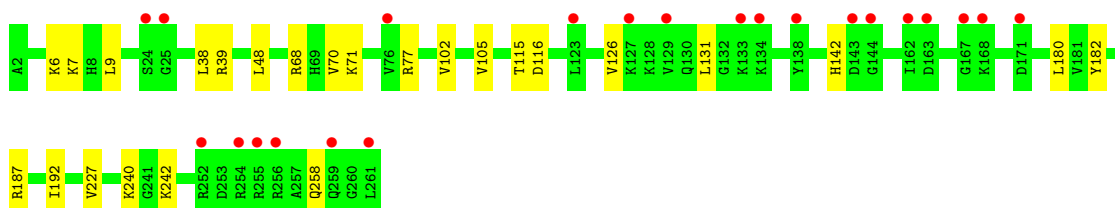
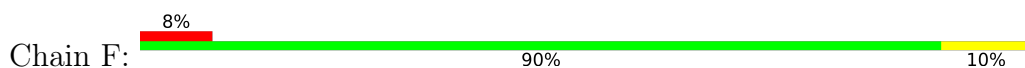
- Molecule 53: 40S ribosomal protein S3



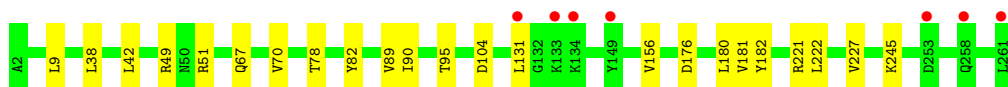
- Molecule 53: 40S ribosomal protein S3



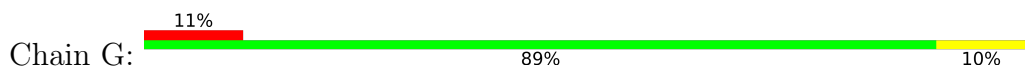
- Molecule 54: 40S ribosomal protein S4-A



- Molecule 54: 40S ribosomal protein S4-A

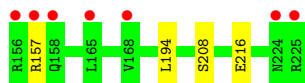
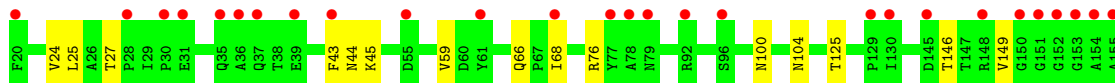


- Molecule 55: 40S ribosomal protein S5

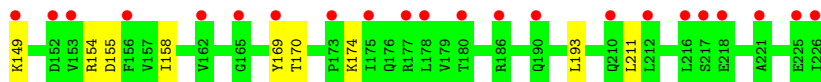
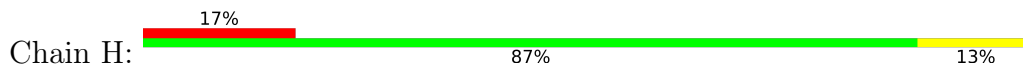




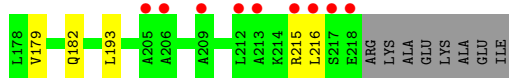
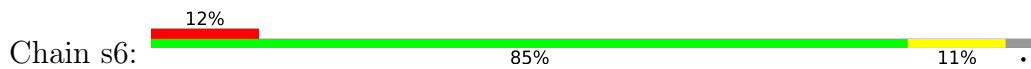
- Molecule 55: 40S ribosomal protein S5



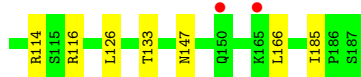
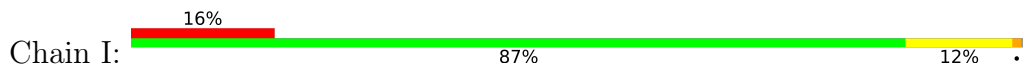
- Molecule 56: 40S ribosomal protein S6-A



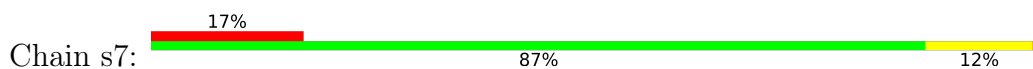
- Molecule 56: 40S ribosomal protein S6-A

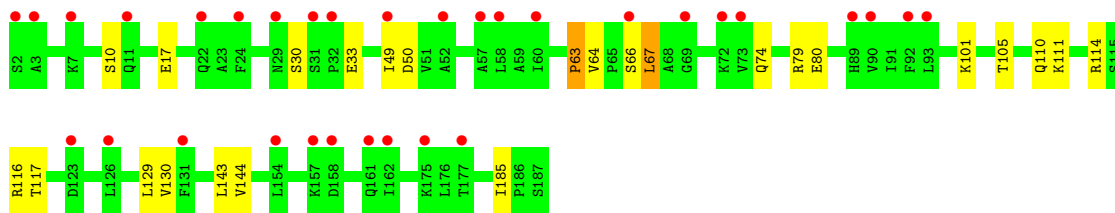


- Molecule 57: 40S ribosomal protein S7-A

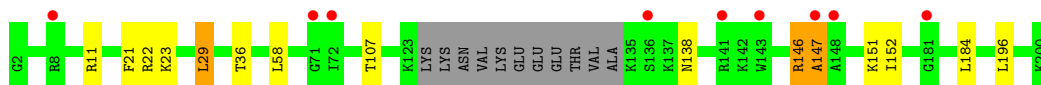
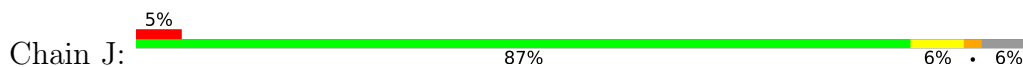


- Molecule 57: 40S ribosomal protein S7-A

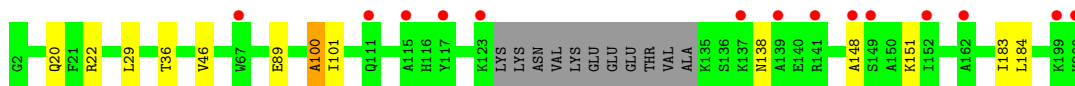
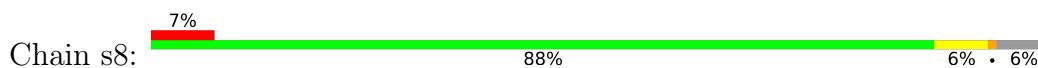




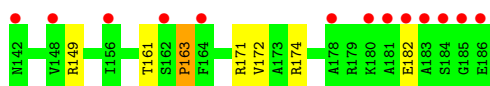
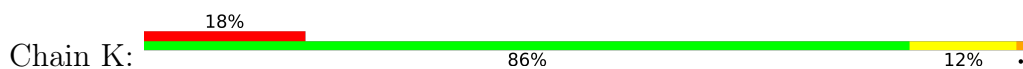
- Molecule 58: 40S ribosomal protein S8-A



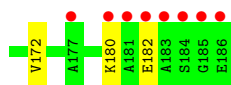
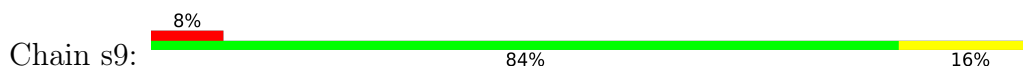
- Molecule 58: 40S ribosomal protein S8-A



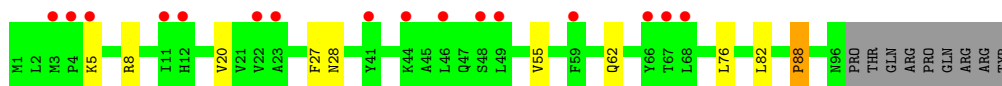
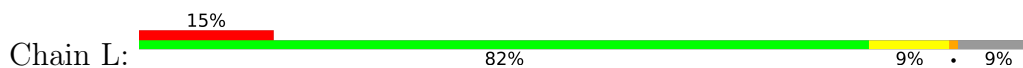
- Molecule 59: 40S ribosomal protein S9-A



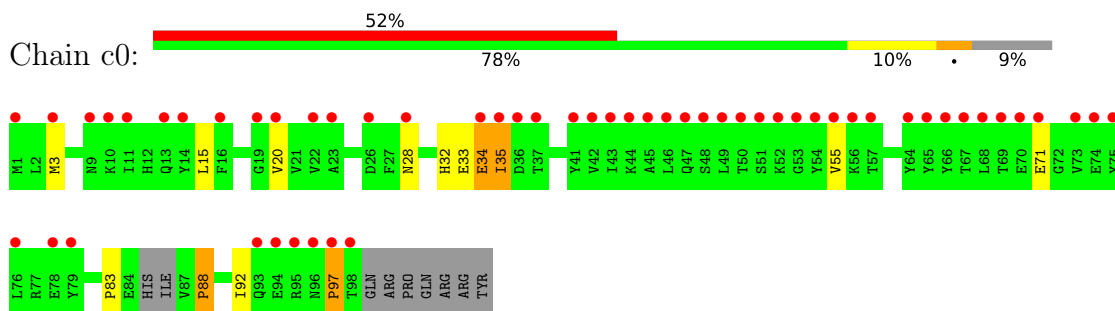
- Molecule 59: 40S ribosomal protein S9-A



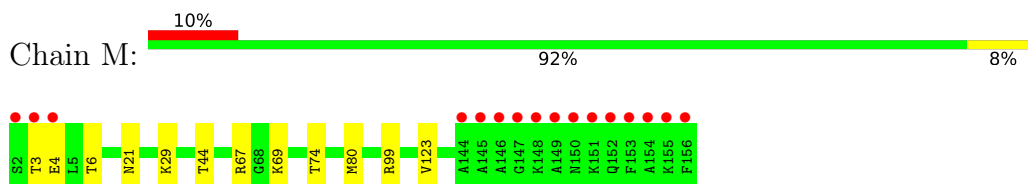
- Molecule 60: 40S ribosomal protein S10-A



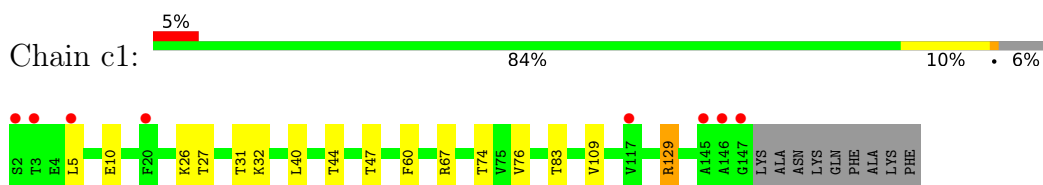
- Molecule 60: 40S ribosomal protein S10-A



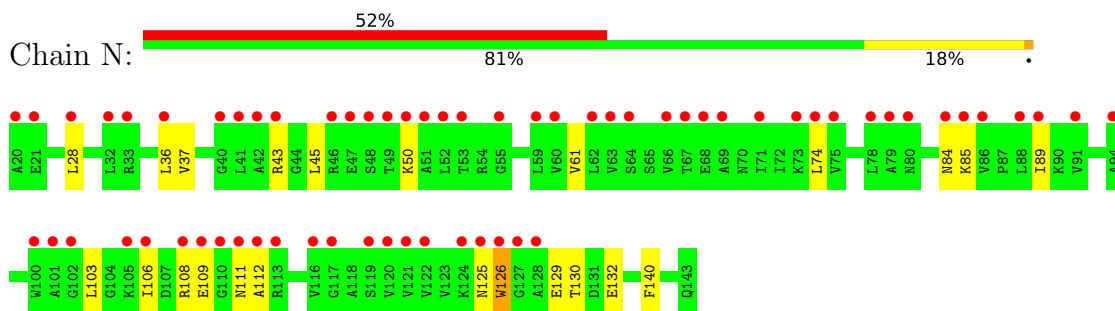
- Molecule 61: 40S ribosomal protein S11-A



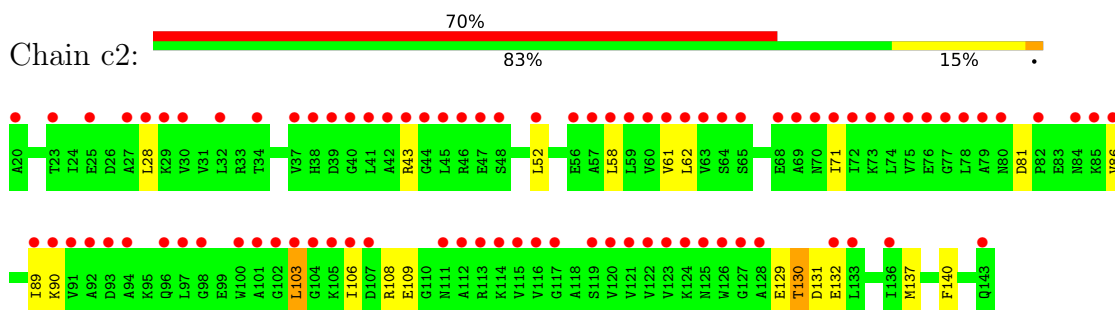
- Molecule 61: 40S ribosomal protein S11-A



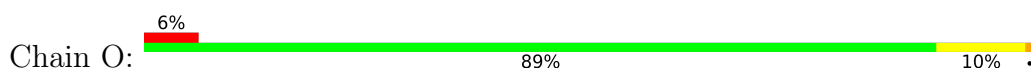
- Molecule 62: 40S ribosomal protein S12



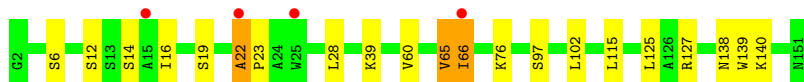
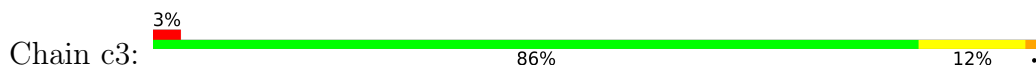
- Molecule 62: 40S ribosomal protein S12



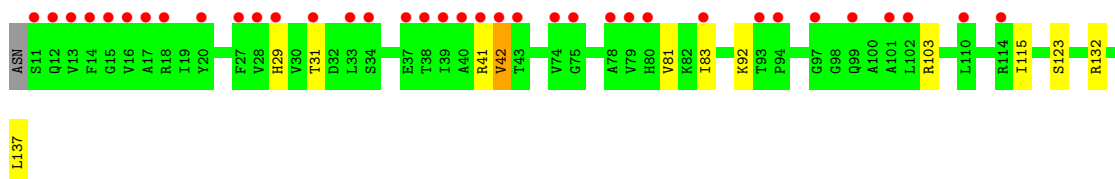
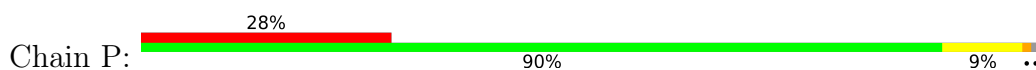
- Molecule 63: 40S ribosomal protein S13



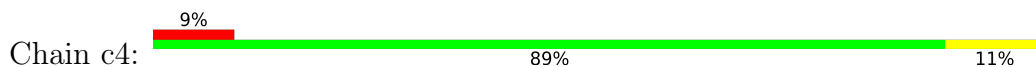
- Molecule 63: 40S ribosomal protein S13



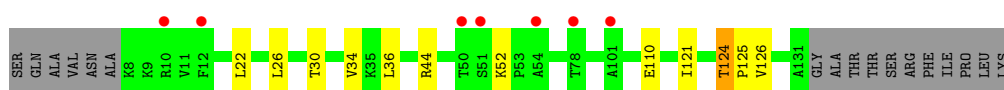
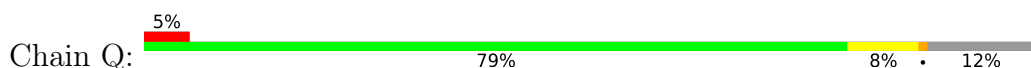
- Molecule 64: 40S ribosomal protein S14-B



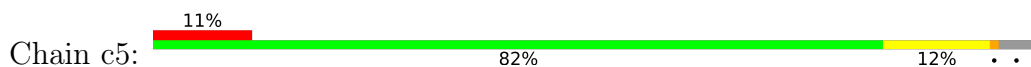
- Molecule 64: 40S ribosomal protein S14-B



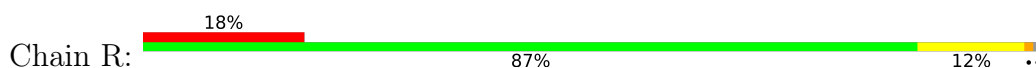
- Molecule 65: 40S ribosomal protein S15

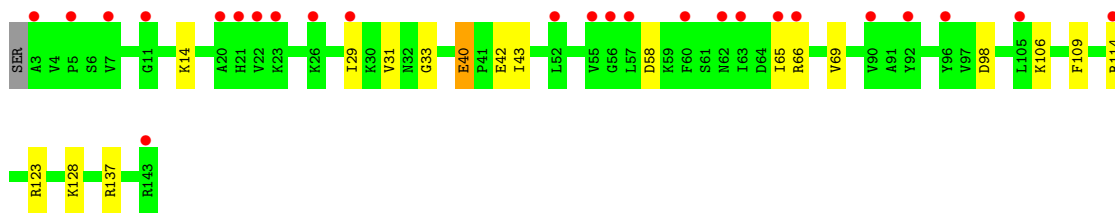


- Molecule 65: 40S ribosomal protein S15

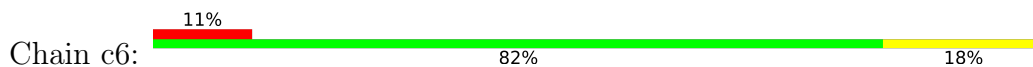


- Molecule 66: 40S ribosomal protein S16-A

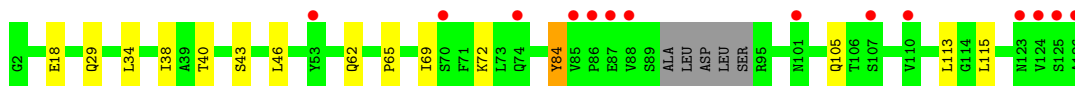
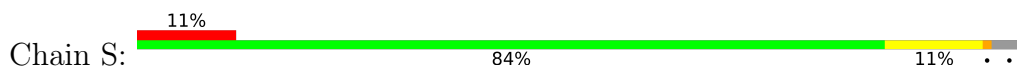




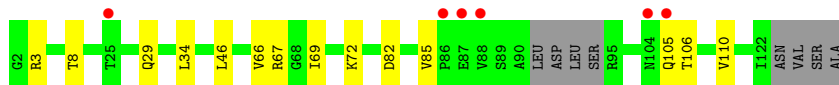
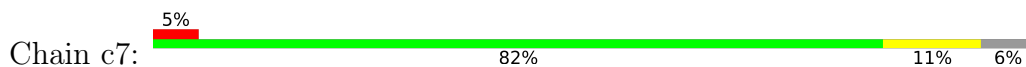
- Molecule 66: 40S ribosomal protein S16-A



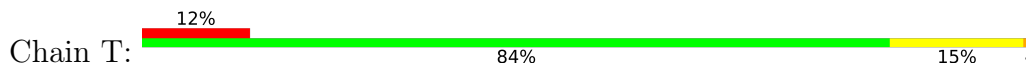
- Molecule 67: 40S ribosomal protein S17-A



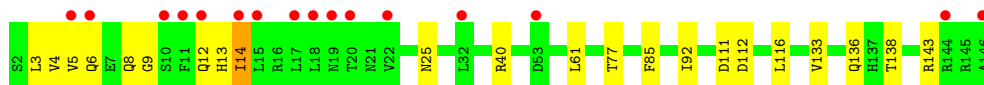
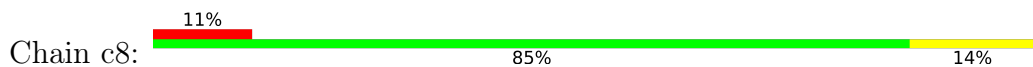
- Molecule 67: 40S ribosomal protein S17-A



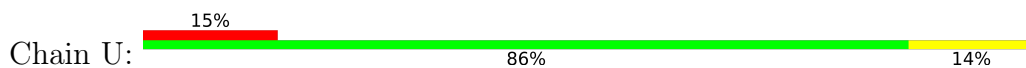
- Molecule 68: 40S ribosomal protein S18-A

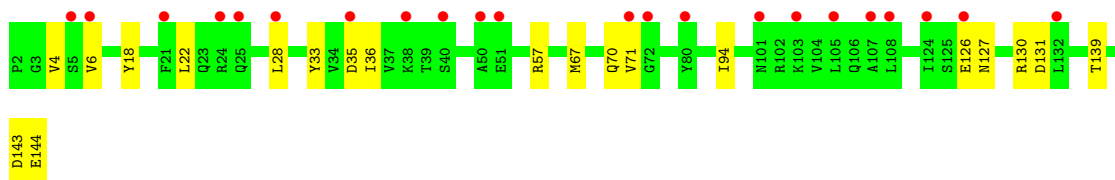


- Molecule 68: 40S ribosomal protein S18-A

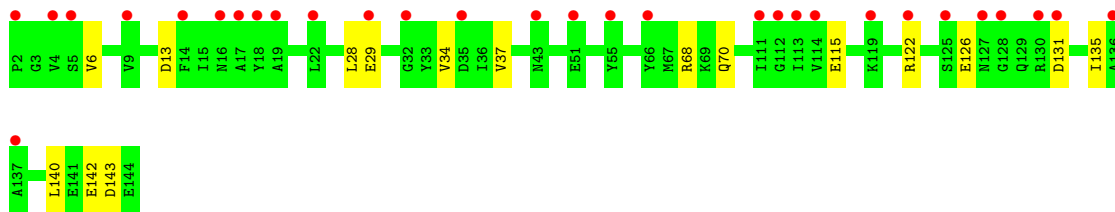
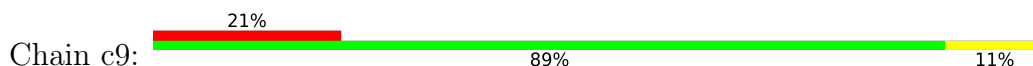


- Molecule 69: 40S ribosomal protein S19-A

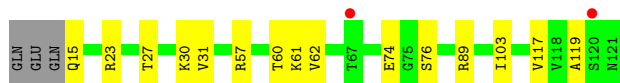
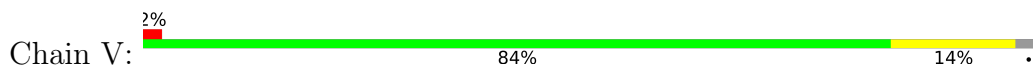




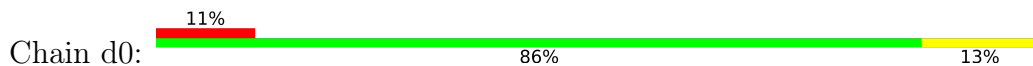
- Molecule 69: 40S ribosomal protein S19-A



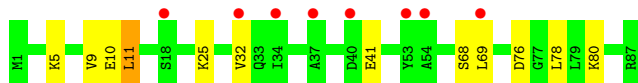
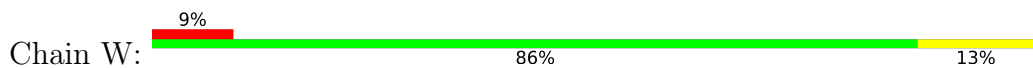
- Molecule 70: 40S ribosomal protein S20



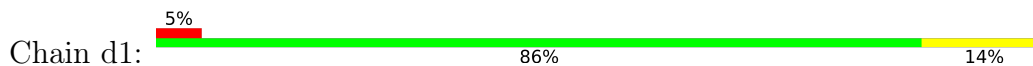
- Molecule 70: 40S ribosomal protein S20



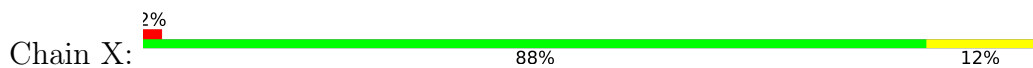
- Molecule 71: 40S ribosomal protein S21-A



- Molecule 71: 40S ribosomal protein S21-A



- Molecule 72: 40S ribosomal protein S22-A



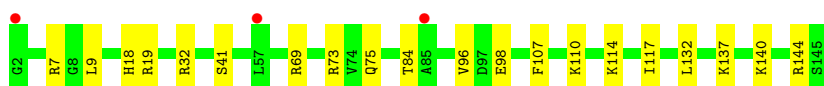
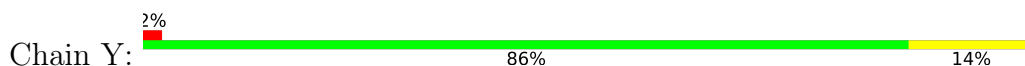




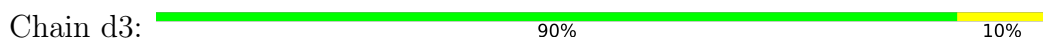
- Molecule 72: 40S ribosomal protein S22-A



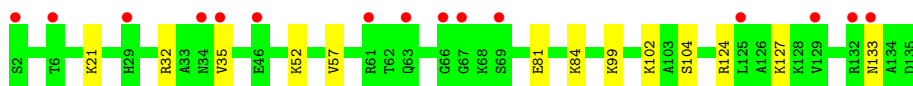
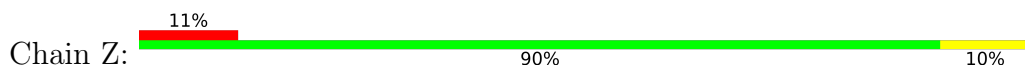
- Molecule 73: 40S ribosomal protein S23-A



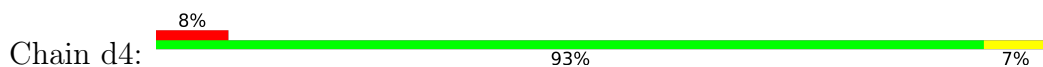
- Molecule 73: 40S ribosomal protein S23-A



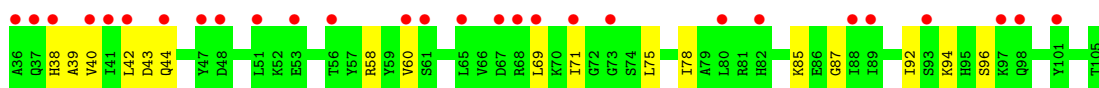
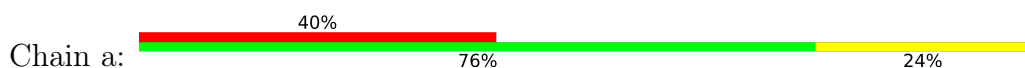
- Molecule 74: 40S ribosomal protein S24-A



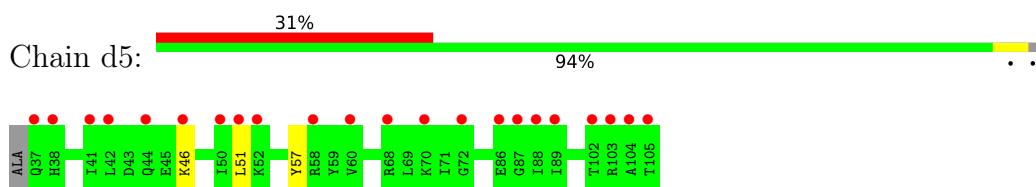
- Molecule 74: 40S ribosomal protein S24-A



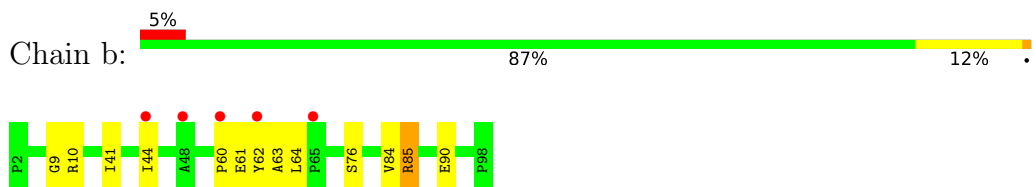
- Molecule 75: 40S ribosomal protein S25-A



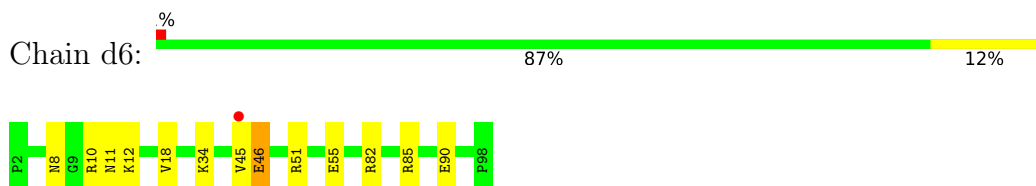
- Molecule 75: 40S ribosomal protein S25-A



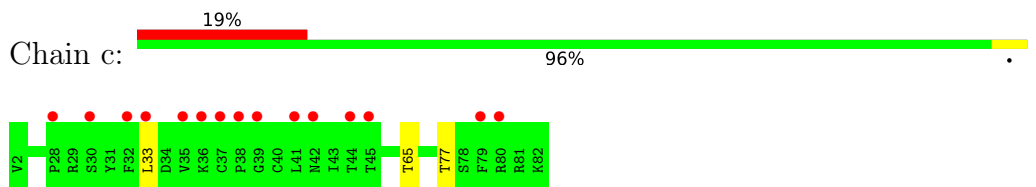
- Molecule 76: 40S ribosomal protein S26-B



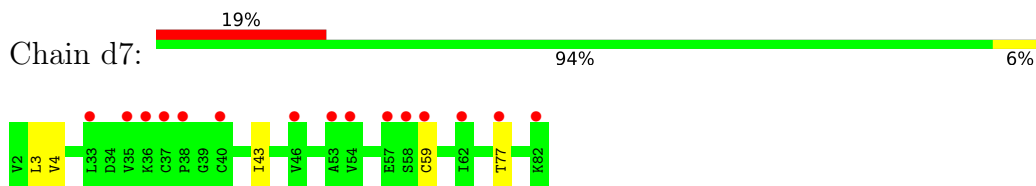
- Molecule 76: 40S ribosomal protein S26-B



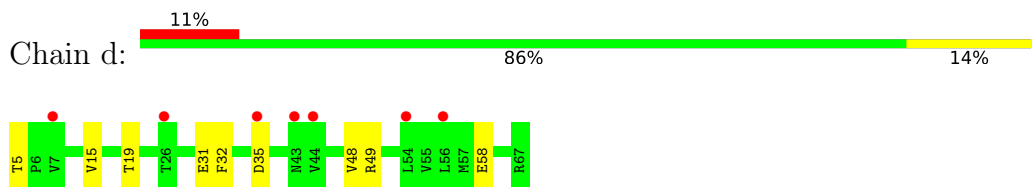
- Molecule 77: 40S ribosomal protein S27-A



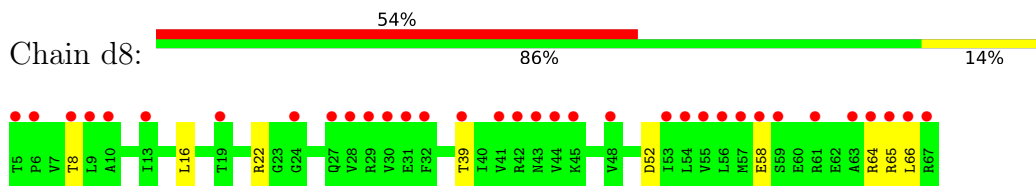
- Molecule 77: 40S ribosomal protein S27-A



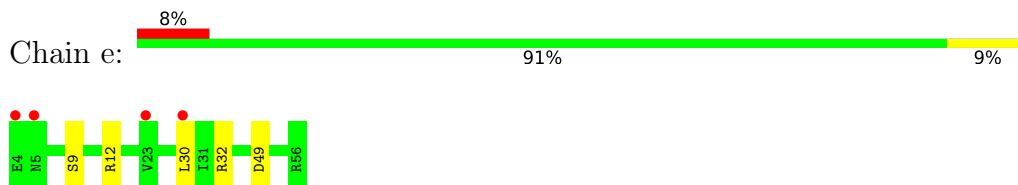
- Molecule 78: 40S ribosomal protein S28-A



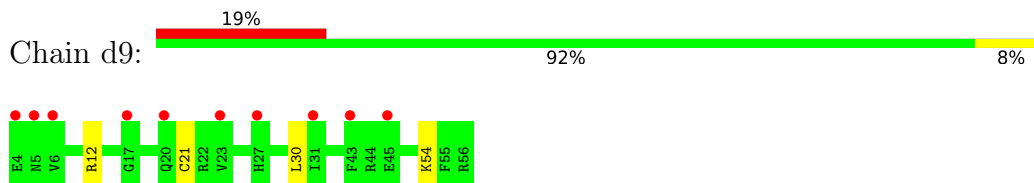
- Molecule 78: 40S ribosomal protein S28-A



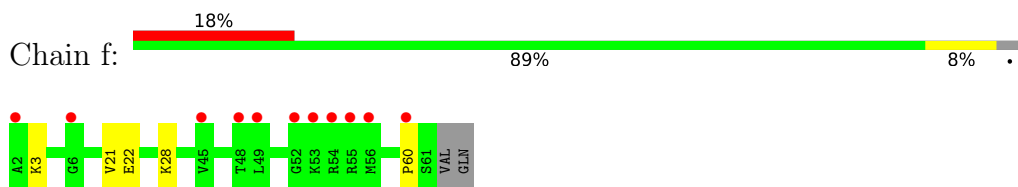
- Molecule 79: 40S ribosomal protein S29-A



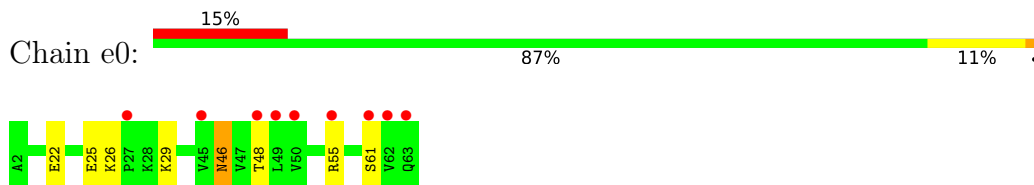
- Molecule 79: 40S ribosomal protein S29-A



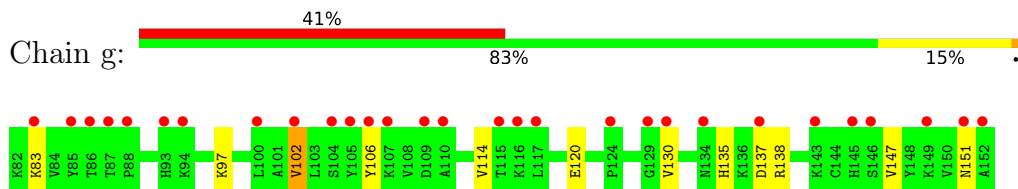
- Molecule 80: 40S ribosomal protein S30-A



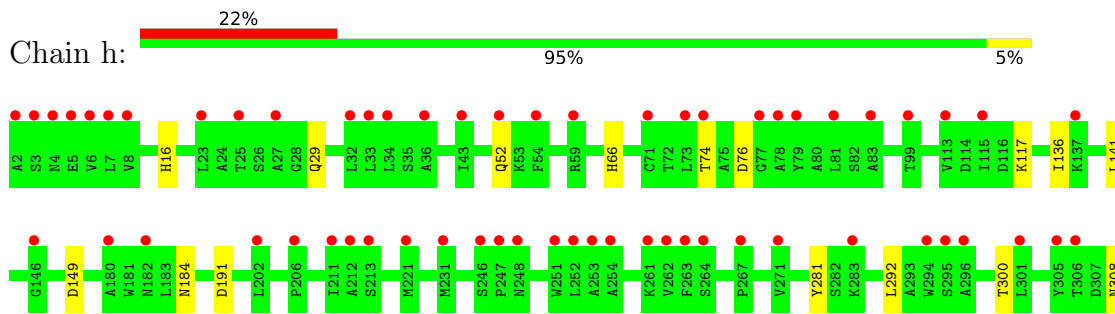
- Molecule 80: 40S ribosomal protein S30-A

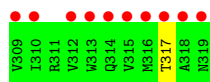


- Molecule 81: Ubiquitin-40S ribosomal protein S31

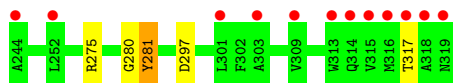


- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein

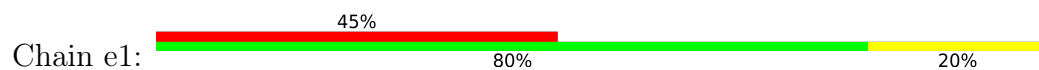




- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 3.13Å)	Xtrriage
Refinement program	PHENIX dev_2450	Depositor
R, $R_{free}$	0.222 , 0.252 0.222 , 0.252	Depositor DCC
$R_{free}$ test set	26196 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.3	Xtrriage
Anisotropy	0.134	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 69.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	410383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage'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.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HN8, OHX, MG, GOL, ZN

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	IR	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(°)	Ideal(°)
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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	34	69
4	j	250/252 (99%)	230 (92%)	19 (8%)	1 (0%)	34	69
5	CE	384/386 (100%)	349 (91%)	31 (8%)	4 (1%)	15	49
5	k	384/386 (100%)	348 (91%)	33 (9%)	3 (1%)	19	54
6	CF	359/361 (99%)	326 (91%)	33 (9%)	0	100	100
6	l	359/361 (99%)	320 (89%)	37 (10%)	2 (1%)	25	59
7	CG	294/296 (99%)	254 (86%)	38 (13%)	2 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	m	294/296 (99%)	263 (90%)	30 (10%)	1 (0%)	41	73
8	CH	152/175 (87%)	139 (91%)	12 (8%)	1 (1%)	22	57
8	n	152/175 (87%)	145 (95%)	6 (4%)	1 (1%)	22	57
9	CI	220/222 (99%)	199 (90%)	16 (7%)	5 (2%)	6	28
9	o	220/222 (99%)	204 (93%)	13 (6%)	3 (1%)	11	40
10	CJ	231/233 (99%)	201 (87%)	28 (12%)	2 (1%)	17	52
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
12	CL	207/220 (94%)	188 (91%)	19 (9%)	0	100	100
12	r	207/220 (94%)	189 (91%)	17 (8%)	1 (0%)	29	64
13	CM	167/169 (99%)	145 (87%)	19 (11%)	3 (2%)	8	34
13	s	167/169 (99%)	137 (82%)	23 (14%)	7 (4%)	3	16
14	CN	191/193 (99%)	168 (88%)	17 (9%)	6 (3%)	4	23
14	t	191/193 (99%)	171 (90%)	13 (7%)	7 (4%)	3	19
15	CO	134/136 (98%)	122 (91%)	11 (8%)	1 (1%)	22	57
15	u	134/136 (98%)	120 (90%)	13 (10%)	1 (1%)	22	57
16	CP	201/203 (99%)	188 (94%)	13 (6%)	0	100	100
16	v	201/203 (99%)	177 (88%)	23 (11%)	1 (0%)	29	64
17	CQ	195/197 (99%)	185 (95%)	8 (4%)	2 (1%)	15	49
17	w	195/197 (99%)	187 (96%)	6 (3%)	2 (1%)	15	49
18	CR	181/183 (99%)	161 (89%)	17 (9%)	3 (2%)	9	36
18	x	181/183 (99%)	164 (91%)	17 (9%)	0	100	100
19	CS	183/185 (99%)	166 (91%)	16 (9%)	1 (0%)	29	64
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%)	25	59
21	CU	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
22	2	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	12	42
22	CV	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	25	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	5	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
23	CW	98/100 (98%)	81 (83%)	16 (16%)	1 (1%)	15	49
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%)	7	30
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
28	DA	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
29	AA	133/135 (98%)	115 (86%)	15 (11%)	3 (2%)	6	28
29	DB	133/135 (98%)	119 (90%)	10 (8%)	4 (3%)	4	23
30	AB	146/148 (99%)	125 (86%)	19 (13%)	2 (1%)	11	40
30	DC	146/148 (99%)	123 (84%)	21 (14%)	2 (1%)	11	40
31	AC	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
31	DD	56/58 (97%)	50 (89%)	5 (9%)	1 (2%)	8	34
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%)	17	52
33	DF	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	17	52
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%)	15	49
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%)	17	52
37	DJ	117/119 (98%)	109 (93%)	7 (6%)	1 (1%)	17	52
38	AJ	97/99 (98%)	83 (86%)	11 (11%)	3 (3%)	4	23
38	DK	97/99 (98%)	84 (87%)	13 (13%)	0	100	100
39	AK	85/87 (98%)	77 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	5	26
48	sM	61/104 (59%)	45 (74%)	14 (23%)	2 (3%)	4	21
49	p0	139/311 (45%)	131 (94%)	8 (6%)	0	100	100
50	B	204/206 (99%)	157 (77%)	40 (20%)	7 (3%)	3	21
50	s0	204/206 (99%)	172 (84%)	30 (15%)	2 (1%)	15	49
51	C	212/216 (98%)	167 (79%)	43 (20%)	2 (1%)	17	52
51	s1	214/216 (99%)	190 (89%)	23 (11%)	1 (0%)	29	64
52	D	215/217 (99%)	189 (88%)	25 (12%)	1 (0%)	29	64
52	s2	215/217 (99%)	190 (88%)	23 (11%)	2 (1%)	17	52
53	E	221/223 (99%)	200 (90%)	19 (9%)	2 (1%)	17	52
53	s3	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	8	34
54	F	258/260 (99%)	233 (90%)	25 (10%)	0	100	100
54	s4	258/260 (99%)	229 (89%)	28 (11%)	1 (0%)	34	69
55	G	204/206 (99%)	166 (81%)	36 (18%)	2 (1%)	15	49
55	s5	204/206 (99%)	168 (82%)	36 (18%)	0	100	100
56	H	224/226 (99%)	202 (90%)	19 (8%)	3 (1%)	12	42
56	s6	216/226 (96%)	199 (92%)	15 (7%)	2 (1%)	17	52
57	I	182/186 (98%)	154 (85%)	25 (14%)	3 (2%)	9	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	s7	184/186 (99%)	158 (86%)	21 (11%)	5 (3%)	5	25
58	J	184/199 (92%)	159 (86%)	21 (11%)	4 (2%)	6	29
58	s8	184/199 (92%)	159 (86%)	23 (12%)	2 (1%)	14	46
59	K	183/185 (99%)	160 (87%)	21 (12%)	2 (1%)	14	46
59	s9	183/185 (99%)	161 (88%)	22 (12%)	0	100	100
60	L	94/105 (90%)	70 (74%)	23 (24%)	1 (1%)	14	46
60	c0	92/105 (88%)	61 (66%)	25 (27%)	6 (6%)	1	8
61	M	153/155 (99%)	137 (90%)	14 (9%)	2 (1%)	12	42
61	c1	144/155 (93%)	128 (89%)	15 (10%)	1 (1%)	22	57
62	N	122/124 (98%)	81 (66%)	33 (27%)	8 (7%)	1	7
62	c2	122/124 (98%)	81 (66%)	37 (30%)	4 (3%)	4	21
63	O	148/150 (99%)	137 (93%)	9 (6%)	2 (1%)	11	40
63	c3	148/150 (99%)	128 (86%)	14 (10%)	6 (4%)	3	16
64	P	125/128 (98%)	103 (82%)	21 (17%)	1 (1%)	19	54
64	c4	126/128 (98%)	110 (87%)	16 (13%)	0	100	100
65	Q	122/141 (86%)	100 (82%)	19 (16%)	3 (2%)	5	27
65	c5	133/141 (94%)	99 (74%)	27 (20%)	7 (5%)	2	12
66	R	139/142 (98%)	122 (88%)	16 (12%)	1 (1%)	22	57
66	c6	140/142 (99%)	124 (89%)	15 (11%)	1 (1%)	22	57
67	S	116/125 (93%)	93 (80%)	22 (19%)	1 (1%)	17	52
67	c7	113/125 (90%)	91 (80%)	21 (19%)	1 (1%)	17	52
68	T	143/145 (99%)	126 (88%)	16 (11%)	1 (1%)	22	57
68	c8	143/145 (99%)	121 (85%)	19 (13%)	3 (2%)	7	30
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%)	15	49
70	d0	108/110 (98%)	92 (85%)	14 (13%)	2 (2%)	8	33
71	W	85/87 (98%)	62 (73%)	22 (26%)	1 (1%)	13	44
71	d1	85/87 (98%)	77 (91%)	7 (8%)	1 (1%)	13	44
72	X	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	54
72	d2	127/129 (98%)	121 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	Y	142/144 (99%)	115 (81%)	24 (17%)	3 (2%)	7	30
73	d3	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
74	Z	132/134 (98%)	120 (91%)	10 (8%)	2 (2%)	10	39
74	d4	132/134 (98%)	114 (86%)	16 (12%)	2 (2%)	10	39
75	a	68/70 (97%)	51 (75%)	14 (21%)	3 (4%)	2	15
75	d5	67/70 (96%)	56 (84%)	11 (16%)	0	100	100
76	b	95/97 (98%)	66 (70%)	24 (25%)	5 (5%)	2	12
76	d6	95/97 (98%)	73 (77%)	20 (21%)	2 (2%)	7	30
77	c	79/81 (98%)	65 (82%)	14 (18%)	0	100	100
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%)	9	36
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%)	41	73
83	e1	49/51 (96%)	30 (61%)	18 (37%)	1 (2%)	7	31
All	All	22260/23067 (96%)	19629 (88%)	2417 (11%)	214 (1%)	15	49

