



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2020 – 03:12 pm BST

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

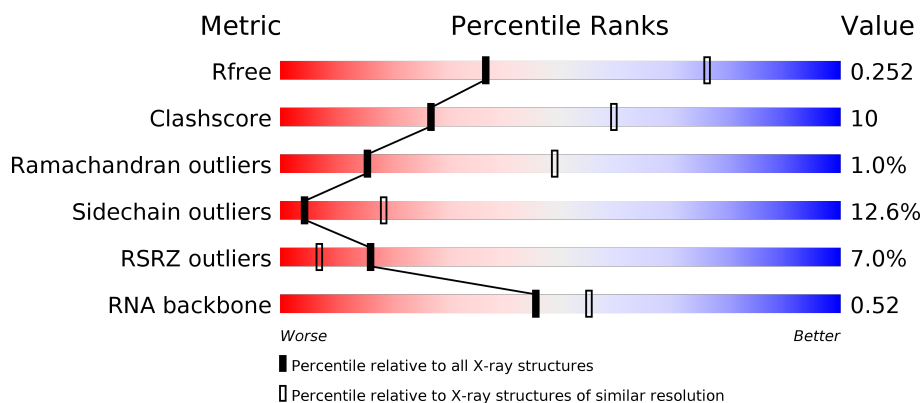
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

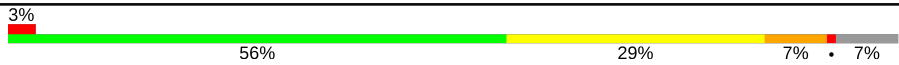



The reported resolution of this entry is 3.10 Å.

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)
Clashscore	141614	1184 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	

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

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

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

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

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

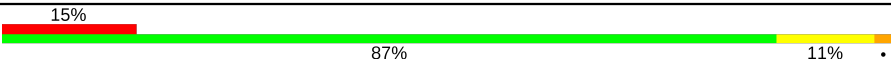


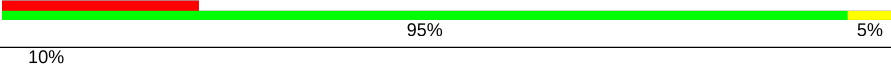
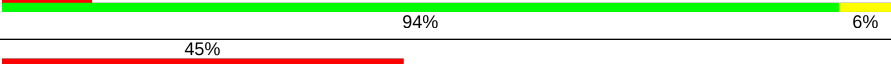
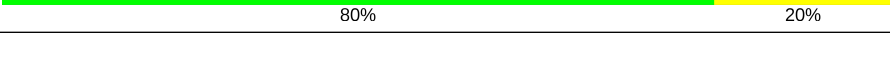
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Mol	Chain	Length	Quality of chain
67	c7	125	
68	T	145	
68	c8	145	
69	U	143	
69	c9	143	
70	V	110	
70	d0	110	
71	W	87	
71	d1	87	
72	X	129	
72	d2	129	
73	Y	144	
73	d3	144	
74	Z	134	
74	d4	134	
75	a	70	
75	d5	70	
76	b	97	
76	d6	97	
77	c	81	
77	d7	81	
78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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	1	3473	-	-	X	-
84	OHX	1	3720	-	-	X	-
84	OHX	6	1975	-	-	X	-
84	OHX	6	2001	-	-	X	-
84	OHX	6	2025	-	-	X	-
84	OHX	A	1909	-	-	X	-
84	OHX	A	2024	-	-	X	-
84	OHX	AR	3443	-	-	X	-
84	OHX	AR	3511	-	-	X	-
84	OHX	AR	3521	-	-	X	-
84	OHX	AR	3696	-	-	X	-
84	OHX	AR	3698	-	-	X	-
84	OHX	AR	3715	-	-	X	-
84	OHX	AR	3731	-	-	X	-
84	OHX	AR	3737	-	-	-	X
84	OHX	AS	203	-	-	X	-
84	OHX	AS	210	-	-	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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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
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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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
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
1	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
1	AR	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	x	183	Total	C	N	O		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
19	y	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
19	CS	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	z	188	Total	C	N	O		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
48	sM	104	Total	C	N	O			
			680	403	140	137	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

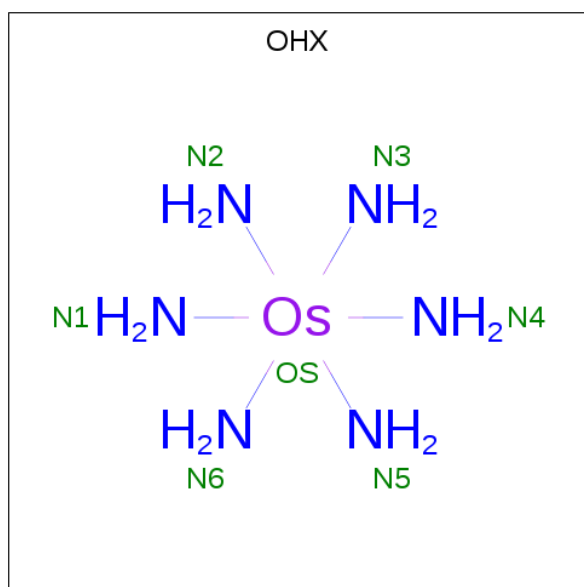
- Molecule 82 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

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

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

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

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



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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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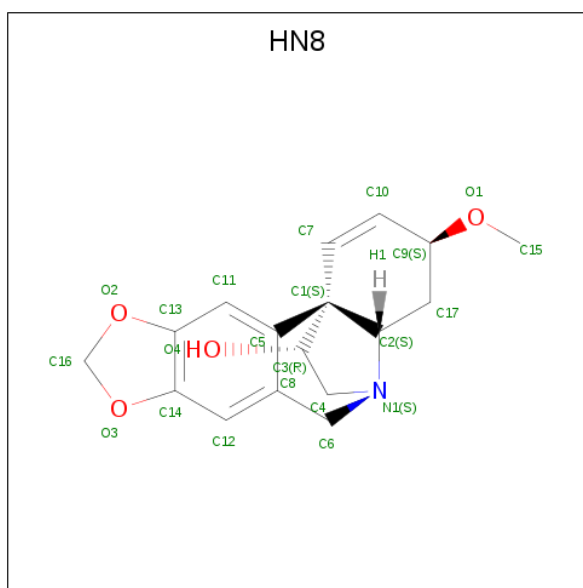
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	n	1	Total 1	Mg 1	0	0
85	x	7	Total 7	Mg 7	0	0
85	T	1	Total 1	Mg 1	0	0
85	AR	515	Total 515	Mg 515	0	0
85	d6	2	Total 2	Mg 2	0	0
85	s6	1	Total 1	Mg 1	0	0
85	s	1	Total 1	Mg 1	0	0
85	DI	2	Total 2	Mg 2	0	0
85	CG	2	Total 2	Mg 2	0	0
85	j	2	Total 2	Mg 2	0	0
85	1	498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

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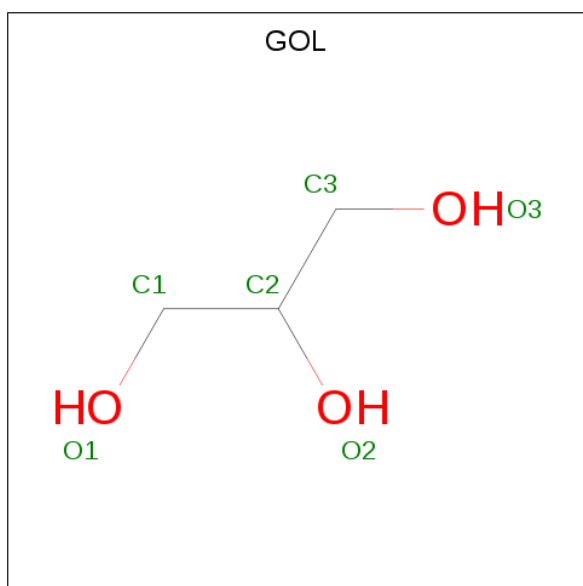
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	U	1	Total 1	Mg 1	0	0
85	r	1	Total 1	Mg 1	0	0
85	CF	1	Total 1	Mg 1	0	0
85	CX	2	Total 2	Mg 2	0	0
85	AG	1	Total 1	Mg 1	0	0
85	DE	1	Total 1	Mg 1	0	0
85	AH	1	Total 1	Mg 1	0	0
85	F	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	CI	1	Total 1	Mg 1	0	0
85	d4	1	Total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

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



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

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



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

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

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

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

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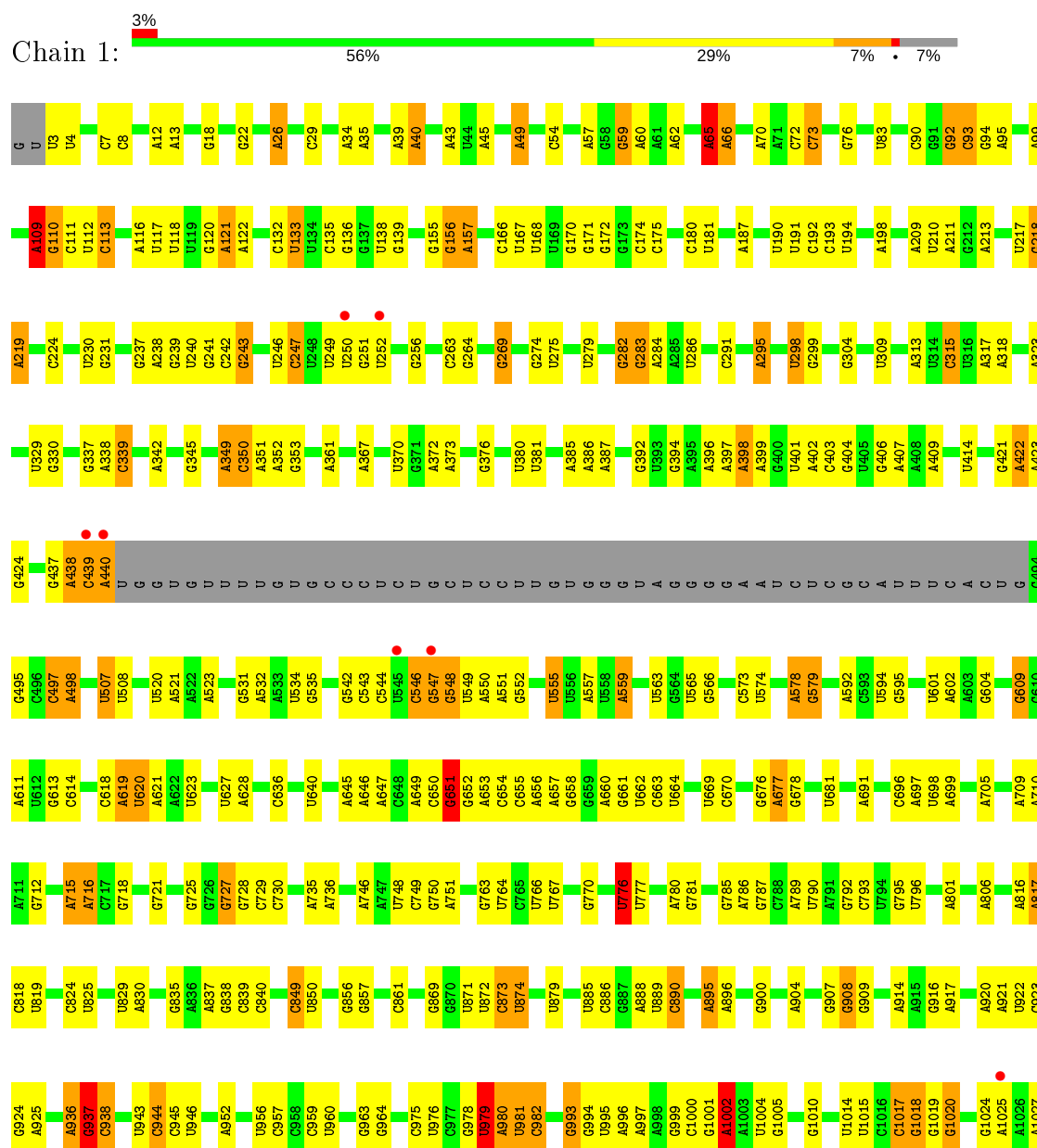
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	d6	1	Total	Zn	0	0
			1	1		

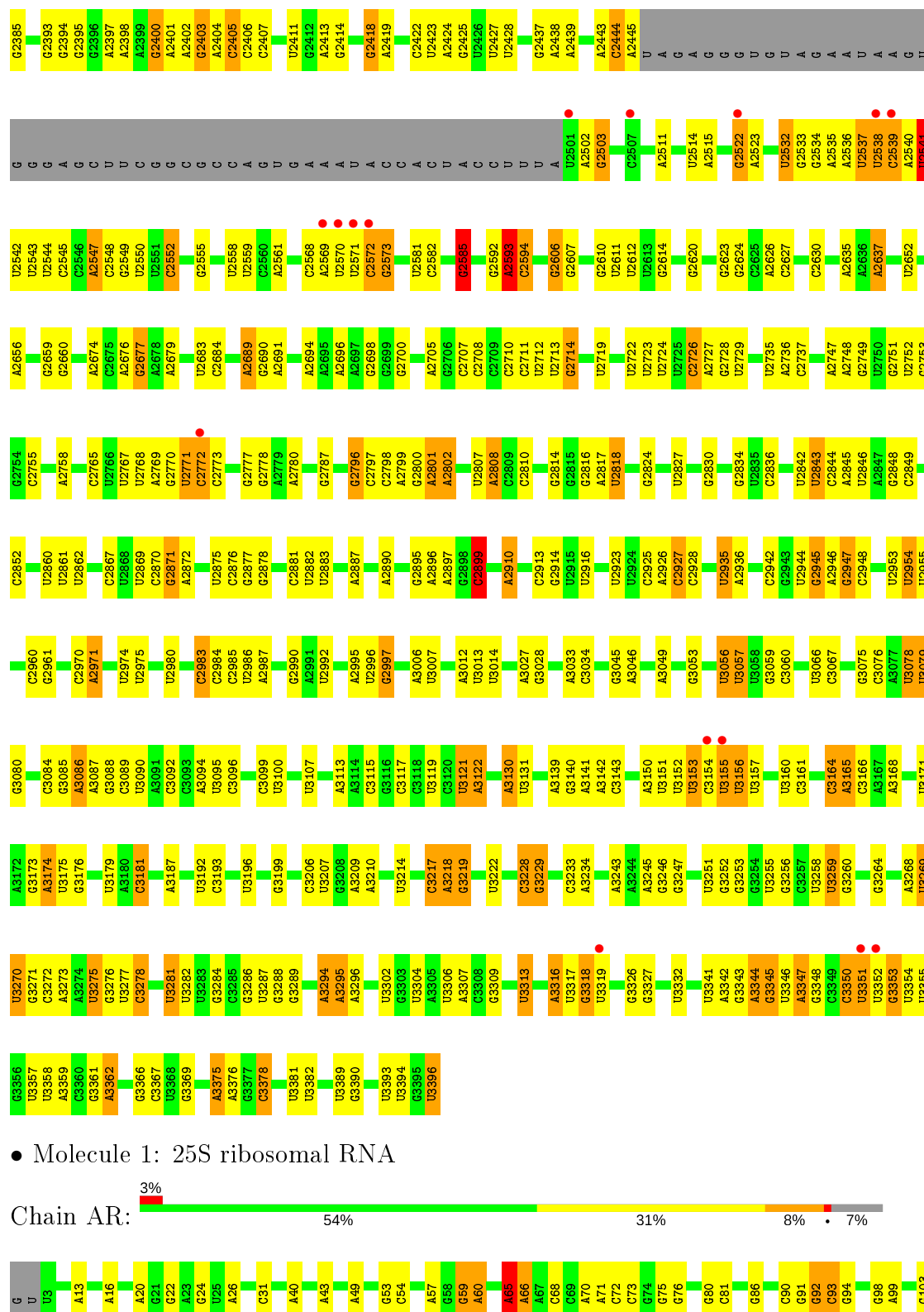
3 Residue-property plots

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

- Molecule 1: 25S ribosomal RNA

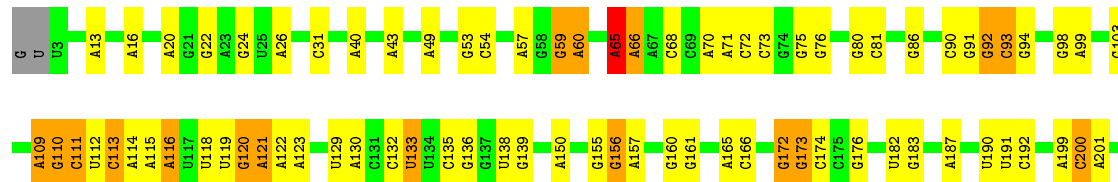


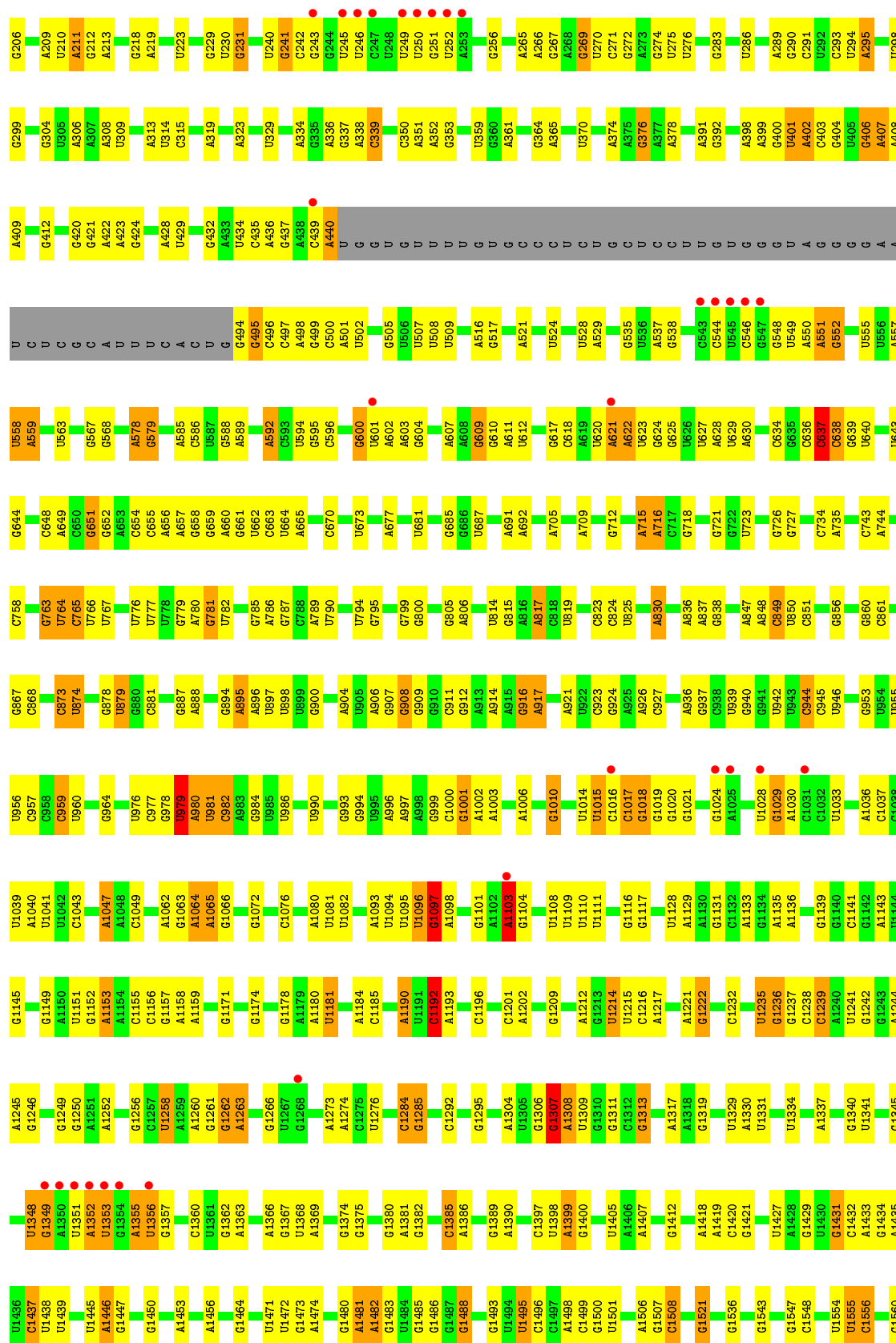
G2273	A2158	G	U1942	U1834	G1748	G1639	U1564	C1437	U1309	A1231	A1120	U1028
A2281	U2159	U	C1951	A1835	A1749	A1643	G1565	G1443	G1313	C1232	U1121	G1029
U2282	G2160	G	G1952	G1838	A1750	A1567	A1566	G1444	G1349	G1233	U1122	A1030
U2286	G2169	A	G1953	A1839	G1751	G1655	U1568	U1445	A1317	U1235	G1127	U1033
C2287	U2170	C	G1954	U1840	C1759	A1656	U1569	U1446	A1318	G1236	U1128	U1034
G2288	U2176	G	U1955	A1841	A1760	G1657	U1570	A1446	G1319	G1237	A1129	G1035
U2298	U2177	U	A	A1842	A1761	G1658	A1571	A1449	C1320	C1238	G1131	A1036
U2301	A2178	C	G	G	A1762	U1659	U1572	G1450	C1327	A1240	A1135	A1047
G2302	G2180	C	U	G	U1763	G1660	C1573	A1460	C1328	G1242	A1048	A1048
A2303	C2181	A	A	A	U1764	G1662	A1575	A1461	U1329	G1243	G1145	C1049
C2304	U2193	C	G	G	G1765	A1667	G1576	A1461	A1330	A1244	G1149	U1052
G2305	G2194	G	G	G	G1766	G1668	A1577	U1472	G1340	G1245	A1153	A1054
C2306	U2199	C	C	C	U1767	G1669	U1580	U1471	U1341	A1246	U1159	A1062
G2307	G2203	U	U	U	U1768	A1676	C1582	A1477	U1348	U1247	G1160	A1064
C2308	U2204	C	C	C	G1770	A1681	A1583	G1478	G1349	G1249	U1168	G1063
A2309	U2205	A	G	G	U1780	U1682	U1584	U1479	A1350	C1255	U1169	A1065
U2310	G2206	U	U	U	U1785	A1683	C1585	U1481	A1352	G1256	U1178	G1066
G2311	A2207	C	C	C	G1786	U1687	A1586	A1482	U1353	C1257	A1179	U1071
A2312	U2208	A	U	U	A1787	U1688	A1587	G1483	G1354	U1258	U1181	U1072
U2313	U2209	G	G	G	C1788	U1689	A1588	U1484	A1355	A1259	G1171	G1067
U2314	G2210	C	A	A	U1792	U1695	A1589	G1485	U1356	A1260	G1178	C1069
G2315	A2213	G	C	C	G1796	U1699	A1593	G1486	G1357	G1261	U1179	U1070
A2324	U2214	U	G	U	U1797	U1699	A1594	G1487	A1362	A1262	A1178	U1071
U2334	G2218	C	C	C	A1798	U1700	U1595	G1488	A1363	G1263	U1180	G1072
G2335	A2219	C	C	C	A1799	C1709	C1596	A1491	C1364	U1265	G1185	U1081
U2336	U2220	U	G	G	U1802	A1803	A1602	G1492	G1367	G1266	U1082	U1082
A2341	G2221	G	G	G	G1803	G1710	A1603	U1494	G1377	U1267	A1190	G1083
U2344	A2222	U	U	U	A1804	G1711	G1604	U1495	G1380	G1268	A1191	A1084
G2345	U2223	C	C	C	C1805	G1712	A1605	C1496	A1386	A1270	G1192	G1087
U2355	U2224	A	U	U	A1806	U1716	C1608	G1497	U1389	A1271	G1193	A1083
A2356	G2225	G	G	G	U1807	U1717	G1609	A1498	G1389	C1272	G1194	U1094
G2357	U2226	C	C	C	G1808	G1718	G1610	C1499	A1390	U1275	A1195	U1095
A2358	C2227	A	U	U	A1809	U1719	A1611	G1507	C1391	C1276	U1201	U1096
C2359	U2228	C	U	U	U1810	U1720	A1612	C1508	G1399	C1277	A1204	A1098
G2360	A2244	G	G	G	G1811	U1724	C1613	G1527	A1399	A1278	U1100	A1099
A2361	G2245	C	G	G	U1812	C1725	C1615	U1533	G1400	C1279	G1209	U1101
C2362	G2246	C	G	G	A1813	G1726	G1618	G1536	A1407	G1285	U1210	A1102
A2368	G2249	U	A	U	A1814	U1727	A1619	G1547	A1418	U1286	U1211	A1103
U2372	G2250	U	C	U	U1815	G1728	A1620	C1548	C1419	A1287	A1212	G1104
A2373	U2255	G	U	U	A1816	A1729	A1621	G1549	A1418	C1292	U1214	U1108
C2374	G2256	A	C	C	U1817	U1923	U1622	C1548	A1419	U1293	U1214	U1109
G2375	U2257	U	U	U	U1818	U1924	U1623	C1548	C1420	U1294	A1217	U1110
U2376	G2261	G	U	U	U1819	G1735	U1629	U1554	G1421	G1295	G1222	U1111
G2377	A2262	C	G	G	U1821	G1736	G1633	U1555	U1427	U1299	G1227	U1114
U2381	U2267	C	U	U	G1825	U1740	C1634	C1556	A1428	G1300	C1227	G1115
G2382	U2268	U	G	G	U1831	A1741	G1635	G1560	G1429	A1433	C1228	G1116
		U	C	C	U1832	G1743	A1636	C1561	A1433	G1307	G1229	G1117
		U	G	G	G1833	G1744	A1638	C1563	A1434	A1308	G1230	



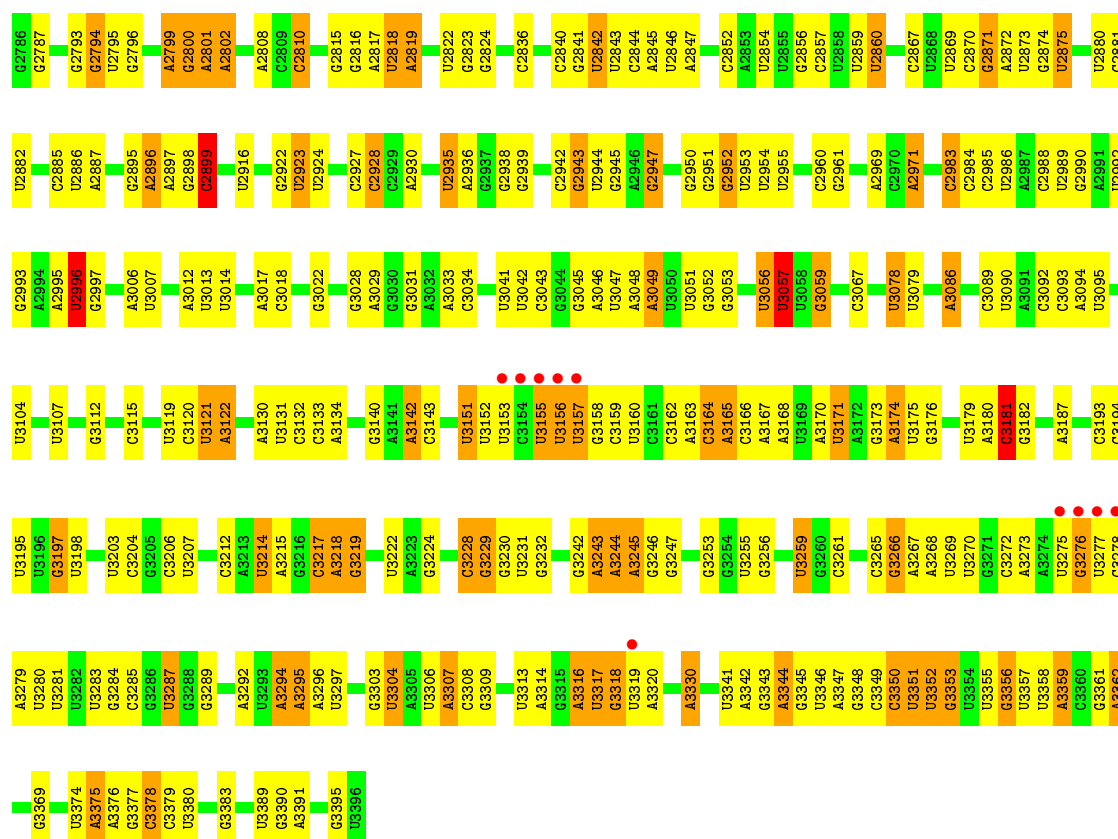
- Molecule 1: 25S ribosomal RNA

Chain AR: 



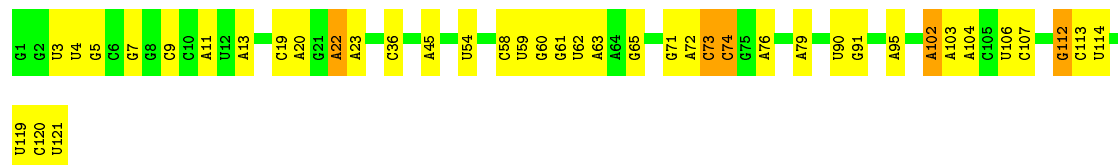






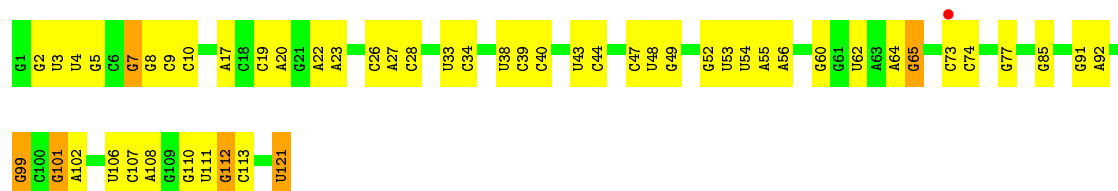
- Molecule 2: 5S ribosomal RNA

Chain 3: 66% 30% .



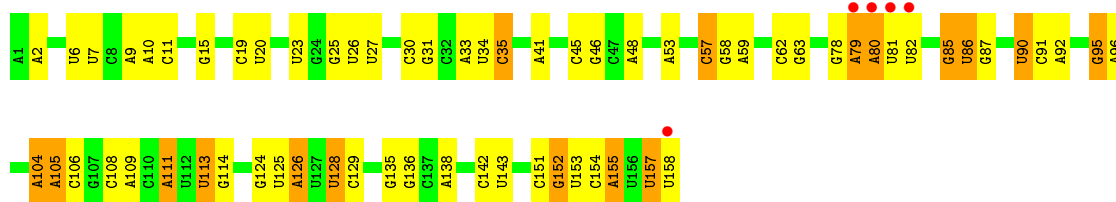
- Molecule 2: 5S ribosomal RNA

Chain AS: 57% 38% 5%

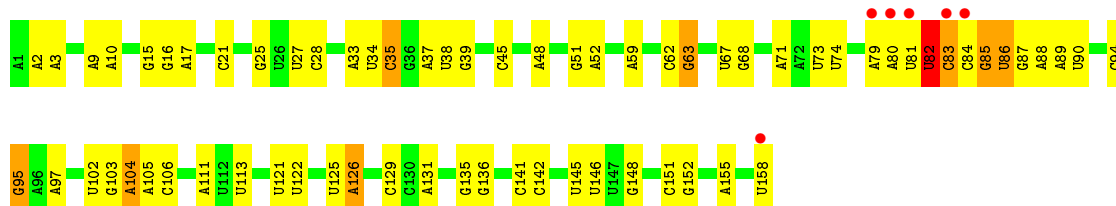


- Molecule 3: 5.8S ribosomal RNA

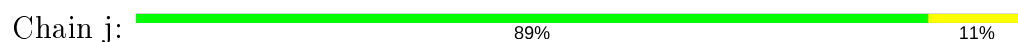
Chain 4: 58% 31% 11%



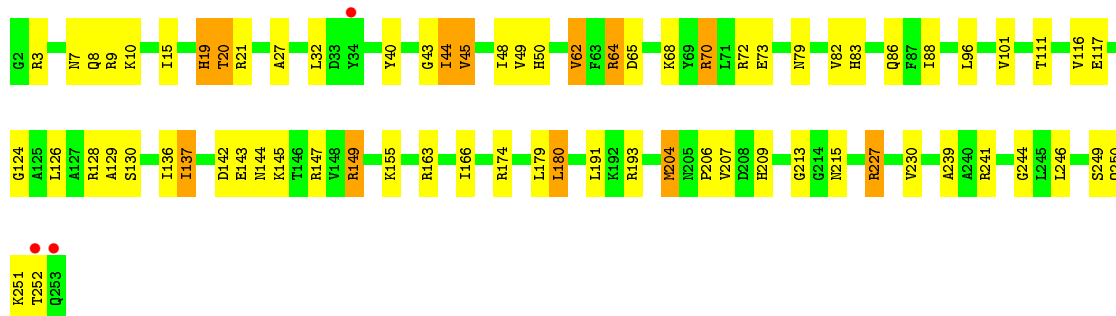
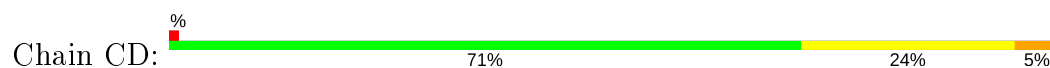
• Molecule 3: 5.8S ribosomal RNA



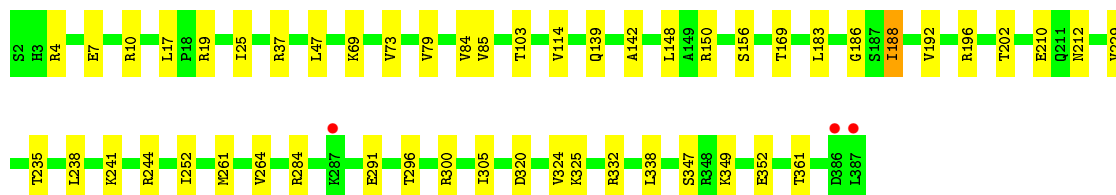
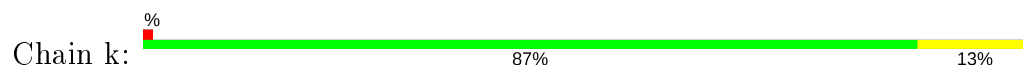
• Molecule 4: 60S ribosomal protein L2-A



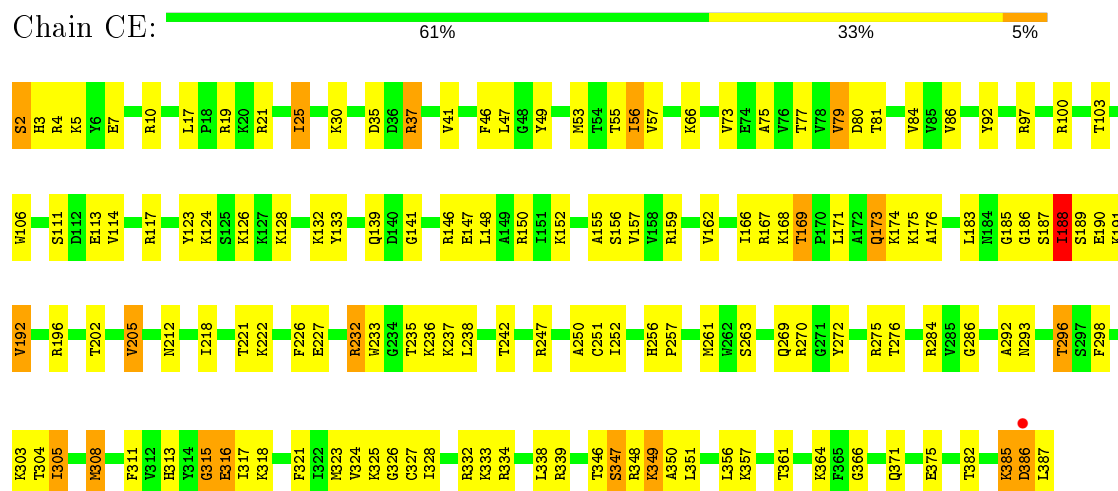
• Molecule 4: 60S ribosomal protein L2-A



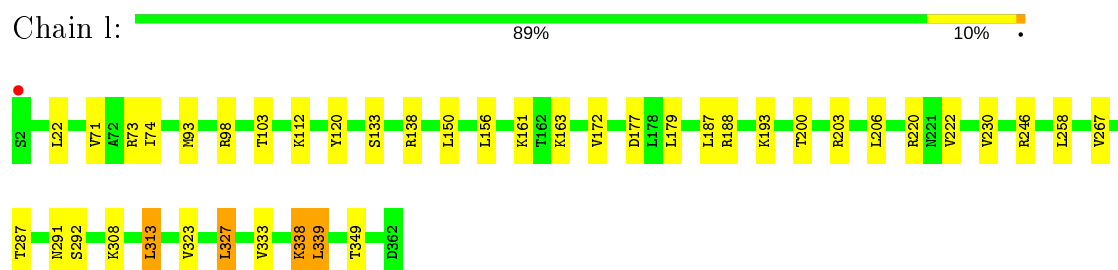
• Molecule 5: 60S ribosomal protein L3



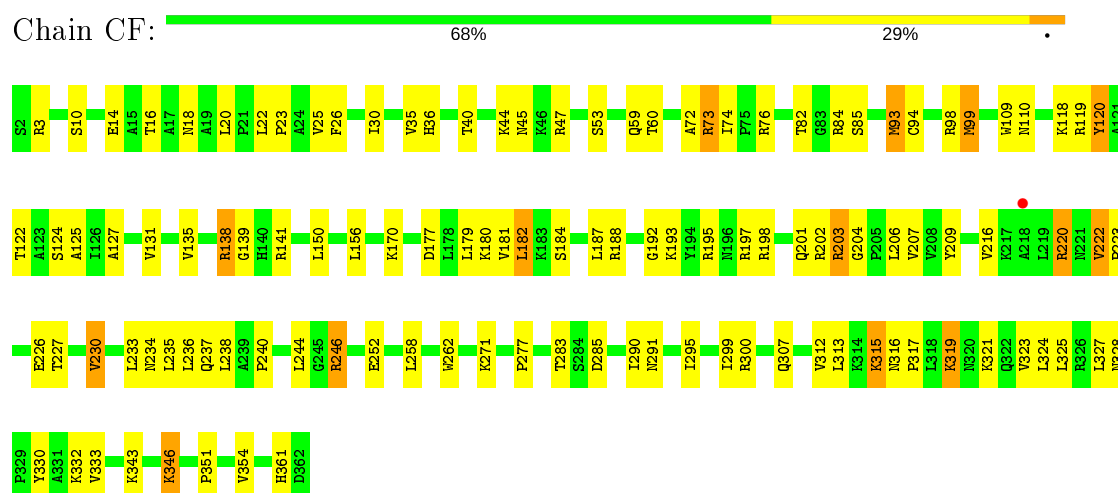
- Molecule 5: 60S ribosomal protein L3



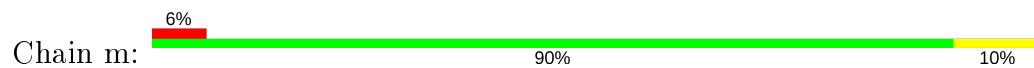
- Molecule 6: 60S ribosomal protein L4-A

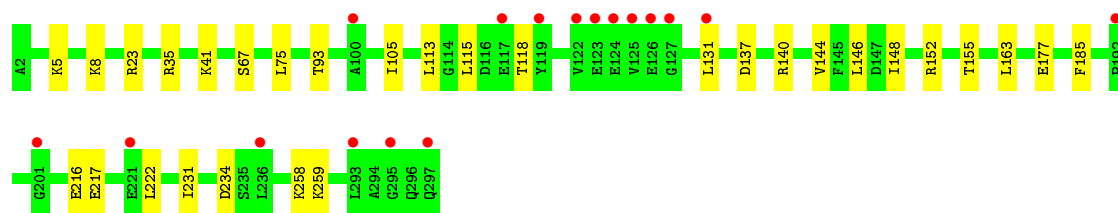


- Molecule 6: 60S ribosomal protein L4-A

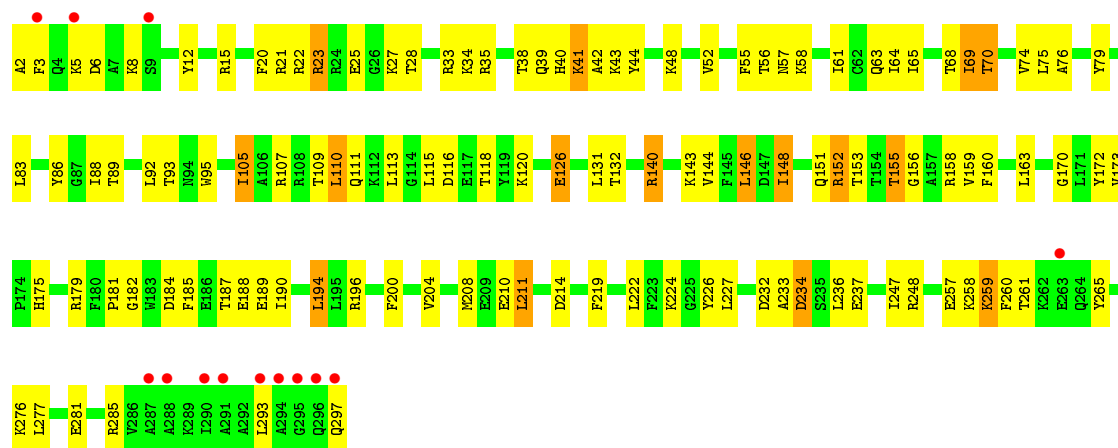


- Molecule 7: 60S ribosomal protein L5

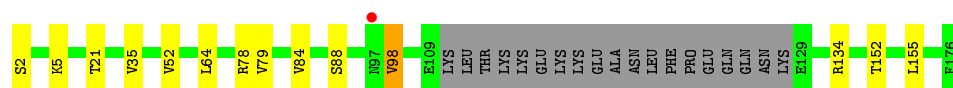
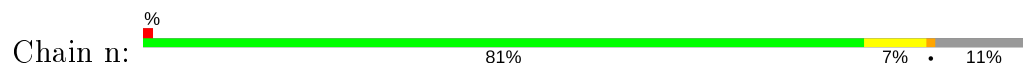




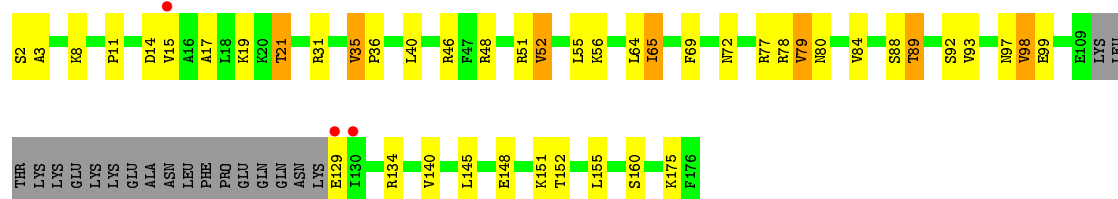
• Molecule 7: 60S ribosomal protein L5



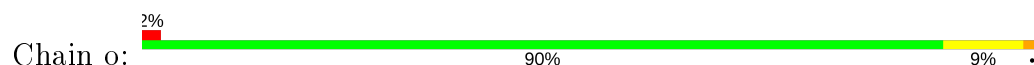
• Molecule 8: 60S ribosomal protein L6-A



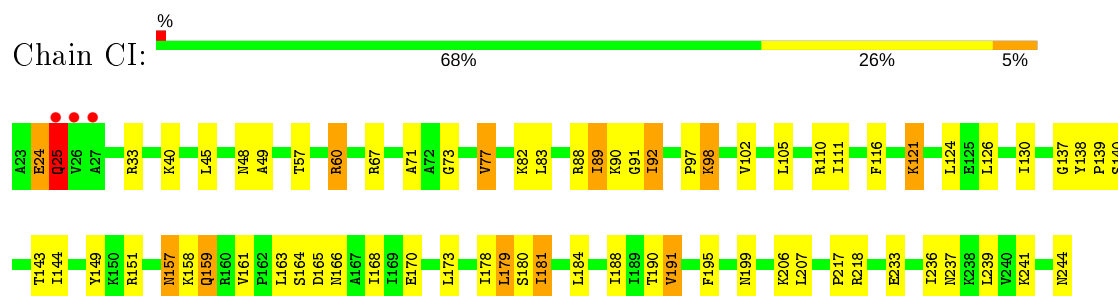
• Molecule 8: 60S ribosomal protein L6-A



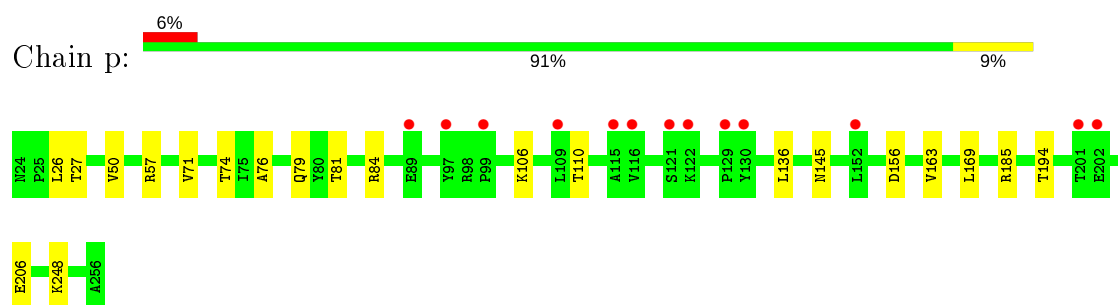
• Molecule 9: 60S ribosomal protein L7-A



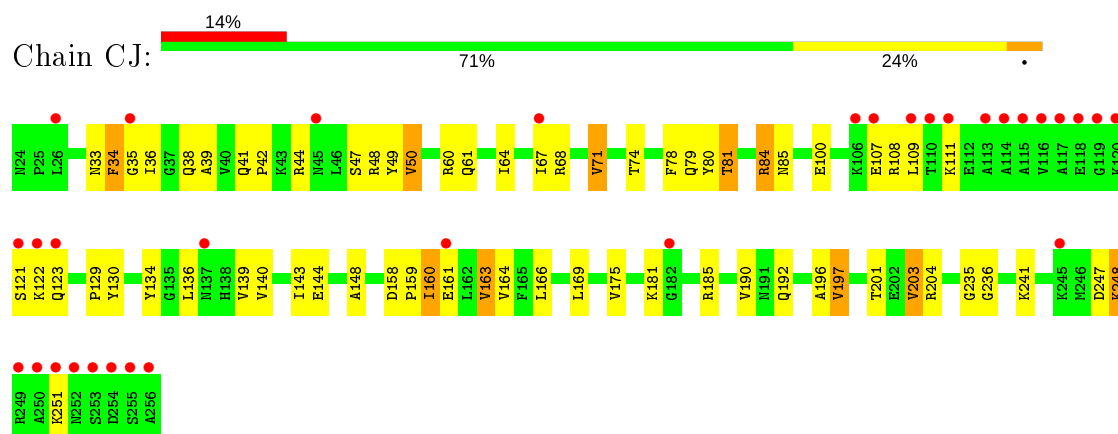
- Molecule 9: 60S ribosomal protein L7-A



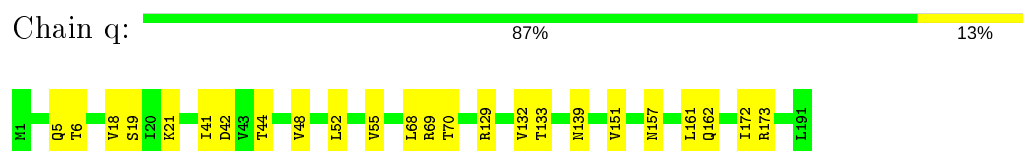
- Molecule 10: 60S ribosomal protein L8-A



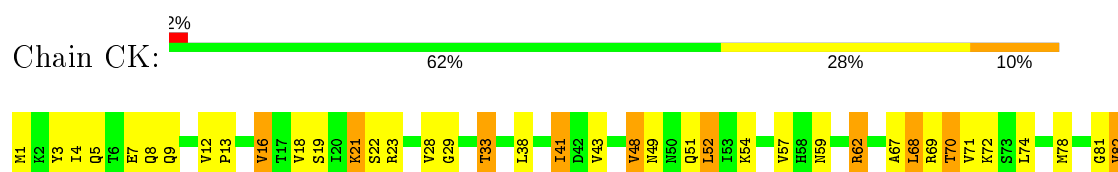
- Molecule 10: 60S ribosomal protein L8-A



- Molecule 11: 60S ribosomal protein L9-A

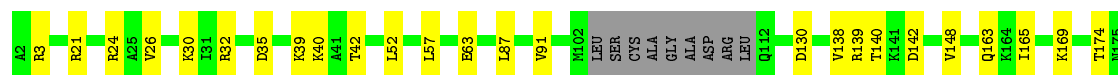
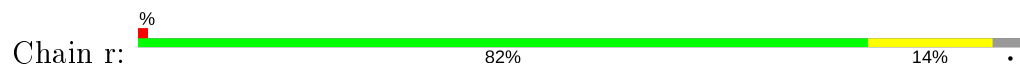


- Molecule 11: 60S ribosomal protein L9-A

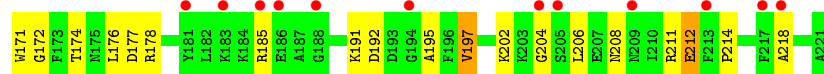
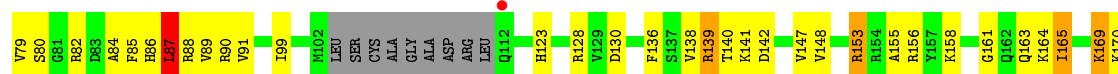




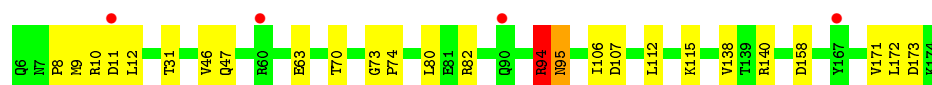
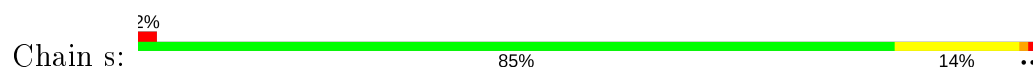
• Molecule 12: 60S ribosomal protein L10



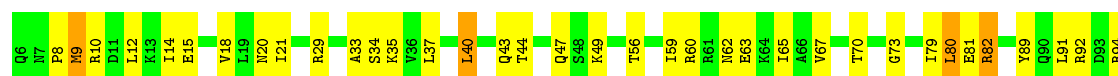
• Molecule 12: 60S ribosomal protein L10



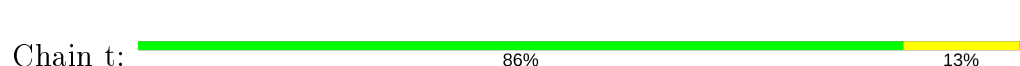
• Molecule 13: 60S ribosomal protein L11-B



• Molecule 13: 60S ribosomal protein L11-B

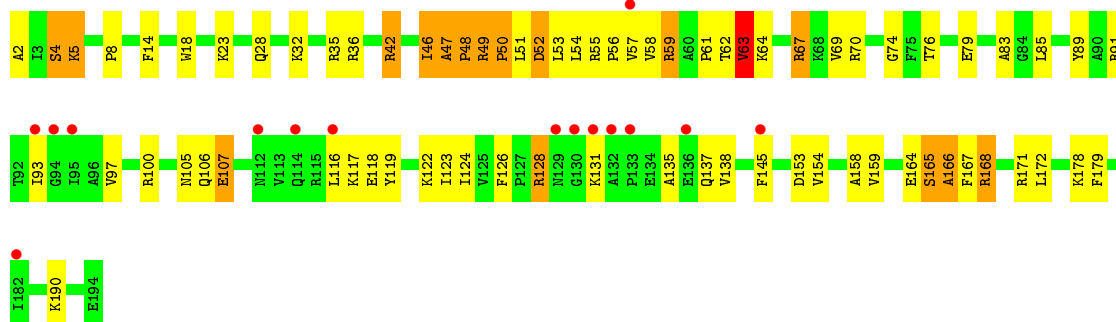


• Molecule 14: 60S ribosomal protein L13-A

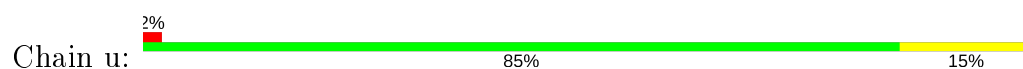




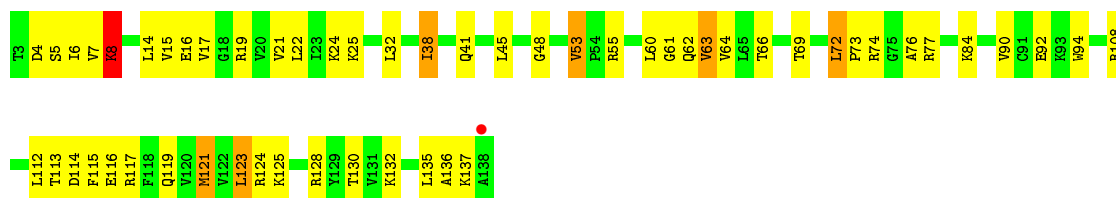
- Molecule 14: 60S ribosomal protein L13-A



- Molecule 15: 60S ribosomal protein L14-A



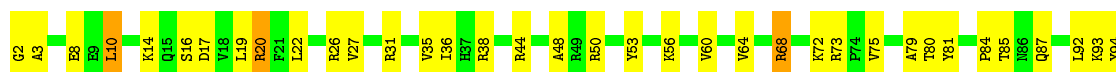
- Molecule 15: 60S ribosomal protein L14-A



- Molecule 16: 60S ribosomal protein L15-A



- Molecule 16: 60S ribosomal protein L15-A





- Molecule 17: 60S ribosomal protein L16-A

Chain w: 88% 11% .