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 [i](#)

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%)	4	19
4	j	193/194 (100%)	166 (86%)	27 (14%)	3	15
5	CE	319/322 (99%)	272 (85%)	47 (15%)	3	13
5	k	321/322 (100%)	274 (85%)	47 (15%)	3	13
6	CF	288/288 (100%)	256 (89%)	32 (11%)	6	24
6	l	288/288 (100%)	249 (86%)	39 (14%)	4	16
7	CG	244/244 (100%)	207 (85%)	37 (15%)	3	12
7	m	244/244 (100%)	216 (88%)	28 (12%)	5	22
8	CH	134/152 (88%)	116 (87%)	18 (13%)	4	16
8	n	134/152 (88%)	120 (90%)	14 (10%)	7	27
9	CI	186/186 (100%)	167 (90%)	19 (10%)	7	27
9	o	186/186 (100%)	165 (89%)	21 (11%)	6	23
10	CJ	187/191 (98%)	172 (92%)	15 (8%)	12	40
10	p	187/191 (98%)	167 (89%)	20 (11%)	6	26
11	CK	171/171 (100%)	143 (84%)	28 (16%)	2	10
11	q	171/171 (100%)	148 (86%)	23 (14%)	4	16
12	CL	177/186 (95%)	151 (85%)	26 (15%)	3	13
12	r	177/186 (95%)	149 (84%)	28 (16%)	2	11
13	CM	147/147 (100%)	125 (85%)	22 (15%)	3	12
13	s	147/147 (100%)	127 (86%)	20 (14%)	3	16
14	CN	154/154 (100%)	128 (83%)	26 (17%)	2	9
14	t	154/154 (100%)	136 (88%)	18 (12%)	5	22
15	CO	107/107 (100%)	93 (87%)	14 (13%)	4	17
15	u	107/107 (100%)	89 (83%)	18 (17%)	2	9
16	CP	175/175 (100%)	160 (91%)	15 (9%)	10	37
16	v	175/175 (100%)	155 (89%)	20 (11%)	5	23
17	CQ	160/160 (100%)	144 (90%)	16 (10%)	7	28
17	w	160/160 (100%)	139 (87%)	21 (13%)	4	17
18	CR	140/145 (97%)	120 (86%)	20 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	x	140/145 (97%)	118 (84%)	22 (16%)	2	11
19	CS	150/150 (100%)	128 (85%)	22 (15%)	3	13
19	y	150/150 (100%)	130 (87%)	20 (13%)	4	16
20	CT	153/153 (100%)	132 (86%)	21 (14%)	3	16
20	z	153/153 (100%)	140 (92%)	13 (8%)	10	37
21	0	156/156 (100%)	131 (84%)	25 (16%)	2	11
21	CU	156/156 (100%)	133 (85%)	23 (15%)	3	13
22	2	136/136 (100%)	116 (85%)	20 (15%)	3	13
22	CV	136/136 (100%)	112 (82%)	24 (18%)	2	8
23	5	87/87 (100%)	80 (92%)	7 (8%)	12	40
23	CW	87/87 (100%)	77 (88%)	10 (12%)	5	22
24	CX	104/104 (100%)	93 (89%)	11 (11%)	6	26
24	IR	104/104 (100%)	89 (86%)	15 (14%)	3	14
26	7	57/86 (66%)	52 (91%)	5 (9%)	10	36
26	CY	57/86 (66%)	47 (82%)	10 (18%)	2	8
27	8	104/105 (99%)	91 (88%)	13 (12%)	4	18
27	CZ	104/105 (99%)	90 (86%)	14 (14%)	4	16
28	9	109/109 (100%)	95 (87%)	14 (13%)	4	18
28	DA	109/109 (100%)	95 (87%)	14 (13%)	4	18
29	AA	115/115 (100%)	104 (90%)	11 (10%)	8	31
29	DB	115/115 (100%)	104 (90%)	11 (10%)	8	31
30	AB	118/118 (100%)	106 (90%)	12 (10%)	7	27
30	DC	118/118 (100%)	103 (87%)	15 (13%)	4	18
31	AC	46/46 (100%)	40 (87%)	6 (13%)	4	18
31	DD	46/46 (100%)	39 (85%)	7 (15%)	3	12
32	AD	81/81 (100%)	70 (86%)	11 (14%)	3	16
32	DE	81/81 (100%)	76 (94%)	5 (6%)	18	49
33	AE	92/96 (96%)	80 (87%)	12 (13%)	4	18
33	DF	92/96 (96%)	75 (82%)	17 (18%)	1	7
34	AF	109/109 (100%)	94 (86%)	15 (14%)	3	16
34	DG	109/109 (100%)	96 (88%)	13 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	AG	90/90 (100%)	81 (90%)	9 (10%)	7	28
35	DH	90/90 (100%)	83 (92%)	7 (8%)	12	40
36	AH	95/95 (100%)	84 (88%)	11 (12%)	5	22
36	DI	95/95 (100%)	85 (90%)	10 (10%)	7	26
37	AI	104/104 (100%)	92 (88%)	12 (12%)	5	22
37	DJ	104/104 (100%)	86 (83%)	18 (17%)	2	9
38	AJ	81/81 (100%)	69 (85%)	12 (15%)	3	13
38	DK	81/81 (100%)	71 (88%)	10 (12%)	4	19
39	AK	70/70 (100%)	63 (90%)	7 (10%)	7	28
39	DL	70/70 (100%)	59 (84%)	11 (16%)	2	11
40	AL	68/68 (100%)	58 (85%)	10 (15%)	3	13
40	DM	68/68 (100%)	61 (90%)	7 (10%)	7	27
41	AM	45/45 (100%)	38 (84%)	7 (16%)	2	11
41	DN	45/45 (100%)	41 (91%)	4 (9%)	9	34
42	AN	47/47 (100%)	39 (83%)	8 (17%)	2	9
42	DO	47/47 (100%)	42 (89%)	5 (11%)	6	26
43	AO	23/23 (100%)	20 (87%)	3 (13%)	4	18
43	DP	23/23 (100%)	19 (83%)	4 (17%)	2	9
44	AP	90/90 (100%)	82 (91%)	8 (9%)	9	34
44	DQ	90/90 (100%)	81 (90%)	9 (10%)	7	28
45	AQ	71/71 (100%)	59 (83%)	12 (17%)	2	9
45	DR	71/71 (100%)	63 (89%)	8 (11%)	6	23
46	i	97/227 (43%)	82 (84%)	15 (16%)	2	11
48	sM	54/54 (100%)	47 (87%)	7 (13%)	4	18
49	p0	105/253 (42%)	91 (87%)	14 (13%)	4	16
50	B	164/173 (95%)	146 (89%)	18 (11%)	6	25
50	s0	165/173 (95%)	140 (85%)	25 (15%)	3	12
51	C	191/192 (100%)	167 (87%)	24 (13%)	4	18
51	s1	192/192 (100%)	164 (85%)	28 (15%)	3	13
52	D	176/176 (100%)	151 (86%)	25 (14%)	3	14
52	s2	176/176 (100%)	144 (82%)	32 (18%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	E	182/182 (100%)	159 (87%)	23 (13%)	4	18
53	s3	182/182 (100%)	164 (90%)	18 (10%)	8	29
54	F	221/221 (100%)	196 (89%)	25 (11%)	6	23
54	s4	221/221 (100%)	200 (90%)	21 (10%)	8	31
55	G	173/173 (100%)	153 (88%)	20 (12%)	5	22
55	s5	173/173 (100%)	155 (90%)	18 (10%)	7	27
56	H	188/193 (97%)	163 (87%)	25 (13%)	4	16
56	s6	187/193 (97%)	163 (87%)	24 (13%)	4	18
57	I	165/166 (99%)	146 (88%)	19 (12%)	5	22
57	s7	165/166 (99%)	145 (88%)	20 (12%)	5	20
58	J	150/160 (94%)	139 (93%)	11 (7%)	14	43
58	s8	150/160 (94%)	140 (93%)	10 (7%)	16	46
59	K	158/158 (100%)	134 (85%)	24 (15%)	3	12
59	s9	158/158 (100%)	129 (82%)	29 (18%)	1	7
60	L	77/98 (79%)	68 (88%)	9 (12%)	5	22
60	c0	73/98 (74%)	65 (89%)	8 (11%)	6	25
61	M	129/136 (95%)	120 (93%)	9 (7%)	15	45
61	c1	129/136 (95%)	113 (88%)	16 (12%)	4	19
62	N	88/100 (88%)	73 (83%)	15 (17%)	2	9
62	c2	88/100 (88%)	73 (83%)	15 (17%)	2	9
63	O	127/127 (100%)	110 (87%)	17 (13%)	4	16
63	c3	127/127 (100%)	111 (87%)	16 (13%)	4	18
64	P	81/97 (84%)	70 (86%)	11 (14%)	3	16
64	c4	97/97 (100%)	85 (88%)	12 (12%)	4	19
65	Q	101/117 (86%)	92 (91%)	9 (9%)	9	34
65	c5	103/117 (88%)	91 (88%)	12 (12%)	5	22
66	R	117/118 (99%)	101 (86%)	16 (14%)	3	16
66	c6	118/118 (100%)	98 (83%)	20 (17%)	2	9
67	S	94/113 (83%)	80 (85%)	14 (15%)	3	13
67	c7	92/113 (81%)	81 (88%)	11 (12%)	5	20
68	T	128/128 (100%)	108 (84%)	20 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	c8	128/128 (100%)	109 (85%)	19 (15%)	3	13
69	U	115/115 (100%)	95 (83%)	20 (17%)	2	9
69	c9	115/115 (100%)	99 (86%)	16 (14%)	3	15
70	V	100/103 (97%)	86 (86%)	14 (14%)	3	15
70	d0	103/103 (100%)	90 (87%)	13 (13%)	4	18
71	W	74/74 (100%)	62 (84%)	12 (16%)	2	10
71	d1	74/74 (100%)	63 (85%)	11 (15%)	3	13
72	X	110/110 (100%)	95 (86%)	15 (14%)	3	16
72	d2	110/110 (100%)	103 (94%)	7 (6%)	17	48
73	Y	119/119 (100%)	102 (86%)	17 (14%)	3	14
73	d3	119/119 (100%)	104 (87%)	15 (13%)	4	18
74	Z	112/112 (100%)	101 (90%)	11 (10%)	8	29
74	d4	112/112 (100%)	105 (94%)	7 (6%)	18	48
75	a	61/61 (100%)	49 (80%)	12 (20%)	1	6
75	d5	61/61 (100%)	58 (95%)	3 (5%)	25	57
76	b	83/83 (100%)	76 (92%)	7 (8%)	11	38
76	d6	83/83 (100%)	71 (86%)	12 (14%)	3	13
77	c	70/70 (100%)	67 (96%)	3 (4%)	29	62
77	d7	70/70 (100%)	65 (93%)	5 (7%)	14	44
78	d	56/56 (100%)	48 (86%)	8 (14%)	3	14
78	d8	56/56 (100%)	47 (84%)	9 (16%)	2	10
79	d9	47/47 (100%)	43 (92%)	4 (8%)	10	37
79	e	47/47 (100%)	42 (89%)	5 (11%)	6	26
80	e0	53/53 (100%)	45 (85%)	8 (15%)	3	12
80	f	51/53 (96%)	47 (92%)	4 (8%)	12	40
81	g	62/62 (100%)	50 (81%)	12 (19%)	1	6
82	h	260/261 (100%)	243 (94%)	17 (6%)	17	47
82	sR	260/261 (100%)	242 (93%)	18 (7%)	15	45
83	e1	43/43 (100%)	35 (81%)	8 (19%)	1	7
All	All	18684/19337 (97%)	16334 (87%)	2350 (13%)	4	18

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

Mol	Chain	Res	Type
82	h	149	ASP
76	d6	46	GLU
51	s1	194	ASN
82	h	136	ILE
59	s9	145	SER

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

Mol	Chain	Res	Type
55	G	103	ASN
62	N	125	ASN
57	s7	71	HIS
59	K	110	GLN
67	S	105	GLN

### 5.3.3 RNA [i](#)

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	2260	U

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Mol	Chain	Res	Type
25	A	73	U
1	AR	2404	A
1	AR	3218	A
25	A	240	U

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	3634	-	0,6,6	-	-	-		
84	OHX	6	1968	-	0,6,6	-	-	-		
84	OHX	AR	3404	-	0,6,6	-	-	-		
84	OHX	AR	3559	-	0,6,6	-	-	-		
84	OHX	6	1972	-	0,6,6	-	-	-		
84	OHX	1	3575	-	0,6,6	-	-	-		
84	OHX	AR	3733	-	0,6,6	-	-	-		
84	OHX	1	3490	-	0,6,6	-	-	-		
84	OHX	AR	3571	-	0,6,6	-	-	-		
84	OHX	AR	3461	-	0,6,6	-	-	-		
84	OHX	AR	3504	-	0,6,6	-	-	-		
84	OHX	1	3522	-	0,6,6	-	-	-		
84	OHX	AR	3575	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1980	-	0,6,6	-	-	-		
84	OHX	M	201	-	0,6,6	-	-	-		
84	OHX	6	1985	-	0,6,6	-	-	-		
84	OHX	1	3658	-	0,6,6	-	-	-		
84	OHX	1	3711	-	0,6,6	-	-	-		
84	OHX	6	1963	-	0,6,6	-	-	-		
84	OHX	AR	3617	-	0,6,6	-	-	-		
84	OHX	1	3643	-	0,6,6	-	-	-		
84	OHX	A	2024	-	0,6,6	-	-	-		
84	OHX	1	3606	-	0,6,6	-	-	-		
84	OHX	AR	3532	-	0,6,6	-	-	-		
84	OHX	AR	3594	-	0,6,6	-	-	-		
84	OHX	1	3481	-	0,6,6	-	-	-		
84	OHX	6	2007	-	0,6,6	-	-	-		
84	OHX	AR	3655	-	0,6,6	-	-	-		
84	OHX	4	206	-	0,6,6	-	-	-		
84	OHX	1	3478	-	0,6,6	-	-	-		
84	OHX	1	3663	-	0,6,6	-	-	-		
84	OHX	AR	3709	-	0,6,6	-	-	-		
84	OHX	AR	3552	-	0,6,6	-	-	-		
84	OHX	1	3436	-	0,6,6	-	-	-		
84	OHX	1	3491	-	0,6,6	-	-	-		
84	OHX	1	3540	-	0,6,6	-	-	-		
84	OHX	1	3582	-	0,6,6	-	-	-		
84	OHX	AR	3707	-	0,6,6	-	-	-		
84	OHX	1	3448	-	0,6,6	-	-	-		
84	OHX	A	1964	-	0,6,6	-	-	-		
84	OHX	A	1966	-	0,6,6	-	-	-		
84	OHX	1	3589	-	0,6,6	-	-	-		
84	OHX	AR	3619	-	0,6,6	-	-	-		
84	OHX	AK	102	-	0,6,6	-	-	-		
84	OHX	1	3603	-	0,6,6	-	-	-		
84	OHX	6	1909	-	0,6,6	-	-	-		
84	OHX	AR	3588	-	0,6,6	-	-	-		
84	OHX	AR	3703	-	0,6,6	-	-	-		
84	OHX	AR	3411	-	0,6,6	-	-	-		
84	OHX	AR	3633	-	0,6,6	-	-	-		
84	OHX	1	3608	-	0,6,6	-	-	-		
84	OHX	AS	206	-	0,6,6	-	-	-		
84	OHX	1	3509	-	0,6,6	-	-	-		
84	OHX	AR	3663	-	0,6,6	-	-	-		
84	OHX	A	1908	-	0,6,6	-	-	-		
84	OHX	A	1990	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3579	-	0,6,6	-	-	-		
84	OHX	AR	3562	-	0,6,6	-	-	-		
84	OHX	A	2031	-	0,6,6	-	-	-		
84	OHX	3	206	-	0,6,6	-	-	-		
84	OHX	1	3460	-	0,6,6	-	-	-		
84	OHX	4	214	-	0,6,6	-	-	-		
84	OHX	AT	211	-	0,6,6	-	-	-		
84	OHX	1	3425	-	0,6,6	-	-	-		
84	OHX	4	202	-	0,6,6	-	-	-		
84	OHX	1	3679	-	0,6,6	-	-	-		
84	OHX	c8	201	-	0,6,6	-	-	-		
84	OHX	AS	209	-	0,6,6	-	-	-		
84	OHX	1	3713	-	0,6,6	-	-	-		
84	OHX	A	1904	-	0,6,6	-	-	-		
84	OHX	CG	302	-	0,6,6	-	-	-		
87	GOL	AR	4262	84	5,5,5	0.26	0	5,5,5	0.53	0
84	OHX	1	3494	-	0,6,6	-	-	-		
84	OHX	1	3417	-	0,6,6	-	-	-		
84	OHX	1	3431	-	0,6,6	-	-	-		
84	OHX	1	3457	-	0,6,6	-	-	-		
84	OHX	1	3653	-	0,6,6	-	-	-		
84	OHX	AR	3402	-	0,6,6	-	-	-		
84	OHX	AR	3452	-	0,6,6	-	-	-		
84	OHX	6	1903	-	0,6,6	-	-	-		
84	OHX	AR	3638	-	0,6,6	-	-	-		
84	OHX	6	1954	-	0,6,6	-	-	-		
86	HN8	AR	4263	-	24,26,26	0.29	0	36,41,41	1.60	4 (11%)
84	OHX	A	1939	-	0,6,6	-	-	-		
84	OHX	1	3480	-	0,6,6	-	-	-		
84	OHX	1	3691	-	0,6,6	-	-	-		
84	OHX	AR	3430	-	0,6,6	-	-	-		
84	OHX	1	3585	-	0,6,6	-	-	-		
84	OHX	1	3707	-	0,6,6	-	-	-		
84	OHX	A	2027	-	0,6,6	-	-	-		
84	OHX	AR	3673	-	0,6,6	-	-	-		
84	OHX	c4	201	-	0,6,6	-	-	-		
84	OHX	6	1970	-	0,6,6	-	-	-		
84	OHX	A	1956	-	0,6,6	-	-	-		
84	OHX	AR	3651	-	0,6,6	-	-	-		
84	OHX	2	201	-	0,6,6	-	-	-		
84	OHX	AT	217	-	0,6,6	-	-	-		
84	OHX	1	3581	-	0,6,6	-	-	-		
84	OHX	DH	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3435	-	0,6,6	-	-	-		
84	OHX	AR	3727	-	0,6,6	-	-	-		
84	OHX	6	1923	-	0,6,6	-	-	-		
84	OHX	T	201	-	0,6,6	-	-	-		
84	OHX	4	209	-	0,6,6	-	-	-		
84	OHX	6	1973	-	0,6,6	-	-	-		
84	OHX	1	3565	-	0,6,6	-	-	-		
84	OHX	A	1963	-	0,6,6	-	-	-		
84	OHX	1	3434	-	0,6,6	-	-	-		
84	OHX	1	3409	-	0,6,6	-	-	-		
84	OHX	6	1943	-	0,6,6	-	-	-		
84	OHX	AR	3565	-	0,6,6	-	-	-		
84	OHX	AR	3596	-	0,6,6	-	-	-		
84	OHX	1	3508	-	0,6,6	-	-	-		
84	OHX	J	301	-	0,6,6	-	-	-		
84	OHX	1	3571	-	0,6,6	-	-	-		
84	OHX	AR	3525	-	0,6,6	-	-	-		
84	OHX	6	1999	-	0,6,6	-	-	-		
84	OHX	AR	3453	-	0,6,6	-	-	-		
84	OHX	1	3418	-	0,6,6	-	-	-		
84	OHX	AR	3529	-	0,6,6	-	-	-		
84	OHX	1	3468	-	0,6,6	-	-	-		
84	OHX	1	3406	-	0,6,6	-	-	-		
84	OHX	1	3721	-	0,6,6	-	-	-		
84	OHX	AR	3449	-	0,6,6	-	-	-		
84	OHX	6	1925	-	0,6,6	-	-	-		
84	OHX	AR	3437	-	0,6,6	-	-	-		
84	OHX	AR	3699	-	0,6,6	-	-	-		
84	OHX	AS	203	-	0,6,6	-	-	-		
84	OHX	AR	3418	-	0,6,6	-	-	-		
84	OHX	DD	101	-	0,6,6	-	-	-		
84	OHX	A	1913	-	0,6,6	-	-	-		
84	OHX	1	3624	-	0,6,6	-	-	-		
84	OHX	6	1953	-	0,6,6	-	-	-		
84	OHX	CE	402	-	0,6,6	-	-	-		
84	OHX	A	1946	-	0,6,6	-	-	-		
84	OHX	AR	3590	-	0,6,6	-	-	-		
84	OHX	AR	3620	-	0,6,6	-	-	-		
84	OHX	6	2001	-	0,6,6	-	-	-		
84	OHX	3	209	-	0,6,6	-	-	-		
84	OHX	6	1910	-	0,6,6	-	-	-		
84	OHX	6	1978	-	0,6,6	-	-	-		
84	OHX	AR	3605	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	2050	-	0,6,6	-	-	-		
84	OHX	AR	3602	-	0,6,6	-	-	-		
84	OHX	6	2051	-	0,6,6	-	-	-		
84	OHX	AR	3424	-	0,6,6	-	-	-		
84	OHX	A	1910	-	0,6,6	-	-	-		
84	OHX	1	401	-	0,6,6	-	-	-		
84	OHX	1	3433	-	0,6,6	-	-	-		
84	OHX	6	2000	-	0,6,6	-	-	-		
84	OHX	6	2015	-	0,6,6	-	-	-		
84	OHX	6	2045	-	0,6,6	-	-	-		
84	OHX	AR	3422	-	0,6,6	-	-	-		
84	OHX	AR	3599	-	0,6,6	-	-	-		
84	OHX	AR	3647	-	0,6,6	-	-	-		
84	OHX	AR	3566	-	0,6,6	-	-	-		
84	OHX	1	3426	-	0,6,6	-	-	-		
84	OHX	1	3577	-	0,6,6	-	-	-		
84	OHX	6	1933	-	0,6,6	-	-	-		
84	OHX	A	1971	-	0,6,6	-	-	-		
84	OHX	6	1947	-	0,6,6	-	-	-		
84	OHX	AR	3446	-	0,6,6	-	-	-		
84	OHX	AR	3505	-	0,6,6	-	-	-		
84	OHX	1	3462	-	0,6,6	-	-	-		
84	OHX	AR	3710	-	0,6,6	-	-	-		
84	OHX	A	1933	-	0,6,6	-	-	-		
84	OHX	A	1924	-	0,6,6	-	-	-		
84	OHX	A	1937	-	0,6,6	-	-	-		
84	OHX	A	1947	-	0,6,6	-	-	-		
84	OHX	1	3401	-	0,6,6	-	-	-		
84	OHX	6	1992	-	0,6,6	-	-	-		
84	OHX	1	3583	-	0,6,6	-	-	-		
84	OHX	AR	3517	-	0,6,6	-	-	-		
84	OHX	AR	3522	-	0,6,6	-	-	-		
84	OHX	AR	3527	-	0,6,6	-	-	-		
84	OHX	AR	3641	-	0,6,6	-	-	-		
84	OHX	AT	206	-	0,6,6	-	-	-		
84	OHX	3	202	-	0,6,6	-	-	-		
84	OHX	AR	3686	-	0,6,6	-	-	-		
84	OHX	AR	3502	-	0,6,6	-	-	-		
84	OHX	AR	3650	-	0,6,6	-	-	-		
84	OHX	AR	3632	-	0,6,6	-	-	-		
84	OHX	AR	3661	-	0,6,6	-	-	-		
84	OHX	A	1950	-	0,6,6	-	-	-		
84	OHX	1	3500	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3553	-	0,6,6	-	-	-		
84	OHX	1	3674	-	0,6,6	-	-	-		
84	OHX	AR	3593	-	0,6,6	-	-	-		
84	OHX	AR	3513	-	0,6,6	-	-	-		
84	OHX	AR	3604	-	0,6,6	-	-	-		
84	OHX	1	3592	-	0,6,6	-	-	-		
84	OHX	1	3550	-	0,6,6	-	-	-		
84	OHX	1	3668	-	0,6,6	-	-	-		
84	OHX	1	3719	-	0,6,6	-	-	-		
84	OHX	AR	3503	-	0,6,6	-	-	-		
84	OHX	AS	207	-	0,6,6	-	-	-		
84	OHX	A	1928	-	0,6,6	-	-	-		
84	OHX	A	1944	-	0,6,6	-	-	-		
84	OHX	1	3619	-	0,6,6	-	-	-		
84	OHX	A	1961	-	0,6,6	-	-	-		
84	OHX	AR	3668	-	0,6,6	-	-	-		
84	OHX	6	1984	-	0,6,6	-	-	-		
84	OHX	6	1913	-	0,6,6	-	-	-		
84	OHX	AR	3492	-	0,6,6	-	-	-		
84	OHX	A	1994	-	0,6,6	-	-	-		
84	OHX	6	1915	-	0,6,6	-	-	-		
84	OHX	1	3718	-	0,6,6	-	-	-		
84	OHX	1	3483	-	0,6,6	-	-	-		
84	OHX	AR	3498	-	0,6,6	-	-	-		
84	OHX	6	2003	-	0,6,6	-	-	-		
84	OHX	AR	3718	-	0,6,6	-	-	-		
84	OHX	AR	3499	-	0,6,6	-	-	-		
84	OHX	A	2020	-	0,6,6	-	-	-		
84	OHX	1	3456	-	0,6,6	-	-	-		
84	OHX	1	3524	-	0,6,6	-	-	-		
84	OHX	1	3420	-	0,6,6	-	-	-		
84	OHX	AR	3613	-	0,6,6	-	-	-		
84	OHX	A	1920	-	0,6,6	-	-	-		
84	OHX	A	1917	-	0,6,6	-	-	-		
84	OHX	sR	401	-	0,6,6	-	-	-		
84	OHX	1	3618	-	0,6,6	-	-	-		
84	OHX	1	3664	-	0,6,6	-	-	-		
84	OHX	6	1950	-	0,6,6	-	-	-		
84	OHX	A	2010	-	0,6,6	-	-	-		
84	OHX	AR	3682	-	0,6,6	-	-	-		
84	OHX	4	208	-	0,6,6	-	-	-		
84	OHX	1	3623	-	0,6,6	-	-	-		
84	OHX	1	3645	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3419	-	0,6,6	-	-	-		
84	OHX	1	3681	-	0,6,6	-	-	-		
84	OHX	AR	3556	-	0,6,6	-	-	-		
84	OHX	1	3534	-	0,6,6	-	-	-		
84	OHX	A	2001	-	0,6,6	-	-	-		
84	OHX	AR	3468	-	0,6,6	-	-	-		
84	OHX	1	3467	-	0,6,6	-	-	-		
84	OHX	1	3428	-	0,6,6	-	-	-		
84	OHX	6	1952	-	0,6,6	-	-	-		
84	OHX	A	2011	-	0,6,6	-	-	-		
84	OHX	A	2017	-	0,6,6	-	-	-		
84	OHX	AR	3546	-	0,6,6	-	-	-		
84	OHX	AR	3685	-	0,6,6	-	-	-		
84	OHX	6	2009	-	0,6,6	-	-	-		
84	OHX	4	213	-	0,6,6	-	-	-		
84	OHX	1	3445	-	0,6,6	-	-	-		
84	OHX	1	3516	-	0,6,6	-	-	-		
84	OHX	1	3622	-	0,6,6	-	-	-		
84	OHX	1	3715	-	0,6,6	-	-	-		
84	OHX	AR	3476	-	0,6,6	-	-	-		
84	OHX	CP	501	-	0,6,6	-	-	-		
87	GOL	A	2160	-	5,5,5	0.10	0	5,5,5	0.29	0
84	OHX	1	3512	-	0,6,6	-	-	-		
84	OHX	6	1934	-	0,6,6	-	-	-		
84	OHX	6	2027	-	0,6,6	-	-	-		
84	OHX	AR	3482	-	0,6,6	-	-	-		
84	OHX	6	1982	-	0,6,6	-	-	-		
84	OHX	1	3528	-	0,6,6	-	-	-		
84	OHX	1	3407	-	0,6,6	-	-	-		
84	OHX	1	3677	-	0,6,6	-	-	-		
84	OHX	A	1903	-	0,6,6	-	-	-		
84	OHX	1	3438	-	0,6,6	-	-	-		
84	OHX	A	1934	-	0,6,6	-	-	-		
84	OHX	A	1975	-	0,6,6	-	-	-		
84	OHX	A	1982	-	0,6,6	-	-	-		
84	OHX	AR	3676	-	0,6,6	-	-	-		
84	OHX	AR	3691	-	0,6,6	-	-	-		
84	OHX	1	3576	-	0,6,6	-	-	-		
84	OHX	6	2006	-	0,6,6	-	-	-		
84	OHX	AR	3537	-	0,6,6	-	-	-		
84	OHX	AR	3569	-	0,6,6	-	-	-		
84	OHX	A	1989	-	0,6,6	-	-	-		
84	OHX	A	2035	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3669	-	0,6,6	-	-	-		
84	OHX	O	201	-	0,6,6	-	-	-		
84	OHX	A	1936	-	0,6,6	-	-	-		
84	OHX	AR	3555	-	0,6,6	-	-	-		
84	OHX	AR	3669	-	0,6,6	-	-	-		
84	OHX	1	3473	-	0,6,6	-	-	-		
84	OHX	1	3432	-	0,6,6	-	-	-		
84	OHX	1	3458	-	0,6,6	-	-	-		
84	OHX	A	1970	-	0,6,6	-	-	-		
84	OHX	6	1997	-	0,6,6	-	-	-		
84	OHX	6	1906	-	0,6,6	-	-	-		
84	OHX	AR	3645	-	0,6,6	-	-	-		
84	OHX	AR	3741	-	0,6,6	-	-	-		
84	OHX	6	2025	-	0,6,6	-	-	-		
84	OHX	AR	3432	-	0,6,6	-	-	-		
84	OHX	6	2039	-	0,6,6	-	-	-		
84	OHX	AR	3470	-	0,6,6	-	-	-		
84	OHX	AR	3631	-	0,6,6	-	-	-		
84	OHX	A	1905	-	0,6,6	-	-	-		
84	OHX	AR	3610	-	0,6,6	-	-	-		
84	OHX	AT	214	-	0,6,6	-	-	-		
84	OHX	y	201	-	0,6,6	-	-	-		
84	OHX	A	1959	-	0,6,6	-	-	-		
84	OHX	1	3444	-	0,6,6	-	-	-		
84	OHX	6	1941	-	0,6,6	-	-	-		
87	GOL	v	305	-	5,5,5	0.18	0	5,5,5	0.54	0
84	OHX	1	3574	-	0,6,6	-	-	-		
84	OHX	A	1941	-	0,6,6	-	-	-		
84	OHX	1	3637	-	0,6,6	-	-	-		
84	OHX	1	3716	-	0,6,6	-	-	-		
84	OHX	6	2016	-	0,6,6	-	-	-		
84	OHX	CX	202	-	0,6,6	-	-	-		
84	OHX	AR	3729	-	0,6,6	-	-	-		
84	OHX	AR	3511	-	0,6,6	-	-	-		
84	OHX	AR	3637	-	0,6,6	-	-	-		
84	OHX	1	3697	84	0,6,6	-	-	-		
84	OHX	6	1917	-	0,6,6	-	-	-		
84	OHX	1	3461	-	0,6,6	-	-	-		
84	OHX	1	3505	-	0,6,6	-	-	-		
84	OHX	AR	3728	-	0,6,6	-	-	-		
84	OHX	A	1901	-	0,6,6	-	-	-		
84	OHX	AR	3665	-	0,6,6	-	-	-		
84	OHX	AR	3702	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3626	-	0,6,6	-	-	-		
84	OHX	1	3465	-	0,6,6	-	-	-		
84	OHX	6	2011	-	0,6,6	-	-	-		
84	OHX	AR	3621	-	0,6,6	-	-	-		
84	OHX	AR	3598	-	0,6,6	-	-	-		
84	OHX	AR	3584	-	0,6,6	-	-	-		
84	OHX	1	3654	-	0,6,6	-	-	-		
84	OHX	1	3698	-	0,6,6	-	-	-		
84	OHX	AR	3704	-	0,6,6	-	-	-		
84	OHX	AR	3472	-	0,6,6	-	-	-		
84	OHX	1	3662	-	0,6,6	-	-	-		
84	OHX	1	3471	-	0,6,6	-	-	-		
84	OHX	A	1988	-	0,6,6	-	-	-		
84	OHX	1	3705	-	0,6,6	-	-	-		
84	OHX	AR	3713	-	0,6,6	-	-	-		
84	OHX	AR	3413	-	0,6,6	-	-	-		
84	OHX	AR	3744	-	0,6,6	-	-	-		
84	OHX	1	3466	-	0,6,6	-	-	-		
84	OHX	AR	3442	-	0,6,6	-	-	-		
84	OHX	1	3586	-	0,6,6	-	-	-		
84	OHX	AR	3587	-	0,6,6	-	-	-		
84	OHX	AR	3722	-	0,6,6	-	-	-		
84	OHX	AR	3410	-	0,6,6	-	-	-		
84	OHX	1	3495	-	0,6,6	-	-	-		
84	OHX	1	3525	-	0,6,6	-	-	-		
84	OHX	1	3594	-	0,6,6	-	-	-		
84	OHX	6	2038	-	0,6,6	-	-	-		
84	OHX	AR	3586	-	0,6,6	-	-	-		
84	OHX	1	3640	-	0,6,6	-	-	-		
84	OHX	AR	3495	-	0,6,6	-	-	-		
84	OHX	1	3513	-	0,6,6	-	-	-		
84	OHX	1	3703	-	0,6,6	-	-	-		
84	OHX	6	1929	-	0,6,6	-	-	-		
84	OHX	1	3625	-	0,6,6	-	-	-		
84	OHX	z	201	-	0,6,6	-	-	-		
84	OHX	6	1931	-	0,6,6	-	-	-		
84	OHX	1	3558	-	0,6,6	-	-	-		
84	OHX	A	1921	-	0,6,6	-	-	-		
84	OHX	6	1939	-	0,6,6	-	-	-		
84	OHX	6	2052	-	0,6,6	-	-	-		
84	OHX	c1	201	-	0,6,6	-	-	-		
84	OHX	6	1977	-	0,6,6	-	-	-		
84	OHX	1	3612	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1919	-	0,6,6	-	-	-		
84	OHX	1	3514	-	0,6,6	-	-	-		
84	OHX	A	1909	-	0,6,6	-	-	-		
84	OHX	1	3633	-	0,6,6	-	-	-		
84	OHX	A	1958	-	0,6,6	-	-	-		
84	OHX	AR	3732	-	0,6,6	-	-	-		
84	OHX	1	3652	-	0,6,6	-	-	-		
84	OHX	1	3523	-	0,6,6	-	-	-		
84	OHX	AR	3460	-	0,6,6	-	-	-		
84	OHX	1	3530	-	0,6,6	-	-	-		
84	OHX	AR	3415	-	0,6,6	-	-	-		
84	OHX	A	1915	-	0,6,6	-	-	-		
84	OHX	c3	201	-	0,6,6	-	-	-		
84	OHX	1	3424	-	0,6,6	-	-	-		
84	OHX	A	1974	-	0,6,6	-	-	-		
84	OHX	1	3591	-	0,6,6	-	-	-		
84	OHX	A	1949	-	0,6,6	-	-	-		
84	OHX	e	101	-	0,6,6	-	-	-		
84	OHX	1	3568	-	0,6,6	-	-	-		
84	OHX	6	1995	-	0,6,6	-	-	-		
84	OHX	3	201	-	0,6,6	-	-	-		
84	OHX	6	2040	-	0,6,6	-	-	-		
84	OHX	1	3717	-	0,6,6	-	-	-		
84	OHX	AR	3521	-	0,6,6	-	-	-		
84	OHX	AM	101	-	0,6,6	-	-	-		
84	OHX	6	1964	-	0,6,6	-	-	-		
84	OHX	AR	3723	-	0,6,6	-	-	-		
84	OHX	1	3411	-	0,6,6	-	-	-		
84	OHX	1	3539	84	0,6,6	-	-	-		
84	OHX	1	3529	-	0,6,6	-	-	-		
84	OHX	AR	3451	-	0,6,6	-	-	-		
84	OHX	A	1930	-	0,6,6	-	-	-		
84	OHX	AR	3683	-	0,6,6	-	-	-		
84	OHX	1	3656	-	0,6,6	-	-	-		
84	OHX	AR	3658	-	0,6,6	-	-	-		
84	OHX	AR	3603	-	0,6,6	-	-	-		
84	OHX	AT	210	-	0,6,6	-	-	-		
84	OHX	CV	201	-	0,6,6	-	-	-		
84	OHX	AR	3608	-	0,6,6	-	-	-		
84	OHX	1	3676	-	0,6,6	-	-	-		
84	OHX	AR	3577	-	0,6,6	-	-	-		
84	OHX	1	3632	-	0,6,6	-	-	-		
84	OHX	AR	3739	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	2040	-	0,6,6	-	-	-		
84	OHX	1	3651	-	0,6,6	-	-	-		
84	OHX	AR	3481	-	0,6,6	-	-	-		
84	OHX	AR	3536	-	0,6,6	-	-	-		
84	OHX	CF	401	-	0,6,6	-	-	-		
84	OHX	AR	3440	-	0,6,6	-	-	-		
84	OHX	1	3590	-	0,6,6	-	-	-		
84	OHX	1	3588	-	0,6,6	-	-	-		
84	OHX	A	2007	-	0,6,6	-	-	-		
84	OHX	1	3616	-	0,6,6	-	-	-		
84	OHX	AR	3646	-	0,6,6	-	-	-		
84	OHX	6	1921	-	0,6,6	-	-	-		
84	OHX	AR	3609	-	0,6,6	-	-	-		
84	OHX	A	2006	-	0,6,6	-	-	-		
84	OHX	AR	3573	-	0,6,6	-	-	-		
84	OHX	1	3596	-	0,6,6	-	-	-		
84	OHX	AR	3582	-	0,6,6	-	-	-		
84	OHX	AR	3475	-	0,6,6	-	-	-		
84	OHX	AR	3740	-	0,6,6	-	-	-		
84	OHX	AR	3447	-	0,6,6	-	-	-		
84	OHX	1	3402	-	0,6,6	-	-	-		
84	OHX	1	3430	-	0,6,6	-	-	-		
84	OHX	6	2034	-	0,6,6	-	-	-		
84	OHX	6	1958	-	0,6,6	-	-	-		
84	OHX	AR	3518	-	0,6,6	-	-	-		
84	OHX	1	3694	-	0,6,6	-	-	-		
84	OHX	1	3695	-	0,6,6	-	-	-		
84	OHX	1	3687	-	0,6,6	-	-	-		
84	OHX	AR	3431	-	0,6,6	-	-	-		
84	OHX	AR	3457	-	0,6,6	-	-	-		
84	OHX	A	2009	-	0,6,6	-	-	-		
84	OHX	A	2039	-	0,6,6	-	-	-		
84	OHX	c5	201	-	0,6,6	-	-	-		
84	OHX	4	203	-	0,6,6	-	-	-		
84	OHX	AH	201	-	0,6,6	-	-	-		
84	OHX	AR	3693	-	0,6,6	-	-	-		
84	OHX	1	3684	-	0,6,6	-	-	-		
84	OHX	3	205	-	0,6,6	-	-	-		
84	OHX	x	201	-	0,6,6	-	-	-		
84	OHX	6	2037	-	0,6,6	-	-	-		
84	OHX	6	1949	-	0,6,6	-	-	-		
84	OHX	AR	3684	-	0,6,6	-	-	-		
84	OHX	1	3720	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3602	-	0,6,6	-	-	-		
84	OHX	1	3666	-	0,6,6	-	-	-		
84	OHX	AR	3601	-	0,6,6	-	-	-		
84	OHX	AR	3642	-	0,6,6	-	-	-		
84	OHX	1	3446	-	0,6,6	-	-	-		
84	OHX	AR	3720	-	0,6,6	-	-	-		
84	OHX	6	2035	-	0,6,6	-	-	-		
84	OHX	x	202	-	0,6,6	-	-	-		
84	OHX	AR	3570	-	0,6,6	-	-	-		
84	OHX	1	3517	-	0,6,6	-	-	-		
84	OHX	6	1960	-	0,6,6	-	-	-		
84	OHX	1	3673	-	0,6,6	-	-	-		
84	OHX	6	1930	-	0,6,6	-	-	-		
84	OHX	1	3630	-	0,6,6	-	-	-		
84	OHX	1	3502	-	0,6,6	-	-	-		
84	OHX	1	3672	-	0,6,6	-	-	-		
84	OHX	A	1960	-	0,6,6	-	-	-		
84	OHX	1	3492	-	0,6,6	-	-	-		
84	OHX	AR	3508	-	0,6,6	-	-	-		
84	OHX	CL	301	-	0,6,6	-	-	-		
84	OHX	1	3476	-	0,6,6	-	-	-		
84	OHX	AR	3560	-	0,6,6	-	-	-		
84	OHX	4	215	-	0,6,6	-	-	-		
84	OHX	1	3688	-	0,6,6	-	-	-		
84	OHX	1	3593	-	0,6,6	-	-	-		
84	OHX	A	2030	-	0,6,6	-	-	-		
84	OHX	AR	3464	-	0,6,6	-	-	-		
84	OHX	AR	3656	-	0,6,6	-	-	-		
84	OHX	6	1981	-	0,6,6	-	-	-		
84	OHX	AR	3423	-	0,6,6	-	-	-		
84	OHX	AR	3671	-	0,6,6	-	-	-		
84	OHX	AR	3688	-	0,6,6	-	-	-		
84	OHX	A	1998	-	0,6,6	-	-	-		
84	OHX	AR	3533	-	0,6,6	-	-	-		
84	OHX	1	3563	-	0,6,6	-	-	-		
84	OHX	A	1943	-	0,6,6	-	-	-		
84	OHX	A	1981	-	0,6,6	-	-	-		
84	OHX	6	2043	-	0,6,6	-	-	-		
84	OHX	1	3569	-	0,6,6	-	-	-		
84	OHX	A	1979	-	0,6,6	-	-	-		
84	OHX	6	2019	-	0,6,6	-	-	-		
84	OHX	AR	3547	-	0,6,6	-	-	-		
84	OHX	6	1912	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	2017	-	0,6,6	-	-	-		
84	OHX	A	2041	-	0,6,6	-	-	-		
84	OHX	AS	205	-	0,6,6	-	-	-		
84	OHX	1	3647	-	0,6,6	-	-	-		
84	OHX	6	2005	-	0,6,6	-	-	-		
84	OHX	AR	3543	-	0,6,6	-	-	-		
84	OHX	AR	3725	-	0,6,6	-	-	-		
84	OHX	A	1999	-	0,6,6	-	-	-		
84	OHX	1	3678	-	0,6,6	-	-	-		
84	OHX	AT	202	-	0,6,6	-	-	-		
84	OHX	AR	3561	-	0,6,6	-	-	-		
84	OHX	1	3648	-	0,6,6	-	-	-		
84	OHX	AS	201	-	0,6,6	-	-	-		
84	OHX	6	1971	-	0,6,6	-	-	-		
84	OHX	1	3690	-	0,6,6	-	-	-		
84	OHX	4	211	-	0,6,6	-	-	-		
84	OHX	A	1923	-	0,6,6	-	-	-		
84	OHX	6	2044	-	0,6,6	-	-	-		
84	OHX	1	3551	-	0,6,6	-	-	-		
84	OHX	A	2003	-	0,6,6	-	-	-		
84	OHX	1	3403	-	0,6,6	-	-	-		
84	OHX	1	3661	-	0,6,6	-	-	-		
84	OHX	AR	3489	87	0,6,6	-	-	-		
84	OHX	1	3510	-	0,6,6	-	-	-		
84	OHX	1	3459	-	0,6,6	-	-	-		
84	OHX	AR	3462	-	0,6,6	-	-	-		
84	OHX	1	3599	-	0,6,6	-	-	-		
84	OHX	AR	3541	-	0,6,6	-	-	-		
84	OHX	AR	3401	-	0,6,6	-	-	-		
84	OHX	A	1940	-	0,6,6	-	-	-		
84	OHX	6	1976	-	0,6,6	-	-	-		
84	OHX	AR	3497	-	0,6,6	-	-	-		
84	OHX	1	3709	-	0,6,6	-	-	-		
84	OHX	6	1920	-	0,6,6	-	-	-		
84	OHX	AR	3549	-	0,6,6	-	-	-		
84	OHX	AR	3743	-	0,6,6	-	-	-		
84	OHX	A	2000	-	0,6,6	-	-	-		
84	OHX	6	1924	-	0,6,6	-	-	-		
84	OHX	A	1911	-	0,6,6	-	-	-		
84	OHX	1	3655	-	0,6,6	-	-	-		
84	OHX	1	3470	-	0,6,6	-	-	-		
84	OHX	6	1987	-	0,6,6	-	-	-		
84	OHX	1	3405	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3674	-	0,6,6	-	-	-		
84	OHX	6	2028	-	0,6,6	-	-	-		
84	OHX	AR	3675	-	0,6,6	-	-	-		
84	OHX	AT	204	-	0,6,6	-	-	-		
84	OHX	1	3421	-	0,6,6	-	-	-		
84	OHX	1	3600	-	0,6,6	-	-	-		
84	OHX	6	2042	-	0,6,6	-	-	-		
84	OHX	AR	3738	-	0,6,6	-	-	-		
84	OHX	1	3427	-	0,6,6	-	-	-		
84	OHX	AR	3568	-	0,6,6	-	-	-		
84	OHX	A	1968	-	0,6,6	-	-	-		
84	OHX	A	1987	-	0,6,6	-	-	-		
84	OHX	A	1995	-	0,6,6	-	-	-		
84	OHX	6	2018	-	0,6,6	-	-	-		
84	OHX	A	1977	-	0,6,6	-	-	-		
84	OHX	A	1986	-	0,6,6	-	-	-		
84	OHX	6	2002	-	0,6,6	-	-	-		
84	OHX	AR	3450	-	0,6,6	-	-	-		
84	OHX	AR	3698	-	0,6,6	-	-	-		
84	OHX	AR	3659	-	0,6,6	-	-	-		
84	OHX	AR	3485	-	0,6,6	-	-	-		
84	OHX	CG	301	-	0,6,6	-	-	-		
84	OHX	A	2002	-	0,6,6	-	-	-		
84	OHX	1	3706	-	0,6,6	-	-	-		
84	OHX	1	3504	-	0,6,6	-	-	-		
84	OHX	6	2036	-	0,6,6	-	-	-		
84	OHX	1	3479	-	0,6,6	-	-	-		
84	OHX	1	3627	-	0,6,6	-	-	-		
84	OHX	AR	3615	-	0,6,6	-	-	-		
84	OHX	6	1919	-	0,6,6	-	-	-		
84	OHX	6	2041	-	0,6,6	-	-	-		
84	OHX	6	1940	-	0,6,6	-	-	-		
84	OHX	AR	3706	-	0,6,6	-	-	-		
84	OHX	AR	3524	-	0,6,6	-	-	-		
84	OHX	A	2028	-	0,6,6	-	-	-		
84	OHX	AR	3479	-	0,6,6	-	-	-		
84	OHX	1	3689	-	0,6,6	-	-	-		
84	OHX	6	1918	-	0,6,6	-	-	-		
84	OHX	AR	3426	-	0,6,6	-	-	-		
84	OHX	AR	3700	-	0,6,6	-	-	-		
84	OHX	1	3561	-	0,6,6	-	-	-		
84	OHX	A	1925	-	0,6,6	-	-	-		
84	OHX	AS	210	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3519	-	0,6,6	-	-	-		
84	OHX	AR	3614	-	0,6,6	-	-	-		
84	OHX	1	3631	-	0,6,6	-	-	-		
84	OHX	6	2026	-	0,6,6	-	-	-		
84	OHX	A	1916	-	0,6,6	-	-	-		
84	OHX	A	1984	-	0,6,6	-	-	-		
84	OHX	AR	3648	-	0,6,6	-	-	-		
84	OHX	1	3644	-	0,6,6	-	-	-		
84	OHX	AR	3712	-	0,6,6	-	-	-		
84	OHX	1	3626	-	0,6,6	-	-	-		
84	OHX	AR	3516	-	0,6,6	-	-	-		
84	OHX	A	1932	-	0,6,6	-	-	-		
84	OHX	1	3443	-	0,6,6	-	-	-		
84	OHX	A	2034	-	0,6,6	-	-	-		
84	OHX	AR	3412	-	0,6,6	-	-	-		
86	HN8	1	4223	-	24,26,26	0.28	0	36,41,41	1.03	2 (5%)
84	OHX	6	1967	-	0,6,6	-	-	-		
84	OHX	6	1975	-	0,6,6	-	-	-		
84	OHX	AR	3443	-	0,6,6	-	-	-		
84	OHX	AR	3528	-	0,6,6	-	-	-		
84	OHX	1	3685	-	0,6,6	-	-	-		
84	OHX	1	3549	-	0,6,6	-	-	-		
84	OHX	AR	3578	-	0,6,6	-	-	-		
84	OHX	A	1935	-	0,6,6	-	-	-		
84	OHX	AR	3708	-	0,6,6	-	-	-		
84	OHX	6	2014	-	0,6,6	-	-	-		
84	OHX	AG	201	-	0,6,6	-	-	-		
84	OHX	1	3469	-	0,6,6	-	-	-		
84	OHX	6	1911	-	0,6,6	-	-	-		
84	OHX	6	1938	-	0,6,6	-	-	-		
84	OHX	AR	3480	-	0,6,6	-	-	-		
84	OHX	AR	3717	-	0,6,6	-	-	-		
84	OHX	AR	3745	-	0,6,6	-	-	-		
84	OHX	6	2031	-	0,6,6	-	-	-		
84	OHX	AR	3428	-	0,6,6	-	-	-		
84	OHX	AR	3467	-	0,6,6	-	-	-		
84	OHX	AR	3473	-	0,6,6	-	-	-		
84	OHX	AR	3662	-	0,6,6	-	-	-		
84	OHX	A	1992	-	0,6,6	-	-	-		
84	OHX	A	2004	-	0,6,6	-	-	-		
84	OHX	AR	3496	-	0,6,6	-	-	-		
84	OHX	AR	3660	-	0,6,6	-	-	-		
84	OHX	1	3537	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3416	-	0,6,6	-	-	-	-	-
84	OHX	6	1994	-	0,6,6	-	-	-	-	-
84	OHX	6	1986	-	0,6,6	-	-	-	-	-
84	OHX	1	3507	-	0,6,6	-	-	-	-	-
84	OHX	AR	3507	-	0,6,6	-	-	-	-	-
84	OHX	AR	3445	-	0,6,6	-	-	-	-	-
84	OHX	AR	3622	-	0,6,6	-	-	-	-	-
84	OHX	AR	3491	-	0,6,6	-	-	-	-	-
84	OHX	1	3422	-	0,6,6	-	-	-	-	-
84	OHX	1	3701	-	0,6,6	-	-	-	-	-
84	OHX	6	1991	-	0,6,6	-	-	-	-	-
84	OHX	AR	3493	-	0,6,6	-	-	-	-	-
84	OHX	1	3613	-	0,6,6	-	-	-	-	-
84	OHX	AP	502	-	0,6,6	-	-	-	-	-
84	OHX	r	301	-	0,6,6	-	-	-	-	-
84	OHX	1	3410	-	0,6,6	-	-	-	-	-
84	OHX	1	3562	-	0,6,6	-	-	-	-	-
84	OHX	AR	3465	-	0,6,6	-	-	-	-	-
84	OHX	6	2032	-	0,6,6	-	-	-	-	-
84	OHX	A	1991	-	0,6,6	-	-	-	-	-
84	OHX	A	1997	-	0,6,6	-	-	-	-	-
84	OHX	AR	3454	-	0,6,6	-	-	-	-	-
84	OHX	AR	3629	-	0,6,6	-	-	-	-	-
84	OHX	6	2021	-	0,6,6	-	-	-	-	-
84	OHX	1	3614	-	0,6,6	-	-	-	-	-
84	OHX	AR	3427	-	0,6,6	-	-	-	-	-
84	OHX	AR	3420	-	0,6,6	-	-	-	-	-
84	OHX	A	2008	-	0,6,6	-	-	-	-	-
84	OHX	1	3548	-	0,6,6	-	-	-	-	-
84	OHX	6	1926	-	0,6,6	-	-	-	-	-
84	OHX	1	3696	-	0,6,6	-	-	-	-	-
84	OHX	A	2016	-	0,6,6	-	-	-	-	-
84	OHX	1	3657	-	0,6,6	-	-	-	-	-
84	OHX	A	2043	-	0,6,6	-	-	-	-	-
84	OHX	1	3559	-	0,6,6	-	-	-	-	-
84	OHX	3	203	-	0,6,6	-	-	-	-	-
84	OHX	6	2012	-	0,6,6	-	-	-	-	-
84	OHX	1	3472	-	0,6,6	-	-	-	-	-
84	OHX	6	2048	-	0,6,6	-	-	-	-	-
84	OHX	1	3499	-	0,6,6	-	-	-	-	-
84	OHX	1	3497	-	0,6,6	-	-	-	-	-
84	OHX	1	3451	-	0,6,6	-	-	-	-	-
84	OHX	4	212	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3667	-	0,6,6	-	-	-		
84	OHX	6	1998	-	0,6,6	-	-	-		
84	OHX	6	1980	-	0,6,6	-	-	-		
84	OHX	1	3710	-	0,6,6	-	-	-		
84	OHX	AR	3471	-	0,6,6	-	-	-		
84	OHX	AR	3444	-	0,6,6	-	-	-		
84	OHX	AR	3439	-	0,6,6	-	-	-		
84	OHX	6	1932	-	0,6,6	-	-	-		
84	OHX	A	1922	-	0,6,6	-	-	-		
84	OHX	1	3503	-	0,6,6	-	-	-		
84	OHX	1	3486	-	0,6,6	-	-	-		
84	OHX	1	3686	-	0,6,6	-	-	-		
84	OHX	A	1965	-	0,6,6	-	-	-		
84	OHX	AR	3526	-	0,6,6	-	-	-		
84	OHX	A	1948	-	0,6,6	-	-	-		
84	OHX	1	3723	1	0,6,6	-	-	-		
84	OHX	AR	3429	-	0,6,6	-	-	-		
84	OHX	AR	3531	-	0,6,6	-	-	-		
84	OHX	AR	3670	-	0,6,6	-	-	-		
84	OHX	1	3453	-	0,6,6	-	-	-		
84	OHX	A	1914	-	0,6,6	-	-	-		
84	OHX	AR	3607	-	0,6,6	-	-	-		
84	OHX	AT	207	-	0,6,6	-	-	-		
84	OHX	1	3567	-	0,6,6	-	-	-		
84	OHX	1	3617	-	0,6,6	-	-	-		
84	OHX	1	3649	-	0,6,6	-	-	-		
84	OHX	6	1946	-	0,6,6	-	-	-		
84	OHX	AR	3640	-	0,6,6	-	-	-		
84	OHX	AR	3459	-	0,6,6	-	-	-		
84	OHX	1	3413	-	0,6,6	-	-	-		
84	OHX	AR	3490	-	0,6,6	-	-	-		
84	OHX	A	1954	-	0,6,6	-	-	-		
84	OHX	1	3692	-	0,6,6	-	-	-		
84	OHX	AR	3635	-	0,6,6	-	-	-		
84	OHX	4	204	-	0,6,6	-	-	-		
84	OHX	A	2014	-	0,6,6	-	-	-		
84	OHX	1	3506	-	0,6,6	-	-	-		
84	OHX	AR	3520	-	0,6,6	-	-	-		
84	OHX	AR	3544	-	0,6,6	-	-	-		
84	OHX	AR	3636	-	0,6,6	-	-	-		
84	OHX	AR	3680	-	0,6,6	-	-	-		
84	OHX	6	2029	-	0,6,6	-	-	-		
84	OHX	6	1916	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3506	-	0,6,6	-	-	-		
84	OHX	A	1902	-	0,6,6	-	-	-		
84	OHX	AT	203	-	0,6,6	-	-	-		
84	OHX	v	301	-	0,6,6	-	-	-		
84	OHX	6	1908	-	0,6,6	-	-	-		
84	OHX	6	1996	-	0,6,6	-	-	-		
84	OHX	AR	3477	84	0,6,6	-	-	-		
84	OHX	AR	3731	-	0,6,6	-	-	-		
84	OHX	A	2025	-	0,6,6	-	-	-		
84	OHX	1	3620	-	0,6,6	-	-	-		
84	OHX	1	3639	-	0,6,6	-	-	-		
84	OHX	1	3560	-	0,6,6	-	-	-		
84	OHX	1	3724	-	0,6,6	-	-	-		
84	OHX	AR	3478	-	0,6,6	-	-	-		
84	OHX	AR	3583	-	0,6,6	-	-	-		
84	OHX	AR	3523	-	0,6,6	-	-	-		
84	OHX	1	3667	-	0,6,6	-	-	-		
84	OHX	AR	3530	-	0,6,6	-	-	-		
84	OHX	1	3621	-	0,6,6	-	-	-		
84	OHX	6	2008	-	0,6,6	-	-	-		
84	OHX	3	204	-	0,6,6	-	-	-		
84	OHX	AR	3724	-	0,6,6	-	-	-		
84	OHX	1	3554	-	0,6,6	-	-	-		
84	OHX	AR	3483	-	0,6,6	-	-	-		
84	OHX	1	3488	-	0,6,6	-	-	-		
84	OHX	AR	3554	-	0,6,6	-	-	-		
84	OHX	1	3556	-	0,6,6	-	-	-		
84	OHX	1	3597	-	0,6,6	-	-	-		
84	OHX	1	3570	-	0,6,6	-	-	-		
84	OHX	1	3642	-	0,6,6	-	-	-		
84	OHX	AR	3597	-	0,6,6	-	-	-		
84	OHX	1	3531	-	0,6,6	-	-	-		
84	OHX	AR	3666	-	0,6,6	-	-	-		
84	OHX	A	1978	-	0,6,6	-	-	-		
84	OHX	AR	3711	-	0,6,6	-	-	-		
84	OHX	K	201	-	0,6,6	-	-	-		
84	OHX	1	3693	-	0,6,6	-	-	-		
84	OHX	AR	3486	-	0,6,6	-	-	-		
84	OHX	AR	3501	-	0,6,6	-	-	-		
84	OHX	A	1931	-	0,6,6	-	-	-		
84	OHX	AR	3595	-	0,6,6	-	-	-		
84	OHX	AR	3652	-	0,6,6	-	-	-		
84	OHX	AR	3545	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	1966	-	0,6,6	-	-	-		
84	OHX	1	3487	-	0,6,6	-	-	-		
84	OHX	1	3498	-	0,6,6	-	-	-		
84	OHX	1	3553	-	0,6,6	-	-	-		
84	OHX	AR	3591	-	0,6,6	-	-	-		
84	OHX	Q	201	-	0,6,6	-	-	-		
84	OHX	AR	3417	-	0,6,6	-	-	-		
84	OHX	1	3475	-	0,6,6	-	-	-		
84	OHX	AR	3487	-	0,6,6	-	-	-		
84	OHX	AR	3515	-	0,6,6	-	-	-		
84	OHX	1	3532	-	0,6,6	-	-	-		
84	OHX	1	3675	-	0,6,6	-	-	-		
84	OHX	AR	3677	-	0,6,6	-	-	-		
84	OHX	AR	3474	-	0,6,6	-	-	-		
84	OHX	6	1902	-	0,6,6	-	-	-		
84	OHX	6	2049	-	0,6,6	-	-	-		
84	OHX	1	3604	-	0,6,6	-	-	-		
84	OHX	AR	3576	-	0,6,6	-	-	-		
84	OHX	6	1969	-	0,6,6	-	-	-		
84	OHX	1	3699	-	0,6,6	-	-	-		
84	OHX	1	3598	-	0,6,6	-	-	-		
84	OHX	AT	213	-	0,6,6	-	-	-		
84	OHX	1	3489	-	0,6,6	-	-	-		
84	OHX	1	3646	-	0,6,6	-	-	-		
84	OHX	1	3671	-	0,6,6	-	-	-		
84	OHX	AR	3694	-	0,6,6	-	-	-		
84	OHX	AR	3687	-	0,6,6	-	-	-		
84	OHX	1	3546	-	0,6,6	-	-	-		
84	OHX	6	1904	-	0,6,6	-	-	-		
84	OHX	6	1922	-	0,6,6	-	-	-		
84	OHX	AR	3695	-	0,6,6	-	-	-		
84	OHX	A	1973	-	0,6,6	-	-	-		
84	OHX	AR	3736	-	0,6,6	-	-	-		
84	OHX	A	1951	-	0,6,6	-	-	-		
84	OHX	1	3452	-	0,6,6	-	-	-		
84	OHX	1	3557	-	0,6,6	-	-	-		
84	OHX	AR	3689	-	0,6,6	-	-	-		
84	OHX	A	1912	-	0,6,6	-	-	-		
84	OHX	1	3518	-	0,6,6	-	-	-		
84	OHX	AR	3540	-	0,6,6	-	-	-		
84	OHX	AR	3425	-	0,6,6	-	-	-		
84	OHX	AR	3514	-	0,6,6	-	-	-		
84	OHX	6	1914	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3441	-	0,6,6	-	-	-		
84	OHX	AR	3519	-	0,6,6	-	-	-		
84	OHX	1	3708	-	0,6,6	-	-	-		
84	OHX	1	3579	-	0,6,6	-	-	-		
84	OHX	1	3714	-	0,6,6	-	-	-		
84	OHX	6	2047	-	0,6,6	-	-	-		
84	OHX	1	3665	-	0,6,6	-	-	-		
84	OHX	1	3542	-	0,6,6	-	-	-		
84	OHX	A	2013	-	0,6,6	-	-	-		
84	OHX	AS	208	-	0,6,6	-	-	-		
84	OHX	AR	3406	-	0,6,6	-	-	-		
84	OHX	6	1935	-	0,6,6	-	-	-		
84	OHX	6	1956	-	0,6,6	-	-	-		
84	OHX	1	3660	-	0,6,6	-	-	-		
84	OHX	1	3601	-	0,6,6	-	-	-		
84	OHX	AR	3630	-	0,6,6	-	-	-		
84	OHX	1	3635	-	0,6,6	-	-	-		
84	OHX	3	208	-	0,6,6	-	-	-		
87	GOL	6	2199	-	5,5,5	0.10	0	5,5,5	0.33	0
84	OHX	CX	201	-	0,6,6	-	-	-		
84	OHX	1	3442	-	0,6,6	-	-	-		
84	OHX	1	3450	-	0,6,6	-	-	-		
84	OHX	1	3659	-	0,6,6	-	-	-		
84	OHX	6	1937	-	0,6,6	-	-	-		
84	OHX	AR	3679	-	0,6,6	-	-	-		
84	OHX	AR	3643	-	0,6,6	-	-	-		
84	OHX	AR	3606	-	0,6,6	-	-	-		
84	OHX	CF	402	-	0,6,6	-	-	-		
84	OHX	1	3609	-	0,6,6	-	-	-		
84	OHX	1	3700	-	0,6,6	-	-	-		
84	OHX	AT	205	-	0,6,6	-	-	-		
84	OHX	1	3580	-	0,6,6	-	-	-		
84	OHX	6	1989	-	0,6,6	-	-	-		
84	OHX	1	3464	-	0,6,6	-	-	-		
84	OHX	AR	3735	-	0,6,6	-	-	-		
84	OHX	4	201	-	0,6,6	-	-	-		
84	OHX	A	1969	-	0,6,6	-	-	-		
84	OHX	AR	3434	-	0,6,6	-	-	-		
84	OHX	1	3533	-	0,6,6	-	-	-		
84	OHX	AR	3409	-	0,6,6	-	-	-		
84	OHX	AR	3611	-	0,6,6	-	-	-		
84	OHX	6	1936	-	0,6,6	-	-	-		
84	OHX	1	3572	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3616	-	0,6,6	-	-	-		
84	OHX	AR	3678	-	0,6,6	-	-	-		
84	OHX	A	2042	-	0,6,6	-	-	-		
84	OHX	AR	3625	-	0,6,6	-	-	-		
84	OHX	AR	3737	-	0,6,6	-	-	-		
84	OHX	1	3702	-	0,6,6	-	-	-		
84	OHX	AR	3572	-	0,6,6	-	-	-		
84	OHX	1	3605	-	0,6,6	-	-	-		
84	OHX	AR	3585	-	0,6,6	-	-	-		
84	OHX	AR	3701	-	0,6,6	-	-	-		
84	OHX	1	3414	-	0,6,6	-	-	-		
84	OHX	6	2022	-	0,6,6	-	-	-		
84	OHX	A	1945	-	0,6,6	-	-	-		
84	OHX	1	3543	-	0,6,6	-	-	-		
84	OHX	AR	3690	-	0,6,6	-	-	-		
84	OHX	AR	3715	-	0,6,6	-	-	-		
84	OHX	AR	3509	-	0,6,6	-	-	-		
84	OHX	AR	3563	-	0,6,6	-	-	-		
84	OHX	A	1938	-	0,6,6	-	-	-		
84	OHX	AR	3403	-	0,6,6	-	-	-		
84	OHX	1	3566	-	0,6,6	-	-	-		
84	OHX	1	3683	-	0,6,6	-	-	-		
84	OHX	DQ	201	-	0,6,6	-	-	-		
84	OHX	h	401	-	0,6,6	-	-	-		
84	OHX	AR	3589	-	0,6,6	-	-	-		
84	OHX	1	3437	-	0,6,6	-	-	-		
84	OHX	1	3712	-	0,6,6	-	-	-		
84	OHX	6	1957	-	0,6,6	-	-	-		
84	OHX	AR	3721	-	0,6,6	-	-	-		
84	OHX	AT	212	-	0,6,6	-	-	-		
84	OHX	A	1927	-	0,6,6	-	-	-		
84	OHX	6	1948	-	0,6,6	-	-	-		
84	OHX	1	3412	-	0,6,6	-	-	-		
84	OHX	AR	3574	-	0,6,6	-	-	-		
84	OHX	1	3535	-	0,6,6	-	-	-		
84	OHX	A	1957	-	0,6,6	-	-	-		
84	OHX	AC	101	-	0,6,6	-	-	-		
84	OHX	1	3541	-	0,6,6	-	-	-		
84	OHX	1	3440	-	0,6,6	-	-	-		
84	OHX	AR	3535	-	0,6,6	-	-	-		
84	OHX	4	207	-	0,6,6	-	-	-		
84	OHX	AR	3405	-	0,6,6	-	-	-		
84	OHX	AR	3624	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	GOL	AR	4261	1	5,5,5	0.14	0	5,5,5	0.33	0
84	OHX	AR	3421	-	0,6,6	-	-	-	-	-
84	OHX	AR	3600	-	0,6,6	-	-	-	-	-
84	OHX	AR	3512	-	0,6,6	-	-	-	-	-
84	OHX	A	2038	-	0,6,6	-	-	-	-	-
84	OHX	AR	3634	-	0,6,6	-	-	-	-	-
84	OHX	6	1945	-	0,6,6	-	-	-	-	-
84	OHX	1	3615	-	0,6,6	-	-	-	-	-
84	OHX	1	3628	-	0,6,6	-	-	-	-	-
84	OHX	AR	3510	-	0,6,6	-	-	-	-	-
84	OHX	AT	215	-	0,6,6	-	-	-	-	-
84	OHX	6	2033	-	0,6,6	-	-	-	-	-
84	OHX	6	1928	-	0,6,6	-	-	-	-	-
84	OHX	6	1944	-	0,6,6	-	-	-	-	-
84	OHX	6	2023	-	0,6,6	-	-	-	-	-
84	OHX	1	3536	-	0,6,6	-	-	-	-	-
84	OHX	1	3587	-	0,6,6	-	-	-	-	-
84	OHX	A	1926	-	0,6,6	-	-	-	-	-
84	OHX	A	2033	-	0,6,6	-	-	-	-	-
84	OHX	AR	3581	-	0,6,6	-	-	-	-	-
84	OHX	AR	3627	-	0,6,6	-	-	-	-	-
84	OHX	6	2046	-	0,6,6	-	-	-	-	-
84	OHX	1	3527	-	0,6,6	-	-	-	-	-
84	OHX	1	3408	-	0,6,6	-	-	-	-	-
84	OHX	4	216	-	0,6,6	-	-	-	-	-
84	OHX	AR	3580	-	0,6,6	-	-	-	-	-
84	OHX	1	3455	-	0,6,6	-	-	-	-	-
84	OHX	AR	3592	-	0,6,6	-	-	-	-	-
84	OHX	1	3650	-	0,6,6	-	-	-	-	-
84	OHX	1	3636	-	0,6,6	-	-	-	-	-
84	OHX	1	3680	-	0,6,6	-	-	-	-	-
84	OHX	6	2020	-	0,6,6	-	-	-	-	-
84	OHX	AR	3455	-	0,6,6	-	-	-	-	-
84	OHX	1	3629	-	0,6,6	-	-	-	-	-
84	OHX	6	2013	-	0,6,6	-	-	-	-	-
84	OHX	AT	208	-	0,6,6	-	-	-	-	-
84	OHX	1	3439	-	0,6,6	-	-	-	-	-
84	OHX	6	2010	-	0,6,6	-	-	-	-	-
84	OHX	1	3447	-	0,6,6	-	-	-	-	-
84	OHX	1	3682	-	0,6,6	-	-	-	-	-
84	OHX	1	3521	-	0,6,6	-	-	-	-	-
84	OHX	AR	3414	-	0,6,6	-	-	-	-	-
84	OHX	A	1955	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3644	-	0,6,6	-	-	-		
84	OHX	CM	201	-	0,6,6	-	-	-		
84	OHX	AR	3484	-	0,6,6	-	-	-		
84	OHX	1	3429	-	0,6,6	-	-	-		
84	OHX	AR	3500	-	0,6,6	-	-	-		
84	OHX	A	1906	-	0,6,6	-	-	-		
84	OHX	1	3454	-	0,6,6	-	-	-		
84	OHX	A	1972	-	0,6,6	-	-	-		
84	OHX	AR	3463	-	0,6,6	-	-	-		
84	OHX	1	3638	-	0,6,6	-	-	-		
84	OHX	AR	3494	-	0,6,6	-	-	-		
84	OHX	6	2024	-	0,6,6	-	-	-		
84	OHX	AR	3730	-	0,6,6	-	-	-		
84	OHX	6	1927	-	0,6,6	-	-	-		
84	OHX	1	3496	-	0,6,6	-	-	-		
84	OHX	6	1962	-	0,6,6	-	-	-		
84	OHX	CK	201	-	0,6,6	-	-	-		
84	OHX	1	3526	-	0,6,6	-	-	-		
84	OHX	AR	3734	-	0,6,6	-	-	-		
84	OHX	AR	3551	-	0,6,6	-	-	-		
84	OHX	AR	3557	-	0,6,6	-	-	-		
84	OHX	AR	3469	-	0,6,6	-	-	-		
84	OHX	A	1962	-	0,6,6	-	-	-		
84	OHX	A	1967	-	0,6,6	-	-	-		
84	OHX	AR	3639	-	0,6,6	-	-	-		
84	OHX	1	3704	-	0,6,6	-	-	-		
84	OHX	A	2036	-	0,6,6	-	-	-		
84	OHX	k	401	-	0,6,6	-	-	-		
84	OHX	1	3416	-	0,6,6	-	-	-		
84	OHX	AR	3441	-	0,6,6	-	-	-		
84	OHX	1	3493	-	0,6,6	-	-	-		
84	OHX	1	3552	-	0,6,6	-	-	-		
84	OHX	AR	3714	-	0,6,6	-	-	-		
84	OHX	1	3578	-	0,6,6	-	-	-		
84	OHX	1	3419	-	0,6,6	-	-	-		
84	OHX	AR	3716	-	0,6,6	-	-	-		
84	OHX	A	1953	-	0,6,6	-	-	-		
84	OHX	AR	3618	-	0,6,6	-	-	-		
84	OHX	1	3555	-	0,6,6	-	-	-		
84	OHX	A	1976	-	0,6,6	-	-	-		
84	OHX	d9	101	-	0,6,6	-	-	-		
84	OHX	1	3544	-	0,6,6	-	-	-		
84	OHX	AR	3681	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1952	-	0,6,6	-	-	-		
84	OHX	6	2004	-	0,6,6	-	-	-		
84	OHX	A	2026	-	0,6,6	-	-	-		
84	OHX	A	1993	-	0,6,6	-	-	-		
84	OHX	1	3610	-	0,6,6	-	-	-		
84	OHX	6	1990	-	0,6,6	-	-	-		
84	OHX	6	1959	-	0,6,6	-	-	-		
84	OHX	6	1901	-	0,6,6	-	-	-		
84	OHX	AR	3550	-	0,6,6	-	-	-		
84	OHX	AR	3742	-	0,6,6	-	-	-		
84	OHX	1	3482	-	0,6,6	-	-	-		
84	OHX	AR	3458	-	0,6,6	-	-	-		
84	OHX	6	1983	-	0,6,6	-	-	-		
84	OHX	AR	3408	-	0,6,6	-	-	-		
84	OHX	AT	209	-	0,6,6	-	-	-		
84	OHX	3	207	-	0,6,6	-	-	-		
84	OHX	6	1993	-	0,6,6	-	-	-		
84	OHX	AR	3548	-	0,6,6	-	-	-		
84	OHX	AR	3696	84	0,6,6	-	-	-		
84	OHX	A	1983	-	0,6,6	-	-	-		
84	OHX	AR	3657	-	0,6,6	-	-	-		
84	OHX	A	2005	-	0,6,6	-	-	-		
84	OHX	AR	3719	-	0,6,6	-	-	-		
84	OHX	6	1955	-	0,6,6	-	-	-		
84	OHX	A	1918	-	0,6,6	-	-	-		
84	OHX	AR	3436	-	0,6,6	-	-	-		
84	OHX	A	1996	-	0,6,6	-	-	-		
84	OHX	1	3404	-	0,6,6	-	-	-		
84	OHX	AR	3448	-	0,6,6	-	-	-		
84	OHX	CE	401	-	0,6,6	-	-	-		
84	OHX	A	2032	-	0,6,6	-	-	-		
84	OHX	AR	3697	-	0,6,6	-	-	-		
84	OHX	A	2022	-	0,6,6	-	-	-		
84	OHX	6	1942	-	0,6,6	-	-	-		
84	OHX	6	1907	-	0,6,6	-	-	-		
84	OHX	A	2021	-	0,6,6	-	-	-		
84	OHX	AR	3558	-	0,6,6	-	-	-		
84	OHX	1	3595	-	0,6,6	-	-	-		
84	OHX	AR	3664	-	0,6,6	-	-	-		
84	OHX	1	3485	-	0,6,6	-	-	-		
84	OHX	A	1942	-	0,6,6	-	-	-		
84	OHX	1	3515	-	0,6,6	-	-	-		
84	OHX	A	1907	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3511	-	0,6,6	-	-	-		
84	OHX	AR	3567	-	0,6,6	-	-	-		
84	OHX	AR	3623	-	0,6,6	-	-	-		
84	OHX	AR	3649	-	0,6,6	-	-	-		
84	OHX	1	3415	-	0,6,6	-	-	-		
84	OHX	6	1979	-	0,6,6	-	-	-		
84	OHX	AR	3534	-	0,6,6	-	-	-		
84	OHX	1	3501	-	0,6,6	-	-	-		
84	OHX	1	3477	-	0,6,6	-	-	-		
84	OHX	AR	3433	-	0,6,6	-	-	-		
84	OHX	A	1985	-	0,6,6	-	-	-		
84	OHX	1	3547	-	0,6,6	-	-	-		
84	OHX	AR	3654	-	0,6,6	-	-	-		
84	OHX	AS	211	-	0,6,6	-	-	-		
84	OHX	A	2012	-	0,6,6	-	-	-		
84	OHX	1	3545	-	0,6,6	-	-	-		
84	OHX	1	3670	-	0,6,6	-	-	-		
84	OHX	6	1988	-	0,6,6	-	-	-		
84	OHX	AR	3456	-	0,6,6	-	-	-		
84	OHX	1	3607	-	0,6,6	-	-	-		
84	OHX	A	2015	-	0,6,6	-	-	-		
84	OHX	1	3564	-	0,6,6	-	-	-		
84	OHX	1	3641	-	0,6,6	-	-	-		
84	OHX	AS	202	-	0,6,6	-	-	-		
84	OHX	6	1951	-	0,6,6	-	-	-		
84	OHX	A	2037	-	0,6,6	-	-	-		
84	OHX	1	3584	-	0,6,6	-	-	-		
84	OHX	AR	3539	-	0,6,6	-	-	-		
84	OHX	1	3423	-	0,6,6	-	-	-		
84	OHX	AR	3564	-	0,6,6	-	-	-		
84	OHX	AT	216	-	0,6,6	-	-	-		
84	OHX	AT	201	-	0,6,6	-	-	-		
84	OHX	s8	301	-	0,6,6	-	-	-		
84	OHX	AR	3542	-	0,6,6	-	-	-		
84	OHX	AR	3672	-	0,6,6	-	-	-		
84	OHX	1	3449	-	0,6,6	-	-	-		
84	OHX	1	3474	-	0,6,6	-	-	-		
84	OHX	AR	3438	-	0,6,6	-	-	-		
84	OHX	AR	3653	-	0,6,6	-	-	-		
84	OHX	1	3520	-	0,6,6	-	-	-		
84	OHX	6	2030	-	0,6,6	-	-	-		
84	OHX	AR	3692	-	0,6,6	-	-	-		
84	OHX	AR	3726	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	1905	-	0,6,6	-	-	-		
84	OHX	4	205	-	0,6,6	-	-	-		
84	OHX	AR	3628	-	0,6,6	-	-	-		
84	OHX	4	210	-	0,6,6	-	-	-		
84	OHX	AR	3705	-	0,6,6	-	-	-		
84	OHX	6	1961	-	0,6,6	-	-	-		
84	OHX	1	3484	-	0,6,6	-	-	-		
84	OHX	A	2023	-	0,6,6	-	-	-		
84	OHX	AR	3466	-	0,6,6	-	-	-		
84	OHX	1	3573	-	0,6,6	-	-	-		
84	OHX	1	3611	-	0,6,6	-	-	-		
84	OHX	1	3463	-	0,6,6	-	-	-		
84	OHX	1	3538	-	0,6,6	-	-	-		
84	OHX	AR	3407	-	0,6,6	-	-	-		
84	OHX	AR	3488	-	0,6,6	-	-	-		
84	OHX	AR	3538	-	0,6,6	-	-	-		
84	OHX	AR	3612	-	0,6,6	-	-	-		
84	OHX	A	2029	-	0,6,6	-	-	-		
84	OHX	6	1974	-	0,6,6	-	-	-		
84	OHX	AR	3435	-	0,6,6	-	-	-		
84	OHX	A	2019	-	0,6,6	-	-	-		
84	OHX	6	1965	-	0,6,6	-	-	-		
84	OHX	A	1929	-	0,6,6	-	-	-		
84	OHX	A	2018	-	0,6,6	-	-	-		
84	OHX	AS	204	-	0,6,6	-	-	-		

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	HN8	AR	4263	-	-	0/2/48/48	0/6/5/5
87	GOL	AR	4261	1	-	2/4/4/4	-
87	GOL	A	2160	-	-	0/4/4/4	-
87	GOL	v	305	-	-	2/4/4/4	-
87	GOL	AR	4262	84	-	1/4/4/4	-
86	HN8	1	4223	-	-	0/2/48/48	0/6/5/5
87	GOL	6	2199	-	-	0/4/4/4	-

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-C3	-5.16	100.15	106.09
86	AR	4263	HN8	C5-C1-C2	-5.00	102.67	106.70
86	AR	4263	HN8	C5-C1-C7	4.00	116.29	114.53
86	1	4223	HN8	C5-C1-C7	3.71	116.17	114.53
86	AR	4263	HN8	C3-C1-C2	2.87	107.05	102.28

There are no chirality outliers.