- Molecule 17: 60S ribosomal protein L16-A

Chain CQ: 2% 69% 27% . .



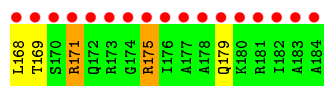
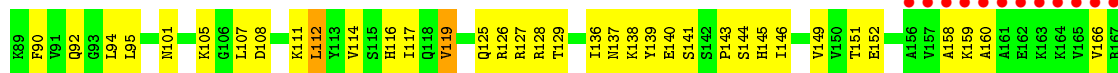
- Molecule 18: 60S ribosomal protein L17-A

Chain x: 11% 87% 12% .



- Molecule 18: 60S ribosomal protein L17-A

Chain CR: 16% 57% 40% .

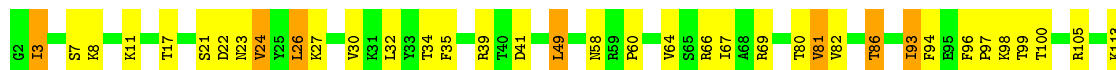


- Molecule 19: 60S ribosomal protein L18-A

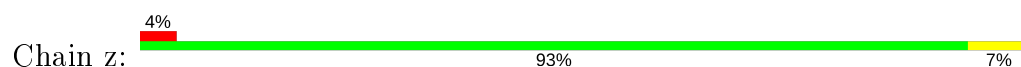
Chain y: 89% 10% .



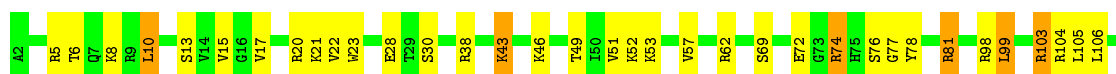
- Molecule 19: 60S ribosomal protein L18-A



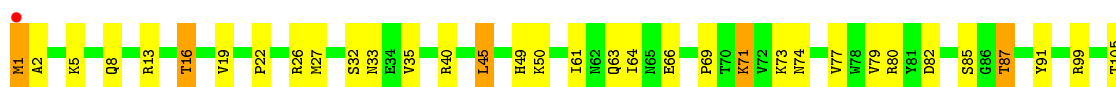
- Molecule 20: 60S ribosomal protein L19-A



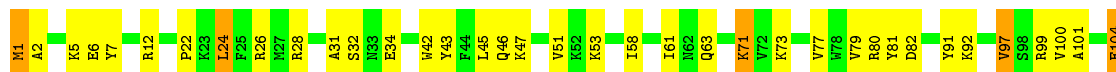
- Molecule 20: 60S ribosomal protein L19-A

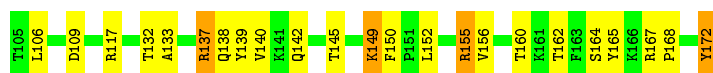


- Molecule 21: 60S ribosomal protein L20-A

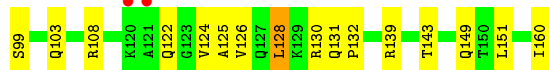


- Molecule 21: 60S ribosomal protein L20-A





- Molecule 22: 60S ribosomal protein L21-A



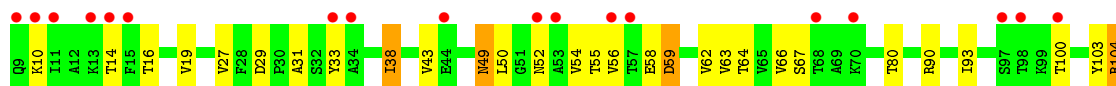
- Molecule 22: 60S ribosomal protein L21-A



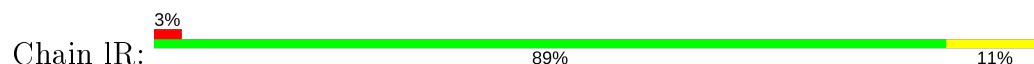
- Molecule 23: 60S ribosomal protein L22-A



- Molecule 23: 60S ribosomal protein L22-A

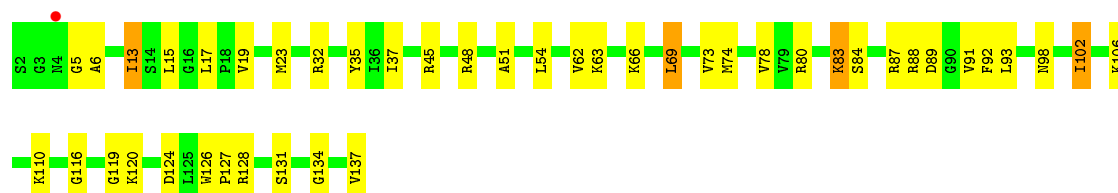


- Molecule 24: 60S ribosomal protein L23-A

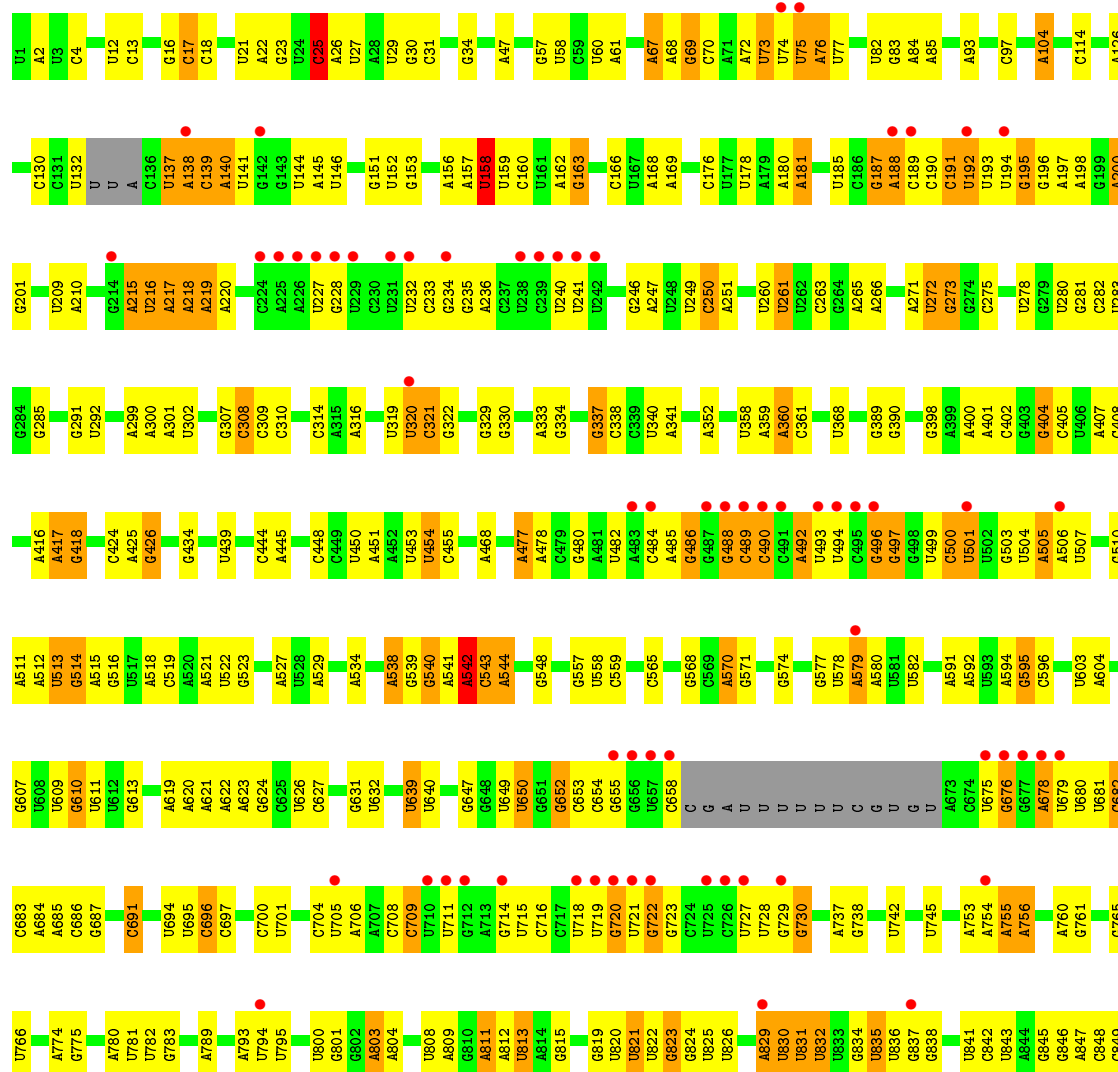


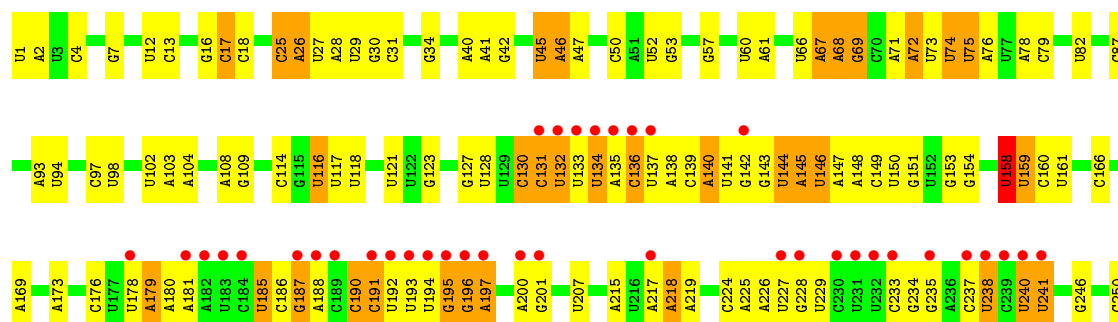
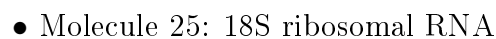


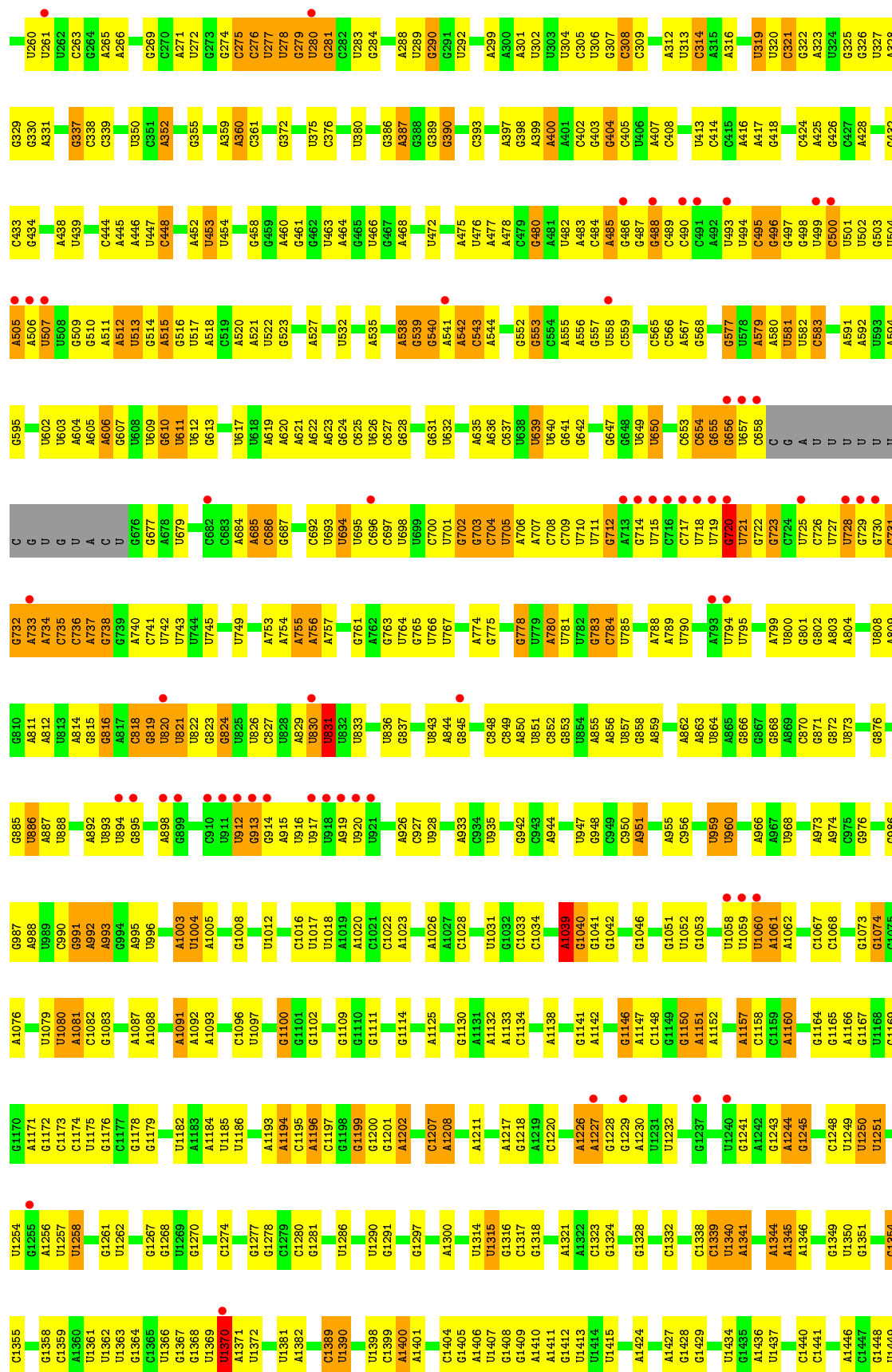
- Molecule 24: 60S ribosomal protein L23-A

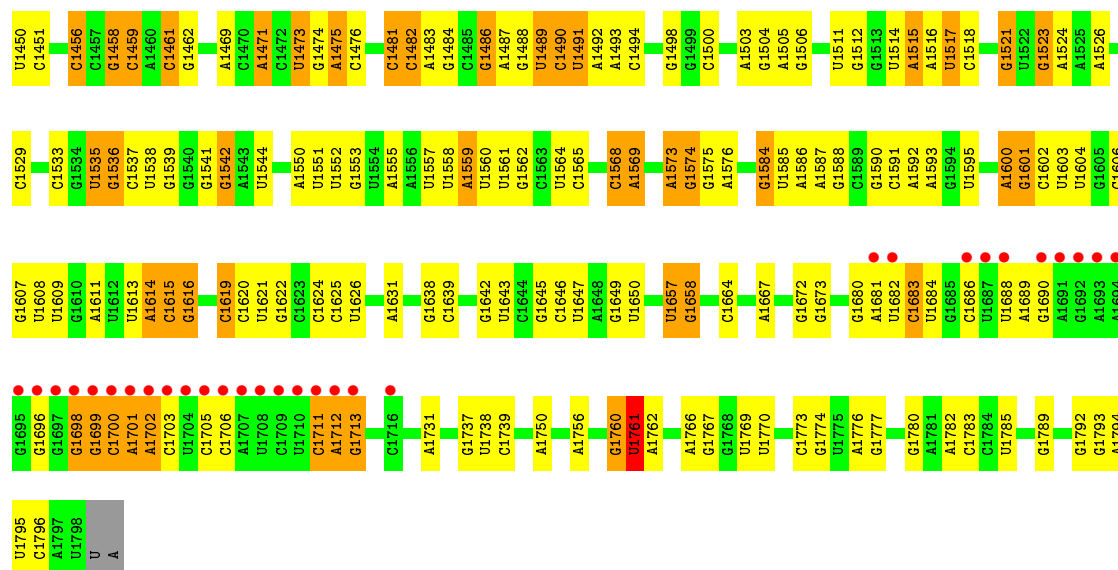


- Molecule 25: 18S ribosomal RNA

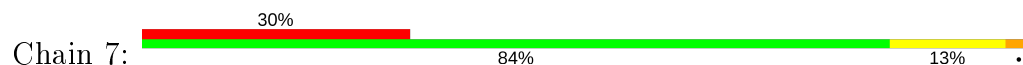




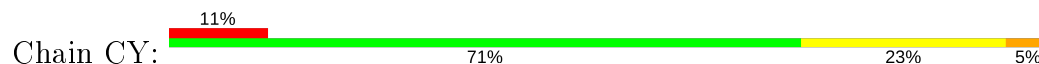




• Molecule 26: 60S ribosomal protein L24-A



• Molecule 26: 60S ribosomal protein L24-A



• Molecule 27: 60S ribosomal protein L25

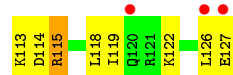
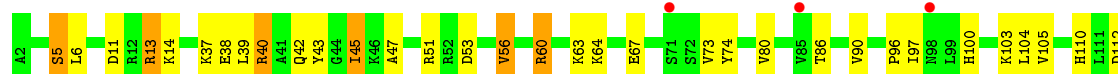


• Molecule 27: 60S ribosomal protein L25

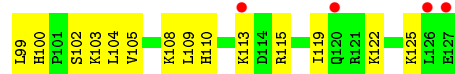
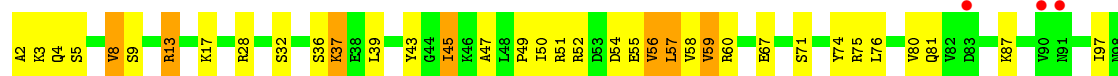




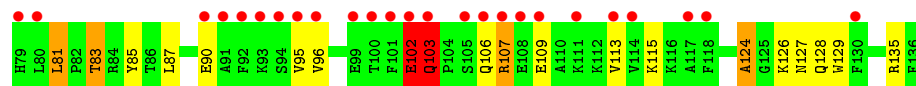
- Molecule 28: 60S ribosomal protein L26-A



- Molecule 28: 60S ribosomal protein L26-A



- Molecule 29: 60S ribosomal protein L27-A

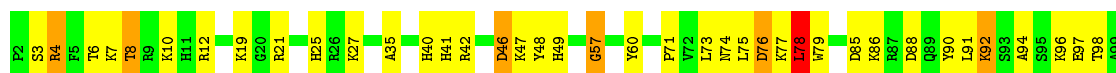


- Molecule 29: 60S ribosomal protein L27-A

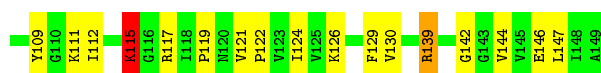
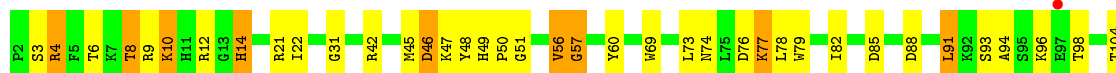


- Molecule 30: 60S ribosomal protein L28





- Molecule 30: 60S ribosomal protein L28



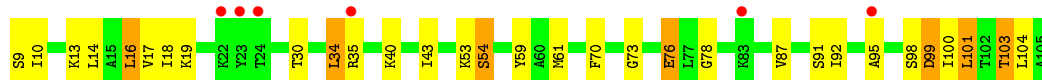
- Molecule 31: 60S ribosomal protein L29



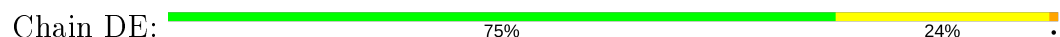
- Molecule 31: 60S ribosomal protein L29



- Molecule 32: 60S ribosomal protein L30

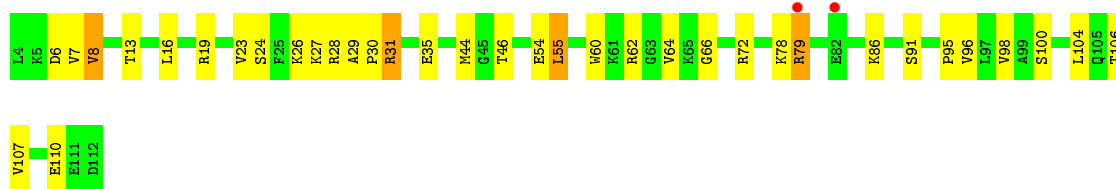


- Molecule 32: 60S ribosomal protein L30

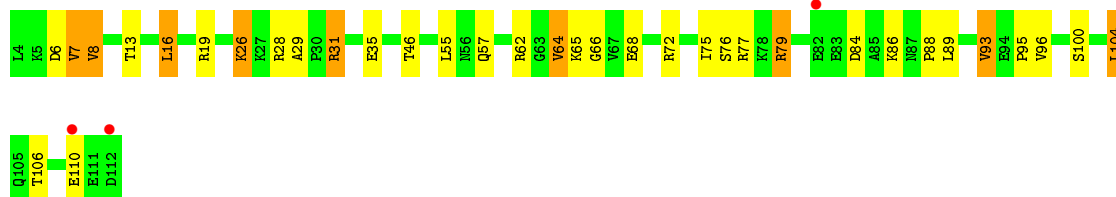


- Molecule 33: 60S ribosomal protein L31-A

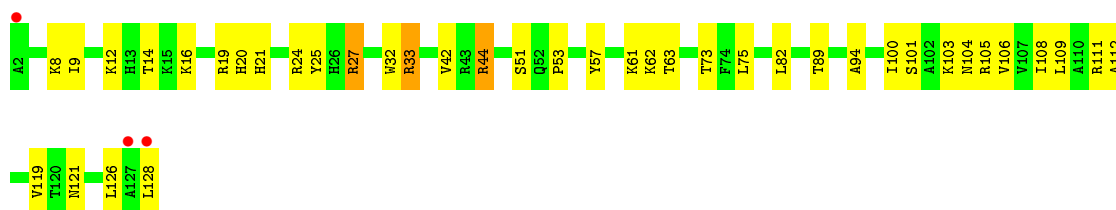




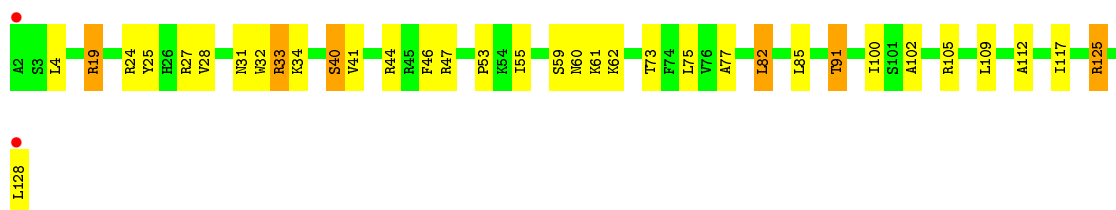
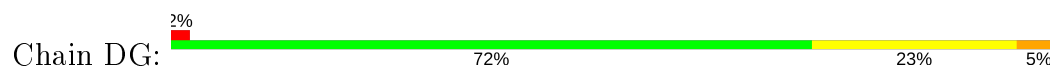
- Molecule 33: 60S ribosomal protein L31-A



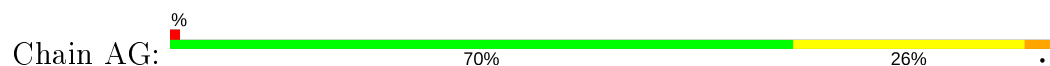
- Molecule 34: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L32



- Molecule 35: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L33-A





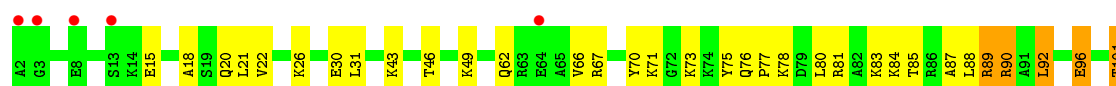
- Molecule 36: 60S ribosomal protein L34-A



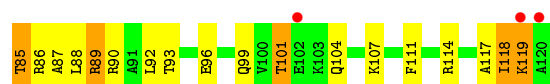
- Molecule 36: 60S ribosomal protein L34-A



- Molecule 37: 60S ribosomal protein L35-A

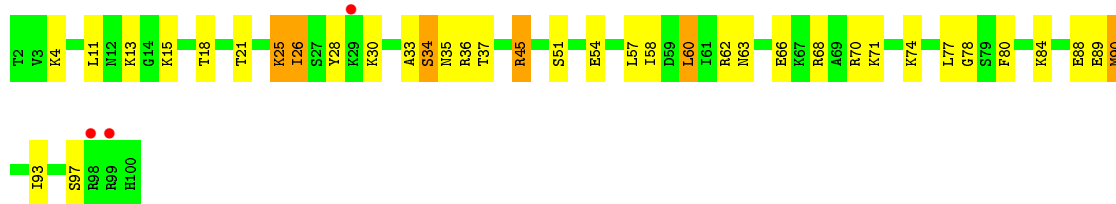


- Molecule 37: 60S ribosomal protein L35-A

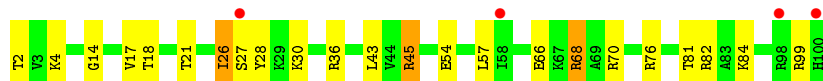
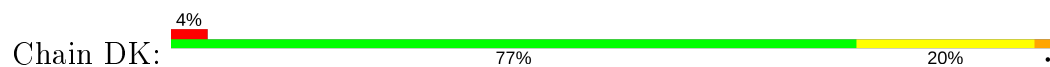


- Molecule 38: 60S ribosomal protein L36-A





- Molecule 38: 60S ribosomal protein L36-A



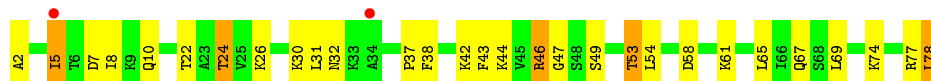
- Molecule 39: 60S ribosomal protein L37-A



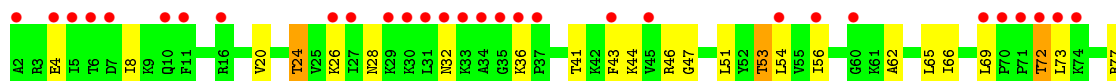
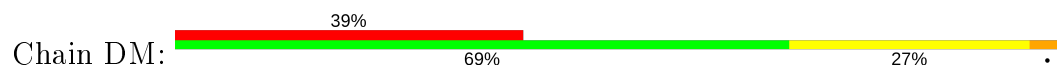
- Molecule 39: 60S ribosomal protein L37-A



- Molecule 40: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L38



L78

- Molecule 41: 60S ribosomal protein L39

Chain AM: 



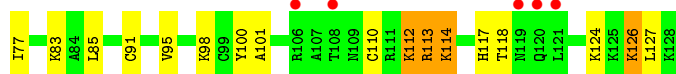
- Molecule 41: 60S ribosomal protein L39

Chain DN: 




- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain AN: 



- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain DO: 



- Molecule 43: 60S ribosomal protein L41-B

Chain AO: 




- Molecule 43: 60S ribosomal protein L41-B

Chain DP: 

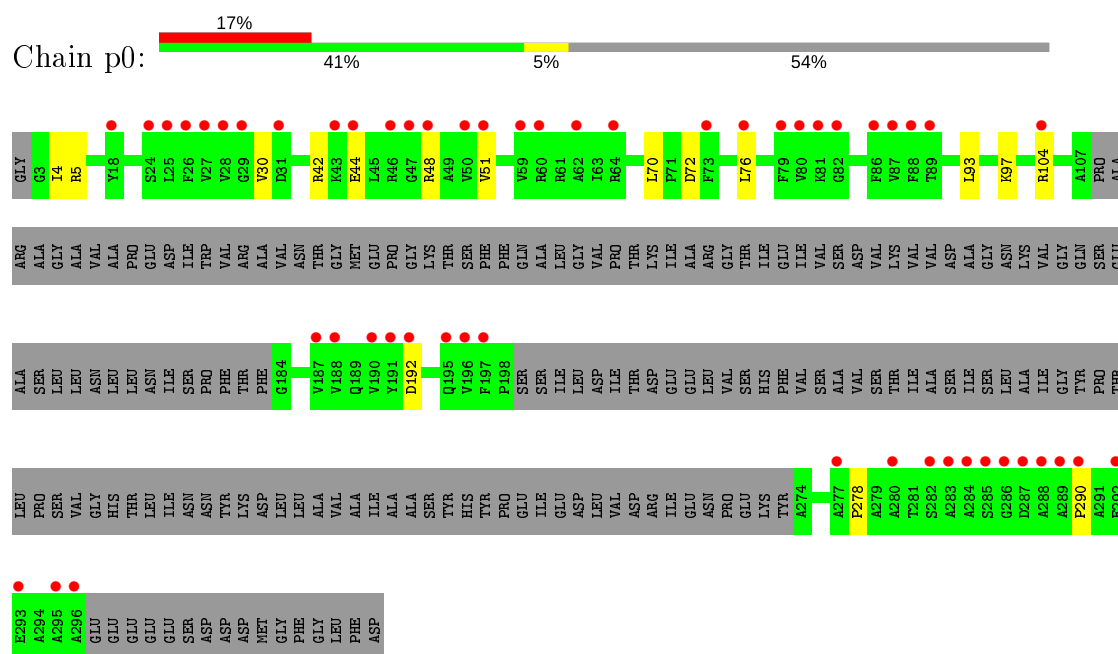


- Molecule 44: 60S ribosomal protein L42-A

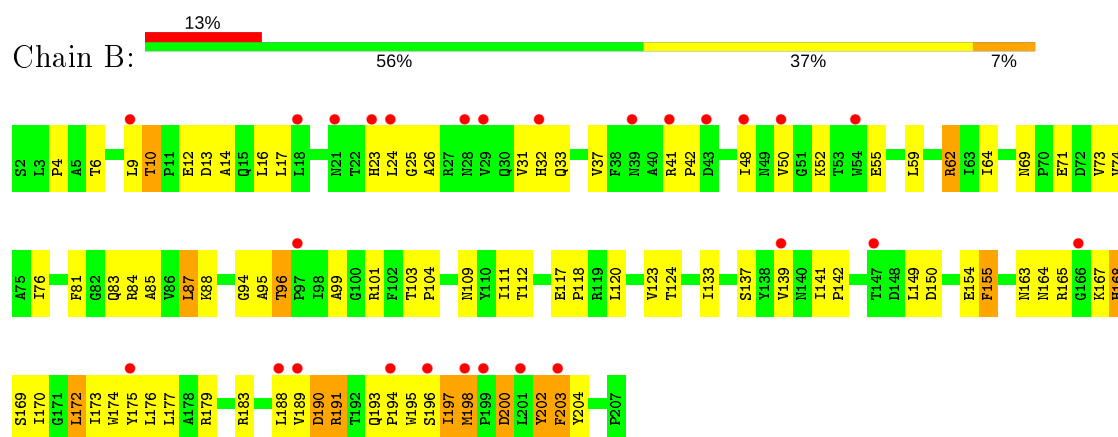
Chain AP: 



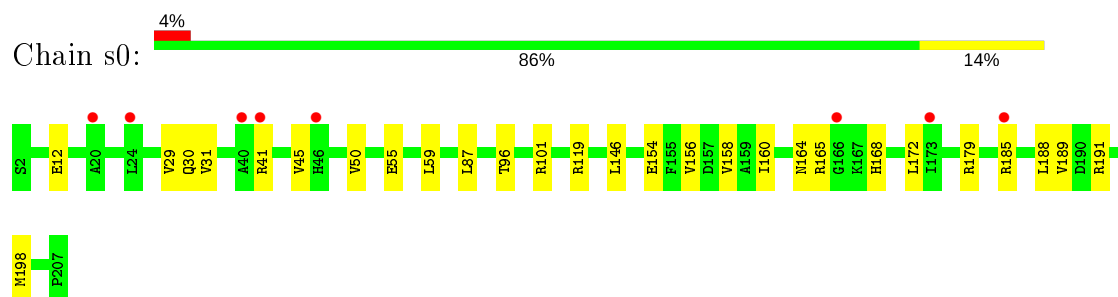
- Molecule 49: 60S acidic ribosomal protein P0



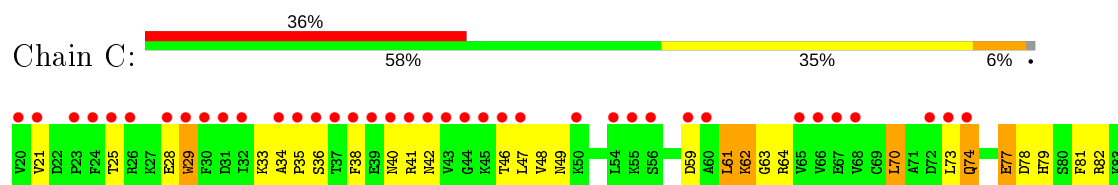
- Molecule 50: 40S ribosomal protein S0-A



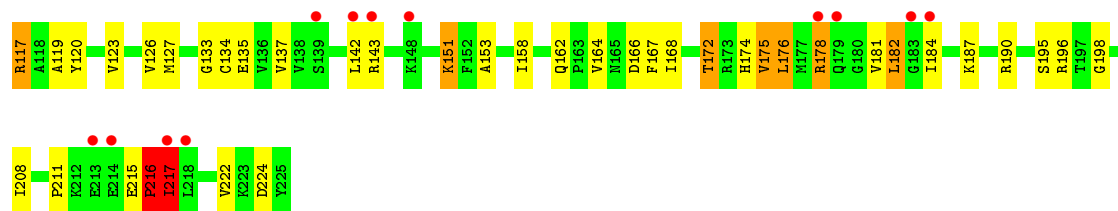
- Molecule 50: 40S ribosomal protein S0-A



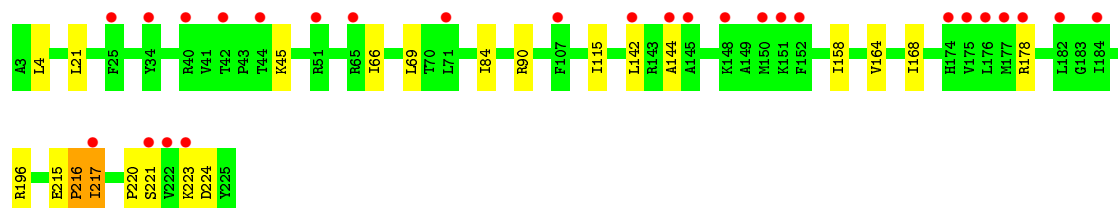
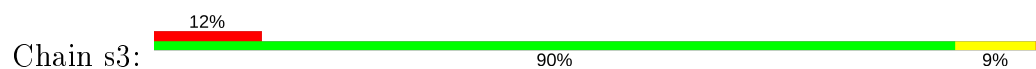
- Molecule 51: 40S ribosomal protein S1-A



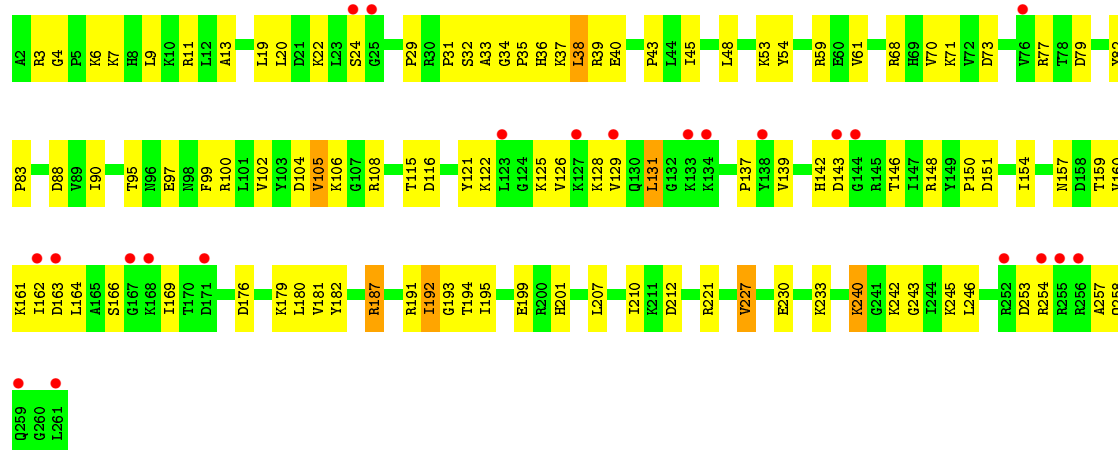




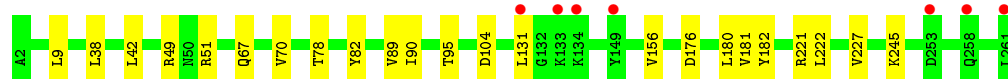
• Molecule 53: 40S ribosomal protein S3



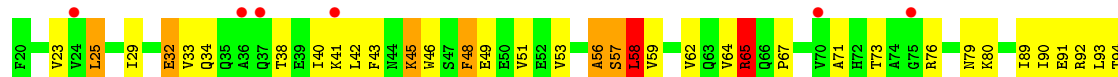
• Molecule 54: 40S ribosomal protein S4-A

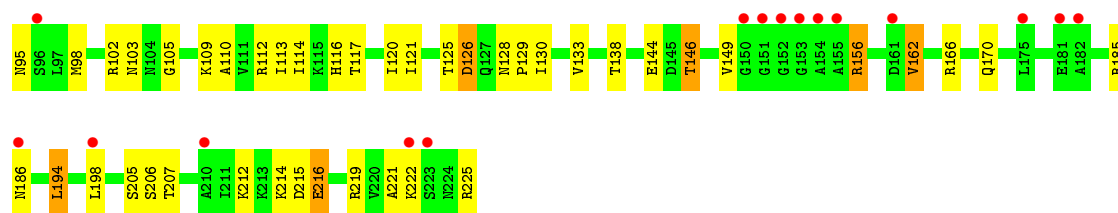


• Molecule 54: 40S ribosomal protein S4-A

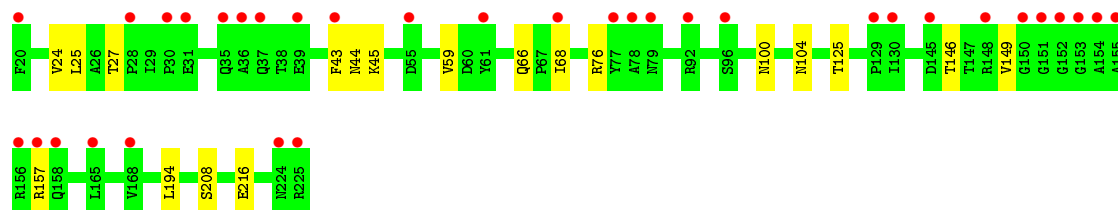


• Molecule 55: 40S ribosomal protein S5

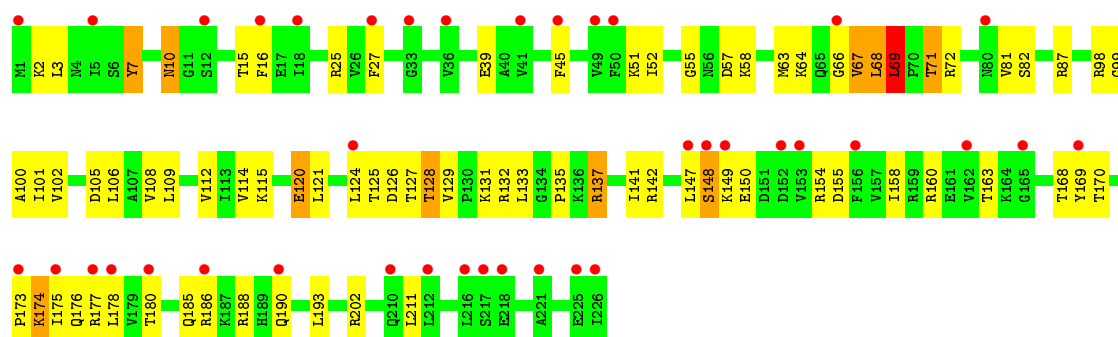




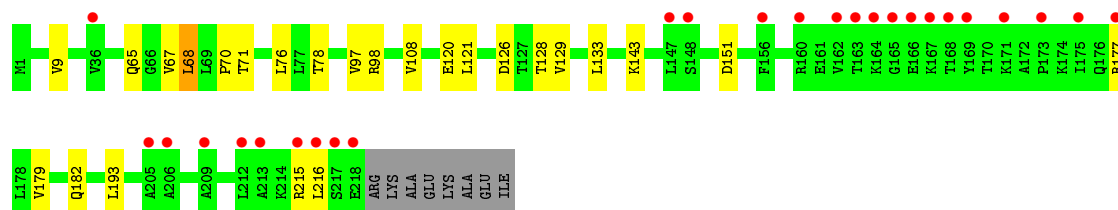
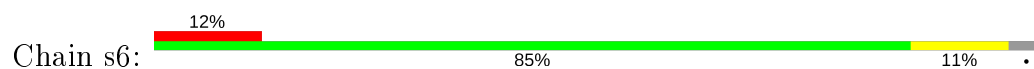
• Molecule 55: 40S ribosomal protein S5



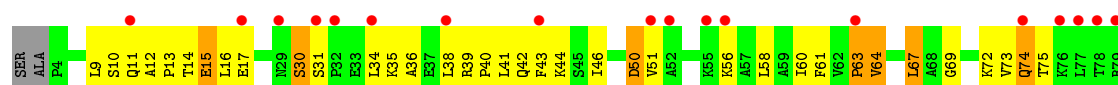
• Molecule 56: 40S ribosomal protein S6-A

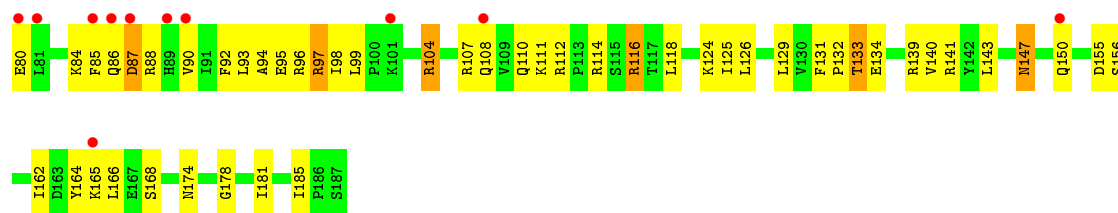


• Molecule 56: 40S ribosomal protein S6-A

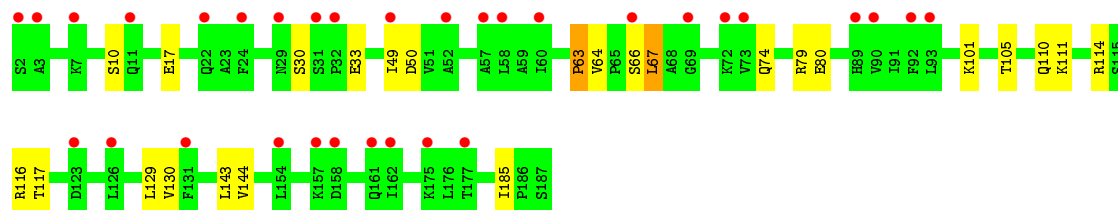
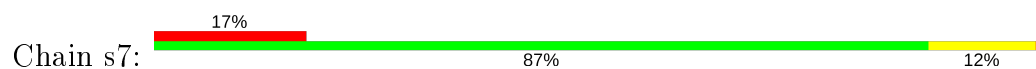


• Molecule 57: 40S ribosomal protein S7-A

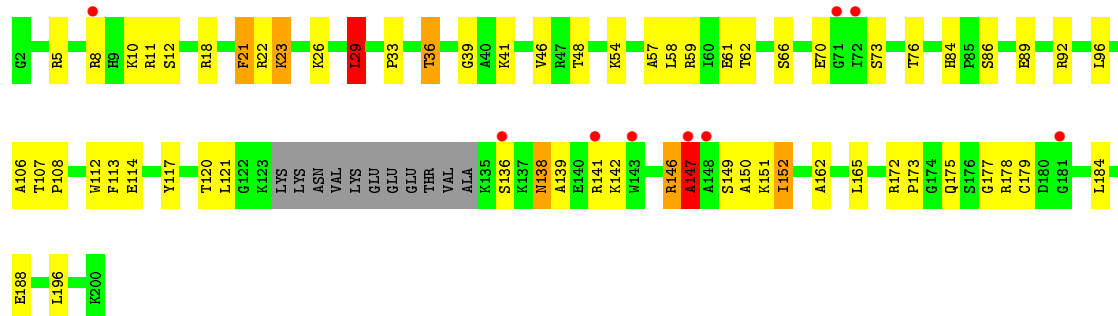




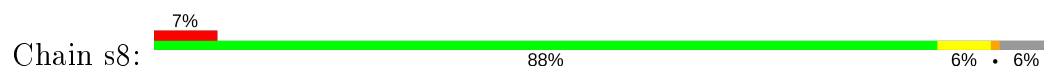
• Molecule 57: 40S ribosomal protein S7-A



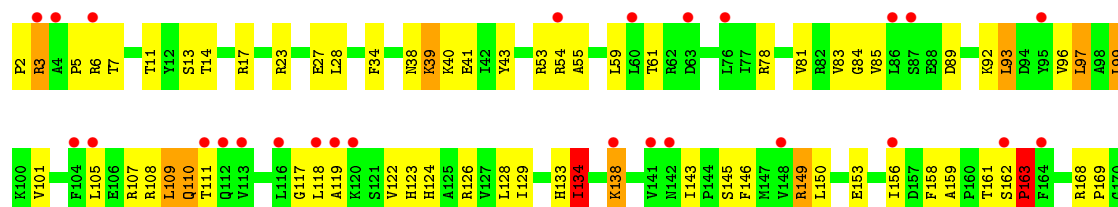
• Molecule 58: 40S ribosomal protein S8-A

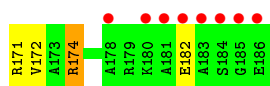


• Molecule 58: 40S ribosomal protein S8-A

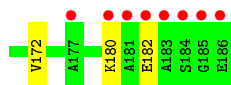
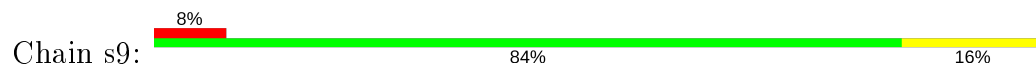


• Molecule 59: 40S ribosomal protein S9-A

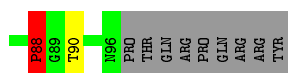
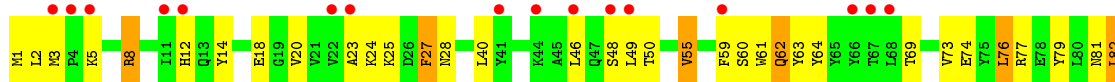




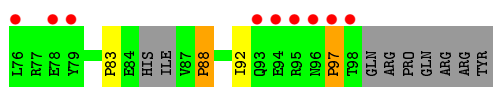
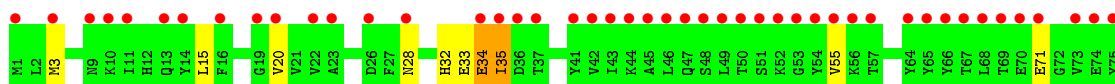
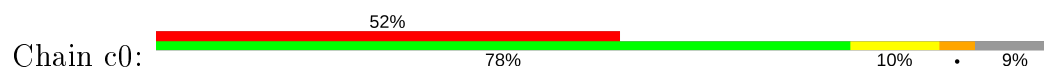
- Molecule 59: 40S ribosomal protein S9-A



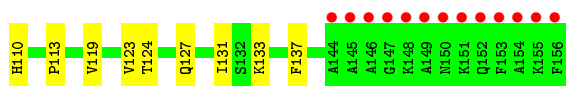
- Molecule 60: 40S ribosomal protein S10-A



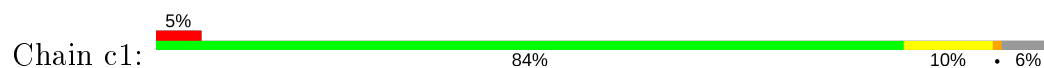
- Molecule 60: 40S ribosomal protein S10-A



- Molecule 61: 40S ribosomal protein S11-A

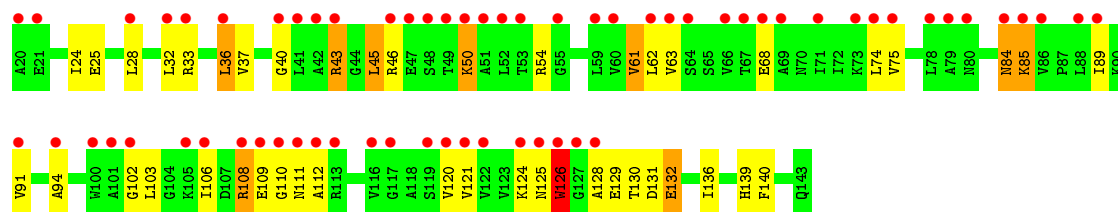


- Molecule 61: 40S ribosomal protein S11-A

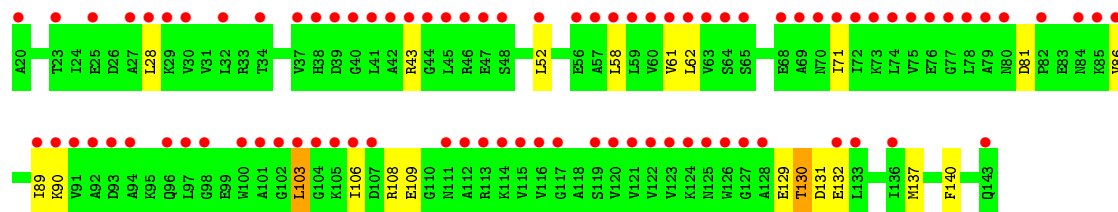
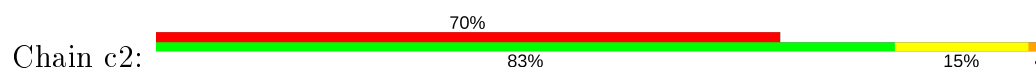