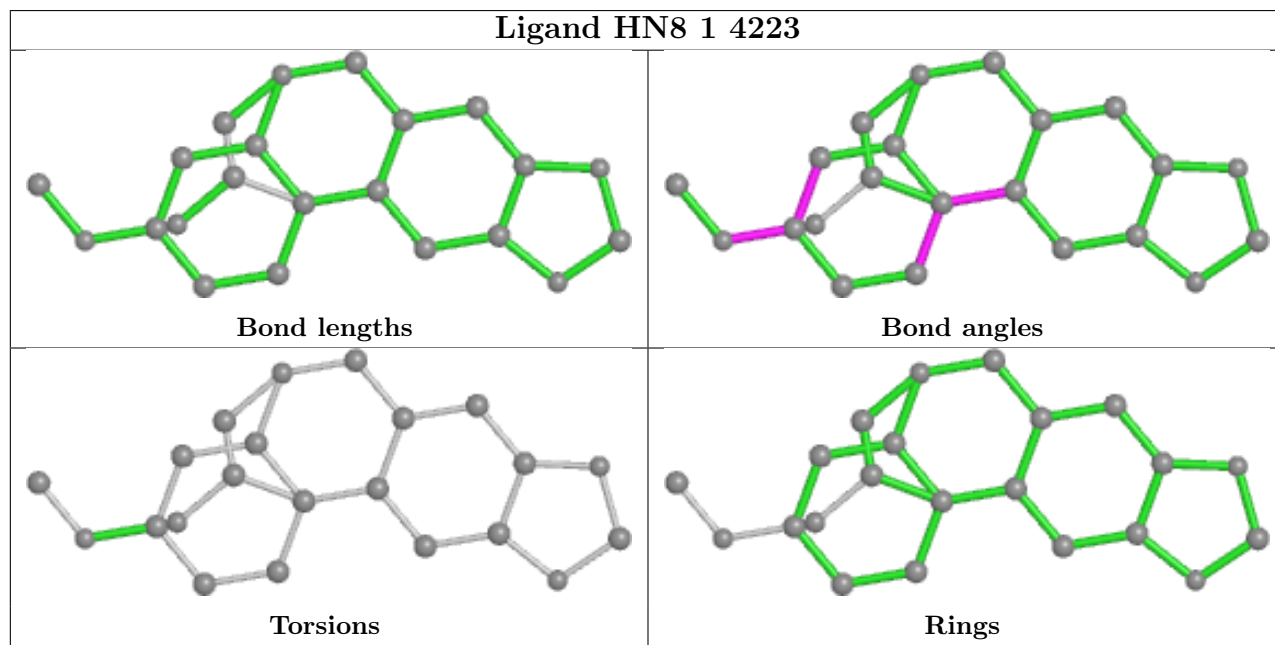
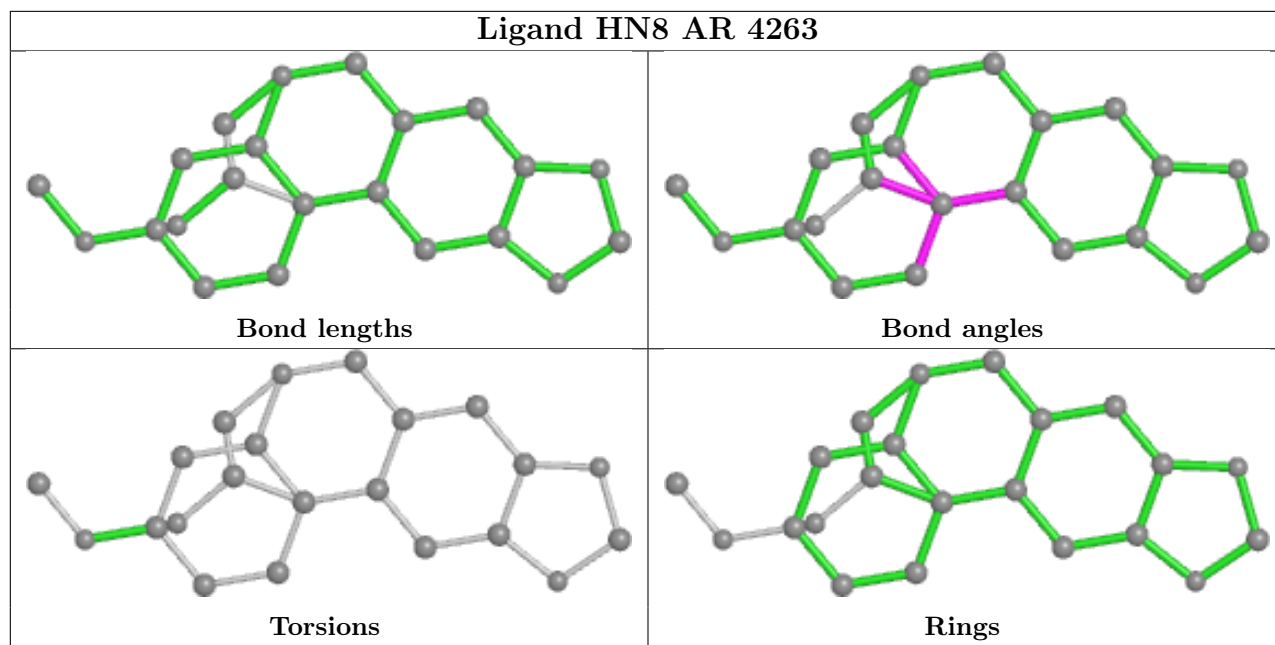
All (5) torsion outliers are listed below:

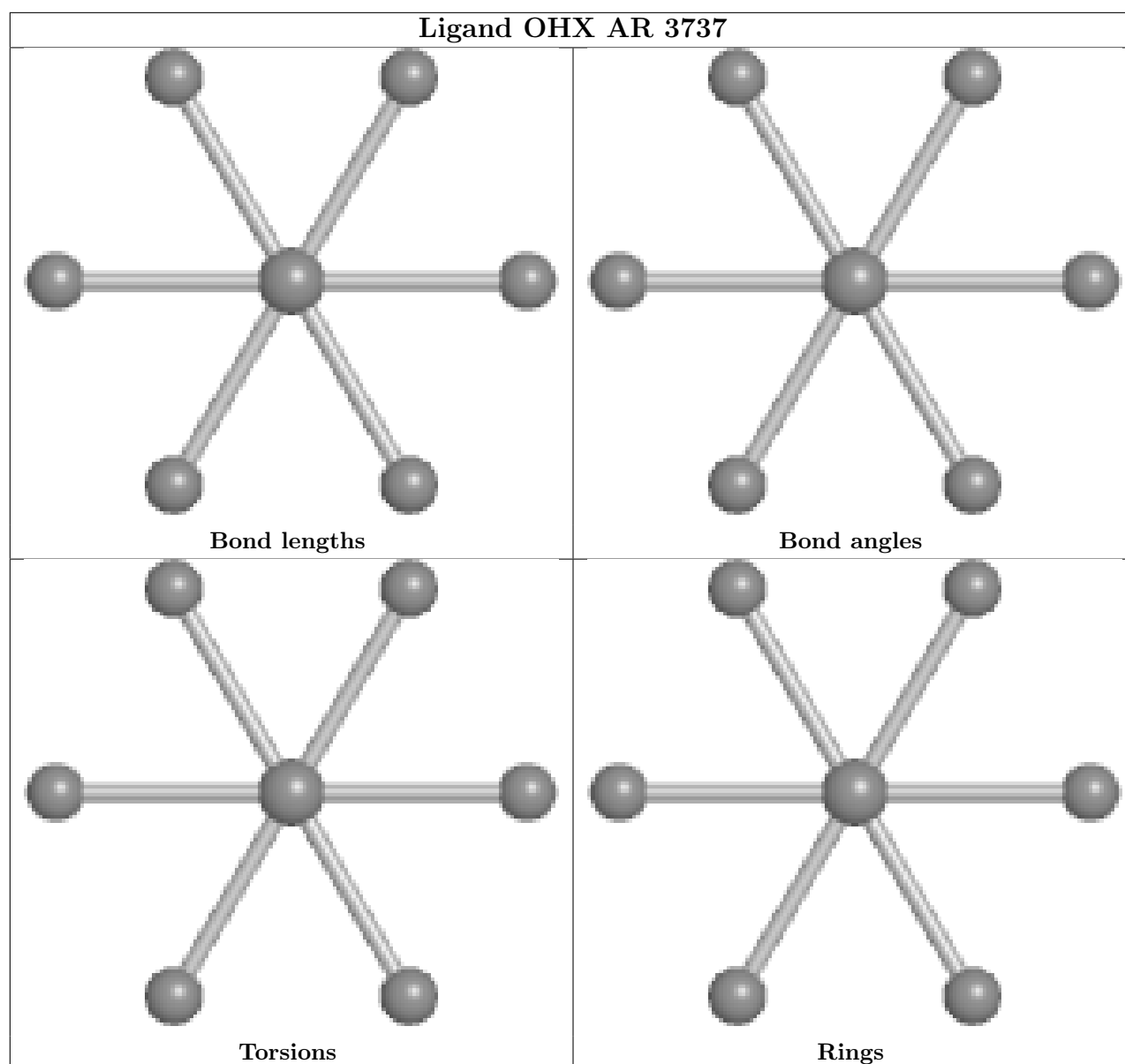
Mol	Chain	Res	Type	Atoms
87	v	305	GOL	O1-C1-C2-C3
87	AR	4261	GOL	C1-C2-C3-O3
87	v	305	GOL	O1-C1-C2-O2
87	AR	4261	GOL	O2-C2-C3-O3
87	AR	4262	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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
25	A	1
47	m2	1

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Mol	Chain	Number of breaks
5	CE	1
50	s0	1
54	s4	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 i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	3149/3396 (92%)	0.22	98 (3%) 49 26	26, 47, 129, 223	0
1	AR	3149/3396 (92%)	0.30	104 (3%) 46 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 72	34, 52, 66, 73	0
3	4	158/158 (100%)	0.21	5 (3%) 47 25	34, 51, 91, 138	0
3	AT	158/158 (100%)	0.25	6 (3%) 40 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%) 94 88	25, 41, 55, 95	0
5	k	386/386 (100%)	-0.02	3 (0%) 86 72	25, 48, 62, 80	0
6	CF	361/361 (100%)	-0.11	1 (0%) 94 88	31, 47, 65, 88	0
6	l	361/361 (100%)	-0.12	1 (0%) 94 88	27, 44, 62, 71	0
7	CG	296/296 (100%)	0.15	13 (4%) 34 17	39, 57, 83, 104	0
7	m	296/296 (100%)	0.48	17 (5%) 23 11	46, 69, 89, 115	0
8	CH	156/175 (89%)	0.07	3 (1%) 66 46	37, 46, 68, 84	0
8	n	156/175 (89%)	0.04	1 (0%) 89 78	36, 43, 66, 86	0
9	CI	222/222 (100%)	-0.13	3 (1%) 75 56	27, 35, 78, 133	0
9	o	222/222 (100%)	-0.16	4 (1%) 68 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%) 24 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%)	-0.25	0 100 100	42, 53, 66, 86	0
12	CL	211/220 (95%)	0.45	13 (6%) 20 9	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 <sup>2</sup> )	Q<0.9
13	CM	169/169 (100%)	-0.19	1 (0%) 89 78	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%) 13 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%)	-0.34	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%)	-0.11	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%) 73 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%) 4 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%) 30 14	48, 63, 158, 169	0
20	z	188/188 (100%)	0.16	7 (3%) 41 21	48, 64, 150, 167	0
21	0	172/172 (100%)	-0.19	1 (0%) 89 78	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	12 (12%) 4 2	79, 93, 105, 123	0
23	CW	100/100 (100%)	1.11	21 (21%) 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%) 51 28	31, 43, 56, 62	0
25	6	1783/1800 (99%)	0.43	115 (6%) 19 8	41, 78, 169, 233	0
25	A	1781/1800 (98%)	0.51	128 (7%) 15 6	49, 87, 186, 250	0
26	7	98/98 (100%)	1.75	29 (29%) 0 0	43, 59, 150, 157	0
26	CY	98/98 (100%)	0.41	11 (11%) 5 2	38, 53, 145, 177	0
27	8	121/121 (100%)	-0.03	1 (0%) 86 72	44, 57, 77, 117	0
27	CZ	121/121 (100%)	0.05	4 (3%) 46 24	48, 64, 85, 100	0
28	9	126/126 (100%)	0.67	6 (4%) 30 14	40, 55, 64, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DA	126/126 (100%)	0.69	7 (5%) 24 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%)	0.90	16 (11%) 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, 88	0
32	AD	97/97 (100%)	0.38	6 (6%) 20 9	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%) 68 47	42, 56, 95, 106	0
33	DF	109/109 (100%)	0.18	3 (2%) 53 30	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%) 25 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%)	0.27	6 (5%) 28 13	46, 61, 70, 77	0
37	DJ	119/119 (100%)	0.27	6 (5%) 28 13	51, 67, 81, 88	0
38	AJ	99/99 (100%)	0.24	3 (3%) 50 27	52, 61, 93, 113	0
38	DK	99/99 (100%)	0.26	4 (4%) 38 19	59, 70, 92, 110	0
39	AK	87/87 (100%)	0.10	3 (3%) 45 24	32, 36, 63, 86	0
39	DL	87/87 (100%)	0.24	3 (3%) 45 24	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	5 (9%) 8 2	37, 43, 61, 69	0
42	DO	52/52 (100%)	0.02	1 (1%) 66 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 <sup>2</sup> )	Q<0.9
44	AP	105/105 (100%)	0.66	9 (8%) 10 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%) 4 2	70, 90, 143, 148	0
47	m2	0/150	-	-	-	-
48	sM	63/104 (60%)	0.77	6 (9%) 8 2	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	27 (13%) 3 1	93, 110, 125, 146	0
50	s0	206/206 (100%)	0.32	8 (3%) 39 20	77, 97, 115, 120	0
51	C	214/216 (99%)	1.64	78 (36%) 0 0	93, 121, 142, 150	0
51	s1	216/216 (100%)	0.53	13 (6%) 21 10	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%)	0.65	19 (8%) 10 4	74, 91, 118, 137	0
53	s3	223/223 (100%)	0.70	27 (12%) 4 1	75, 103, 134, 148	0
54	F	260/260 (100%)	0.62	22 (8%) 10 4	63, 87, 97, 121	0
54	s4	260/260 (100%)	0.16	7 (2%) 54 31	53, 84, 98, 128	0
55	G	206/206 (100%)	0.77	22 (10%) 6 2	92, 112, 131, 141	0
55	s5	206/206 (100%)	0.95	34 (16%) 1 1	74, 95, 114, 122	0
56	H	226/226 (100%)	0.87	39 (17%) 1 0	61, 94, 116, 143	0
56	s6	218/226 (96%)	0.63	26 (11%) 4 2	52, 83, 111, 124	0
57	I	184/186 (98%)	1.03	29 (15%) 2 1	87, 119, 148, 156	0
57	s7	186/186 (100%)	1.00	32 (17%) 1 0	77, 112, 147, 152	0
58	J	188/199 (94%)	0.29	9 (4%) 30 14	53, 70, 111, 126	0
58	s8	188/199 (94%)	0.57	14 (7%) 14 5	49, 73, 124, 140	0
59	K	185/185 (100%)	1.06	34 (18%) 1 0	77, 95, 129, 158	0
59	s9	185/185 (100%)	0.68	15 (8%) 12 5	67, 85, 116, 151	0
60	L	96/105 (91%)	1.12	16 (16%) 1 1	81, 102, 129, 139	0
60	c0	96/105 (91%)	2.34	55 (57%) 0 0	96, 126, 139, 147	0
61	M	155/155 (100%)	0.82	16 (10%) 6 2	56, 70, 126, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
61	c1	146/155 (94%)	0.46	8 (5%) 25 11	55, 70, 104, 131	0
62	N	124/124 (100%)	1.99	64 (51%) 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%) 21 10	64, 85, 100, 104	0
63	c3	150/150 (100%)	0.16	4 (2%) 54 31	59, 78, 96, 111	0
64	P	127/128 (99%)	1.40	36 (28%) 0 0	66, 119, 135, 138	0
64	c4	128/128 (100%)	0.63	11 (8%) 10 4	57, 81, 91, 94	0
65	Q	124/141 (87%)	0.49	7 (5%) 24 11	75, 89, 126, 146	0
65	c5	135/141 (95%)	0.80	16 (11%) 4 2	82, 97, 118, 131	0
66	R	141/142 (99%)	1.05	25 (17%) 1 0	81, 107, 115, 120	0
66	c6	142/142 (100%)	0.69	15 (10%) 6 2	67, 91, 106, 127	0
67	S	120/125 (96%)	0.56	14 (11%) 4 2	90, 109, 134, 138	0
67	c7	117/125 (93%)	0.13	6 (5%) 28 13	78, 97, 122, 130	0
68	T	145/145 (100%)	0.79	17 (11%) 4 2	71, 99, 129, 140	0
68	c8	145/145 (100%)	0.71	16 (11%) 5 2	79, 91, 116, 127	0
69	U	143/143 (100%)	1.00	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%) 66 46	73, 109, 141, 145	0
70	d0	110/110 (100%)	0.46	12 (10%) 5 2	70, 111, 154, 172	0
71	W	87/87 (100%)	0.61	8 (9%) 9 3	90, 96, 115, 124	0
71	d1	87/87 (100%)	0.14	4 (4%) 32 16	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%)	0.05	1 (0%) 86 72	57, 70, 81, 97	0
73	Y	144/144 (100%)	0.22	3 (2%) 63 43	57, 62, 73, 88	0
73	d3	144/144 (100%)	-0.08	0 100 100	46, 52, 66, 78	0
74	Z	134/134 (100%)	0.47	15 (11%) 5 2	69, 97, 114, 125	0
74	d4	134/134 (100%)	0.23	11 (8%) 11 4	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%)	0.42	5 (5%) 27 12	67, 83, 135, 138	0
76	d6	97/97 (100%)	0.14	1 (1%) 82 67	51, 63, 95, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
77	c	81/81 (100%)	1.03	15 (18%) 1 0	82, 95, 127, 134	0
77	d7	81/81 (100%)	1.14	15 (18%) 1 0	72, 87, 126, 132	0
78	d	63/63 (100%)	0.96	7 (11%) 5 2	104, 121, 132, 134	0
78	d8	63/63 (100%)	1.97	34 (53%) 0 0	91, 107, 121, 125	0
79	d9	53/53 (100%)	1.20	10 (18%) 1 0	71, 82, 120, 128	0
79	e	53/53 (100%)	0.69	4 (7%) 14 5	75, 80, 96, 104	0
80	e0	62/62 (100%)	0.97	9 (14%) 2 1	59, 83, 113, 125	0
80	f	60/62 (96%)	1.14	11 (18%) 1 0	63, 92, 131, 134	0
81	g	71/71 (100%)	1.75	29 (40%) 0 0	105, 124, 144, 150	0
82	h	318/318 (100%)	1.11	70 (22%) 0 0	97, 115, 135, 147	0
82	sR	318/318 (100%)	0.61	32 (10%) 7 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%)	0.39	2308 (6%) 16 7	24, 66, 132, 250	0

The worst 5 of 2308 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	CR	161	ALA	24.1
18	CR	162	GLU	20.5
26	7	76	VAL	18.1
18	CR	160	ALA	16.2
26	7	75	THR	15.8

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	6	2176	1/1	0.31	0.68	93,93,93,93	0
85	MG	1	3951	1/1	0.45	0.33	69,69,69,69	0
85	MG	6	2158	1/1	0.46	0.75	74,74,74,74	0
85	MG	1	4140	1/1	0.46	0.29	187,187,187,187	0
85	MG	A	2130	1/1	0.46	0.62	74,74,74,74	0
85	MG	1	3813	1/1	0.48	0.37	61,61,61,61	0
85	MG	1	3958	1/1	0.49	0.38	44,44,44,44	0
85	MG	1	4053	1/1	0.49	0.41	74,74,74,74	0
85	MG	1	3965	1/1	0.51	0.57	94,94,94,94	0
85	MG	A	2121	1/1	0.52	0.31	62,62,62,62	0
85	MG	1	3948	1/1	0.55	0.23	73,73,73,73	0
85	MG	AR	4196	1/1	0.55	0.43	43,43,43,43	0
85	MG	4	229	1/1	0.56	0.41	54,54,54,54	0
85	MG	AS	228	1/1	0.56	0.42	84,84,84,84	0
85	MG	AR	4102	1/1	0.57	0.98	30,30,30,30	0
85	MG	AR	4104	1/1	0.57	0.39	66,66,66,66	0
85	MG	1	4150	1/1	0.57	0.26	49,49,49,49	0
85	MG	A	2150	1/1	0.57	0.16	86,86,86,86	0
85	MG	1	4152	1/1	0.59	0.80	111,111,111,111	0
85	MG	AR	4122	1/1	0.60	0.25	68,68,68,68	0
85	MG	1	4104	1/1	0.60	0.45	53,53,53,53	0
85	MG	AR	3890	1/1	0.60	0.42	29,29,29,29	0
85	MG	AR	4013	1/1	0.60	0.29	65,65,65,65	0
85	MG	1	3989	1/1	0.60	0.26	55,55,55,55	0
85	MG	6	2168	1/1	0.60	0.31	132,132,132,132	0
85	MG	1	3772	1/1	0.61	0.20	35,35,35,35	0
85	MG	6	2180	1/1	0.61	0.60	64,64,64,64	0
85	MG	A	2124	1/1	0.61	0.30	68,68,68,68	0
85	MG	6	2185	1/1	0.61	0.46	89,89,89,89	0
85	MG	AR	4254	1/1	0.61	0.38	56,56,56,56	0
85	MG	A	2155	1/1	0.61	0.46	75,75,75,75	0
85	MG	6	2194	1/1	0.62	0.15	108,108,108,108	0
85	MG	6	2160	1/1	0.62	0.38	85,85,85,85	0
85	MG	4	221	1/1	0.63	0.54	51,51,51,51	0
85	MG	1	4004	1/1	0.64	0.26	44,44,44,44	0
85	MG	AR	4125	1/1	0.64	0.29	82,82,82,82	0
85	MG	AS	220	1/1	0.64	0.36	68,68,68,68	0
85	MG	AR	3950	1/1	0.65	0.27	47,47,47,47	0
85	MG	1	3823	1/1	0.65	0.27	41,41,41,41	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	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3955	1/1	0.66	0.17	34,34,34,34	0
85	MG	AR	4255	1/1	0.67	0.64	57,57,57,57	0
85	MG	1	4124	1/1	0.68	0.22	48,48,48,48	0
85	MG	t	202	1/1	0.68	0.26	101,101,101,101	0
85	MG	AR	4219	1/1	0.68	0.17	67,67,67,67	0
85	MG	AR	4074	1/1	0.68	0.23	77,77,77,77	0
85	MG	AR	4174	1/1	0.69	0.42	39,39,39,39	0
85	MG	AT	218	1/1	0.69	0.34	30,30,30,30	0
85	MG	A	2099	1/1	0.69	0.69	71,71,71,71	0
85	MG	A	2103	1/1	0.69	0.55	73,73,73,73	0
85	MG	AR	3833	1/1	0.69	0.30	49,49,49,49	0
85	MG	1	3930	1/1	0.69	0.57	40,40,40,40	0
85	MG	1	3952	1/1	0.69	0.24	77,77,77,77	0
85	MG	1	3820	1/1	0.69	0.60	65,65,65,65	0
85	MG	6	2086	1/1	0.69	0.25	82,82,82,82	0
85	MG	A	2117	1/1	0.70	0.19	71,71,71,71	0
85	MG	6	2133	1/1	0.70	0.66	61,61,61,61	0
85	MG	A	2085	1/1	0.70	0.40	63,63,63,63	0
85	MG	AR	4170	1/1	0.70	0.27	32,32,32,32	0
85	MG	A	2139	1/1	0.70	0.36	64,64,64,64	0
85	MG	6	2174	1/1	0.70	0.44	58,58,58,58	0
85	MG	A	2151	1/1	0.70	0.69	52,52,52,52	0
85	MG	A	2112	1/1	0.70	0.37	86,86,86,86	0
85	MG	Y	201	1/1	0.70	0.20	61,61,61,61	0
85	MG	6	2154	1/1	0.71	0.41	54,54,54,54	0
85	MG	1	403	1/1	0.71	0.47	37,37,37,37	0
85	MG	1	4061	1/1	0.71	0.31	54,54,54,54	0
85	MG	AR	4119	1/1	0.71	0.39	91,91,91,91	0
84	OHX	AR	3737	7/7	0.71	0.46	158,158,158,159	0
85	MG	4	233	1/1	0.71	0.20	48,48,48,48	0
85	MG	AR	4037	1/1	0.71	0.34	70,70,70,70	0
85	MG	AR	4003	1/1	0.72	0.43	45,45,45,45	0
85	MG	AR	4222	1/1	0.72	0.39	58,58,58,58	0
85	MG	1	3814	1/1	0.72	0.22	77,77,77,77	0
85	MG	AR	4030	1/1	0.72	0.57	59,59,59,59	0
85	MG	s	300	1/1	0.72	0.27	70,70,70,70	0
85	MG	AR	4049	1/1	0.72	0.19	50,50,50,50	0
85	MG	1	4101	1/1	0.72	0.51	38,38,38,38	0
85	MG	A	2046	1/1	0.72	0.29	67,67,67,67	0
85	MG	A	2062	1/1	0.72	0.71	65,65,65,65	0
85	MG	AR	4181	1/1	0.72	0.24	50,50,50,50	0
85	MG	AR	3817	1/1	0.72	0.24	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4034	1/1	0.73	0.45	60,60,60,60	0
85	MG	AR	4214	1/1	0.73	0.24	55,55,55,55	0
85	MG	AT	224	1/1	0.73	0.23	68,68,68,68	0
85	MG	CD	302	1/1	0.73	0.49	36,36,36,36	0
85	MG	A	2128	1/1	0.73	0.50	78,78,78,78	0
85	MG	DC	203	1/1	0.73	0.31	47,47,47,47	0
85	MG	6	2124	1/1	0.73	0.28	66,66,66,66	0
85	MG	A	2146	1/1	0.73	0.16	120,120,120,120	0
85	MG	1	4161	1/1	0.73	0.25	69,69,69,69	0
85	MG	AR	4011	1/1	0.73	0.39	58,58,58,58	0
85	MG	1	4190	1/1	0.73	0.56	25,25,25,25	0
85	MG	1	3988	1/1	0.73	0.37	34,34,34,34	0
85	MG	AR	4024	1/1	0.74	0.78	53,53,53,53	0
85	MG	AS	225	1/1	0.74	0.35	58,58,58,58	0
85	MG	AR	4161	1/1	0.74	0.27	39,39,39,39	0
85	MG	AR	3783	1/1	0.74	0.32	44,44,44,44	0
85	MG	1	3983	1/1	0.74	0.52	55,55,55,55	0
85	MG	1	4151	1/1	0.74	0.28	41,41,41,41	0
85	MG	A	2131	1/1	0.74	0.43	64,64,64,64	0
85	MG	A	2135	1/1	0.74	0.56	55,55,55,55	0
85	MG	1	4081	1/1	0.74	0.39	29,29,29,29	0
85	MG	1	4129	1/1	0.74	0.43	33,33,33,33	0
85	MG	1	4131	1/1	0.74	0.32	48,48,48,48	0
85	MG	6	2192	1/1	0.74	0.67	74,74,74,74	0
85	MG	1	4056	1/1	0.74	0.30	51,51,51,51	0
85	MG	AR	3782	1/1	0.74	0.35	36,36,36,36	0
85	MG	A	2118	1/1	0.75	0.92	80,80,80,80	0
85	MG	AR	4215	1/1	0.75	0.28	70,70,70,70	0
85	MG	AR	3995	1/1	0.75	0.34	65,65,65,65	0
85	MG	AR	3827	1/1	0.75	0.35	58,58,58,58	0
85	MG	A	2045	1/1	0.75	0.79	58,58,58,58	0
85	MG	1	4158	1/1	0.75	0.46	47,47,47,47	0
85	MG	A	2054	1/1	0.75	0.23	66,66,66,66	0
85	MG	A	2136	1/1	0.75	0.71	74,74,74,74	0
85	MG	6	2083	1/1	0.75	0.46	63,63,63,63	0
85	MG	AR	4022	1/1	0.75	0.44	30,30,30,30	0
85	MG	1	3816	1/1	0.75	0.34	44,44,44,44	0
85	MG	AR	4117	1/1	0.75	0.31	64,64,64,64	0
85	MG	6	2117	1/1	0.75	0.28	65,65,65,65	0
85	MG	AT	222	1/1	0.75	0.34	43,43,43,43	0
85	MG	4	235	1/1	0.76	0.50	70,70,70,70	0
85	MG	CM	202	1/1	0.76	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3790	1/1	0.76	0.12	43,43,43,43	0
85	MG	1	3857	1/1	0.76	0.25	56,56,56,56	0
85	MG	1	4093	1/1	0.76	0.37	57,57,57,57	0
85	MG	6	2188	1/1	0.76	0.54	66,66,66,66	0
85	MG	AR	4257	1/1	0.76	0.32	51,51,51,51	0
85	MG	6	2189	1/1	0.76	0.34	63,63,63,63	0
85	MG	1	4155	1/1	0.76	0.23	53,53,53,53	0
85	MG	1	4148	1/1	0.76	0.18	53,53,53,53	0
85	MG	6	2088	1/1	0.76	0.35	82,82,82,82	0
85	MG	AR	4087	1/1	0.76	0.36	63,63,63,63	0
85	MG	AR	3776	1/1	0.76	0.33	76,76,76,76	0
85	MG	AS	219	1/1	0.77	0.24	58,58,58,58	0
85	MG	6	2162	1/1	0.77	0.26	60,60,60,60	0
85	MG	6	2163	1/1	0.77	0.42	48,48,48,48	0
85	MG	AR	4171	1/1	0.77	0.17	88,88,88,88	0
85	MG	AR	4085	1/1	0.77	0.46	35,35,35,35	0
85	MG	6	2081	1/1	0.77	0.25	55,55,55,55	0
84	OHX	1	3691	7/7	0.77	0.31	201,201,201,201	0
85	MG	1	3744	1/1	0.77	0.42	83,83,83,83	0
85	MG	AR	3921	1/1	0.77	0.31	38,38,38,38	0
85	MG	1	3801	1/1	0.77	0.54	37,37,37,37	0
85	MG	6	2074	1/1	0.77	0.37	62,62,62,62	0
85	MG	AR	4225	1/1	0.77	0.35	34,34,34,34	0
85	MG	AR	4244	1/1	0.77	0.40	45,45,45,45	0
85	MG	AR	3976	1/1	0.77	0.44	81,81,81,81	0
85	MG	A	2084	1/1	0.77	0.22	72,72,72,72	0
85	MG	AR	4156	1/1	0.77	1.08	72,72,72,72	0
85	MG	V	201	1/1	0.77	0.50	70,70,70,70	0
85	MG	AR	4160	1/1	0.77	0.26	78,78,78,78	0
85	MG	b	101	1/1	0.77	0.45	65,65,65,65	0
85	MG	1	3811	1/1	0.78	0.30	44,44,44,44	0
85	MG	6	2197	1/1	0.78	0.57	56,56,56,56	0
85	MG	AF	202	1/1	0.78	0.27	28,28,28,28	0
85	MG	AR	4123	1/1	0.78	0.36	57,57,57,57	0
85	MG	AR	4005	1/1	0.78	0.62	40,40,40,40	0
85	MG	AR	4141	1/1	0.78	0.36	37,37,37,37	0
85	MG	1	3976	1/1	0.78	0.14	61,61,61,61	0
85	MG	1	3941	1/1	0.78	0.41	78,78,78,78	0
85	MG	1	4012	1/1	0.78	0.44	50,50,50,50	0
85	MG	AR	3803	1/1	0.78	0.51	35,35,35,35	0
85	MG	1	4087	1/1	0.78	0.23	59,59,59,59	0
85	MG	1	4092	1/1	0.78	0.64	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	4187	1/1	0.78	0.35	43,43,43,43	0
85	MG	x	206	1/1	0.78	0.58	35,35,35,35	0
85	MG	6	2157	1/1	0.78	0.28	56,56,56,56	0
85	MG	1	4046	1/1	0.78	0.34	37,37,37,37	0
85	MG	6	2076	1/1	0.78	0.58	105,105,105,105	0
85	MG	AR	4220	1/1	0.78	0.39	44,44,44,44	0
85	MG	AR	3968	1/1	0.78	0.32	30,30,30,30	0
85	MG	AR	3971	1/1	0.78	0.42	57,57,57,57	0
87	GOL	AR	4261	6/6	0.78	0.34	48,48,48,48	0
85	MG	6	2183	1/1	0.79	0.58	71,71,71,71	0
85	MG	AR	4097	1/1	0.79	0.58	40,40,40,40	0
85	MG	4	236	1/1	0.79	0.19	50,50,50,50	0
85	MG	4	238	1/1	0.79	0.26	35,35,35,35	0
85	MG	AR	4110	1/1	0.79	0.50	46,46,46,46	0
85	MG	1	3751	1/1	0.79	0.35	40,40,40,40	0
85	MG	1	3800	1/1	0.79	0.61	45,45,45,45	0
85	MG	DI	202	1/1	0.79	0.36	56,56,56,56	0
85	MG	6	2092	1/1	0.79	0.58	93,93,93,93	0
85	MG	6	2193	1/1	0.79	0.45	55,55,55,55	0
85	MG	6	2167	1/1	0.79	0.50	53,53,53,53	0
85	MG	1	4023	1/1	0.79	0.48	57,57,57,57	0
85	MG	AR	3964	1/1	0.79	0.29	35,35,35,35	0
85	MG	1	3750	1/1	0.79	0.18	55,55,55,55	0
85	MG	AR	4063	1/1	0.79	0.12	54,54,54,54	0
85	MG	1	3994	1/1	0.79	0.27	47,47,47,47	0
85	MG	1	4001	1/1	0.79	0.45	47,47,47,47	0
87	GOL	6	2199	6/6	0.79	0.44	49,49,49,49	0
85	MG	A	2116	1/1	0.79	0.61	67,67,67,67	0
88	ZN	d7	101	1/1	0.79	0.47	143,143,143,143	0
85	MG	AT	231	1/1	0.80	0.83	52,52,52,52	0
85	MG	1	3807	1/1	0.80	0.18	41,41,41,41	0
85	MG	1	4040	1/1	0.80	0.30	74,74,74,74	0
85	MG	AR	3986	1/1	0.80	0.21	56,56,56,56	0
85	MG	AR	4223	1/1	0.80	0.30	61,61,61,61	0
85	MG	1	4074	1/1	0.80	0.24	37,37,37,37	0
85	MG	AR	3998	1/1	0.80	0.45	40,40,40,40	0
85	MG	1	4044	1/1	0.80	0.32	47,47,47,47	0
85	MG	1	4127	1/1	0.80	0.26	45,45,45,45	0
85	MG	6	2130	1/1	0.80	0.31	66,66,66,66	0
85	MG	4	232	1/1	0.80	0.28	37,37,37,37	0
85	MG	A	2091	1/1	0.80	0.43	71,71,71,71	0
85	MG	1	3852	1/1	0.80	0.33	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4194	1/1	0.80	0.27	53,53,53,53	0
85	MG	1	4014	1/1	0.80	0.37	57,57,57,57	0
85	MG	AR	4198	1/1	0.80	0.59	51,51,51,51	0
85	MG	AR	3779	1/1	0.80	0.38	73,73,73,73	0
87	GOL	AR	4262	6/6	0.80	0.34	48,48,48,48	0
85	MG	1	4159	1/1	0.80	0.39	43,43,43,43	0
85	MG	A	2083	1/1	0.81	0.18	68,68,68,68	0
85	MG	6	2146	1/1	0.81	1.00	80,80,80,80	0
84	OHX	1	3668	7/7	0.81	0.45	124,124,124,124	0
85	MG	AR	4128	1/1	0.81	0.21	55,55,55,55	0
85	MG	1	4027	1/1	0.81	0.39	35,35,35,35	0
85	MG	AR	4155	1/1	0.81	0.45	34,34,34,34	0
85	MG	1	4203	1/1	0.81	0.24	31,31,31,31	0
85	MG	A	2114	1/1	0.81	0.39	76,76,76,76	0
85	MG	1	4088	1/1	0.81	0.25	44,44,44,44	0
85	MG	AS	217	1/1	0.81	0.47	44,44,44,44	0
85	MG	1	3963	1/1	0.81	0.25	45,45,45,45	0
85	MG	AR	4169	1/1	0.81	0.29	46,46,46,46	0
85	MG	1	3840	1/1	0.81	0.31	78,78,78,78	0
85	MG	1	3998	1/1	0.81	0.34	36,36,36,36	0
85	MG	AR	3760	1/1	0.81	0.14	53,53,53,53	0
85	MG	AR	3761	1/1	0.81	0.33	31,31,31,31	0
85	MG	AR	4182	1/1	0.81	0.37	79,79,79,79	0
85	MG	1	3966	1/1	0.81	0.18	69,69,69,69	0
84	OHX	1	3717	7/7	0.81	0.54	144,144,144,145	0
85	MG	CE	407	1/1	0.81	0.59	41,41,41,41	0
85	MG	CG	304	1/1	0.81	0.25	56,56,56,56	0
85	MG	CJ	301	1/1	0.81	0.22	78,78,78,78	0
85	MG	A	2152	1/1	0.81	0.70	43,43,43,43	0
85	MG	AR	3780	1/1	0.81	0.17	88,88,88,88	0
85	MG	AR	4200	1/1	0.81	0.25	48,48,48,48	0
85	MG	DE	201	1/1	0.81	0.28	72,72,72,72	0
85	MG	AR	4206	1/1	0.81	0.28	33,33,33,33	0
85	MG	1	3954	1/1	0.81	0.15	46,46,46,46	0
85	MG	j	302	1/1	0.81	0.25	35,35,35,35	0
85	MG	1	3987	1/1	0.81	0.68	65,65,65,65	0
85	MG	1	4170	1/1	0.81	0.49	41,41,41,41	0
85	MG	AR	4039	1/1	0.82	0.38	56,56,56,56	0
85	MG	6	2152	1/1	0.82	0.43	62,62,62,62	0
85	MG	AR	4056	1/1	0.82	0.38	44,44,44,44	0
85	MG	AR	4060	1/1	0.82	0.27	70,70,70,70	0
85	MG	AR	3836	1/1	0.82	0.45	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3985	1/1	0.82	0.60	50,50,50,50	0
85	MG	AR	3903	1/1	0.82	0.69	39,39,39,39	0
85	MG	6	2072	1/1	0.82	0.70	40,40,40,40	0
85	MG	AR	3944	1/1	0.82	0.17	38,38,38,38	0
85	MG	A	2098	1/1	0.82	0.48	65,65,65,65	0
85	MG	AR	4101	1/1	0.82	0.25	48,48,48,48	0
85	MG	AR	4224	1/1	0.82	0.49	47,47,47,47	0
85	MG	A	2107	1/1	0.82	0.31	80,80,80,80	0
85	MG	AR	3945	1/1	0.82	0.15	40,40,40,40	0
85	MG	AR	4239	1/1	0.82	0.42	39,39,39,39	0
85	MG	1	4045	1/1	0.82	0.34	39,39,39,39	0
85	MG	1	3925	1/1	0.82	0.13	46,46,46,46	0
85	MG	1	3855	1/1	0.82	0.32	44,44,44,44	0
85	MG	AR	3749	1/1	0.82	0.19	42,42,42,42	0
85	MG	AR	3751	1/1	0.82	0.36	36,36,36,36	0
85	MG	AR	3756	1/1	0.82	0.36	36,36,36,36	0
85	MG	AR	3984	1/1	0.82	0.65	50,50,50,50	0
85	MG	1	4013	1/1	0.82	0.33	52,52,52,52	0
85	MG	1	4119	1/1	0.82	0.28	35,35,35,35	0
85	MG	1	4060	1/1	0.82	0.36	44,44,44,44	0
85	MG	AT	221	1/1	0.82	0.76	52,52,52,52	0
85	MG	A	2140	1/1	0.82	0.82	82,82,82,82	0
85	MG	1	3863	1/1	0.82	0.20	55,55,55,55	0
85	MG	6	2099	1/1	0.82	0.39	51,51,51,51	0
85	MG	AT	228	1/1	0.82	0.37	47,47,47,47	0
85	MG	1	4165	1/1	0.82	0.40	24,24,24,24	0
85	MG	1	3955	1/1	0.82	0.43	51,51,51,51	0
85	MG	CE	403	1/1	0.82	0.32	22,22,22,22	0
85	MG	AR	4014	1/1	0.82	0.39	57,57,57,57	0
85	MG	AR	3794	1/1	0.82	0.24	34,34,34,34	0
85	MG	c6	201	1/1	0.82	0.22	89,89,89,89	0
85	MG	c9	201	1/1	0.82	0.10	79,79,79,79	0
85	MG	1	3997	1/1	0.82	0.17	54,54,54,54	0
85	MG	AR	3811	1/1	0.82	0.20	50,50,50,50	0
85	MG	1	3866	1/1	0.82	0.39	34,34,34,34	0
87	GOL	A	2160	6/6	0.82	0.35	60,60,60,60	0
85	MG	x	203	1/1	0.82	0.39	63,63,63,63	0
85	MG	1	3761	1/1	0.83	0.30	41,41,41,41	0
85	MG	6	2178	1/1	0.83	0.36	57,57,57,57	0
85	MG	AR	3812	1/1	0.83	0.42	32,32,32,32	0
85	MG	AR	3816	1/1	0.83	0.24	39,39,39,39	0
85	MG	A	2048	1/1	0.83	0.33	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	2034	7/7	0.83	0.20	231,232,232,232	0
85	MG	4	234	1/1	0.83	0.43	44,44,44,44	0
85	MG	A	2081	1/1	0.83	0.31	66,66,66,66	0
85	MG	1	3779	1/1	0.83	0.48	55,55,55,55	0
85	MG	6	2186	1/1	0.83	0.31	107,107,107,107	0
85	MG	1	3739	1/1	0.83	0.32	51,51,51,51	0
85	MG	6	2111	1/1	0.83	0.42	61,61,61,61	0
85	MG	A	2094	1/1	0.83	0.38	110,110,110,110	0
85	MG	AR	3911	1/1	0.83	0.42	40,40,40,40	0
85	MG	AR	4075	1/1	0.83	0.31	36,36,36,36	0
85	MG	AR	4221	1/1	0.83	0.28	35,35,35,35	0
85	MG	AR	4076	1/1	0.83	0.32	48,48,48,48	0
85	MG	1	3993	1/1	0.83	0.62	42,42,42,42	0
85	MG	1	4098	1/1	0.83	0.27	47,47,47,47	0
85	MG	AR	4089	1/1	0.83	0.10	62,62,62,62	0
85	MG	AR	4232	1/1	0.83	0.43	28,28,28,28	0
85	MG	AR	4090	1/1	0.83	0.49	57,57,57,57	0
85	MG	AR	4240	1/1	0.83	0.55	70,70,70,70	0
85	MG	AR	4094	1/1	0.83	0.31	43,43,43,43	0
85	MG	A	2127	1/1	0.83	0.29	83,83,83,83	0
85	MG	AR	4245	1/1	0.83	0.22	26,26,26,26	0
85	MG	1	3819	1/1	0.83	0.40	27,27,27,27	0
85	MG	1	3870	1/1	0.83	0.28	47,47,47,47	0
85	MG	6	2138	1/1	0.83	0.30	73,73,73,73	0
85	MG	6	2140	1/1	0.83	0.40	69,69,69,69	0
85	MG	1	4118	1/1	0.83	0.34	43,43,43,43	0
85	MG	AR	4116	1/1	0.83	0.30	99,99,99,99	0
85	MG	v	303	1/1	0.83	0.24	44,44,44,44	0
85	MG	AR	3973	1/1	0.83	0.23	40,40,40,40	0
85	MG	AR	3975	1/1	0.83	0.27	31,31,31,31	0
85	MG	AR	3752	1/1	0.83	0.21	37,37,37,37	0
85	MG	1	4050	1/1	0.83	0.36	31,31,31,31	0
84	OHX	AR	3664	7/7	0.83	0.43	180,180,181,181	0
85	MG	AR	3994	1/1	0.83	0.32	25,25,25,25	0
85	MG	6	2064	1/1	0.83	0.68	53,53,53,53	0
85	MG	6	2068	1/1	0.83	0.46	61,61,61,61	0
85	MG	6	2070	1/1	0.83	0.39	73,73,73,73	0
84	OHX	AR	3686	7/7	0.83	0.38	156,156,156,157	0
85	MG	1	3972	1/1	0.83	0.85	45,45,45,45	0
84	OHX	6	2045	7/7	0.83	0.34	141,141,142,142	0
85	MG	1	3843	1/1	0.83	0.41	24,24,24,24	0
85	MG	AR	4173	1/1	0.83	0.31	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3841	1/1	0.84	0.29	54,54,54,54	0
85	MG	1	4145	1/1	0.84	0.33	42,42,42,42	0
85	MG	1	4070	1/1	0.84	0.20	68,68,68,68	0
85	MG	1	3853	1/1	0.84	0.55	48,48,48,48	0
85	MG	AR	4086	1/1	0.84	0.40	42,42,42,42	0
85	MG	1	4202	1/1	0.84	0.56	19,19,19,19	0
85	MG	1	4003	1/1	0.84	0.35	79,79,79,79	0
85	MG	AR	4188	1/1	0.84	1.10	31,31,31,31	0
84	OHX	AR	3719	7/7	0.84	0.42	133,133,133,133	0
85	MG	1	4006	1/1	0.84	0.57	47,47,47,47	0
85	MG	AR	4019	1/1	0.84	0.27	45,45,45,45	0
85	MG	AT	226	1/1	0.84	0.30	63,63,63,63	0
85	MG	AR	4021	1/1	0.84	0.17	82,82,82,82	0
85	MG	1	4091	1/1	0.84	0.32	47,47,47,47	0
85	MG	AR	3960	1/1	0.84	0.21	41,41,41,41	0
85	MG	6	2118	1/1	0.84	0.14	93,93,93,93	0
85	MG	AR	4113	1/1	0.84	0.58	37,37,37,37	0
85	MG	AR	4032	1/1	0.84	0.37	48,48,48,48	0
85	MG	1	3931	1/1	0.84	0.53	32,32,32,32	0
85	MG	AR	4035	1/1	0.84	0.38	43,43,43,43	0
85	MG	CP	502	1/1	0.84	0.42	45,45,45,45	0
85	MG	CQ	204	1/1	0.84	0.41	30,30,30,30	0
85	MG	CR	202	1/1	0.84	0.28	29,29,29,29	0
85	MG	AB	207	1/1	0.84	0.24	34,34,34,34	0
85	MG	6	2173	1/1	0.84	0.73	48,48,48,48	0
85	MG	AR	4044	1/1	0.84	0.56	60,60,60,60	0
85	MG	AR	4045	1/1	0.84	0.30	55,55,55,55	0
85	MG	A	2159	1/1	0.84	0.93	64,64,64,64	0
85	MG	AR	4234	1/1	0.84	0.45	32,32,32,32	0
85	MG	A	2047	1/1	0.84	0.65	55,55,55,55	0
85	MG	AR	4046	1/1	0.84	0.26	46,46,46,46	0
85	MG	1	4160	1/1	0.84	0.32	34,34,34,34	0
84	OHX	AR	3717	7/7	0.84	0.42	144,144,144,144	0
85	MG	A	2068	1/1	0.84	0.56	84,84,84,84	0
85	MG	A	2069	1/1	0.84	0.49	58,58,58,58	0
85	MG	1	4163	1/1	0.84	0.24	44,44,44,44	0
85	MG	AR	4253	1/1	0.84	0.17	41,41,41,41	0
85	MG	1	4065	1/1	0.84	0.31	48,48,48,48	0
85	MG	1	3940	1/1	0.85	0.37	43,43,43,43	0
85	MG	A	2089	1/1	0.85	0.19	90,90,90,90	0
85	MG	1	3967	1/1	0.85	0.20	38,38,38,38	0
85	MG	1	3799	1/1	0.85	0.41	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2095	1/1	0.85	0.25	96,96,96,96	0
85	MG	1	3754	1/1	0.85	0.52	37,37,37,37	0
85	MG	1	4111	1/1	0.85	0.55	44,44,44,44	0
85	MG	A	2101	1/1	0.85	0.38	64,64,64,64	0
85	MG	AS	226	1/1	0.85	0.21	67,67,67,67	0
84	OHX	AR	3705	7/7	0.85	0.36	141,142,142,142	0
85	MG	AR	3988	1/1	0.85	0.81	50,50,50,50	0
85	MG	1	3984	1/1	0.85	0.27	70,70,70,70	0
85	MG	6	2145	1/1	0.85	0.20	59,59,59,59	0
85	MG	1	4064	1/1	0.85	0.30	58,58,58,58	0
85	MG	AR	4183	1/1	0.85	0.23	55,55,55,55	0
85	MG	1	3805	1/1	0.85	0.20	29,29,29,29	0
84	OHX	A	1971	7/7	0.85	0.23	149,150,151,151	0
85	MG	1	3874	1/1	0.85	0.55	49,49,49,49	0
85	MG	AR	4093	1/1	0.85	0.37	46,46,46,46	0
85	MG	AR	3862	1/1	0.85	0.21	56,56,56,56	0
85	MG	AR	4096	1/1	0.85	0.32	54,54,54,54	0
85	MG	AR	3873	1/1	0.85	0.46	31,31,31,31	0
85	MG	AR	4017	1/1	0.85	0.31	95,95,95,95	0
85	MG	4	220	1/1	0.85	0.34	64,64,64,64	0
85	MG	AR	4103	1/1	0.85	0.19	47,47,47,47	0
85	MG	A	2142	1/1	0.85	0.13	80,80,80,80	0
85	MG	1	4135	1/1	0.85	0.48	51,51,51,51	0
85	MG	1	4077	1/1	0.85	0.27	33,33,33,33	0
84	OHX	AR	3728	7/7	0.85	0.42	151,152,152,152	0
85	MG	AR	4025	1/1	0.85	0.25	31,31,31,31	0
85	MG	1	4082	1/1	0.85	0.30	35,35,35,35	0
85	MG	AR	3759	1/1	0.85	0.62	34,34,34,34	0
85	MG	1	3959	1/1	0.85	0.27	66,66,66,66	0
85	MG	AR	4238	1/1	0.85	0.38	36,36,36,36	0
85	MG	A	2050	1/1	0.85	0.39	67,67,67,67	0
85	MG	1	4042	1/1	0.85	0.41	48,48,48,48	0
85	MG	AR	3958	1/1	0.85	0.56	38,38,38,38	0
85	MG	1	3731	1/1	0.85	0.49	36,36,36,36	0
85	MG	AR	4140	1/1	0.85	0.49	44,44,44,44	0
85	MG	6	2110	1/1	0.85	0.54	54,54,54,54	0
85	MG	AR	4142	1/1	0.85	0.31	46,46,46,46	0
85	MG	1	3797	1/1	0.85	0.18	79,79,79,79	0
85	MG	DC	202	1/1	0.86	0.30	48,48,48,48	0
85	MG	6	2066	1/1	0.86	0.35	74,74,74,74	0
85	MG	AR	3954	1/1	0.86	0.30	44,44,44,44	0
85	MG	1	4038	1/1	0.86	0.72	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	DQ	203	1/1	0.86	0.22	45,45,45,45	0
85	MG	AR	4187	1/1	0.86	0.43	36,36,36,36	0
85	MG	AR	3957	1/1	0.86	0.13	55,55,55,55	0
85	MG	AR	4071	1/1	0.86	0.27	39,39,39,39	0
85	MG	3	216	1/1	0.86	0.40	58,58,58,58	0
85	MG	1	3759	1/1	0.86	0.12	41,41,41,41	0
85	MG	1	3926	1/1	0.86	0.16	37,37,37,37	0
84	OHX	1	3709	7/7	0.86	0.35	157,158,158,158	0
85	MG	6	2161	1/1	0.86	0.49	58,58,58,58	0
84	OHX	6	2046	7/7	0.86	0.36	151,152,152,152	0
85	MG	A	2075	1/1	0.86	0.43	74,74,74,74	0
85	MG	1	3936	1/1	0.86	0.54	61,61,61,61	0
84	OHX	1	3714	7/7	0.86	0.51	146,147,147,148	0
85	MG	AR	4092	1/1	0.86	0.32	47,47,47,47	0
85	MG	AR	3982	1/1	0.86	0.24	53,53,53,53	0
85	MG	6	2087	1/1	0.86	0.30	56,56,56,56	0
84	OHX	AR	3734	7/7	0.86	0.55	148,148,148,149	0
85	MG	A	2092	1/1	0.86	0.27	91,91,91,91	0
85	MG	6	2090	1/1	0.86	0.31	49,49,49,49	0
85	MG	AR	3991	1/1	0.86	0.14	98,98,98,98	0
84	OHX	1	3702	7/7	0.86	0.22	219,219,219,219	0
85	MG	1	3981	1/1	0.86	0.50	50,50,50,50	0
85	MG	6	2105	1/1	0.86	0.48	64,64,64,64	0
85	MG	AR	3814	1/1	0.86	0.31	105,105,105,105	0
85	MG	1	4007	1/1	0.86	0.42	29,29,29,29	0
85	MG	A	2109	1/1	0.86	0.41	60,60,60,60	0
85	MG	A	2110	1/1	0.86	0.67	116,116,116,116	0
85	MG	1	4009	1/1	0.86	0.66	42,42,42,42	0
85	MG	AR	4248	1/1	0.86	0.94	45,45,45,45	0
85	MG	6	2115	1/1	0.86	0.41	85,85,85,85	0
85	MG	AR	4118	1/1	0.86	0.41	31,31,31,31	0
85	MG	AR	3829	1/1	0.86	0.66	66,66,66,66	0
85	MG	AR	4120	1/1	0.86	0.27	31,31,31,31	0
84	OHX	A	1946	7/7	0.86	0.22	165,166,166,167	0
85	MG	1	3752	1/1	0.86	0.42	57,57,57,57	0
85	MG	AR	3840	1/1	0.86	0.31	47,47,47,47	0
85	MG	AR	4127	1/1	0.86	0.17	77,77,77,77	0
85	MG	6	2122	1/1	0.86	0.48	61,61,61,61	0
85	MG	AR	3852	1/1	0.86	0.24	37,37,37,37	0
85	MG	1	4183	1/1	0.86	0.17	44,44,44,44	0
85	MG	AR	4029	1/1	0.86	0.22	42,42,42,42	0
85	MG	AR	4145	1/1	0.86	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4146	1/1	0.86	0.19	34,34,34,34	0
85	MG	AT	225	1/1	0.86	0.91	53,53,53,53	0
85	MG	v	304	1/1	0.86	0.62	52,52,52,52	0
85	MG	AT	227	1/1	0.86	0.89	79,79,79,79	0
85	MG	1	3953	1/1	0.86	0.20	46,46,46,46	0
85	MG	AR	4157	1/1	0.86	0.28	75,75,75,75	0
85	MG	A	2156	1/1	0.86	0.62	45,45,45,45	0
85	MG	AR	4159	1/1	0.86	0.38	36,36,36,36	0
85	MG	T	202	1/1	0.86	0.09	97,97,97,97	0
85	MG	U	201	1/1	0.86	0.42	76,76,76,76	0
85	MG	AR	3894	1/1	0.86	0.53	45,45,45,45	0
85	MG	6	2195	1/1	0.86	0.65	35,35,35,35	0
85	MG	AR	4164	1/1	0.86	0.23	41,41,41,41	0
84	OHX	1	3724	7/7	0.86	0.22	113,113,113,113	0
85	MG	AB	202	1/1	0.86	0.31	29,29,29,29	0
87	GOL	v	305	6/6	0.86	0.26	38,38,38,38	0
85	MG	AR	3935	1/1	0.86	0.62	49,49,49,49	0
85	MG	6	2059	1/1	0.86	0.43	70,70,70,70	0
85	MG	1	3832	1/1	0.86	0.41	26,26,26,26	0
85	MG	CR	203	1/1	0.86	0.15	95,95,95,95	0
85	MG	CR	204	1/1	0.86	0.21	46,46,46,46	0
85	MG	1	3908	1/1	0.87	0.50	62,62,62,62	0
85	MG	1	3961	1/1	0.87	0.19	40,40,40,40	0
85	MG	A	2088	1/1	0.87	0.53	59,59,59,59	0
85	MG	1	4000	1/1	0.87	0.23	43,43,43,43	0
84	OHX	AR	3741	7/7	0.87	0.38	207,208,208,208	0
85	MG	1	4193	1/1	0.87	0.37	23,23,23,23	0
84	OHX	1	3708	7/7	0.87	0.39	134,134,134,134	0
85	MG	1	4128	1/1	0.87	0.45	51,51,51,51	0
85	MG	1	4210	1/1	0.87	0.30	24,24,24,24	0
85	MG	6	2079	1/1	0.87	0.24	45,45,45,45	0
85	MG	6	2164	1/1	0.87	0.35	53,53,53,53	0
85	MG	AR	4080	1/1	0.87	0.51	32,32,32,32	0
85	MG	1	4211	1/1	0.87	0.63	42,42,42,42	0
84	OHX	z	201	7/7	0.87	0.39	155,156,157,157	0
85	MG	6	2169	1/1	0.87	0.63	49,49,49,49	0
84	OHX	A	2007	7/7	0.87	0.26	200,200,201,201	0
85	MG	1	3971	1/1	0.87	0.46	35,35,35,35	0
85	MG	1	4138	1/1	0.87	0.28	33,33,33,33	0
85	MG	1	3845	1/1	0.87	0.40	18,18,18,18	0
84	OHX	A	2025	7/7	0.87	0.48	173,173,173,173	0
84	OHX	AR	3640	7/7	0.87	0.32	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	CF	403	1/1	0.87	0.40	34,34,34,34	0
85	MG	1	3944	1/1	0.87	0.48	32,32,32,32	0
85	MG	1	3767	1/1	0.87	0.12	60,60,60,60	0
85	MG	A	2129	1/1	0.87	0.30	57,57,57,57	0
85	MG	CL	302	1/1	0.87	0.36	68,68,68,68	0
84	OHX	AR	3652	7/7	0.87	0.44	112,112,113,113	0
85	MG	A	2134	1/1	0.87	0.35	70,70,70,70	0
85	MG	AR	4207	1/1	0.87	0.50	48,48,48,48	0
85	MG	1	4154	1/1	0.87	0.21	46,46,46,46	0
85	MG	AR	3842	1/1	0.87	0.16	47,47,47,47	0
85	MG	AR	3845	1/1	0.87	0.41	23,23,23,23	0
85	MG	AR	3851	1/1	0.87	0.29	38,38,38,38	0
85	MG	CU	201	1/1	0.87	0.40	38,38,38,38	0
85	MG	DA	201	1/1	0.87	0.28	48,48,48,48	0
85	MG	1	3778	1/1	0.87	0.46	49,49,49,49	0
85	MG	AR	4020	1/1	0.87	0.23	41,41,41,41	0
85	MG	n	201	1/1	0.87	0.26	43,43,43,43	0
85	MG	6	2120	1/1	0.87	0.42	69,69,69,69	0
84	OHX	6	1960	7/7	0.87	0.22	118,118,118,118	0
85	MG	1	3786	1/1	0.87	0.20	40,40,40,40	0
84	OHX	6	2040	7/7	0.87	0.29	184,184,185,185	0
85	MG	AR	4124	1/1	0.87	0.18	39,39,39,39	0
85	MG	1	3892	1/1	0.87	0.41	23,23,23,23	0
85	MG	AR	3913	1/1	0.87	0.43	26,26,26,26	0
85	MG	s6	301	1/1	0.87	0.29	77,77,77,77	0
85	MG	A	2053	1/1	0.87	0.72	57,57,57,57	0
85	MG	1	3996	1/1	0.87	0.44	64,64,64,64	0
85	MG	d4	201	1/1	0.87	0.38	53,53,53,53	0
85	MG	1	4108	1/1	0.87	0.21	42,42,42,42	0
85	MG	AR	4246	1/1	0.87	0.41	22,22,22,22	0
85	MG	6	2141	1/1	0.87	0.32	52,52,52,52	0
85	MG	AR	4250	1/1	0.87	0.80	59,59,59,59	0
85	MG	x	209	1/1	0.87	0.66	39,39,39,39	0
85	MG	AR	3947	1/1	0.87	0.50	44,44,44,44	0
85	MG	AS	215	1/1	0.88	0.36	58,58,58,58	0
85	MG	3	220	1/1	0.88	0.17	68,68,68,68	0
85	MG	A	2087	1/1	0.88	0.50	78,78,78,78	0
85	MG	AR	4051	1/1	0.88	0.38	40,40,40,40	0
85	MG	1	3803	1/1	0.88	0.42	41,41,41,41	0
85	MG	AS	223	1/1	0.88	0.28	41,41,41,41	0
85	MG	AS	224	1/1	0.88	0.24	55,55,55,55	0
85	MG	A	2093	1/1	0.88	0.14	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4137	1/1	0.88	0.17	55,55,55,55	0
85	MG	6	2171	1/1	0.88	0.25	56,56,56,56	0
85	MG	4	222	1/1	0.88	0.28	33,33,33,33	0
85	MG	1	3939	1/1	0.88	0.29	39,39,39,39	0
84	OHX	A	2036	7/7	0.88	0.15	252,253,253,253	0
84	OHX	A	2041	7/7	0.88	0.46	139,139,140,140	0
85	MG	6	2103	1/1	0.88	0.33	69,69,69,69	0
85	MG	1	4084	1/1	0.88	0.27	32,32,32,32	0
84	OHX	1	3687	7/7	0.88	0.42	149,149,150,150	0
85	MG	AR	4175	1/1	0.88	0.25	35,35,35,35	0
85	MG	1	3945	1/1	0.88	0.29	57,57,57,57	0
85	MG	AR	3838	1/1	0.88	0.37	27,27,27,27	0
85	MG	1	4033	1/1	0.88	0.21	58,58,58,58	0
84	OHX	AR	3707	7/7	0.88	0.25	129,129,130,130	0
85	MG	CE	404	1/1	0.88	0.29	27,27,27,27	0
84	OHX	AR	3517	7/7	0.88	0.16	145,146,146,146	0
85	MG	AR	3999	1/1	0.88	0.30	44,44,44,44	0
85	MG	1	3785	1/1	0.88	0.45	25,25,25,25	0
84	OHX	6	2018	7/7	0.88	0.23	189,189,189,189	0
85	MG	1	3787	1/1	0.88	0.46	46,46,46,46	0
85	MG	AR	3861	1/1	0.88	0.37	30,30,30,30	0
85	MG	A	2133	1/1	0.88	0.20	72,72,72,72	0
85	MG	1	3897	1/1	0.88	0.21	46,46,46,46	0
85	MG	AR	3868	1/1	0.88	0.46	25,25,25,25	0
85	MG	1	4162	1/1	0.88	0.25	40,40,40,40	0
85	MG	1	4110	1/1	0.88	0.24	30,30,30,30	0
84	OHX	AR	3720	7/7	0.88	0.33	152,152,152,152	0
85	MG	x	208	1/1	0.88	0.33	46,46,46,46	0
85	MG	AR	4023	1/1	0.88	0.23	31,31,31,31	0
85	MG	AR	3907	1/1	0.88	0.63	25,25,25,25	0
85	MG	1	4113	1/1	0.88	0.26	57,57,57,57	0
85	MG	1	4115	1/1	0.88	0.23	36,36,36,36	0
84	OHX	AR	3722	7/7	0.88	0.31	140,141,141,141	0
85	MG	DL	102	1/1	0.88	0.50	39,39,39,39	0
84	OHX	AR	3726	7/7	0.88	0.42	118,118,118,118	0
85	MG	1	3927	1/1	0.88	0.24	42,42,42,42	0
85	MG	AR	4126	1/1	0.88	0.69	83,83,83,83	0
85	MG	1	4125	1/1	0.88	0.38	23,23,23,23	0
85	MG	1	3758	1/1	0.88	0.50	32,32,32,32	0
85	MG	AR	4130	1/1	0.88	0.15	31,31,31,31	0
84	OHX	AR	3690	7/7	0.88	0.47	117,118,118,118	0
85	MG	1	3933	1/1	0.88	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	3	212	1/1	0.88	0.44	62,62,62,62	0
85	MG	AR	4251	1/1	0.88	0.41	59,59,59,59	0
85	MG	1	3934	1/1	0.88	0.44	54,54,54,54	0
85	MG	A	2070	1/1	0.88	0.53	79,79,79,79	0
85	MG	AR	4047	1/1	0.88	0.14	54,54,54,54	0
85	MG	A	2080	1/1	0.88	0.39	65,65,65,65	0
85	MG	AR	4149	1/1	0.88	0.38	66,66,66,66	0
85	MG	AR	4150	1/1	0.88	0.18	44,44,44,44	0
85	MG	DI	201	1/1	0.89	0.22	68,68,68,68	0
85	MG	AR	4050	1/1	0.89	0.31	91,91,91,91	0
85	MG	3	211	1/1	0.89	0.35	38,38,38,38	0
85	MG	AR	4186	1/1	0.89	0.21	33,33,33,33	0
85	MG	1	3873	1/1	0.89	0.23	48,48,48,48	0
85	MG	AR	4059	1/1	0.89	0.20	47,47,47,47	0
85	MG	1	3777	1/1	0.89	0.17	30,30,30,30	0
85	MG	6	2190	1/1	0.89	0.48	66,66,66,66	0
85	MG	AR	4067	1/1	0.89	0.34	34,34,34,34	0
85	MG	AR	4069	1/1	0.89	0.23	26,26,26,26	0
85	MG	1	3881	1/1	0.89	0.55	31,31,31,31	0
85	MG	AR	4073	1/1	0.89	0.39	40,40,40,40	0
85	MG	AR	4210	1/1	0.89	0.72	54,54,54,54	0
85	MG	3	221	1/1	0.89	0.47	34,34,34,34	0
85	MG	AR	3943	1/1	0.89	0.10	41,41,41,41	0
85	MG	1	3886	1/1	0.89	0.41	21,21,21,21	0
85	MG	1	4130	1/1	0.89	0.27	45,45,45,45	0
85	MG	AR	4083	1/1	0.89	0.28	31,31,31,31	0
85	MG	1	3995	1/1	0.89	0.31	34,34,34,34	0
85	MG	4	228	1/1	0.89	0.26	54,54,54,54	0
84	OHX	AR	3733	7/7	0.89	0.33	187,188,188,188	0
84	OHX	c4	201	7/7	0.89	0.53	152,152,153,153	0
85	MG	1	3726	1/1	0.89	0.84	54,54,54,54	0
85	MG	1	3999	1/1	0.89	0.33	41,41,41,41	0
85	MG	1	4073	1/1	0.89	0.38	40,40,40,40	0
85	MG	1	3956	1/1	0.89	0.54	34,34,34,34	0
85	MG	AR	3967	1/1	0.89	0.55	42,42,42,42	0
85	MG	6	2123	1/1	0.89	0.24	69,69,69,69	0
85	MG	AR	4099	1/1	0.89	0.16	41,41,41,41	0
85	MG	4	237	1/1	0.89	0.20	38,38,38,38	0
85	MG	1	3915	1/1	0.89	0.12	36,36,36,36	0
85	MG	4	240	1/1	0.89	0.57	32,32,32,32	0
85	MG	AR	3764	1/1	0.89	0.34	33,33,33,33	0
85	MG	6	2134	1/1	0.89	0.22	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3777	1/1	0.89	0.31	37,37,37,37	0
85	MG	1	4080	1/1	0.89	0.22	35,35,35,35	0
84	OHX	6	2051	7/7	0.89	0.29	172,172,172,173	0
85	MG	1	3960	1/1	0.89	0.21	33,33,33,33	0
85	MG	6	2144	1/1	0.89	0.38	74,74,74,74	0
85	MG	r	302	1/1	0.89	0.22	37,37,37,37	0
85	MG	1	4005	1/1	0.89	0.35	36,36,36,36	0
85	MG	6	2149	1/1	0.89	0.32	46,46,46,46	0
85	MG	6	2150	1/1	0.89	0.13	77,77,77,77	0
85	MG	A	2125	1/1	0.89	0.85	56,56,56,56	0
84	OHX	6	1975	7/7	0.89	0.43	120,120,120,120	0
84	OHX	AR	3602	7/7	0.89	0.18	143,143,144,144	0
85	MG	1	3928	1/1	0.89	0.27	34,34,34,34	0
84	OHX	CF	401	7/7	0.89	0.31	146,146,147,147	0
84	OHX	6	2006	7/7	0.89	0.29	151,151,152,152	0
85	MG	AR	4135	1/1	0.89	0.18	62,62,62,62	0
85	MG	x	207	1/1	0.89	0.31	33,33,33,33	0
85	MG	AR	3834	1/1	0.89	0.47	33,33,33,33	0
85	MG	1	3932	1/1	0.89	0.19	55,55,55,55	0
84	OHX	1	3723	7/7	0.89	0.35	113,113,113,113	0
84	OHX	A	1985	7/7	0.89	0.31	140,140,141,141	0
85	MG	AT	229	1/1	0.89	0.42	55,55,55,55	0
85	MG	AR	4148	1/1	0.89	0.28	43,43,43,43	0
85	MG	A	2149	1/1	0.89	0.25	60,60,60,60	0
85	MG	1	4029	1/1	0.89	0.11	47,47,47,47	0
85	MG	1	4184	1/1	0.89	0.26	36,36,36,36	0
85	MG	AR	4153	1/1	0.89	0.19	88,88,88,88	0
85	MG	AR	4154	1/1	0.89	0.32	39,39,39,39	0
85	MG	AR	4028	1/1	0.89	0.19	41,41,41,41	0
84	OHX	1	3620	7/7	0.89	0.35	118,118,118,118	0
85	MG	D	301	1/1	0.89	0.58	58,58,58,58	0
85	MG	1	4036	1/1	0.89	0.42	70,70,70,70	0
85	MG	1	3982	1/1	0.89	0.37	32,32,32,32	0
84	OHX	A	2015	7/7	0.89	0.41	169,170,171,172	0