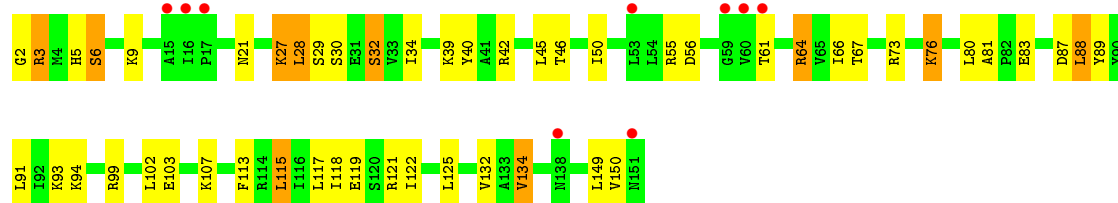
- Molecule 62: 40S ribosomal protein S12



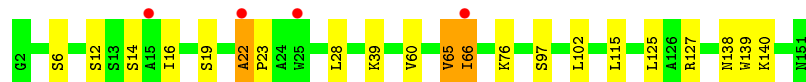
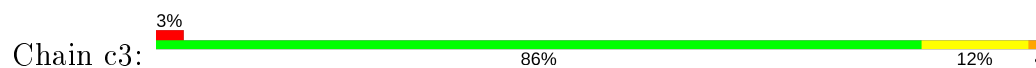
- Molecule 62: 40S ribosomal protein S12



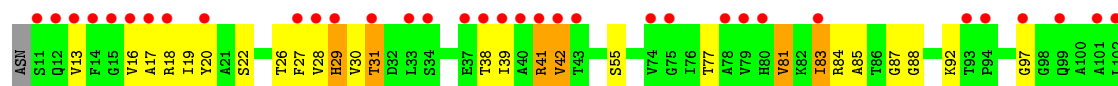
- Molecule 63: 40S ribosomal protein S13

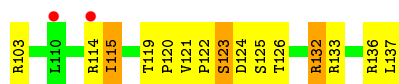


- Molecule 63: 40S ribosomal protein S13

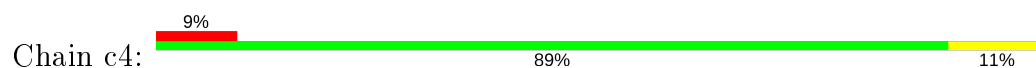


- Molecule 64: 40S ribosomal protein S14-B

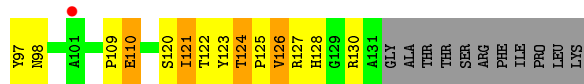




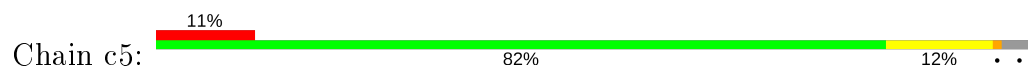
- Molecule 64: 40S ribosomal protein S14-B



- Molecule 65: 40S ribosomal protein S15



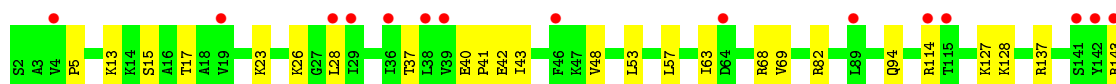
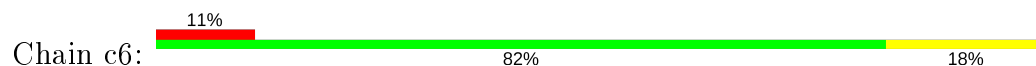
- Molecule 65: 40S ribosomal protein S15



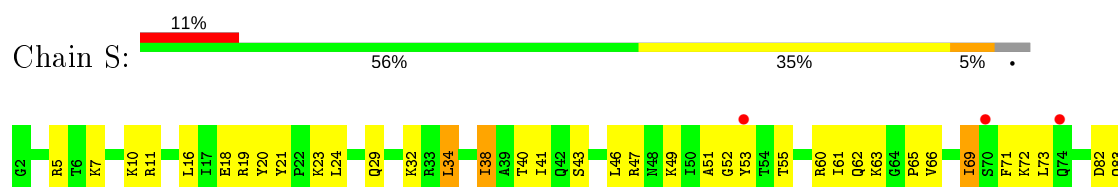
- Molecule 66: 40S ribosomal protein S16-A



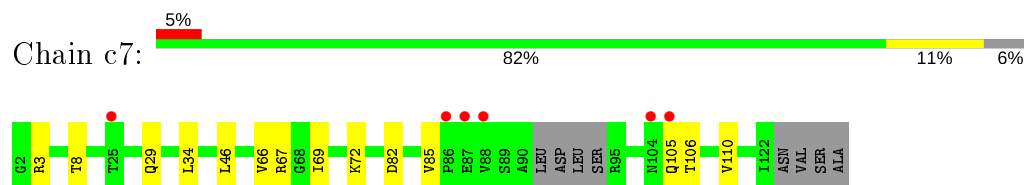
- Molecule 66: 40S ribosomal protein S16-A



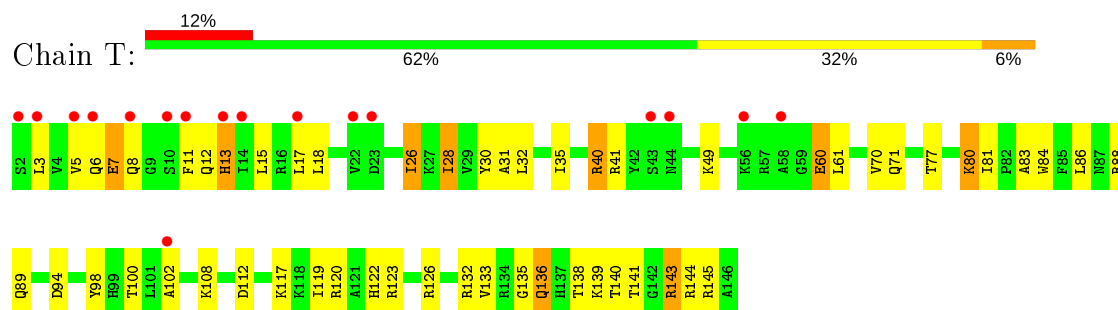
- Molecule 67: 40S ribosomal protein S17-A



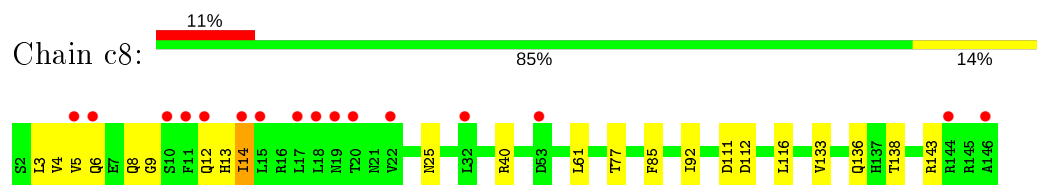
- Molecule 67: 40S ribosomal protein S17-A



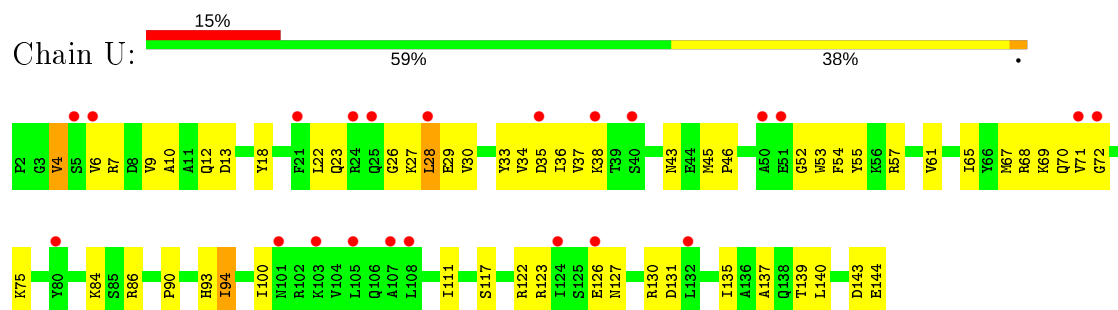
- Molecule 68: 40S ribosomal protein S18-A



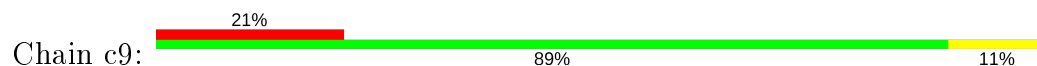
- Molecule 68: 40S ribosomal protein S18-A

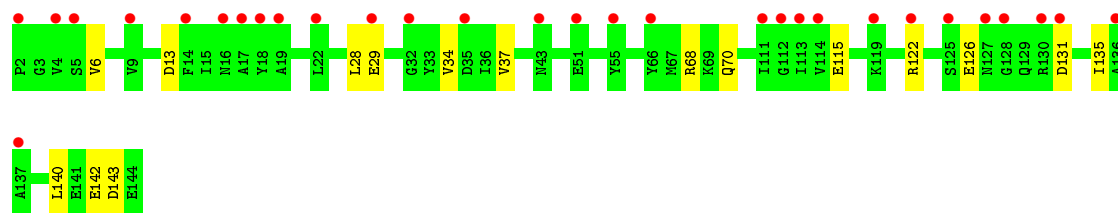


- Molecule 69: 40S ribosomal protein S19-A

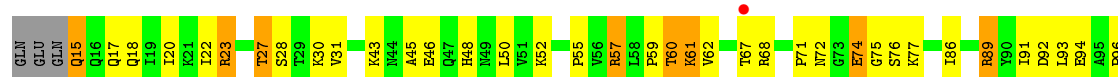


- Molecule 69: 40S ribosomal protein S19-A

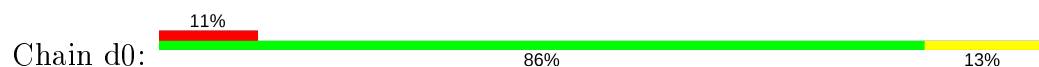




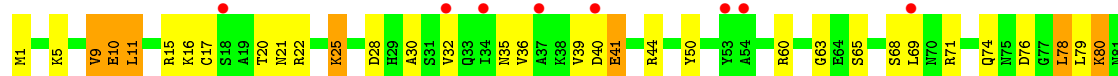
- Molecule 70: 40S ribosomal protein S20



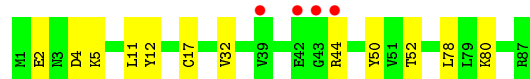
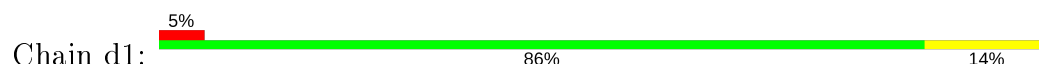
- Molecule 70: 40S ribosomal protein S20



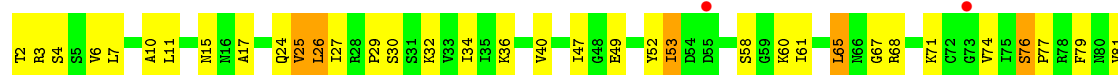
- Molecule 71: 40S ribosomal protein S21-A



- Molecule 71: 40S ribosomal protein S21-A



- Molecule 72: 40S ribosomal protein S22-A





- Molecule 72: 40S ribosomal protein S22-A



- Molecule 73: 40S ribosomal protein S23-A



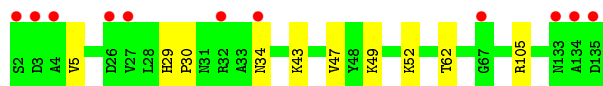
- Molecule 73: 40S ribosomal protein S23-A



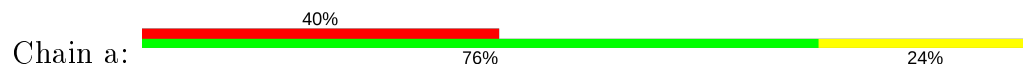
- Molecule 74: 40S ribosomal protein S24-A

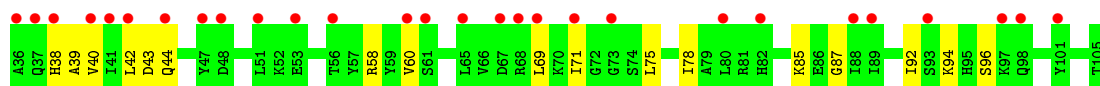


- Molecule 74: 40S ribosomal protein S24-A

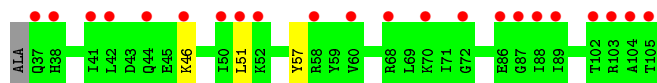


- Molecule 75: 40S ribosomal protein S25-A

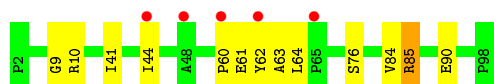
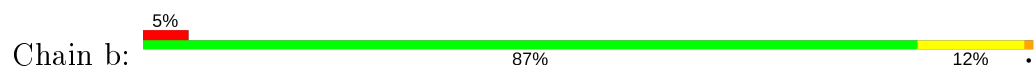




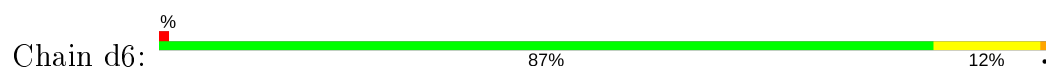
- Molecule 75: 40S ribosomal protein S25-A



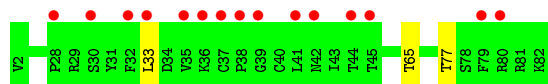
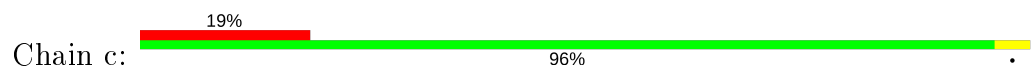
- Molecule 76: 40S ribosomal protein S26-B



- Molecule 76: 40S ribosomal protein S26-B



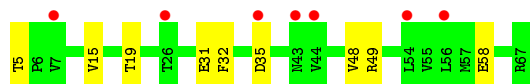
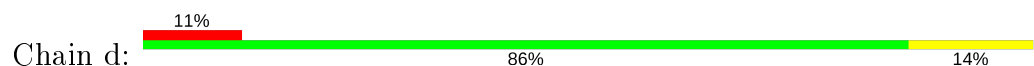
- Molecule 77: 40S ribosomal protein S27-A



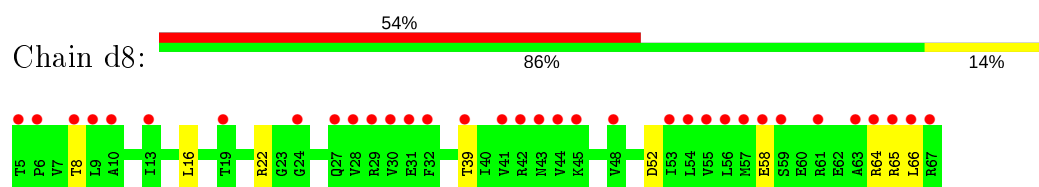
- Molecule 77: 40S ribosomal protein S27-A



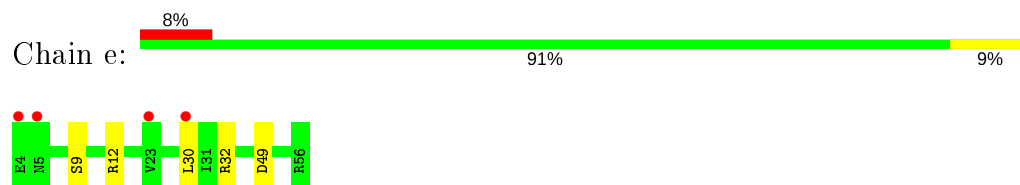
- Molecule 78: 40S ribosomal protein S28-A



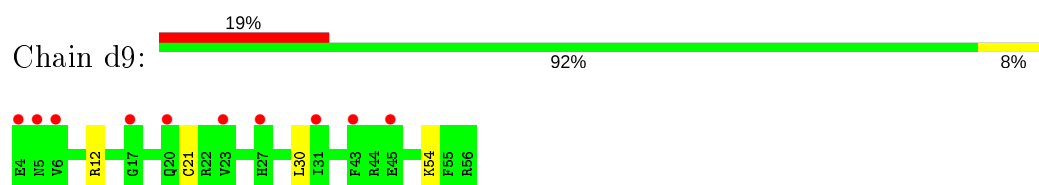
- Molecule 78: 40S ribosomal protein S28-A



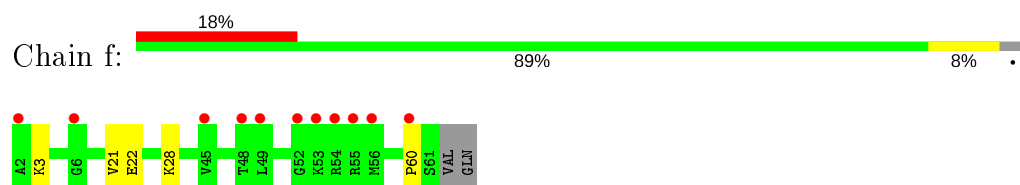
- Molecule 79: 40S ribosomal protein S29-A



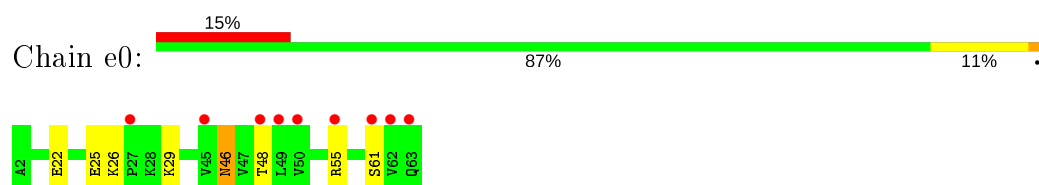
- Molecule 79: 40S ribosomal protein S29-A



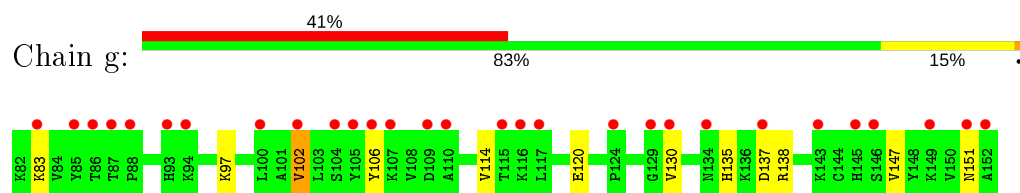
- Molecule 80: 40S ribosomal protein S30-A



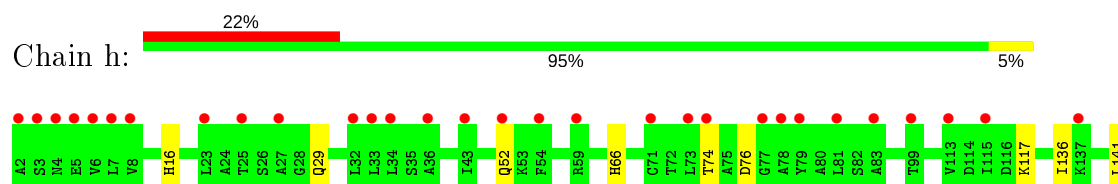
- Molecule 80: 40S ribosomal protein S30-A

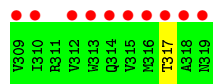
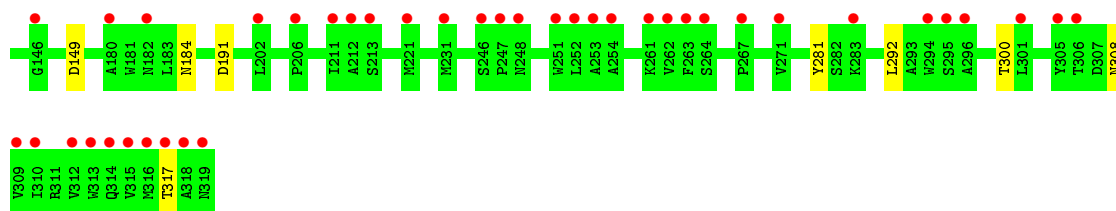


- Molecule 81: Ubiquitin-40S ribosomal protein S31

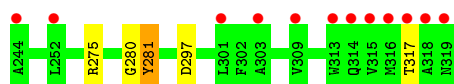


- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein

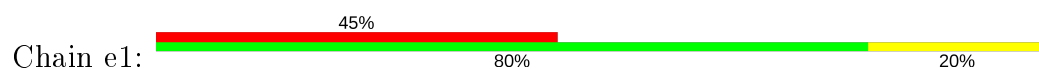




- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 83: Ubiquitin-40S ribosomal protein S31



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	303.13Å 286.50Å 435.66Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	99.84 – 3.10 99.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (99.84-3.10) 99.5 (99.94-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.13Å)	Xtriage
Refinement program	PHENIX dev_2450	Depositor
R, R_{free}	0.222 , 0.252 0.222 , 0.252	Depositor DCC
R_{free} test set	26196 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	410383	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
62	c2	0.35	1/898 (0.1%)	0.62	1/1220 (0.1%)
63	O	0.31	0/1215	0.49	0/1638
63	c3	0.32	0/1215	0.53	0/1638
64	P	0.28	0/901	0.54	0/1217
64	c4	0.32	0/960	0.55	0/1290
65	Q	0.31	0/998	0.49	0/1341
65	c5	0.29	0/1060	0.60	0/1426
66	R	0.29	0/1125	0.55	0/1510
66	c6	0.29	0/1131	0.54	0/1518
67	S	0.29	0/935	0.52	0/1254
67	c7	0.28	0/914	0.48	0/1224
68	T	0.29	0/1211	0.50	0/1628
68	c8	0.29	0/1211	0.50	0/1628
69	U	0.29	0/1130	0.46	0/1517
69	c9	0.29	0/1130	0.46	0/1517
70	V	0.27	0/865	0.51	0/1169
70	d0	0.29	0/892	0.52	0/1205
71	W	0.31	0/693	0.50	0/935
71	d1	0.30	0/693	0.51	0/935
72	X	0.30	0/1038	0.55	0/1395
72	d2	0.31	0/1038	0.52	0/1395
73	Y	0.33	0/1139	0.55	0/1518
73	d3	0.35	0/1139	0.54	0/1518
74	Z	0.31	0/1087	0.49	0/1449
74	d4	0.32	0/1087	0.54	0/1449
75	a	0.29	0/571	0.53	0/768
75	d5	0.27	0/566	0.46	0/761
76	b	0.34	0/782	0.61	0/1047
76	d6	0.33	0/782	0.60	0/1047
77	c	0.27	0/620	0.54	0/838
77	d7	0.28	0/620	0.54	0/838
78	d	0.43	1/499 (0.2%)	0.53	0/670
78	d8	0.28	0/499	0.62	0/670
79	d9	0.33	0/452	0.51	0/600
79	e	0.30	0/452	0.50	0/600
80	e0	0.32	0/499	0.49	0/665
80	f	0.29	0/483	0.48	0/643
81	g	0.29	0/577	0.58	0/770
82	h	0.26	0/2494	0.49	0/3393
82	sR	0.27	0/2495	0.50	0/3395
83	e1	0.27	0/404	0.56	0/542
All	All	0.47	11/429967 (0.0%)	0.83	346/631328 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	3
5	k	0	2
6	l	0	2
7	CG	0	3
7	m	0	1
9	CI	0	2
9	o	0	2
10	CJ	0	2
10	p	0	1
11	CK	0	1
11	q	0	1
12	CL	0	1
13	CM	0	2
13	s	0	2
14	CN	0	1
14	t	0	2
15	CO	0	1
15	u	0	1
16	CP	0	1
17	CQ	0	1
17	w	0	1
18	x	0	1
19	CS	0	1
21	CU	0	2
26	CY	0	1
29	AA	0	2
30	DC	0	2
31	AC	0	1
31	DD	0	1
37	AI	0	1
37	DJ	0	1
50	B	0	1
51	s1	0	1
53	E	0	2
53	s3	0	2
55	G	0	3
55	s5	0	1
56	H	0	2
57	I	0	2

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

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

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

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	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 ⓘ

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

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

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

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

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

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

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	s	1	0	0	0	0
85	s4	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	1	0	0	0	0
85	sM	2	0	0	0	0
85	t	3	0	0	0	0
85	v	3	0	0	0	0
85	w	2	0	0	0	0
85	x	7	0	0	0	0
85	z	1	0	0	0	0
86	1	22	0	0	0	0
86	AR	22	0	0	0	0
87	6	6	0	8	0	0
87	A	6	0	8	0	0
87	AR	12	0	14	3	0
87	v	6	0	8	0	0
88	AK	1	0	0	0	0
88	AN	1	0	0	0	0
88	AP	1	0	0	0	0
88	AQ	1	0	0	0	0
88	DL	1	0	0	0	0
88	DO	1	0	0	0	0
88	DQ	1	0	0	0	0
88	DR	1	0	0	0	0
88	b	1	0	0	0	0
88	c	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e	1	0	0	0	0
88	e1	1	0	0	0	0
88	g	1	0	0	0	0
All	All	410383	0	296944	4796	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4796 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1481:A:O2'	1:1:1858:A:N3	1.96	0.98

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	250/252 (99%)	226 (90%)	23 (9%)	1 (0%)	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	CL	207/220 (94%)	188 (91%)	19 (9%)	0	100	100
12	r	207/220 (94%)	189 (91%)	17 (8%)	1 (0%)	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	DA	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
29	AA	133/135 (98%)	115 (86%)	15 (11%)	3 (2%)	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
39	DL	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
40	AL	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
40	DM	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
41	AM	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
41	DN	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
42	AN	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
42	DO	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
43	AO	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
43	DP	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	AP	103/105 (98%)	84 (82%)	19 (18%)	0	100	100
44	DQ	103/105 (98%)	88 (85%)	15 (15%)	0	100	100
45	AQ	89/91 (98%)	79 (89%)	10 (11%)	0	100	100
45	DR	89/91 (98%)	82 (92%)	7 (8%)	0	100	100
46	i	155/272 (57%)	121 (78%)	30 (19%)	4 (3%)	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	d7	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
78	d	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
78	d8	61/63 (97%)	47 (77%)	14 (23%)	0	100	100
79	d9	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
79	e	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
80	e0	60/62 (97%)	52 (87%)	8 (13%)	0	100	100
80	f	58/62 (94%)	47 (81%)	10 (17%)	1 (2%)	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 ⓘ

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
20	CT	22	VAL
40	DM	69	LEU
66	c6	43	ILE
21	CU	132	THR
29	DB	66	THR

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

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

5.3.3 RNA ⓘ

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

5 of 2006 RNA backbone outliers are listed below:

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

5 of 186 RNA pucker outliers are listed below:

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

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2548 ligands modelled in this entry, 1 is modelled with single atom and 1477 are monoatomic - leaving 1070 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
84	OHX	AR	3631	-	0,6,6	0.00	-	-		
84	OHX	AR	3665	-	0,6,6	0.00	-	-		
84	OHX	AR	3460	-	0,6,6	0.00	-	-		
84	OHX	AR	3578	-	0,6,6	0.00	-	-		
84	OHX	6	1988	-	0,6,6	0.00	-	-		
84	OHX	AR	3542	-	0,6,6	0.00	-	-		
84	OHX	6	1938	-	0,6,6	0.00	-	-		
84	OHX	4	202	-	0,6,6	0.00	-	-		
84	OHX	AR	3476	-	0,6,6	0.00	-	-		
84	OHX	1	3700	-	0,6,6	0.00	-	-		
84	OHX	CL	301	-	0,6,6	0.00	-	-		
84	OHX	1	3571	-	0,6,6	0.00	-	-		
84	OHX	AR	3742	-	0,6,6	0.00	-	-		
84	OHX	AR	3605	-	0,6,6	0.00	-	-		
84	OHX	1	3500	-	0,6,6	0.00	-	-		
84	OHX	AR	3588	-	0,6,6	0.00	-	-		
84	OHX	1	3546	-	0,6,6	0.00	-	-		
84	OHX	1	3426	-	0,6,6	0.00	-	-		
84	OHX	6	1941	-	0,6,6	0.00	-	-		
84	OHX	1	3675	-	0,6,6	0.00	-	-		
84	OHX	AR	3710	-	0,6,6	0.00	-	-		
84	OHX	1	3501	-	0,6,6	0.00	-	-		
84	OHX	AR	3642	-	0,6,6	0.00	-	-		
84	OHX	1	3409	-	0,6,6	0.00	-	-		
84	OHX	AR	3480	-	0,6,6	0.00	-	-		
84	OHX	AR	3591	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3420	-	0,6,6	0.00	-	-		
84	OHX	AR	3699	-	0,6,6	0.00	-	-		
84	OHX	6	1930	-	0,6,6	0.00	-	-		
84	OHX	A	2025	-	0,6,6	0.00	-	-		
84	OHX	AR	3646	-	0,6,6	0.00	-	-		
84	OHX	1	3484	-	0,6,6	0.00	-	-		
84	OHX	A	1968	-	0,6,6	0.00	-	-		
84	OHX	AR	3568	-	0,6,6	0.00	-	-		
84	OHX	AR	3598	-	0,6,6	0.00	-	-		
84	OHX	1	3671	-	0,6,6	0.00	-	-		
84	OHX	1	3681	-	0,6,6	0.00	-	-		
84	OHX	A	1963	-	0,6,6	0.00	-	-		
84	OHX	k	401	-	0,6,6	0.00	-	-		
84	OHX	A	1953	-	0,6,6	0.00	-	-		
84	OHX	A	1956	-	0,6,6	0.00	-	-		
84	OHX	AR	3529	-	0,6,6	0.00	-	-		
84	OHX	e	101	-	0,6,6	0.00	-	-		
84	OHX	1	3574	-	0,6,6	0.00	-	-		
84	OHX	AR	3704	-	0,6,6	0.00	-	-		
84	OHX	1	3536	-	0,6,6	0.00	-	-		
84	OHX	1	3545	-	0,6,6	0.00	-	-		
84	OHX	1	3430	-	0,6,6	0.00	-	-		
84	OHX	1	3612	-	0,6,6	0.00	-	-		
84	OHX	4	216	-	0,6,6	0.00	-	-		
84	OHX	A	2020	-	0,6,6	0.00	-	-		
84	OHX	AR	3569	-	0,6,6	0.00	-	-		
84	OHX	AR	3562	-	0,6,6	0.00	-	-		
84	OHX	6	1928	-	0,6,6	0.00	-	-		
84	OHX	6	1910	-	0,6,6	0.00	-	-		
84	OHX	AR	3672	-	0,6,6	0.00	-	-		
84	OHX	AR	3430	-	0,6,6	0.00	-	-		
84	OHX	AT	214	-	0,6,6	0.00	-	-		
84	OHX	A	1943	-	0,6,6	0.00	-	-		
84	OHX	1	3557	-	0,6,6	0.00	-	-		
84	OHX	AR	3509	-	0,6,6	0.00	-	-		
84	OHX	6	1919	-	0,6,6	0.00	-	-		
84	OHX	AR	3406	-	0,6,6	0.00	-	-		
84	OHX	AR	3548	-	0,6,6	0.00	-	-		
84	OHX	AR	3426	-	0,6,6	0.00	-	-		
84	OHX	AR	3645	-	0,6,6	0.00	-	-		
84	OHX	6	1952	-	0,6,6	0.00	-	-		
84	OHX	1	3616	-	0,6,6	0.00	-	-		
84	OHX	1	3497	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3621	-	0,6,6	0.00	-	-		
84	OHX	AR	3487	-	0,6,6	0.00	-	-		
84	OHX	AR	3421	-	0,6,6	0.00	-	-		
84	OHX	6	2001	-	0,6,6	0.00	-	-		
84	OHX	A	2024	-	0,6,6	0.00	-	-		
84	OHX	1	3414	-	0,6,6	0.00	-	-		
84	OHX	AR	3669	-	0,6,6	0.00	-	-		
84	OHX	A	2033	-	0,6,6	0.00	-	-		
84	OHX	AR	3485	-	0,6,6	0.00	-	-		
84	OHX	v	301	-	0,6,6	0.00	-	-		
84	OHX	4	204	-	0,6,6	0.00	-	-		
84	OHX	1	3686	-	0,6,6	0.00	-	-		
84	OHX	3	207	-	0,6,6	0.00	-	-		
84	OHX	AR	3711	-	0,6,6	0.00	-	-		
84	OHX	1	3709	-	0,6,6	0.00	-	-		
84	OHX	1	3494	-	0,6,6	0.00	-	-		
84	OHX	AR	3436	-	0,6,6	0.00	-	-		
84	OHX	1	3720	-	0,6,6	0.00	-	-		
84	OHX	6	2030	-	0,6,6	0.00	-	-		
84	OHX	CM	201	-	0,6,6	0.00	-	-		
84	OHX	AS	202	-	0,6,6	0.00	-	-		
84	OHX	A	2034	-	0,6,6	0.00	-	-		
84	OHX	AR	3620	-	0,6,6	0.00	-	-		
84	OHX	1	3626	-	0,6,6	0.00	-	-		
84	OHX	AR	3729	-	0,6,6	0.00	-	-		
84	OHX	1	3544	-	0,6,6	0.00	-	-		
84	OHX	6	2006	-	0,6,6	0.00	-	-		
84	OHX	AS	207	-	0,6,6	0.00	-	-		
84	OHX	AR	3684	-	0,6,6	0.00	-	-		
84	OHX	CG	301	-	0,6,6	0.00	-	-		
84	OHX	6	1992	-	0,6,6	0.00	-	-		
84	OHX	DD	101	-	0,6,6	0.00	-	-		
84	OHX	AR	3477	84	0,6,6	0.00	-	-		
84	OHX	1	3418	-	0,6,6	0.00	-	-		
84	OHX	1	3573	-	0,6,6	0.00	-	-		
84	OHX	6	2031	-	0,6,6	0.00	-	-		
84	OHX	A	2037	-	0,6,6	0.00	-	-		
84	OHX	AR	3611	-	0,6,6	0.00	-	-		
84	OHX	1	3606	-	0,6,6	0.00	-	-		
84	OHX	A	1902	-	0,6,6	0.00	-	-		
84	OHX	A	1979	-	0,6,6	0.00	-	-		
84	OHX	1	3516	-	0,6,6	0.00	-	-		
84	OHX	A	1989	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3528	-	0,6,6	0.00	-	-		
84	OHX	1	3691	-	0,6,6	0.00	-	-		
84	OHX	6	1940	-	0,6,6	0.00	-	-		
84	OHX	1	3650	-	0,6,6	0.00	-	-		
84	OHX	A	1990	-	0,6,6	0.00	-	-		
84	OHX	1	3716	-	0,6,6	0.00	-	-		
84	OHX	1	3651	-	0,6,6	0.00	-	-		
84	OHX	A	1937	-	0,6,6	0.00	-	-		
84	OHX	AR	3535	-	0,6,6	0.00	-	-		
84	OHX	AT	215	-	0,6,6	0.00	-	-		
84	OHX	6	1983	-	0,6,6	0.00	-	-		
84	OHX	AR	3687	-	0,6,6	0.00	-	-		
84	OHX	AR	3440	-	0,6,6	0.00	-	-		
84	OHX	AR	3700	-	0,6,6	0.00	-	-		
84	OHX	1	3622	-	0,6,6	0.00	-	-		
84	OHX	1	3412	-	0,6,6	0.00	-	-		
84	OHX	AR	3471	-	0,6,6	0.00	-	-		
84	OHX	1	3637	-	0,6,6	0.00	-	-		
84	OHX	1	3701	-	0,6,6	0.00	-	-		
84	OHX	1	3542	-	0,6,6	0.00	-	-		
84	OHX	AR	3447	-	0,6,6	0.00	-	-		
84	OHX	AS	208	-	0,6,6	0.00	-	-		
84	OHX	6	1961	-	0,6,6	0.00	-	-		
84	OHX	AR	3461	-	0,6,6	0.00	-	-		
84	OHX	AR	3675	-	0,6,6	0.00	-	-		
84	OHX	1	3684	-	0,6,6	0.00	-	-		
84	OHX	6	2040	-	0,6,6	0.00	-	-		
84	OHX	1	3593	-	0,6,6	0.00	-	-		
84	OHX	6	1937	-	0,6,6	0.00	-	-		
84	OHX	AS	209	-	0,6,6	0.00	-	-		
84	OHX	A	1915	-	0,6,6	0.00	-	-		
84	OHX	A	1986	-	0,6,6	0.00	-	-		
84	OHX	1	3699	-	0,6,6	0.00	-	-		
84	OHX	1	3423	-	0,6,6	0.00	-	-		
84	OHX	A	1971	-	0,6,6	0.00	-	-		
84	OHX	A	1907	-	0,6,6	0.00	-	-		
84	OHX	6	1936	-	0,6,6	0.00	-	-		
84	OHX	AR	3515	-	0,6,6	0.00	-	-		
84	OHX	AR	3662	-	0,6,6	0.00	-	-		
84	OHX	6	1911	-	0,6,6	0.00	-	-		
84	OHX	AG	201	-	0,6,6	0.00	-	-		
84	OHX	A	1969	-	0,6,6	0.00	-	-		
84	OHX	A	1964	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3469	-	0,6,6	0.00	-	-		
84	OHX	1	3415	-	0,6,6	0.00	-	-		
84	OHX	AR	3522	-	0,6,6	0.00	-	-		
84	OHX	A	2042	-	0,6,6	0.00	-	-		
84	OHX	1	3450	-	0,6,6	0.00	-	-		
84	OHX	6	1994	-	0,6,6	0.00	-	-		
84	OHX	AR	3695	-	0,6,6	0.00	-	-		
84	OHX	AR	3670	-	0,6,6	0.00	-	-		
84	OHX	AR	3540	-	0,6,6	0.00	-	-		
84	OHX	AR	3495	-	0,6,6	0.00	-	-		
84	OHX	1	3534	-	0,6,6	0.00	-	-		
84	OHX	A	2002	-	0,6,6	0.00	-	-		
84	OHX	AR	3624	-	0,6,6	0.00	-	-		
84	OHX	AR	3554	-	0,6,6	0.00	-	-		
84	OHX	AR	3606	-	0,6,6	0.00	-	-		
84	OHX	6	1905	-	0,6,6	0.00	-	-		
84	OHX	1	3632	-	0,6,6	0.00	-	-		
84	OHX	6	2025	-	0,6,6	0.00	-	-		
84	OHX	1	3665	-	0,6,6	0.00	-	-		
84	OHX	1	3441	-	0,6,6	0.00	-	-		
84	OHX	1	3466	-	0,6,6	0.00	-	-		
84	OHX	AR	3636	-	0,6,6	0.00	-	-		
84	OHX	AR	3607	-	0,6,6	0.00	-	-		
84	OHX	AR	3735	-	0,6,6	0.00	-	-		
84	OHX	1	3623	-	0,6,6	0.00	-	-		
84	OHX	AR	3527	-	0,6,6	0.00	-	-		
84	OHX	3	206	-	0,6,6	0.00	-	-		
84	OHX	AR	3639	-	0,6,6	0.00	-	-		
84	OHX	1	3587	-	0,6,6	0.00	-	-		
84	OHX	AR	3712	-	0,6,6	0.00	-	-		
84	OHX	1	3630	-	0,6,6	0.00	-	-		
84	OHX	1	3452	-	0,6,6	0.00	-	-		
84	OHX	1	3576	-	0,6,6	0.00	-	-		
84	OHX	A	2030	-	0,6,6	0.00	-	-		
84	OHX	6	1964	-	0,6,6	0.00	-	-		
84	OHX	3	205	-	0,6,6	0.00	-	-		
84	OHX	AR	3423	-	0,6,6	0.00	-	-		
84	OHX	1	3717	-	0,6,6	0.00	-	-		
84	OHX	1	3493	-	0,6,6	0.00	-	-		
84	OHX	1	3619	-	0,6,6	0.00	-	-		
84	OHX	AR	3622	-	0,6,6	0.00	-	-		
84	OHX	1	3692	-	0,6,6	0.00	-	-		
84	OHX	AP	502	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	2014	-	0,6,6	0.00	-	-		
84	OHX	4	213	-	0,6,6	0.00	-	-		
84	OHX	AR	3403	-	0,6,6	0.00	-	-		
84	OHX	A	1951	-	0,6,6	0.00	-	-		
84	OHX	AR	3610	-	0,6,6	0.00	-	-		
84	OHX	1	3475	-	0,6,6	0.00	-	-		
84	OHX	1	3683	-	0,6,6	0.00	-	-		
84	OHX	1	3525	-	0,6,6	0.00	-	-		
84	OHX	A	1970	-	0,6,6	0.00	-	-		
84	OHX	AR	3693	-	0,6,6	0.00	-	-		
84	OHX	6	1950	-	0,6,6	0.00	-	-		
84	OHX	1	3643	-	0,6,6	0.00	-	-		
84	OHX	AR	3583	-	0,6,6	0.00	-	-		
84	OHX	AR	3413	-	0,6,6	0.00	-	-		
84	OHX	A	1948	-	0,6,6	0.00	-	-		
84	OHX	1	3566	-	0,6,6	0.00	-	-		
84	OHX	1	3538	-	0,6,6	0.00	-	-		
84	OHX	4	207	-	0,6,6	0.00	-	-		
84	OHX	AT	217	-	0,6,6	0.00	-	-		
84	OHX	AR	3479	-	0,6,6	0.00	-	-		
84	OHX	AR	3656	-	0,6,6	0.00	-	-		
84	OHX	AR	3575	-	0,6,6	0.00	-	-		
84	OHX	1	3667	-	0,6,6	0.00	-	-		
84	OHX	1	3668	-	0,6,6	0.00	-	-		
84	OHX	AR	3635	-	0,6,6	0.00	-	-		
84	OHX	1	3421	-	0,6,6	0.00	-	-		
84	OHX	1	3451	-	0,6,6	0.00	-	-		
84	OHX	AR	3691	-	0,6,6	0.00	-	-		
84	OHX	AR	3705	-	0,6,6	0.00	-	-		
84	OHX	A	1917	-	0,6,6	0.00	-	-		
84	OHX	AR	3719	-	0,6,6	0.00	-	-		
84	OHX	6	1943	-	0,6,6	0.00	-	-		
84	OHX	A	1931	-	0,6,6	0.00	-	-		
84	OHX	AR	3572	-	0,6,6	0.00	-	-		
84	OHX	A	1945	-	0,6,6	0.00	-	-		
84	OHX	6	1963	-	0,6,6	0.00	-	-		
84	OHX	3	208	-	0,6,6	0.00	-	-		
84	OHX	1	3514	-	0,6,6	0.00	-	-		
84	OHX	AR	3594	-	0,6,6	0.00	-	-		
84	OHX	6	1906	-	0,6,6	0.00	-	-		
84	OHX	DH	201	-	0,6,6	0.00	-	-		
84	OHX	A	1999	-	0,6,6	0.00	-	-		
84	OHX	A	2001	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3637	-	0,6,6	0.00	-	-		
84	OHX	1	3456	-	0,6,6	0.00	-	-		
84	OHX	A	1955	-	0,6,6	0.00	-	-		
84	OHX	A	1936	-	0,6,6	0.00	-	-		
84	OHX	1	3669	-	0,6,6	0.00	-	-		
84	OHX	1	3581	-	0,6,6	0.00	-	-		
84	OHX	6	1934	-	0,6,6	0.00	-	-		
84	OHX	AR	3445	-	0,6,6	0.00	-	-		
84	OHX	AR	3538	-	0,6,6	0.00	-	-		
84	OHX	6	1931	-	0,6,6	0.00	-	-		
84	OHX	1	3535	-	0,6,6	0.00	-	-		
84	OHX	AR	3553	-	0,6,6	0.00	-	-		
84	OHX	6	2047	-	0,6,6	0.00	-	-		
84	OHX	1	3526	-	0,6,6	0.00	-	-		
84	OHX	A	1941	-	0,6,6	0.00	-	-		
84	OHX	6	2007	-	0,6,6	0.00	-	-		
84	OHX	c4	201	-	0,6,6	0.00	-	-		
84	OHX	6	1981	-	0,6,6	0.00	-	-		
84	OHX	AR	3422	-	0,6,6	0.00	-	-		
84	OHX	AR	3733	-	0,6,6	0.00	-	-		
84	OHX	1	3715	-	0,6,6	0.00	-	-		
84	OHX	AR	3589	-	0,6,6	0.00	-	-		
84	OHX	1	3710	-	0,6,6	0.00	-	-		
84	OHX	1	3556	-	0,6,6	0.00	-	-		
84	OHX	1	3549	-	0,6,6	0.00	-	-		
84	OHX	6	1970	-	0,6,6	0.00	-	-		
84	OHX	4	211	-	0,6,6	0.00	-	-		
84	OHX	1	3706	-	0,6,6	0.00	-	-		
84	OHX	1	3617	-	0,6,6	0.00	-	-		
84	OHX	1	3527	-	0,6,6	0.00	-	-		
84	OHX	1	3575	-	0,6,6	0.00	-	-		
84	OHX	1	3486	-	0,6,6	0.00	-	-		
84	OHX	AT	202	-	0,6,6	0.00	-	-		
84	OHX	AR	3612	-	0,6,6	0.00	-	-		
84	OHX	A	1920	-	0,6,6	0.00	-	-		
84	OHX	1	3541	-	0,6,6	0.00	-	-		
84	OHX	AR	3536	-	0,6,6	0.00	-	-		
84	OHX	h	401	-	0,6,6	0.00	-	-		
84	OHX	6	1998	-	0,6,6	0.00	-	-		
84	OHX	1	3435	-	0,6,6	0.00	-	-		
84	OHX	AR	3402	-	0,6,6	0.00	-	-		
84	OHX	6	2050	-	0,6,6	0.00	-	-		
84	OHX	AR	3524	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3447	-	0,6,6	0.00	-	-		
84	OHX	6	2015	-	0,6,6	0.00	-	-		
84	OHX	6	1972	-	0,6,6	0.00	-	-		
84	OHX	AR	3723	-	0,6,6	0.00	-	-		
84	OHX	1	3629	-	0,6,6	0.00	-	-		
84	OHX	AR	3401	-	0,6,6	0.00	-	-		
84	OHX	6	1989	-	0,6,6	0.00	-	-		
84	OHX	AR	3633	-	0,6,6	0.00	-	-		
84	OHX	1	3679	-	0,6,6	0.00	-	-		
84	OHX	6	1982	-	0,6,6	0.00	-	-		
84	OHX	A	1988	-	0,6,6	0.00	-	-		
84	OHX	4	212	-	0,6,6	0.00	-	-		
84	OHX	1	3676	-	0,6,6	0.00	-	-		
84	OHX	A	1977	-	0,6,6	0.00	-	-		
84	OHX	1	3443	-	0,6,6	0.00	-	-		
84	OHX	AR	3619	-	0,6,6	0.00	-	-		
84	OHX	6	2009	-	0,6,6	0.00	-	-		
84	OHX	1	3491	-	0,6,6	0.00	-	-		
84	OHX	1	3433	-	0,6,6	0.00	-	-		
84	OHX	3	209	-	0,6,6	0.00	-	-		
84	OHX	AR	3706	-	0,6,6	0.00	-	-		
84	OHX	AR	3648	-	0,6,6	0.00	-	-		
84	OHX	AR	3427	-	0,6,6	0.00	-	-		
84	OHX	1	3488	-	0,6,6	0.00	-	-		
84	OHX	1	3713	-	0,6,6	0.00	-	-		
84	OHX	A	2000	-	0,6,6	0.00	-	-		
84	OHX	6	1957	-	0,6,6	0.00	-	-		
84	OHX	AR	3494	-	0,6,6	0.00	-	-		
84	OHX	AS	203	-	0,6,6	0.00	-	-		
84	OHX	AR	3489	87	0,6,6	0.00	-	-		
84	OHX	6	2021	-	0,6,6	0.00	-	-		
84	OHX	6	2052	-	0,6,6	0.00	-	-		
84	OHX	AT	203	-	0,6,6	0.00	-	-		
84	OHX	A	1926	-	0,6,6	0.00	-	-		
84	OHX	A	2007	-	0,6,6	0.00	-	-		
84	OHX	AR	3547	-	0,6,6	0.00	-	-		
84	OHX	6	2011	-	0,6,6	0.00	-	-		
84	OHX	AR	3444	-	0,6,6	0.00	-	-		
84	OHX	1	3424	-	0,6,6	0.00	-	-		
84	OHX	AC	101	-	0,6,6	0.00	-	-		
84	OHX	AR	3731	-	0,6,6	0.00	-	-		
84	OHX	1	3648	-	0,6,6	0.00	-	-		
84	OHX	1	3649	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	A	1918	-	0,6,6	0.00	-	-		
84	OHX	A	1928	-	0,6,6	0.00	-	-		
84	OHX	AR	3481	-	0,6,6	0.00	-	-		
84	OHX	6	2010	-	0,6,6	0.00	-	-		
84	OHX	1	3440	-	0,6,6	0.00	-	-		
84	OHX	AR	3419	-	0,6,6	0.00	-	-		
84	OHX	4	205	-	0,6,6	0.00	-	-		
84	OHX	AR	3557	-	0,6,6	0.00	-	-		
84	OHX	6	2039	-	0,6,6	0.00	-	-		
84	OHX	AR	3676	-	0,6,6	0.00	-	-		
84	OHX	1	3620	-	0,6,6	0.00	-	-		
84	OHX	AR	3744	-	0,6,6	0.00	-	-		
84	OHX	1	3721	-	0,6,6	0.00	-	-		
84	OHX	1	3449	-	0,6,6	0.00	-	-		
84	OHX	1	3417	-	0,6,6	0.00	-	-		
84	OHX	1	3680	-	0,6,6	0.00	-	-		
84	OHX	AR	3475	-	0,6,6	0.00	-	-		
84	OHX	6	1977	-	0,6,6	0.00	-	-		
84	OHX	6	2035	-	0,6,6	0.00	-	-		
84	OHX	6	1927	-	0,6,6	0.00	-	-		
84	OHX	6	1922	-	0,6,6	0.00	-	-		
84	OHX	AR	3741	-	0,6,6	0.00	-	-		
84	OHX	AR	3566	-	0,6,6	0.00	-	-		
84	OHX	AR	3466	-	0,6,6	0.00	-	-		
84	OHX	A	1935	-	0,6,6	0.00	-	-		
84	OHX	r	301	-	0,6,6	0.00	-	-		
84	OHX	6	1993	-	0,6,6	0.00	-	-		
84	OHX	AT	207	-	0,6,6	0.00	-	-		
84	OHX	AR	3528	-	0,6,6	0.00	-	-		
84	OHX	A	1978	-	0,6,6	0.00	-	-		
84	OHX	1	3519	-	0,6,6	0.00	-	-		
84	OHX	AR	3438	-	0,6,6	0.00	-	-		
84	OHX	AR	3437	-	0,6,6	0.00	-	-		
84	OHX	AR	3563	-	0,6,6	0.00	-	-		
84	OHX	A	1962	-	0,6,6	0.00	-	-		
84	OHX	1	3512	-	0,6,6	0.00	-	-		
84	OHX	CF	402	-	0,6,6	0.00	-	-		
84	OHX	6	1925	-	0,6,6	0.00	-	-		
84	OHX	AR	3499	-	0,6,6	0.00	-	-		
84	OHX	AR	3720	-	0,6,6	0.00	-	-		
84	OHX	1	3638	-	0,6,6	0.00	-	-		
84	OHX	A	2021	-	0,6,6	0.00	-	-		
84	OHX	AR	3654	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3713	-	0,6,6	0.00	-	-		
84	OHX	1	3631	-	0,6,6	0.00	-	-		
84	OHX	1	3490	-	0,6,6	0.00	-	-		
87	GOL	AR	4261	1	5,5,5	0.14	0	5,5,5	0.33	0
84	OHX	A	1919	-	0,6,6	0.00	-	-		
84	OHX	1	3693	-	0,6,6	0.00	-	-		
84	OHX	1	3457	-	0,6,6	0.00	-	-		
84	OHX	1	3625	-	0,6,6	0.00	-	-		
84	OHX	AR	3680	-	0,6,6	0.00	-	-		
84	OHX	AR	3686	-	0,6,6	0.00	-	-		
84	OHX	A	2031	-	0,6,6	0.00	-	-		
84	OHX	AR	3504	-	0,6,6	0.00	-	-		
84	OHX	1	3401	-	0,6,6	0.00	-	-		
84	OHX	A	1913	-	0,6,6	0.00	-	-		
84	OHX	AR	3627	-	0,6,6	0.00	-	-		
84	OHX	A	1952	-	0,6,6	0.00	-	-		
84	OHX	A	1908	-	0,6,6	0.00	-	-		
84	OHX	6	1944	-	0,6,6	0.00	-	-		
84	OHX	3	201	-	0,6,6	0.00	-	-		
84	OHX	1	3442	-	0,6,6	0.00	-	-		
84	OHX	AR	3414	-	0,6,6	0.00	-	-		
84	OHX	AR	3531	-	0,6,6	0.00	-	-		
84	OHX	AR	3664	-	0,6,6	0.00	-	-		
84	OHX	1	3615	-	0,6,6	0.00	-	-		
84	OHX	1	3453	-	0,6,6	0.00	-	-		
84	OHX	A	1985	-	0,6,6	0.00	-	-		
84	OHX	c8	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3451	-	0,6,6	0.00	-	-		
84	OHX	AR	3596	-	0,6,6	0.00	-	-		
84	OHX	AR	3433	-	0,6,6	0.00	-	-		
84	OHX	AR	3530	-	0,6,6	0.00	-	-		
84	OHX	AR	3696	84	0,6,6	0.00	-	-		
84	OHX	A	1946	-	0,6,6	0.00	-	-		
84	OHX	1	3605	-	0,6,6	0.00	-	-		
84	OHX	AR	3483	-	0,6,6	0.00	-	-		
84	OHX	1	3666	-	0,6,6	0.00	-	-		
84	OHX	1	3524	-	0,6,6	0.00	-	-		
84	OHX	A	1947	-	0,6,6	0.00	-	-		
84	OHX	AR	3728	-	0,6,6	0.00	-	-		
84	OHX	1	3655	-	0,6,6	0.00	-	-		
84	OHX	6	2029	-	0,6,6	0.00	-	-		
84	OHX	6	1999	-	0,6,6	0.00	-	-		
84	OHX	A	2035	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3503	-	0,6,6	0.00	-	-		
84	OHX	1	3405	-	0,6,6	0.00	-	-		
84	OHX	AR	3448	-	0,6,6	0.00	-	-		
84	OHX	1	3480	-	0,6,6	0.00	-	-		
84	OHX	A	1994	-	0,6,6	0.00	-	-		
84	OHX	A	1927	-	0,6,6	0.00	-	-		
84	OHX	AR	3458	-	0,6,6	0.00	-	-		
84	OHX	AR	3640	-	0,6,6	0.00	-	-		
84	OHX	1	3580	-	0,6,6	0.00	-	-		
84	OHX	1	3608	-	0,6,6	0.00	-	-		
84	OHX	1	3660	-	0,6,6	0.00	-	-		
84	OHX	AR	3503	-	0,6,6	0.00	-	-		
84	OHX	6	2005	-	0,6,6	0.00	-	-		
84	OHX	1	3532	-	0,6,6	0.00	-	-		
84	OHX	A	1957	-	0,6,6	0.00	-	-		
84	OHX	A	1958	-	0,6,6	0.00	-	-		
84	OHX	1	3614	-	0,6,6	0.00	-	-		
84	OHX	AR	3585	-	0,6,6	0.00	-	-		
84	OHX	1	3654	-	0,6,6	0.00	-	-		
84	OHX	AR	3638	-	0,6,6	0.00	-	-		
84	OHX	6	1955	-	0,6,6	0.00	-	-		
84	OHX	AR	3709	-	0,6,6	0.00	-	-		
84	OHX	1	3601	-	0,6,6	0.00	-	-		
84	OHX	AR	3545	-	0,6,6	0.00	-	-		
84	OHX	A	1950	-	0,6,6	0.00	-	-		
84	OHX	3	204	-	0,6,6	0.00	-	-		
84	OHX	6	1986	-	0,6,6	0.00	-	-		
84	OHX	A	2036	-	0,6,6	0.00	-	-		
84	OHX	AR	3655	-	0,6,6	0.00	-	-		
84	OHX	1	3658	-	0,6,6	0.00	-	-		
84	OHX	AR	3579	-	0,6,6	0.00	-	-		
84	OHX	6	1990	-	0,6,6	0.00	-	-		
84	OHX	AR	3603	-	0,6,6	0.00	-	-		
84	OHX	1	3458	-	0,6,6	0.00	-	-		
84	OHX	A	1934	-	0,6,6	0.00	-	-		
84	OHX	AR	3502	-	0,6,6	0.00	-	-		
84	OHX	1	3561	-	0,6,6	0.00	-	-		
84	OHX	1	3613	-	0,6,6	0.00	-	-		
84	OHX	6	1912	-	0,6,6	0.00	-	-		
84	OHX	6	2036	-	0,6,6	0.00	-	-		
84	OHX	AT	204	-	0,6,6	0.00	-	-		
84	OHX	A	2009	-	0,6,6	0.00	-	-		
84	OHX	AR	3488	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3521	-	0,6,6	0.00	-	-		
84	OHX	1	3520	-	0,6,6	0.00	-	-		
84	OHX	1	3445	-	0,6,6	0.00	-	-		
84	OHX	AR	3484	-	0,6,6	0.00	-	-		
84	OHX	A	1922	-	0,6,6	0.00	-	-		
84	OHX	AR	3498	-	0,6,6	0.00	-	-		
84	OHX	AR	3424	-	0,6,6	0.00	-	-		
84	OHX	AR	3597	-	0,6,6	0.00	-	-		
84	OHX	1	3479	-	0,6,6	0.00	-	-		
84	OHX	1	3682	-	0,6,6	0.00	-	-		
84	OHX	AR	3452	-	0,6,6	0.00	-	-		
84	OHX	AR	3641	-	0,6,6	0.00	-	-		
84	OHX	AR	3573	-	0,6,6	0.00	-	-		
84	OHX	AR	3492	-	0,6,6	0.00	-	-		
84	OHX	1	3663	-	0,6,6	0.00	-	-		
84	OHX	AR	3623	-	0,6,6	0.00	-	-		
84	OHX	AR	3666	-	0,6,6	0.00	-	-		
84	OHX	AR	3409	-	0,6,6	0.00	-	-		
84	OHX	1	3642	-	0,6,6	0.00	-	-		
84	OHX	4	208	-	0,6,6	0.00	-	-		
84	OHX	AR	3404	-	0,6,6	0.00	-	-		
84	OHX	A	1998	-	0,6,6	0.00	-	-		
84	OHX	1	3567	-	0,6,6	0.00	-	-		
84	OHX	1	3492	-	0,6,6	0.00	-	-		
84	OHX	AR	3434	-	0,6,6	0.00	-	-		
84	OHX	AR	3592	-	0,6,6	0.00	-	-		
84	OHX	6	1917	-	0,6,6	0.00	-	-		
84	OHX	1	3588	-	0,6,6	0.00	-	-		
84	OHX	1	3582	-	0,6,6	0.00	-	-		
84	OHX	A	2010	-	0,6,6	0.00	-	-		
84	OHX	AR	3626	-	0,6,6	0.00	-	-		
84	OHX	AR	3449	-	0,6,6	0.00	-	-		
84	OHX	6	1926	-	0,6,6	0.00	-	-		
84	OHX	1	3531	-	0,6,6	0.00	-	-		
84	OHX	A	1974	-	0,6,6	0.00	-	-		
84	OHX	1	3419	-	0,6,6	0.00	-	-		
84	OHX	1	3543	-	0,6,6	0.00	-	-		
84	OHX	1	3454	-	0,6,6	0.00	-	-		
84	OHX	6	1971	-	0,6,6	0.00	-	-		
84	OHX	AR	3454	-	0,6,6	0.00	-	-		
84	OHX	A	1916	-	0,6,6	0.00	-	-		
84	OHX	AR	3546	-	0,6,6	0.00	-	-		
84	OHX	6	1901	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	1904	-	0,6,6	0.00	-	-		
84	OHX	A	2040	-	0,6,6	0.00	-	-		
84	OHX	A	1921	-	0,6,6	0.00	-	-		
84	OHX	3	203	-	0,6,6	0.00	-	-		
84	OHX	AR	3417	-	0,6,6	0.00	-	-		
84	OHX	A	2017	-	0,6,6	0.00	-	-		
84	OHX	6	2024	-	0,6,6	0.00	-	-		
84	OHX	AR	3617	-	0,6,6	0.00	-	-		
84	OHX	AR	3643	-	0,6,6	0.00	-	-		
84	OHX	AR	3677	-	0,6,6	0.00	-	-		
84	OHX	1	3590	-	0,6,6	0.00	-	-		
84	OHX	1	3533	-	0,6,6	0.00	-	-		
84	OHX	A	1972	-	0,6,6	0.00	-	-		
84	OHX	A	1960	-	0,6,6	0.00	-	-		
84	OHX	AR	3601	-	0,6,6	0.00	-	-		
84	OHX	A	1938	-	0,6,6	0.00	-	-		
84	OHX	AR	3410	-	0,6,6	0.00	-	-		
84	OHX	A	2011	-	0,6,6	0.00	-	-		
84	OHX	AR	3739	-	0,6,6	0.00	-	-		
84	OHX	AR	3532	-	0,6,6	0.00	-	-		
84	OHX	6	1946	-	0,6,6	0.00	-	-		
84	OHX	AR	3736	-	0,6,6	0.00	-	-		
84	OHX	AR	3537	-	0,6,6	0.00	-	-		
84	OHX	A	1995	-	0,6,6	0.00	-	-		
84	OHX	AR	3608	-	0,6,6	0.00	-	-		
84	OHX	c1	201	-	0,6,6	0.00	-	-		
84	OHX	AS	206	-	0,6,6	0.00	-	-		
84	OHX	x	201	-	0,6,6	0.00	-	-		
84	OHX	1	3428	-	0,6,6	0.00	-	-		
84	OHX	1	3600	-	0,6,6	0.00	-	-		
84	OHX	AR	3730	-	0,6,6	0.00	-	-		
84	OHX	4	203	-	0,6,6	0.00	-	-		
84	OHX	6	1979	-	0,6,6	0.00	-	-		
84	OHX	AR	3657	-	0,6,6	0.00	-	-		
84	OHX	A	1984	-	0,6,6	0.00	-	-		
84	OHX	AR	3628	-	0,6,6	0.00	-	-		
84	OHX	AR	3652	-	0,6,6	0.00	-	-		
84	OHX	A	1959	-	0,6,6	0.00	-	-		
84	OHX	AS	205	-	0,6,6	0.00	-	-		
84	OHX	A	1949	-	0,6,6	0.00	-	-		
84	OHX	A	1903	-	0,6,6	0.00	-	-		
84	OHX	AR	3734	-	0,6,6	0.00	-	-		
84	OHX	1	3577	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3559	-	0,6,6	0.00	-	-		
84	OHX	1	3594	-	0,6,6	0.00	-	-		
84	OHX	AR	3609	-	0,6,6	0.00	-	-		
84	OHX	AR	3702	-	0,6,6	0.00	-	-		
84	OHX	1	3403	-	0,6,6	0.00	-	-		
84	OHX	1	3540	-	0,6,6	0.00	-	-		
84	OHX	A	1905	-	0,6,6	0.00	-	-		
84	OHX	A	2028	-	0,6,6	0.00	-	-		
84	OHX	AR	3517	-	0,6,6	0.00	-	-		
84	OHX	1	3570	-	0,6,6	0.00	-	-		
84	OHX	1	3407	-	0,6,6	0.00	-	-		
84	OHX	AR	3407	-	0,6,6	0.00	-	-		
84	OHX	6	2018	-	0,6,6	0.00	-	-		
84	OHX	AR	3473	-	0,6,6	0.00	-	-		
84	OHX	DQ	201	-	0,6,6	0.00	-	-		
84	OHX	1	3472	-	0,6,6	0.00	-	-		
84	OHX	1	3477	-	0,6,6	0.00	-	-		
84	OHX	1	3696	-	0,6,6	0.00	-	-		
84	OHX	AR	3689	-	0,6,6	0.00	-	-		
84	OHX	AT	209	-	0,6,6	0.00	-	-		
84	OHX	sR	401	-	0,6,6	0.00	-	-		
84	OHX	1	3537	-	0,6,6	0.00	-	-		
84	OHX	A	1911	-	0,6,6	0.00	-	-		
84	OHX	A	1914	-	0,6,6	0.00	-	-		
84	OHX	AR	3558	-	0,6,6	0.00	-	-		
84	OHX	A	2003	-	0,6,6	0.00	-	-		
84	OHX	AR	3425	-	0,6,6	0.00	-	-		
84	OHX	1	3498	-	0,6,6	0.00	-	-		
84	OHX	AR	3506	-	0,6,6	0.00	-	-		
84	OHX	AR	3590	-	0,6,6	0.00	-	-		
84	OHX	1	3677	-	0,6,6	0.00	-	-		
84	OHX	AR	3658	-	0,6,6	0.00	-	-		
84	OHX	AR	3582	-	0,6,6	0.00	-	-		
84	OHX	A	1933	-	0,6,6	0.00	-	-		
84	OHX	1	3485	-	0,6,6	0.00	-	-		
84	OHX	1	3618	-	0,6,6	0.00	-	-		
84	OHX	6	1960	-	0,6,6	0.00	-	-		
84	OHX	AR	3561	-	0,6,6	0.00	-	-		
84	OHX	6	2046	-	0,6,6	0.00	-	-		
84	OHX	AR	3457	-	0,6,6	0.00	-	-		
84	OHX	AR	3745	-	0,6,6	0.00	-	-		
84	OHX	1	3644	-	0,6,6	0.00	-	-		
84	OHX	1	3404	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3455	-	0,6,6	0.00	-	-		
84	OHX	AR	3418	-	0,6,6	0.00	-	-		
84	OHX	AR	3428	-	0,6,6	0.00	-	-		
84	OHX	z	201	-	0,6,6	0.00	-	-		
84	OHX	6	1947	-	0,6,6	0.00	-	-		
84	OHX	AR	3737	-	0,6,6	0.00	-	-		
84	OHX	A	2006	-	0,6,6	0.00	-	-		
84	OHX	1	3425	-	0,6,6	0.00	-	-		
84	OHX	1	3589	-	0,6,6	0.00	-	-		
84	OHX	AT	210	-	0,6,6	0.00	-	-		
84	OHX	A	1966	-	0,6,6	0.00	-	-		
84	OHX	1	3406	-	0,6,6	0.00	-	-		
84	OHX	1	3518	-	0,6,6	0.00	-	-		
84	OHX	AR	3743	-	0,6,6	0.00	-	-		
84	OHX	A	1929	-	0,6,6	0.00	-	-		
84	OHX	6	2032	-	0,6,6	0.00	-	-		
84	OHX	AR	3604	-	0,6,6	0.00	-	-		
87	GOL	A	2160	-	5,5,5	0.10	0	5,5,5	0.29	0
84	OHX	1	3702	-	0,6,6	0.00	-	-		
84	OHX	AR	3724	-	0,6,6	0.00	-	-		
84	OHX	1	3708	-	0,6,6	0.00	-	-		
84	OHX	6	2016	-	0,6,6	0.00	-	-		
84	OHX	6	1920	-	0,6,6	0.00	-	-		
84	OHX	A	2039	-	0,6,6	0.00	-	-		
84	OHX	1	3673	-	0,6,6	0.00	-	-		
84	OHX	1	3446	-	0,6,6	0.00	-	-		
84	OHX	1	3448	-	0,6,6	0.00	-	-		
84	OHX	6	1956	-	0,6,6	0.00	-	-		
84	OHX	1	3611	-	0,6,6	0.00	-	-		
84	OHX	y	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3602	-	0,6,6	0.00	-	-		
84	OHX	AR	3541	-	0,6,6	0.00	-	-		
84	OHX	A	2014	-	0,6,6	0.00	-	-		
84	OHX	1	3657	-	0,6,6	0.00	-	-		
84	OHX	1	3502	-	0,6,6	0.00	-	-		
84	OHX	1	3659	-	0,6,6	0.00	-	-		
84	OHX	AR	3550	-	0,6,6	0.00	-	-		
84	OHX	1	3460	-	0,6,6	0.00	-	-		
84	OHX	6	2048	-	0,6,6	0.00	-	-		
84	OHX	6	1978	-	0,6,6	0.00	-	-		
84	OHX	A	1930	-	0,6,6	0.00	-	-		
84	OHX	6	2028	-	0,6,6	0.00	-	-		
84	OHX	1	3661	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3727	-	0,6,6	0.00	-	-		
84	OHX	A	1975	-	0,6,6	0.00	-	-		
84	OHX	AR	3722	-	0,6,6	0.00	-	-		
84	OHX	1	3427	-	0,6,6	0.00	-	-		
84	OHX	1	3690	-	0,6,6	0.00	-	-		
84	OHX	6	1965	-	0,6,6	0.00	-	-		
84	OHX	1	3705	-	0,6,6	0.00	-	-		
84	OHX	1	3602	-	0,6,6	0.00	-	-		
84	OHX	AR	3415	-	0,6,6	0.00	-	-		
84	OHX	AR	3634	-	0,6,6	0.00	-	-		
84	OHX	6	2003	-	0,6,6	0.00	-	-		
84	OHX	1	3553	-	0,6,6	0.00	-	-		
84	OHX	AR	3659	-	0,6,6	0.00	-	-		
84	OHX	AR	3465	-	0,6,6	0.00	-	-		
84	OHX	1	3510	-	0,6,6	0.00	-	-		
84	OHX	A	2005	-	0,6,6	0.00	-	-		
84	OHX	1	3603	-	0,6,6	0.00	-	-		
84	OHX	1	3628	-	0,6,6	0.00	-	-		
84	OHX	AR	3673	-	0,6,6	0.00	-	-		
84	OHX	1	3411	-	0,6,6	0.00	-	-		
84	OHX	6	1935	-	0,6,6	0.00	-	-		
84	OHX	6	2049	-	0,6,6	0.00	-	-		
84	OHX	AR	3629	-	0,6,6	0.00	-	-		
84	OHX	AR	3470	-	0,6,6	0.00	-	-		
84	OHX	CX	202	-	0,6,6	0.00	-	-		
84	OHX	4	206	-	0,6,6	0.00	-	-		
84	OHX	A	2032	-	0,6,6	0.00	-	-		
84	OHX	AR	3688	-	0,6,6	0.00	-	-		
84	OHX	1	3685	-	0,6,6	0.00	-	-		
84	OHX	1	3635	-	0,6,6	0.00	-	-		
84	OHX	A	1940	-	0,6,6	0.00	-	-		
84	OHX	1	3596	-	0,6,6	0.00	-	-		
84	OHX	1	3434	-	0,6,6	0.00	-	-		
84	OHX	AR	3625	-	0,6,6	0.00	-	-		
84	OHX	A	1906	-	0,6,6	0.00	-	-		
84	OHX	1	3465	-	0,6,6	0.00	-	-		
84	OHX	A	1967	-	0,6,6	0.00	-	-		
84	OHX	AR	3615	-	0,6,6	0.00	-	-		
84	OHX	1	3422	-	0,6,6	0.00	-	-		
84	OHX	CK	201	-	0,6,6	0.00	-	-		
84	OHX	1	3511	-	0,6,6	0.00	-	-		
84	OHX	1	3634	-	0,6,6	0.00	-	-		
84	OHX	1	3578	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3712	-	0,6,6	0.00	-	-		
84	OHX	6	1980	-	0,6,6	0.00	-	-		
84	OHX	1	3724	-	0,6,6	0.00	-	-		
84	OHX	1	3627	-	0,6,6	0.00	-	-		
84	OHX	1	3463	-	0,6,6	0.00	-	-		
84	OHX	AR	3717	-	0,6,6	0.00	-	-		
84	OHX	6	2012	-	0,6,6	0.00	-	-		
84	OHX	AR	3556	-	0,6,6	0.00	-	-		
86	HN8	1	4223	-	24,26,26	0.28	0	36,41,41	1.03	2 (5%)
84	OHX	AR	3525	-	0,6,6	0.00	-	-		
84	OHX	AR	3513	-	0,6,6	0.00	-	-		
84	OHX	T	201	-	0,6,6	0.00	-	-		
84	OHX	6	1962	-	0,6,6	0.00	-	-		
84	OHX	1	3568	-	0,6,6	0.00	-	-		
84	OHX	6	2045	-	0,6,6	0.00	-	-		
84	OHX	AR	3692	-	0,6,6	0.00	-	-		
84	OHX	6	1996	-	0,6,6	0.00	-	-		
84	OHX	AR	3560	-	0,6,6	0.00	-	-		
84	OHX	AR	3526	-	0,6,6	0.00	-	-		
84	OHX	A	2018	-	0,6,6	0.00	-	-		
84	OHX	6	1984	-	0,6,6	0.00	-	-		
84	OHX	A	1992	-	0,6,6	0.00	-	-		
84	OHX	AR	3514	-	0,6,6	0.00	-	-		
84	OHX	1	3723	1	0,6,6	0.00	-	-		
84	OHX	AR	3660	-	0,6,6	0.00	-	-		
84	OHX	6	2004	-	0,6,6	0.00	-	-		
84	OHX	AR	3446	-	0,6,6	0.00	-	-		
84	OHX	2	201	-	0,6,6	0.00	-	-		
84	OHX	4	214	-	0,6,6	0.00	-	-		
84	OHX	6	1909	-	0,6,6	0.00	-	-		
84	OHX	A	2004	-	0,6,6	0.00	-	-		
84	OHX	AR	3685	-	0,6,6	0.00	-	-		
84	OHX	AR	3716	-	0,6,6	0.00	-	-		
84	OHX	AR	3539	-	0,6,6	0.00	-	-		
84	OHX	AR	3497	-	0,6,6	0.00	-	-		
84	OHX	1	3410	-	0,6,6	0.00	-	-		
84	OHX	6	1932	-	0,6,6	0.00	-	-		
84	OHX	AR	3519	-	0,6,6	0.00	-	-		
84	OHX	s8	301	-	0,6,6	0.00	-	-		
84	OHX	1	3468	-	0,6,6	0.00	-	-		
84	OHX	6	1903	-	0,6,6	0.00	-	-		
84	OHX	AT	213	-	0,6,6	0.00	-	-		
84	OHX	CF	401	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	1914	-	0,6,6	0.00	-	-		
84	OHX	AR	3491	-	0,6,6	0.00	-	-		
84	OHX	6	1953	-	0,6,6	0.00	-	-		
84	OHX	AR	3616	-	0,6,6	0.00	-	-		
84	OHX	6	1949	-	0,6,6	0.00	-	-		
84	OHX	3	202	-	0,6,6	0.00	-	-		
84	OHX	CE	401	-	0,6,6	0.00	-	-		
84	OHX	6	1987	-	0,6,6	0.00	-	-		
84	OHX	x	202	-	0,6,6	0.00	-	-		
84	OHX	6	1915	-	0,6,6	0.00	-	-		
84	OHX	6	2037	-	0,6,6	0.00	-	-		
84	OHX	AR	3671	-	0,6,6	0.00	-	-		
84	OHX	1	3598	-	0,6,6	0.00	-	-		
84	OHX	1	3645	-	0,6,6	0.00	-	-		
84	OHX	1	3694	-	0,6,6	0.00	-	-		
84	OHX	A	1954	-	0,6,6	0.00	-	-		
84	OHX	c3	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3570	-	0,6,6	0.00	-	-		
84	OHX	AR	3614	-	0,6,6	0.00	-	-		
84	OHX	1	3674	-	0,6,6	0.00	-	-		
84	OHX	1	3444	-	0,6,6	0.00	-	-		
84	OHX	AR	3698	-	0,6,6	0.00	-	-		
84	OHX	A	2008	-	0,6,6	0.00	-	-		
84	OHX	A	2023	-	0,6,6	0.00	-	-		
84	OHX	1	3586	-	0,6,6	0.00	-	-		
84	OHX	A	1942	-	0,6,6	0.00	-	-		
84	OHX	AR	3647	-	0,6,6	0.00	-	-		
84	OHX	AS	201	-	0,6,6	0.00	-	-		
84	OHX	A	1924	-	0,6,6	0.00	-	-		
84	OHX	A	2012	-	0,6,6	0.00	-	-		
84	OHX	1	3646	-	0,6,6	0.00	-	-		
84	OHX	1	3508	-	0,6,6	0.00	-	-		
84	OHX	4	209	-	0,6,6	0.00	-	-		
84	OHX	6	1976	-	0,6,6	0.00	-	-		
84	OHX	AR	3707	-	0,6,6	0.00	-	-		
84	OHX	6	1973	-	0,6,6	0.00	-	-		
84	OHX	1	3459	-	0,6,6	0.00	-	-		
84	OHX	AR	3462	-	0,6,6	0.00	-	-		
84	OHX	A	1991	-	0,6,6	0.00	-	-		
84	OHX	AR	3593	-	0,6,6	0.00	-	-		
84	OHX	A	1904	-	0,6,6	0.00	-	-		
84	OHX	AR	3455	-	0,6,6	0.00	-	-		
84	OHX	A	1909	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	2041	-	0,6,6	0.00	-	-		
84	OHX	AR	3490	-	0,6,6	0.00	-	-		
84	OHX	AT	208	-	0,6,6	0.00	-	-		
84	OHX	4	215	-	0,6,6	0.00	-	-		
84	OHX	AR	3429	-	0,6,6	0.00	-	-		
84	OHX	AR	3644	-	0,6,6	0.00	-	-		
84	OHX	1	3656	-	0,6,6	0.00	-	-		
84	OHX	6	1942	-	0,6,6	0.00	-	-		
84	OHX	AR	3459	-	0,6,6	0.00	-	-		
84	OHX	CG	302	-	0,6,6	0.00	-	-		
84	OHX	6	2023	-	0,6,6	0.00	-	-		
84	OHX	1	3555	-	0,6,6	0.00	-	-		
84	OHX	6	1974	-	0,6,6	0.00	-	-		
84	OHX	AR	3584	-	0,6,6	0.00	-	-		
84	OHX	6	2022	-	0,6,6	0.00	-	-		
84	OHX	AR	3564	-	0,6,6	0.00	-	-		
84	OHX	CE	402	-	0,6,6	0.00	-	-		
84	OHX	1	3697	84	0,6,6	0.00	-	-		
84	OHX	6	1975	-	0,6,6	0.00	-	-		
84	OHX	6	1959	-	0,6,6	0.00	-	-		
84	OHX	A	1993	-	0,6,6	0.00	-	-		
84	OHX	AR	3595	-	0,6,6	0.00	-	-		
84	OHX	AR	3508	-	0,6,6	0.00	-	-		
84	OHX	1	3471	-	0,6,6	0.00	-	-		
84	OHX	1	3474	-	0,6,6	0.00	-	-		
84	OHX	AR	3432	-	0,6,6	0.00	-	-		
84	OHX	1	3552	-	0,6,6	0.00	-	-		
84	OHX	1	3579	-	0,6,6	0.00	-	-		
84	OHX	1	3636	-	0,6,6	0.00	-	-		
84	OHX	1	3633	-	0,6,6	0.00	-	-		
84	OHX	6	1991	-	0,6,6	0.00	-	-		
84	OHX	A	2041	-	0,6,6	0.00	-	-		
84	OHX	A	1987	-	0,6,6	0.00	-	-		
84	OHX	AR	3580	-	0,6,6	0.00	-	-		
84	OHX	AR	3740	-	0,6,6	0.00	-	-		
84	OHX	1	3461	-	0,6,6	0.00	-	-		
84	OHX	1	3547	-	0,6,6	0.00	-	-		
84	OHX	6	1902	-	0,6,6	0.00	-	-		
84	OHX	6	1916	-	0,6,6	0.00	-	-		
84	OHX	A	1996	-	0,6,6	0.00	-	-		
84	OHX	AS	204	-	0,6,6	0.00	-	-		
84	OHX	AR	3668	-	0,6,6	0.00	-	-		
84	OHX	A	1932	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3429	-	0,6,6	0.00	-	-		
84	OHX	AR	3442	-	0,6,6	0.00	-	-		
84	OHX	1	3652	-	0,6,6	0.00	-	-		
84	OHX	AR	3576	-	0,6,6	0.00	-	-		
84	OHX	AR	3474	-	0,6,6	0.00	-	-		
84	OHX	AR	3478	-	0,6,6	0.00	-	-		
84	OHX	6	1907	-	0,6,6	0.00	-	-		
84	OHX	1	3647	-	0,6,6	0.00	-	-		
84	OHX	1	3707	-	0,6,6	0.00	-	-		
84	OHX	AR	3405	-	0,6,6	0.00	-	-		
84	OHX	6	1921	-	0,6,6	0.00	-	-		
84	OHX	A	1976	-	0,6,6	0.00	-	-		
84	OHX	1	3562	-	0,6,6	0.00	-	-		
84	OHX	AR	3453	-	0,6,6	0.00	-	-		
84	OHX	AR	3694	-	0,6,6	0.00	-	-		
84	OHX	1	3509	-	0,6,6	0.00	-	-		
84	OHX	1	3703	-	0,6,6	0.00	-	-		
84	OHX	1	3481	-	0,6,6	0.00	-	-		
84	OHX	AR	3408	-	0,6,6	0.00	-	-		
84	OHX	AR	3649	-	0,6,6	0.00	-	-		
84	OHX	1	3522	-	0,6,6	0.00	-	-		
84	OHX	AR	3463	-	0,6,6	0.00	-	-		
84	OHX	AR	3567	-	0,6,6	0.00	-	-		
84	OHX	6	2043	-	0,6,6	0.00	-	-		
84	OHX	AR	3732	-	0,6,6	0.00	-	-		
84	OHX	AR	3518	-	0,6,6	0.00	-	-		
84	OHX	AR	3574	-	0,6,6	0.00	-	-		
84	OHX	AR	3472	-	0,6,6	0.00	-	-		
84	OHX	1	3607	-	0,6,6	0.00	-	-		
84	OHX	AR	3411	-	0,6,6	0.00	-	-		
84	OHX	1	3515	-	0,6,6	0.00	-	-		
84	OHX	1	3478	-	0,6,6	0.00	-	-		
84	OHX	AR	3701	-	0,6,6	0.00	-	-		
84	OHX	AR	3501	-	0,6,6	0.00	-	-		
84	OHX	AR	3469	-	0,6,6	0.00	-	-		
84	OHX	6	1929	-	0,6,6	0.00	-	-		
84	OHX	AR	3632	-	0,6,6	0.00	-	-		
84	OHX	A	1997	-	0,6,6	0.00	-	-		
84	OHX	l	401	-	0,6,6	0.00	-	-		
84	OHX	1	3640	-	0,6,6	0.00	-	-		
84	OHX	1	3704	-	0,6,6	0.00	-	-		
84	OHX	A	1910	-	0,6,6	0.00	-	-		
84	OHX	1	3483	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	A	2015	-	0,6,6	0.00	-	-		
84	OHX	AR	3651	-	0,6,6	0.00	-	-		
84	OHX	AR	3613	-	0,6,6	0.00	-	-		
84	OHX	1	3591	-	0,6,6	0.00	-	-		
84	OHX	1	3507	-	0,6,6	0.00	-	-		
84	OHX	M	201	-	0,6,6	0.00	-	-		
84	OHX	1	3719	-	0,6,6	0.00	-	-		
84	OHX	A	1912	-	0,6,6	0.00	-	-		
84	OHX	AR	3549	-	0,6,6	0.00	-	-		
84	OHX	6	1958	-	0,6,6	0.00	-	-		
84	OHX	AS	210	-	0,6,6	0.00	-	-		
84	OHX	A	1982	-	0,6,6	0.00	-	-		
84	OHX	AT	212	-	0,6,6	0.00	-	-		
84	OHX	AR	3581	-	0,6,6	0.00	-	-		
84	OHX	A	1939	-	0,6,6	0.00	-	-		
84	OHX	6	1985	-	0,6,6	0.00	-	-		
84	OHX	1	3564	-	0,6,6	0.00	-	-		
84	OHX	1	3467	-	0,6,6	0.00	-	-		
84	OHX	1	3688	-	0,6,6	0.00	-	-		
84	OHX	AR	3500	-	0,6,6	0.00	-	-		
84	OHX	1	3597	-	0,6,6	0.00	-	-		
84	OHX	A	1901	-	0,6,6	0.00	-	-		
84	OHX	6	1997	-	0,6,6	0.00	-	-		
84	OHX	1	3495	-	0,6,6	0.00	-	-		
84	OHX	A	1981	-	0,6,6	0.00	-	-		
84	OHX	6	2027	-	0,6,6	0.00	-	-		
84	OHX	1	3439	-	0,6,6	0.00	-	-		
84	OHX	A	2019	-	0,6,6	0.00	-	-		
84	OHX	1	3402	-	0,6,6	0.00	-	-		
84	OHX	1	3689	-	0,6,6	0.00	-	-		
84	OHX	6	2038	-	0,6,6	0.00	-	-		
84	OHX	AR	3507	-	0,6,6	0.00	-	-		
84	OHX	1	3470	-	0,6,6	0.00	-	-		
84	OHX	6	1995	-	0,6,6	0.00	-	-		
84	OHX	AT	211	-	0,6,6	0.00	-	-		
84	OHX	AR	3412	-	0,6,6	0.00	-	-		
86	HN8	AR	4263	-	24,26,26	0.29	0	36,41,41	1.60	4 (11%)
84	OHX	AS	211	-	0,6,6	0.00	-	-		
84	OHX	A	1961	-	0,6,6	0.00	-	-		
84	OHX	AR	3523	-	0,6,6	0.00	-	-		
84	OHX	AR	3667	-	0,6,6	0.00	-	-		
84	OHX	6	2019	-	0,6,6	0.00	-	-		
84	OHX	6	2017	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3571	-	0,6,6	0.00	-	-		
84	OHX	AR	3435	-	0,6,6	0.00	-	-		
84	OHX	1	3592	-	0,6,6	0.00	-	-		
84	OHX	1	3621	-	0,6,6	0.00	-	-		
84	OHX	AR	3708	-	0,6,6	0.00	-	-		
84	OHX	AR	3703	-	0,6,6	0.00	-	-		
84	OHX	AT	201	-	0,6,6	0.00	-	-		
84	OHX	CX	201	-	0,6,6	0.00	-	-		
84	OHX	6	2051	-	0,6,6	0.00	-	-		
87	GOL	v	305	-	5,5,5	0.18	0	5,5,5	0.54	0
84	OHX	AR	3715	-	0,6,6	0.00	-	-		
84	OHX	A	2043	-	0,6,6	0.00	-	-		
84	OHX	A	2022	-	0,6,6	0.00	-	-		
84	OHX	1	3551	-	0,6,6	0.00	-	-		
84	OHX	AR	3551	-	0,6,6	0.00	-	-		
84	OHX	1	3584	-	0,6,6	0.00	-	-		
84	OHX	6	2002	-	0,6,6	0.00	-	-		
84	OHX	6	1924	-	0,6,6	0.00	-	-		
84	OHX	J	301	-	0,6,6	0.00	-	-		
84	OHX	1	3548	-	0,6,6	0.00	-	-		
84	OHX	6	2013	-	0,6,6	0.00	-	-		
84	OHX	1	3513	-	0,6,6	0.00	-	-		
84	OHX	AR	3496	-	0,6,6	0.00	-	-		
84	OHX	1	3695	-	0,6,6	0.00	-	-		
84	OHX	AR	3420	-	0,6,6	0.00	-	-		
84	OHX	AR	3544	-	0,6,6	0.00	-	-		
84	OHX	AT	206	-	0,6,6	0.00	-	-		
84	OHX	AR	3443	-	0,6,6	0.00	-	-		
84	OHX	1	3604	-	0,6,6	0.00	-	-		
84	OHX	1	3530	-	0,6,6	0.00	-	-		
84	OHX	1	3672	-	0,6,6	0.00	-	-		
84	OHX	1	3678	-	0,6,6	0.00	-	-		
84	OHX	6	1933	-	0,6,6	0.00	-	-		
84	OHX	6	1918	-	0,6,6	0.00	-	-		
84	OHX	1	3408	-	0,6,6	0.00	-	-		
84	OHX	1	3438	-	0,6,6	0.00	-	-		
84	OHX	1	3583	-	0,6,6	0.00	-	-		
84	OHX	1	3499	-	0,6,6	0.00	-	-		
84	OHX	6	1923	-	0,6,6	0.00	-	-		
84	OHX	AR	3441	-	0,6,6	0.00	-	-		
84	OHX	AR	3679	-	0,6,6	0.00	-	-		
84	OHX	AR	3456	-	0,6,6	0.00	-	-		
84	OHX	c5	201	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3533	-	0,6,6	0.00	-	-		
84	OHX	AR	3482	-	0,6,6	0.00	-	-		
84	OHX	1	3432	-	0,6,6	0.00	-	-		
84	OHX	AR	3543	-	0,6,6	0.00	-	-		
84	OHX	AR	3600	-	0,6,6	0.00	-	-		
84	OHX	1	3464	-	0,6,6	0.00	-	-		
84	OHX	AR	3682	-	0,6,6	0.00	-	-		
84	OHX	4	210	-	0,6,6	0.00	-	-		
84	OHX	6	2034	-	0,6,6	0.00	-	-		
84	OHX	1	3554	-	0,6,6	0.00	-	-		
84	OHX	1	3610	-	0,6,6	0.00	-	-		
84	OHX	A	1980	-	0,6,6	0.00	-	-		
84	OHX	AR	3663	-	0,6,6	0.00	-	-		
84	OHX	AR	3493	-	0,6,6	0.00	-	-		
84	OHX	1	3505	-	0,6,6	0.00	-	-		
84	OHX	1	3585	-	0,6,6	0.00	-	-		
84	OHX	AH	201	-	0,6,6	0.00	-	-		
84	OHX	6	2042	-	0,6,6	0.00	-	-		
84	OHX	AR	3587	-	0,6,6	0.00	-	-		
84	OHX	AR	3650	-	0,6,6	0.00	-	-		
84	OHX	AR	3721	-	0,6,6	0.00	-	-		
84	OHX	AR	3586	-	0,6,6	0.00	-	-		
84	OHX	AR	3718	-	0,6,6	0.00	-	-		
84	OHX	AR	3565	-	0,6,6	0.00	-	-		
84	OHX	A	2013	-	0,6,6	0.00	-	-		
84	OHX	6	2033	-	0,6,6	0.00	-	-		
84	OHX	1	3462	-	0,6,6	0.00	-	-		
84	OHX	AR	3516	-	0,6,6	0.00	-	-		
84	OHX	6	1967	-	0,6,6	0.00	-	-		
84	OHX	AR	3690	-	0,6,6	0.00	-	-		
84	OHX	AR	3725	-	0,6,6	0.00	-	-		
84	OHX	AR	3520	-	0,6,6	0.00	-	-		
84	OHX	AR	3486	-	0,6,6	0.00	-	-		
84	OHX	6	1908	-	0,6,6	0.00	-	-		
84	OHX	K	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3630	-	0,6,6	0.00	-	-		
84	OHX	AR	3534	-	0,6,6	0.00	-	-		
84	OHX	1	3565	-	0,6,6	0.00	-	-		
84	OHX	AR	3738	-	0,6,6	0.00	-	-		
84	OHX	AR	3431	-	0,6,6	0.00	-	-		
84	OHX	6	2044	-	0,6,6	0.00	-	-		
84	OHX	1	3558	-	0,6,6	0.00	-	-		
84	OHX	1	3670	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3687	-	0,6,6	0.00	-	-		
84	OHX	1	3711	-	0,6,6	0.00	-	-		
84	OHX	6	1948	-	0,6,6	0.00	-	-		
84	OHX	1	3476	-	0,6,6	0.00	-	-		
84	OHX	6	2000	-	0,6,6	0.00	-	-		
84	OHX	AR	3697	-	0,6,6	0.00	-	-		
84	OHX	1	3529	-	0,6,6	0.00	-	-		
84	OHX	A	1944	-	0,6,6	0.00	-	-		
84	OHX	6	1945	-	0,6,6	0.00	-	-		
84	OHX	1	3609	-	0,6,6	0.00	-	-		
84	OHX	6	1966	-	0,6,6	0.00	-	-		
84	OHX	1	3662	-	0,6,6	0.00	-	-		
84	OHX	1	3595	-	0,6,6	0.00	-	-		
84	OHX	AR	3599	-	0,6,6	0.00	-	-		
84	OHX	A	2027	-	0,6,6	0.00	-	-		
84	OHX	d9	101	-	0,6,6	0.00	-	-		
84	OHX	O	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3555	-	0,6,6	0.00	-	-		
84	OHX	1	3698	-	0,6,6	0.00	-	-		
84	OHX	6	2008	-	0,6,6	0.00	-	-		
84	OHX	AR	3521	-	0,6,6	0.00	-	-		
84	OHX	AR	3505	-	0,6,6	0.00	-	-		
84	OHX	AR	3726	-	0,6,6	0.00	-	-		
84	OHX	1	3496	-	0,6,6	0.00	-	-		
84	OHX	AR	3416	-	0,6,6	0.00	-	-		
84	OHX	AR	3552	-	0,6,6	0.00	-	-		
84	OHX	1	3523	-	0,6,6	0.00	-	-		
84	OHX	CP	501	-	0,6,6	0.00	-	-		
84	OHX	1	3550	-	0,6,6	0.00	-	-		
84	OHX	6	1939	-	0,6,6	0.00	-	-		
84	OHX	AR	3464	-	0,6,6	0.00	-	-		
84	OHX	A	1923	-	0,6,6	0.00	-	-		
84	OHX	1	3413	-	0,6,6	0.00	-	-		
84	OHX	AR	3678	-	0,6,6	0.00	-	-		
84	OHX	AR	3450	-	0,6,6	0.00	-	-		
84	OHX	6	1951	-	0,6,6	0.00	-	-		
84	OHX	AR	3674	-	0,6,6	0.00	-	-		
84	OHX	1	3517	-	0,6,6	0.00	-	-		
84	OHX	1	3416	-	0,6,6	0.00	-	-		
84	OHX	AR	3467	-	0,6,6	0.00	-	-		
84	OHX	1	3431	-	0,6,6	0.00	-	-		
84	OHX	6	1969	-	0,6,6	0.00	-	-		
84	OHX	1	3560	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	4	201	-	0,6,6	0.00	-	-		
84	OHX	AT	216	-	0,6,6	0.00	-	-		
84	OHX	AR	3510	-	0,6,6	0.00	-	-		
84	OHX	1	3599	-	0,6,6	0.00	-	-		
84	OHX	AR	3511	-	0,6,6	0.00	-	-		
84	OHX	AR	3681	-	0,6,6	0.00	-	-		
84	OHX	AM	101	-	0,6,6	0.00	-	-		
84	OHX	AR	3653	-	0,6,6	0.00	-	-		
84	OHX	1	3482	-	0,6,6	0.00	-	-		
84	OHX	1	3487	-	0,6,6	0.00	-	-		
84	OHX	A	1965	-	0,6,6	0.00	-	-		
84	OHX	1	3569	-	0,6,6	0.00	-	-		
84	OHX	AR	3439	-	0,6,6	0.00	-	-		
84	OHX	A	1925	-	0,6,6	0.00	-	-		
84	OHX	1	3714	-	0,6,6	0.00	-	-		
84	OHX	6	2020	-	0,6,6	0.00	-	-		
84	OHX	AK	102	-	0,6,6	0.00	-	-		
84	OHX	AR	3468	-	0,6,6	0.00	-	-		
84	OHX	1	3572	-	0,6,6	0.00	-	-		
84	OHX	AT	205	-	0,6,6	0.00	-	-		
87	GOL	AR	4262	84	5,5,5	0.26	0	5,5,5	0.53	0
84	OHX	1	3653	-	0,6,6	0.00	-	-		
84	OHX	AR	3577	-	0,6,6	0.00	-	-		
84	OHX	CV	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3512	-	0,6,6	0.00	-	-		
84	OHX	1	3436	-	0,6,6	0.00	-	-		
84	OHX	1	3437	-	0,6,6	0.00	-	-		
84	OHX	1	3624	-	0,6,6	0.00	-	-		
84	OHX	1	3489	-	0,6,6	0.00	-	-		
84	OHX	A	2016	-	0,6,6	0.00	-	-		
84	OHX	AR	3714	-	0,6,6	0.00	-	-		
84	OHX	A	2029	-	0,6,6	0.00	-	-		
84	OHX	1	3504	-	0,6,6	0.00	-	-		
84	OHX	1	3563	-	0,6,6	0.00	-	-		
84	OHX	6	1913	-	0,6,6	0.00	-	-		
84	OHX	AR	3618	-	0,6,6	0.00	-	-		
84	OHX	1	3506	-	0,6,6	0.00	-	-		
84	OHX	6	2026	-	0,6,6	0.00	-	-		
84	OHX	AR	3661	-	0,6,6	0.00	-	-		
84	OHX	1	3641	-	0,6,6	0.00	-	-		
84	OHX	6	1968	-	0,6,6	0.00	-	-		
84	OHX	A	1973	-	0,6,6	0.00	-	-		
84	OHX	1	3473	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3639	-	0,6,6	0.00	-	-		
84	OHX	1	3539	84	0,6,6	0.00	-	-		
84	OHX	1	3559	-	0,6,6	0.00	-	-		
84	OHX	AR	3683	-	0,6,6	0.00	-	-		
84	OHX	A	1983	-	0,6,6	0.00	-	-		
84	OHX	6	1954	-	0,6,6	0.00	-	-		
84	OHX	1	3718	-	0,6,6	0.00	-	-		
84	OHX	Q	201	-	0,6,6	0.00	-	-		
84	OHX	A	2026	-	0,6,6	0.00	-	-		
84	OHX	1	3664	-	0,6,6	0.00	-	-		
84	OHX	A	2038	-	0,6,6	0.00	-	-		
87	GOL	6	2199	-	5,5,5	0.10	0	5,5,5	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	HN8	AR	4263	-	-	0/2/48/48	0/6/5/5
87	GOL	A	2160	-	-	0/4/4/4	-
87	GOL	v	305	-	-	2/4/4/4	-
87	GOL	AR	4261	1	-	2/4/4/4	-
86	HN8	1	4223	-	-	0/2/48/48	0/6/5/5
87	GOL	AR	4262	84	-	1/4/4/4	-
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	AR	4261	GOL	C1-C2-C3-O3
87	v	305	GOL	O1-C1-C2-C3
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.