84	OHX	1	3712	7/7	0.89	0.34	133,133,133,133	0
85	MG	AR	4163	1/1	0.89	0.23	62,62,62,62	0
84	OHX	1	3721	7/7	0.89	0.35	127,127,127,128	0
84	OHX	AR	3729	7/7	0.89	0.46	120,120,120,121	0
85	MG	AR	4043	1/1	0.89	0.38	37,37,37,37	0
85	MG	CR	205	1/1	0.89	0.40	31,31,31,31	0
85	MG	d5	201	1/1	0.89	0.09	71,71,71,71	0
85	MG	AR	3882	1/1	0.89	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	4219	1/1	0.89	0.26	98,98,98,98	0
85	MG	DC	201	1/1	0.89	0.45	30,30,30,30	0
85	MG	AR	3891	1/1	0.89	0.27	69,69,69,69	0
85	MG	6	2085	1/1	0.89	0.47	75,75,75,75	0
85	MG	AR	3899	1/1	0.89	0.60	45,45,45,45	0
85	MG	AR	3765	1/1	0.90	0.39	71,71,71,71	0
85	MG	AR	3773	1/1	0.90	0.29	41,41,41,41	0
84	OHX	A	2042	7/7	0.90	0.21	172,173,173,174	0
84	OHX	A	2043	7/7	0.90	0.19	155,156,156,157	0
85	MG	1	4102	1/1	0.90	0.37	57,57,57,57	0
84	OHX	AR	3692	7/7	0.90	0.31	170,171,171,171	0
84	OHX	1	3656	7/7	0.90	0.50	143,143,143,144	0
85	MG	1	3818	1/1	0.90	0.43	39,39,39,39	0
84	OHX	6	2001	7/7	0.90	0.28	119,120,120,120	0
85	MG	1	3737	1/1	0.90	0.93	57,57,57,57	0
85	MG	AR	3807	1/1	0.90	0.38	25,25,25,25	0
84	OHX	1	3710	7/7	0.90	0.33	136,137,137,137	0
85	MG	AR	4166	1/1	0.90	0.16	38,38,38,38	0
85	MG	1	4116	1/1	0.90	0.52	44,44,44,44	0
85	MG	4	231	1/1	0.90	0.23	58,58,58,58	0
85	MG	6	2139	1/1	0.90	0.22	45,45,45,45	0
85	MG	AR	4033	1/1	0.90	0.26	40,40,40,40	0
85	MG	1	4117	1/1	0.90	0.31	41,41,41,41	0
85	MG	AR	3821	1/1	0.90	0.21	42,42,42,42	0
85	MG	A	2051	1/1	0.90	0.47	67,67,67,67	0
85	MG	1	3830	1/1	0.90	0.22	44,44,44,44	0
84	OHX	1	3501	7/7	0.90	0.17	126,126,127,127	0
85	MG	AR	4040	1/1	0.90	0.26	43,43,43,43	0
85	MG	A	2065	1/1	0.90	0.73	57,57,57,57	0
85	MG	AR	4042	1/1	0.90	0.12	57,57,57,57	0
85	MG	1	4015	1/1	0.90	0.37	67,67,67,67	0
85	MG	1	4020	1/1	0.90	0.39	34,34,34,34	0
84	OHX	6	2021	7/7	0.90	0.25	181,181,182,182	0
84	OHX	6	2039	7/7	0.90	0.62	132,133,133,134	0
85	MG	AR	4197	1/1	0.90	0.27	35,35,35,35	0
85	MG	1	4028	1/1	0.90	0.16	46,46,46,46	0
84	OHX	1	3626	7/7	0.90	0.35	124,124,124,124	0
85	MG	1	3851	1/1	0.90	0.36	34,34,34,34	0
84	OHX	6	2041	7/7	0.90	0.34	143,144,145,145	0
84	OHX	1	3642	7/7	0.90	0.45	135,135,136,136	0
84	OHX	1	3718	7/7	0.90	0.39	149,149,149,149	0
85	MG	t	201	1/1	0.90	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3962	1/1	0.90	0.41	39,39,39,39	0
85	MG	AR	4064	1/1	0.90	0.24	38,38,38,38	0
84	OHX	1	3719	7/7	0.90	0.52	120,120,121,121	0
85	MG	6	2166	1/1	0.90	0.49	53,53,53,53	0
85	MG	AR	4070	1/1	0.90	0.19	50,50,50,50	0
85	MG	1	4147	1/1	0.90	0.21	48,48,48,48	0
85	MG	1	3762	1/1	0.90	0.56	30,30,30,30	0
85	MG	A	2102	1/1	0.90	0.49	58,58,58,58	0
85	MG	x	205	1/1	0.90	0.66	33,33,33,33	0
85	MG	A	2106	1/1	0.90	0.50	58,58,58,58	0
85	MG	1	3766	1/1	0.90	0.16	73,73,73,73	0
85	MG	1	3869	1/1	0.90	0.49	34,34,34,34	0
84	OHX	6	2052	7/7	0.90	0.33	143,144,144,144	0
85	MG	1	4055	1/1	0.90	0.17	33,33,33,33	0
85	MG	A	2113	1/1	0.90	0.48	73,73,73,73	0
85	MG	AR	4084	1/1	0.90	0.22	34,34,34,34	0
85	MG	1	3771	1/1	0.90	0.42	33,33,33,33	0
85	MG	1	4156	1/1	0.90	0.19	44,44,44,44	0
85	MG	AR	3914	1/1	0.90	0.43	32,32,32,32	0
84	OHX	AR	3738	7/7	0.90	0.15	141,142,142,142	0
85	MG	A	2122	1/1	0.90	0.17	86,86,86,86	0
84	OHX	AM	101	7/7	0.90	0.43	121,121,121,121	0
85	MG	AR	4252	1/1	0.90	0.37	50,50,50,50	0
84	OHX	1	3696	7/7	0.90	0.39	146,146,147,147	0
84	OHX	1	3700	7/7	0.90	0.36	148,148,149,149	0
84	OHX	AR	3604	7/7	0.90	0.19	158,159,159,159	0
85	MG	AR	3946	1/1	0.90	0.30	59,59,59,59	0
85	MG	AS	213	1/1	0.90	0.45	26,26,26,26	0
85	MG	A	2132	1/1	0.90	0.26	98,98,98,98	0
85	MG	1	3898	1/1	0.90	0.46	33,33,33,33	0
85	MG	AR	4098	1/1	0.90	0.20	46,46,46,46	0
85	MG	AS	218	1/1	0.90	0.30	33,33,33,33	0
85	MG	AR	3948	1/1	0.90	0.54	40,40,40,40	0
85	MG	6	2078	1/1	0.90	0.45	42,42,42,42	0
84	OHX	AR	3631	7/7	0.90	0.18	175,176,177,177	0
85	MG	6	2080	1/1	0.90	0.64	69,69,69,69	0
85	MG	AR	3956	1/1	0.90	0.22	29,29,29,29	0
84	OHX	1	3644	7/7	0.90	0.25	166,167,167,167	0
85	MG	6	2082	1/1	0.90	0.48	54,54,54,54	0
84	OHX	AR	3646	7/7	0.90	0.37	108,108,108,108	0
85	MG	6	2198	1/1	0.90	0.56	49,49,49,49	0
85	MG	1	3793	1/1	0.90	0.30	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AB	204	1/1	0.90	0.29	52,52,52,52	0
84	OHX	3	209	7/7	0.90	0.28	152,152,152,152	0
84	OHX	A	2026	7/7	0.90	0.40	123,123,124,124	0
85	MG	AG	202	1/1	0.90	0.20	43,43,43,43	0
85	MG	AH	202	1/1	0.90	0.15	58,58,58,58	0
85	MG	1	4085	1/1	0.90	0.39	51,51,51,51	0
85	MG	AR	3750	1/1	0.90	0.41	27,27,27,27	0
85	MG	CD	301	1/1	0.90	0.36	34,34,34,34	0
85	MG	s4	301	1/1	0.90	0.23	59,59,59,59	0
85	MG	1	4198	1/1	0.90	0.60	43,43,43,43	0
84	OHX	A	2029	7/7	0.90	0.20	184,184,184,184	0
85	MG	AR	3753	1/1	0.90	0.33	26,26,26,26	0
85	MG	AR	4134	1/1	0.90	0.27	44,44,44,44	0
85	MG	AR	3755	1/1	0.90	0.18	56,56,56,56	0
84	OHX	A	2030	7/7	0.90	0.47	142,143,143,144	0
85	MG	1	4209	1/1	0.90	0.67	48,48,48,48	0
84	OHX	x	201	7/7	0.90	0.39	110,110,110,110	0
84	OHX	1	3707	7/7	0.90	0.40	125,125,126,126	0
84	OHX	1	3653	7/7	0.90	0.29	133,133,133,133	0
85	MG	AR	4009	1/1	0.90	0.34	37,37,37,37	0
85	MG	1	4035	1/1	0.91	0.60	47,47,47,47	0
85	MG	1	3746	1/1	0.91	0.41	26,26,26,26	0
85	MG	1	4037	1/1	0.91	0.30	30,30,30,30	0
85	MG	6	2196	1/1	0.91	0.76	48,48,48,48	0
84	OHX	AR	3665	7/7	0.91	0.39	133,133,133,133	0
84	OHX	AR	3745	7/7	0.91	0.34	128,128,128,128	0
85	MG	AB	201	1/1	0.91	0.28	34,34,34,34	0
84	OHX	AS	211	7/7	0.91	0.29	141,141,142,142	0
85	MG	AB	203	1/1	0.91	0.34	32,32,32,32	0
84	OHX	AT	213	7/7	0.91	0.25	137,137,137,137	0
85	MG	AB	205	1/1	0.91	0.22	40,40,40,40	0
85	MG	AR	4136	1/1	0.91	0.27	36,36,36,36	0
85	MG	AR	4137	1/1	0.91	0.48	79,79,79,79	0
85	MG	AR	4139	1/1	0.91	0.35	46,46,46,46	0
85	MG	1	3847	1/1	0.91	0.54	28,28,28,28	0
85	MG	1	3848	1/1	0.91	0.40	60,60,60,60	0
85	MG	CX	204	1/1	0.91	0.21	46,46,46,46	0
85	MG	AR	3979	1/1	0.91	0.57	41,41,41,41	0
85	MG	1	3849	1/1	0.91	0.44	23,23,23,23	0
84	OHX	AR	3677	7/7	0.91	0.38	110,111,111,111	0
85	MG	AR	4147	1/1	0.91	0.23	31,31,31,31	0
84	OHX	4	215	7/7	0.91	0.28	137,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	A	1970	7/7	0.91	0.35	132,132,133,133	0
85	MG	1	4174	1/1	0.91	0.83	55,55,55,55	0
85	MG	1	4058	1/1	0.91	0.31	51,51,51,51	0
84	OHX	1	3596	7/7	0.91	0.49	143,144,144,144	0
85	MG	DQ	204	1/1	0.91	0.35	32,32,32,32	0
85	MG	1	3765	1/1	0.91	0.49	21,21,21,21	0
85	MG	1	3861	1/1	0.91	0.24	34,34,34,34	0
84	OHX	1	3695	7/7	0.91	0.61	154,154,155,155	0
85	MG	1	3865	1/1	0.91	0.32	45,45,45,45	0
85	MG	6	2109	1/1	0.91	0.42	56,56,56,56	0
84	OHX	A	1993	7/7	0.91	0.38	151,151,152,152	0
84	OHX	AR	3695	7/7	0.91	0.30	122,122,123,123	0
85	MG	AR	3770	1/1	0.91	0.44	32,32,32,32	0
85	MG	A	2056	1/1	0.91	0.34	65,65,65,65	0
85	MG	AR	3771	1/1	0.91	0.36	42,42,42,42	0
85	MG	1	3979	1/1	0.91	0.31	39,39,39,39	0
85	MG	A	2067	1/1	0.91	0.81	64,64,64,64	0
84	OHX	6	2048	7/7	0.91	0.35	173,174,174,174	0
84	OHX	A	2021	7/7	0.91	0.43	133,133,134,134	0
85	MG	AR	3778	1/1	0.91	0.26	42,42,42,42	0
85	MG	1	4213	1/1	0.91	0.64	50,50,50,50	0
84	OHX	A	2023	7/7	0.91	0.26	144,145,145,145	0
85	MG	AR	4176	1/1	0.91	0.23	33,33,33,33	0
85	MG	AR	4177	1/1	0.91	0.30	32,32,32,32	0
85	MG	AR	4180	1/1	0.91	0.39	48,48,48,48	0
84	OHX	1	3673	7/7	0.91	0.56	133,133,133,133	0
85	MG	A	2086	1/1	0.91	0.24	66,66,66,66	0
85	MG	AR	4026	1/1	0.91	0.33	60,60,60,60	0
85	MG	1	3884	1/1	0.91	0.34	29,29,29,29	0
85	MG	AR	4184	1/1	0.91	0.16	69,69,69,69	0
85	MG	AR	3789	1/1	0.91	0.39	36,36,36,36	0
85	MG	6	2127	1/1	0.91	0.47	54,54,54,54	0
85	MG	AR	3796	1/1	0.91	0.41	64,64,64,64	0
85	MG	6	2129	1/1	0.91	0.38	62,62,62,62	0
85	MG	1	3782	1/1	0.91	0.45	58,58,58,58	0
85	MG	3	217	1/1	0.91	0.36	40,40,40,40	0
84	OHX	1	3720	7/7	0.91	0.28	128,128,129,129	0
84	OHX	AR	3718	7/7	0.91	0.47	166,167,167,167	0
85	MG	AR	4205	1/1	0.91	0.24	59,59,59,59	0
85	MG	AR	3815	1/1	0.91	0.24	32,32,32,32	0
85	MG	1	3992	1/1	0.91	0.24	40,40,40,40	0
84	OHX	1	3676	7/7	0.91	0.30	149,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3899	1/1	0.91	0.35	39,39,39,39	0
85	MG	AR	3824	1/1	0.91	0.13	77,77,77,77	0
85	MG	AR	4216	1/1	0.91	0.20	44,44,44,44	0
85	MG	6	2142	1/1	0.91	0.24	83,83,83,83	0
85	MG	6	2143	1/1	0.91	0.31	75,75,75,75	0
85	MG	AR	3832	1/1	0.91	0.53	30,30,30,30	0
85	MG	4	227	1/1	0.91	0.40	52,52,52,52	0
85	MG	1	4100	1/1	0.91	0.27	53,53,53,53	0
85	MG	1	3901	1/1	0.91	0.49	39,39,39,39	0
85	MG	1	3789	1/1	0.91	0.17	42,42,42,42	0
85	MG	AR	4231	1/1	0.91	0.35	32,32,32,32	0
85	MG	1	3913	1/1	0.91	0.59	28,28,28,28	0
84	OHX	6	2002	7/7	0.91	0.27	132,133,133,134	0
85	MG	AR	4236	1/1	0.91	0.42	23,23,23,23	0
85	MG	1	4109	1/1	0.91	0.14	66,66,66,66	0
85	MG	1	3917	1/1	0.91	0.26	30,30,30,30	0
85	MG	AR	4068	1/1	0.91	0.12	99,99,99,99	0
85	MG	1	3920	1/1	0.91	0.10	41,41,41,41	0
84	OHX	A	2035	7/7	0.91	0.48	130,131,131,131	0
84	OHX	6	2004	7/7	0.91	0.40	157,157,158,158	0
84	OHX	A	2038	7/7	0.91	0.34	146,147,147,147	0
84	OHX	A	2039	7/7	0.91	0.41	166,167,168,168	0
85	MG	k	402	1/1	0.91	0.37	37,37,37,37	0
85	MG	6	2165	1/1	0.91	0.35	51,51,51,51	0
85	MG	AR	3889	1/1	0.91	0.36	35,35,35,35	0
85	MG	1	3929	1/1	0.91	0.30	34,34,34,34	0
84	OHX	1	3701	7/7	0.91	0.31	139,139,140,140	0
85	MG	AR	4256	1/1	0.91	0.43	49,49,49,49	0
85	MG	AR	3892	1/1	0.91	0.48	31,31,31,31	0
84	OHX	AR	3727	7/7	0.91	0.23	187,188,188,188	0
85	MG	AR	3896	1/1	0.91	0.55	36,36,36,36	0
85	MG	AR	3897	1/1	0.91	0.44	51,51,51,51	0
85	MG	1	4011	1/1	0.91	0.37	44,44,44,44	0
84	OHX	6	2008	7/7	0.91	0.18	136,136,136,136	0
85	MG	H	301	1/1	0.91	0.10	83,83,83,83	0
84	OHX	s8	301	7/7	0.91	0.32	167,167,168,168	0
84	OHX	c3	201	7/7	0.91	0.24	155,156,156,157	0
84	OHX	AR	3639	7/7	0.91	0.22	138,139,139,139	0
85	MG	w	202	1/1	0.91	0.32	31,31,31,31	0
84	OHX	AR	3730	7/7	0.91	0.33	176,176,176,176	0
85	MG	AR	3922	1/1	0.91	0.49	31,31,31,31	0
85	MG	AR	4100	1/1	0.91	0.28	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3929	1/1	0.91	0.37	25,25,25,25	0
85	MG	c8	202	1/1	0.91	0.33	79,79,79,79	0
85	MG	AR	3934	1/1	0.91	0.31	32,32,32,32	0
85	MG	1	4021	1/1	0.91	0.15	44,44,44,44	0
85	MG	1	4022	1/1	0.91	0.59	53,53,53,53	0
85	MG	d6	101	1/1	0.91	0.34	49,49,49,49	0
84	OHX	1	3659	7/7	0.91	0.32	140,140,140,141	0
85	MG	1	3732	1/1	0.91	0.44	26,26,26,26	0
84	OHX	3	205	7/7	0.91	0.21	127,128,128,128	0
84	OHX	1	3716	7/7	0.91	0.45	138,138,139,139	0
85	MG	1	4030	1/1	0.91	0.73	72,72,72,72	0
84	OHX	4	213	7/7	0.91	0.31	117,117,117,117	0
84	OHX	CF	402	7/7	0.92	0.34	145,146,146,146	0
85	MG	AT	220	1/1	0.92	0.47	53,53,53,53	0
84	OHX	CG	302	7/7	0.92	0.38	147,147,147,148	0
85	MG	1	3755	1/1	0.92	0.42	36,36,36,36	0
85	MG	1	4079	1/1	0.92	0.21	97,97,97,97	0
85	MG	1	3969	1/1	0.92	0.21	41,41,41,41	0
85	MG	1	3970	1/1	0.92	0.30	31,31,31,31	0
85	MG	4	225	1/1	0.92	0.32	25,25,25,25	0
84	OHX	AR	3668	7/7	0.92	0.37	131,132,132,132	0
85	MG	1	3862	1/1	0.92	0.46	52,52,52,52	0
85	MG	1	3974	1/1	0.92	0.22	28,28,28,28	0
85	MG	AR	3902	1/1	0.92	0.57	42,42,42,42	0
84	OHX	6	2033	7/7	0.92	0.39	150,151,151,152	0
85	MG	1	3864	1/1	0.92	0.25	38,38,38,38	0
85	MG	1	4089	1/1	0.92	0.21	42,42,42,42	0
84	OHX	1	3627	7/7	0.92	0.28	141,142,142,143	0
84	OHX	A	1981	7/7	0.92	0.16	194,195,195,195	0
85	MG	1	3764	1/1	0.92	0.58	41,41,41,41	0
84	OHX	1	3692	7/7	0.92	0.29	113,113,113,113	0
85	MG	AR	3924	1/1	0.92	0.49	27,27,27,27	0
85	MG	AR	3927	1/1	0.92	0.45	35,35,35,35	0
85	MG	1	4099	1/1	0.92	0.23	44,44,44,44	0
85	MG	1	3871	1/1	0.92	0.47	30,30,30,30	0
84	OHX	1	401	7/7	0.92	0.41	143,143,144,144	0
84	OHX	A	2006	7/7	0.92	0.31	149,150,150,150	0
85	MG	1	402	1/1	0.92	0.33	57,57,57,57	0
85	MG	1	3877	1/1	0.92	0.71	36,36,36,36	0
85	MG	1	4107	1/1	0.92	0.16	40,40,40,40	0
85	MG	o	302	1/1	0.92	0.21	39,39,39,39	0
85	MG	1	3990	1/1	0.92	0.30	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	DA	202	1/1	0.92	0.20	45,45,45,45	0
84	OHX	AR	3694	7/7	0.92	0.33	146,147,147,147	0
84	OHX	A	2011	7/7	0.92	0.23	149,149,150,150	0
84	OHX	A	2012	7/7	0.92	0.37	139,140,140,140	0
85	MG	t	203	1/1	0.92	0.42	29,29,29,29	0
84	OHX	1	3665	7/7	0.92	0.36	129,129,129,129	0
84	OHX	A	2017	7/7	0.92	0.31	158,159,160,160	0
84	OHX	A	2019	7/7	0.92	0.29	176,176,176,176	0
85	MG	AR	3961	1/1	0.92	0.53	43,43,43,43	0
84	OHX	1	3666	7/7	0.92	0.42	117,118,118,118	0
85	MG	x	204	1/1	0.92	0.35	28,28,28,28	0
84	OHX	1	3698	7/7	0.92	0.30	162,163,163,163	0
85	MG	1	3905	1/1	0.92	0.47	38,38,38,38	0
84	OHX	AR	3709	7/7	0.92	0.28	110,111,111,111	0
85	MG	1	4002	1/1	0.92	0.56	37,37,37,37	0
84	OHX	AR	3716	7/7	0.92	0.37	143,143,143,143	0
85	MG	AR	3977	1/1	0.92	0.41	41,41,41,41	0
85	MG	6	2056	1/1	0.92	0.22	77,77,77,77	0
85	MG	AR	3980	1/1	0.92	0.86	40,40,40,40	0
85	MG	A	2057	1/1	0.92	0.46	70,70,70,70	0
85	MG	A	2061	1/1	0.92	0.50	59,59,59,59	0
84	OHX	6	2050	7/7	0.92	0.47	159,159,160,160	0
85	MG	6	2060	1/1	0.92	0.34	47,47,47,47	0
84	OHX	1	3651	7/7	0.92	0.26	130,130,131,131	0
84	OHX	6	1977	7/7	0.92	0.25	150,151,151,152	0
85	MG	AR	3747	1/1	0.92	0.30	23,23,23,23	0
85	MG	AR	3992	1/1	0.92	0.64	67,67,67,67	0
85	MG	AR	4165	1/1	0.92	0.21	43,43,43,43	0
84	OHX	1	3672	7/7	0.92	0.41	147,147,147,148	0
85	MG	1	4008	1/1	0.92	0.29	37,37,37,37	0
85	MG	AR	3996	1/1	0.92	0.33	56,56,56,56	0
84	OHX	AR	3721	7/7	0.92	0.38	139,139,140,140	0
84	OHX	A	2037	7/7	0.92	0.44	153,154,154,155	0
85	MG	1	3802	1/1	0.92	0.18	86,86,86,86	0
85	MG	6	2077	1/1	0.92	0.54	39,39,39,39	0
84	OHX	AR	3506	7/7	0.92	0.21	112,112,112,112	0
85	MG	1	4146	1/1	0.92	0.17	48,48,48,48	0
85	MG	AR	4178	1/1	0.92	0.19	24,24,24,24	0
84	OHX	1	3652	7/7	0.92	0.33	110,110,110,110	0
84	OHX	AR	3599	7/7	0.92	0.24	136,136,136,136	0
84	OHX	1	3722	1/7	0.92	0.12	136,136,136,136	0
85	MG	AR	4018	1/1	0.92	0.21	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	6	2005	7/7	0.92	0.42	126,126,127,127	0
84	OHX	1	3488	7/7	0.92	0.17	109,109,109,110	0
85	MG	A	2100	1/1	0.92	0.44	92,92,92,92	0
84	OHX	AR	3732	7/7	0.92	0.52	146,146,147,147	0
85	MG	1	4026	1/1	0.92	0.41	65,65,65,65	0
85	MG	AR	4189	1/1	0.92	1.14	32,32,32,32	0
85	MG	AR	4192	1/1	0.92	0.19	29,29,29,29	0
85	MG	1	3937	1/1	0.92	0.12	68,68,68,68	0
85	MG	1	3938	1/1	0.92	0.21	34,34,34,34	0
85	MG	6	2091	1/1	0.92	0.41	61,61,61,61	0
84	OHX	6	2007	7/7	0.92	0.28	145,146,146,146	0
85	MG	AR	4027	1/1	0.92	0.23	76,76,76,76	0
85	MG	6	2095	1/1	0.92	0.43	41,41,41,41	0
85	MG	A	2115	1/1	0.92	0.38	83,83,83,83	0
84	OHX	c5	201	7/7	0.92	0.19	161,161,161,161	0
85	MG	6	2100	1/1	0.92	0.51	36,36,36,36	0
85	MG	AR	4209	1/1	0.92	0.40	74,74,74,74	0
85	MG	AR	4031	1/1	0.92	0.20	39,39,39,39	0
85	MG	AR	3785	1/1	0.92	0.47	57,57,57,57	0
84	OHX	d9	101	7/7	0.92	0.48	153,153,154,154	0
85	MG	AR	3792	1/1	0.92	0.51	43,43,43,43	0
85	MG	A	2126	1/1	0.92	0.68	64,64,64,64	0
85	MG	1	3942	1/1	0.92	0.26	32,32,32,32	0
85	MG	6	2106	1/1	0.92	0.39	50,50,50,50	0
85	MG	AR	4038	1/1	0.92	0.23	35,35,35,35	0
85	MG	1	3943	1/1	0.92	0.54	37,37,37,37	0
85	MG	AR	3804	1/1	0.92	0.45	27,27,27,27	0
85	MG	1	3821	1/1	0.92	0.52	66,66,66,66	0
85	MG	AR	3808	1/1	0.92	0.34	28,28,28,28	0
85	MG	AR	4226	1/1	0.92	0.41	24,24,24,24	0
85	MG	AR	4230	1/1	0.92	0.55	18,18,18,18	0
84	OHX	1	3643	7/7	0.92	0.39	114,114,114,114	0
85	MG	1	4039	1/1	0.92	0.48	40,40,40,40	0
85	MG	AR	4233	1/1	0.92	0.33	31,31,31,31	0
85	MG	1	3947	1/1	0.92	0.21	26,26,26,26	0
85	MG	A	2143	1/1	0.92	0.38	106,106,106,106	0
85	MG	1	3728	1/1	0.92	0.61	52,52,52,52	0
85	MG	1	3949	1/1	0.92	0.47	44,44,44,44	0
85	MG	6	2121	1/1	0.92	0.28	41,41,41,41	0
85	MG	AR	3820	1/1	0.92	0.26	43,43,43,43	0
85	MG	AR	4055	1/1	0.92	0.17	40,40,40,40	0
84	OHX	AR	3644	7/7	0.92	0.31	126,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3833	1/1	0.92	0.70	24,24,24,24	0
85	MG	A	2157	1/1	0.92	0.79	75,75,75,75	0
85	MG	1	3834	1/1	0.92	0.51	22,22,22,22	0
85	MG	AR	4061	1/1	0.92	0.53	50,50,50,50	0
85	MG	F	301	1/1	0.92	0.33	64,64,64,64	0
84	OHX	1	3688	7/7	0.92	0.25	129,130,130,130	0
85	MG	1	4054	1/1	0.92	0.21	56,56,56,56	0
84	OHX	AR	3647	7/7	0.92	0.29	126,126,127,127	0
85	MG	6	2132	1/1	0.92	0.35	42,42,42,42	0
85	MG	AR	3835	1/1	0.92	0.41	45,45,45,45	0
84	OHX	1	3690	7/7	0.92	0.41	122,123,123,123	0
85	MG	1	3740	1/1	0.92	0.36	30,30,30,30	0
85	MG	AR	4072	1/1	0.92	0.25	70,70,70,70	0
85	MG	AS	214	1/1	0.92	0.30	52,52,52,52	0
84	OHX	AS	210	7/7	0.92	0.24	115,115,116,116	0
85	MG	1	4214	1/1	0.92	0.39	43,43,43,43	0
85	MG	1	4218	1/1	0.92	0.14	32,32,32,32	0
84	OHX	AR	3657	7/7	0.92	0.39	114,114,115,115	0
85	MG	3	210	1/1	0.92	0.39	59,59,59,59	0
85	MG	1	3850	1/1	0.92	0.48	31,31,31,31	0
84	OHX	6	2023	7/7	0.92	0.38	161,161,162,162	0
85	MG	3	214	1/1	0.92	0.52	34,34,34,34	0
85	MG	AR	3864	1/1	0.92	0.29	40,40,40,40	0
85	MG	AS	227	1/1	0.92	0.32	45,45,45,45	0
84	OHX	6	2030	7/7	0.92	0.29	118,118,118,119	0
85	MG	AR	4058	1/1	0.93	0.53	61,61,61,61	0
85	MG	1	4017	1/1	0.93	0.21	101,101,101,101	0
85	MG	1	4018	1/1	0.93	0.33	38,38,38,38	0
84	OHX	AR	3739	7/7	0.93	0.51	148,149,149,150	0
85	MG	6	2112	1/1	0.93	0.53	46,46,46,46	0
85	MG	AR	3823	1/1	0.93	0.51	39,39,39,39	0
84	OHX	AR	3740	7/7	0.93	0.25	161,161,161,162	0
85	MG	6	2116	1/1	0.93	0.21	62,62,62,62	0
84	OHX	1	3614	7/7	0.93	0.28	133,133,133,134	0
84	OHX	1	3618	7/7	0.93	0.19	190,190,190,190	0
85	MG	1	4178	1/1	0.93	0.40	28,28,28,28	0
85	MG	1	4025	1/1	0.93	0.48	32,32,32,32	0
85	MG	1	3921	1/1	0.93	0.12	57,57,57,57	0
84	OHX	AS	209	7/7	0.93	0.31	140,140,140,140	0
85	MG	1	4189	1/1	0.93	0.36	27,27,27,27	0
85	MG	AR	3839	1/1	0.93	0.43	33,33,33,33	0
85	MG	AR	4077	1/1	0.93	0.32	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	4078	1/1	0.93	0.52	60,60,60,60	0
85	MG	AT	223	1/1	0.93	0.79	45,45,45,45	0
85	MG	6	2125	1/1	0.93	0.32	75,75,75,75	0
84	OHX	AR	3606	7/7	0.93	0.31	113,113,114,114	0
84	OHX	1	3552	7/7	0.93	0.10	150,150,151,151	0
85	MG	1	3773	1/1	0.93	0.21	38,38,38,38	0
85	MG	AR	3847	1/1	0.93	0.16	38,38,38,38	0
84	OHX	AR	3635	7/7	0.93	0.22	137,138,138,138	0
84	OHX	AT	217	7/7	0.93	0.37	128,128,128,128	0
84	OHX	CE	402	7/7	0.93	0.38	138,139,139,139	0
85	MG	6	2137	1/1	0.93	0.12	82,82,82,82	0
84	OHX	AR	3636	7/7	0.93	0.48	133,133,134,134	0
84	OHX	1	3556	7/7	0.93	0.27	117,117,117,117	0
84	OHX	1	3704	7/7	0.93	0.33	116,117,117,117	0
84	OHX	A	1918	7/7	0.93	0.23	128,129,129,129	0
85	MG	CG	303	1/1	0.93	0.13	62,62,62,62	0
85	MG	1	4217	1/1	0.93	0.92	58,58,58,58	0
85	MG	1	4041	1/1	0.93	0.16	45,45,45,45	0
84	OHX	AR	3641	7/7	0.93	0.48	133,133,133,133	0
84	OHX	A	1966	7/7	0.93	0.19	131,131,132,132	0
84	OHX	1	3686	7/7	0.93	0.58	156,156,157,157	0
85	MG	CQ	201	1/1	0.93	0.38	34,34,34,34	0
84	OHX	1	3655	7/7	0.93	0.37	138,138,138,139	0
84	OHX	6	2013	7/7	0.93	0.32	121,122,122,122	0
85	MG	AR	4109	1/1	0.93	0.16	39,39,39,39	0
84	OHX	AR	3649	7/7	0.93	0.50	144,144,144,144	0
84	OHX	AR	3650	7/7	0.93	0.44	118,118,118,118	0
84	OHX	A	1996	7/7	0.93	0.32	139,140,140,141	0
85	MG	AR	3905	1/1	0.93	0.48	29,29,29,29	0
84	OHX	1	3563	7/7	0.93	0.24	114,114,115,115	0
85	MG	3	222	1/1	0.93	0.38	52,52,52,52	0
85	MG	4	217	1/1	0.93	0.56	52,52,52,52	0
85	MG	1	3946	1/1	0.93	0.28	34,34,34,34	0
85	MG	AR	3920	1/1	0.93	0.50	27,27,27,27	0
85	MG	1	3804	1/1	0.93	0.50	35,35,35,35	0
84	OHX	1	3636	7/7	0.93	0.32	126,126,126,126	0
85	MG	1	4062	1/1	0.93	0.16	45,45,45,45	0
85	MG	AR	3925	1/1	0.93	0.41	34,34,34,34	0
85	MG	DO	202	1/1	0.93	0.25	42,42,42,42	0
84	OHX	AR	3663	7/7	0.93	0.29	147,148,148,148	0
85	MG	AR	3928	1/1	0.93	0.46	39,39,39,39	0
85	MG	sM	201	1/1	0.93	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	A	2044	1/1	0.93	0.80	50,50,50,50	0
84	OHX	6	2022	7/7	0.93	0.29	153,154,154,155	0
85	MG	1	4068	1/1	0.93	0.46	42,42,42,42	0
85	MG	4	230	1/1	0.93	0.34	35,35,35,35	0
84	OHX	1	3711	7/7	0.93	0.59	119,120,120,120	0
84	OHX	6	2024	7/7	0.93	0.35	151,152,152,153	0
84	OHX	AR	3670	7/7	0.93	0.19	143,143,144,144	0
85	MG	A	2052	1/1	0.93	0.42	53,53,53,53	0
84	OHX	A	2020	7/7	0.93	0.23	147,148,148,148	0
84	OHX	AR	3674	7/7	0.93	0.46	130,130,130,131	0
85	MG	A	2055	1/1	0.93	0.47	71,71,71,71	0
85	MG	AR	4143	1/1	0.93	0.26	34,34,34,34	0
85	MG	AR	4144	1/1	0.93	0.33	41,41,41,41	0
85	MG	A	2060	1/1	0.93	0.62	55,55,55,55	0
84	OHX	AR	3675	7/7	0.93	0.33	138,139,139,139	0
84	OHX	4	216	7/7	0.93	0.26	126,126,126,126	0
84	OHX	AR	3678	7/7	0.93	0.42	137,137,137,138	0
85	MG	1	3826	1/1	0.93	0.25	33,33,33,33	0
85	MG	j	301	1/1	0.93	0.21	29,29,29,29	0
85	MG	1	3828	1/1	0.93	0.55	30,30,30,30	0
85	MG	AR	4152	1/1	0.93	0.23	38,38,38,38	0
85	MG	A	2072	1/1	0.93	0.39	66,66,66,66	0
85	MG	1	4086	1/1	0.93	0.29	32,32,32,32	0
85	MG	A	2076	1/1	0.93	0.35	51,51,51,51	0
85	MG	A	2078	1/1	0.93	0.68	54,54,54,54	0
84	OHX	6	2032	7/7	0.93	0.50	131,131,132,132	0
85	MG	1	3964	1/1	0.93	0.47	68,68,68,68	0
85	MG	AR	3962	1/1	0.93	0.19	93,93,93,93	0
84	OHX	1	3661	7/7	0.93	0.32	119,120,120,120	0
85	MG	AR	4158	1/1	0.93	0.20	29,29,29,29	0
85	MG	AR	3965	1/1	0.93	0.25	50,50,50,50	0
85	MG	AR	3966	1/1	0.93	0.45	38,38,38,38	0
85	MG	o	301	1/1	0.93	0.19	34,34,34,34	0
84	OHX	6	2035	7/7	0.93	0.36	142,142,143,143	0
85	MG	A	2090	1/1	0.93	0.20	57,57,57,57	0
84	OHX	6	2036	7/7	0.93	0.40	135,135,136,136	0
85	MG	1	3837	1/1	0.93	0.33	26,26,26,26	0
84	OHX	6	2037	7/7	0.93	0.40	137,137,138,138	0
85	MG	AR	4167	1/1	0.93	0.25	71,71,71,71	0
84	OHX	AR	3701	7/7	0.93	0.29	128,128,128,128	0
84	OHX	AR	3704	7/7	0.93	0.38	133,133,133,133	0
85	MG	1	3973	1/1	0.93	0.47	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	2038	7/7	0.93	0.41	148,148,148,148	0
85	MG	1	3975	1/1	0.93	0.33	42,42,42,42	0
84	OHX	A	2040	7/7	0.93	0.37	162,162,162,162	0
85	MG	AF	201	1/1	0.93	0.30	41,41,41,41	0
85	MG	A	2104	1/1	0.93	0.15	137,137,137,137	0
85	MG	A	2105	1/1	0.93	0.43	94,94,94,94	0
84	OHX	AR	3706	7/7	0.93	0.34	155,155,155,156	0
84	OHX	1	3713	7/7	0.93	0.26	138,138,138,139	0
84	OHX	AR	3708	7/7	0.93	0.26	138,138,139,139	0
84	OHX	K	201	7/7	0.93	0.51	137,137,138,138	0
85	MG	AR	3748	1/1	0.93	0.38	44,44,44,44	0
84	OHX	x	202	7/7	0.93	0.36	144,144,145,145	0
84	OHX	AR	3711	7/7	0.93	0.37	144,144,145,145	0
85	MG	AR	4185	1/1	0.93	0.37	38,38,38,38	0
84	OHX	1	3664	7/7	0.93	0.35	124,124,124,124	0
85	MG	AR	4002	1/1	0.93	0.50	28,28,28,28	0
84	OHX	6	2043	7/7	0.93	0.31	145,145,146,146	0
84	OHX	6	1932	7/7	0.93	0.23	132,132,133,133	0
85	MG	AR	3754	1/1	0.93	0.31	40,40,40,40	0
85	MG	A	2123	1/1	0.93	0.51	55,55,55,55	0
85	MG	AR	4193	1/1	0.93	0.32	38,38,38,38	0
84	OHX	6	1950	7/7	0.93	0.21	135,135,136,136	0
85	MG	6	2065	1/1	0.93	0.58	40,40,40,40	0
85	MG	AR	3757	1/1	0.93	0.41	31,31,31,31	0
85	MG	AR	4015	1/1	0.93	0.16	45,45,45,45	0
85	MG	AR	4016	1/1	0.93	0.36	33,33,33,33	0
85	MG	AR	4201	1/1	0.93	0.27	35,35,35,35	0
85	MG	AR	4204	1/1	0.93	0.30	38,38,38,38	0
85	MG	AR	3758	1/1	0.93	0.30	37,37,37,37	0
84	OHX	1	3694	7/7	0.93	0.41	116,116,117,117	0
85	MG	6	2067	1/1	0.93	0.30	45,45,45,45	0
85	MG	1	3729	1/1	0.93	0.32	90,90,90,90	0
84	OHX	6	2049	7/7	0.93	0.33	170,171,171,171	0
85	MG	AR	4211	1/1	0.93	0.14	73,73,73,73	0
85	MG	1	3868	1/1	0.93	0.42	29,29,29,29	0
85	MG	AR	3767	1/1	0.93	0.58	35,35,35,35	0
85	MG	AR	3769	1/1	0.93	0.26	59,59,59,59	0
85	MG	AR	4218	1/1	0.93	0.27	54,54,54,54	0
85	MG	A	2147	1/1	0.93	0.26	79,79,79,79	0
84	OHX	6	1961	7/7	0.93	0.19	128,129,129,130	0
85	MG	1	3734	1/1	0.93	0.34	43,43,43,43	0
84	OHX	AR	3723	7/7	0.93	0.28	146,146,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3725	7/7	0.93	0.20	165,165,165,165	0
85	MG	1	4136	1/1	0.93	0.27	40,40,40,40	0
84	OHX	1	3485	7/7	0.93	0.16	120,121,121,121	0
84	OHX	1	3609	7/7	0.93	0.40	119,120,120,120	0
85	MG	A	2158	1/1	0.93	0.34	67,67,67,67	0
84	OHX	6	1986	7/7	0.93	0.32	147,148,148,148	0
84	OHX	6	1987	7/7	0.93	0.28	137,137,138,138	0
84	OHX	6	1989	7/7	0.93	0.43	143,144,144,145	0
84	OHX	AR	3527	7/7	0.93	0.20	112,112,112,112	0
85	MG	AR	3788	1/1	0.93	0.50	28,28,28,28	0
85	MG	1	3896	1/1	0.93	0.30	36,36,36,36	0
84	OHX	AR	3571	7/7	0.93	0.18	125,125,125,125	0
84	OHX	AR	3596	7/7	0.93	0.24	121,121,122,122	0
85	MG	AR	4041	1/1	0.93	0.36	34,34,34,34	0
85	MG	1	3756	1/1	0.93	0.42	32,32,32,32	0
85	MG	AR	4242	1/1	0.93	0.46	35,35,35,35	0
85	MG	c1	202	1/1	0.93	0.41	67,67,67,67	0
85	MG	AR	4243	1/1	0.93	0.59	30,30,30,30	0
85	MG	AR	3798	1/1	0.93	0.33	33,33,33,33	0
85	MG	1	4153	1/1	0.93	0.18	39,39,39,39	0
85	MG	6	2094	1/1	0.93	0.22	37,37,37,37	0
85	MG	AR	3805	1/1	0.93	0.44	36,36,36,36	0
84	OHX	AR	3736	7/7	0.93	0.28	132,132,132,133	0
84	OHX	AR	3597	7/7	0.93	0.30	150,151,151,151	0
85	MG	1	3906	1/1	0.93	0.36	42,42,42,42	0
84	OHX	6	1992	7/7	0.93	0.23	137,137,138,138	0
85	MG	1	3912	1/1	0.93	0.59	22,22,22,22	0
85	MG	1	4016	1/1	0.93	0.18	39,39,39,39	0
88	ZN	c	101	1/1	0.93	0.34	145,145,145,145	0
85	MG	AR	4057	1/1	0.93	0.39	41,41,41,41	0
85	MG	AR	4227	1/1	0.94	0.33	22,22,22,22	0
84	OHX	AR	3685	7/7	0.94	0.33	120,121,121,121	0
84	OHX	A	2032	7/7	0.94	0.20	154,154,155,155	0
84	OHX	A	2033	7/7	0.94	0.25	146,146,147,147	0
85	MG	AR	3997	1/1	0.94	0.12	44,44,44,44	0
84	OHX	6	1940	7/7	0.94	0.13	149,150,151,151	0
84	OHX	AR	3689	7/7	0.94	0.34	118,118,119,119	0
85	MG	AR	4001	1/1	0.94	0.22	38,38,38,38	0
84	OHX	1	3641	7/7	0.94	0.36	141,141,141,141	0
84	OHX	AR	3691	7/7	0.94	0.41	116,116,116,117	0
85	MG	AR	4004	1/1	0.94	0.16	32,32,32,32	0
84	OHX	6	2042	7/7	0.94	0.34	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4006	1/1	0.94	0.55	47,47,47,47	0
85	MG	AR	4008	1/1	0.94	0.25	26,26,26,26	0
84	OHX	1	3498	7/7	0.94	0.21	115,116,116,116	0
85	MG	AR	4010	1/1	0.94	0.30	30,30,30,30	0
84	OHX	1	3675	7/7	0.94	0.30	140,141,141,141	0
84	OHX	AR	3698	7/7	0.94	0.41	123,123,123,124	0
84	OHX	6	1962	7/7	0.94	0.30	136,137,137,137	0
84	OHX	AR	3702	7/7	0.94	0.40	139,139,140,140	0
85	MG	4	223	1/1	0.94	0.59	27,27,27,27	0
85	MG	1	3880	1/1	0.94	0.59	31,31,31,31	0
85	MG	AB	206	1/1	0.94	0.27	26,26,26,26	0
84	OHX	6	2047	7/7	0.94	0.32	161,162,162,162	0
84	OHX	Q	201	7/7	0.94	0.26	165,165,165,165	0
84	OHX	6	1969	7/7	0.94	0.15	127,127,128,128	0
85	MG	1	3890	1/1	0.94	0.47	34,34,34,34	0
84	OHX	6	1971	7/7	0.94	0.24	136,136,136,137	0
84	OHX	1	3610	7/7	0.94	0.23	130,130,131,131	0
84	OHX	1	3679	7/7	0.94	0.30	131,131,132,132	0
84	OHX	6	1979	7/7	0.94	0.46	135,135,136,136	0
84	OHX	AR	3710	7/7	0.94	0.34	137,137,137,138	0
85	MG	1	3727	1/1	0.94	0.28	37,37,37,37	0
84	OHX	1	3462	7/7	0.94	0.21	119,120,120,120	0
85	MG	1	4049	1/1	0.94	0.25	32,32,32,32	0
84	OHX	AR	3712	7/7	0.94	0.27	109,109,109,109	0
85	MG	4	241	1/1	0.94	0.58	45,45,45,45	0
85	MG	AS	230	1/1	0.94	0.42	36,36,36,36	0
85	MG	1	3730	1/1	0.94	0.35	36,36,36,36	0
84	OHX	AR	3713	7/7	0.94	0.24	178,178,179,179	0
84	OHX	1	3648	7/7	0.94	0.25	119,120,120,120	0
85	MG	AR	4036	1/1	0.94	0.27	41,41,41,41	0
85	MG	k	403	1/1	0.94	0.20	30,30,30,30	0
84	OHX	1	3650	7/7	0.94	0.27	128,128,128,128	0
85	MG	1	4057	1/1	0.94	0.23	26,26,26,26	0
85	MG	1	3735	1/1	0.94	0.35	24,24,24,24	0
84	OHX	AR	3524	7/7	0.94	0.29	118,119,119,119	0
85	MG	1	3738	1/1	0.94	0.35	28,28,28,28	0
85	MG	AR	3768	1/1	0.94	0.18	39,39,39,39	0
85	MG	1	3922	1/1	0.94	0.45	45,45,45,45	0
85	MG	1	3923	1/1	0.94	0.39	51,51,51,51	0
84	OHX	1	3689	7/7	0.94	0.52	140,140,141,141	0
85	MG	1	4066	1/1	0.94	0.27	20,20,20,20	0
84	OHX	AR	3528	7/7	0.94	0.21	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	CE	406	1/1	0.94	0.19	25,25,25,25	0
85	MG	1	3742	1/1	0.94	0.47	38,38,38,38	0
84	OHX	AR	3531	7/7	0.94	0.19	115,115,115,115	0
84	OHX	AR	3552	7/7	0.94	0.28	114,114,114,114	0
85	MG	1	3747	1/1	0.94	0.34	37,37,37,37	0
85	MG	CI	301	1/1	0.94	0.26	33,33,33,33	0
84	OHX	AR	3563	7/7	0.94	0.17	122,122,123,123	0
84	OHX	AR	3564	7/7	0.94	0.14	155,155,155,155	0
85	MG	AR	3784	1/1	0.94	0.24	51,51,51,51	0
84	OHX	6	1993	7/7	0.94	0.28	134,135,135,135	0
85	MG	1	3753	1/1	0.94	0.54	35,35,35,35	0
85	MG	CQ	202	1/1	0.94	0.33	32,32,32,32	0
85	MG	1	4083	1/1	0.94	0.29	41,41,41,41	0
85	MG	CR	201	1/1	0.94	0.65	29,29,29,29	0
85	MG	AR	3791	1/1	0.94	0.26	34,34,34,34	0
84	OHX	AR	3590	7/7	0.94	0.37	113,113,113,113	0
85	MG	6	2054	1/1	0.94	0.39	49,49,49,49	0
84	OHX	AR	3593	7/7	0.94	0.23	113,114,114,114	0
84	OHX	6	1999	7/7	0.94	0.26	138,139,139,140	0
85	MG	AR	3800	1/1	0.94	0.65	33,33,33,33	0
85	MG	AR	3801	1/1	0.94	0.38	32,32,32,32	0
84	OHX	1	3615	7/7	0.94	0.38	133,133,133,134	0
84	OHX	1	3514	7/7	0.94	0.18	112,112,112,112	0
84	OHX	AR	3600	7/7	0.94	0.33	119,119,119,119	0
85	MG	1	4090	1/1	0.94	0.21	42,42,42,42	0
85	MG	DC	204	1/1	0.94	0.14	35,35,35,35	0
84	OHX	1	3619	7/7	0.94	0.22	127,127,127,127	0
85	MG	AR	3809	1/1	0.94	0.65	37,37,37,37	0
85	MG	1	3763	1/1	0.94	0.65	29,29,29,29	0
85	MG	AR	4082	1/1	0.94	0.34	24,24,24,24	0
85	MG	6	2069	1/1	0.94	0.35	65,65,65,65	0
85	MG	AR	3813	1/1	0.94	0.16	55,55,55,55	0
84	OHX	AR	3735	7/7	0.94	0.30	129,129,129,129	0
84	OHX	1	3591	7/7	0.94	0.28	109,109,109,109	0
85	MG	sM	202	1/1	0.94	0.54	42,42,42,42	0
84	OHX	1	3594	7/7	0.94	0.20	131,131,132,132	0
84	OHX	AR	3607	7/7	0.94	0.30	113,113,113,113	0
85	MG	1	3768	1/1	0.94	0.41	36,36,36,36	0
85	MG	1	3770	1/1	0.94	0.25	29,29,29,29	0
85	MG	1	3950	1/1	0.94	0.14	38,38,38,38	0
85	MG	A	2049	1/1	0.94	0.50	54,54,54,54	0
84	OHX	AR	3608	7/7	0.94	0.34	131,131,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3825	1/1	0.94	0.27	33,33,33,33	0
84	OHX	AR	3611	7/7	0.94	0.23	126,126,126,126	0
84	OHX	AR	3615	7/7	0.94	0.36	132,133,133,133	0
85	MG	AR	3831	1/1	0.94	0.23	44,44,44,44	0