57 monomers are involved in 85 short contacts:

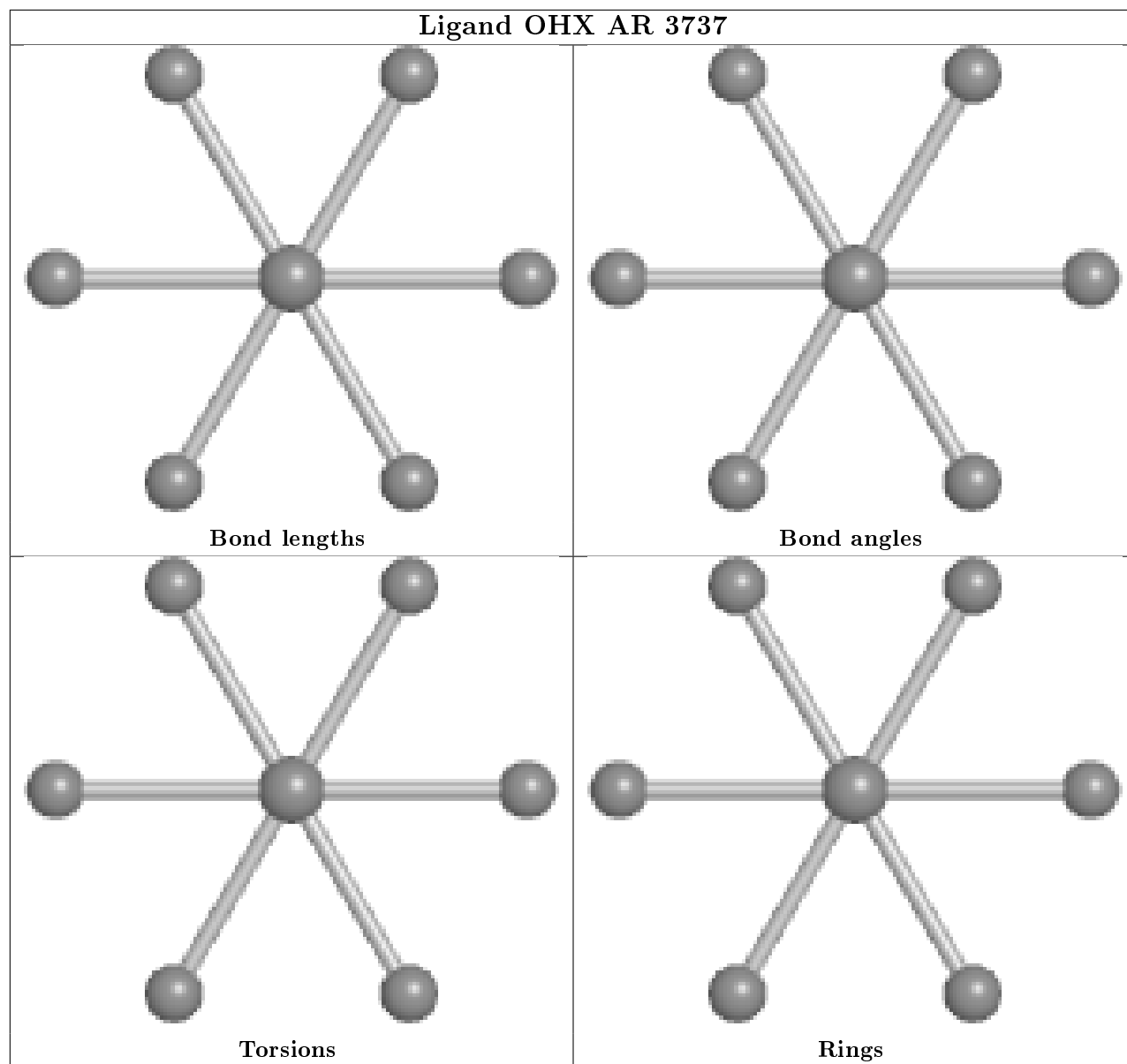
Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3642	OHX	2	0
84	AR	3591	OHX	1	0
84	A	1968	OHX	3	0
84	AR	3645	OHX	1	0
84	6	2001	OHX	4	0
84	A	2024	OHX	6	0
84	1	3720	OHX	6	0
84	AR	3477	OHX	2	0
84	AR	3687	OHX	2	0
84	AR	3554	OHX	1	0
84	6	2025	OHX	4	0
84	1	3493	OHX	2	0
84	1	3683	OHX	1	0
84	AR	3693	OHX	1	0
84	AR	3413	OHX	1	0
84	1	3575	OHX	1	0
84	AS	203	OHX	5	0
84	AT	203	OHX	2	0
84	AR	3731	OHX	6	0
84	AR	3566	OHX	2	0
87	AR	4261	GOL	1	0
84	AR	3627	OHX	1	0
84	AR	3696	OHX	4	0
84	1	3666	OHX	1	0
84	AR	3502	OHX	2	0
84	A	2009	OHX	3	0
84	1	3682	OHX	1	0
84	AR	3689	OHX	1	0
84	A	1914	OHX	1	0
84	AR	3590	OHX	2	0
84	AR	3743	OHX	2	0
84	1	3661	OHX	1	0
84	1	3510	OHX	1	0

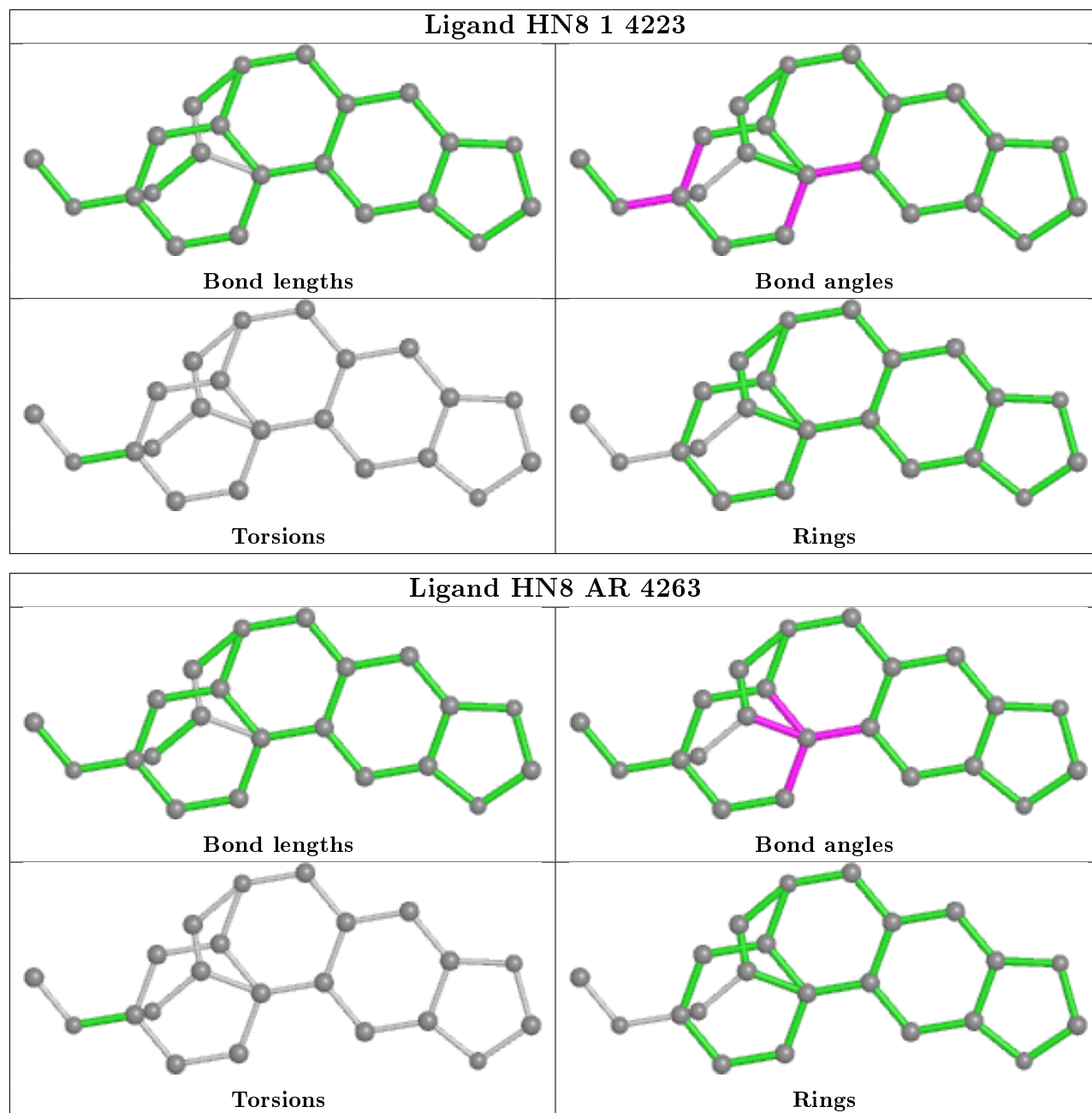
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	CX	202	OHX	1	0
84	6	1915	OHX	3	0
84	AR	3671	OHX	1	0
84	AR	3698	OHX	4	0
84	A	1909	OHX	6	0
84	CG	302	OHX	1	0
84	1	3697	OHX	2	0
84	6	1975	OHX	4	0
84	AR	3501	OHX	2	0
84	1	3704	OHX	1	0
84	AS	210	OHX	5	0
84	AT	212	OHX	2	0
84	AR	3715	OHX	4	0
84	6	2013	OHX	1	0
84	AR	3443	OHX	6	0
84	1	3604	OHX	1	0
84	AR	3534	OHX	2	0
84	AR	3521	OHX	4	0
84	AR	3511	OHX	4	0
87	AR	4262	GOL	2	0
84	1	3506	OHX	1	0
84	1	3473	OHX	6	0
84	1	3539	OHX	2	0
84	1	3559	OHX	1	0

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

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Mol	Chain	Number of breaks
50	s0	1
47	m2	1
25	A	1
54	s4	1
5	CE	1

The worst 5 of 7 chain breaks are listed below:

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

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	3149/3396 (92%)	0.22	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 ²)	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 ²)	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, 89	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 ²)	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 ²)	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, 119, 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 ²)	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	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	A	2130	1/1	0.46	0.62	74,74,74,74	0
85	MG	1	4140	1/1	0.46	0.29	187,187,187,187	0
85	MG	6	2158	1/1	0.46	0.75	74,74,74,74	0
85	MG	1	3813	1/1	0.48	0.37	61,61,61,61	0
85	MG	1	4053	1/1	0.49	0.41	74,74,74,74	0
85	MG	1	3958	1/1	0.49	0.38	44,44,44,44	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	AS	228	1/1	0.56	0.42	84,84,84,84	0
85	MG	4	229	1/1	0.56	0.41	54,54,54,54	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	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	AR	4122	1/1	0.60	0.25	68,68,68,68	0
85	MG	6	2168	1/1	0.60	0.31	132,132,132,132	0
85	MG	1	3989	1/1	0.60	0.26	55,55,55,55	0
85	MG	1	4104	1/1	0.60	0.45	53,53,53,53	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	AR	4254	1/1	0.61	0.38	56,56,56,56	0
85	MG	1	3772	1/1	0.61	0.20	35,35,35,35	0
85	MG	A	2155	1/1	0.61	0.46	75,75,75,75	0
85	MG	6	2185	1/1	0.61	0.46	89,89,89,89	0
85	MG	6	2160	1/1	0.62	0.38	85,85,85,85	0
85	MG	6	2194	1/1	0.62	0.15	108,108,108,108	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	1	3823	1/1	0.65	0.27	41,41,41,41	0
85	MG	AR	3950	1/1	0.65	0.27	47,47,47,47	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(\AA^2)	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	AR	4074	1/1	0.68	0.23	77,77,77,77	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	A	2099	1/1	0.69	0.69	71,71,71,71	0
85	MG	1	3952	1/1	0.69	0.24	77,77,77,77	0
85	MG	AR	3833	1/1	0.69	0.30	49,49,49,49	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	2103	1/1	0.69	0.55	73,73,73,73	0
85	MG	AT	218	1/1	0.69	0.34	30,30,30,30	0
85	MG	AR	4174	1/1	0.69	0.42	39,39,39,39	0
85	MG	1	3930	1/1	0.69	0.57	40,40,40,40	0
85	MG	Y	201	1/1	0.70	0.20	61,61,61,61	0
85	MG	6	2133	1/1	0.70	0.66	61,61,61,61	0
85	MG	A	2117	1/1	0.70	0.19	71,71,71,71	0
85	MG	AR	4170	1/1	0.70	0.27	32,32,32,32	0
85	MG	6	2174	1/1	0.70	0.44	58,58,58,58	0
85	MG	A	2139	1/1	0.70	0.36	64,64,64,64	0
85	MG	A	2085	1/1	0.70	0.40	63,63,63,63	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	AR	4037	1/1	0.71	0.34	70,70,70,70	0
85	MG	6	2154	1/1	0.71	0.41	54,54,54,54	0
85	MG	1	4061	1/1	0.71	0.31	54,54,54,54	0
85	MG	4	233	1/1	0.71	0.20	48,48,48,48	0
84	OHX	AR	3737	7/7	0.71	0.46	158,158,158,159	0
85	MG	l	403	1/1	0.71	0.47	37,37,37,37	0
85	MG	AR	4119	1/1	0.71	0.39	91,91,91,91	0
85	MG	AR	4049	1/1	0.72	0.19	50,50,50,50	0
85	MG	AR	4003	1/1	0.72	0.43	45,45,45,45	0
85	MG	AR	3817	1/1	0.72	0.24	112,112,112,112	0
85	MG	AR	4181	1/1	0.72	0.24	50,50,50,50	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	A	2062	1/1	0.72	0.71	65,65,65,65	0
85	MG	AR	4030	1/1	0.72	0.57	59,59,59,59	0
85	MG	1	4101	1/1	0.72	0.51	38,38,38,38	0
85	MG	s	300	1/1	0.72	0.27	70,70,70,70	0
85	MG	A	2046	1/1	0.72	0.29	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	CD	302	1/1	0.73	0.49	36,36,36,36	0
85	MG	6	2124	1/1	0.73	0.28	66,66,66,66	0
85	MG	1	4161	1/1	0.73	0.25	69,69,69,69	0
85	MG	A	2146	1/1	0.73	0.16	120,120,120,120	0
85	MG	AR	4034	1/1	0.73	0.45	60,60,60,60	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	1	4190	1/1	0.73	0.56	25,25,25,25	0
85	MG	AR	4011	1/1	0.73	0.39	58,58,58,58	0
85	MG	AR	4214	1/1	0.73	0.24	55,55,55,55	0
85	MG	1	3988	1/1	0.73	0.37	34,34,34,34	0
85	MG	AT	224	1/1	0.73	0.23	68,68,68,68	0
85	MG	AR	4161	1/1	0.74	0.27	39,39,39,39	0
85	MG	1	4129	1/1	0.74	0.43	33,33,33,33	0
85	MG	A	2131	1/1	0.74	0.43	64,64,64,64	0
85	MG	6	2192	1/1	0.74	0.67	74,74,74,74	0
85	MG	AR	4024	1/1	0.74	0.78	53,53,53,53	0
85	MG	AR	3783	1/1	0.74	0.32	44,44,44,44	0
85	MG	1	4131	1/1	0.74	0.32	48,48,48,48	0
85	MG	A	2135	1/1	0.74	0.56	55,55,55,55	0
85	MG	1	4151	1/1	0.74	0.28	41,41,41,41	0
85	MG	AR	3782	1/1	0.74	0.35	36,36,36,36	0
85	MG	AS	225	1/1	0.74	0.35	58,58,58,58	0
85	MG	1	4056	1/1	0.74	0.30	51,51,51,51	0
85	MG	1	3983	1/1	0.74	0.52	55,55,55,55	0
85	MG	1	4081	1/1	0.74	0.39	29,29,29,29	0
85	MG	AR	4022	1/1	0.75	0.44	30,30,30,30	0
85	MG	6	2117	1/1	0.75	0.28	65,65,65,65	0
85	MG	1	3816	1/1	0.75	0.34	44,44,44,44	0
85	MG	A	2136	1/1	0.75	0.71	74,74,74,74	0
85	MG	AR	4215	1/1	0.75	0.28	70,70,70,70	0
85	MG	AR	4117	1/1	0.75	0.31	64,64,64,64	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	AT	222	1/1	0.75	0.34	43,43,43,43	0
85	MG	A	2118	1/1	0.75	0.92	80,80,80,80	0
85	MG	6	2083	1/1	0.75	0.46	63,63,63,63	0
85	MG	A	2045	1/1	0.75	0.79	58,58,58,58	0
85	MG	A	2054	1/1	0.75	0.23	66,66,66,66	0
85	MG	1	4158	1/1	0.75	0.46	47,47,47,47	0
85	MG	1	4148	1/1	0.76	0.18	53,53,53,53	0
85	MG	AR	4257	1/1	0.76	0.32	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	6	2188	1/1	0.76	0.54	66,66,66,66	0
85	MG	AR	3776	1/1	0.76	0.33	76,76,76,76	0
85	MG	AR	4087	1/1	0.76	0.36	63,63,63,63	0
85	MG	6	2088	1/1	0.76	0.35	82,82,82,82	0
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	4155	1/1	0.76	0.23	53,53,53,53	0
85	MG	CM	202	1/1	0.76	0.15	62,62,62,62	0
85	MG	6	2189	1/1	0.76	0.34	63,63,63,63	0
85	MG	1	4093	1/1	0.76	0.37	57,57,57,57	0
85	MG	4	235	1/1	0.76	0.50	70,70,70,70	0
85	MG	AR	4085	1/1	0.77	0.46	35,35,35,35	0
85	MG	AR	4160	1/1	0.77	0.26	78,78,78,78	0
85	MG	1	3801	1/1	0.77	0.54	37,37,37,37	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	AS	219	1/1	0.77	0.24	58,58,58,58	0
85	MG	6	2081	1/1	0.77	0.25	55,55,55,55	0
85	MG	AR	4244	1/1	0.77	0.40	45,45,45,45	0
85	MG	AR	4171	1/1	0.77	0.17	88,88,88,88	0
85	MG	AR	4156	1/1	0.77	1.08	72,72,72,72	0
84	OHX	1	3691	7/7	0.77	0.31	201,201,201,201	0
85	MG	6	2162	1/1	0.77	0.26	60,60,60,60	0
85	MG	AR	4225	1/1	0.77	0.35	34,34,34,34	0
85	MG	6	2074	1/1	0.77	0.37	62,62,62,62	0
85	MG	V	201	1/1	0.77	0.50	70,70,70,70	0
85	MG	6	2163	1/1	0.77	0.42	48,48,48,48	0
85	MG	A	2084	1/1	0.77	0.22	72,72,72,72	0
85	MG	b	101	1/1	0.77	0.45	65,65,65,65	0
85	MG	AR	3976	1/1	0.77	0.44	81,81,81,81	0
85	MG	AR	3971	1/1	0.78	0.42	57,57,57,57	0
85	MG	6	2157	1/1	0.78	0.28	56,56,56,56	0
85	MG	1	4187	1/1	0.78	0.35	43,43,43,43	0
85	MG	6	2076	1/1	0.78	0.58	105,105,105,105	0
85	MG	AF	202	1/1	0.78	0.27	28,28,28,28	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	AR	3968	1/1	0.78	0.32	30,30,30,30	0
85	MG	AR	4005	1/1	0.78	0.62	40,40,40,40	0
85	MG	AR	4123	1/1	0.78	0.36	57,57,57,57	0
85	MG	x	206	1/1	0.78	0.58	35,35,35,35	0
85	MG	AR	4141	1/1	0.78	0.36	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	GOL	AR	4261	6/6	0.78	0.34	48,48,48,48	0
85	MG	1	4092	1/1	0.78	0.64	54,54,54,54	0
85	MG	1	3976	1/1	0.78	0.14	61,61,61,61	0
85	MG	1	4046	1/1	0.78	0.34	37,37,37,37	0
85	MG	1	3811	1/1	0.78	0.30	44,44,44,44	0
85	MG	1	4087	1/1	0.78	0.23	59,59,59,59	0
85	MG	AR	4220	1/1	0.78	0.39	44,44,44,44	0
85	MG	1	3941	1/1	0.78	0.41	78,78,78,78	0
85	MG	6	2197	1/1	0.78	0.57	56,56,56,56	0
85	MG	1	3800	1/1	0.79	0.61	45,45,45,45	0
85	MG	1	3994	1/1	0.79	0.27	47,47,47,47	0
85	MG	DI	202	1/1	0.79	0.36	56,56,56,56	0
85	MG	AR	4063	1/1	0.79	0.12	54,54,54,54	0
85	MG	6	2167	1/1	0.79	0.50	53,53,53,53	0
88	ZN	d7	101	1/1	0.79	0.47	143,143,143,143	0
85	MG	4	236	1/1	0.79	0.19	50,50,50,50	0
85	MG	AR	3964	1/1	0.79	0.29	35,35,35,35	0
85	MG	1	3751	1/1	0.79	0.35	40,40,40,40	0
85	MG	A	2116	1/1	0.79	0.61	67,67,67,67	0
85	MG	6	2183	1/1	0.79	0.58	71,71,71,71	0
85	MG	1	4023	1/1	0.79	0.48	57,57,57,57	0
85	MG	4	238	1/1	0.79	0.26	35,35,35,35	0
85	MG	6	2193	1/1	0.79	0.45	55,55,55,55	0
85	MG	1	4001	1/1	0.79	0.45	47,47,47,47	0
85	MG	1	3750	1/1	0.79	0.18	55,55,55,55	0
85	MG	AR	4097	1/1	0.79	0.58	40,40,40,40	0
85	MG	AR	4110	1/1	0.79	0.50	46,46,46,46	0
87	GOL	6	2199	6/6	0.79	0.44	49,49,49,49	0
85	MG	6	2092	1/1	0.79	0.58	93,93,93,93	0
85	MG	1	4044	1/1	0.80	0.32	47,47,47,47	0
85	MG	AR	3986	1/1	0.80	0.21	56,56,56,56	0
85	MG	AR	4194	1/1	0.80	0.27	53,53,53,53	0
85	MG	1	4159	1/1	0.80	0.39	43,43,43,43	0
85	MG	4	232	1/1	0.80	0.28	37,37,37,37	0
85	MG	1	4074	1/1	0.80	0.24	37,37,37,37	0
85	MG	1	3852	1/1	0.80	0.33	38,38,38,38	0
85	MG	1	4040	1/1	0.80	0.30	74,74,74,74	0
85	MG	1	4127	1/1	0.80	0.26	45,45,45,45	0
85	MG	AT	231	1/1	0.80	0.83	52,52,52,52	0
85	MG	AR	4198	1/1	0.80	0.59	51,51,51,51	0
85	MG	AR	4223	1/1	0.80	0.30	61,61,61,61	0
87	GOL	AR	4262	6/6	0.80	0.34	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	A	2091	1/1	0.80	0.43	71,71,71,71	0
85	MG	AR	3998	1/1	0.80	0.45	40,40,40,40	0
85	MG	6	2130	1/1	0.80	0.31	66,66,66,66	0
85	MG	1	3807	1/1	0.80	0.18	41,41,41,41	0
85	MG	1	4014	1/1	0.80	0.37	57,57,57,57	0
85	MG	AR	3779	1/1	0.80	0.38	73,73,73,73	0
85	MG	AR	4206	1/1	0.81	0.28	33,33,33,33	0
85	MG	1	3987	1/1	0.81	0.68	65,65,65,65	0
85	MG	1	3998	1/1	0.81	0.34	36,36,36,36	0
85	MG	1	3966	1/1	0.81	0.18	69,69,69,69	0
85	MG	AR	4169	1/1	0.81	0.29	46,46,46,46	0
85	MG	AR	3761	1/1	0.81	0.33	31,31,31,31	0
85	MG	A	2114	1/1	0.81	0.39	76,76,76,76	0
85	MG	CJ	301	1/1	0.81	0.22	78,78,78,78	0
85	MG	CG	304	1/1	0.81	0.25	56,56,56,56	0
85	MG	AR	3760	1/1	0.81	0.14	53,53,53,53	0
84	OHX	1	3668	7/7	0.81	0.45	124,124,124,124	0
85	MG	6	2146	1/1	0.81	1.00	80,80,80,80	0
85	MG	1	4088	1/1	0.81	0.25	44,44,44,44	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	1	3840	1/1	0.81	0.31	78,78,78,78	0
85	MG	A	2083	1/1	0.81	0.18	68,68,68,68	0
85	MG	AR	4200	1/1	0.81	0.25	48,48,48,48	0
85	MG	A	2152	1/1	0.81	0.70	43,43,43,43	0
85	MG	1	3954	1/1	0.81	0.15	46,46,46,46	0
85	MG	1	3963	1/1	0.81	0.25	45,45,45,45	0
85	MG	1	4170	1/1	0.81	0.49	41,41,41,41	0
85	MG	1	4203	1/1	0.81	0.24	31,31,31,31	0
85	MG	j	302	1/1	0.81	0.25	35,35,35,35	0
85	MG	1	4027	1/1	0.81	0.39	35,35,35,35	0
85	MG	AS	217	1/1	0.81	0.47	44,44,44,44	0
85	MG	AR	4182	1/1	0.81	0.37	79,79,79,79	0
85	MG	DE	201	1/1	0.81	0.28	72,72,72,72	0
85	MG	AR	4155	1/1	0.81	0.45	34,34,34,34	0
85	MG	AR	4128	1/1	0.81	0.21	55,55,55,55	0
85	MG	AR	3780	1/1	0.81	0.17	88,88,88,88	0
85	MG	AR	4224	1/1	0.82	0.49	47,47,47,47	0
85	MG	AR	3944	1/1	0.82	0.17	38,38,38,38	0
85	MG	AT	228	1/1	0.82	0.37	47,47,47,47	0
85	MG	1	3997	1/1	0.82	0.17	54,54,54,54	0
85	MG	6	2099	1/1	0.82	0.39	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	A	2107	1/1	0.82	0.31	80,80,80,80	0
87	GOL	A	2160	6/6	0.82	0.35	60,60,60,60	0
85	MG	AR	3749	1/1	0.82	0.19	42,42,42,42	0
85	MG	AR	4101	1/1	0.82	0.25	48,48,48,48	0
85	MG	1	4013	1/1	0.82	0.33	52,52,52,52	0
85	MG	A	2140	1/1	0.82	0.82	82,82,82,82	0
85	MG	6	2072	1/1	0.82	0.70	40,40,40,40	0
85	MG	AR	4014	1/1	0.82	0.39	57,57,57,57	0
85	MG	1	4060	1/1	0.82	0.36	44,44,44,44	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	AR	4056	1/1	0.82	0.38	44,44,44,44	0
85	MG	6	2152	1/1	0.82	0.43	62,62,62,62	0
85	MG	AR	3903	1/1	0.82	0.69	39,39,39,39	0
85	MG	c6	201	1/1	0.82	0.22	89,89,89,89	0
85	MG	1	3855	1/1	0.82	0.32	44,44,44,44	0
85	MG	CE	403	1/1	0.82	0.32	22,22,22,22	0
85	MG	AR	3794	1/1	0.82	0.24	34,34,34,34	0
85	MG	AR	4039	1/1	0.82	0.38	56,56,56,56	0
85	MG	1	3985	1/1	0.82	0.60	50,50,50,50	0
85	MG	AR	3756	1/1	0.82	0.36	36,36,36,36	0
85	MG	AR	3811	1/1	0.82	0.20	50,50,50,50	0
85	MG	AR	3751	1/1	0.82	0.36	36,36,36,36	0
85	MG	AR	4239	1/1	0.82	0.42	39,39,39,39	0
85	MG	1	3863	1/1	0.82	0.20	55,55,55,55	0
85	MG	1	4165	1/1	0.82	0.40	24,24,24,24	0
85	MG	A	2098	1/1	0.82	0.48	65,65,65,65	0
85	MG	AR	3836	1/1	0.82	0.45	48,48,48,48	0
85	MG	1	3866	1/1	0.82	0.39	34,34,34,34	0
85	MG	c9	201	1/1	0.82	0.10	79,79,79,79	0
85	MG	AR	4060	1/1	0.82	0.27	70,70,70,70	0
85	MG	1	4119	1/1	0.82	0.28	35,35,35,35	0
85	MG	AR	3984	1/1	0.82	0.65	50,50,50,50	0
85	MG	AT	221	1/1	0.82	0.76	52,52,52,52	0
85	MG	1	3955	1/1	0.82	0.43	51,51,51,51	0
85	MG	x	203	1/1	0.82	0.39	63,63,63,63	0
85	MG	AR	3945	1/1	0.82	0.15	40,40,40,40	0
85	MG	v	303	1/1	0.83	0.24	44,44,44,44	0
85	MG	AR	4075	1/1	0.83	0.31	36,36,36,36	0
85	MG	AR	3994	1/1	0.83	0.32	25,25,25,25	0
85	MG	6	2186	1/1	0.83	0.31	107,107,107,107	0
85	MG	1	4050	1/1	0.83	0.36	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4116	1/1	0.83	0.30	99,99,99,99	0
85	MG	6	2178	1/1	0.83	0.36	57,57,57,57	0
85	MG	1	3972	1/1	0.83	0.85	45,45,45,45	0
85	MG	AR	4240	1/1	0.83	0.55	70,70,70,70	0
85	MG	A	2048	1/1	0.83	0.33	52,52,52,52	0
85	MG	6	2140	1/1	0.83	0.40	69,69,69,69	0
85	MG	A	2081	1/1	0.83	0.31	66,66,66,66	0
85	MG	AR	4076	1/1	0.83	0.32	48,48,48,48	0
85	MG	1	4118	1/1	0.83	0.34	43,43,43,43	0
85	MG	AR	4090	1/1	0.83	0.49	57,57,57,57	0
85	MG	AR	3911	1/1	0.83	0.42	40,40,40,40	0
85	MG	6	2068	1/1	0.83	0.46	61,61,61,61	0
85	MG	AR	4221	1/1	0.83	0.28	35,35,35,35	0
85	MG	AR	4173	1/1	0.83	0.31	53,53,53,53	0
85	MG	AR	4245	1/1	0.83	0.22	26,26,26,26	0
84	OHX	6	2045	7/7	0.83	0.34	141,141,142,142	0
85	MG	4	234	1/1	0.83	0.43	44,44,44,44	0
85	MG	1	3779	1/1	0.83	0.48	55,55,55,55	0
85	MG	6	2070	1/1	0.83	0.39	73,73,73,73	0
84	OHX	AR	3664	7/7	0.83	0.43	180,180,181,181	0
85	MG	1	3993	1/1	0.83	0.62	42,42,42,42	0
85	MG	AR	4232	1/1	0.83	0.43	28,28,28,28	0
85	MG	AR	3752	1/1	0.83	0.21	37,37,37,37	0
85	MG	1	3761	1/1	0.83	0.30	41,41,41,41	0
85	MG	6	2111	1/1	0.83	0.42	61,61,61,61	0
85	MG	1	3819	1/1	0.83	0.40	27,27,27,27	0
85	MG	AR	3975	1/1	0.83	0.27	31,31,31,31	0
85	MG	AR	4094	1/1	0.83	0.31	43,43,43,43	0
85	MG	1	3739	1/1	0.83	0.32	51,51,51,51	0
84	OHX	A	2034	7/7	0.83	0.20	231,232,232,232	0
85	MG	6	2138	1/1	0.83	0.30	73,73,73,73	0
85	MG	1	3870	1/1	0.83	0.28	47,47,47,47	0
85	MG	1	3843	1/1	0.83	0.41	24,24,24,24	0
85	MG	AR	3812	1/1	0.83	0.42	32,32,32,32	0
85	MG	6	2064	1/1	0.83	0.68	53,53,53,53	0
85	MG	A	2127	1/1	0.83	0.29	83,83,83,83	0
85	MG	AR	3816	1/1	0.83	0.24	39,39,39,39	0
85	MG	AR	4089	1/1	0.83	0.10	62,62,62,62	0
85	MG	A	2094	1/1	0.83	0.38	110,110,110,110	0
85	MG	AR	3973	1/1	0.83	0.23	40,40,40,40	0
84	OHX	AR	3686	7/7	0.83	0.38	156,156,156,157	0
85	MG	1	4098	1/1	0.83	0.27	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3717	7/7	0.84	0.42	144,144,144,144	0
85	MG	1	4065	1/1	0.84	0.31	48,48,48,48	0
85	MG	A	2047	1/1	0.84	0.65	55,55,55,55	0
85	MG	1	4202	1/1	0.84	0.56	19,19,19,19	0
85	MG	1	4160	1/1	0.84	0.32	34,34,34,34	0
85	MG	AR	4046	1/1	0.84	0.26	46,46,46,46	0
85	MG	AR	4113	1/1	0.84	0.58	37,37,37,37	0
85	MG	A	2068	1/1	0.84	0.56	84,84,84,84	0
85	MG	1	4091	1/1	0.84	0.32	47,47,47,47	0
85	MG	AR	4234	1/1	0.84	0.45	32,32,32,32	0
85	MG	AR	4188	1/1	0.84	1.10	31,31,31,31	0
85	MG	AR	4021	1/1	0.84	0.17	82,82,82,82	0
85	MG	1	4070	1/1	0.84	0.20	68,68,68,68	0
85	MG	1	4006	1/1	0.84	0.57	47,47,47,47	0
85	MG	6	2118	1/1	0.84	0.14	93,93,93,93	0
85	MG	AT	226	1/1	0.84	0.30	63,63,63,63	0
85	MG	CP	502	1/1	0.84	0.42	45,45,45,45	0
85	MG	AR	3841	1/1	0.84	0.29	54,54,54,54	0
85	MG	AR	4086	1/1	0.84	0.40	42,42,42,42	0
85	MG	AR	4044	1/1	0.84	0.56	60,60,60,60	0
85	MG	AR	3960	1/1	0.84	0.21	41,41,41,41	0
85	MG	AR	4019	1/1	0.84	0.27	45,45,45,45	0
85	MG	1	4163	1/1	0.84	0.24	44,44,44,44	0
85	MG	A	2159	1/1	0.84	0.93	64,64,64,64	0
85	MG	1	3853	1/1	0.84	0.55	48,48,48,48	0
85	MG	CR	202	1/1	0.84	0.28	29,29,29,29	0
85	MG	A	2069	1/1	0.84	0.49	58,58,58,58	0
85	MG	AR	4035	1/1	0.84	0.38	43,43,43,43	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	6	2173	1/1	0.84	0.73	48,48,48,48	0
85	MG	AB	207	1/1	0.84	0.24	34,34,34,34	0
85	MG	CQ	204	1/1	0.84	0.41	30,30,30,30	0
85	MG	1	4145	1/1	0.84	0.33	42,42,42,42	0
84	OHX	AR	3719	7/7	0.84	0.42	133,133,133,133	0
85	MG	AR	4045	1/1	0.84	0.30	55,55,55,55	0
85	MG	AR	4253	1/1	0.84	0.17	41,41,41,41	0
85	MG	1	4003	1/1	0.84	0.35	79,79,79,79	0
85	MG	A	2089	1/1	0.85	0.19	90,90,90,90	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	4111	1/1	0.85	0.55	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3799	1/1	0.85	0.41	37,37,37,37	0
85	MG	1	4135	1/1	0.85	0.48	51,51,51,51	0
85	MG	AS	226	1/1	0.85	0.21	67,67,67,67	0
85	MG	1	3967	1/1	0.85	0.20	38,38,38,38	0
85	MG	AR	3958	1/1	0.85	0.56	38,38,38,38	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	AR	3873	1/1	0.85	0.46	31,31,31,31	0
85	MG	1	4082	1/1	0.85	0.30	35,35,35,35	0
85	MG	A	2142	1/1	0.85	0.13	80,80,80,80	0
84	OHX	AR	3728	7/7	0.85	0.42	151,152,152,152	0
84	OHX	A	1971	7/7	0.85	0.23	149,150,151,151	0
85	MG	4	220	1/1	0.85	0.34	64,64,64,64	0
85	MG	AR	4093	1/1	0.85	0.37	46,46,46,46	0
85	MG	AR	3759	1/1	0.85	0.62	34,34,34,34	0
85	MG	1	4042	1/1	0.85	0.41	48,48,48,48	0
85	MG	AR	4025	1/1	0.85	0.25	31,31,31,31	0
85	MG	1	4077	1/1	0.85	0.27	33,33,33,33	0
85	MG	1	3754	1/1	0.85	0.52	37,37,37,37	0
85	MG	AR	4103	1/1	0.85	0.19	47,47,47,47	0
85	MG	AR	4096	1/1	0.85	0.32	54,54,54,54	0
85	MG	1	3731	1/1	0.85	0.49	36,36,36,36	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
85	MG	AR	4238	1/1	0.85	0.38	36,36,36,36	0
85	MG	1	3984	1/1	0.85	0.27	70,70,70,70	0
85	MG	A	2050	1/1	0.85	0.39	67,67,67,67	0
85	MG	AR	4017	1/1	0.85	0.31	95,95,95,95	0
85	MG	1	4064	1/1	0.85	0.30	58,58,58,58	0
85	MG	1	3959	1/1	0.85	0.27	66,66,66,66	0
85	MG	AR	4140	1/1	0.85	0.49	44,44,44,44	0
85	MG	1	3940	1/1	0.85	0.37	43,43,43,43	0
85	MG	AR	3862	1/1	0.85	0.21	56,56,56,56	0
85	MG	1	3797	1/1	0.85	0.18	79,79,79,79	0
85	MG	A	2095	1/1	0.85	0.25	96,96,96,96	0
85	MG	6	2145	1/1	0.85	0.20	59,59,59,59	0
85	MG	A	2101	1/1	0.85	0.38	64,64,64,64	0
85	MG	1	3874	1/1	0.85	0.55	49,49,49,49	0
85	MG	T	202	1/1	0.86	0.09	97,97,97,97	0
85	MG	6	2059	1/1	0.86	0.43	70,70,70,70	0
85	MG	AR	4029	1/1	0.86	0.22	42,42,42,42	0
85	MG	6	2115	1/1	0.86	0.41	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3981	1/1	0.86	0.50	50,50,50,50	0
85	MG	AT	225	1/1	0.86	0.91	53,53,53,53	0
85	MG	6	2122	1/1	0.86	0.48	61,61,61,61	0
85	MG	1	3953	1/1	0.86	0.20	46,46,46,46	0
85	MG	AR	4248	1/1	0.86	0.94	45,45,45,45	0
84	OHX	1	3702	7/7	0.86	0.22	219,219,219,219	0
85	MG	AR	4146	1/1	0.86	0.19	34,34,34,34	0
85	MG	1	3752	1/1	0.86	0.42	57,57,57,57	0
85	MG	AB	202	1/1	0.86	0.31	29,29,29,29	0
85	MG	AT	227	1/1	0.86	0.89	79,79,79,79	0
85	MG	CR	203	1/1	0.86	0.15	95,95,95,95	0
85	MG	AR	4120	1/1	0.86	0.27	31,31,31,31	0
85	MG	3	216	1/1	0.86	0.40	58,58,58,58	0
85	MG	6	2195	1/1	0.86	0.65	35,35,35,35	0
84	OHX	AR	3734	7/7	0.86	0.55	148,148,148,149	0
85	MG	AR	3840	1/1	0.86	0.31	47,47,47,47	0
84	OHX	1	3724	7/7	0.86	0.22	113,113,113,113	0
85	MG	DC	202	1/1	0.86	0.30	48,48,48,48	0
85	MG	6	2161	1/1	0.86	0.49	58,58,58,58	0
85	MG	A	2110	1/1	0.86	0.67	116,116,116,116	0
85	MG	AR	4092	1/1	0.86	0.32	47,47,47,47	0
85	MG	AR	4187	1/1	0.86	0.43	36,36,36,36	0
85	MG	AR	3982	1/1	0.86	0.24	53,53,53,53	0
85	MG	AR	3814	1/1	0.86	0.31	105,105,105,105	0
84	OHX	1	3709	7/7	0.86	0.35	157,158,158,158	0
85	MG	AR	4145	1/1	0.86	0.20	70,70,70,70	0
85	MG	AR	4157	1/1	0.86	0.28	75,75,75,75	0
85	MG	AR	4071	1/1	0.86	0.27	39,39,39,39	0
85	MG	U	201	1/1	0.86	0.42	76,76,76,76	0
85	MG	6	2066	1/1	0.86	0.35	74,74,74,74	0
85	MG	AR	4118	1/1	0.86	0.41	31,31,31,31	0
85	MG	1	3926	1/1	0.86	0.16	37,37,37,37	0
85	MG	6	2087	1/1	0.86	0.30	56,56,56,56	0
85	MG	1	4007	1/1	0.86	0.42	29,29,29,29	0
85	MG	AR	4164	1/1	0.86	0.23	41,41,41,41	0
85	MG	1	4009	1/1	0.86	0.66	42,42,42,42	0
85	MG	AR	4127	1/1	0.86	0.17	77,77,77,77	0
85	MG	AR	3852	1/1	0.86	0.24	37,37,37,37	0
85	MG	1	3936	1/1	0.86	0.54	61,61,61,61	0
85	MG	AR	3829	1/1	0.86	0.66	66,66,66,66	0
85	MG	v	304	1/1	0.86	0.62	52,52,52,52	0
84	OHX	1	3714	7/7	0.86	0.51	146,147,147,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3954	1/1	0.86	0.30	44,44,44,44	0
85	MG	A	2092	1/1	0.86	0.27	91,91,91,91	0
85	MG	DQ	203	1/1	0.86	0.22	45,45,45,45	0
85	MG	1	3832	1/1	0.86	0.41	26,26,26,26	0
85	MG	6	2090	1/1	0.86	0.31	49,49,49,49	0
85	MG	6	2105	1/1	0.86	0.48	64,64,64,64	0
85	MG	1	4038	1/1	0.86	0.72	41,41,41,41	0
85	MG	AR	3935	1/1	0.86	0.62	49,49,49,49	0
85	MG	AR	3957	1/1	0.86	0.13	55,55,55,55	0
85	MG	A	2156	1/1	0.86	0.62	45,45,45,45	0
84	OHX	6	2046	7/7	0.86	0.36	151,152,152,152	0
85	MG	AR	3894	1/1	0.86	0.53	45,45,45,45	0
85	MG	A	2075	1/1	0.86	0.43	74,74,74,74	0
85	MG	CR	204	1/1	0.86	0.21	46,46,46,46	0
85	MG	A	2109	1/1	0.86	0.41	60,60,60,60	0
87	GOL	v	305	6/6	0.86	0.26	38,38,38,38	0
85	MG	1	4183	1/1	0.86	0.17	44,44,44,44	0
85	MG	1	3759	1/1	0.86	0.12	41,41,41,41	0
85	MG	AR	4159	1/1	0.86	0.38	36,36,36,36	0
84	OHX	A	1946	7/7	0.86	0.22	165,166,166,167	0
85	MG	AR	3991	1/1	0.86	0.14	98,98,98,98	0
85	MG	1	3971	1/1	0.87	0.46	35,35,35,35	0
85	MG	1	3845	1/1	0.87	0.40	18,18,18,18	0
85	MG	A	2134	1/1	0.87	0.35	70,70,70,70	0
84	OHX	z	201	7/7	0.87	0.39	155,156,157,157	0
85	MG	1	3786	1/1	0.87	0.20	40,40,40,40	0
85	MG	A	2053	1/1	0.87	0.72	57,57,57,57	0
84	OHX	AR	3741	7/7	0.87	0.38	207,208,208,208	0
85	MG	s6	301	1/1	0.87	0.29	77,77,77,77	0
85	MG	1	3961	1/1	0.87	0.19	40,40,40,40	0
85	MG	1	4211	1/1	0.87	0.63	42,42,42,42	0
85	MG	1	3767	1/1	0.87	0.12	60,60,60,60	0
85	MG	6	2169	1/1	0.87	0.63	49,49,49,49	0
85	MG	AR	3913	1/1	0.87	0.43	26,26,26,26	0
85	MG	1	4193	1/1	0.87	0.37	23,23,23,23	0
85	MG	AR	3851	1/1	0.87	0.29	38,38,38,38	0
85	MG	AR	3845	1/1	0.87	0.41	23,23,23,23	0
85	MG	x	209	1/1	0.87	0.66	39,39,39,39	0
84	OHX	A	2025	7/7	0.87	0.48	173,173,173,173	0
85	MG	AR	4246	1/1	0.87	0.41	22,22,22,22	0
85	MG	A	2088	1/1	0.87	0.53	59,59,59,59	0
85	MG	AR	3947	1/1	0.87	0.50	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4128	1/1	0.87	0.45	51,51,51,51	0
85	MG	6	2141	1/1	0.87	0.32	52,52,52,52	0
85	MG	6	2164	1/1	0.87	0.35	53,53,53,53	0
85	MG	1	3944	1/1	0.87	0.48	32,32,32,32	0
85	MG	n	201	1/1	0.87	0.26	43,43,43,43	0
84	OHX	A	2007	7/7	0.87	0.26	200,200,201,201	0
85	MG	AR	4250	1/1	0.87	0.80	59,59,59,59	0
85	MG	AR	4020	1/1	0.87	0.23	41,41,41,41	0
85	MG	1	4154	1/1	0.87	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	4108	1/1	0.87	0.21	42,42,42,42	0
85	MG	AR	3842	1/1	0.87	0.16	47,47,47,47	0
85	MG	1	4000	1/1	0.87	0.23	43,43,43,43	0
84	OHX	AR	3640	7/7	0.87	0.32	126,126,126,126	0
85	MG	6	2079	1/1	0.87	0.24	45,45,45,45	0
85	MG	CU	201	1/1	0.87	0.40	38,38,38,38	0
85	MG	CL	302	1/1	0.87	0.36	68,68,68,68	0
84	OHX	1	3708	7/7	0.87	0.39	134,134,134,134	0
85	MG	AR	4080	1/1	0.87	0.51	32,32,32,32	0
85	MG	CF	403	1/1	0.87	0.40	34,34,34,34	0
85	MG	1	3892	1/1	0.87	0.41	23,23,23,23	0
84	OHX	6	1960	7/7	0.87	0.22	118,118,118,118	0
84	OHX	6	2040	7/7	0.87	0.29	184,184,185,185	0
85	MG	1	4138	1/1	0.87	0.28	33,33,33,33	0
85	MG	1	3996	1/1	0.87	0.44	64,64,64,64	0
85	MG	6	2120	1/1	0.87	0.42	69,69,69,69	0
85	MG	AR	4124	1/1	0.87	0.18	39,39,39,39	0
85	MG	1	3778	1/1	0.87	0.46	49,49,49,49	0
84	OHX	AR	3652	7/7	0.87	0.44	112,112,113,113	0
85	MG	1	4210	1/1	0.87	0.30	24,24,24,24	0
85	MG	d4	201	1/1	0.87	0.38	53,53,53,53	0
85	MG	DA	201	1/1	0.87	0.28	48,48,48,48	0
85	MG	AR	4207	1/1	0.87	0.50	48,48,48,48	0
85	MG	A	2129	1/1	0.87	0.30	57,57,57,57	0
84	OHX	AR	3707	7/7	0.88	0.25	129,129,130,130	0
85	MG	AS	215	1/1	0.88	0.36	58,58,58,58	0
85	MG	AR	4149	1/1	0.88	0.38	66,66,66,66	0
85	MG	1	3787	1/1	0.88	0.46	46,46,46,46	0
85	MG	1	4162	1/1	0.88	0.25	40,40,40,40	0
85	MG	1	4115	1/1	0.88	0.23	36,36,36,36	0
84	OHX	1	3687	7/7	0.88	0.42	149,149,150,150	0
84	OHX	AR	3722	7/7	0.88	0.31	140,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	3	220	1/1	0.88	0.17	68,68,68,68	0
85	MG	6	2171	1/1	0.88	0.25	56,56,56,56	0
85	MG	1	3927	1/1	0.88	0.24	42,42,42,42	0
85	MG	3	212	1/1	0.88	0.44	62,62,62,62	0
85	MG	1	4084	1/1	0.88	0.27	32,32,32,32	0
84	OHX	A	2036	7/7	0.88	0.15	252,253,253,253	0
85	MG	AR	3907	1/1	0.88	0.63	25,25,25,25	0
85	MG	AR	4130	1/1	0.88	0.15	31,31,31,31	0
85	MG	1	3933	1/1	0.88	0.11	49,49,49,49	0
85	MG	1	3939	1/1	0.88	0.29	39,39,39,39	0
84	OHX	A	2041	7/7	0.88	0.46	139,139,140,140	0
85	MG	AR	4126	1/1	0.88	0.69	83,83,83,83	0
85	MG	AR	4251	1/1	0.88	0.41	59,59,59,59	0
85	MG	1	3758	1/1	0.88	0.50	32,32,32,32	0
85	MG	AR	3861	1/1	0.88	0.37	30,30,30,30	0
85	MG	AR	3868	1/1	0.88	0.46	25,25,25,25	0
85	MG	AR	3999	1/1	0.88	0.30	44,44,44,44	0
85	MG	1	4110	1/1	0.88	0.24	30,30,30,30	0
85	MG	A	2080	1/1	0.88	0.39	65,65,65,65	0
85	MG	AS	224	1/1	0.88	0.24	55,55,55,55	0
85	MG	AR	4175	1/1	0.88	0.25	35,35,35,35	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
85	MG	A	2087	1/1	0.88	0.50	78,78,78,78	0
85	MG	DL	102	1/1	0.88	0.50	39,39,39,39	0
85	MG	1	4113	1/1	0.88	0.26	57,57,57,57	0
85	MG	AR	4047	1/1	0.88	0.14	54,54,54,54	0
85	MG	4	222	1/1	0.88	0.28	33,33,33,33	0
85	MG	A	2133	1/1	0.88	0.20	72,72,72,72	0
85	MG	AR	4150	1/1	0.88	0.18	44,44,44,44	0
85	MG	1	3934	1/1	0.88	0.44	54,54,54,54	0
85	MG	6	2103	1/1	0.88	0.33	69,69,69,69	0
84	OHX	AR	3517	7/7	0.88	0.16	145,146,146,146	0
85	MG	A	2070	1/1	0.88	0.53	79,79,79,79	0
85	MG	AR	4051	1/1	0.88	0.38	40,40,40,40	0
85	MG	A	2093	1/1	0.88	0.14	100,100,100,100	0
84	OHX	6	2018	7/7	0.88	0.23	189,189,189,189	0
84	OHX	AR	3690	7/7	0.88	0.47	117,118,118,118	0
85	MG	CE	404	1/1	0.88	0.29	27,27,27,27	0
85	MG	1	3803	1/1	0.88	0.42	41,41,41,41	0
85	MG	1	3945	1/1	0.88	0.29	57,57,57,57	0
85	MG	x	208	1/1	0.88	0.33	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4125	1/1	0.88	0.38	23,23,23,23	0
84	OHX	AR	3726	7/7	0.88	0.42	118,118,118,118	0
85	MG	1	3785	1/1	0.88	0.45	25,25,25,25	0
85	MG	AR	4023	1/1	0.88	0.23	31,31,31,31	0
85	MG	AS	223	1/1	0.88	0.28	41,41,41,41	0
85	MG	1	3897	1/1	0.88	0.21	46,46,46,46	0
84	OHX	AR	3720	7/7	0.88	0.33	152,152,152,152	0
85	MG	1	4137	1/1	0.88	0.17	55,55,55,55	0
85	MG	AR	4083	1/1	0.89	0.28	31,31,31,31	0
85	MG	3	211	1/1	0.89	0.35	38,38,38,38	0
85	MG	6	2144	1/1	0.89	0.38	74,74,74,74	0
85	MG	AR	3943	1/1	0.89	0.10	41,41,41,41	0
84	OHX	A	2015	7/7	0.89	0.41	169,170,171,172	0
85	MG	AR	4210	1/1	0.89	0.72	54,54,54,54	0
85	MG	AR	4186	1/1	0.89	0.21	33,33,33,33	0
85	MG	1	3999	1/1	0.89	0.33	41,41,41,41	0
85	MG	1	3932	1/1	0.89	0.19	55,55,55,55	0
84	OHX	6	2006	7/7	0.89	0.29	151,151,152,152	0
85	MG	AR	3834	1/1	0.89	0.47	33,33,33,33	0
85	MG	1	3982	1/1	0.89	0.37	32,32,32,32	0
85	MG	D	301	1/1	0.89	0.58	58,58,58,58	0
85	MG	1	3873	1/1	0.89	0.23	48,48,48,48	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	AR	4028	1/1	0.89	0.19	41,41,41,41	0
84	OHX	c4	201	7/7	0.89	0.53	152,152,153,153	0
85	MG	1	3956	1/1	0.89	0.54	34,34,34,34	0
85	MG	1	3726	1/1	0.89	0.84	54,54,54,54	0
85	MG	AR	4073	1/1	0.89	0.39	40,40,40,40	0
85	MG	AR	3764	1/1	0.89	0.34	33,33,33,33	0
85	MG	1	4219	1/1	0.89	0.26	98,98,98,98	0
85	MG	1	4184	1/1	0.89	0.26	36,36,36,36	0
84	OHX	1	3723	7/7	0.89	0.35	113,113,113,113	0
85	MG	6	2190	1/1	0.89	0.48	66,66,66,66	0
84	OHX	CF	401	7/7	0.89	0.31	146,146,147,147	0
84	OHX	1	3620	7/7	0.89	0.35	118,118,118,118	0
85	MG	4	240	1/1	0.89	0.57	32,32,32,32	0
85	MG	A	2149	1/1	0.89	0.25	60,60,60,60	0
85	MG	1	4130	1/1	0.89	0.27	45,45,45,45	0
84	OHX	1	3721	7/7	0.89	0.35	127,127,127,128	0
85	MG	1	4005	1/1	0.89	0.35	36,36,36,36	0
85	MG	AR	4163	1/1	0.89	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4036	1/1	0.89	0.42	70,70,70,70	0
85	MG	CR	205	1/1	0.89	0.40	31,31,31,31	0
85	MG	AR	3899	1/1	0.89	0.60	45,45,45,45	0
85	MG	1	4073	1/1	0.89	0.38	40,40,40,40	0
84	OHX	1	3712	7/7	0.89	0.34	133,133,133,133	0
85	MG	r	302	1/1	0.89	0.22	37,37,37,37	0
84	OHX	AR	3602	7/7	0.89	0.18	143,143,144,144	0
85	MG	6	2149	1/1	0.89	0.32	46,46,46,46	0
85	MG	AR	4050	1/1	0.89	0.31	91,91,91,91	0
85	MG	1	3960	1/1	0.89	0.21	33,33,33,33	0
85	MG	AR	4059	1/1	0.89	0.20	47,47,47,47	0
85	MG	x	207	1/1	0.89	0.31	33,33,33,33	0
85	MG	1	4029	1/1	0.89	0.11	47,47,47,47	0
84	OHX	6	1975	7/7	0.89	0.43	120,120,120,120	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
84	OHX	6	2051	7/7	0.89	0.29	172,172,172,173	0
85	MG	6	2134	1/1	0.89	0.22	80,80,80,80	0
85	MG	1	3915	1/1	0.89	0.12	36,36,36,36	0
85	MG	1	3777	1/1	0.89	0.17	30,30,30,30	0
85	MG	AR	4154	1/1	0.89	0.32	39,39,39,39	0
85	MG	1	4080	1/1	0.89	0.22	35,35,35,35	0
85	MG	1	3995	1/1	0.89	0.31	34,34,34,34	0
85	MG	6	2150	1/1	0.89	0.13	77,77,77,77	0
85	MG	AR	3882	1/1	0.89	0.14	47,47,47,47	0
85	MG	d5	201	1/1	0.89	0.09	71,71,71,71	0
85	MG	AR	4069	1/1	0.89	0.23	26,26,26,26	0
85	MG	AR	4153	1/1	0.89	0.19	88,88,88,88	0
85	MG	1	3886	1/1	0.89	0.41	21,21,21,21	0
85	MG	AR	4043	1/1	0.89	0.38	37,37,37,37	0
85	MG	A	2125	1/1	0.89	0.85	56,56,56,56	0
85	MG	DI	201	1/1	0.89	0.22	68,68,68,68	0
85	MG	AR	4148	1/1	0.89	0.28	43,43,43,43	0
84	OHX	A	1985	7/7	0.89	0.31	140,140,141,141	0
85	MG	AR	3777	1/1	0.89	0.31	37,37,37,37	0
85	MG	AR	3891	1/1	0.89	0.27	69,69,69,69	0
85	MG	3	221	1/1	0.89	0.47	34,34,34,34	0
85	MG	AR	4067	1/1	0.89	0.34	34,34,34,34	0
85	MG	1	3881	1/1	0.89	0.55	31,31,31,31	0
85	MG	DC	201	1/1	0.89	0.45	30,30,30,30	0
84	OHX	AR	3729	7/7	0.89	0.46	120,120,120,121	0
85	MG	6	2085	1/1	0.89	0.47	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	4	228	1/1	0.89	0.26	54,54,54,54	0
85	MG	AR	4135	1/1	0.89	0.18	62,62,62,62	0
85	MG	AT	229	1/1	0.89	0.42	55,55,55,55	0
84	OHX	AR	3733	7/7	0.89	0.33	187,188,188,188	0
85	MG	1	3928	1/1	0.89	0.27	34,34,34,34	0
85	MG	AR	3765	1/1	0.90	0.39	71,71,71,71	0
85	MG	6	2139	1/1	0.90	0.22	45,45,45,45	0
85	MG	A	2051	1/1	0.90	0.47	67,67,67,67	0
84	OHX	1	3718	7/7	0.90	0.39	149,149,149,149	0
84	OHX	AR	3604	7/7	0.90	0.19	158,159,159,159	0
85	MG	AR	4042	1/1	0.90	0.12	57,57,57,57	0
84	OHX	A	2026	7/7	0.90	0.40	123,123,124,124	0
85	MG	1	3851	1/1	0.90	0.36	34,34,34,34	0
85	MG	x	205	1/1	0.90	0.66	33,33,33,33	0
85	MG	s4	301	1/1	0.90	0.23	59,59,59,59	0
84	OHX	AR	3738	7/7	0.90	0.15	141,142,142,142	0
84	OHX	1	3707	7/7	0.90	0.40	125,125,126,126	0
85	MG	AR	3946	1/1	0.90	0.30	59,59,59,59	0
85	MG	AR	3755	1/1	0.90	0.18	56,56,56,56	0
85	MG	1	4085	1/1	0.90	0.39	51,51,51,51	0
84	OHX	6	2041	7/7	0.90	0.34	143,144,145,145	0
84	OHX	AM	101	7/7	0.90	0.43	121,121,121,121	0
85	MG	A	2132	1/1	0.90	0.26	98,98,98,98	0
85	MG	AR	4033	1/1	0.90	0.26	40,40,40,40	0
85	MG	6	2198	1/1	0.90	0.56	49,49,49,49	0
85	MG	4	231	1/1	0.90	0.23	58,58,58,58	0
85	MG	t	201	1/1	0.90	0.17	51,51,51,51	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	1	3710	7/7	0.90	0.33	136,137,137,137	0
85	MG	A	2102	1/1	0.90	0.49	58,58,58,58	0
85	MG	1	3737	1/1	0.90	0.93	57,57,57,57	0
85	MG	1	3793	1/1	0.90	0.30	37,37,37,37	0
84	OHX	1	3700	7/7	0.90	0.36	148,148,149,149	0
85	MG	1	3830	1/1	0.90	0.22	44,44,44,44	0
84	OHX	3	209	7/7	0.90	0.28	152,152,152,152	0
84	OHX	x	201	7/7	0.90	0.39	110,110,110,110	0
84	OHX	1	3501	7/7	0.90	0.17	126,126,127,127	0
85	MG	AR	3753	1/1	0.90	0.33	26,26,26,26	0
85	MG	1	4117	1/1	0.90	0.31	41,41,41,41	0
85	MG	AH	202	1/1	0.90	0.15	58,58,58,58	0
85	MG	AR	4197	1/1	0.90	0.27	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	6	2080	1/1	0.90	0.64	69,69,69,69	0
85	MG	AR	4134	1/1	0.90	0.27	44,44,44,44	0
84	OHX	AR	3646	7/7	0.90	0.37	108,108,108,108	0
85	MG	AR	4009	1/1	0.90	0.34	37,37,37,37	0
84	OHX	1	3696	7/7	0.90	0.39	146,146,147,147	0
85	MG	1	4156	1/1	0.90	0.19	44,44,44,44	0
85	MG	AR	4070	1/1	0.90	0.19	50,50,50,50	0
85	MG	1	3766	1/1	0.90	0.16	73,73,73,73	0
85	MG	A	2065	1/1	0.90	0.73	57,57,57,57	0
84	OHX	1	3656	7/7	0.90	0.50	143,143,143,144	0
85	MG	AR	4166	1/1	0.90	0.16	38,38,38,38	0
84	OHX	A	2029	7/7	0.90	0.20	184,184,184,184	0
85	MG	AR	3956	1/1	0.90	0.22	29,29,29,29	0
85	MG	AR	4252	1/1	0.90	0.37	50,50,50,50	0
84	OHX	6	2001	7/7	0.90	0.28	119,120,120,120	0
85	MG	AR	3773	1/1	0.90	0.29	41,41,41,41	0
85	MG	1	4055	1/1	0.90	0.17	33,33,33,33	0
84	OHX	1	3642	7/7	0.90	0.45	135,135,136,136	0
85	MG	AR	4098	1/1	0.90	0.20	46,46,46,46	0
85	MG	1	4209	1/1	0.90	0.67	48,48,48,48	0
84	OHX	AR	3692	7/7	0.90	0.31	170,171,171,171	0
84	OHX	AR	3631	7/7	0.90	0.18	175,176,177,177	0
85	MG	6	2078	1/1	0.90	0.45	42,42,42,42	0
84	OHX	A	2043	7/7	0.90	0.19	155,156,156,157	0
85	MG	1	4116	1/1	0.90	0.52	44,44,44,44	0
85	MG	1	4102	1/1	0.90	0.37	57,57,57,57	0
85	MG	1	3898	1/1	0.90	0.46	33,33,33,33	0
85	MG	1	3771	1/1	0.90	0.42	33,33,33,33	0
85	MG	6	2166	1/1	0.90	0.49	53,53,53,53	0
84	OHX	1	3626	7/7	0.90	0.35	124,124,124,124	0
84	OHX	1	3653	7/7	0.90	0.29	133,133,133,133	0
85	MG	A	2122	1/1	0.90	0.17	86,86,86,86	0
85	MG	AB	204	1/1	0.90	0.29	52,52,52,52	0
85	MG	AR	3750	1/1	0.90	0.41	27,27,27,27	0
85	MG	A	2106	1/1	0.90	0.50	58,58,58,58	0
85	MG	AR	4084	1/1	0.90	0.22	34,34,34,34	0
84	OHX	6	2052	7/7	0.90	0.33	143,144,144,144	0
85	MG	AR	3821	1/1	0.90	0.21	42,42,42,42	0
85	MG	A	2113	1/1	0.90	0.48	73,73,73,73	0
84	OHX	A	2030	7/7	0.90	0.47	142,143,143,144	0
85	MG	AS	218	1/1	0.90	0.30	33,33,33,33	0
85	MG	1	3962	1/1	0.90	0.41	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AG	202	1/1	0.90	0.20	43,43,43,43	0
85	MG	AR	3807	1/1	0.90	0.38	25,25,25,25	0
85	MG	1	4147	1/1	0.90	0.21	48,48,48,48	0
84	OHX	6	2039	7/7	0.90	0.62	132,133,133,134	0
85	MG	AR	4040	1/1	0.90	0.26	43,43,43,43	0
85	MG	AR	3914	1/1	0.90	0.43	32,32,32,32	0
84	OHX	1	3644	7/7	0.90	0.25	166,167,167,167	0
85	MG	AR	3948	1/1	0.90	0.54	40,40,40,40	0
85	MG	1	4028	1/1	0.90	0.16	46,46,46,46	0
85	MG	1	4015	1/1	0.90	0.37	67,67,67,67	0
85	MG	6	2082	1/1	0.90	0.48	54,54,54,54	0
85	MG	1	3869	1/1	0.90	0.49	34,34,34,34	0
84	OHX	A	2042	7/7	0.90	0.21	172,173,173,174	0
85	MG	AS	213	1/1	0.90	0.45	26,26,26,26	0
84	OHX	1	3719	7/7	0.90	0.52	120,120,121,121	0
85	MG	CD	301	1/1	0.90	0.36	34,34,34,34	0
85	MG	AR	4064	1/1	0.90	0.24	38,38,38,38	0
85	MG	1	4198	1/1	0.90	0.60	43,43,43,43	0
85	MG	1	3818	1/1	0.90	0.43	39,39,39,39	0
85	MG	1	3762	1/1	0.90	0.56	30,30,30,30	0
85	MG	d6	101	1/1	0.91	0.34	49,49,49,49	0
84	OHX	4	213	7/7	0.91	0.31	117,117,117,117	0
85	MG	AR	4177	1/1	0.91	0.30	32,32,32,32	0
84	OHX	1	3596	7/7	0.91	0.49	143,144,144,144	0
85	MG	AR	3771	1/1	0.91	0.36	42,42,42,42	0
85	MG	AR	3778	1/1	0.91	0.26	42,42,42,42	0
84	OHX	A	2039	7/7	0.91	0.41	166,167,168,168	0
85	MG	1	3913	1/1	0.91	0.59	28,28,28,28	0
84	OHX	AR	3730	7/7	0.91	0.33	176,176,176,176	0
85	MG	AR	3892	1/1	0.91	0.48	31,31,31,31	0
85	MG	1	4100	1/1	0.91	0.27	53,53,53,53	0
85	MG	AR	3789	1/1	0.91	0.39	36,36,36,36	0
85	MG	1	4035	1/1	0.91	0.60	47,47,47,47	0
85	MG	6	2196	1/1	0.91	0.76	48,48,48,48	0
84	OHX	1	3720	7/7	0.91	0.28	128,128,129,129	0
85	MG	1	3929	1/1	0.91	0.30	34,34,34,34	0
85	MG	A	2086	1/1	0.91	0.24	66,66,66,66	0
84	OHX	3	205	7/7	0.91	0.21	127,128,128,128	0
85	MG	AR	4137	1/1	0.91	0.48	79,79,79,79	0
85	MG	c8	202	1/1	0.91	0.33	79,79,79,79	0
85	MG	1	3782	1/1	0.91	0.45	58,58,58,58	0
85	MG	AR	4231	1/1	0.91	0.35	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4068	1/1	0.91	0.12	99,99,99,99	0
85	MG	4	227	1/1	0.91	0.40	52,52,52,52	0
85	MG	1	4058	1/1	0.91	0.31	51,51,51,51	0
85	MG	AR	3796	1/1	0.91	0.41	64,64,64,64	0
85	MG	1	4213	1/1	0.91	0.64	50,50,50,50	0
85	MG	AR	3929	1/1	0.91	0.37	25,25,25,25	0
84	OHX	6	2008	7/7	0.91	0.18	136,136,136,136	0
84	OHX	AR	3727	7/7	0.91	0.23	187,188,188,188	0
85	MG	1	3765	1/1	0.91	0.49	21,21,21,21	0
84	OHX	A	2038	7/7	0.91	0.34	146,147,147,147	0
85	MG	DQ	204	1/1	0.91	0.35	32,32,32,32	0
85	MG	AR	4180	1/1	0.91	0.39	48,48,48,48	0
85	MG	1	3849	1/1	0.91	0.44	23,23,23,23	0
84	OHX	AT	213	7/7	0.91	0.25	137,137,137,137	0
84	OHX	A	2035	7/7	0.91	0.48	130,131,131,131	0
85	MG	1	3746	1/1	0.91	0.41	26,26,26,26	0
85	MG	AR	4176	1/1	0.91	0.23	33,33,33,33	0
85	MG	AR	4139	1/1	0.91	0.35	46,46,46,46	0
85	MG	AR	3770	1/1	0.91	0.44	32,32,32,32	0
84	OHX	A	1970	7/7	0.91	0.35	132,132,133,133	0
84	OHX	6	2004	7/7	0.91	0.40	157,157,158,158	0
84	OHX	A	1993	7/7	0.91	0.38	151,151,152,152	0
85	MG	1	3884	1/1	0.91	0.34	29,29,29,29	0
85	MG	AR	4236	1/1	0.91	0.42	23,23,23,23	0
85	MG	6	2142	1/1	0.91	0.24	83,83,83,83	0
85	MG	AR	3922	1/1	0.91	0.49	31,31,31,31	0
85	MG	AB	203	1/1	0.91	0.34	32,32,32,32	0
85	MG	AR	3934	1/1	0.91	0.31	32,32,32,32	0
85	MG	6	2129	1/1	0.91	0.38	62,62,62,62	0
85	MG	AR	4147	1/1	0.91	0.23	31,31,31,31	0
85	MG	1	3979	1/1	0.91	0.31	39,39,39,39	0
85	MG	A	2056	1/1	0.91	0.34	65,65,65,65	0
84	OHX	1	3673	7/7	0.91	0.56	133,133,133,133	0
85	MG	1	4037	1/1	0.91	0.30	30,30,30,30	0
85	MG	1	3861	1/1	0.91	0.24	34,34,34,34	0
84	OHX	4	215	7/7	0.91	0.28	137,138,138,138	0
84	OHX	s8	301	7/7	0.91	0.32	167,167,168,168	0
85	MG	1	4022	1/1	0.91	0.59	53,53,53,53	0
84	OHX	1	3716	7/7	0.91	0.45	138,138,139,139	0
85	MG	6	2127	1/1	0.91	0.47	54,54,54,54	0
84	OHX	c3	201	7/7	0.91	0.24	155,156,156,157	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(\AA^2)	Q<0.9
85	MG	1	3848	1/1	0.91	0.40	60,60,60,60	0
85	MG	6	2165	1/1	0.91	0.35	51,51,51,51	0
84	OHX	AR	3718	7/7	0.91	0.47	166,167,167,167	0
84	OHX	AR	3639	7/7	0.91	0.22	138,139,139,139	0
85	MG	AB	205	1/1	0.91	0.22	40,40,40,40	0
84	OHX	AR	3677	7/7	0.91	0.38	110,111,111,111	0
84	OHX	A	2023	7/7	0.91	0.26	144,145,145,145	0
85	MG	AR	4216	1/1	0.91	0.20	44,44,44,44	0
84	OHX	A	2021	7/7	0.91	0.43	133,133,134,134	0
85	MG	1	3917	1/1	0.91	0.26	30,30,30,30	0
85	MG	6	2143	1/1	0.91	0.31	75,75,75,75	0
84	OHX	1	3695	7/7	0.91	0.61	154,154,155,155	0
85	MG	1	3847	1/1	0.91	0.54	28,28,28,28	0
85	MG	6	2109	1/1	0.91	0.42	56,56,56,56	0
85	MG	AR	3979	1/1	0.91	0.57	41,41,41,41	0
85	MG	1	4021	1/1	0.91	0.15	44,44,44,44	0
84	OHX	6	2002	7/7	0.91	0.27	132,133,133,134	0
85	MG	AR	3897	1/1	0.91	0.44	51,51,51,51	0
85	MG	AR	4184	1/1	0.91	0.16	69,69,69,69	0
85	MG	CX	204	1/1	0.91	0.21	46,46,46,46	0
85	MG	AR	4100	1/1	0.91	0.28	57,57,57,57	0
85	MG	AR	3896	1/1	0.91	0.55	36,36,36,36	0
85	MG	1	3920	1/1	0.91	0.10	41,41,41,41	0
85	MG	AR	3832	1/1	0.91	0.53	30,30,30,30	0
84	OHX	AR	3695	7/7	0.91	0.30	122,122,123,123	0
85	MG	AR	4205	1/1	0.91	0.24	59,59,59,59	0
85	MG	AB	201	1/1	0.91	0.28	34,34,34,34	0
85	MG	k	402	1/1	0.91	0.37	37,37,37,37	0
85	MG	A	2067	1/1	0.91	0.81	64,64,64,64	0
85	MG	AR	4256	1/1	0.91	0.43	49,49,49,49	0
85	MG	1	4030	1/1	0.91	0.73	72,72,72,72	0
84	OHX	AR	3745	7/7	0.91	0.34	128,128,128,128	0
84	OHX	1	3701	7/7	0.91	0.31	139,139,140,140	0
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	3	217	1/1	0.91	0.36	40,40,40,40	0
85	MG	AR	3889	1/1	0.91	0.36	35,35,35,35	0
85	MG	AR	4026	1/1	0.91	0.33	60,60,60,60	0
84	OHX	1	3659	7/7	0.91	0.32	140,140,140,141	0
85	MG	H	301	1/1	0.91	0.10	83,83,83,83	0
84	OHX	6	2048	7/7	0.91	0.35	173,174,174,174	0
85	MG	1	3901	1/1	0.91	0.49	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4011	1/1	0.91	0.37	44,44,44,44	0
85	MG	1	3789	1/1	0.91	0.17	42,42,42,42	0
85	MG	1	3992	1/1	0.91	0.24	40,40,40,40	0
85	MG	1	4109	1/1	0.91	0.14	66,66,66,66	0
85	MG	1	4174	1/1	0.91	0.83	55,55,55,55	0
84	OHX	AS	211	7/7	0.91	0.29	141,141,142,142	0
85	MG	AR	3815	1/1	0.91	0.24	32,32,32,32	0
85	MG	AR	4136	1/1	0.91	0.27	36,36,36,36	0
85	MG	1	3865	1/1	0.91	0.32	45,45,45,45	0
84	OHX	AR	3665	7/7	0.91	0.39	133,133,133,133	0
85	MG	w	202	1/1	0.91	0.32	31,31,31,31	0
85	MG	1	3732	1/1	0.91	0.44	26,26,26,26	0
85	MG	AS	227	1/1	0.92	0.32	45,45,45,45	0
85	MG	1	3938	1/1	0.92	0.21	34,34,34,34	0
85	MG	AT	220	1/1	0.92	0.47	53,53,53,53	0
85	MG	1	3755	1/1	0.92	0.42	36,36,36,36	0
85	MG	6	2100	1/1	0.92	0.51	36,36,36,36	0
85	MG	1	3834	1/1	0.92	0.51	22,22,22,22	0
85	MG	t	203	1/1	0.92	0.42	29,29,29,29	0
84	OHX	A	2011	7/7	0.92	0.23	149,149,150,150	0
85	MG	AR	3835	1/1	0.92	0.41	45,45,45,45	0
85	MG	1	3990	1/1	0.92	0.30	24,24,24,24	0
85	MG	1	3802	1/1	0.92	0.18	86,86,86,86	0
85	MG	6	2060	1/1	0.92	0.34	47,47,47,47	0
85	MG	1	4026	1/1	0.92	0.41	65,65,65,65	0
85	MG	1	3862	1/1	0.92	0.46	52,52,52,52	0
85	MG	AR	3980	1/1	0.92	0.86	40,40,40,40	0
85	MG	A	2143	1/1	0.92	0.38	106,106,106,106	0
85	MG	AR	3804	1/1	0.92	0.45	27,27,27,27	0
85	MG	F	301	1/1	0.92	0.33	64,64,64,64	0
85	MG	AR	4226	1/1	0.92	0.41	24,24,24,24	0
85	MG	1	3970	1/1	0.92	0.30	31,31,31,31	0
85	MG	AR	3808	1/1	0.92	0.34	28,28,28,28	0
84	OHX	CF	402	7/7	0.92	0.34	145,146,146,146	0
84	OHX	A	2006	7/7	0.92	0.31	149,150,150,150	0
85	MG	AR	4055	1/1	0.92	0.17	40,40,40,40	0
85	MG	A	2057	1/1	0.92	0.46	70,70,70,70	0
85	MG	1	4218	1/1	0.92	0.14	32,32,32,32	0
85	MG	AR	4018	1/1	0.92	0.21	36,36,36,36	0
85	MG	1	3833	1/1	0.92	0.70	24,24,24,24	0
84	OHX	6	2030	7/7	0.92	0.29	118,118,118,119	0
84	OHX	AS	210	7/7	0.92	0.24	115,115,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3647	7/7	0.92	0.29	126,126,127,127	0
84	OHX	A	2012	7/7	0.92	0.37	139,140,140,140	0
85	MG	l	402	1/1	0.92	0.33	57,57,57,57	0
85	MG	1	4054	1/1	0.92	0.21	56,56,56,56	0
85	MG	AR	3820	1/1	0.92	0.26	43,43,43,43	0
85	MG	1	3871	1/1	0.92	0.47	30,30,30,30	0
85	MG	1	3850	1/1	0.92	0.48	31,31,31,31	0
85	MG	3	210	1/1	0.92	0.39	59,59,59,59	0
84	OHX	6	2023	7/7	0.92	0.38	161,161,162,162	0
84	OHX	1	3690	7/7	0.92	0.41	122,123,123,123	0
85	MG	x	204	1/1	0.92	0.35	28,28,28,28	0
85	MG	AR	3785	1/1	0.92	0.47	57,57,57,57	0
85	MG	A	2100	1/1	0.92	0.44	92,92,92,92	0
84	OHX	A	2037	7/7	0.92	0.44	153,154,154,155	0
85	MG	AR	3747	1/1	0.92	0.30	23,23,23,23	0
85	MG	AR	4178	1/1	0.92	0.19	24,24,24,24	0
84	OHX	AR	3732	7/7	0.92	0.52	146,146,147,147	0
84	OHX	1	3692	7/7	0.92	0.29	113,113,113,113	0
84	OHX	AR	3716	7/7	0.92	0.37	143,143,143,143	0
85	MG	AR	4038	1/1	0.92	0.23	35,35,35,35	0
84	OHX	AR	3657	7/7	0.92	0.39	114,114,115,115	0
85	MG	AR	4027	1/1	0.92	0.23	76,76,76,76	0
85	MG	A	2157	1/1	0.92	0.79	75,75,75,75	0
85	MG	1	4039	1/1	0.92	0.48	40,40,40,40	0
84	OHX	AR	3668	7/7	0.92	0.37	131,132,132,132	0
84	OHX	1	3666	7/7	0.92	0.42	117,118,118,118	0
84	OHX	6	2005	7/7	0.92	0.42	126,126,127,127	0
84	OHX	AR	3694	7/7	0.92	0.33	146,147,147,147	0
85	MG	AR	4209	1/1	0.92	0.40	74,74,74,74	0
85	MG	1	3969	1/1	0.92	0.21	41,41,41,41	0
84	OHX	A	1981	7/7	0.92	0.16	194,195,195,195	0
84	OHX	A	2019	7/7	0.92	0.29	176,176,176,176	0
85	MG	6	2095	1/1	0.92	0.43	41,41,41,41	0
85	MG	1	3947	1/1	0.92	0.21	26,26,26,26	0
85	MG	6	2121	1/1	0.92	0.28	41,41,41,41	0
84	OHX	1	3627	7/7	0.92	0.28	141,142,142,143	0
84	OHX	1	3665	7/7	0.92	0.36	129,129,129,129	0
84	OHX	CG	302	7/7	0.92	0.38	147,147,147,148	0
85	MG	1	4002	1/1	0.92	0.56	37,37,37,37	0
85	MG	AR	3927	1/1	0.92	0.45	35,35,35,35	0
85	MG	1	3949	1/1	0.92	0.47	44,44,44,44	0
85	MG	1	3937	1/1	0.92	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3961	1/1	0.92	0.53	43,43,43,43	0
85	MG	1	3764	1/1	0.92	0.58	41,41,41,41	0
84	OHX	AR	3721	7/7	0.92	0.38	139,139,140,140	0
85	MG	1	3728	1/1	0.92	0.61	52,52,52,52	0
85	MG	A	2126	1/1	0.92	0.68	64,64,64,64	0
85	MG	AR	3992	1/1	0.92	0.64	67,67,67,67	0
85	MG	AR	4061	1/1	0.92	0.53	50,50,50,50	0
84	OHX	1	3488	7/7	0.92	0.17	109,109,109,110	0
85	MG	AR	3902	1/1	0.92	0.57	42,42,42,42	0
85	MG	AR	3792	1/1	0.92	0.51	43,43,43,43	0
85	MG	AR	3864	1/1	0.92	0.29	40,40,40,40	0
85	MG	1	4107	1/1	0.92	0.16	40,40,40,40	0
85	MG	4	225	1/1	0.92	0.32	25,25,25,25	0
85	MG	AR	3977	1/1	0.92	0.41	41,41,41,41	0
85	MG	AS	214	1/1	0.92	0.30	52,52,52,52	0
84	OHX	1	3688	7/7	0.92	0.25	129,130,130,130	0
85	MG	AR	4230	1/1	0.92	0.55	18,18,18,18	0
84	OHX	d9	101	7/7	0.92	0.48	153,153,154,154	0
84	OHX	6	1977	7/7	0.92	0.25	150,151,151,152	0
85	MG	1	3864	1/1	0.92	0.25	38,38,38,38	0
84	OHX	AR	3709	7/7	0.92	0.28	110,111,111,111	0
85	MG	1	3740	1/1	0.92	0.36	30,30,30,30	0
85	MG	AR	4031	1/1	0.92	0.20	39,39,39,39	0
84	OHX	1	3672	7/7	0.92	0.41	147,147,147,148	0
85	MG	1	3877	1/1	0.92	0.71	36,36,36,36	0
85	MG	1	3942	1/1	0.92	0.26	32,32,32,32	0
84	OHX	1	3722	1/7	0.92	0.12	136,136,136,136	0
85	MG	AR	4165	1/1	0.92	0.21	43,43,43,43	0
85	MG	1	4146	1/1	0.92	0.17	48,48,48,48	0
85	MG	DA	202	1/1	0.92	0.20	45,45,45,45	0
84	OHX	1	3651	7/7	0.92	0.26	130,130,131,131	0
85	MG	6	2091	1/1	0.92	0.41	61,61,61,61	0
84	OHX	6	2050	7/7	0.92	0.47	159,159,160,160	0
84	OHX	c5	201	7/7	0.92	0.19	161,161,161,161	0
84	OHX	6	2033	7/7	0.92	0.39	150,151,151,152	0
85	MG	AR	3924	1/1	0.92	0.49	27,27,27,27	0
85	MG	6	2077	1/1	0.92	0.54	39,39,39,39	0
85	MG	A	2061	1/1	0.92	0.50	59,59,59,59	0
85	MG	6	2132	1/1	0.92	0.35	42,42,42,42	0
84	OHX	1	3643	7/7	0.92	0.39	114,114,114,114	0
85	MG	3	214	1/1	0.92	0.52	34,34,34,34	0
85	MG	AR	3996	1/1	0.92	0.33	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4214	1/1	0.92	0.39	43,43,43,43	0
85	MG	1	4079	1/1	0.92	0.21	97,97,97,97	0
85	MG	6	2106	1/1	0.92	0.39	50,50,50,50	0
85	MG	1	4089	1/1	0.92	0.21	42,42,42,42	0
84	OHX	l	401	7/7	0.92	0.41	143,143,144,144	0
85	MG	AR	4233	1/1	0.92	0.33	31,31,31,31	0
85	MG	1	3974	1/1	0.92	0.22	28,28,28,28	0
84	OHX	6	2007	7/7	0.92	0.28	145,146,146,146	0
84	OHX	AR	3506	7/7	0.92	0.21	112,112,112,112	0
85	MG	6	2056	1/1	0.92	0.22	77,77,77,77	0
85	MG	AR	4072	1/1	0.92	0.25	70,70,70,70	0
85	MG	1	4008	1/1	0.92	0.29	37,37,37,37	0
84	OHX	AR	3644	7/7	0.92	0.31	126,127,127,127	0
84	OHX	AR	3599	7/7	0.92	0.24	136,136,136,136	0
85	MG	AR	4189	1/1	0.92	1.14	32,32,32,32	0
85	MG	A	2115	1/1	0.92	0.38	83,83,83,83	0
84	OHX	1	3698	7/7	0.92	0.30	162,163,163,163	0
85	MG	AR	4192	1/1	0.92	0.19	29,29,29,29	0
84	OHX	A	2017	7/7	0.92	0.31	158,159,160,160	0
85	MG	1	4099	1/1	0.92	0.23	44,44,44,44	0
84	OHX	1	3652	7/7	0.92	0.33	110,110,110,110	0
85	MG	o	302	1/1	0.92	0.21	39,39,39,39	0
85	MG	1	3821	1/1	0.92	0.52	66,66,66,66	0
85	MG	1	3943	1/1	0.92	0.54	37,37,37,37	0
85	MG	1	3905	1/1	0.92	0.47	38,38,38,38	0
85	MG	A	2052	1/1	0.93	0.42	53,53,53,53	0
84	OHX	1	3563	7/7	0.93	0.24	114,114,115,115	0
84	OHX	AR	3708	7/7	0.93	0.26	138,138,139,139	0
85	MG	AR	3798	1/1	0.93	0.33	33,33,33,33	0
84	OHX	6	1932	7/7	0.93	0.23	132,132,133,133	0
85	MG	A	2044	1/1	0.93	0.80	50,50,50,50	0
84	OHX	AR	3527	7/7	0.93	0.20	112,112,112,112	0
84	OHX	A	2040	7/7	0.93	0.37	162,162,162,162	0
84	OHX	6	2032	7/7	0.93	0.50	131,131,132,132	0
85	MG	A	2090	1/1	0.93	0.20	57,57,57,57	0
85	MG	1	4041	1/1	0.93	0.16	45,45,45,45	0
85	MG	sM	201	1/1	0.93	0.12	41,41,41,41	0
84	OHX	1	3664	7/7	0.93	0.35	124,124,124,124	0
85	MG	A	2076	1/1	0.93	0.35	51,51,51,51	0
85	MG	o	301	1/1	0.93	0.19	34,34,34,34	0
85	MG	AR	4243	1/1	0.93	0.59	30,30,30,30	0
85	MG	AR	3805	1/1	0.93	0.44	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3754	1/1	0.93	0.31	40,40,40,40	0
84	OHX	1	3655	7/7	0.93	0.37	138,138,138,139	0
85	MG	1	3921	1/1	0.93	0.12	57,57,57,57	0
85	MG	AR	3758	1/1	0.93	0.30	37,37,37,37	0
85	MG	AR	3962	1/1	0.93	0.19	93,93,93,93	0
84	OHX	6	2024	7/7	0.93	0.35	151,152,152,153	0
84	OHX	6	2038	7/7	0.93	0.41	148,148,148,148	0
85	MG	CG	303	1/1	0.93	0.13	62,62,62,62	0
84	OHX	AR	3596	7/7	0.93	0.24	121,121,122,122	0
85	MG	1	4178	1/1	0.93	0.40	28,28,28,28	0
85	MG	DO	202	1/1	0.93	0.25	42,42,42,42	0
84	OHX	6	1987	7/7	0.93	0.28	137,137,138,138	0
85	MG	AT	223	1/1	0.93	0.79	45,45,45,45	0
84	OHX	x	202	7/7	0.93	0.36	144,144,145,145	0
85	MG	6	2065	1/1	0.93	0.58	40,40,40,40	0
84	OHX	1	3556	7/7	0.93	0.27	117,117,117,117	0
85	MG	AR	3920	1/1	0.93	0.50	27,27,27,27	0
85	MG	1	3975	1/1	0.93	0.33	42,42,42,42	0
85	MG	A	2158	1/1	0.93	0.34	67,67,67,67	0
84	OHX	1	3661	7/7	0.93	0.32	119,120,120,120	0
85	MG	1	4062	1/1	0.93	0.16	45,45,45,45	0
85	MG	AR	4015	1/1	0.93	0.16	45,45,45,45	0
84	OHX	1	3694	7/7	0.93	0.41	116,116,117,117	0
84	OHX	AR	3723	7/7	0.93	0.28	146,146,147,147	0
84	OHX	AR	3635	7/7	0.93	0.22	137,138,138,138	0
84	OHX	6	2049	7/7	0.93	0.33	170,171,171,171	0
85	MG	AR	4144	1/1	0.93	0.33	41,41,41,41	0
85	MG	1	3896	1/1	0.93	0.30	36,36,36,36	0
85	MG	AR	3748	1/1	0.93	0.38	44,44,44,44	0
85	MG	A	2147	1/1	0.93	0.26	79,79,79,79	0
85	MG	AR	3788	1/1	0.93	0.50	28,28,28,28	0
88	ZN	c	101	1/1	0.93	0.34	145,145,145,145	0
85	MG	1	3734	1/1	0.93	0.34	43,43,43,43	0
84	OHX	AS	209	7/7	0.93	0.31	140,140,140,140	0
85	MG	4	230	1/1	0.93	0.34	35,35,35,35	0
85	MG	AR	3769	1/1	0.93	0.26	59,59,59,59	0
84	OHX	1	3713	7/7	0.93	0.26	138,138,138,139	0
85	MG	AR	4078	1/1	0.93	0.52	60,60,60,60	0
84	OHX	6	2037	7/7	0.93	0.40	137,137,138,138	0
84	OHX	AR	3663	7/7	0.93	0.29	147,148,148,148	0
85	MG	AR	4057	1/1	0.93	0.39	41,41,41,41	0
84	OHX	4	216	7/7	0.93	0.26	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3670	7/7	0.93	0.19	143,143,144,144	0
85	MG	1	4153	1/1	0.93	0.18	39,39,39,39	0
84	OHX	6	1989	7/7	0.93	0.43	143,144,144,145	0
84	OHX	AR	3736	7/7	0.93	0.28	132,132,132,133	0
85	MG	AR	3757	1/1	0.93	0.41	31,31,31,31	0
84	OHX	A	2020	7/7	0.93	0.23	147,148,148,148	0
84	OHX	AR	3641	7/7	0.93	0.48	133,133,133,133	0
85	MG	1	3964	1/1	0.93	0.47	68,68,68,68	0
85	MG	1	3906	1/1	0.93	0.36	42,42,42,42	0
85	MG	AR	4167	1/1	0.93	0.25	71,71,71,71	0
85	MG	AR	4193	1/1	0.93	0.32	38,38,38,38	0
85	MG	1	3826	1/1	0.93	0.25	33,33,33,33	0
85	MG	CQ	201	1/1	0.93	0.38	34,34,34,34	0
84	OHX	6	2022	7/7	0.93	0.29	153,154,154,155	0
84	OHX	CE	402	7/7	0.93	0.38	138,139,139,139	0
85	MG	1	3756	1/1	0.93	0.42	32,32,32,32	0
84	OHX	6	1950	7/7	0.93	0.21	135,135,136,136	0
84	OHX	1	3485	7/7	0.93	0.16	120,121,121,121	0
85	MG	1	3828	1/1	0.93	0.55	30,30,30,30	0
84	OHX	AT	217	7/7	0.93	0.37	128,128,128,128	0
85	MG	A	2078	1/1	0.93	0.68	54,54,54,54	0
85	MG	j	301	1/1	0.93	0.21	29,29,29,29	0
85	MG	AR	3966	1/1	0.93	0.45	38,38,38,38	0
84	OHX	1	3552	7/7	0.93	0.10	150,150,151,151	0
84	OHX	1	3636	7/7	0.93	0.32	126,126,126,126	0
85	MG	1	4217	1/1	0.93	0.92	58,58,58,58	0
84	OHX	AR	3704	7/7	0.93	0.38	133,133,133,133	0
84	OHX	1	3614	7/7	0.93	0.28	133,133,133,134	0
85	MG	AR	4058	1/1	0.93	0.53	61,61,61,61	0
85	MG	4	217	1/1	0.93	0.56	52,52,52,52	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
84	OHX	AR	3706	7/7	0.93	0.34	155,155,155,156	0
85	MG	3	222	1/1	0.93	0.38	52,52,52,52	0
85	MG	AR	3925	1/1	0.93	0.41	34,34,34,34	0
85	MG	AR	3928	1/1	0.93	0.46	39,39,39,39	0
84	OHX	A	1966	7/7	0.93	0.19	131,131,132,132	0
85	MG	1	4068	1/1	0.93	0.46	42,42,42,42	0
85	MG	A	2104	1/1	0.93	0.15	137,137,137,137	0
85	MG	AR	4242	1/1	0.93	0.46	35,35,35,35	0
84	OHX	6	2035	7/7	0.93	0.36	142,142,143,143	0
84	OHX	AR	3649	7/7	0.93	0.50	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	6	2043	7/7	0.93	0.31	145,145,146,146	0
84	OHX	A	1996	7/7	0.93	0.32	139,140,140,141	0
84	OHX	AR	3701	7/7	0.93	0.29	128,128,128,128	0
85	MG	6	2116	1/1	0.93	0.21	62,62,62,62	0
84	OHX	1	3704	7/7	0.93	0.33	116,117,117,117	0
85	MG	AR	4152	1/1	0.93	0.23	38,38,38,38	0
84	OHX	1	3686	7/7	0.93	0.58	156,156,157,157	0
85	MG	AR	4211	1/1	0.93	0.14	73,73,73,73	0
85	MG	A	2055	1/1	0.93	0.47	71,71,71,71	0
85	MG	A	2072	1/1	0.93	0.39	66,66,66,66	0
84	OHX	AR	3711	7/7	0.93	0.37	144,144,145,145	0
85	MG	A	2105	1/1	0.93	0.43	94,94,94,94	0
84	OHX	A	1918	7/7	0.93	0.23	128,129,129,129	0
85	MG	1	4136	1/1	0.93	0.27	40,40,40,40	0
85	MG	1	3912	1/1	0.93	0.59	22,22,22,22	0
84	OHX	AR	3571	7/7	0.93	0.18	125,125,125,125	0
84	OHX	6	1992	7/7	0.93	0.23	137,137,138,138	0
85	MG	A	2123	1/1	0.93	0.51	55,55,55,55	0
85	MG	AR	4109	1/1	0.93	0.16	39,39,39,39	0
85	MG	1	4086	1/1	0.93	0.29	32,32,32,32	0
85	MG	1	3868	1/1	0.93	0.42	29,29,29,29	0
84	OHX	6	2013	7/7	0.93	0.32	121,122,122,122	0
85	MG	AR	4201	1/1	0.93	0.27	35,35,35,35	0
84	OHX	AR	3678	7/7	0.93	0.42	137,137,137,138	0
85	MG	c1	202	1/1	0.93	0.41	67,67,67,67	0
85	MG	6	2067	1/1	0.93	0.30	45,45,45,45	0
85	MG	AR	3767	1/1	0.93	0.58	35,35,35,35	0
84	OHX	6	1986	7/7	0.93	0.32	147,148,148,148	0
85	MG	1	3804	1/1	0.93	0.50	35,35,35,35	0
85	MG	AR	4016	1/1	0.93	0.36	33,33,33,33	0
84	OHX	6	1961	7/7	0.93	0.19	128,129,129,130	0
84	OHX	AR	3675	7/7	0.93	0.33	138,139,139,139	0
85	MG	1	3837	1/1	0.93	0.33	26,26,26,26	0
85	MG	1	4016	1/1	0.93	0.18	39,39,39,39	0
84	OHX	AR	3597	7/7	0.93	0.30	150,151,151,151	0
85	MG	AR	4158	1/1	0.93	0.20	29,29,29,29	0
85	MG	6	2137	1/1	0.93	0.12	82,82,82,82	0
85	MG	AR	4218	1/1	0.93	0.27	54,54,54,54	0
85	MG	AR	3847	1/1	0.93	0.16	38,38,38,38	0
85	MG	1	3946	1/1	0.93	0.28	34,34,34,34	0
85	MG	1	4025	1/1	0.93	0.48	32,32,32,32	0
84	OHX	AR	3740	7/7	0.93	0.25	161,161,161,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3650	7/7	0.93	0.44	118,118,118,118	0
85	MG	1	3973	1/1	0.93	0.47	37,37,37,37	0
85	MG	AR	3839	1/1	0.93	0.43	33,33,33,33	0
84	OHX	AR	3725	7/7	0.93	0.20	165,165,165,165	0
85	MG	1	3729	1/1	0.93	0.32	90,90,90,90	0
84	OHX	K	201	7/7	0.93	0.51	137,137,138,138	0
85	MG	AR	4002	1/1	0.93	0.50	28,28,28,28	0
85	MG	6	2094	1/1	0.93	0.22	37,37,37,37	0
85	MG	AR	4041	1/1	0.93	0.36	34,34,34,34	0
85	MG	A	2060	1/1	0.93	0.62	55,55,55,55	0
85	MG	AR	4077	1/1	0.93	0.32	40,40,40,40	0
84	OHX	AR	3606	7/7	0.93	0.31	113,113,114,114	0
85	MG	1	4189	1/1	0.93	0.36	27,27,27,27	0
85	MG	AF	201	1/1	0.93	0.30	41,41,41,41	0
85	MG	AR	4204	1/1	0.93	0.30	38,38,38,38	0
84	OHX	1	3609	7/7	0.93	0.40	119,120,120,120	0
84	OHX	1	3711	7/7	0.93	0.59	119,120,120,120	0
85	MG	1	3773	1/1	0.93	0.21	38,38,38,38	0
85	MG	AR	3965	1/1	0.93	0.25	50,50,50,50	0
85	MG	AR	3905	1/1	0.93	0.48	29,29,29,29	0
85	MG	6	2112	1/1	0.93	0.53	46,46,46,46	0
85	MG	1	4017	1/1	0.93	0.21	101,101,101,101	0
84	OHX	1	3618	7/7	0.93	0.19	190,190,190,190	0
85	MG	AR	4143	1/1	0.93	0.26	34,34,34,34	0
85	MG	6	2125	1/1	0.93	0.32	75,75,75,75	0
84	OHX	AR	3674	7/7	0.93	0.46	130,130,130,131	0
84	OHX	6	2036	7/7	0.93	0.40	135,135,136,136	0
85	MG	AR	3823	1/1	0.93	0.51	39,39,39,39	0
85	MG	AR	4185	1/1	0.93	0.37	38,38,38,38	0
84	OHX	AR	3636	7/7	0.93	0.48	133,133,134,134	0
84	OHX	AR	3655	7/7	0.94	0.24	129,129,130,130	0
85	MG	1	3794	1/1	0.94	0.53	34,34,34,34	0
85	MG	A	2096	1/1	0.94	0.41	62,62,62,62	0
84	OHX	A	1974	7/7	0.94	0.14	167,167,168,168	0
84	OHX	6	1962	7/7	0.94	0.30	136,137,137,137	0
85	MG	1	3829	1/1	0.94	0.53	16,16,16,16	0
85	MG	AR	3949	1/1	0.94	0.19	32,32,32,32	0
84	OHX	A	2022	7/7	0.94	0.36	167,167,167,167	0
84	OHX	1	3631	7/7	0.94	0.32	116,116,117,117	0
84	OHX	6	2047	7/7	0.94	0.32	161,162,162,162	0
84	OHX	AR	3666	7/7	0.94	0.27	130,131,131,131	0
84	OHX	A	1953	7/7	0.94	0.41	146,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3784	1/1	0.94	0.24	51,51,51,51	0
84	OHX	6	1940	7/7	0.94	0.13	149,150,151,151	0
85	MG	6	2096	1/1	0.94	0.57	68,68,68,68	0
85	MG	AR	4006	1/1	0.94	0.55	47,47,47,47	0
85	MG	1	4010	1/1	0.94	0.46	30,30,30,30	0
84	OHX	AT	215	7/7	0.94	0.20	137,138,138,138	0
84	OHX	AR	3681	7/7	0.94	0.23	140,140,140,141	0
85	MG	1	4194	1/1	0.94	0.50	22,22,22,22	0
85	MG	A	2071	1/1	0.94	0.33	64,64,64,64	0
85	MG	1	4181	1/1	0.94	0.35	23,23,23,23	0
85	MG	AR	4036	1/1	0.94	0.27	41,41,41,41	0
84	OHX	AR	3531	7/7	0.94	0.19	115,115,115,115	0
85	MG	AR	3981	1/1	0.94	0.14	33,33,33,33	0
84	OHX	AR	3710	7/7	0.94	0.34	137,137,137,138	0
84	OHX	4	214	7/7	0.94	0.46	140,140,140,140	0
85	MG	AR	4203	1/1	0.94	0.24	29,29,29,29	0
85	MG	AR	3923	1/1	0.94	0.66	38,38,38,38	0
84	OHX	CM	201	7/7	0.94	0.34	150,150,151,151	0
85	MG	1	4169	1/1	0.94	0.27	30,30,30,30	0
85	MG	AR	3912	1/1	0.94	0.54	23,23,23,23	0
84	OHX	6	1993	7/7	0.94	0.28	134,135,135,135	0
84	OHX	AR	3528	7/7	0.94	0.21	108,108,108,108	0
84	OHX	AR	3698	7/7	0.94	0.41	123,123,123,124	0
85	MG	AR	3875	1/1	0.94	0.16	45,45,45,45	0
84	OHX	Q	201	7/7	0.94	0.26	165,165,165,165	0
84	OHX	1	3462	7/7	0.94	0.21	119,120,120,120	0
84	OHX	1	3594	7/7	0.94	0.20	131,131,132,132	0
85	MG	1	4167	1/1	0.94	0.23	23,23,23,23	0
84	OHX	6	1979	7/7	0.94	0.46	135,135,136,136	0
84	OHX	1	3498	7/7	0.94	0.21	115,116,116,116	0
85	MG	1	3890	1/1	0.94	0.47	34,34,34,34	0
85	MG	AR	3825	1/1	0.94	0.27	33,33,33,33	0
85	MG	AR	3993	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
84	OHX	A	2013	7/7	0.94	0.34	132,133,133,133	0
84	OHX	6	2031	7/7	0.94	0.31	125,126,126,126	0
84	OHX	1	3591	7/7	0.94	0.28	109,109,109,109	0
85	MG	AR	3801	1/1	0.94	0.38	32,32,32,32	0
85	MG	AR	3809	1/1	0.94	0.65	37,37,37,37	0
84	OHX	AR	3735	7/7	0.94	0.30	129,129,129,129	0
84	OHX	AR	3685	7/7	0.94	0.33	120,121,121,121	0
84	OHX	1	3514	7/7	0.94	0.18	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3900	1/1	0.94	0.81	37,37,37,37	0
85	MG	AR	3843	1/1	0.94	0.35	30,30,30,30	0
84	OHX	6	2028	7/7	0.94	0.40	123,124,124,124	0
84	OHX	AR	3712	7/7	0.94	0.27	109,109,109,109	0
84	OHX	6	2016	7/7	0.94	0.25	120,120,121,121	0
84	OHX	1	3632	7/7	0.94	0.34	156,156,156,156	0
84	OHX	6	1969	7/7	0.94	0.15	127,127,128,128	0
84	OHX	AR	3563	7/7	0.94	0.17	122,122,123,123	0
85	MG	1	3753	1/1	0.94	0.54	35,35,35,35	0
84	OHX	A	1959	7/7	0.94	0.20	137,138,139,139	0
85	MG	sM	202	1/1	0.94	0.54	42,42,42,42	0
85	MG	1	3738	1/1	0.94	0.35	28,28,28,28	0
84	OHX	AR	3702	7/7	0.94	0.40	139,139,140,140	0
84	OHX	A	2014	7/7	0.94	0.35	127,128,128,128	0
85	MG	6	2102	1/1	0.94	0.46	45,45,45,45	0
85	MG	1	3923	1/1	0.94	0.39	51,51,51,51	0
84	OHX	6	2025	7/7	0.94	0.39	120,120,121,121	0
84	OHX	1	3540	7/7	0.94	0.18	111,111,111,111	0
84	OHX	AR	3654	7/7	0.94	0.50	137,137,138,138	0
84	OHX	1	3705	7/7	0.94	0.38	131,131,132,132	0
85	MG	1	3860	1/1	0.94	0.47	36,36,36,36	0
84	OHX	3	206	7/7	0.94	0.20	127,127,128,128	0
84	OHX	AR	3659	7/7	0.94	0.54	136,136,137,137	0
85	MG	6	2069	1/1	0.94	0.35	65,65,65,65	0
85	MG	AR	3854	1/1	0.94	0.40	48,48,48,48	0
84	OHX	A	2032	7/7	0.94	0.20	154,154,155,155	0
85	MG	1	3768	1/1	0.94	0.41	36,36,36,36	0
85	MG	6	2097	1/1	0.94	0.42	46,46,46,46	0
84	OHX	AR	3608	7/7	0.94	0.34	131,131,132,132	0
84	OHX	AR	3667	7/7	0.94	0.38	146,147,147,147	0
84	OHX	1	3650	7/7	0.94	0.27	128,128,128,128	0
84	OHX	AR	3713	7/7	0.94	0.24	178,178,179,179	0
85	MG	AR	4213	1/1	0.94	0.14	53,53,53,53	0
85	MG	A	2049	1/1	0.94	0.50	54,54,54,54	0
85	MG	1	4083	1/1	0.94	0.29	41,41,41,41	0
85	MG	AR	3883	1/1	0.94	0.54	32,32,32,32	0
84	OHX	AR	3660	7/7	0.94	0.43	123,123,124,124	0
85	MG	AR	4001	1/1	0.94	0.22	38,38,38,38	0
85	MG	1	3880	1/1	0.94	0.59	31,31,31,31	0
84	OHX	AR	3600	7/7	0.94	0.33	119,119,119,119	0
85	MG	1	4123	1/1	0.94	0.22	51,51,51,51	0
85	MG	AR	4114	1/1	0.94	0.28	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	4	241	1/1	0.94	0.58	45,45,45,45	0
85	MG	AR	3969	1/1	0.94	0.13	60,60,60,60	0
84	OHX	AR	3564	7/7	0.94	0.14	155,155,155,155	0
85	MG	A	2082	1/1	0.94	0.23	61,61,61,61	0
85	MG	6	2159	1/1	0.94	0.08	82,82,82,82	0
85	MG	CR	201	1/1	0.94	0.65	29,29,29,29	0
85	MG	AB	206	1/1	0.94	0.27	26,26,26,26	0
85	MG	AR	3791	1/1	0.94	0.26	34,34,34,34	0
85	MG	1	4126	1/1	0.94	0.98	33,33,33,33	0
85	MG	1	3742	1/1	0.94	0.47	38,38,38,38	0
84	OHX	A	1963	7/7	0.94	0.18	150,151,152,152	0
85	MG	6	2155	1/1	0.94	0.86	58,58,58,58	0
85	MG	1	3957	1/1	0.94	0.39	37,37,37,37	0
84	OHX	A	1991	7/7	0.94	0.24	157,157,158,158	0
84	OHX	AR	3593	7/7	0.94	0.23	113,114,114,114	0
85	MG	AS	230	1/1	0.94	0.42	36,36,36,36	0
84	OHX	6	2019	7/7	0.94	0.30	140,140,141,141	0
84	OHX	A	2028	7/7	0.94	0.34	157,157,158,158	0
85	MG	1	4057	1/1	0.94	0.23	26,26,26,26	0
85	MG	1	3950	1/1	0.94	0.14	38,38,38,38	0
84	OHX	AR	3689	7/7	0.94	0.34	118,118,119,119	0
85	MG	AR	4008	1/1	0.94	0.25	26,26,26,26	0
85	MG	AR	3813	1/1	0.94	0.16	55,55,55,55	0
85	MG	A	2111	1/1	0.94	0.26	90,90,90,90	0
84	OHX	1	3669	7/7	0.94	0.39	131,131,131,131	0
84	OHX	y	201	7/7	0.94	0.32	128,129,129,129	0
84	OHX	AR	3590	7/7	0.94	0.37	113,113,113,113	0
85	MG	1	3808	1/1	0.94	0.47	43,43,43,43	0
85	MG	CQ	202	1/1	0.94	0.33	32,32,32,32	0
85	MG	1	4220	1/1	0.94	0.57	35,35,35,35	0
85	MG	AR	4107	1/1	0.94	0.13	78,78,78,78	0
84	OHX	A	2033	7/7	0.94	0.25	146,146,147,147	0
85	MG	1	3770	1/1	0.94	0.25	29,29,29,29	0
84	OHX	AR	3691	7/7	0.94	0.41	116,116,116,117	0
85	MG	d3	201	1/1	0.94	0.25	49,49,49,49	0
85	MG	AR	4162	1/1	0.94	0.60	56,56,56,56	0
84	OHX	1	3610	7/7	0.94	0.23	130,130,131,131	0
85	MG	AR	3831	1/1	0.94	0.23	44,44,44,44	0
85	MG	6	2108	1/1	0.94	0.56	50,50,50,50	0
84	OHX	1	3629	7/7	0.94	0.22	148,148,148,149	0
84	OHX	1	3679	7/7	0.94	0.30	131,131,132,132	0
85	MG	1	4090	1/1	0.94	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3997	1/1	0.94	0.12	44,44,44,44	0
85	MG	1	4206	1/1	0.94	0.30	30,30,30,30	0
85	MG	AR	3888	1/1	0.94	0.67	24,24,24,24	0
85	MG	1	3730	1/1	0.94	0.35	36,36,36,36	0
85	MG	1	4212	1/1	0.94	0.42	39,39,39,39	0
84	OHX	6	1929	7/7	0.94	0.11	157,158,159,159	0
85	MG	DC	204	1/1	0.94	0.14	35,35,35,35	0
84	OHX	AR	3524	7/7	0.94	0.29	118,119,119,119	0
85	MG	AR	3879	1/1	0.94	0.64	22,22,22,22	0
85	MG	1	3986	1/1	0.94	0.26	42,42,42,42	0
84	OHX	AR	3651	7/7	0.94	0.31	150,151,151,151	0
85	MG	AR	4227	1/1	0.94	0.33	22,22,22,22	0
85	MG	CI	301	1/1	0.94	0.26	33,33,33,33	0
84	OHX	6	1919	7/7	0.94	0.21	121,121,122,122	0
85	MG	1	4166	1/1	0.94	0.16	47,47,47,47	0
85	MG	1	4195	1/1	0.94	0.46	29,29,29,29	0
85	MG	AR	4004	1/1	0.94	0.16	32,32,32,32	0
84	OHX	AT	212	7/7	0.94	0.30	128,128,128,128	0
85	MG	1	3978	1/1	0.94	0.35	46,46,46,46	0
84	OHX	1	3663	7/7	0.94	0.19	111,111,111,111	0
85	MG	AR	3800	1/1	0.94	0.65	33,33,33,33	0
85	MG	AR	3872	1/1	0.94	0.34	43,43,43,43	0
85	MG	1	3922	1/1	0.94	0.45	45,45,45,45	0
85	MG	1	3795	1/1	0.94	0.29	26,26,26,26	0
85	MG	CE	406	1/1	0.94	0.19	25,25,25,25	0
84	OHX	AR	3607	7/7	0.94	0.30	113,113,113,113	0
84	OHX	AR	3634	7/7	0.94	0.26	112,112,113,113	0
85	MG	1	4139	1/1	0.94	0.28	31,31,31,31	0
84	OHX	1	3639	7/7	0.94	0.32	132,132,132,132	0
85	MG	1	4201	1/1	0.94	0.49	28,28,28,28	0
85	MG	1	3763	1/1	0.94	0.65	29,29,29,29	0
85	MG	1	4066	1/1	0.94	0.27	20,20,20,20	0
85	MG	1	3791	1/1	0.94	0.60	54,54,54,54	0
85	MG	6	2113	1/1	0.94	0.23	77,77,77,77	0
84	OHX	1	3648	7/7	0.94	0.25	119,120,120,120	0
85	MG	4	223	1/1	0.94	0.59	27,27,27,27	0
85	MG	6	2054	1/1	0.94	0.39	49,49,49,49	0
84	OHX	1	3689	7/7	0.94	0.52	140,140,141,141	0
84	OHX	1	3615	7/7	0.94	0.38	133,133,133,134	0
84	OHX	r	301	7/7	0.94	0.20	115,115,115,115	0
84	OHX	AR	3611	7/7	0.94	0.23	126,126,126,126	0
85	MG	AR	4010	1/1	0.94	0.30	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3615	7/7	0.94	0.36	132,133,133,133	0
85	MG	1	3735	1/1	0.94	0.35	24,24,24,24	0
85	MG	k	403	1/1	0.94	0.20	30,30,30,30	0
85	MG	AR	4082	1/1	0.94	0.34	24,24,24,24	0
84	OHX	6	2010	7/7	0.94	0.33	154,155,155,155	0
84	OHX	1	3660	7/7	0.94	0.28	153,153,154,154	0
85	MG	AR	3893	1/1	0.94	0.95	50,50,50,50	0
85	MG	AR	3963	1/1	0.94	0.20	49,49,49,49	0
84	OHX	6	1971	7/7	0.94	0.24	136,136,136,137	0
84	OHX	1	3619	7/7	0.94	0.22	127,127,127,127	0
85	MG	AR	4108	1/1	0.94	0.19	36,36,36,36	0
84	OHX	AR	3552	7/7	0.94	0.28	114,114,114,114	0
85	MG	AR	3978	1/1	0.94	0.36	49,49,49,49	0
85	MG	A	2097	1/1	0.94	0.57	53,53,53,53	0
84	OHX	A	2018	7/7	0.94	0.34	155,155,156,156	0
84	OHX	1	3605	7/7	0.94	0.33	129,130,130,130	0
85	MG	1	3727	1/1	0.94	0.28	37,37,37,37	0
85	MG	AR	3959	1/1	0.94	0.28	32,32,32,32	0
84	OHX	AR	3742	7/7	0.94	0.25	128,129,129,129	0
85	MG	AR	3917	1/1	0.94	0.50	42,42,42,42	0
84	OHX	6	1999	7/7	0.94	0.26	138,139,139,140	0
84	OHX	1	3675	7/7	0.94	0.30	140,141,141,141	0
84	OHX	AR	3622	7/7	0.94	0.24	130,131,131,131	0
85	MG	1	4049	1/1	0.94	0.25	32,32,32,32	0
85	MG	1	3747	1/1	0.94	0.34	37,37,37,37	0
84	OHX	1	3641	7/7	0.94	0.36	141,141,141,141	0
84	OHX	6	2042	7/7	0.94	0.34	151,151,151,151	0
85	MG	1	3831	1/1	0.94	0.47	26,26,26,26	0
85	MG	AR	3859	1/1	0.94	0.49	29,29,29,29	0
85	MG	A	2153	1/1	0.94	0.58	51,51,51,51	0
84	OHX	CG	301	7/7	0.94	0.16	142,143,143,144	0
84	OHX	1	3606	7/7	0.95	0.40	138,138,138,138	0
85	MG	AR	4138	1/1	0.95	0.47	28,28,28,28	0
84	OHX	A	1973	7/7	0.95	0.28	167,168,169,169	0
84	OHX	A	1960	7/7	0.95	0.18	151,151,151,152	0
84	OHX	1	3539	7/7	0.95	0.28	119,119,119,119	0
85	MG	1	3841	1/1	0.95	0.59	29,29,29,29	0
85	MG	AR	3942	1/1	0.95	0.56	31,31,31,31	0
85	MG	6	2126	1/1	0.95	0.29	53,53,53,53	0
84	OHX	CL	301	7/7	0.95	0.21	121,122,122,122	0
86	HN8	AR	4263	22/22	0.95	0.26	27,27,27,27	22
85	MG	1	4075	1/1	0.95	0.43	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AH	201	7/7	0.95	0.44	129,129,129,130	0
85	MG	1	3977	1/1	0.95	0.14	48,48,48,48	0
84	OHX	AR	3474	7/7	0.95	0.19	114,114,114,115	0
85	MG	AR	3853	1/1	0.95	0.26	43,43,43,43	0
85	MG	1	3859	1/1	0.95	0.44	28,28,28,28	0
84	OHX	A	1958	7/7	0.95	0.22	173,173,173,173	0
84	OHX	1	3616	7/7	0.95	0.31	146,146,147,147	0
84	OHX	A	1995	7/7	0.95	0.17	151,152,152,152	0
84	OHX	6	1956	7/7	0.95	0.12	174,174,175,175	0
85	MG	1	3809	1/1	0.95	0.27	39,39,39,39	0
85	MG	AR	4066	1/1	0.95	0.14	56,56,56,56	0
84	OHX	A	1986	7/7	0.95	0.29	168,169,170,170	0
84	OHX	A	1969	7/7	0.95	0.34	144,144,145,145	0
85	MG	1	3846	1/1	0.95	0.28	39,39,39,39	0
85	MG	A	2064	1/1	0.95	0.34	65,65,65,65	0
84	OHX	AR	3544	7/7	0.95	0.16	109,109,110,110	0
85	MG	4	219	1/1	0.95	0.68	42,42,42,42	0
84	OHX	1	3604	7/7	0.95	0.34	116,116,117,117	0
84	OHX	AR	3495	7/7	0.95	0.17	113,113,114,114	0
85	MG	6	2179	1/1	0.95	0.36	43,43,43,43	0
85	MG	AR	3989	1/1	0.95	0.23	44,44,44,44	0
85	MG	AR	4202	1/1	0.95	0.56	29,29,29,29	0
85	MG	CE	405	1/1	0.95	0.89	26,26,26,26	0
84	OHX	AK	102	7/7	0.95	0.18	105,105,105,105	0
84	OHX	AR	3575	7/7	0.95	0.28	119,120,120,120	0
85	MG	l	404	1/1	0.95	0.34	35,35,35,35	0
85	MG	1	4141	1/1	0.95	0.38	64,64,64,64	0
85	MG	AR	3880	1/1	0.95	0.47	42,42,42,42	0
85	MG	1	3894	1/1	0.95	0.48	22,22,22,22	0
85	MG	k	404	1/1	0.95	0.67	32,32,32,32	0
84	OHX	1	3544	7/7	0.95	0.16	116,117,117,117	0
84	OHX	1	3583	7/7	0.95	0.16	131,132,132,132	0
84	OHX	1	3657	7/7	0.95	0.28	123,123,124,124	0
84	OHX	1	3487	7/7	0.95	0.17	115,115,116,116	0
84	OHX	AR	3503	7/7	0.95	0.17	120,120,121,121	0
85	MG	AR	3904	1/1	0.95	0.52	21,21,21,21	0
85	MG	AS	212	1/1	0.95	0.33	41,41,41,41	0
84	OHX	AR	3579	7/7	0.95	0.35	130,130,130,130	0
85	MG	6	2073	1/1	0.95	0.52	48,48,48,48	0
85	MG	A	2059	1/1	0.95	0.61	53,53,53,53	0
85	MG	1	3902	1/1	0.95	0.50	35,35,35,35	0
84	OHX	1	3577	7/7	0.95	0.31	118,118,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3724	7/7	0.95	0.27	130,130,131,131	0
85	MG	1	3872	1/1	0.95	0.59	32,32,32,32	0
84	OHX	1	3554	7/7	0.95	0.24	129,129,130,130	0
84	OHX	AR	3577	7/7	0.95	0.09	156,157,158,158	0
85	MG	AR	4062	1/1	0.95	0.17	42,42,42,42	0
85	MG	AR	3972	1/1	0.95	0.53	39,39,39,39	0
85	MG	AR	4111	1/1	0.95	0.35	37,37,37,37	0
84	OHX	6	2027	7/7	0.95	0.47	146,147,147,148	0
84	OHX	6	1984	7/7	0.95	0.26	150,150,151,151	0
85	MG	1	3749	1/1	0.95	0.26	24,24,24,24	0
85	MG	AR	4105	1/1	0.95	0.14	42,42,42,42	0
85	MG	AR	3915	1/1	0.95	0.61	28,28,28,28	0
84	OHX	6	2015	7/7	0.95	0.35	135,135,136,136	0
85	MG	6	2089	1/1	0.95	0.44	44,44,44,44	0
85	MG	4	218	1/1	0.95	0.60	49,49,49,49	0
85	MG	AR	4088	1/1	0.95	0.40	25,25,25,25	0
84	OHX	A	1964	7/7	0.95	0.28	122,122,123,123	0
84	OHX	AR	3673	7/7	0.95	0.19	125,125,125,125	0
84	OHX	6	1954	7/7	0.95	0.09	178,178,178,178	0
84	OHX	1	3559	7/7	0.95	0.17	143,143,143,144	0
84	OHX	AR	3688	7/7	0.95	0.29	136,136,137,137	0
84	OHX	6	2020	7/7	0.95	0.18	135,136,136,137	0
84	OHX	6	2014	7/7	0.95	0.34	129,129,129,130	0
85	MG	6	2062	1/1	0.95	0.42	51,51,51,51	0
84	OHX	A	1915	7/7	0.95	0.21	142,143,143,144	0
85	MG	1	4179	1/1	0.95	0.23	38,38,38,38	0
84	OHX	6	2012	7/7	0.95	0.21	136,136,137,137	0
85	MG	AR	3865	1/1	0.95	0.41	24,24,24,24	0
85	MG	1	4144	1/1	0.95	0.16	53,53,53,53	0
84	OHX	1	3517	7/7	0.95	0.26	119,119,120,120	0
84	OHX	AR	3460	7/7	0.95	0.20	112,112,112,112	0
85	MG	1	3788	1/1	0.95	0.53	45,45,45,45	0
84	OHX	AR	3637	7/7	0.95	0.40	129,129,129,129	0
85	MG	A	2063	1/1	0.95	0.50	51,51,51,51	0
84	OHX	1	3525	7/7	0.95	0.21	114,114,114,115	0
84	OHX	1	3612	7/7	0.95	0.31	122,122,122,122	0
84	OHX	AR	3605	7/7	0.95	0.16	128,128,128,129	0
85	MG	6	2128	1/1	0.95	0.23	47,47,47,47	0
84	OHX	1	3469	7/7	0.95	0.21	117,117,118,118	0
84	OHX	1	3649	7/7	0.95	0.35	113,113,113,113	0
84	OHX	AR	3610	7/7	0.95	0.38	137,138,138,138	0
84	OHX	AR	3714	7/7	0.95	0.33	132,132,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	w	201	1/1	0.95	0.42	37,37,37,37	0
84	OHX	AR	3595	7/7	0.95	0.31	131,131,131,132	0
84	OHX	1	3667	7/7	0.95	0.30	127,127,128,128	0
84	OHX	1	3581	7/7	0.95	0.22	112,113,113,113	0
85	MG	AR	3856	1/1	0.95	0.71	27,27,27,27	0
84	OHX	1	3674	7/7	0.95	0.28	136,136,137,137	0
85	MG	1	3919	1/1	0.95	0.27	33,33,33,33	0
84	OHX	6	1973	7/7	0.95	0.22	137,138,138,138	0
85	MG	4	224	1/1	0.95	0.40	33,33,33,33	0
84	OHX	AR	3499	7/7	0.95	0.15	125,126,126,126	0
85	MG	6	2148	1/1	0.95	0.43	48,48,48,48	0
85	MG	AR	4199	1/1	0.95	0.36	45,45,45,45	0
85	MG	AS	221	1/1	0.95	0.16	60,60,60,60	0
85	MG	1	3796	1/1	0.95	0.54	18,18,18,18	0
85	MG	1	4024	1/1	0.95	0.21	61,61,61,61	0
85	MG	AR	3857	1/1	0.95	0.53	20,20,20,20	0
85	MG	AR	3881	1/1	0.95	0.29	30,30,30,30	0
88	ZN	g	501	1/1	0.95	0.06	119,119,119,119	0
85	MG	A	2120	1/1	0.95	0.22	85,85,85,85	0
85	MG	1	4173	1/1	0.95	0.54	36,36,36,36	0
85	MG	AR	3802	1/1	0.95	0.12	40,40,40,40	0
84	OHX	A	1977	7/7	0.95	0.25	153,154,154,155	0
85	MG	1	3924	1/1	0.95	0.37	60,60,60,60	0
85	MG	AR	4212	1/1	0.95	0.27	31,31,31,31	0
84	OHX	1	3527	7/7	0.95	0.12	135,135,136,136	0
85	MG	1	3914	1/1	0.95	0.50	19,19,19,19	0
84	OHX	AR	3592	7/7	0.95	0.34	114,114,114,114	0
85	MG	AR	3793	1/1	0.95	0.31	29,29,29,29	0
84	OHX	1	3588	7/7	0.95	0.19	128,128,128,128	0
84	OHX	AR	3603	7/7	0.95	0.24	107,107,107,107	0
84	OHX	A	2031	7/7	0.95	0.35	159,160,161,161	0
86	HN8	1	4223	22/22	0.95	0.24	32,32,32,32	0
85	MG	AR	4259	1/1	0.95	0.49	16,16,16,16	0
85	MG	1	3824	1/1	0.95	0.39	25,25,25,25	0
84	OHX	AR	3568	7/7	0.95	0.25	117,117,117,117	0
85	MG	1	3867	1/1	0.95	0.43	35,35,35,35	0
85	MG	DH	203	1/1	0.95	0.28	31,31,31,31	0
84	OHX	AR	3472	7/7	0.95	0.16	111,111,111,112	0
85	MG	1	3839	1/1	0.95	0.19	27,27,27,27	0
84	OHX	AR	3532	7/7	0.95	0.14	135,136,136,137	0
84	OHX	1	3671	7/7	0.95	0.24	149,150,150,150	0
85	MG	CP	504	1/1	0.95	0.23	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3511	7/7	0.95	0.26	108,108,108,108	0
84	OHX	1	3545	7/7	0.95	0.21	120,120,120,120	0
85	MG	AR	3822	1/1	0.95	0.31	46,46,46,46	0
84	OHX	A	1909	7/7	0.95	0.24	151,151,152,153	0
85	MG	6	2156	1/1	0.95	0.16	101,101,101,101	0
84	OHX	6	2009	7/7	0.95	0.18	126,127,127,128	0
84	OHX	1	3634	7/7	0.95	0.17	132,132,132,133	0
84	OHX	AR	3427	7/7	0.95	0.29	110,110,111,111	0
84	OHX	6	1997	7/7	0.95	0.36	132,132,133,133	0
85	MG	AR	3886	1/1	0.95	0.70	30,30,30,30	0
84	OHX	AR	3638	7/7	0.95	0.42	119,119,119,119	0
84	OHX	AR	3703	7/7	0.95	0.51	136,136,136,136	0
85	MG	1	4175	1/1	0.95	0.44	39,39,39,39	0
84	OHX	1	3715	7/7	0.95	0.09	166,166,167,167	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
85	MG	1	3733	1/1	0.95	0.49	26,26,26,26	0
84	OHX	AR	3538	7/7	0.95	0.17	123,123,124,124	0
84	OHX	1	3706	7/7	0.95	0.30	136,137,137,138	0
85	MG	AR	3877	1/1	0.95	0.34	22,22,22,22	0
85	MG	AR	4247	1/1	0.95	0.46	22,22,22,22	0
84	OHX	A	1935	7/7	0.95	0.23	140,140,141,141	0
85	MG	AR	4228	1/1	0.95	0.38	27,27,27,27	0
84	OHX	AT	214	7/7	0.95	0.33	131,131,131,132	0
84	OHX	A	2002	7/7	0.95	0.31	147,148,149,149	0
85	MG	AR	3746	1/1	0.95	0.26	58,58,58,58	0
84	OHX	1	3567	7/7	0.95	0.24	128,129,129,129	0
85	MG	AR	4065	1/1	0.95	0.25	31,31,31,31	0
85	MG	AR	3937	1/1	0.95	0.67	27,27,27,27	0
85	MG	CM	203	1/1	0.95	0.21	55,55,55,55	0
85	MG	AR	4151	1/1	0.95	0.10	148,148,148,148	0
85	MG	1	4208	1/1	0.95	0.32	37,37,37,37	0
85	MG	1	4171	1/1	0.95	0.24	85,85,85,85	0
85	MG	AR	3855	1/1	0.95	0.43	33,33,33,33	0
84	OHX	AR	3624	7/7	0.95	0.33	150,150,151,151	0
84	OHX	A	2024	7/7	0.95	0.24	151,152,153,153	0
85	MG	1	3774	1/1	0.95	0.54	43,43,43,43	0
84	OHX	6	1972	7/7	0.95	0.42	142,143,143,144	0
85	MG	1	4186	1/1	0.95	0.52	25,25,25,25	0
85	MG	6	2107	1/1	0.95	0.55	43,43,43,43	0
84	OHX	1	3481	7/7	0.95	0.19	116,117,117,117	0
85	MG	AR	4012	1/1	0.95	0.35	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3918	1/1	0.95	0.48	27,27,27,27	0
84	OHX	AR	3565	7/7	0.95	0.20	113,113,113,113	0
85	MG	1	3741	1/1	0.95	0.25	37,37,37,37	0
85	MG	1	3879	1/1	0.95	0.38	45,45,45,45	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	3537	7/7	0.95	0.15	131,132,132,132	0
85	MG	1	4071	1/1	0.95	0.20	40,40,40,40	0
84	OHX	1	3681	7/7	0.95	0.32	127,127,127,128	0
84	OHX	6	1966	7/7	0.95	0.15	133,133,134,134	0
85	MG	AR	3901	1/1	0.95	0.45	29,29,29,29	0
84	OHX	AR	3587	7/7	0.95	0.24	126,126,126,126	0
84	OHX	1	3662	7/7	0.95	0.31	116,116,116,116	0
85	MG	6	2135	1/1	0.95	0.24	49,49,49,49	0
84	OHX	A	2027	7/7	0.95	0.33	159,160,161,161	0
84	OHX	4	210	7/7	0.95	0.27	108,108,108,108	0
85	MG	6	2153	1/1	0.95	0.27	97,97,97,97	0
84	OHX	AR	3658	7/7	0.95	0.35	122,123,123,123	0
85	MG	1	3907	1/1	0.95	0.33	40,40,40,40	0
84	OHX	1	3575	7/7	0.95	0.27	116,117,117,117	0
84	OHX	AT	216	7/7	0.95	0.40	132,132,132,132	0
84	OHX	1	3550	7/7	0.95	0.18	115,115,115,116	0
85	MG	6	2147	1/1	0.95	0.12	57,57,57,57	0
84	OHX	AR	3583	7/7	0.95	0.22	113,114,114,114	0
85	MG	AR	4129	1/1	0.95	0.36	26,26,26,26	0
85	MG	1	4207	1/1	0.95	0.28	36,36,36,36	0
84	OHX	AR	3700	7/7	0.95	0.47	135,135,135,135	0
85	MG	1	4106	1/1	0.95	0.34	67,67,67,67	0
85	MG	AR	3867	1/1	0.95	0.55	18,18,18,18	0
84	OHX	1	3599	7/7	0.95	0.43	115,116,116,116	0
85	MG	AR	3826	1/1	0.95	0.32	23,23,23,23	0
84	OHX	A	2000	7/7	0.95	0.24	140,141,141,141	0
85	MG	AR	4121	1/1	0.95	0.30	27,27,27,27	0
85	MG	1	4048	1/1	0.95	0.83	33,33,33,33	0
85	MG	AR	3990	1/1	0.95	0.08	39,39,39,39	0
84	OHX	AR	3618	7/7	0.95	0.21	113,113,114,114	0
84	OHX	AR	3601	7/7	0.95	0.42	127,127,128,128	0
85	MG	AR	4237	1/1	0.95	0.21	39,39,39,39	0
84	OHX	1	3537	7/7	0.95	0.25	115,115,115,116	0
85	MG	1	3769	1/1	0.95	0.19	45,45,45,45	0
84	OHX	6	2026	7/7	0.95	0.25	146,146,147,147	0
85	MG	A	2148	1/1	0.95	0.37	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3941	1/1	0.96	0.46	36,36,36,36	0
84	OHX	A	1944	7/7	0.96	0.12	138,139,139,140	0
85	MG	AR	4112	1/1	0.96	0.15	54,54,54,54	0
84	OHX	1	3582	7/7	0.96	0.29	121,121,121,121	0
85	MG	CP	505	1/1	0.96	0.27	71,71,71,71	0
84	OHX	1	3595	7/7	0.96	0.11	140,140,140,140	0
84	OHX	AR	3466	7/7	0.96	0.18	120,120,121,121	0
84	OHX	1	3703	7/7	0.96	0.46	131,131,132,132	0
84	OHX	1	3531	7/7	0.96	0.19	114,114,114,114	0
84	OHX	AR	3546	7/7	0.96	0.21	123,124,124,124	0
84	OHX	AR	3548	7/7	0.96	0.16	121,121,122,122	0
84	OHX	A	1955	7/7	0.96	0.13	145,146,147,147	0
85	MG	1	3856	1/1	0.96	0.68	24,24,24,24	0
85	MG	AR	4079	1/1	0.96	0.31	34,34,34,34	0
84	OHX	1	3497	7/7	0.96	0.11	125,125,126,126	0
85	MG	AR	3931	1/1	0.96	0.29	17,17,17,17	0
84	OHX	6	2029	7/7	0.96	0.41	152,153,153,154	0
84	OHX	A	1999	7/7	0.96	0.24	146,146,147,147	0
85	MG	AR	3895	1/1	0.96	0.28	43,43,43,43	0
85	MG	1	4176	1/1	0.96	0.62	34,34,34,34	0
84	OHX	AR	3617	7/7	0.96	0.28	123,123,123,123	0
85	MG	lR	201	1/1	0.96	0.36	26,26,26,26	0
85	MG	3	219	1/1	0.96	0.21	56,56,56,56	0
85	MG	AS	229	1/1	0.96	0.24	46,46,46,46	0
85	MG	d3	202	1/1	0.96	0.33	47,47,47,47	0
84	OHX	AR	3598	7/7	0.96	0.18	117,118,118,118	0
84	OHX	1	3543	7/7	0.96	0.22	119,119,120,120	0
84	OHX	1	3677	7/7	0.96	0.33	116,116,117,117	0
84	OHX	1	3489	7/7	0.96	0.21	113,113,114,114	0
85	MG	1	4052	1/1	0.96	0.29	21,21,21,21	0
84	OHX	AR	3543	7/7	0.96	0.24	123,123,123,123	0
84	OHX	k	401	7/7	0.96	0.27	118,118,118,118	0
84	OHX	A	1936	7/7	0.96	0.17	126,127,127,128	0
84	OHX	AR	3699	7/7	0.96	0.36	117,117,117,117	0
84	OHX	T	201	7/7	0.96	0.19	145,146,146,147	0
84	OHX	AR	3580	7/7	0.96	0.20	117,118,118,118	0
85	MG	1	3757	1/1	0.96	0.19	38,38,38,38	0
84	OHX	AR	3693	7/7	0.96	0.41	131,131,131,131	0
84	OHX	6	1946	7/7	0.96	0.17	127,128,128,129	0
85	MG	AS	216	1/1	0.96	0.50	23,23,23,23	0
84	OHX	A	1994	7/7	0.96	0.28	142,143,144,144	0
85	MG	3	213	1/1	0.96	0.45	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4143	1/1	0.96	0.21	29,29,29,29	0
85	MG	6	2104	1/1	0.96	0.20	70,70,70,70	0
84	OHX	1	3455	7/7	0.96	0.16	127,127,127,128	0
84	OHX	AR	3586	7/7	0.96	0.24	119,119,120,120	0
85	MG	AP	503	1/1	0.96	0.28	27,27,27,27	0
84	OHX	1	3541	7/7	0.96	0.26	119,119,120,120	0
84	OHX	6	1947	7/7	0.96	0.14	121,122,122,122	0
85	MG	A	2137	1/1	0.96	0.48	58,58,58,58	0
84	OHX	1	3509	7/7	0.96	0.14	119,120,120,120	0
84	OHX	AR	3743	7/7	0.96	0.33	109,109,109,109	0
84	OHX	A	1997	7/7	0.96	0.28	139,140,140,140	0
85	MG	4	239	1/1	0.96	0.69	43,43,43,43	0
85	MG	1	3775	1/1	0.96	0.29	32,32,32,32	0
85	MG	AR	3926	1/1	0.96	0.37	33,33,33,33	0
85	MG	AR	3844	1/1	0.96	0.40	27,27,27,27	0
85	MG	AR	4091	1/1	0.96	0.31	35,35,35,35	0
84	OHX	AR	3687	7/7	0.96	0.37	121,121,122,122	0
85	MG	1	4120	1/1	0.96	0.40	27,27,27,27	0
84	OHX	AR	3715	7/7	0.96	0.29	118,118,119,119	0
84	OHX	1	3684	7/7	0.96	0.41	141,141,141,141	0
84	OHX	AR	3662	7/7	0.96	0.22	111,111,112,112	0
84	OHX	AR	3632	7/7	0.96	0.35	117,117,118,118	0
84	OHX	AR	3522	7/7	0.96	0.13	114,114,115,115	0
84	OHX	1	3451	7/7	0.96	0.22	111,111,111,111	0
84	OHX	1	3640	7/7	0.96	0.35	124,124,124,125	0
84	OHX	AT	210	7/7	0.96	0.20	119,119,120,120	0
84	OHX	AR	3697	7/7	0.96	0.25	114,115,115,115	0
84	OHX	1	3611	7/7	0.96	0.21	119,119,119,120	0
84	OHX	AR	3562	7/7	0.96	0.24	124,124,124,124	0
84	OHX	AR	3541	7/7	0.96	0.19	125,125,125,125	0
84	OHX	CX	202	7/7	0.96	0.27	117,118,118,118	0
85	MG	CK	202	1/1	0.96	0.20	44,44,44,44	0
85	MG	6	2114	1/1	0.96	0.47	46,46,46,46	0
85	MG	1	4221	1/1	0.96	0.52	35,35,35,35	0
84	OHX	6	1921	7/7	0.96	0.17	141,141,142,143	0
84	OHX	1	3446	7/7	0.96	0.19	116,116,116,116	0
85	MG	AR	4000	1/1	0.96	0.43	25,25,25,25	0
85	MG	AR	3936	1/1	0.96	0.52	20,20,20,20	0
84	OHX	1	3507	7/7	0.96	0.23	113,113,114,114	0
84	OHX	A	1933	7/7	0.96	0.13	122,122,122,123	0
84	OHX	A	1976	7/7	0.96	0.18	123,124,124,124	0
84	OHX	6	1978	7/7	0.96	0.29	117,117,117,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3597	7/7	0.96	0.39	117,117,118,118	0
84	OHX	AR	3534	7/7	0.96	0.16	109,109,109,109	0
85	MG	AK	103	1/1	0.96	0.44	36,36,36,36	0
85	MG	AR	3787	1/1	0.96	0.69	31,31,31,31	0
85	MG	1	4188	1/1	0.96	0.36	28,28,28,28	0
85	MG	1	4197	1/1	0.96	0.34	32,32,32,32	0
84	OHX	6	1995	7/7	0.96	0.24	133,134,134,135	0
85	MG	1	3854	1/1	0.96	0.62	34,34,34,34	0
84	OHX	AT	211	7/7	0.96	0.11	137,138,138,138	0
84	OHX	A	1989	7/7	0.96	0.37	154,155,155,155	0
85	MG	1	3876	1/1	0.96	0.40	37,37,37,37	0
84	OHX	1	3637	7/7	0.96	0.15	140,140,140,141	0
84	OHX	AR	3682	7/7	0.96	0.52	144,144,144,145	0
85	MG	1	4103	1/1	0.96	0.27	60,60,60,60	0
85	MG	AR	3933	1/1	0.96	0.47	24,24,24,24	0
84	OHX	1	3685	7/7	0.96	0.41	121,121,121,121	0
84	OHX	1	3593	7/7	0.96	0.15	166,167,167,167	0
84	OHX	CK	201	7/7	0.96	0.21	118,118,119,119	0
84	OHX	AR	3581	7/7	0.96	0.18	109,109,109,109	0
84	OHX	6	2011	7/7	0.96	0.43	146,146,147,147	0
84	OHX	AR	3555	7/7	0.96	0.21	115,115,115,115	0
84	OHX	1	3592	7/7	0.96	0.33	117,117,117,117	0
85	MG	AR	3790	1/1	0.96	0.34	22,22,22,22	0
84	OHX	AR	3731	7/7	0.96	0.19	117,117,117,117	0
85	MG	AR	3919	1/1	0.96	0.43	34,34,34,34	0
84	OHX	6	1996	7/7	0.96	0.20	154,154,155,155	0
84	OHX	1	3526	7/7	0.96	0.29	114,115,115,115	0
85	MG	AR	4217	1/1	0.96	0.60	80,80,80,80	0
84	OHX	AR	3669	7/7	0.96	0.17	175,176,176,176	0
84	OHX	A	1983	7/7	0.96	0.24	142,142,143,143	0
84	OHX	1	3518	7/7	0.96	0.15	109,110,110,110	0
85	MG	6	2172	1/1	0.96	0.26	38,38,38,38	0
85	MG	1	4032	1/1	0.96	0.31	42,42,42,42	0
84	OHX	A	2003	7/7	0.96	0.32	129,130,130,130	0
84	OHX	AR	3514	7/7	0.96	0.19	112,112,112,113	0
84	OHX	1	3654	7/7	0.96	0.14	136,136,136,137	0
85	MG	4	226	1/1	0.96	0.59	42,42,42,42	0
84	OHX	AR	3557	7/7	0.96	0.17	123,123,124,124	0
85	MG	6	2075	1/1	0.96	0.14	76,76,76,76	0
84	OHX	1	3589	7/7	0.96	0.23	113,113,113,113	0
85	MG	A	2074	1/1	0.96	0.41	55,55,55,55	0
84	OHX	AR	3553	7/7	0.96	0.29	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	3	215	1/1	0.96	0.57	31,31,31,31	0
84	OHX	AR	3441	7/7	0.96	0.18	116,117,117,117	0
85	MG	1	4216	1/1	0.96	0.39	23,23,23,23	0
84	OHX	AR	3545	7/7	0.96	0.24	108,108,108,108	0
85	MG	AR	3772	1/1	0.96	0.52	37,37,37,37	0
85	MG	1	3968	1/1	0.96	0.47	29,29,29,29	0
84	OHX	AR	3671	7/7	0.96	0.28	113,113,113,113	0
85	MG	6	2055	1/1	0.96	0.73	49,49,49,49	0
84	OHX	AR	3676	7/7	0.96	0.29	122,122,123,123	0
84	OHX	AR	3614	7/7	0.96	0.20	114,114,114,114	0
84	OHX	6	1952	7/7	0.96	0.14	148,148,148,148	0
85	MG	1	4094	1/1	0.96	0.15	78,78,78,78	0
85	MG	1	3792	1/1	0.96	0.52	37,37,37,37	0
84	OHX	6	1990	7/7	0.96	0.29	129,130,130,130	0
84	OHX	AR	3612	7/7	0.96	0.34	111,111,111,111	0
84	OHX	AR	3570	7/7	0.96	0.25	120,121,121,121	0
84	OHX	6	1976	7/7	0.96	0.13	146,147,147,148	0
84	OHX	1	3510	7/7	0.96	0.16	111,111,111,111	0
85	MG	A	2144	1/1	0.96	0.39	69,69,69,69	0
84	OHX	1	3458	7/7	0.96	0.20	116,116,116,117	0
84	OHX	AR	3628	7/7	0.96	0.32	147,148,148,148	0
85	MG	1	4177	1/1	0.96	0.44	27,27,27,27	0
84	OHX	AR	3633	7/7	0.96	0.28	124,125,125,125	0
85	MG	AR	4095	1/1	0.96	0.22	25,25,25,25	0
84	OHX	1	3693	7/7	0.96	0.27	118,118,118,118	0
84	OHX	1	3547	7/7	0.96	0.11	120,121,121,121	0
84	OHX	AR	3629	7/7	0.96	0.14	141,141,141,142	0
84	OHX	c1	201	7/7	0.96	0.41	147,148,148,149	0
85	MG	1	4222	1/1	0.96	0.65	13,13,13,13	0
84	OHX	1	3431	7/7	0.96	0.30	114,114,114,114	0
84	OHX	AR	3512	7/7	0.96	0.18	118,118,119,119	0
84	OHX	A	2001	7/7	0.96	0.20	136,137,137,138	0
84	OHX	AR	3621	7/7	0.96	0.35	135,135,136,136	0
84	OHX	3	207	7/7	0.96	0.20	137,138,138,138	0
85	MG	DH	202	1/1	0.96	0.26	40,40,40,40	0
84	OHX	1	3471	7/7	0.96	0.21	112,112,113,113	0
85	MG	1	3781	1/1	0.96	0.39	33,33,33,33	0
84	OHX	1	3617	7/7	0.96	0.23	122,122,122,122	0
84	OHX	A	1975	7/7	0.96	0.10	156,158,158,158	0
84	OHX	A	2005	7/7	0.96	0.32	131,132,132,132	0
85	MG	6	2177	1/1	0.96	0.19	68,68,68,68	0
84	OHX	AR	3613	7/7	0.96	0.29	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3624	7/7	0.96	0.20	136,136,136,137	0
85	MG	6	2187	1/1	0.96	0.18	82,82,82,82	0
84	OHX	6	1998	7/7	0.96	0.33	146,146,147,147	0
84	OHX	AR	3556	7/7	0.96	0.21	109,109,109,109	0
85	MG	6	2151	1/1	0.96	0.15	60,60,60,60	0
84	OHX	6	1985	7/7	0.96	0.33	130,130,131,131	0
84	OHX	1	3520	7/7	0.96	0.18	123,123,124,124	0
85	MG	1	3842	1/1	0.96	0.55	25,25,25,25	0
85	MG	A	2138	1/1	0.96	0.46	66,66,66,66	0
84	OHX	1	3680	7/7	0.96	0.32	122,122,122,122	0
84	OHX	AR	3567	7/7	0.96	0.15	121,121,121,121	0
84	OHX	1	3579	7/7	0.96	0.17	119,120,120,120	0
85	MG	AR	4007	1/1	0.96	0.28	29,29,29,29	0
84	OHX	AR	3648	7/7	0.96	0.55	130,131,131,131	0
84	OHX	6	2017	7/7	0.96	0.29	135,135,136,136	0
85	MG	1	4095	1/1	0.96	0.20	61,61,61,61	0
84	OHX	6	1980	7/7	0.96	0.34	116,116,116,116	0
84	OHX	1	3483	7/7	0.96	0.12	113,113,113,113	0
84	OHX	AR	3551	7/7	0.96	0.14	129,129,130,130	0
84	OHX	AR	3526	7/7	0.96	0.18	117,117,117,118	0
85	MG	1	4105	1/1	0.96	0.49	26,26,26,26	0
84	OHX	1	3628	7/7	0.96	0.26	144,145,145,145	0
84	OHX	AR	3536	7/7	0.96	0.22	123,124,124,124	0
84	OHX	A	2016	7/7	0.96	0.28	142,143,143,144	0
84	OHX	AR	3619	7/7	0.96	0.35	122,123,123,124	0
85	MG	AR	3874	1/1	0.96	0.60	27,27,27,27	0
84	OHX	6	1988	7/7	0.96	0.14	133,133,133,134	0
84	OHX	6	2034	7/7	0.96	0.19	155,155,155,155	0
85	MG	6	2093	1/1	0.96	0.33	47,47,47,47	0
85	MG	CO	201	1/1	0.96	0.19	44,44,44,44	0
84	OHX	AR	3627	7/7	0.96	0.32	127,128,128,128	0
85	MG	1	4096	1/1	0.96	0.41	27,27,27,27	0
85	MG	1	3838	1/1	0.96	0.57	33,33,33,33	0
85	MG	AR	3952	1/1	0.96	0.36	28,28,28,28	0
85	MG	AR	3951	1/1	0.96	0.53	29,29,29,29	0
85	MG	1	3743	1/1	0.96	0.28	79,79,79,79	0
85	MG	1	3812	1/1	0.96	0.64	64,64,64,64	0
84	OHX	1	3622	7/7	0.96	0.27	153,154,154,154	0
84	OHX	AR	3530	7/7	0.96	0.17	112,113,113,113	0
85	MG	1	3916	1/1	0.96	0.29	26,26,26,26	0
84	OHX	1	3683	7/7	0.96	0.33	118,118,118,118	0
84	OHX	6	1949	7/7	0.96	0.11	135,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4249	1/1	0.96	0.44	24,24,24,24	0
84	OHX	6	2044	7/7	0.96	0.35	140,141,141,141	0
85	MG	1	4069	1/1	0.96	0.43	46,46,46,46	0
84	OHX	1	3584	7/7	0.96	0.25	114,114,114,114	0
85	MG	1	4199	1/1	0.96	0.59	24,24,24,24	0
84	OHX	1	3500	7/7	0.96	0.16	119,120,120,120	0
85	MG	6	2101	1/1	0.96	0.51	53,53,53,53	0
84	OHX	A	1978	7/7	0.96	0.26	143,144,144,145	0
85	MG	AR	4258	1/1	0.96	0.54	34,34,34,34	0
84	OHX	AR	3588	7/7	0.96	0.27	112,112,112,113	0
84	OHX	1	3519	7/7	0.96	0.22	116,116,116,116	0
85	MG	A	2066	1/1	0.96	0.59	79,79,79,79	0
85	MG	AR	3828	1/1	0.96	0.61	60,60,60,60	0
85	MG	AR	3916	1/1	0.96	0.58	19,19,19,19	0
84	OHX	1	3670	7/7	0.96	0.24	111,111,111,111	0
84	OHX	AR	3684	7/7	0.96	0.52	124,125,125,125	0
84	OHX	6	2000	7/7	0.96	0.17	130,130,131,131	0
84	OHX	6	1941	7/7	0.96	0.13	120,120,121,121	0
85	MG	6	2061	1/1	0.96	0.32	100,100,100,100	0
88	ZN	e1	501	1/1	0.96	0.06	153,153,153,153	0
85	MG	A	2119	1/1	0.96	0.35	57,57,57,57	0
84	OHX	1	3623	7/7	0.96	0.23	114,114,115,115	0
84	OHX	AR	3679	7/7	0.96	0.25	153,153,153,154	0
85	MG	1	3980	1/1	0.96	0.26	73,73,73,73	0
84	OHX	O	201	7/7	0.96	0.28	158,159,159,160	0
84	OHX	1	3553	7/7	0.96	0.29	121,122,122,122	0
84	OHX	AR	3521	7/7	0.96	0.28	117,118,118,118	0
84	OHX	4	211	7/7	0.96	0.14	138,139,139,140	0
84	OHX	1	3473	7/7	0.96	0.15	114,115,115,115	0
85	MG	1	4172	1/1	0.96	0.41	67,67,67,67	0
85	MG	AR	3939	1/1	0.96	0.31	31,31,31,31	0
85	MG	AR	4133	1/1	0.96	0.27	25,25,25,25	0
84	OHX	A	1980	7/7	0.96	0.26	137,137,138,138	0
85	MG	1	4168	1/1	0.96	0.45	20,20,20,20	0
84	OHX	1	3586	7/7	0.96	0.23	121,122,122,122	0
84	OHX	A	2009	7/7	0.96	0.38	126,126,127,127	0
84	OHX	e	101	7/7	0.96	0.41	143,144,145,145	0
85	MG	AR	3766	1/1	0.96	0.14	96,96,96,96	0
84	OHX	A	1947	7/7	0.96	0.27	129,129,130,130	0
84	OHX	AR	3623	7/7	0.96	0.29	138,139,139,139	0
84	OHX	1	3445	7/7	0.96	0.26	111,112,112,112	0
85	MG	6	2084	1/1	0.96	0.22	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3795	1/1	0.96	0.66	49,49,49,49	0
84	OHX	1	3601	7/7	0.96	0.30	112,112,112,112	0
84	OHX	1	3435	7/7	0.96	0.27	114,114,114,114	0
85	MG	AR	3871	1/1	0.96	0.40	28,28,28,28	0
84	OHX	AR	3626	7/7	0.96	0.30	122,123,123,123	0
85	MG	AR	3846	1/1	0.96	0.56	33,33,33,33	0
84	OHX	6	1994	7/7	0.96	0.25	170,170,170,170	0
84	OHX	4	206	7/7	0.96	0.16	116,116,116,116	0
84	OHX	1	3565	7/7	0.96	0.25	131,131,131,131	0
84	OHX	6	1982	7/7	0.96	0.17	147,147,148,148	0
84	OHX	A	1941	7/7	0.97	0.12	136,137,137,137	0
85	MG	6	2058	1/1	0.97	0.43	45,45,45,45	0
84	OHX	4	203	7/7	0.97	0.16	106,107,107,107	0
85	MG	AR	3850	1/1	0.97	0.28	24,24,24,24	0
84	OHX	1	3646	7/7	0.97	0.25	117,118,118,118	0
84	OHX	6	1905	7/7	0.97	0.34	132,133,133,134	0
88	ZN	d9	102	1/1	0.97	0.13	83,83,83,83	0
84	OHX	A	1982	7/7	0.97	0.30	121,122,122,122	0
84	OHX	6	1935	7/7	0.97	0.14	121,121,121,122	0
85	MG	AR	4132	1/1	0.97	0.15	49,49,49,49	0
84	OHX	AR	3542	7/7	0.97	0.11	152,152,152,153	0
85	MG	AR	3806	1/1	0.97	0.29	57,57,57,57	0
84	OHX	1	3635	7/7	0.97	0.28	122,122,123,123	0
84	OHX	6	1938	7/7	0.97	0.13	130,131,131,131	0
84	OHX	AR	3458	7/7	0.97	0.19	114,114,114,115	0
85	MG	A	2108	1/1	0.97	0.62	57,57,57,57	0
85	MG	1	3815	1/1	0.97	0.14	40,40,40,40	0
84	OHX	1	3558	7/7	0.97	0.17	134,134,135,135	0
85	MG	AR	3908	1/1	0.97	0.53	25,25,25,25	0
84	OHX	1	3608	7/7	0.97	0.25	118,119,119,119	0
84	OHX	3	202	7/7	0.97	0.12	115,116,116,116	0
84	OHX	AR	3594	7/7	0.97	0.20	114,114,115,115	0
85	MG	1	4182	1/1	0.97	0.30	25,25,25,25	0
84	OHX	A	1943	7/7	0.97	0.21	133,133,134,134	0
84	OHX	4	205	7/7	0.97	0.17	106,106,106,106	0
84	OHX	AR	3520	7/7	0.97	0.31	112,112,113,113	0
84	OHX	AR	3569	7/7	0.97	0.29	137,137,137,138	0
84	OHX	A	1911	7/7	0.97	0.22	139,140,141,141	0
84	OHX	AR	3661	7/7	0.97	0.46	112,112,112,113	0
84	OHX	1	3449	7/7	0.97	0.23	117,117,118,118	0
84	OHX	AR	3561	7/7	0.97	0.24	110,110,110,111	0
84	OHX	A	1988	7/7	0.97	0.23	139,140,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3616	7/7	0.97	0.34	109,110,110,110	0
84	OHX	4	204	7/7	0.97	0.15	108,108,108,108	0
85	MG	AR	3869	1/1	0.97	0.40	31,31,31,31	0
84	OHX	AR	3559	7/7	0.97	0.31	121,121,121,121	0
84	OHX	6	1927	7/7	0.97	0.22	124,124,125,125	0
84	OHX	6	1974	7/7	0.97	0.15	121,121,122,122	0
84	OHX	1	3600	7/7	0.97	0.15	150,150,150,150	0
84	OHX	AT	203	7/7	0.97	0.14	117,117,117,117	0
84	OHX	6	1983	7/7	0.97	0.18	128,129,129,129	0
85	MG	A	2079	1/1	0.97	0.64	58,58,58,58	0
84	OHX	AR	3473	7/7	0.97	0.11	111,111,112,112	0
85	MG	1	3883	1/1	0.97	0.41	22,22,22,22	0
84	OHX	AR	3539	7/7	0.97	0.14	127,128,128,128	0
84	OHX	1	3576	7/7	0.97	0.14	131,131,132,132	0
84	OHX	AR	3585	7/7	0.97	0.20	117,117,117,117	0
84	OHX	1	3603	7/7	0.97	0.17	123,123,124,124	0
84	OHX	AR	3540	7/7	0.97	0.16	108,108,108,108	0
84	OHX	A	1910	7/7	0.97	0.23	138,139,139,140	0
85	MG	1	3836	1/1	0.97	0.39	36,36,36,36	0
85	MG	6	2063	1/1	0.97	0.20	82,82,82,82	0
84	OHX	AP	502	7/7	0.97	0.17	112,113,113,113	0
85	MG	AR	3898	1/1	0.97	0.63	28,28,28,28	0
84	OHX	1	3546	7/7	0.97	0.17	127,127,127,127	0
84	OHX	c8	201	7/7	0.97	0.20	146,147,147,148	0
85	MG	1	3806	1/1	0.97	0.46	51,51,51,51	0
85	MG	1	3780	1/1	0.97	0.33	17,17,17,17	0
84	OHX	1	3572	7/7	0.97	0.27	118,119,119,119	0
85	MG	1	3760	1/1	0.97	0.35	27,27,27,27	0
84	OHX	AR	3494	7/7	0.97	0.15	124,125,125,125	0
84	OHX	A	1937	7/7	0.97	0.16	153,154,155,155	0
84	OHX	1	3425	7/7	0.97	0.25	108,109,109,109	0
84	OHX	A	1913	7/7	0.97	0.20	126,126,127,127	0
84	OHX	1	3502	7/7	0.97	0.18	114,114,114,114	0
84	OHX	AS	208	7/7	0.97	0.10	138,139,139,139	0
84	OHX	AR	3642	7/7	0.97	0.24	122,122,122,122	0
84	OHX	AR	3566	7/7	0.97	0.24	115,115,115,116	0
85	MG	AR	3762	1/1	0.97	0.17	24,24,24,24	0
84	OHX	A	2008	7/7	0.97	0.16	132,132,133,133	0
85	MG	A	2058	1/1	0.97	0.66	46,46,46,46	0
84	OHX	AR	3493	7/7	0.97	0.25	114,114,114,114	0
85	MG	1	4185	1/1	0.97	0.50	27,27,27,27	0
84	OHX	1	3536	7/7	0.97	0.22	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	6	1955	7/7	0.97	0.13	179,179,179,179	0
85	MG	AR	3848	1/1	0.97	0.28	31,31,31,31	0
84	OHX	AT	207	7/7	0.97	0.15	117,117,117,117	0
84	OHX	A	1930	7/7	0.97	0.10	122,122,123,123	0
84	OHX	6	1925	7/7	0.97	0.20	122,122,122,123	0
84	OHX	A	1956	7/7	0.97	0.14	133,133,134,134	0
84	OHX	AT	208	7/7	0.97	0.32	114,114,114,114	0
84	OHX	3	203	7/7	0.97	0.11	118,118,118,119	0
84	OHX	1	3574	7/7	0.97	0.28	116,116,117,117	0
84	OHX	1	3573	7/7	0.97	0.18	131,131,132,132	0
85	MG	1	4051	1/1	0.97	0.22	44,44,44,44	0
85	MG	AR	3849	1/1	0.97	0.45	35,35,35,35	0
85	MG	1	4043	1/1	0.97	0.32	27,27,27,27	0
84	OHX	AR	3554	7/7	0.97	0.15	112,112,112,112	0
84	OHX	1	3607	7/7	0.97	0.17	122,122,122,122	0
85	MG	AR	3786	1/1	0.97	0.48	25,25,25,25	0
84	OHX	6	1943	7/7	0.97	0.09	124,124,125,125	0
84	OHX	1	3625	7/7	0.97	0.22	135,135,135,135	0
84	OHX	6	1959	7/7	0.97	0.17	137,138,138,139	0
84	OHX	1	3566	7/7	0.97	0.18	113,113,114,114	0
85	MG	AR	4179	1/1	0.97	0.27	43,43,43,43	0
84	OHX	A	1940	7/7	0.97	0.28	137,138,138,139	0
84	OHX	AR	3625	7/7	0.97	0.36	134,134,134,134	0
84	OHX	AR	3504	7/7	0.97	0.18	110,110,110,110	0
84	OHX	AR	3591	7/7	0.97	0.25	112,112,112,112	0
85	MG	AR	3906	1/1	0.97	0.36	33,33,33,33	0
84	OHX	A	1968	7/7	0.97	0.34	125,125,126,126	0
84	OHX	1	3463	7/7	0.97	0.13	121,121,122,122	0
84	OHX	AR	3653	7/7	0.97	0.30	120,120,121,121	0
85	MG	s8	302	1/1	0.97	0.33	51,51,51,51	0
84	OHX	AR	3479	7/7	0.97	0.15	110,110,110,110	0
84	OHX	AR	3463	7/7	0.97	0.17	110,110,111,111	0
84	OHX	AR	3656	7/7	0.97	0.31	134,134,134,134	0
85	MG	AR	3987	1/1	0.97	0.30	31,31,31,31	0
84	OHX	1	3585	7/7	0.97	0.23	115,115,116,116	0
84	OHX	1	3466	7/7	0.97	0.16	114,115,115,115	0
85	MG	AR	4115	1/1	0.97	0.33	46,46,46,46	0
84	OHX	AR	3560	7/7	0.97	0.19	135,135,136,136	0
84	OHX	1	3442	7/7	0.97	0.24	120,121,121,121	0
84	OHX	A	2004	7/7	0.97	0.22	139,139,140,140	0
84	OHX	AR	3455	7/7	0.97	0.22	111,112,112,112	0
85	MG	1	4205	1/1	0.97	0.24	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	6	1907	7/7	0.97	0.32	135,136,136,137	0
84	OHX	1	3647	7/7	0.97	0.23	118,118,118,118	0
85	MG	AR	3775	1/1	0.97	0.23	22,22,22,22	0
85	MG	AR	3930	1/1	0.97	0.62	29,29,29,29	0
84	OHX	6	1953	7/7	0.97	0.12	132,133,133,134	0
84	OHX	1	3562	7/7	0.97	0.14	121,121,121,121	0
85	MG	1	3878	1/1	0.97	0.58	24,24,24,24	0
84	OHX	A	1951	7/7	0.97	0.24	145,145,146,146	0
84	OHX	A	1917	7/7	0.97	0.17	130,131,131,131	0
85	MG	1	3909	1/1	0.97	0.57	25,25,25,25	0
84	OHX	1	3598	7/7	0.97	0.27	127,127,127,127	0
84	OHX	1	3480	7/7	0.97	0.14	119,119,119,120	0
84	OHX	A	1927	7/7	0.97	0.14	138,138,139,139	0
85	MG	1	4072	1/1	0.97	0.18	46,46,46,46	0
84	OHX	AR	3513	7/7	0.97	0.09	150,151,151,151	0
85	MG	AR	4229	1/1	0.97	0.70	34,34,34,34	0
84	OHX	AR	3484	7/7	0.97	0.19	114,114,114,114	0
84	OHX	4	209	7/7	0.97	0.23	113,113,113,113	0
84	OHX	AR	3492	7/7	0.97	0.15	116,116,117,117	0
85	MG	1	3895	1/1	0.97	0.42	28,28,28,28	0
84	OHX	AR	3683	7/7	0.97	0.36	126,127,127,127	0
84	OHX	AR	3696	7/7	0.97	0.18	112,113,113,113	0
84	OHX	A	1945	7/7	0.97	0.18	143,144,144,145	0
84	OHX	3	208	7/7	0.97	0.30	116,116,116,116	0
84	OHX	AR	3549	7/7	0.97	0.20	116,117,117,117	0
85	MG	1	3776	1/1	0.97	0.50	43,43,43,43	0
84	OHX	AR	3519	7/7	0.97	0.15	108,109,109,109	0
85	MG	AR	3970	1/1	0.97	0.23	50,50,50,50	0
84	OHX	AR	3445	7/7	0.97	0.18	107,107,107,107	0
84	OHX	AR	3483	7/7	0.97	0.17	111,111,111,111	0
85	MG	1	4114	1/1	0.97	0.23	52,52,52,52	0
84	OHX	A	1939	7/7	0.97	0.11	140,141,141,142	0
85	MG	1	3835	1/1	0.97	0.47	30,30,30,30	0
85	MG	AR	3938	1/1	0.97	0.39	34,34,34,34	0
85	MG	1	4192	1/1	0.97	0.66	21,21,21,21	0
84	OHX	A	1931	7/7	0.97	0.10	139,140,140,140	0
84	OHX	6	1939	7/7	0.97	0.10	131,132,132,133	0
85	MG	1	4019	1/1	0.97	0.24	42,42,42,42	0
85	MG	AR	3810	1/1	0.97	0.51	27,27,27,27	0
84	OHX	1	3658	7/7	0.97	0.34	142,143,143,143	0
85	MG	1	4112	1/1	0.97	0.43	32,32,32,32	0
84	OHX	AR	3584	7/7	0.97	0.13	131,131,131,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3613	7/7	0.97	0.47	120,120,121,121	0
84	OHX	6	1909	7/7	0.97	0.26	137,138,138,139	0
84	OHX	A	1932	7/7	0.97	0.18	141,142,142,143	0
85	MG	1	4204	1/1	0.97	0.51	34,34,34,34	0
84	OHX	1	3503	7/7	0.97	0.10	127,128,128,129	0
84	OHX	6	1967	7/7	0.97	0.17	126,127,127,127	0
85	MG	1	3887	1/1	0.97	0.83	42,42,42,42	0
85	MG	AR	4048	1/1	0.97	0.23	34,34,34,34	0
84	OHX	1	3494	7/7	0.97	0.13	119,119,120,120	0
84	OHX	AR	3574	7/7	0.97	0.17	112,113,113,113	0
84	OHX	A	1948	7/7	0.97	0.13	139,140,140,140	0
84	OHX	A	1987	7/7	0.97	0.15	128,128,129,129	0
84	OHX	A	1990	7/7	0.97	0.27	135,135,136,136	0
84	OHX	4	208	7/7	0.97	0.36	106,106,106,106	0
84	OHX	AR	3535	7/7	0.97	0.13	114,115,115,115	0
85	MG	AR	3932	1/1	0.97	0.28	63,63,63,63	0
84	OHX	1	3538	7/7	0.97	0.09	125,125,125,126	0
84	OHX	AR	3459	7/7	0.97	0.26	114,114,115,115	0
85	MG	A	2077	1/1	0.97	0.59	48,48,48,48	0
85	MG	AR	4053	1/1	0.97	0.40	30,30,30,30	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	AT	206	7/7	0.97	0.11	123,124,124,124	0
84	OHX	1	3564	7/7	0.97	0.24	126,126,127,127	0
84	OHX	AR	3478	7/7	0.97	0.17	110,110,110,111	0
84	OHX	A	1979	7/7	0.97	0.22	142,143,144,144	0
84	OHX	3	204	7/7	0.97	0.15	124,125,125,125	0
84	OHX	6	1933	7/7	0.97	0.13	116,116,117,117	0
84	OHX	1	3495	7/7	0.97	0.14	114,115,115,115	0
85	MG	3	218	1/1	0.97	0.22	54,54,54,54	0
85	MG	1	3918	1/1	0.97	0.20	31,31,31,31	0
84	OHX	A	1926	7/7	0.97	0.08	127,127,127,128	0
84	OHX	AR	3547	7/7	0.97	0.28	116,116,116,117	0
84	OHX	1	3438	7/7	0.97	0.25	117,117,117,117	0
84	OHX	1	3602	7/7	0.97	0.23	128,128,128,129	0
84	OHX	A	1921	7/7	0.97	0.22	142,143,144,144	0
84	OHX	A	1928	7/7	0.97	0.13	125,126,126,126	0
85	MG	CP	503	1/1	0.97	0.41	38,38,38,38	0
84	OHX	1	3542	7/7	0.97	0.17	119,119,120,120	0
84	OHX	AR	3533	7/7	0.97	0.18	111,111,111,111	0
84	OHX	A	1934	7/7	0.97	0.12	132,132,133,133	0
85	MG	1	4059	1/1	0.97	0.42	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3953	1/1	0.97	0.19	34,34,34,34	0
84	OHX	AR	3501	7/7	0.97	0.31	113,113,114,114	0
85	MG	6	2136	1/1	0.97	0.23	52,52,52,52	0
84	OHX	1	3569	7/7	0.97	0.28	111,111,111,111	0
84	OHX	6	1911	7/7	0.97	0.24	134,135,135,135	0
84	OHX	J	301	7/7	0.97	0.25	157,157,158,158	0
84	OHX	1	3548	7/7	0.97	0.11	134,134,134,134	0
84	OHX	1	3633	7/7	0.97	0.30	134,134,135,135	0
85	MG	AR	3797	1/1	0.97	0.27	31,31,31,31	0
84	OHX	AR	3496	7/7	0.97	0.24	112,113,113,113	0
84	OHX	AR	3620	7/7	0.97	0.33	143,144,144,144	0
85	MG	6	2071	1/1	0.97	0.49	45,45,45,45	0
84	OHX	1	3528	7/7	0.97	0.12	119,120,120,120	0
85	MG	v	302	1/1	0.97	0.34	36,36,36,36	0
85	MG	6	2057	1/1	0.97	0.56	51,51,51,51	0
84	OHX	1	3504	7/7	0.97	0.19	127,127,127,128	0
84	OHX	1	3534	7/7	0.97	0.19	113,113,113,113	0
85	MG	AS	231	1/1	0.97	0.19	56,56,56,56	0
85	MG	6	2053	1/1	0.97	0.57	41,41,41,41	0
84	OHX	1	3682	7/7	0.97	0.14	110,110,111,111	0
84	OHX	1	3638	7/7	0.97	0.33	122,123,123,123	0
84	OHX	1	3678	7/7	0.97	0.15	117,117,118,118	0
85	MG	CX	203	1/1	0.97	0.39	19,19,19,19	0
84	OHX	A	1998	7/7	0.97	0.25	158,159,160,160	0
84	OHX	1	3476	7/7	0.97	0.14	111,111,111,112	0
84	OHX	1	3568	7/7	0.97	0.28	115,116,116,116	0
84	OHX	1	3492	7/7	0.97	0.19	117,118,118,118	0
85	MG	AR	3985	1/1	0.97	0.49	35,35,35,35	0
85	MG	1	4122	1/1	0.97	0.25	78,78,78,78	0
85	MG	AR	4235	1/1	0.97	0.37	26,26,26,26	0
85	MG	AR	3885	1/1	0.97	0.37	33,33,33,33	0
84	OHX	h	401	7/7	0.97	0.15	175,176,177,177	0
84	OHX	6	1964	7/7	0.97	0.12	123,123,124,124	0
84	OHX	6	1965	7/7	0.97	0.24	116,117,117,117	0
84	OHX	AR	3630	7/7	0.97	0.13	124,125,125,125	0
84	OHX	AT	209	7/7	0.97	0.11	121,121,122,122	0
84	OHX	1	3549	7/7	0.97	0.15	120,120,120,120	0
84	OHX	AR	3558	7/7	0.97	0.16	137,137,137,137	0
84	OHX	6	1936	7/7	0.97	0.15	116,116,117,117	0
84	OHX	A	1992	7/7	0.97	0.21	140,141,142,142	0
85	MG	1	3784	1/1	0.97	0.45	26,26,26,26	0
84	OHX	1	3529	7/7	0.97	0.17	115,115,115,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	6	1957	7/7	0.97	0.14	129,130,130,131	0
85	MG	AR	3974	1/1	0.97	0.42	81,81,81,81	0
84	OHX	AR	3447	7/7	0.97	0.25	112,112,112,112	0
84	OHX	AR	3516	7/7	0.97	0.15	112,112,112,112	0
84	OHX	AR	3442	7/7	0.97	0.22	112,112,112,112	0
84	OHX	6	2003	7/7	0.97	0.13	126,126,127,127	0
85	MG	1	4157	1/1	0.97	0.48	60,60,60,60	0
84	OHX	1	3580	7/7	0.97	0.35	115,116,116,116	0
84	OHX	1	3578	7/7	0.97	0.19	107,107,107,107	0
84	OHX	A	1965	7/7	0.97	0.16	134,135,135,136	0
84	OHX	AR	3643	7/7	0.97	0.30	120,121,121,121	0
85	MG	d6	102	1/1	0.97	0.50	38,38,38,38	0
84	OHX	AR	3491	7/7	0.97	0.13	108,108,109,109	0
84	OHX	1	3571	7/7	0.97	0.18	111,111,112,112	0
84	OHX	4	212	7/7	0.97	0.28	128,128,128,128	0
84	OHX	v	301	7/7	0.97	0.20	113,113,114,114	0
85	MG	1	3822	1/1	0.97	0.49	18,18,18,18	0
84	OHX	AR	3469	7/7	0.97	0.14	121,122,122,122	0
85	MG	1	4200	1/1	0.97	0.49	22,22,22,22	0
84	OHX	AR	3456	7/7	0.97	0.19	117,117,117,117	0
84	OHX	AR	3576	7/7	0.97	0.32	128,128,129,129	0
84	OHX	1	3699	7/7	0.97	0.40	130,131,131,131	0
85	MG	A	2154	1/1	0.97	0.93	45,45,45,45	0
84	OHX	AR	3467	7/7	0.97	0.13	108,109,109,109	0
84	OHX	AR	3432	7/7	0.97	0.27	117,117,117,118	0
84	OHX	AT	205	7/7	0.97	0.15	108,108,108,108	0
84	OHX	1	3645	7/7	0.97	0.34	125,126,126,126	0
84	OHX	1	3561	7/7	0.97	0.26	124,124,125,125	0
84	OHX	AG	201	7/7	0.97	0.21	114,115,115,115	0
84	OHX	1	3506	7/7	0.97	0.29	109,109,110,110	0
85	MG	1	4191	1/1	0.97	0.44	29,29,29,29	0
84	OHX	AS	206	7/7	0.97	0.13	124,124,125,125	0
85	MG	1	3736	1/1	0.97	0.60	31,31,31,31	0
84	OHX	6	1968	7/7	0.97	0.26	122,122,123,123	0
85	MG	1	3900	1/1	0.97	0.34	42,42,42,42	0
85	MG	AR	3837	1/1	0.97	0.59	19,19,19,19	0
84	OHX	6	1934	7/7	0.97	0.13	139,139,140,140	0
84	OHX	A	1954	7/7	0.97	0.17	135,136,136,136	0
84	OHX	AR	3480	7/7	0.97	0.12	113,114,114,114	0
85	MG	AT	230	1/1	0.98	0.42	39,39,39,39	0
84	OHX	A	2010	7/7	0.98	0.14	157,158,158,159	0
84	OHX	4	207	7/7	0.98	0.12	118,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AS	202	7/7	0.98	0.22	124,124,125,125	0
84	OHX	1	3530	7/7	0.98	0.13	138,138,139,139	0
85	MG	1	3817	1/1	0.98	0.26	23,23,23,23	0
84	OHX	1	3447	7/7	0.98	0.20	113,113,113,113	0
84	OHX	6	1923	7/7	0.98	0.17	121,121,122,122	0
84	OHX	6	1918	7/7	0.98	0.17	116,117,117,117	0
84	OHX	6	1910	7/7	0.98	0.26	119,120,120,120	0
84	OHX	AR	3453	7/7	0.98	0.10	106,106,107,107	0
84	OHX	1	3512	7/7	0.98	0.17	110,110,110,110	0
84	OHX	AR	3457	7/7	0.98	0.18	108,108,108,109	0
84	OHX	1	3557	7/7	0.98	0.16	117,118,118,118	0
84	OHX	AT	204	7/7	0.98	0.11	105,105,105,106	0
84	OHX	6	1913	7/7	0.98	0.26	133,134,135,135	0
84	OHX	1	3407	7/7	0.98	0.31	106,106,107,107	0
85	MG	1	3991	1/1	0.98	0.17	66,66,66,66	0
84	OHX	AS	205	7/7	0.98	0.12	113,113,114,114	0
84	OHX	A	1949	7/7	0.98	0.08	148,149,149,149	0
84	OHX	AR	3490	7/7	0.98	0.12	112,112,112,113	0
84	OHX	6	1920	7/7	0.98	0.14	133,133,134,134	0
84	OHX	A	1903	7/7	0.98	0.35	149,149,150,150	0
84	OHX	1	3448	7/7	0.98	0.21	117,117,117,117	0
84	OHX	AR	3487	7/7	0.98	0.13	107,107,107,107	0
85	MG	1	4180	1/1	0.98	0.35	45,45,45,45	0
84	OHX	AR	3465	7/7	0.98	0.17	118,118,118,118	0
84	OHX	6	1924	7/7	0.98	0.15	134,135,135,135	0
84	OHX	AR	3482	7/7	0.98	0.19	111,112,112,112	0
84	OHX	AR	3550	7/7	0.98	0.14	107,107,107,107	0
84	OHX	1	3460	7/7	0.98	0.16	118,118,118,119	0
84	OHX	1	3459	7/7	0.98	0.19	108,108,108,108	0
84	OHX	A	1919	7/7	0.98	0.17	121,122,122,122	0
85	MG	6	2119	1/1	0.98	0.47	74,74,74,74	0
85	MG	1	3798	1/1	0.98	0.23	32,32,32,32	0
85	MG	AR	3830	1/1	0.98	0.46	42,42,42,42	0
84	OHX	AR	3508	7/7	0.98	0.21	109,109,109,109	0
84	OHX	AR	3417	7/7	0.98	0.26	111,112,112,112	0
84	OHX	1	3486	7/7	0.98	0.14	116,117,117,117	0
85	MG	1	4149	1/1	0.98	0.18	54,54,54,54	0
84	OHX	1	3434	7/7	0.98	0.25	126,127,127,127	0
85	MG	6	2131	1/1	0.98	0.24	44,44,44,44	0
84	OHX	AR	3451	7/7	0.98	0.20	114,114,114,114	0
84	OHX	6	1981	7/7	0.98	0.29	139,140,140,140	0
85	MG	AR	3781	1/1	0.98	0.25	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3443	7/7	0.98	0.14	116,116,117,117	0
84	OHX	A	1984	7/7	0.98	0.10	130,130,131,131	0
84	OHX	CP	501	7/7	0.98	0.20	126,126,126,127	0
84	OHX	6	1922	7/7	0.98	0.18	121,122,122,122	0
84	OHX	1	3443	7/7	0.98	0.19	119,120,120,120	0
85	MG	1	4196	1/1	0.98	0.42	30,30,30,30	0
85	MG	1	4063	1/1	0.98	0.09	38,38,38,38	0
84	OHX	1	3477	7/7	0.98	0.12	109,109,109,109	0
84	OHX	6	1963	7/7	0.98	0.16	125,125,126,126	0
84	OHX	AR	3437	7/7	0.98	0.23	108,108,108,108	0
84	OHX	A	1962	7/7	0.98	0.21	132,133,133,134	0
85	MG	6	2170	1/1	0.98	0.17	64,64,64,64	0
84	OHX	1	3697	7/7	0.98	0.25	119,119,120,120	0
84	OHX	A	1942	7/7	0.98	0.19	133,133,134,134	0
84	OHX	A	1952	7/7	0.98	0.20	128,129,129,129	0
85	MG	AR	3884	1/1	0.98	0.45	22,22,22,22	0
84	OHX	A	1908	7/7	0.98	0.24	141,142,143,143	0
84	OHX	AR	3450	7/7	0.98	0.16	127,127,127,128	0
84	OHX	AR	3497	7/7	0.98	0.09	124,125,125,126	0
84	OHX	1	3499	7/7	0.98	0.23	111,111,111,111	0
84	OHX	AR	3498	7/7	0.98	0.15	123,123,123,124	0
85	MG	1	4132	1/1	0.98	0.13	86,86,86,86	0
84	OHX	AR	3448	7/7	0.98	0.17	115,115,115,115	0
84	OHX	A	1972	7/7	0.98	0.22	148,148,148,148	0
84	OHX	1	3491	7/7	0.98	0.18	120,120,121,121	0
84	OHX	1	3560	7/7	0.98	0.12	111,112,112,112	0
85	MG	1	3893	1/1	0.98	0.26	26,26,26,26	0
84	OHX	1	3439	7/7	0.98	0.19	109,109,109,109	0
84	OHX	AR	3510	7/7	0.98	0.13	117,118,118,118	0
84	OHX	1	3468	7/7	0.98	0.20	116,117,117,117	0
84	OHX	3	201	7/7	0.98	0.19	121,121,121,122	0
84	OHX	AS	203	7/7	0.98	0.16	116,116,116,116	0
84	OHX	AR	3489	7/7	0.98	0.15	114,114,114,114	0
85	MG	1	4047	1/1	0.98	0.12	57,57,57,57	0
85	MG	1	3889	1/1	0.98	0.54	23,23,23,23	0
84	OHX	AC	101	7/7	0.98	0.30	114,115,115,115	0
84	OHX	1	3516	7/7	0.98	0.12	116,117,117,117	0
84	OHX	AS	201	7/7	0.98	0.24	119,119,119,120	0
84	OHX	AR	3461	7/7	0.98	0.14	110,111,111,111	0
84	OHX	1	3508	7/7	0.98	0.10	113,114,114,114	0
84	OHX	6	1931	7/7	0.98	0.10	115,116,116,116	0
84	OHX	AR	3525	7/7	0.98	0.06	119,119,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3535	7/7	0.98	0.17	111,111,111,112	0
84	OHX	AR	3502	7/7	0.98	0.17	113,114,114,114	0
85	MG	AR	4131	1/1	0.98	0.09	39,39,39,39	0
84	OHX	AR	3471	7/7	0.98	0.13	109,109,109,109	0
84	OHX	6	1944	7/7	0.98	0.10	143,143,144,144	0
84	OHX	1	3404	7/7	0.98	0.35	120,120,121,121	0
84	OHX	AR	3475	7/7	0.98	0.14	116,116,116,116	0
84	OHX	AR	3486	7/7	0.98	0.19	111,111,111,111	0
84	OHX	AR	3433	7/7	0.98	0.21	110,110,110,111	0
85	MG	1	3904	1/1	0.98	0.53	25,25,25,25	0
84	OHX	6	1928	7/7	0.98	0.08	126,126,127,127	0
84	OHX	1	3456	7/7	0.98	0.16	111,111,111,111	0
84	OHX	AS	207	7/7	0.98	0.16	122,122,122,123	0
85	MG	1	3827	1/1	0.98	0.73	32,32,32,32	0
85	MG	AR	3863	1/1	0.98	0.57	21,21,21,21	0
84	OHX	1	3410	7/7	0.98	0.32	112,112,112,112	0
85	MG	1	3885	1/1	0.98	0.49	20,20,20,20	0
84	OHX	1	3555	7/7	0.98	0.17	111,111,112,112	0
84	OHX	A	1938	7/7	0.98	0.15	126,127,127,127	0
84	OHX	1	3524	7/7	0.98	0.21	116,117,117,117	0
84	OHX	1	3479	7/7	0.98	0.17	108,109,109,109	0
84	OHX	6	1937	7/7	0.98	0.11	119,120,120,120	0
84	OHX	AT	202	7/7	0.98	0.30	106,106,106,106	0
84	OHX	1	3403	7/7	0.98	0.30	113,113,113,114	0
85	MG	AR	4054	1/1	0.98	0.14	55,55,55,55	0
84	OHX	A	1929	7/7	0.98	0.14	123,123,124,124	0
85	MG	AR	3860	1/1	0.98	0.51	23,23,23,23	0
84	OHX	CE	401	7/7	0.98	0.17	114,114,115,115	0
84	OHX	AR	3485	7/7	0.98	0.15	114,114,115,115	0
85	MG	1	3888	1/1	0.98	0.40	29,29,29,29	0
84	OHX	1	3457	7/7	0.98	0.18	126,127,127,128	0
84	OHX	1	3522	7/7	0.98	0.13	120,121,121,121	0
84	OHX	1	3453	7/7	0.98	0.14	120,120,120,120	0
84	OHX	AR	3476	7/7	0.98	0.17	109,109,109,109	0
84	OHX	1	3474	7/7	0.98	0.16	122,122,123,123	0
85	MG	1	3891	1/1	0.98	0.60	17,17,17,17	0
84	OHX	1	3515	7/7	0.98	0.10	110,110,110,110	0
85	MG	1	3910	1/1	0.98	0.58	19,19,19,19	0
84	OHX	AR	3444	7/7	0.98	0.15	112,112,112,112	0
84	OHX	AR	3464	7/7	0.98	0.17	106,106,106,106	0
84	OHX	1	3417	7/7	0.98	0.31	116,117,117,117	0
84	OHX	1	3415	7/7	0.98	0.32	123,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3420	7/7	0.98	0.29	118,118,118,118	0
84	OHX	AR	3523	7/7	0.98	0.15	107,108,108,108	0
84	OHX	A	1950	7/7	0.98	0.13	127,128,128,128	0
84	OHX	1	3532	7/7	0.98	0.07	159,159,159,159	0
85	MG	1	3783	1/1	0.98	0.46	18,18,18,18	0
85	MG	1	3935	1/1	0.98	0.23	47,47,47,47	0
84	OHX	4	201	7/7	0.98	0.35	108,108,108,108	0
85	MG	6	2098	1/1	0.98	0.52	68,68,68,68	0
84	OHX	AR	3470	7/7	0.98	0.17	115,116,116,116	0
84	OHX	1	3587	7/7	0.98	0.23	133,133,133,134	0
84	OHX	AR	3672	7/7	0.98	0.29	109,110,110,110	0
85	MG	1	3875	1/1	0.98	0.46	23,23,23,23	0
84	OHX	1	3511	7/7	0.98	0.14	109,109,109,109	0
85	MG	1	4133	1/1	0.98	0.09	51,51,51,51	0
84	OHX	DD	101	7/7	0.98	0.29	113,114,114,114	0
84	OHX	AR	3645	7/7	0.98	0.35	118,118,118,118	0
85	MG	AR	3876	1/1	0.98	0.55	27,27,27,27	0
84	OHX	AR	3414	7/7	0.98	0.30	113,113,114,114	0
85	MG	6	2184	1/1	0.98	0.22	83,83,83,83	0
84	OHX	6	1930	7/7	0.98	0.21	121,121,122,122	0
84	OHX	AR	3488	7/7	0.98	0.09	118,118,119,119	0
84	OHX	1	3452	7/7	0.98	0.16	109,109,109,109	0
84	OHX	A	1957	7/7	0.98	0.23	133,134,134,134	0
84	OHX	AR	3401	7/7	0.98	0.39	121,121,121,122	0
84	OHX	AS	204	7/7	0.98	0.15	113,113,113,113	0
84	OHX	A	1922	7/7	0.98	0.11	123,124,124,124	0
84	OHX	A	1967	7/7	0.98	0.12	119,119,120,120	0
84	OHX	1	3493	7/7	0.98	0.17	115,116,116,116	0
84	OHX	AR	3582	7/7	0.98	0.27	114,114,114,114	0
84	OHX	AR	3468	7/7	0.98	0.16	124,124,125,125	0
85	MG	AR	4260	1/1	0.98	0.52	6,6,6,6	0
85	MG	AR	3763	1/1	0.98	0.59	17,17,17,17	0
85	MG	AR	3870	1/1	0.98	0.70	33,33,33,33	0
85	MG	1	4121	1/1	0.98	0.10	64,64,64,64	0
85	MG	AT	219	1/1	0.98	0.35	36,36,36,36	0
84	OHX	6	1991	7/7	0.98	0.29	133,134,134,135	0
85	MG	AS	222	1/1	0.98	0.21	44,44,44,44	0
84	OHX	1	3521	7/7	0.98	0.14	116,117,117,117	0
84	OHX	1	3441	7/7	0.98	0.20	116,116,116,117	0
84	OHX	AR	3415	7/7	0.98	0.35	109,109,110,110	0
84	OHX	AR	3411	7/7	0.98	0.30	106,106,106,106	0
84	OHX	AR	3477	7/7	0.98	0.20	112,112,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3432	7/7	0.98	0.27	117,117,117,117	0
85	MG	AR	4208	1/1	0.98	0.21	57,57,57,57	0
85	MG	1	4215	1/1	0.98	0.62	27,27,27,27	0
84	OHX	1	3470	7/7	0.98	0.18	115,115,115,115	0
84	OHX	AR	3435	7/7	0.98	0.22	112,113,113,113	0
84	OHX	AR	3430	7/7	0.98	0.14	107,107,107,107	0
84	OHX	AR	3572	7/7	0.98	0.28	118,119,119,119	0
84	OHX	AR	3452	7/7	0.98	0.18	121,121,122,122	0
84	OHX	AR	3573	7/7	0.98	0.21	123,123,123,123	0
84	OHX	1	3461	7/7	0.98	0.18	110,110,111,111	0
85	MG	1	4142	1/1	0.98	0.26	38,38,38,38	0
84	OHX	AR	3454	7/7	0.98	0.17	112,112,113,113	0
84	OHX	A	1916	7/7	0.98	0.18	136,137,137,138	0
85	MG	AR	4106	1/1	0.98	0.07	46,46,46,46	0
84	OHX	AR	3518	7/7	0.98	0.10	118,119,119,119	0
84	OHX	1	3630	7/7	0.98	0.33	113,113,114,114	0
84	OHX	6	1926	7/7	0.98	0.12	120,121,121,121	0
84	OHX	6	1942	7/7	0.98	0.16	135,135,136,136	0
84	OHX	A	1923	7/7	0.98	0.13	124,125,125,125	0
84	OHX	1	3482	7/7	0.98	0.18	117,117,117,117	0
84	OHX	1	3444	7/7	0.98	0.23	116,116,117,117	0
85	MG	AR	3774	1/1	0.98	0.15	30,30,30,30	0
85	MG	6	2182	1/1	0.98	0.14	83,83,83,83	0
84	OHX	1	3454	7/7	0.98	0.18	111,111,111,111	0
84	OHX	6	1916	7/7	0.98	0.21	119,120,120,120	0
84	OHX	1	3465	7/7	0.98	0.18	117,117,117,117	0
84	OHX	DH	201	7/7	0.98	0.13	113,113,113,113	0
84	OHX	1	3590	7/7	0.98	0.12	137,138,138,138	0
84	OHX	A	1912	7/7	0.98	0.19	137,137,138,138	0
84	OHX	AR	3515	7/7	0.98	0.22	113,113,114,114	0
84	OHX	6	1945	7/7	0.98	0.17	126,127,127,128	0
85	MG	AR	3858	1/1	0.98	0.32	36,36,36,36	0
85	MG	1	4078	1/1	0.98	0.29	24,24,24,24	0
85	MG	z	202	1/1	0.98	0.28	59,59,59,59	0
84	OHX	AR	3481	7/7	0.98	0.20	106,106,107,107	0
84	OHX	CX	201	7/7	0.98	0.17	116,116,116,116	0
85	MG	1	3810	1/1	0.98	0.12	32,32,32,32	0
85	MG	AR	4190	1/1	0.98	0.19	30,30,30,30	0
84	OHX	6	1958	7/7	0.98	0.15	126,127,127,127	0
84	OHX	A	1901	7/7	0.98	0.29	127,127,127,128	0
84	OHX	1	3440	7/7	0.98	0.22	110,110,111,111	0
84	OHX	AR	3505	7/7	0.98	0.20	114,114,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3844	1/1	0.98	0.41	28,28,28,28	0
84	OHX	1	3496	7/7	0.98	0.16	115,115,115,115	0
84	OHX	1	3533	7/7	0.98	0.13	149,149,150,150	0
84	OHX	AR	3589	7/7	0.98	0.13	109,110,110,110	0
84	OHX	AR	3507	7/7	0.98	0.08	123,123,123,123	0
84	OHX	1	3523	7/7	0.98	0.19	119,119,120,120	0
85	MG	AR	3819	1/1	0.98	0.36	37,37,37,37	0
84	OHX	1	3484	7/7	0.98	0.10	125,126,126,126	0
84	OHX	AR	3436	7/7	0.98	0.24	109,109,109,109	0
84	OHX	1	3513	7/7	0.98	0.11	113,113,114,114	0
84	OHX	6	1951	7/7	0.98	0.14	134,134,135,135	0
84	OHX	1	3570	7/7	0.98	0.09	144,144,145,145	0
84	OHX	A	1961	7/7	0.98	0.11	149,150,151,151	0
84	OHX	6	1970	7/7	0.98	0.26	126,126,127,127	0
84	OHX	6	1948	7/7	0.98	0.13	127,128,128,128	0
85	MG	1	4034	1/1	0.98	0.25	42,42,42,42	0
84	OHX	AR	3439	7/7	0.98	0.25	119,120,120,120	0
84	OHX	1	3472	7/7	0.98	0.17	110,111,111,111	0
85	MG	1	4067	1/1	0.98	0.09	40,40,40,40	0
84	OHX	AR	3529	7/7	0.98	0.12	108,109,109,109	0
84	OHX	AR	3407	7/7	0.98	0.34	113,113,113,113	0
84	OHX	AR	3406	7/7	0.98	0.34	112,112,113,113	0
84	OHX	DQ	201	7/7	0.98	0.15	111,111,111,111	0
84	OHX	AR	3425	7/7	0.98	0.23	105,106,106,106	0
84	OHX	1	3430	7/7	0.98	0.19	110,110,110,110	0
84	OHX	AR	3412	7/7	0.98	0.28	109,109,109,109	0
84	OHX	1	3505	7/7	0.98	0.18	116,116,117,117	0
84	OHX	1	3467	7/7	0.98	0.17	123,123,124,124	0
84	OHX	sR	401	7/7	0.98	0.22	161,161,162,162	0
85	MG	AR	3818	1/1	0.98	0.78	37,37,37,37	0
84	OHX	AR	3500	7/7	0.98	0.12	115,115,115,115	0
84	OHX	1	3475	7/7	0.98	0.14	117,117,118,118	0
84	OHX	A	1914	7/7	0.98	0.23	126,127,127,127	0
84	OHX	AR	3744	7/7	0.98	0.17	109,110,110,110	0
85	MG	AR	4081	1/1	0.98	0.24	55,55,55,55	0
84	OHX	1	3416	7/7	0.99	0.24	109,109,109,109	0
85	MG	AR	4195	1/1	0.99	0.18	63,63,63,63	0
84	OHX	1	3411	7/7	0.99	0.29	111,112,112,112	0
85	MG	AR	3866	1/1	0.99	0.23	34,34,34,34	0
85	MG	1	4076	1/1	0.99	0.24	64,64,64,64	0
84	OHX	1	3402	7/7	0.99	0.35	114,115,115,115	0
84	OHX	4	202	7/7	0.99	0.33	112,112,112,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	A	2145	1/1	0.99	0.21	92,92,92,92	0
84	OHX	A	1902	7/7	0.99	0.26	122,122,123,123	0
88	ZN	DR	501	1/1	0.99	0.15	59,59,59,59	0
85	MG	1	4134	1/1	0.99	0.20	63,63,63,63	0
84	OHX	A	1906	7/7	0.99	0.23	142,143,143,143	0
84	OHX	AR	3434	7/7	0.99	0.22	111,111,111,111	0
84	OHX	6	1917	7/7	0.99	0.16	131,131,132,132	0
85	MG	AR	3887	1/1	0.99	0.46	21,21,21,21	0
85	MG	1	3745	1/1	0.99	0.67	31,31,31,31	0
85	MG	1	3858	1/1	0.99	0.37	25,25,25,25	0
84	OHX	6	1912	7/7	0.99	0.18	122,122,123,123	0
84	OHX	1	3428	7/7	0.99	0.28	126,126,127,127	0
84	OHX	A	1920	7/7	0.99	0.14	128,128,129,129	0
85	MG	1	4031	1/1	0.99	0.55	21,21,21,21	0
84	OHX	1	3412	7/7	0.99	0.30	114,114,115,115	0
85	MG	1	4097	1/1	0.99	0.22	70,70,70,70	0
84	OHX	1	3406	7/7	0.99	0.33	108,108,108,108	0
85	MG	AR	3878	1/1	0.99	0.36	31,31,31,31	0
84	OHX	AR	3410	7/7	0.99	0.31	109,109,109,110	0
84	OHX	1	3408	7/7	0.99	0.32	112,112,112,113	0
84	OHX	AR	3413	7/7	0.99	0.26	107,107,107,107	0
85	MG	AR	3940	1/1	0.99	0.49	21,21,21,21	0
85	MG	1	4164	1/1	0.99	0.22	58,58,58,58	0
85	MG	6	2181	1/1	0.99	0.11	95,95,95,95	0
84	OHX	AR	3424	7/7	0.99	0.27	112,112,113,113	0
84	OHX	1	3436	7/7	0.99	0.28	115,115,115,115	0
84	OHX	2	201	7/7	0.99	0.31	119,119,120,120	0
88	ZN	DO	201	1/1	0.99	0.15	32,32,32,32	0
84	OHX	6	1903	7/7	0.99	0.29	117,118,118,118	0
84	OHX	1	3414	7/7	0.99	0.27	109,109,109,109	0
85	MG	AR	4241	1/1	0.99	0.39	17,17,17,17	0
84	OHX	1	3464	7/7	0.99	0.20	109,109,109,109	0
84	OHX	6	1902	7/7	0.99	0.34	136,136,137,137	0
84	OHX	AR	3409	7/7	0.99	0.34	120,120,120,121	0
84	OHX	AR	3426	7/7	0.99	0.27	111,112,112,112	0
84	OHX	AR	3404	7/7	0.99	0.33	112,112,112,112	0
85	MG	AR	3799	1/1	0.99	0.36	22,22,22,22	0
84	OHX	AR	3440	7/7	0.99	0.18	125,125,125,126	0
84	OHX	1	3418	7/7	0.99	0.27	114,115,115,115	0
84	OHX	AR	3421	7/7	0.99	0.25	113,113,113,113	0
84	OHX	AR	3416	7/7	0.99	0.29	114,114,115,115	0
84	OHX	A	1905	7/7	0.99	0.29	128,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3825	1/1	0.99	0.41	31,31,31,31	0
84	OHX	AR	3449	7/7	0.99	0.14	116,117,117,117	0
84	OHX	1	3490	7/7	0.99	0.17	113,113,113,113	0
84	OHX	AR	3446	7/7	0.99	0.17	112,113,113,113	0
84	OHX	1	3409	7/7	0.99	0.30	116,116,117,117	0
84	OHX	AR	3509	7/7	0.99	0.10	106,106,106,106	0
88	ZN	e	102	1/1	0.99	0.08	79,79,79,79	0
84	OHX	1	3419	7/7	0.99	0.26	107,107,107,107	0
84	OHX	AR	3419	7/7	0.99	0.27	122,122,123,123	0
84	OHX	AR	3402	7/7	0.99	0.39	113,113,113,113	0
84	OHX	AR	3423	7/7	0.99	0.28	110,111,111,111	0
84	OHX	6	1914	7/7	0.99	0.20	133,133,134,134	0
84	OHX	6	1901	7/7	0.99	0.34	119,120,120,120	0
84	OHX	AR	3462	7/7	0.99	0.16	116,116,116,116	0
85	MG	6	2175	1/1	0.99	0.10	118,118,118,118	0
84	OHX	A	1924	7/7	0.99	0.09	132,132,133,133	0
84	OHX	6	1904	7/7	0.99	0.27	124,124,124,125	0
85	MG	AR	4172	1/1	0.99	0.12	65,65,65,65	0
84	OHX	AT	201	7/7	0.99	0.33	109,109,110,110	0
84	OHX	6	1906	7/7	0.99	0.29	122,123,123,124	0
84	OHX	6	1908	7/7	0.99	0.25	120,120,121,121	0
84	OHX	AR	3429	7/7	0.99	0.19	112,112,112,112	0
84	OHX	AR	3609	7/7	0.99	0.16	107,107,107,107	0
85	MG	AR	4052	1/1	0.99	0.12	86,86,86,86	0
84	OHX	AR	3418	7/7	0.99	0.30	116,116,117,117	0
85	MG	AR	3910	1/1	0.99	0.32	23,23,23,23	0
84	OHX	1	3478	7/7	0.99	0.14	125,125,125,126	0
85	MG	1	3725	1/1	0.99	0.38	34,34,34,34	0
84	OHX	A	1904	7/7	0.99	0.23	133,134,134,134	0
84	OHX	AR	3428	7/7	0.99	0.21	115,115,115,116	0
84	OHX	AR	3431	7/7	0.99	0.24	109,109,110,110	0
84	OHX	1	3405	7/7	0.99	0.37	124,125,125,125	0
84	OHX	1	3450	7/7	0.99	0.17	121,122,122,123	0
84	OHX	1	3426	7/7	0.99	0.28	120,120,120,120	0
84	OHX	1	3427	7/7	0.99	0.26	112,113,113,113	0
85	MG	AR	3909	1/1	0.99	0.57	25,25,25,25	0
84	OHX	AR	3438	7/7	0.99	0.22	108,108,108,108	0
84	OHX	1	3422	7/7	0.99	0.26	116,116,117,117	0
84	OHX	AR	3420	7/7	0.99	0.29	113,114,114,114	0
84	OHX	1	3401	7/7	0.99	0.38	114,114,115,115	0
84	OHX	1	3413	7/7	0.99	0.32	112,113,113,113	0
84	OHX	AR	3578	7/7	0.99	0.14	109,109,110,110	0