84	OHX	AR	3742	7/7	0.94	0.25	128,129,129,129	0
84	OHX	AR	3622	7/7	0.94	0.24	130,131,131,131	0
84	OHX	1	3540	7/7	0.94	0.18	111,111,111,111	0
85	MG	1	3957	1/1	0.94	0.39	37,37,37,37	0
84	OHX	AR	3634	7/7	0.94	0.26	112,112,113,113	0
85	MG	AR	4107	1/1	0.94	0.13	78,78,78,78	0
85	MG	AR	4108	1/1	0.94	0.19	36,36,36,36	0
84	OHX	3	206	7/7	0.94	0.20	127,127,128,128	0
84	OHX	AT	212	7/7	0.94	0.30	128,128,128,128	0
84	OHX	6	2010	7/7	0.94	0.33	154,155,155,155	0
85	MG	AR	4114	1/1	0.94	0.28	40,40,40,40	0
85	MG	A	2071	1/1	0.94	0.33	64,64,64,64	0
85	MG	1	4123	1/1	0.94	0.22	51,51,51,51	0
84	OHX	AT	215	7/7	0.94	0.20	137,138,138,138	0
85	MG	AR	3843	1/1	0.94	0.35	30,30,30,30	0
85	MG	6	2096	1/1	0.94	0.57	68,68,68,68	0
85	MG	6	2097	1/1	0.94	0.42	46,46,46,46	0
84	OHX	1	3660	7/7	0.94	0.28	153,153,154,154	0
85	MG	A	2082	1/1	0.94	0.23	61,61,61,61	0
85	MG	1	4126	1/1	0.94	0.98	33,33,33,33	0
85	MG	AR	3854	1/1	0.94	0.40	48,48,48,48	0
85	MG	AR	3859	1/1	0.94	0.49	29,29,29,29	0
85	MG	6	2102	1/1	0.94	0.46	45,45,45,45	0
85	MG	1	3791	1/1	0.94	0.60	54,54,54,54	0
84	OHX	6	2016	7/7	0.94	0.25	120,120,121,121	0
85	MG	1	3794	1/1	0.94	0.53	34,34,34,34	0
85	MG	AR	3872	1/1	0.94	0.34	43,43,43,43	0
85	MG	6	2108	1/1	0.94	0.56	50,50,50,50	0
85	MG	AR	3875	1/1	0.94	0.16	45,45,45,45	0
85	MG	AR	3879	1/1	0.94	0.64	22,22,22,22	0
85	MG	1	3795	1/1	0.94	0.29	26,26,26,26	0
85	MG	AR	3883	1/1	0.94	0.54	32,32,32,32	0
85	MG	A	2096	1/1	0.94	0.41	62,62,62,62	0
85	MG	A	2097	1/1	0.94	0.57	53,53,53,53	0
85	MG	AR	3888	1/1	0.94	0.67	24,24,24,24	0
84	OHX	1	3629	7/7	0.94	0.22	148,148,148,149	0
84	OHX	6	2019	7/7	0.94	0.30	140,140,141,141	0
84	OHX	CG	301	7/7	0.94	0.16	142,143,143,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2113	1/1	0.94	0.23	77,77,77,77	0
85	MG	AR	3893	1/1	0.94	0.95	50,50,50,50	0
84	OHX	4	214	7/7	0.94	0.46	140,140,140,140	0
84	OHX	CM	201	7/7	0.94	0.34	150,150,151,151	0
85	MG	1	4139	1/1	0.94	0.28	31,31,31,31	0
84	OHX	1	3663	7/7	0.94	0.19	111,111,111,111	0
85	MG	AR	3900	1/1	0.94	0.81	37,37,37,37	0
84	OHX	1	3631	7/7	0.94	0.32	116,116,117,117	0
85	MG	A	2111	1/1	0.94	0.26	90,90,90,90	0
84	OHX	A	1953	7/7	0.94	0.41	146,147,147,147	0
85	MG	1	3978	1/1	0.94	0.35	46,46,46,46	0
84	OHX	A	1959	7/7	0.94	0.20	137,138,139,139	0
85	MG	1	3808	1/1	0.94	0.47	43,43,43,43	0
85	MG	AR	3912	1/1	0.94	0.54	23,23,23,23	0
84	OHX	A	1963	7/7	0.94	0.18	150,151,152,152	0
84	OHX	1	3632	7/7	0.94	0.34	156,156,156,156	0
85	MG	AR	3917	1/1	0.94	0.50	42,42,42,42	0
85	MG	AR	4162	1/1	0.94	0.60	56,56,56,56	0
84	OHX	AR	3651	7/7	0.94	0.31	150,151,151,151	0
84	OHX	6	2025	7/7	0.94	0.39	120,120,121,121	0
85	MG	1	3986	1/1	0.94	0.26	42,42,42,42	0
85	MG	AR	3923	1/1	0.94	0.66	38,38,38,38	0
84	OHX	A	1974	7/7	0.94	0.14	167,167,168,168	0
84	OHX	AR	3654	7/7	0.94	0.50	137,137,138,138	0
84	OHX	AR	3655	7/7	0.94	0.24	129,129,130,130	0
84	OHX	A	1991	7/7	0.94	0.24	157,157,158,158	0
84	OHX	6	2028	7/7	0.94	0.40	123,124,124,124	0
84	OHX	AR	3659	7/7	0.94	0.54	136,136,137,137	0
84	OHX	AR	3660	7/7	0.94	0.43	123,123,124,124	0
85	MG	1	3829	1/1	0.94	0.53	16,16,16,16	0
85	MG	1	4166	1/1	0.94	0.16	47,47,47,47	0
85	MG	1	4167	1/1	0.94	0.23	23,23,23,23	0
85	MG	1	4169	1/1	0.94	0.27	30,30,30,30	0
84	OHX	r	301	7/7	0.94	0.20	115,115,115,115	0
85	MG	1	3831	1/1	0.94	0.47	26,26,26,26	0
85	MG	AR	3949	1/1	0.94	0.19	32,32,32,32	0
84	OHX	6	2031	7/7	0.94	0.31	125,126,126,126	0
85	MG	1	4181	1/1	0.94	0.35	23,23,23,23	0
84	OHX	1	3705	7/7	0.94	0.38	131,131,132,132	0
85	MG	6	2155	1/1	0.94	0.86	58,58,58,58	0
84	OHX	A	2013	7/7	0.94	0.34	132,133,133,133	0
84	OHX	A	2014	7/7	0.94	0.35	127,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	A	2153	1/1	0.94	0.58	51,51,51,51	0
85	MG	AR	3959	1/1	0.94	0.28	32,32,32,32	0
85	MG	6	2159	1/1	0.94	0.08	82,82,82,82	0
84	OHX	AR	3666	7/7	0.94	0.27	130,131,131,131	0
84	OHX	AR	3667	7/7	0.94	0.38	146,147,147,147	0
85	MG	AR	3963	1/1	0.94	0.20	49,49,49,49	0
84	OHX	A	2018	7/7	0.94	0.34	155,155,156,156	0
85	MG	1	4194	1/1	0.94	0.50	22,22,22,22	0
85	MG	1	4195	1/1	0.94	0.46	29,29,29,29	0
85	MG	AR	4203	1/1	0.94	0.24	29,29,29,29	0
84	OHX	1	3605	7/7	0.94	0.33	129,130,130,130	0
85	MG	1	4201	1/1	0.94	0.49	28,28,28,28	0
85	MG	AR	3969	1/1	0.94	0.13	60,60,60,60	0
84	OHX	y	201	7/7	0.94	0.32	128,129,129,129	0
84	OHX	1	3639	7/7	0.94	0.32	132,132,132,132	0
85	MG	1	4206	1/1	0.94	0.30	30,30,30,30	0
84	OHX	A	2022	7/7	0.94	0.36	167,167,167,167	0
85	MG	AR	4213	1/1	0.94	0.14	53,53,53,53	0
84	OHX	6	1919	7/7	0.94	0.21	121,121,122,122	0
85	MG	AR	3978	1/1	0.94	0.36	49,49,49,49	0
85	MG	d3	201	1/1	0.94	0.25	49,49,49,49	0
85	MG	1	4010	1/1	0.94	0.46	30,30,30,30	0
85	MG	1	4212	1/1	0.94	0.42	39,39,39,39	0
85	MG	AR	3981	1/1	0.94	0.14	33,33,33,33	0
84	OHX	6	1929	7/7	0.94	0.11	157,158,159,159	0
84	OHX	1	3669	7/7	0.94	0.39	131,131,131,131	0
84	OHX	A	2028	7/7	0.94	0.34	157,157,158,158	0
84	OHX	AR	3681	7/7	0.94	0.23	140,140,140,141	0
85	MG	1	3860	1/1	0.94	0.47	36,36,36,36	0
85	MG	1	4220	1/1	0.94	0.57	35,35,35,35	0
85	MG	AR	3993	1/1	0.94	0.35	28,28,28,28	0
85	MG	AR	4012	1/1	0.95	0.35	30,30,30,30	0
85	MG	1	404	1/1	0.95	0.34	35,35,35,35	0
85	MG	1	4071	1/1	0.95	0.20	40,40,40,40	0
84	OHX	AR	3605	7/7	0.95	0.16	128,128,128,129	0
84	OHX	1	3604	7/7	0.95	0.34	116,116,117,117	0
85	MG	1	4075	1/1	0.95	0.43	41,41,41,41	0
85	MG	1	3924	1/1	0.95	0.37	60,60,60,60	0
85	MG	AR	4247	1/1	0.95	0.46	22,22,22,22	0
85	MG	1	3749	1/1	0.95	0.26	24,24,24,24	0
84	OHX	6	2020	7/7	0.95	0.18	135,136,136,137	0
84	OHX	1	3539	7/7	0.95	0.28	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3610	7/7	0.95	0.38	137,138,138,138	0
84	OHX	1	3606	7/7	0.95	0.40	138,138,138,138	0
85	MG	w	201	1/1	0.95	0.42	37,37,37,37	0
84	OHX	1	3469	7/7	0.95	0.21	117,117,118,118	0
84	OHX	AR	3618	7/7	0.95	0.21	113,113,114,114	0
84	OHX	1	3544	7/7	0.95	0.16	116,117,117,117	0
85	MG	AR	4259	1/1	0.95	0.49	16,16,16,16	0
85	MG	AS	212	1/1	0.95	0.33	41,41,41,41	0
84	OHX	AR	3624	7/7	0.95	0.33	150,150,151,151	0
84	OHX	1	3612	7/7	0.95	0.31	122,122,122,122	0
84	OHX	6	2026	7/7	0.95	0.25	146,146,147,147	0
84	OHX	6	2027	7/7	0.95	0.47	146,147,147,148	0
84	OHX	1	3657	7/7	0.95	0.28	123,123,124,124	0
84	OHX	AT	214	7/7	0.95	0.33	131,131,131,132	0
84	OHX	AR	3637	7/7	0.95	0.40	129,129,129,129	0
85	MG	AS	221	1/1	0.95	0.16	60,60,60,60	0
84	OHX	AT	216	7/7	0.95	0.40	132,132,132,132	0
84	OHX	AR	3638	7/7	0.95	0.42	119,119,119,119	0
85	MG	AR	3793	1/1	0.95	0.31	29,29,29,29	0
85	MG	6	2062	1/1	0.95	0.42	51,51,51,51	0
84	OHX	1	3545	7/7	0.95	0.21	120,120,120,120	0
85	MG	1	3769	1/1	0.95	0.19	45,45,45,45	0
84	OHX	1	3550	7/7	0.95	0.18	115,115,115,116	0
84	OHX	1	3706	7/7	0.95	0.30	136,137,137,138	0
85	MG	AR	3802	1/1	0.95	0.12	40,40,40,40	0
85	MG	1	4106	1/1	0.95	0.34	67,67,67,67	0
84	OHX	1	3616	7/7	0.95	0.31	146,146,147,147	0
84	OHX	6	1954	7/7	0.95	0.09	178,178,178,178	0
85	MG	1	3774	1/1	0.95	0.54	43,43,43,43	0
85	MG	6	2073	1/1	0.95	0.52	48,48,48,48	0
84	OHX	CL	301	7/7	0.95	0.21	121,122,122,122	0
84	OHX	6	1956	7/7	0.95	0.12	174,174,175,175	0
84	OHX	A	1909	7/7	0.95	0.24	151,151,152,153	0
84	OHX	A	1915	7/7	0.95	0.21	142,143,143,144	0
84	OHX	1	3662	7/7	0.95	0.31	116,116,116,116	0
84	OHX	A	1935	7/7	0.95	0.23	140,140,141,141	0
84	OHX	1	3487	7/7	0.95	0.17	115,115,116,116	0
85	MG	1	3788	1/1	0.95	0.53	45,45,45,45	0
84	OHX	1	3554	7/7	0.95	0.24	129,129,130,130	0
85	MG	CE	405	1/1	0.95	0.89	26,26,26,26	0
85	MG	AR	4062	1/1	0.95	0.17	42,42,42,42	0
84	OHX	A	1958	7/7	0.95	0.22	173,173,173,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3822	1/1	0.95	0.31	46,46,46,46	0
85	MG	AR	4065	1/1	0.95	0.25	31,31,31,31	0
85	MG	AR	4066	1/1	0.95	0.14	56,56,56,56	0
84	OHX	6	1966	7/7	0.95	0.15	133,133,134,134	0
84	OHX	A	1960	7/7	0.95	0.18	151,151,151,152	0
84	OHX	1	3481	7/7	0.95	0.19	116,117,117,117	0
85	MG	AR	3826	1/1	0.95	0.32	23,23,23,23	0
85	MG	CM	203	1/1	0.95	0.21	55,55,55,55	0
85	MG	6	2089	1/1	0.95	0.44	44,44,44,44	0
85	MG	CP	504	1/1	0.95	0.23	46,46,46,46	0
84	OHX	A	1964	7/7	0.95	0.28	122,122,123,123	0
85	MG	1	3796	1/1	0.95	0.54	18,18,18,18	0
85	MG	CQ	203	1/1	0.95	0.15	34,34,34,34	0
84	OHX	1	3621	7/7	0.95	0.23	125,126,126,126	0
84	OHX	A	1969	7/7	0.95	0.34	144,144,145,145	0
84	OHX	6	1972	7/7	0.95	0.42	142,143,143,144	0
84	OHX	AR	3658	7/7	0.95	0.35	122,123,123,123	0
84	OHX	A	1973	7/7	0.95	0.28	167,168,169,169	0
84	OHX	6	1973	7/7	0.95	0.22	137,138,138,138	0
84	OHX	A	1977	7/7	0.95	0.25	153,154,154,155	0
84	OHX	1	3667	7/7	0.95	0.30	127,127,128,128	0
85	MG	1	4141	1/1	0.95	0.38	64,64,64,64	0
85	MG	1	4144	1/1	0.95	0.16	53,53,53,53	0
84	OHX	1	3559	7/7	0.95	0.17	143,143,143,144	0
85	MG	6	2107	1/1	0.95	0.55	43,43,43,43	0
85	MG	AR	4088	1/1	0.95	0.40	25,25,25,25	0
84	OHX	A	1986	7/7	0.95	0.29	168,169,170,170	0
85	MG	1	3809	1/1	0.95	0.27	39,39,39,39	0
85	MG	DH	203	1/1	0.95	0.28	31,31,31,31	0
85	MG	1	3977	1/1	0.95	0.14	48,48,48,48	0
85	MG	AR	3853	1/1	0.95	0.26	43,43,43,43	0
84	OHX	1	3715	7/7	0.95	0.09	166,166,167,167	0
85	MG	AR	3855	1/1	0.95	0.43	33,33,33,33	0
85	MG	AR	3856	1/1	0.95	0.71	27,27,27,27	0
85	MG	AR	3857	1/1	0.95	0.53	20,20,20,20	0
84	OHX	6	1984	7/7	0.95	0.26	150,150,151,151	0
84	OHX	A	1995	7/7	0.95	0.17	151,152,152,152	0
84	OHX	1	3517	7/7	0.95	0.26	119,119,120,120	0
84	OHX	A	2000	7/7	0.95	0.24	140,141,141,141	0
85	MG	AR	3865	1/1	0.95	0.41	24,24,24,24	0
85	MG	AR	3867	1/1	0.95	0.55	18,18,18,18	0
85	MG	AR	4105	1/1	0.95	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	A	2002	7/7	0.95	0.31	147,148,149,149	0
84	OHX	1	3671	7/7	0.95	0.24	149,150,150,150	0
84	OHX	1	3567	7/7	0.95	0.24	128,129,129,129	0
84	OHX	AH	201	7/7	0.95	0.44	129,129,129,130	0
85	MG	AR	4111	1/1	0.95	0.35	37,37,37,37	0
85	MG	AR	3877	1/1	0.95	0.34	22,22,22,22	0
85	MG	1	3824	1/1	0.95	0.39	25,25,25,25	0
85	MG	AR	3880	1/1	0.95	0.47	42,42,42,42	0
85	MG	AR	3881	1/1	0.95	0.29	30,30,30,30	0
85	MG	A	2059	1/1	0.95	0.61	53,53,53,53	0
84	OHX	AR	3673	7/7	0.95	0.19	125,125,125,125	0
84	OHX	AK	102	7/7	0.95	0.18	105,105,105,105	0
85	MG	AR	3886	1/1	0.95	0.70	30,30,30,30	0
85	MG	A	2063	1/1	0.95	0.50	51,51,51,51	0
85	MG	A	2064	1/1	0.95	0.34	65,65,65,65	0
85	MG	AR	4121	1/1	0.95	0.30	27,27,27,27	0
84	OHX	1	3575	7/7	0.95	0.27	116,117,117,117	0
85	MG	6	2126	1/1	0.95	0.29	53,53,53,53	0
84	OHX	AR	3427	7/7	0.95	0.29	110,110,111,111	0
85	MG	6	2128	1/1	0.95	0.23	47,47,47,47	0
84	OHX	AR	3460	7/7	0.95	0.20	112,112,112,112	0
84	OHX	AR	3680	7/7	0.95	0.42	141,141,142,142	0
85	MG	A	2073	1/1	0.95	0.57	50,50,50,50	0
84	OHX	AR	3472	7/7	0.95	0.16	111,111,111,112	0
85	MG	AR	4129	1/1	0.95	0.36	26,26,26,26	0
84	OHX	AR	3474	7/7	0.95	0.19	114,114,114,115	0
85	MG	1	4171	1/1	0.95	0.24	85,85,85,85	0
85	MG	6	2135	1/1	0.95	0.24	49,49,49,49	0
85	MG	1	4173	1/1	0.95	0.54	36,36,36,36	0
85	MG	AR	3901	1/1	0.95	0.45	29,29,29,29	0
85	MG	AR	4138	1/1	0.95	0.47	28,28,28,28	0
84	OHX	AR	3495	7/7	0.95	0.17	113,113,114,114	0
85	MG	1	4175	1/1	0.95	0.44	39,39,39,39	0
85	MG	AR	3904	1/1	0.95	0.52	21,21,21,21	0
85	MG	1	3839	1/1	0.95	0.19	27,27,27,27	0
85	MG	1	4179	1/1	0.95	0.23	38,38,38,38	0
84	OHX	AR	3688	7/7	0.95	0.29	136,136,137,137	0
85	MG	1	3841	1/1	0.95	0.59	29,29,29,29	0
84	OHX	AR	3499	7/7	0.95	0.15	125,126,126,126	0
85	MG	1	4186	1/1	0.95	0.52	25,25,25,25	0
85	MG	AR	3915	1/1	0.95	0.61	28,28,28,28	0
84	OHX	A	2024	7/7	0.95	0.24	151,152,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3918	1/1	0.95	0.48	27,27,27,27	0
85	MG	AR	4151	1/1	0.95	0.10	148,148,148,148	0
85	MG	6	2147	1/1	0.95	0.12	57,57,57,57	0
85	MG	6	2148	1/1	0.95	0.43	48,48,48,48	0
85	MG	1	3846	1/1	0.95	0.28	39,39,39,39	0
84	OHX	AR	3503	7/7	0.95	0.17	120,120,121,121	0
84	OHX	1	3674	7/7	0.95	0.28	136,136,137,137	0
85	MG	6	2153	1/1	0.95	0.27	97,97,97,97	0
84	OHX	A	2027	7/7	0.95	0.33	159,160,161,161	0
84	OHX	AR	3511	7/7	0.95	0.26	108,108,108,108	0
85	MG	6	2156	1/1	0.95	0.16	101,101,101,101	0
84	OHX	6	1997	7/7	0.95	0.36	132,132,133,133	0
84	OHX	1	3577	7/7	0.95	0.31	118,118,119,119	0
85	MG	AR	3937	1/1	0.95	0.67	27,27,27,27	0
85	MG	AR	3942	1/1	0.95	0.56	31,31,31,31	0
84	OHX	A	2031	7/7	0.95	0.35	159,160,161,161	0
84	OHX	1	3634	7/7	0.95	0.17	132,132,132,133	0
84	OHX	AR	3700	7/7	0.95	0.47	135,135,135,135	0
85	MG	1	4207	1/1	0.95	0.28	36,36,36,36	0
85	MG	1	4208	1/1	0.95	0.32	37,37,37,37	0
85	MG	1	3859	1/1	0.95	0.44	28,28,28,28	0
84	OHX	1	3581	7/7	0.95	0.22	112,113,113,113	0
85	MG	A	2120	1/1	0.95	0.22	85,85,85,85	0
84	OHX	1	3681	7/7	0.95	0.32	127,127,127,128	0
84	OHX	AR	3703	7/7	0.95	0.51	136,136,136,136	0
84	OHX	AR	3532	7/7	0.95	0.14	135,136,136,137	0
84	OHX	AR	3537	7/7	0.95	0.15	131,132,132,132	0
84	OHX	AR	3538	7/7	0.95	0.17	123,123,124,124	0
84	OHX	AR	3544	7/7	0.95	0.16	109,109,110,110	0
85	MG	1	3867	1/1	0.95	0.43	35,35,35,35	0
85	MG	1	4024	1/1	0.95	0.21	61,61,61,61	0
84	OHX	1	3583	7/7	0.95	0.16	131,132,132,132	0
85	MG	6	2179	1/1	0.95	0.36	43,43,43,43	0
84	OHX	1	3588	7/7	0.95	0.19	128,128,128,128	0
84	OHX	1	3525	7/7	0.95	0.21	114,114,114,115	0
84	OHX	AR	3565	7/7	0.95	0.20	113,113,113,113	0
85	MG	1	3872	1/1	0.95	0.59	32,32,32,32	0
84	OHX	AR	3568	7/7	0.95	0.25	117,117,117,117	0
84	OHX	4	210	7/7	0.95	0.27	108,108,108,108	0
84	OHX	AR	3714	7/7	0.95	0.33	132,132,133,133	0
85	MG	1	3879	1/1	0.95	0.38	45,45,45,45	0
85	MG	AR	3972	1/1	0.95	0.53	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3575	7/7	0.95	0.28	119,120,120,120	0
85	MG	4	218	1/1	0.95	0.60	49,49,49,49	0
85	MG	AR	4199	1/1	0.95	0.36	45,45,45,45	0
85	MG	A	2148	1/1	0.95	0.37	64,64,64,64	0
85	MG	4	219	1/1	0.95	0.68	42,42,42,42	0
84	OHX	AR	3577	7/7	0.95	0.09	156,157,158,158	0
85	MG	AR	4202	1/1	0.95	0.56	29,29,29,29	0
84	OHX	AR	3579	7/7	0.95	0.35	130,130,130,130	0
84	OHX	AR	3583	7/7	0.95	0.22	113,114,114,114	0
84	OHX	AR	3587	7/7	0.95	0.24	126,126,126,126	0
85	MG	4	224	1/1	0.95	0.40	33,33,33,33	0
84	OHX	6	2009	7/7	0.95	0.18	126,127,127,128	0
85	MG	1	3894	1/1	0.95	0.48	22,22,22,22	0
84	OHX	AR	3592	7/7	0.95	0.34	114,114,114,114	0
84	OHX	1	3527	7/7	0.95	0.12	135,135,136,136	0
85	MG	AR	4212	1/1	0.95	0.27	31,31,31,31	0
85	MG	AR	3989	1/1	0.95	0.23	44,44,44,44	0
85	MG	AR	3990	1/1	0.95	0.08	39,39,39,39	0
85	MG	1	4048	1/1	0.95	0.83	33,33,33,33	0
84	OHX	AR	3724	7/7	0.95	0.27	130,130,131,131	0
84	OHX	AR	3595	7/7	0.95	0.31	131,131,131,132	0
85	MG	1	3733	1/1	0.95	0.49	26,26,26,26	0
85	MG	1	3902	1/1	0.95	0.50	35,35,35,35	0
84	OHX	6	2012	7/7	0.95	0.21	136,136,137,137	0
85	MG	AR	3746	1/1	0.95	0.26	58,58,58,58	0
84	OHX	1	3537	7/7	0.95	0.25	115,115,115,116	0
85	MG	1	3907	1/1	0.95	0.33	40,40,40,40	0
84	OHX	6	2014	7/7	0.95	0.34	129,129,129,130	0
84	OHX	6	2015	7/7	0.95	0.35	135,135,136,136	0
84	OHX	AR	3601	7/7	0.95	0.42	127,127,128,128	0
85	MG	AR	4228	1/1	0.95	0.38	27,27,27,27	0
85	MG	1	3914	1/1	0.95	0.50	19,19,19,19	0
86	HN8	1	4223	22/22	0.95	0.24	32,32,32,32	0
86	HN8	AR	4263	22/22	0.95	0.26	27,27,27,27	22
84	OHX	1	3599	7/7	0.95	0.43	115,116,116,116	0
85	MG	1	3741	1/1	0.95	0.25	37,37,37,37	0
85	MG	1	3919	1/1	0.95	0.27	33,33,33,33	0
85	MG	k	404	1/1	0.95	0.67	32,32,32,32	0
84	OHX	AR	3603	7/7	0.95	0.24	107,107,107,107	0
85	MG	AR	4237	1/1	0.95	0.21	39,39,39,39	0
88	ZN	g	501	1/1	0.95	0.06	119,119,119,119	0
84	OHX	1	3649	7/7	0.95	0.35	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3682	7/7	0.96	0.52	144,144,144,145	0
84	OHX	AR	3684	7/7	0.96	0.52	124,125,125,125	0
84	OHX	1	3519	7/7	0.96	0.22	116,116,116,116	0
84	OHX	O	201	7/7	0.96	0.28	158,159,159,160	0
84	OHX	6	1978	7/7	0.96	0.29	117,117,117,118	0
85	MG	AR	4217	1/1	0.96	0.60	80,80,80,80	0
84	OHX	T	201	7/7	0.96	0.19	145,146,146,147	0
85	MG	AR	3951	1/1	0.96	0.53	29,29,29,29	0
85	MG	AR	3952	1/1	0.96	0.36	28,28,28,28	0
84	OHX	e	101	7/7	0.96	0.41	143,144,145,145	0
84	OHX	AR	3687	7/7	0.96	0.37	121,121,122,122	0
85	MG	1	4143	1/1	0.96	0.21	29,29,29,29	0
84	OHX	c1	201	7/7	0.96	0.41	147,148,148,149	0
84	OHX	1	3703	7/7	0.96	0.46	131,131,132,132	0
84	OHX	6	1980	7/7	0.96	0.34	116,116,116,116	0
84	OHX	AR	3512	7/7	0.96	0.18	118,118,119,119	0
84	OHX	AR	3514	7/7	0.96	0.19	112,112,112,113	0
84	OHX	6	1982	7/7	0.96	0.17	147,147,148,148	0
84	OHX	AR	3693	7/7	0.96	0.41	131,131,131,131	0
84	OHX	AR	3521	7/7	0.96	0.28	117,118,118,118	0
84	OHX	AR	3522	7/7	0.96	0.13	114,114,115,115	0
85	MG	6	2151	1/1	0.96	0.15	60,60,60,60	0
84	OHX	AR	3697	7/7	0.96	0.25	114,115,115,115	0
84	OHX	1	3584	7/7	0.96	0.25	114,114,114,114	0
84	OHX	AR	3699	7/7	0.96	0.36	117,117,117,117	0
84	OHX	AR	3526	7/7	0.96	0.18	117,117,117,118	0
84	OHX	6	1985	7/7	0.96	0.33	130,130,131,131	0
84	OHX	1	3586	7/7	0.96	0.23	121,122,122,122	0
84	OHX	AR	3530	7/7	0.96	0.17	112,113,113,113	0
84	OHX	1	3520	7/7	0.96	0.18	123,123,124,124	0
84	OHX	6	1988	7/7	0.96	0.14	133,133,133,134	0
84	OHX	AR	3534	7/7	0.96	0.16	109,109,109,109	0
84	OHX	AR	3536	7/7	0.96	0.22	123,124,124,124	0
84	OHX	1	3589	7/7	0.96	0.23	113,113,113,113	0
85	MG	AR	4249	1/1	0.96	0.44	24,24,24,24	0
85	MG	1	4168	1/1	0.96	0.45	20,20,20,20	0
85	MG	1	3743	1/1	0.96	0.28	79,79,79,79	0
84	OHX	6	1990	7/7	0.96	0.29	129,130,130,130	0
84	OHX	AR	3541	7/7	0.96	0.19	125,125,125,125	0
85	MG	1	4172	1/1	0.96	0.41	67,67,67,67	0
84	OHX	AR	3543	7/7	0.96	0.24	123,123,123,123	0
84	OHX	1	3473	7/7	0.96	0.15	114,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	6	2172	1/1	0.96	0.26	38,38,38,38	0
85	MG	AR	4258	1/1	0.96	0.54	34,34,34,34	0
84	OHX	AR	3545	7/7	0.96	0.24	108,108,108,108	0
85	MG	1	4176	1/1	0.96	0.62	34,34,34,34	0
85	MG	1	4177	1/1	0.96	0.44	27,27,27,27	0
85	MG	6	2177	1/1	0.96	0.19	68,68,68,68	0
84	OHX	AR	3546	7/7	0.96	0.21	123,124,124,124	0
85	MG	AS	216	1/1	0.96	0.50	23,23,23,23	0
84	OHX	AR	3715	7/7	0.96	0.29	118,118,119,119	0
84	OHX	AR	3548	7/7	0.96	0.16	121,121,122,122	0
84	OHX	AR	3551	7/7	0.96	0.14	129,129,130,130	0
85	MG	AR	4000	1/1	0.96	0.43	25,25,25,25	0
84	OHX	1	3592	7/7	0.96	0.33	117,117,117,117	0
84	OHX	AR	3553	7/7	0.96	0.29	113,113,113,113	0
85	MG	6	2187	1/1	0.96	0.18	82,82,82,82	0
85	MG	1	3968	1/1	0.96	0.47	29,29,29,29	0
85	MG	1	4188	1/1	0.96	0.36	28,28,28,28	0
85	MG	1	3757	1/1	0.96	0.19	38,38,38,38	0
85	MG	AR	4007	1/1	0.96	0.28	29,29,29,29	0
85	MG	AS	229	1/1	0.96	0.24	46,46,46,46	0
84	OHX	AR	3555	7/7	0.96	0.21	115,115,115,115	0
84	OHX	AR	3556	7/7	0.96	0.21	109,109,109,109	0
84	OHX	AR	3557	7/7	0.96	0.17	123,123,124,124	0
84	OHX	AR	3562	7/7	0.96	0.24	124,124,124,124	0
85	MG	1	4197	1/1	0.96	0.34	32,32,32,32	0
84	OHX	6	1994	7/7	0.96	0.25	170,170,170,170	0
85	MG	1	4199	1/1	0.96	0.59	24,24,24,24	0
84	OHX	6	1995	7/7	0.96	0.24	133,134,134,135	0
84	OHX	6	1996	7/7	0.96	0.20	154,154,155,155	0
84	OHX	AR	3567	7/7	0.96	0.15	121,121,121,121	0
84	OHX	1	3593	7/7	0.96	0.15	166,167,167,167	0
84	OHX	AR	3570	7/7	0.96	0.25	120,121,121,121	0
85	MG	1	3980	1/1	0.96	0.26	73,73,73,73	0
84	OHX	6	1998	7/7	0.96	0.33	146,146,147,147	0
84	OHX	AR	3731	7/7	0.96	0.19	117,117,117,117	0
84	OHX	1	3526	7/7	0.96	0.29	114,115,115,115	0
84	OHX	6	2000	7/7	0.96	0.17	130,130,131,131	0
84	OHX	1	3654	7/7	0.96	0.14	136,136,136,137	0
84	OHX	AR	3580	7/7	0.96	0.20	117,118,118,118	0
85	MG	AK	103	1/1	0.96	0.44	36,36,36,36	0
85	MG	AP	503	1/1	0.96	0.28	27,27,27,27	0
85	MG	1	4216	1/1	0.96	0.39	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3775	1/1	0.96	0.29	32,32,32,32	0
84	OHX	AR	3581	7/7	0.96	0.18	109,109,109,109	0
84	OHX	1	3595	7/7	0.96	0.11	140,140,140,140	0
85	MG	CK	202	1/1	0.96	0.20	44,44,44,44	0
84	OHX	AR	3586	7/7	0.96	0.24	119,119,120,120	0
85	MG	1	4221	1/1	0.96	0.52	35,35,35,35	0
85	MG	1	4222	1/1	0.96	0.65	13,13,13,13	0
85	MG	CO	201	1/1	0.96	0.19	44,44,44,44	0
85	MG	1	3781	1/1	0.96	0.39	33,33,33,33	0
84	OHX	1	3445	7/7	0.96	0.26	111,112,112,112	0
85	MG	CP	505	1/1	0.96	0.27	71,71,71,71	0
84	OHX	AR	3588	7/7	0.96	0.27	112,112,112,113	0
85	MG	3	213	1/1	0.96	0.45	48,48,48,48	0
84	OHX	1	3597	7/7	0.96	0.39	117,117,118,118	0
85	MG	3	215	1/1	0.96	0.57	31,31,31,31	0
84	OHX	1	3531	7/7	0.96	0.19	114,114,114,114	0
84	OHX	AR	3743	7/7	0.96	0.33	109,109,109,109	0
85	MG	3	219	1/1	0.96	0.21	56,56,56,56	0
84	OHX	1	3601	7/7	0.96	0.30	112,112,112,112	0
84	OHX	1	3483	7/7	0.96	0.12	113,113,113,113	0
85	MG	AR	3766	1/1	0.96	0.14	96,96,96,96	0
84	OHX	1	3446	7/7	0.96	0.19	116,116,116,116	0
85	MG	1	3792	1/1	0.96	0.52	37,37,37,37	0
84	OHX	1	3451	7/7	0.96	0.22	111,111,111,111	0
84	OHX	AT	210	7/7	0.96	0.20	119,119,120,120	0
84	OHX	AT	211	7/7	0.96	0.11	137,138,138,138	0
85	MG	AR	3772	1/1	0.96	0.52	37,37,37,37	0
84	OHX	AR	3598	7/7	0.96	0.18	117,118,118,118	0
84	OHX	6	2011	7/7	0.96	0.43	146,146,147,147	0
85	MG	DH	202	1/1	0.96	0.26	40,40,40,40	0
84	OHX	1	3541	7/7	0.96	0.26	119,119,120,120	0
84	OHX	1	3543	7/7	0.96	0.22	119,119,120,120	0
84	OHX	1	3611	7/7	0.96	0.21	119,119,119,120	0
85	MG	4	226	1/1	0.96	0.59	42,42,42,42	0
84	OHX	1	3455	7/7	0.96	0.16	127,127,127,128	0
84	OHX	1	3489	7/7	0.96	0.21	113,113,114,114	0
84	OHX	6	2017	7/7	0.96	0.29	135,135,136,136	0
84	OHX	1	3547	7/7	0.96	0.11	120,121,121,121	0
85	MG	AR	3787	1/1	0.96	0.69	31,31,31,31	0
84	OHX	3	207	7/7	0.96	0.20	137,138,138,138	0
84	OHX	1	3670	7/7	0.96	0.24	111,111,111,111	0
85	MG	AR	3790	1/1	0.96	0.34	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	CK	201	7/7	0.96	0.21	118,118,119,119	0
84	OHX	4	206	7/7	0.96	0.16	116,116,116,116	0
85	MG	1	3812	1/1	0.96	0.64	64,64,64,64	0
84	OHX	1	3497	7/7	0.96	0.11	125,125,126,126	0
85	MG	AR	3795	1/1	0.96	0.66	49,49,49,49	0
84	OHX	CX	202	7/7	0.96	0.27	117,118,118,118	0
84	OHX	AR	3612	7/7	0.96	0.34	111,111,111,111	0
85	MG	AR	4079	1/1	0.96	0.31	34,34,34,34	0
85	MG	4	239	1/1	0.96	0.69	43,43,43,43	0
84	OHX	AR	3613	7/7	0.96	0.29	112,112,112,112	0
84	OHX	AR	3614	7/7	0.96	0.20	114,114,114,114	0
84	OHX	A	1933	7/7	0.96	0.13	122,122,122,123	0
84	OHX	4	211	7/7	0.96	0.14	138,139,139,140	0
84	OHX	A	1936	7/7	0.96	0.17	126,127,127,128	0
84	OHX	A	1944	7/7	0.96	0.12	138,139,139,140	0
84	OHX	AR	3617	7/7	0.96	0.28	123,123,123,123	0
84	OHX	A	1947	7/7	0.96	0.27	129,129,130,130	0
85	MG	1	4032	1/1	0.96	0.31	42,42,42,42	0
85	MG	A	2066	1/1	0.96	0.59	79,79,79,79	0
85	MG	AR	4091	1/1	0.96	0.31	35,35,35,35	0
84	OHX	1	3617	7/7	0.96	0.23	122,122,122,122	0
84	OHX	A	1955	7/7	0.96	0.13	145,146,147,147	0
84	OHX	AR	3619	7/7	0.96	0.35	122,123,123,124	0
85	MG	AR	4095	1/1	0.96	0.22	25,25,25,25	0
84	OHX	AR	3621	7/7	0.96	0.35	135,135,136,136	0
84	OHX	1	3458	7/7	0.96	0.20	116,116,116,117	0
85	MG	A	2074	1/1	0.96	0.41	55,55,55,55	0
84	OHX	AR	3623	7/7	0.96	0.29	138,139,139,139	0
84	OHX	1	3553	7/7	0.96	0.29	121,122,122,122	0
85	MG	1	3838	1/1	0.96	0.57	33,33,33,33	0
84	OHX	AR	3626	7/7	0.96	0.30	122,123,123,123	0
84	OHX	AR	3627	7/7	0.96	0.32	127,128,128,128	0
84	OHX	AR	3628	7/7	0.96	0.32	147,148,148,148	0
85	MG	1	3842	1/1	0.96	0.55	25,25,25,25	0
84	OHX	AR	3629	7/7	0.96	0.14	141,141,141,142	0
84	OHX	1	3500	7/7	0.96	0.16	119,120,120,120	0
85	MG	AR	3828	1/1	0.96	0.61	60,60,60,60	0
84	OHX	AR	3632	7/7	0.96	0.35	117,117,118,118	0
85	MG	1	4052	1/1	0.96	0.29	21,21,21,21	0
84	OHX	A	1975	7/7	0.96	0.10	156,158,158,158	0
85	MG	AR	4112	1/1	0.96	0.15	54,54,54,54	0
84	OHX	A	1976	7/7	0.96	0.18	123,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3633	7/7	0.96	0.28	124,125,125,125	0
84	OHX	A	1978	7/7	0.96	0.26	143,144,144,145	0
85	MG	lR	201	1/1	0.96	0.36	26,26,26,26	0
84	OHX	A	1980	7/7	0.96	0.26	137,137,138,138	0
85	MG	6	2055	1/1	0.96	0.73	49,49,49,49	0
84	OHX	k	401	7/7	0.96	0.27	118,118,118,118	0
84	OHX	A	1983	7/7	0.96	0.24	142,142,143,143	0
85	MG	1	3854	1/1	0.96	0.62	34,34,34,34	0
85	MG	6	2061	1/1	0.96	0.32	100,100,100,100	0
85	MG	AR	3844	1/1	0.96	0.40	27,27,27,27	0
84	OHX	6	2029	7/7	0.96	0.41	152,153,153,154	0
85	MG	AR	3846	1/1	0.96	0.56	33,33,33,33	0
85	MG	1	3856	1/1	0.96	0.68	24,24,24,24	0
84	OHX	1	3431	7/7	0.96	0.30	114,114,114,114	0
84	OHX	A	1989	7/7	0.96	0.37	154,155,155,155	0
84	OHX	1	3677	7/7	0.96	0.33	116,116,117,117	0
85	MG	AR	4133	1/1	0.96	0.27	25,25,25,25	0
85	MG	1	4069	1/1	0.96	0.43	46,46,46,46	0
84	OHX	1	3622	7/7	0.96	0.27	153,154,154,154	0
84	OHX	A	1994	7/7	0.96	0.28	142,143,144,144	0
84	OHX	1	3680	7/7	0.96	0.32	122,122,122,122	0
84	OHX	6	2034	7/7	0.96	0.19	155,155,155,155	0
84	OHX	A	1997	7/7	0.96	0.28	139,140,140,140	0
85	MG	6	2075	1/1	0.96	0.14	76,76,76,76	0
84	OHX	A	1999	7/7	0.96	0.24	146,146,147,147	0
84	OHX	1	3623	7/7	0.96	0.23	114,114,115,115	0
85	MG	A	2119	1/1	0.96	0.35	57,57,57,57	0
84	OHX	A	2001	7/7	0.96	0.20	136,137,137,138	0
84	OHX	1	3683	7/7	0.96	0.33	118,118,118,118	0
85	MG	AR	3871	1/1	0.96	0.40	28,28,28,28	0
84	OHX	A	2003	7/7	0.96	0.32	129,130,130,130	0
84	OHX	A	2005	7/7	0.96	0.32	131,132,132,132	0
85	MG	AR	3874	1/1	0.96	0.60	27,27,27,27	0
84	OHX	1	3684	7/7	0.96	0.41	141,141,141,141	0
84	OHX	6	1921	7/7	0.96	0.17	141,141,142,143	0
85	MG	6	2084	1/1	0.96	0.22	48,48,48,48	0
84	OHX	A	2009	7/7	0.96	0.38	126,126,127,127	0
85	MG	1	3876	1/1	0.96	0.40	37,37,37,37	0
84	OHX	AR	3648	7/7	0.96	0.55	130,131,131,131	0
84	OHX	1	3685	7/7	0.96	0.41	121,121,121,121	0
84	OHX	1	3624	7/7	0.96	0.20	136,136,136,137	0
84	OHX	1	3507	7/7	0.96	0.23	113,113,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	6	1941	7/7	0.96	0.13	120,120,121,121	0
84	OHX	A	2016	7/7	0.96	0.28	142,143,143,144	0
85	MG	A	2137	1/1	0.96	0.48	58,58,58,58	0
85	MG	A	2138	1/1	0.96	0.46	66,66,66,66	0
85	MG	6	2093	1/1	0.96	0.33	47,47,47,47	0
85	MG	1	4094	1/1	0.96	0.15	78,78,78,78	0
85	MG	1	4095	1/1	0.96	0.20	61,61,61,61	0
85	MG	1	4096	1/1	0.96	0.41	27,27,27,27	0
85	MG	A	2144	1/1	0.96	0.39	69,69,69,69	0
85	MG	AR	3895	1/1	0.96	0.28	43,43,43,43	0
84	OHX	6	1946	7/7	0.96	0.17	127,128,128,129	0
84	OHX	6	2044	7/7	0.96	0.35	140,141,141,141	0
84	OHX	6	1947	7/7	0.96	0.14	121,122,122,122	0
85	MG	6	2101	1/1	0.96	0.51	53,53,53,53	0
84	OHX	6	1949	7/7	0.96	0.11	135,136,136,136	0
84	OHX	1	3509	7/7	0.96	0.14	119,120,120,120	0
85	MG	6	2104	1/1	0.96	0.20	70,70,70,70	0
85	MG	1	4103	1/1	0.96	0.27	60,60,60,60	0
84	OHX	6	1952	7/7	0.96	0.14	148,148,148,148	0
85	MG	1	4105	1/1	0.96	0.49	26,26,26,26	0
84	OHX	AR	3662	7/7	0.96	0.22	111,111,112,112	0
84	OHX	1	3628	7/7	0.96	0.26	144,145,145,145	0
84	OHX	1	3565	7/7	0.96	0.25	131,131,131,131	0
84	OHX	1	3510	7/7	0.96	0.16	111,111,111,111	0
84	OHX	1	3435	7/7	0.96	0.27	114,114,114,114	0
85	MG	AR	3916	1/1	0.96	0.58	19,19,19,19	0
84	OHX	1	3693	7/7	0.96	0.27	118,118,118,118	0
85	MG	6	2114	1/1	0.96	0.47	46,46,46,46	0
85	MG	AR	3919	1/1	0.96	0.43	34,34,34,34	0
84	OHX	1	3471	7/7	0.96	0.21	112,112,113,113	0
84	OHX	AR	3669	7/7	0.96	0.17	175,176,176,176	0
84	OHX	1	3579	7/7	0.96	0.17	119,120,120,120	0
84	OHX	AR	3671	7/7	0.96	0.28	113,113,113,113	0
84	OHX	1	3637	7/7	0.96	0.15	140,140,140,141	0
85	MG	1	3916	1/1	0.96	0.29	26,26,26,26	0
85	MG	AR	3926	1/1	0.96	0.37	33,33,33,33	0
85	MG	1	4120	1/1	0.96	0.40	27,27,27,27	0
85	MG	d3	202	1/1	0.96	0.33	47,47,47,47	0
84	OHX	AR	3441	7/7	0.96	0.18	116,117,117,117	0
84	OHX	1	3518	7/7	0.96	0.15	109,110,110,110	0
85	MG	AR	3931	1/1	0.96	0.29	17,17,17,17	0
85	MG	AR	3933	1/1	0.96	0.47	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3676	7/7	0.96	0.29	122,122,123,123	0
84	OHX	AR	3466	7/7	0.96	0.18	120,120,121,121	0
85	MG	AR	3936	1/1	0.96	0.52	20,20,20,20	0
84	OHX	1	3640	7/7	0.96	0.35	124,124,124,125	0
85	MG	AR	3939	1/1	0.96	0.31	31,31,31,31	0
85	MG	AR	3941	1/1	0.96	0.46	36,36,36,36	0
84	OHX	AR	3679	7/7	0.96	0.25	153,153,153,154	0
84	OHX	1	3582	7/7	0.96	0.29	121,121,121,121	0
84	OHX	6	1976	7/7	0.96	0.13	146,147,147,148	0
88	ZN	e1	501	1/1	0.96	0.06	153,153,153,153	0
84	OHX	AR	3625	7/7	0.97	0.36	134,134,134,134	0
84	OHX	A	1968	7/7	0.97	0.34	125,125,126,126	0
84	OHX	1	3506	7/7	0.97	0.29	109,109,110,110	0
84	OHX	1	3466	7/7	0.97	0.16	114,115,115,115	0
84	OHX	6	1953	7/7	0.97	0.12	132,133,133,134	0
85	MG	AR	3930	1/1	0.97	0.62	29,29,29,29	0
84	OHX	1	3638	7/7	0.97	0.33	122,123,123,123	0
85	MG	AR	3932	1/1	0.97	0.28	63,63,63,63	0
84	OHX	AR	3630	7/7	0.97	0.13	124,125,125,125	0
84	OHX	AG	201	7/7	0.97	0.21	114,115,115,115	0
84	OHX	6	1955	7/7	0.97	0.13	179,179,179,179	0
84	OHX	1	3585	7/7	0.97	0.23	115,115,116,116	0
84	OHX	6	1957	7/7	0.97	0.14	129,130,130,131	0
85	MG	AR	3938	1/1	0.97	0.39	34,34,34,34	0
84	OHX	A	1979	7/7	0.97	0.22	142,143,144,144	0
84	OHX	AP	502	7/7	0.97	0.17	112,113,113,113	0
84	OHX	6	1959	7/7	0.97	0.17	137,138,138,139	0
85	MG	1	4112	1/1	0.97	0.43	32,32,32,32	0
84	OHX	A	1982	7/7	0.97	0.30	121,122,122,122	0
85	MG	1	4114	1/1	0.97	0.23	52,52,52,52	0
84	OHX	AR	3432	7/7	0.97	0.27	117,117,117,118	0
84	OHX	1	3542	7/7	0.97	0.17	119,119,120,120	0
84	OHX	AR	3442	7/7	0.97	0.22	112,112,112,112	0
85	MG	AR	4229	1/1	0.97	0.70	34,34,34,34	0
84	OHX	A	1987	7/7	0.97	0.15	128,128,129,129	0
84	OHX	A	1988	7/7	0.97	0.23	139,140,141,141	0
84	OHX	AR	3445	7/7	0.97	0.18	107,107,107,107	0
85	MG	6	2136	1/1	0.97	0.23	52,52,52,52	0
85	MG	AR	3953	1/1	0.97	0.19	34,34,34,34	0
85	MG	AR	4235	1/1	0.97	0.37	26,26,26,26	0
85	MG	1	4122	1/1	0.97	0.25	78,78,78,78	0
85	MG	1	3878	1/1	0.97	0.58	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	A	1990	7/7	0.97	0.27	135,135,136,136	0
84	OHX	AR	3447	7/7	0.97	0.25	112,112,112,112	0