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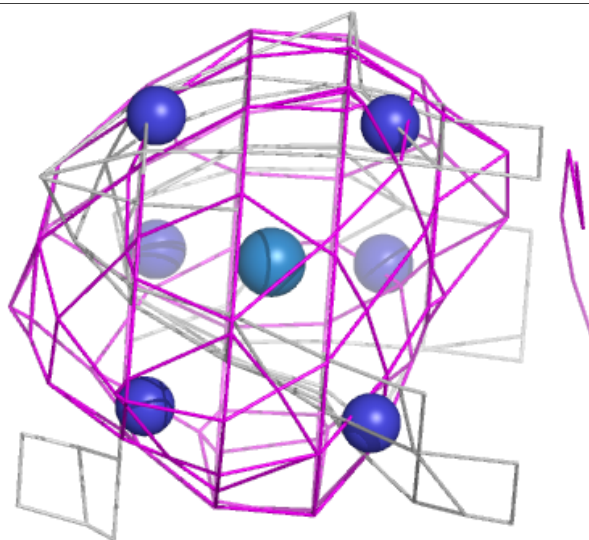
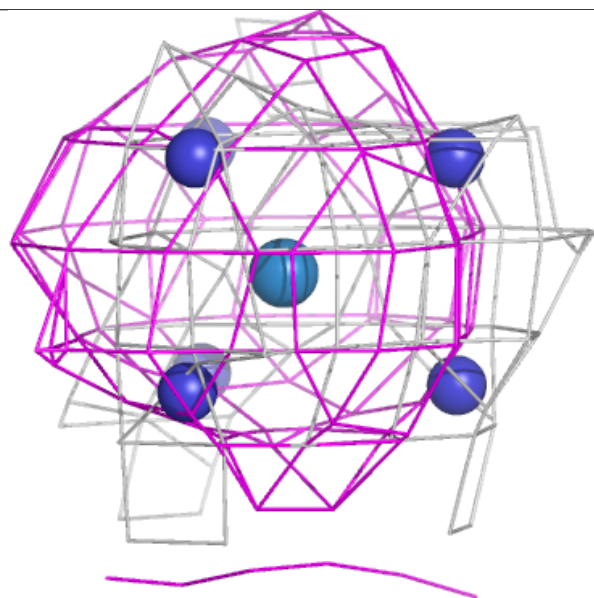
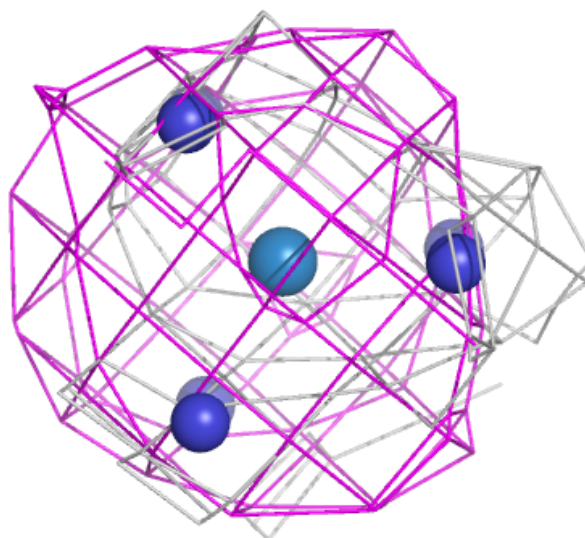
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3983	1/1	0.99	0.12	33,33,33,33	0
84	OHX	AR	3408	7/7	0.99	0.33	107,107,107,107	0
88	ZN	b	102	1/1	0.99	0.16	71,71,71,71	0
85	MG	1	3882	1/1	0.99	0.45	32,32,32,32	0
84	OHX	1	3421	7/7	0.99	0.29	115,115,116,116	0
84	OHX	A	1925	7/7	0.99	0.12	136,137,137,137	0
88	ZN	AP	501	1/1	0.99	0.04	61,61,61,61	0
84	OHX	1	3433	7/7	0.99	0.26	118,119,119,119	0
85	MG	1	3903	1/1	0.99	0.67	21,21,21,21	0
84	OHX	AR	3403	7/7	0.99	0.28	110,110,110,110	0
84	OHX	1	3423	7/7	0.99	0.26	120,120,121,121	0
85	MG	AR	4191	1/1	0.99	0.17	58,58,58,58	0
84	OHX	A	1907	7/7	0.99	0.19	133,134,134,134	0
84	OHX	1	3437	7/7	0.99	0.24	116,117,117,117	0
85	MG	A	2141	1/1	0.99	0.31	101,101,101,101	0
84	OHX	AR	3422	7/7	0.99	0.28	112,112,112,112	0
84	OHX	6	1915	7/7	0.99	0.17	119,119,120,120	0
84	OHX	1	3424	7/7	0.99	0.23	115,115,115,115	0
88	ZN	DQ	202	1/1	0.99	0.03	63,63,63,63	0
84	OHX	CV	201	7/7	0.99	0.31	117,117,117,117	0
85	MG	1	3748	1/1	0.99	0.34	44,44,44,44	0
84	OHX	AR	3405	7/7	0.99	0.34	119,119,120,120	0
85	MG	1	3911	1/1	0.99	0.65	21,21,21,21	0
88	ZN	DL	101	1/1	0.99	0.20	41,41,41,41	0
84	OHX	1	3429	7/7	0.99	0.22	110,110,110,110	0
85	MG	AR	4168	1/1	1.00	0.19	65,65,65,65	0
88	ZN	AK	101	1/1	1.00	0.15	34,34,34,34	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	AN	500	1/1	1.00	0.13	38,38,38,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

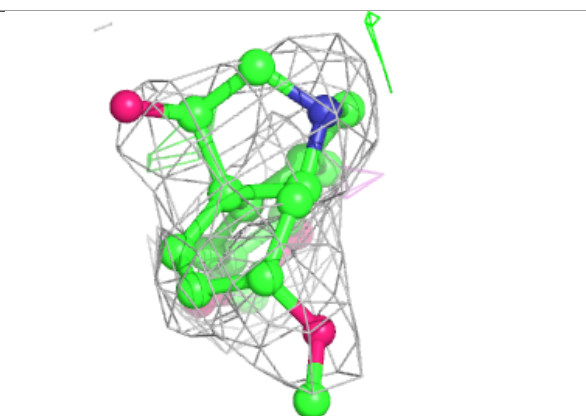
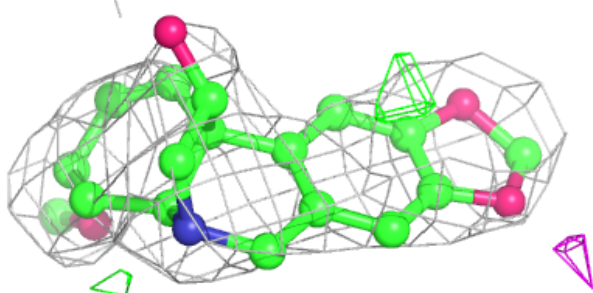
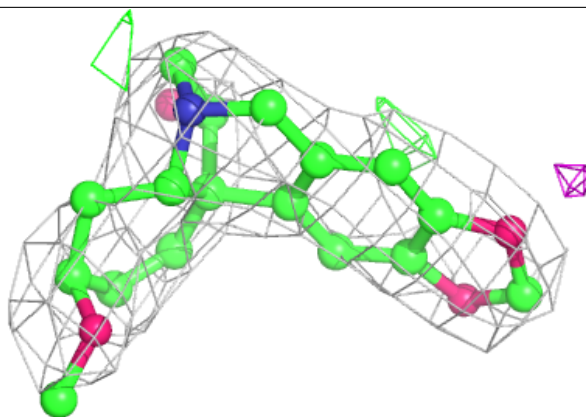
Electron density around OHX AR 3737:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

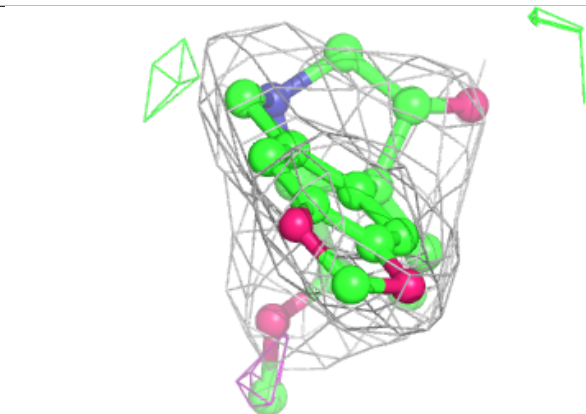
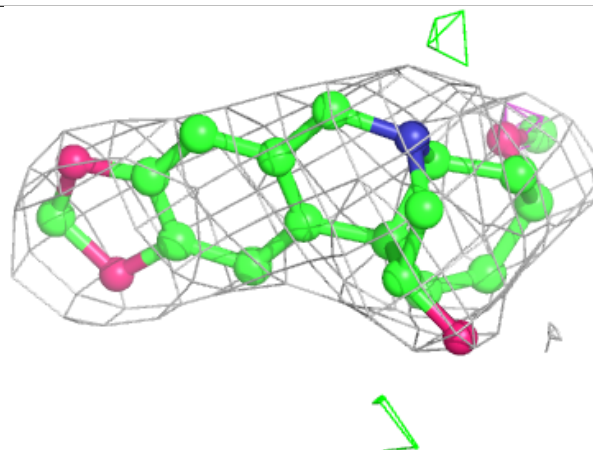
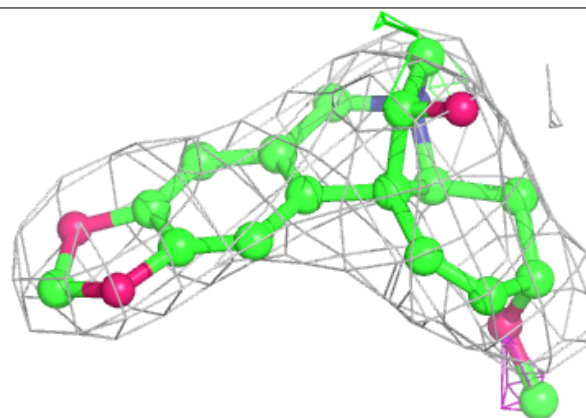


Electron density around HN8 AR 4263:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HN8 1 4223:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.