84	OHX	A	1992	7/7	0.97	0.21	140,141,142,142	0
85	MG	1	3883	1/1	0.97	0.41	22,22,22,22	0
84	OHX	AR	3642	7/7	0.97	0.24	122,122,122,122	0
84	OHX	AR	3643	7/7	0.97	0.30	120,121,121,121	0
85	MG	1	3887	1/1	0.97	0.83	42,42,42,42	0
84	OHX	AR	3455	7/7	0.97	0.22	111,112,112,112	0
84	OHX	AR	3456	7/7	0.97	0.19	117,117,117,117	0
84	OHX	AR	3458	7/7	0.97	0.19	114,114,114,115	0
85	MG	1	3895	1/1	0.97	0.42	28,28,28,28	0
84	OHX	A	1998	7/7	0.97	0.25	158,159,160,160	0
84	OHX	AR	3459	7/7	0.97	0.26	114,114,115,115	0
84	OHX	1	3699	7/7	0.97	0.40	130,131,131,131	0
85	MG	AR	3970	1/1	0.97	0.23	50,50,50,50	0
84	OHX	AR	3463	7/7	0.97	0.17	110,110,111,111	0
85	MG	1	3900	1/1	0.97	0.34	42,42,42,42	0
84	OHX	1	3442	7/7	0.97	0.24	120,121,121,121	0
85	MG	AR	3974	1/1	0.97	0.42	81,81,81,81	0
84	OHX	AR	3467	7/7	0.97	0.13	108,109,109,109	0
84	OHX	A	2004	7/7	0.97	0.22	139,139,140,140	0
84	OHX	AR	3653	7/7	0.97	0.30	120,120,121,121	0
84	OHX	AR	3469	7/7	0.97	0.14	121,122,122,122	0
84	OHX	6	1964	7/7	0.97	0.12	123,123,124,124	0
85	MG	1	3909	1/1	0.97	0.57	25,25,25,25	0
84	OHX	A	2008	7/7	0.97	0.16	132,132,133,133	0
84	OHX	AR	3656	7/7	0.97	0.31	134,134,134,134	0
84	OHX	AR	3473	7/7	0.97	0.11	111,111,112,112	0
85	MG	AR	3985	1/1	0.97	0.49	35,35,35,35	0
84	OHX	6	1965	7/7	0.97	0.24	116,117,117,117	0
85	MG	AR	3987	1/1	0.97	0.30	31,31,31,31	0
84	OHX	AR	3478	7/7	0.97	0.17	110,110,110,111	0
85	MG	1	4157	1/1	0.97	0.48	60,60,60,60	0
84	OHX	AR	3479	7/7	0.97	0.15	110,110,110,110	0
85	MG	1	3918	1/1	0.97	0.20	31,31,31,31	0
84	OHX	AR	3661	7/7	0.97	0.46	112,112,112,113	0
84	OHX	AR	3480	7/7	0.97	0.12	113,114,114,114	0
84	OHX	AR	3483	7/7	0.97	0.17	111,111,111,111	0
84	OHX	AR	3484	7/7	0.97	0.19	114,114,114,114	0
85	MG	AS	231	1/1	0.97	0.19	56,56,56,56	0
84	OHX	AR	3491	7/7	0.97	0.13	108,108,109,109	0
84	OHX	AR	3492	7/7	0.97	0.15	116,116,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3493	7/7	0.97	0.25	114,114,114,114	0
84	OHX	AR	3494	7/7	0.97	0.15	124,125,125,125	0
84	OHX	1	3425	7/7	0.97	0.25	108,109,109,109	0
84	OHX	AR	3496	7/7	0.97	0.24	112,113,113,113	0
84	OHX	6	1967	7/7	0.97	0.17	126,127,127,127	0
84	OHX	AR	3501	7/7	0.97	0.31	113,113,114,114	0
84	OHX	6	1968	7/7	0.97	0.26	122,122,123,123	0
84	OHX	AR	3504	7/7	0.97	0.18	110,110,110,110	0
84	OHX	1	3438	7/7	0.97	0.25	117,117,117,117	0
84	OHX	1	3546	7/7	0.97	0.17	127,127,127,127	0
84	OHX	1	3645	7/7	0.97	0.34	125,126,126,126	0
84	OHX	AR	3513	7/7	0.97	0.09	150,151,151,151	0
84	OHX	1	3646	7/7	0.97	0.25	117,118,118,118	0
84	OHX	AR	3516	7/7	0.97	0.15	112,112,112,112	0
85	MG	1	4182	1/1	0.97	0.30	25,25,25,25	0
84	OHX	6	1974	7/7	0.97	0.15	121,121,122,122	0
84	OHX	AR	3683	7/7	0.97	0.36	126,127,127,127	0
85	MG	1	4185	1/1	0.97	0.50	27,27,27,27	0
84	OHX	AR	3519	7/7	0.97	0.15	108,109,109,109	0
84	OHX	AR	3520	7/7	0.97	0.31	112,112,113,113	0
84	OHX	1	3647	7/7	0.97	0.23	118,118,118,118	0
84	OHX	1	3492	7/7	0.97	0.19	117,118,118,118	0
84	OHX	1	3548	7/7	0.97	0.11	134,134,134,134	0
85	MG	1	4191	1/1	0.97	0.44	29,29,29,29	0
85	MG	1	4192	1/1	0.97	0.66	21,21,21,21	0
84	OHX	1	3549	7/7	0.97	0.15	120,120,120,120	0
84	OHX	1	3494	7/7	0.97	0.13	119,119,120,120	0
84	OHX	J	301	7/7	0.97	0.25	157,157,158,158	0
85	MG	CP	503	1/1	0.97	0.41	38,38,38,38	0
84	OHX	1	3551	7/7	0.97	0.27	118,118,119,119	0
84	OHX	M	201	7/7	0.97	0.38	137,137,138,138	0
84	OHX	1	3598	7/7	0.97	0.27	127,127,127,127	0
85	MG	1	4200	1/1	0.97	0.49	22,22,22,22	0
84	OHX	6	1983	7/7	0.97	0.18	128,129,129,129	0
84	OHX	1	3495	7/7	0.97	0.14	114,115,115,115	0
84	OHX	AR	3533	7/7	0.97	0.18	111,111,111,111	0
85	MG	1	4204	1/1	0.97	0.51	34,34,34,34	0
85	MG	1	4205	1/1	0.97	0.24	31,31,31,31	0
84	OHX	h	401	7/7	0.97	0.15	175,176,177,177	0
84	OHX	AR	3696	7/7	0.97	0.18	112,113,113,113	0
84	OHX	1	3600	7/7	0.97	0.15	150,150,150,150	0
85	MG	CX	203	1/1	0.97	0.39	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3535	7/7	0.97	0.13	114,115,115,115	0
84	OHX	1	3476	7/7	0.97	0.14	111,111,111,112	0
84	OHX	1	3602	7/7	0.97	0.23	128,128,128,129	0
84	OHX	c8	201	7/7	0.97	0.20	146,147,147,148	0
84	OHX	1	3658	7/7	0.97	0.34	142,143,143,143	0
84	OHX	AR	3539	7/7	0.97	0.14	127,128,128,128	0
84	OHX	AR	3540	7/7	0.97	0.16	108,108,108,108	0
85	MG	AR	3762	1/1	0.97	0.17	24,24,24,24	0
84	OHX	1	3603	7/7	0.97	0.17	123,123,124,124	0
84	OHX	AR	3542	7/7	0.97	0.11	152,152,152,153	0
85	MG	AR	4048	1/1	0.97	0.23	34,34,34,34	0
84	OHX	1	3480	7/7	0.97	0.14	119,119,119,120	0
84	OHX	1	3449	7/7	0.97	0.23	117,117,118,118	0
84	OHX	1	3558	7/7	0.97	0.17	134,134,135,135	0
85	MG	AR	4053	1/1	0.97	0.40	30,30,30,30	0
84	OHX	1	3607	7/7	0.97	0.17	122,122,122,122	0
84	OHX	AR	3547	7/7	0.97	0.28	116,116,116,117	0
84	OHX	1	3608	7/7	0.97	0.25	118,119,119,119	0
85	MG	1	3736	1/1	0.97	0.60	31,31,31,31	0
84	OHX	AR	3549	7/7	0.97	0.20	116,117,117,117	0
85	MG	AR	3775	1/1	0.97	0.23	22,22,22,22	0
84	OHX	1	3463	7/7	0.97	0.13	121,121,122,122	0
84	OHX	3	202	7/7	0.97	0.12	115,116,116,116	0
84	OHX	3	203	7/7	0.97	0.11	118,118,118,119	0
84	OHX	AR	3554	7/7	0.97	0.15	112,112,112,112	0
85	MG	3	218	1/1	0.97	0.22	54,54,54,54	0
84	OHX	3	204	7/7	0.97	0.15	124,125,125,125	0
84	OHX	1	3561	7/7	0.97	0.26	124,124,125,125	0
84	OHX	1	3562	7/7	0.97	0.14	121,121,121,121	0
84	OHX	AR	3558	7/7	0.97	0.16	137,137,137,137	0
85	MG	AR	3786	1/1	0.97	0.48	25,25,25,25	0
84	OHX	AR	3559	7/7	0.97	0.31	121,121,121,121	0
85	MG	A	2058	1/1	0.97	0.66	46,46,46,46	0
84	OHX	AR	3560	7/7	0.97	0.19	135,135,136,136	0
84	OHX	AR	3561	7/7	0.97	0.24	110,110,110,111	0
84	OHX	1	3528	7/7	0.97	0.12	119,120,120,120	0
84	OHX	6	2003	7/7	0.97	0.13	126,126,127,127	0
84	OHX	3	208	7/7	0.97	0.30	116,116,116,116	0
84	OHX	1	3613	7/7	0.97	0.47	120,120,121,121	0
84	OHX	AR	3566	7/7	0.97	0.24	115,115,115,116	0
84	OHX	4	203	7/7	0.97	0.16	106,107,107,107	0
84	OHX	4	204	7/7	0.97	0.15	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3797	1/1	0.97	0.27	31,31,31,31	0
84	OHX	AR	3569	7/7	0.97	0.29	137,137,137,138	0
84	OHX	4	205	7/7	0.97	0.17	106,106,106,106	0
85	MG	1	3760	1/1	0.97	0.35	27,27,27,27	0
84	OHX	1	3564	7/7	0.97	0.24	126,126,127,127	0
84	OHX	AR	3574	7/7	0.97	0.17	112,113,113,113	0
84	OHX	4	208	7/7	0.97	0.36	106,106,106,106	0
84	OHX	AR	3576	7/7	0.97	0.32	128,128,129,129	0
85	MG	AR	3806	1/1	0.97	0.29	57,57,57,57	0
85	MG	A	2077	1/1	0.97	0.59	48,48,48,48	0
84	OHX	4	209	7/7	0.97	0.23	113,113,113,113	0
85	MG	A	2079	1/1	0.97	0.64	58,58,58,58	0
84	OHX	1	3529	7/7	0.97	0.17	115,115,115,116	0
84	OHX	1	3566	7/7	0.97	0.18	113,113,114,114	0
85	MG	AR	3810	1/1	0.97	0.51	27,27,27,27	0
84	OHX	4	212	7/7	0.97	0.28	128,128,128,128	0
84	OHX	1	3502	7/7	0.97	0.18	114,114,114,114	0
84	OHX	AR	3584	7/7	0.97	0.13	131,131,131,132	0
84	OHX	AR	3585	7/7	0.97	0.20	117,117,117,117	0
84	OHX	1	3568	7/7	0.97	0.28	115,116,116,116	0
84	OHX	AS	206	7/7	0.97	0.13	124,124,125,125	0
84	OHX	AS	208	7/7	0.97	0.10	138,139,139,139	0
84	OHX	1	3569	7/7	0.97	0.28	111,111,111,111	0
85	MG	1	3776	1/1	0.97	0.50	43,43,43,43	0
84	OHX	1	3571	7/7	0.97	0.18	111,111,112,112	0
84	OHX	1	3572	7/7	0.97	0.27	118,119,119,119	0
84	OHX	AT	203	7/7	0.97	0.14	117,117,117,117	0
85	MG	1	3780	1/1	0.97	0.33	17,17,17,17	0
84	OHX	AT	205	7/7	0.97	0.15	108,108,108,108	0
85	MG	1	4019	1/1	0.97	0.24	42,42,42,42	0
84	OHX	AT	206	7/7	0.97	0.11	123,124,124,124	0
85	MG	1	3784	1/1	0.97	0.45	26,26,26,26	0
84	OHX	AT	207	7/7	0.97	0.15	117,117,117,117	0
84	OHX	AT	208	7/7	0.97	0.32	114,114,114,114	0
85	MG	AR	4115	1/1	0.97	0.33	46,46,46,46	0
84	OHX	AT	209	7/7	0.97	0.11	121,121,122,122	0
84	OHX	AR	3591	7/7	0.97	0.25	112,112,112,112	0
85	MG	v	302	1/1	0.97	0.34	36,36,36,36	0
84	OHX	1	3678	7/7	0.97	0.15	117,117,118,118	0
85	MG	AR	3837	1/1	0.97	0.59	19,19,19,19	0
85	MG	A	2108	1/1	0.97	0.62	57,57,57,57	0
84	OHX	1	3573	7/7	0.97	0.18	131,131,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3594	7/7	0.97	0.20	114,114,115,115	0
84	OHX	v	301	7/7	0.97	0.20	113,113,114,114	0
84	OHX	1	3574	7/7	0.97	0.28	116,116,117,117	0
84	OHX	1	3534	7/7	0.97	0.19	113,113,113,113	0
84	OHX	1	3682	7/7	0.97	0.14	110,110,111,111	0
84	OHX	1	3625	7/7	0.97	0.22	135,135,135,135	0
84	OHX	6	1905	7/7	0.97	0.34	132,133,133,134	0
84	OHX	6	1907	7/7	0.97	0.32	135,136,136,137	0
84	OHX	6	1909	7/7	0.97	0.26	137,138,138,139	0
85	MG	AR	4132	1/1	0.97	0.15	49,49,49,49	0
85	MG	AR	3848	1/1	0.97	0.28	31,31,31,31	0
85	MG	AR	3849	1/1	0.97	0.45	35,35,35,35	0
85	MG	AR	3850	1/1	0.97	0.28	24,24,24,24	0
84	OHX	6	1911	7/7	0.97	0.24	134,135,135,135	0
85	MG	6	2053	1/1	0.97	0.57	41,41,41,41	0
84	OHX	1	3576	7/7	0.97	0.14	131,131,132,132	0
84	OHX	1	3536	7/7	0.97	0.22	109,109,109,109	0
84	OHX	6	1925	7/7	0.97	0.20	122,122,122,123	0
85	MG	6	2057	1/1	0.97	0.56	51,51,51,51	0
85	MG	6	2058	1/1	0.97	0.43	45,45,45,45	0
85	MG	1	4043	1/1	0.97	0.32	27,27,27,27	0
84	OHX	6	1927	7/7	0.97	0.22	124,124,125,125	0
85	MG	1	3806	1/1	0.97	0.46	51,51,51,51	0
84	OHX	1	3578	7/7	0.97	0.19	107,107,107,107	0
85	MG	6	2063	1/1	0.97	0.20	82,82,82,82	0
84	OHX	A	1910	7/7	0.97	0.23	138,139,139,140	0
84	OHX	A	1911	7/7	0.97	0.22	139,140,141,141	0
85	MG	AR	3869	1/1	0.97	0.40	31,31,31,31	0
84	OHX	A	1913	7/7	0.97	0.20	126,126,127,127	0
85	MG	1	4051	1/1	0.97	0.22	44,44,44,44	0
84	OHX	1	3503	7/7	0.97	0.10	127,128,128,129	0
84	OHX	A	1917	7/7	0.97	0.17	130,131,131,131	0
84	OHX	6	1933	7/7	0.97	0.13	116,116,117,117	0
85	MG	6	2071	1/1	0.97	0.49	45,45,45,45	0
85	MG	1	3815	1/1	0.97	0.14	40,40,40,40	0
84	OHX	A	1921	7/7	0.97	0.22	142,143,144,144	0
84	OHX	A	1926	7/7	0.97	0.08	127,127,127,128	0
84	OHX	A	1927	7/7	0.97	0.14	138,138,139,139	0
85	MG	1	4059	1/1	0.97	0.42	51,51,51,51	0
85	MG	AR	3885	1/1	0.97	0.37	33,33,33,33	0
84	OHX	A	1928	7/7	0.97	0.13	125,126,126,126	0
84	OHX	A	1930	7/7	0.97	0.10	122,122,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2154	1/1	0.97	0.93	45,45,45,45	0
85	MG	1	3822	1/1	0.97	0.49	18,18,18,18	0
84	OHX	A	1931	7/7	0.97	0.10	139,140,140,140	0
84	OHX	A	1932	7/7	0.97	0.18	141,142,142,143	0
84	OHX	6	1934	7/7	0.97	0.13	139,139,140,140	0
84	OHX	A	1934	7/7	0.97	0.12	132,132,133,133	0
84	OHX	6	1935	7/7	0.97	0.14	121,121,121,122	0
84	OHX	6	1936	7/7	0.97	0.15	116,116,117,117	0
84	OHX	A	1937	7/7	0.97	0.16	153,154,155,155	0
85	MG	1	4072	1/1	0.97	0.18	46,46,46,46	0
85	MG	AR	3898	1/1	0.97	0.63	28,28,28,28	0
84	OHX	A	1939	7/7	0.97	0.11	140,141,141,142	0
84	OHX	A	1940	7/7	0.97	0.28	137,138,138,139	0
85	MG	AR	4179	1/1	0.97	0.27	43,43,43,43	0
84	OHX	A	1941	7/7	0.97	0.12	136,137,137,137	0
85	MG	1	3835	1/1	0.97	0.47	30,30,30,30	0
85	MG	s8	302	1/1	0.97	0.33	51,51,51,51	0
85	MG	1	3836	1/1	0.97	0.39	36,36,36,36	0
84	OHX	A	1943	7/7	0.97	0.21	133,133,134,134	0
84	OHX	6	1938	7/7	0.97	0.13	130,131,131,131	0
85	MG	AR	3906	1/1	0.97	0.36	33,33,33,33	0
84	OHX	A	1945	7/7	0.97	0.18	143,144,144,145	0
85	MG	AR	3908	1/1	0.97	0.53	25,25,25,25	0
84	OHX	AR	3616	7/7	0.97	0.34	109,110,110,110	0
84	OHX	6	1939	7/7	0.97	0.10	131,132,132,133	0
84	OHX	A	1948	7/7	0.97	0.13	139,140,140,140	0
85	MG	d6	102	1/1	0.97	0.50	38,38,38,38	0
84	OHX	A	1951	7/7	0.97	0.24	145,145,146,146	0
84	OHX	1	3580	7/7	0.97	0.35	115,116,116,116	0
84	OHX	A	1954	7/7	0.97	0.17	135,136,136,136	0
84	OHX	1	3538	7/7	0.97	0.09	125,125,125,126	0
84	OHX	A	1956	7/7	0.97	0.14	133,133,134,134	0
84	OHX	AR	3620	7/7	0.97	0.33	143,144,144,144	0
84	OHX	6	1943	7/7	0.97	0.09	124,124,125,125	0
84	OHX	1	3633	7/7	0.97	0.30	134,134,135,135	0
84	OHX	1	3504	7/7	0.97	0.19	127,127,127,128	0
84	OHX	1	3635	7/7	0.97	0.28	122,122,123,123	0
88	ZN	d9	102	1/1	0.97	0.13	83,83,83,83	0
84	OHX	A	1965	7/7	0.97	0.16	134,135,135,136	0
84	OHX	1	3496	7/7	0.98	0.16	115,115,115,115	0
84	OHX	1	3454	7/7	0.98	0.18	111,111,111,111	0
84	OHX	AR	3481	7/7	0.98	0.20	106,106,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3482	7/7	0.98	0.19	111,112,112,112	0
84	OHX	1	3404	7/7	0.98	0.35	120,120,121,121	0
84	OHX	1	3555	7/7	0.98	0.17	111,111,112,112	0
84	OHX	AR	3485	7/7	0.98	0.15	114,114,115,115	0
84	OHX	AR	3486	7/7	0.98	0.19	111,111,111,111	0
84	OHX	A	1938	7/7	0.98	0.15	126,127,127,127	0
85	MG	1	3798	1/1	0.98	0.23	32,32,32,32	0
84	OHX	AR	3487	7/7	0.98	0.13	107,107,107,107	0
84	OHX	AR	3488	7/7	0.98	0.09	118,118,119,119	0
84	OHX	AR	3489	7/7	0.98	0.15	114,114,114,114	0
84	OHX	A	1942	7/7	0.98	0.19	133,133,134,134	0
84	OHX	AR	3490	7/7	0.98	0.12	112,112,112,113	0
85	MG	AR	3763	1/1	0.98	0.59	17,17,17,17	0
85	MG	AR	4260	1/1	0.98	0.52	6,6,6,6	0
84	OHX	6	1991	7/7	0.98	0.29	133,134,134,135	0
84	OHX	AR	3645	7/7	0.98	0.35	118,118,118,118	0
84	OHX	1	3499	7/7	0.98	0.23	111,111,111,111	0
84	OHX	1	3557	7/7	0.98	0.16	117,118,118,118	0
84	OHX	1	3456	7/7	0.98	0.16	111,111,111,111	0
84	OHX	A	1949	7/7	0.98	0.08	148,149,149,149	0
85	MG	1	3810	1/1	0.98	0.12	32,32,32,32	0
84	OHX	A	1950	7/7	0.98	0.13	127,128,128,128	0
84	OHX	1	3457	7/7	0.98	0.18	126,127,127,128	0
84	OHX	A	1952	7/7	0.98	0.20	128,129,129,129	0
85	MG	AS	222	1/1	0.98	0.21	44,44,44,44	0
85	MG	AR	3774	1/1	0.98	0.15	30,30,30,30	0
84	OHX	1	3560	7/7	0.98	0.12	111,112,112,112	0
84	OHX	AR	3497	7/7	0.98	0.09	124,125,125,126	0
84	OHX	AR	3498	7/7	0.98	0.15	123,123,123,124	0
85	MG	1	3817	1/1	0.98	0.26	23,23,23,23	0
84	OHX	1	3432	7/7	0.98	0.27	117,117,117,117	0
84	OHX	A	1957	7/7	0.98	0.23	133,134,134,134	0
85	MG	AR	3781	1/1	0.98	0.25	23,23,23,23	0
84	OHX	AR	3500	7/7	0.98	0.12	115,115,115,115	0
84	OHX	1	3459	7/7	0.98	0.19	108,108,108,108	0
85	MG	AT	219	1/1	0.98	0.35	36,36,36,36	0
85	MG	1	4034	1/1	0.98	0.25	42,42,42,42	0
84	OHX	AR	3502	7/7	0.98	0.17	113,114,114,114	0
84	OHX	A	1961	7/7	0.98	0.11	149,150,151,151	0
84	OHX	A	1962	7/7	0.98	0.21	132,133,133,134	0
84	OHX	1	3460	7/7	0.98	0.16	118,118,118,119	0
85	MG	1	3827	1/1	0.98	0.73	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	1	3505	7/7	0.98	0.18	116,116,117,117	0
84	OHX	AR	3505	7/7	0.98	0.20	114,114,115,115	0
84	OHX	1	3461	7/7	0.98	0.18	110,110,111,111	0
84	OHX	A	1967	7/7	0.98	0.12	119,119,120,120	0
85	MG	AT	230	1/1	0.98	0.42	39,39,39,39	0
84	OHX	AR	3507	7/7	0.98	0.08	123,123,123,123	0
84	OHX	AR	3508	7/7	0.98	0.21	109,109,109,109	0
84	OHX	AR	3510	7/7	0.98	0.13	117,118,118,118	0
85	MG	1	4047	1/1	0.98	0.12	57,57,57,57	0
84	OHX	1	3434	7/7	0.98	0.25	126,127,127,127	0
84	OHX	A	1972	7/7	0.98	0.22	148,148,148,148	0
84	OHX	1	3508	7/7	0.98	0.10	113,114,114,114	0
84	OHX	6	1910	7/7	0.98	0.26	119,120,120,120	0
84	OHX	1	3630	7/7	0.98	0.33	113,113,114,114	0
84	OHX	AR	3515	7/7	0.98	0.22	113,113,114,114	0
84	OHX	6	1913	7/7	0.98	0.26	133,134,135,135	0
84	OHX	6	1916	7/7	0.98	0.21	119,120,120,120	0
84	OHX	AR	3518	7/7	0.98	0.10	118,119,119,119	0
85	MG	AR	4054	1/1	0.98	0.14	55,55,55,55	0
85	MG	1	3844	1/1	0.98	0.41	28,28,28,28	0
84	OHX	AR	3672	7/7	0.98	0.29	109,110,110,110	0
84	OHX	6	1918	7/7	0.98	0.17	116,117,117,117	0
84	OHX	1	3407	7/7	0.98	0.31	106,106,107,107	0
84	OHX	6	1920	7/7	0.98	0.14	133,133,134,134	0
84	OHX	A	1984	7/7	0.98	0.10	130,130,131,131	0
85	MG	1	4063	1/1	0.98	0.09	38,38,38,38	0
84	OHX	1	3465	7/7	0.98	0.18	117,117,117,117	0
84	OHX	AR	3523	7/7	0.98	0.15	107,108,108,108	0
85	MG	z	202	1/1	0.98	0.28	59,59,59,59	0
85	MG	AR	3818	1/1	0.98	0.78	37,37,37,37	0
85	MG	AR	3819	1/1	0.98	0.36	37,37,37,37	0
84	OHX	6	1922	7/7	0.98	0.18	121,122,122,122	0
85	MG	1	4067	1/1	0.98	0.09	40,40,40,40	0
84	OHX	AR	3525	7/7	0.98	0.06	119,119,120,120	0
84	OHX	6	1923	7/7	0.98	0.17	121,121,122,122	0
84	OHX	6	1924	7/7	0.98	0.15	134,135,135,135	0
84	OHX	1	3570	7/7	0.98	0.09	144,144,145,145	0
84	OHX	AR	3529	7/7	0.98	0.12	108,109,109,109	0
84	OHX	6	1926	7/7	0.98	0.12	120,121,121,121	0
84	OHX	1	3697	7/7	0.98	0.25	119,119,120,120	0
84	OHX	6	1928	7/7	0.98	0.08	126,126,127,127	0
85	MG	AR	3830	1/1	0.98	0.46	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	1	3511	7/7	0.98	0.14	109,109,109,109	0
85	MG	1	4078	1/1	0.98	0.29	24,24,24,24	0
84	OHX	6	1930	7/7	0.98	0.21	121,121,122,122	0
85	MG	AR	4081	1/1	0.98	0.24	55,55,55,55	0
84	OHX	6	1931	7/7	0.98	0.10	115,116,116,116	0
84	OHX	1	3512	7/7	0.98	0.17	110,110,110,110	0
84	OHX	1	3513	7/7	0.98	0.11	113,113,114,114	0
84	OHX	1	3410	7/7	0.98	0.32	112,112,112,112	0
84	OHX	1	3515	7/7	0.98	0.10	110,110,110,110	0
84	OHX	1	3516	7/7	0.98	0.12	116,117,117,117	0
84	OHX	6	1937	7/7	0.98	0.11	119,120,120,120	0
84	OHX	1	3467	7/7	0.98	0.17	123,123,124,124	0
84	OHX	1	3468	7/7	0.98	0.20	116,117,117,117	0
84	OHX	1	3439	7/7	0.98	0.19	109,109,109,109	0
84	OHX	1	3470	7/7	0.98	0.18	115,115,115,115	0
85	MG	1	3875	1/1	0.98	0.46	23,23,23,23	0
84	OHX	6	1942	7/7	0.98	0.16	135,135,136,136	0
84	OHX	A	2010	7/7	0.98	0.14	157,158,158,159	0
84	OHX	1	3521	7/7	0.98	0.14	116,117,117,117	0
84	OHX	6	1944	7/7	0.98	0.10	143,143,144,144	0
84	OHX	6	1945	7/7	0.98	0.17	126,127,127,128	0
84	OHX	AR	3550	7/7	0.98	0.14	107,107,107,107	0
84	OHX	1	3522	7/7	0.98	0.13	120,121,121,121	0
84	OHX	1	3523	7/7	0.98	0.19	119,119,120,120	0
85	MG	1	3885	1/1	0.98	0.49	20,20,20,20	0
84	OHX	6	1948	7/7	0.98	0.13	127,128,128,128	0
84	OHX	1	3524	7/7	0.98	0.21	116,117,117,117	0
85	MG	1	3888	1/1	0.98	0.40	29,29,29,29	0
85	MG	AR	4106	1/1	0.98	0.07	46,46,46,46	0
85	MG	AR	3858	1/1	0.98	0.32	36,36,36,36	0
85	MG	1	3889	1/1	0.98	0.54	23,23,23,23	0
85	MG	AR	3860	1/1	0.98	0.51	23,23,23,23	0
84	OHX	1	3440	7/7	0.98	0.22	110,110,111,111	0
85	MG	1	3891	1/1	0.98	0.60	17,17,17,17	0
85	MG	AR	3863	1/1	0.98	0.57	21,21,21,21	0
84	OHX	6	1951	7/7	0.98	0.14	134,134,135,135	0
85	MG	1	3893	1/1	0.98	0.26	26,26,26,26	0
84	OHX	1	3472	7/7	0.98	0.17	110,111,111,111	0
84	OHX	1	3587	7/7	0.98	0.23	133,133,133,134	0
84	OHX	1	3441	7/7	0.98	0.20	116,116,116,117	0
85	MG	AR	3870	1/1	0.98	0.70	33,33,33,33	0
84	OHX	1	3474	7/7	0.98	0.16	122,122,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	6	2098	1/1	0.98	0.52	68,68,68,68	0
84	OHX	1	3590	7/7	0.98	0.12	137,138,138,138	0
84	OHX	1	3475	7/7	0.98	0.14	117,117,118,118	0
84	OHX	6	1958	7/7	0.98	0.15	126,127,127,127	0
85	MG	AR	3876	1/1	0.98	0.55	27,27,27,27	0
84	OHX	1	3530	7/7	0.98	0.13	138,138,139,139	0
84	OHX	1	3415	7/7	0.98	0.32	123,124,124,124	0
85	MG	1	3904	1/1	0.98	0.53	25,25,25,25	0
84	OHX	1	3532	7/7	0.98	0.07	159,159,159,159	0
85	MG	1	4121	1/1	0.98	0.10	64,64,64,64	0
84	OHX	1	3533	7/7	0.98	0.13	149,149,150,150	0
85	MG	AR	4131	1/1	0.98	0.09	39,39,39,39	0
85	MG	AR	3884	1/1	0.98	0.45	22,22,22,22	0
84	OHX	AC	101	7/7	0.98	0.30	114,115,115,115	0
84	OHX	6	1963	7/7	0.98	0.16	125,125,126,126	0
84	OHX	1	3477	7/7	0.98	0.12	109,109,109,109	0
85	MG	1	3910	1/1	0.98	0.58	19,19,19,19	0
84	OHX	1	3535	7/7	0.98	0.17	111,111,111,112	0
84	OHX	AR	3572	7/7	0.98	0.28	118,119,119,119	0
84	OHX	AR	3573	7/7	0.98	0.21	123,123,123,123	0
84	OHX	3	201	7/7	0.98	0.19	121,121,121,122	0
84	OHX	1	3479	7/7	0.98	0.17	108,109,109,109	0
85	MG	1	4132	1/1	0.98	0.13	86,86,86,86	0
85	MG	1	4133	1/1	0.98	0.09	51,51,51,51	0
85	MG	6	2119	1/1	0.98	0.47	74,74,74,74	0
84	OHX	AR	3401	7/7	0.98	0.39	121,121,121,122	0
84	OHX	AR	3406	7/7	0.98	0.34	112,112,113,113	0
84	OHX	AR	3407	7/7	0.98	0.34	113,113,113,113	0
84	OHX	AR	3411	7/7	0.98	0.30	106,106,106,106	0
84	OHX	AR	3412	7/7	0.98	0.28	109,109,109,109	0
84	OHX	AR	3582	7/7	0.98	0.27	114,114,114,114	0
84	OHX	AR	3414	7/7	0.98	0.30	113,113,114,114	0
85	MG	1	4142	1/1	0.98	0.26	38,38,38,38	0
84	OHX	AR	3415	7/7	0.98	0.35	109,109,110,110	0
84	OHX	AR	3417	7/7	0.98	0.26	111,112,112,112	0
84	OHX	AR	3425	7/7	0.98	0.23	105,106,106,106	0
85	MG	6	2131	1/1	0.98	0.24	44,44,44,44	0
84	OHX	1	3443	7/7	0.98	0.19	119,120,120,120	0
84	OHX	AR	3430	7/7	0.98	0.14	107,107,107,107	0
84	OHX	AR	3589	7/7	0.98	0.13	109,110,110,110	0
85	MG	1	4149	1/1	0.98	0.18	54,54,54,54	0
84	OHX	1	3444	7/7	0.98	0.23	116,116,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3744	7/7	0.98	0.17	109,110,110,110	0
84	OHX	AR	3433	7/7	0.98	0.21	110,110,110,111	0
84	OHX	AS	201	7/7	0.98	0.24	119,119,119,120	0
84	OHX	AS	202	7/7	0.98	0.22	124,124,125,125	0
85	MG	1	3935	1/1	0.98	0.23	47,47,47,47	0
84	OHX	AS	203	7/7	0.98	0.16	116,116,116,116	0
84	OHX	sR	401	7/7	0.98	0.22	161,161,162,162	0
84	OHX	AS	204	7/7	0.98	0.15	113,113,113,113	0
84	OHX	AS	205	7/7	0.98	0.12	113,113,114,114	0
84	OHX	AR	3435	7/7	0.98	0.22	112,113,113,113	0
84	OHX	AS	207	7/7	0.98	0.16	122,122,122,123	0
84	OHX	AR	3436	7/7	0.98	0.24	109,109,109,109	0
84	OHX	AR	3437	7/7	0.98	0.23	108,108,108,108	0
84	OHX	AR	3439	7/7	0.98	0.25	119,120,120,120	0
84	OHX	6	1970	7/7	0.98	0.26	126,126,127,127	0
84	OHX	AT	202	7/7	0.98	0.30	106,106,106,106	0
84	OHX	1	3482	7/7	0.98	0.18	117,117,117,117	0
84	OHX	AT	204	7/7	0.98	0.11	105,105,105,106	0
84	OHX	AR	3443	7/7	0.98	0.14	116,116,117,117	0
84	OHX	AR	3444	7/7	0.98	0.15	112,112,112,112	0
84	OHX	1	3417	7/7	0.98	0.31	116,117,117,117	0
84	OHX	1	3484	7/7	0.98	0.10	125,126,126,126	0
84	OHX	AR	3448	7/7	0.98	0.17	115,115,115,115	0
84	OHX	AR	3450	7/7	0.98	0.16	127,127,127,128	0
84	OHX	AR	3451	7/7	0.98	0.20	114,114,114,114	0
84	OHX	AR	3452	7/7	0.98	0.18	121,121,122,122	0
85	MG	AR	4190	1/1	0.98	0.19	30,30,30,30	0
84	OHX	AR	3453	7/7	0.98	0.10	106,106,107,107	0
84	OHX	AR	3454	7/7	0.98	0.17	112,112,113,113	0
85	MG	1	4180	1/1	0.98	0.35	45,45,45,45	0
84	OHX	1	3420	7/7	0.98	0.29	118,118,118,118	0
84	OHX	1	3486	7/7	0.98	0.14	116,117,117,117	0
84	OHX	AR	3457	7/7	0.98	0.18	108,108,108,109	0
84	OHX	CE	401	7/7	0.98	0.17	114,114,115,115	0
85	MG	6	2170	1/1	0.98	0.17	64,64,64,64	0
84	OHX	4	201	7/7	0.98	0.35	108,108,108,108	0
84	OHX	1	3447	7/7	0.98	0.20	113,113,113,113	0
84	OHX	1	3448	7/7	0.98	0.21	117,117,117,117	0
84	OHX	AR	3461	7/7	0.98	0.14	110,111,111,111	0
84	OHX	1	3403	7/7	0.98	0.30	113,113,113,114	0
84	OHX	AR	3464	7/7	0.98	0.17	106,106,106,106	0
84	OHX	AR	3465	7/7	0.98	0.17	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4208	1/1	0.98	0.21	57,57,57,57	0
84	OHX	1	3491	7/7	0.98	0.18	120,120,121,121	0
84	OHX	CP	501	7/7	0.98	0.20	126,126,126,127	0
85	MG	6	2182	1/1	0.98	0.14	83,83,83,83	0
84	OHX	CX	201	7/7	0.98	0.17	116,116,116,116	0
85	MG	6	2184	1/1	0.98	0.22	83,83,83,83	0
84	OHX	6	1981	7/7	0.98	0.29	139,140,140,140	0
85	MG	1	4196	1/1	0.98	0.42	30,30,30,30	0
84	OHX	DD	101	7/7	0.98	0.29	113,114,114,114	0
84	OHX	DH	201	7/7	0.98	0.13	113,113,113,113	0
84	OHX	DQ	201	7/7	0.98	0.15	111,111,111,111	0
84	OHX	A	1901	7/7	0.98	0.29	127,127,127,128	0
84	OHX	A	1903	7/7	0.98	0.35	149,149,150,150	0
84	OHX	A	1908	7/7	0.98	0.24	141,142,143,143	0
84	OHX	AR	3468	7/7	0.98	0.16	124,124,125,125	0
84	OHX	4	207	7/7	0.98	0.12	118,119,119,119	0
84	OHX	AR	3470	7/7	0.98	0.17	115,116,116,116	0
84	OHX	A	1912	7/7	0.98	0.19	137,137,138,138	0
84	OHX	AR	3471	7/7	0.98	0.13	109,109,109,109	0
84	OHX	A	1914	7/7	0.98	0.23	126,127,127,127	0
84	OHX	1	3430	7/7	0.98	0.19	110,110,110,110	0
84	OHX	A	1916	7/7	0.98	0.18	136,137,137,138	0
84	OHX	1	3493	7/7	0.98	0.17	115,116,116,116	0
84	OHX	1	3452	7/7	0.98	0.16	109,109,109,109	0
84	OHX	A	1919	7/7	0.98	0.17	121,122,122,122	0
85	MG	1	3991	1/1	0.98	0.17	66,66,66,66	0
85	MG	1	4215	1/1	0.98	0.62	27,27,27,27	0
84	OHX	AR	3475	7/7	0.98	0.14	116,116,116,116	0
84	OHX	A	1922	7/7	0.98	0.11	123,124,124,124	0
85	MG	1	3783	1/1	0.98	0.46	18,18,18,18	0
84	OHX	A	1923	7/7	0.98	0.13	124,125,125,125	0
84	OHX	AR	3476	7/7	0.98	0.17	109,109,109,109	0
84	OHX	AR	3477	7/7	0.98	0.20	112,112,113,113	0
84	OHX	1	3453	7/7	0.98	0.14	120,120,120,120	0
84	OHX	A	1929	7/7	0.98	0.14	123,123,124,124	0
84	OHX	1	3408	7/7	0.99	0.32	112,112,112,113	0
85	MG	AR	4172	1/1	0.99	0.12	65,65,65,65	0
84	OHX	1	3450	7/7	0.99	0.17	121,122,122,123	0
84	OHX	AR	3402	7/7	0.99	0.39	113,113,113,113	0
85	MG	AR	3866	1/1	0.99	0.23	34,34,34,34	0
84	OHX	AR	3403	7/7	0.99	0.28	110,110,110,110	0
84	OHX	AR	3404	7/7	0.99	0.33	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3405	7/7	0.99	0.34	119,119,120,120	0
84	OHX	2	201	7/7	0.99	0.31	119,119,120,120	0
84	OHX	6	1901	7/7	0.99	0.34	119,120,120,120	0
84	OHX	AR	3609	7/7	0.99	0.16	107,107,107,107	0
84	OHX	AR	3408	7/7	0.99	0.33	107,107,107,107	0
84	OHX	AR	3409	7/7	0.99	0.34	120,120,120,121	0
84	OHX	AR	3410	7/7	0.99	0.31	109,109,109,110	0
84	OHX	6	1902	7/7	0.99	0.34	136,136,137,137	0
84	OHX	6	1903	7/7	0.99	0.29	117,118,118,118	0
85	MG	AR	3878	1/1	0.99	0.36	31,31,31,31	0
84	OHX	AR	3413	7/7	0.99	0.26	107,107,107,107	0
84	OHX	6	1904	7/7	0.99	0.27	124,124,124,125	0
84	OHX	1	3426	7/7	0.99	0.28	120,120,120,120	0
85	MG	AR	4191	1/1	0.99	0.17	58,58,58,58	0
85	MG	AR	3983	1/1	0.99	0.12	33,33,33,33	0
84	OHX	AR	3416	7/7	0.99	0.29	114,114,115,115	0
84	OHX	AT	201	7/7	0.99	0.33	109,109,110,110	0
85	MG	AR	4195	1/1	0.99	0.18	63,63,63,63	0
85	MG	1	4031	1/1	0.99	0.55	21,21,21,21	0
84	OHX	6	1906	7/7	0.99	0.29	122,123,123,124	0
85	MG	1	3858	1/1	0.99	0.37	25,25,25,25	0
85	MG	AR	3887	1/1	0.99	0.46	21,21,21,21	0
84	OHX	AR	3418	7/7	0.99	0.30	116,116,117,117	0
84	OHX	AR	3419	7/7	0.99	0.27	122,122,123,123	0
84	OHX	AR	3420	7/7	0.99	0.29	113,114,114,114	0
84	OHX	AR	3421	7/7	0.99	0.25	113,113,113,113	0
84	OHX	AR	3422	7/7	0.99	0.28	112,112,112,112	0
84	OHX	AR	3423	7/7	0.99	0.28	110,111,111,111	0
84	OHX	AR	3424	7/7	0.99	0.27	112,112,113,113	0
84	OHX	1	3478	7/7	0.99	0.14	125,125,125,126	0
84	OHX	AR	3426	7/7	0.99	0.27	111,112,112,112	0
85	MG	AR	3799	1/1	0.99	0.36	22,22,22,22	0
84	OHX	6	1908	7/7	0.99	0.25	120,120,121,121	0
85	MG	1	4134	1/1	0.99	0.20	63,63,63,63	0
84	OHX	AR	3428	7/7	0.99	0.21	115,115,115,116	0
84	OHX	AR	3429	7/7	0.99	0.19	112,112,112,112	0
85	MG	6	2175	1/1	0.99	0.10	118,118,118,118	0
84	OHX	1	3427	7/7	0.99	0.26	112,113,113,113	0
84	OHX	AR	3431	7/7	0.99	0.24	109,109,110,110	0
84	OHX	1	3428	7/7	0.99	0.28	126,126,127,127	0
84	OHX	1	3429	7/7	0.99	0.22	110,110,110,110	0
84	OHX	AR	3434	7/7	0.99	0.22	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	6	2181	1/1	0.99	0.11	95,95,95,95	0
85	MG	AR	3909	1/1	0.99	0.57	25,25,25,25	0
85	MG	AR	3910	1/1	0.99	0.32	23,23,23,23	0
84	OHX	6	1912	7/7	0.99	0.18	122,122,123,123	0
84	OHX	1	3409	7/7	0.99	0.30	116,116,117,117	0
84	OHX	6	1914	7/7	0.99	0.20	133,133,134,134	0
84	OHX	AR	3438	7/7	0.99	0.22	108,108,108,108	0
84	OHX	6	1915	7/7	0.99	0.17	119,119,120,120	0
85	MG	A	2141	1/1	0.99	0.31	101,101,101,101	0
84	OHX	AR	3440	7/7	0.99	0.18	125,125,125,126	0
85	MG	1	3882	1/1	0.99	0.45	32,32,32,32	0
84	OHX	4	202	7/7	0.99	0.33	112,112,112,113	0
85	MG	A	2145	1/1	0.99	0.21	92,92,92,92	0
84	OHX	6	1917	7/7	0.99	0.16	131,131,132,132	0
84	OHX	CV	201	7/7	0.99	0.31	117,117,117,117	0
84	OHX	AR	3509	7/7	0.99	0.10	106,106,106,106	0
84	OHX	1	3402	7/7	0.99	0.35	114,115,115,115	0
84	OHX	AR	3578	7/7	0.99	0.14	109,109,110,110	0
84	OHX	1	3411	7/7	0.99	0.29	111,112,112,112	0
84	OHX	1	3433	7/7	0.99	0.26	118,119,119,119	0
84	OHX	AR	3446	7/7	0.99	0.17	112,113,113,113	0
85	MG	1	3725	1/1	0.99	0.38	34,34,34,34	0
84	OHX	A	1902	7/7	0.99	0.26	122,122,123,123	0
85	MG	AR	4241	1/1	0.99	0.39	17,17,17,17	0
84	OHX	1	3412	7/7	0.99	0.30	114,114,115,115	0
84	OHX	A	1904	7/7	0.99	0.23	133,134,134,134	0
84	OHX	A	1905	7/7	0.99	0.29	128,129,129,129	0
84	OHX	A	1906	7/7	0.99	0.23	142,143,143,143	0
85	MG	1	4164	1/1	0.99	0.22	58,58,58,58	0
84	OHX	A	1907	7/7	0.99	0.19	133,134,134,134	0
84	OHX	1	3413	7/7	0.99	0.32	112,113,113,113	0
84	OHX	AR	3449	7/7	0.99	0.14	116,117,117,117	0
85	MG	1	4076	1/1	0.99	0.24	64,64,64,64	0
84	OHX	1	3436	7/7	0.99	0.28	115,115,115,115	0
84	OHX	1	3437	7/7	0.99	0.24	116,117,117,117	0
85	MG	AR	3940	1/1	0.99	0.49	21,21,21,21	0
85	MG	1	3903	1/1	0.99	0.67	21,21,21,21	0
84	OHX	1	3490	7/7	0.99	0.17	113,113,113,113	0
84	OHX	1	3414	7/7	0.99	0.27	109,109,109,109	0
84	OHX	1	3464	7/7	0.99	0.20	109,109,109,109	0
84	OHX	1	3405	7/7	0.99	0.37	124,125,125,125	0
84	OHX	1	3416	7/7	0.99	0.24	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	1	3406	7/7	0.99	0.33	108,108,108,108	0
84	OHX	1	3418	7/7	0.99	0.27	114,115,115,115	0
85	MG	1	3911	1/1	0.99	0.65	21,21,21,21	0
85	MG	AR	4052	1/1	0.99	0.12	86,86,86,86	0
85	MG	1	3825	1/1	0.99	0.41	31,31,31,31	0
84	OHX	1	3419	7/7	0.99	0.26	107,107,107,107	0
84	OHX	A	1920	7/7	0.99	0.14	128,128,129,129	0
85	MG	1	3745	1/1	0.99	0.67	31,31,31,31	0
84	OHX	1	3401	7/7	0.99	0.38	114,114,115,115	0
84	OHX	1	3421	7/7	0.99	0.29	115,115,116,116	0
85	MG	1	3748	1/1	0.99	0.34	44,44,44,44	0
84	OHX	AR	3462	7/7	0.99	0.16	116,116,116,116	0
84	OHX	A	1924	7/7	0.99	0.09	132,132,133,133	0
88	ZN	AP	501	1/1	0.99	0.04	61,61,61,61	0
88	ZN	DL	101	1/1	0.99	0.20	41,41,41,41	0
88	ZN	DO	201	1/1	0.99	0.15	32,32,32,32	0
88	ZN	DQ	202	1/1	0.99	0.03	63,63,63,63	0
88	ZN	DR	501	1/1	0.99	0.15	59,59,59,59	0
88	ZN	b	102	1/1	0.99	0.16	71,71,71,71	0
85	MG	1	4097	1/1	0.99	0.22	70,70,70,70	0
88	ZN	e	102	1/1	0.99	0.08	79,79,79,79	0
84	OHX	A	1925	7/7	0.99	0.12	136,137,137,137	0
84	OHX	1	3422	7/7	0.99	0.26	116,116,117,117	0
84	OHX	1	3423	7/7	0.99	0.26	120,120,121,121	0
84	OHX	1	3424	7/7	0.99	0.23	115,115,115,115	0
88	ZN	AQ	501	1/1	1.00	0.13	56,56,56,56	0
88	ZN	d6	103	1/1	1.00	0.13	53,53,53,53	0
88	ZN	AK	101	1/1	1.00	0.15	34,34,34,34	0
88	ZN	AN	500	1/1	1.00	0.13	38,38,38,38	0
85	MG	AR	4168	1/1	1.00	0.19	65,65,65,65	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.