



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 01:54 AM EDT

PDB ID : 5MEI / pdb_00005mei
Title : Crystal structure of Agelastatin A bound to the 80S ribosome
Authors : McClary, B.; Zinshteyn, B.; Meyer, M.; Jouanneau, M.; Pellegrino, S.;
Yusupova, G.; Schuller, A.; Reyes, J.C.P.; Lu, J.; Luo, C.; Dang, Y.; Romo,
D.; Yusupov, M.; Green, R.; Liu, J.O.
Deposited on : 2016-11-15
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

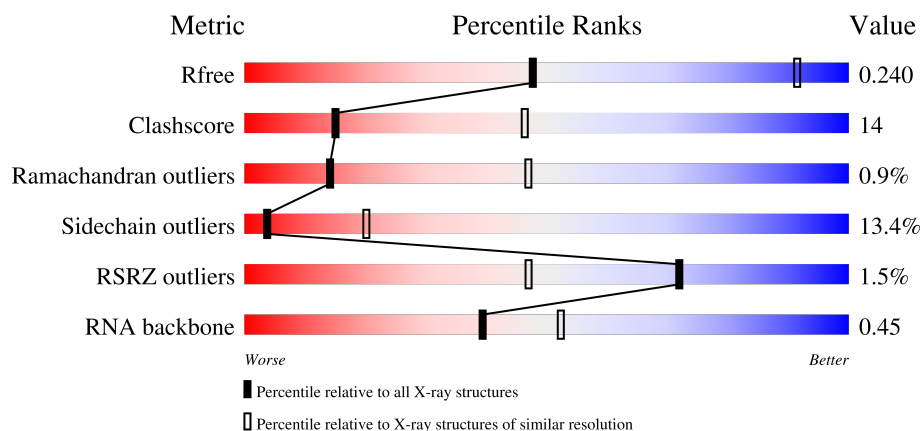
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	

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Mol	Chain	Length	Quality of chain
2	AS	121	
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	

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Mol	Chain	Length	Quality of chain
15	CO	136	
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	l2	136	
25	6	1800	
25	A	1800	
26	7	98	
26	CY	98	
27	8	121	

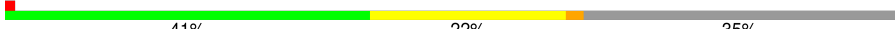
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Mol	Chain	Length	Quality of chain
27	CZ	121	
28	9	126	
28	DA	126	
29	AA	135	
29	DB	135	
30	AB	148	
30	DC	148	
31	AC	58	
31	DD	58	
32	AD	97	
32	DE	97	
33	AE	109	
33	DF	109	
34	AF	127	
34	DG	127	
35	AG	106	
35	DH	106	
36	AH	112	
36	DI	112	
37	AI	119	
37	DJ	119	
38	AJ	99	
38	DK	99	
39	AK	87	
39	DL	87	

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Mol	Chain	Length	Quality of chain
40	AL	77	
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	168	
47	p0	220	
48	sM	104	
49	B	206	
49	s0	206	
50	C	216	
50	s1	216	
51	D	217	
51	s2	217	
52	E	223	
52	s3	223	
53	F	260	
53	s4	260	

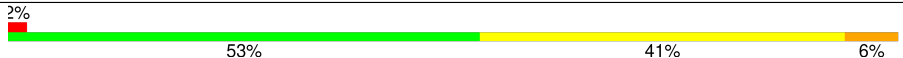
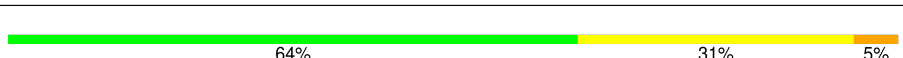
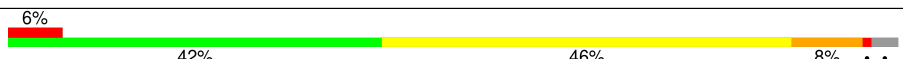
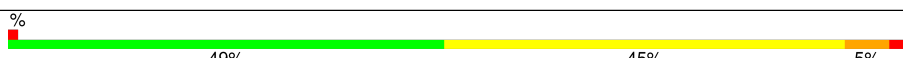
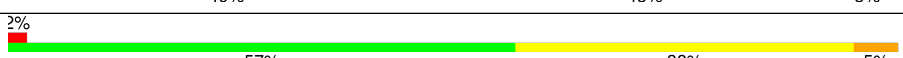
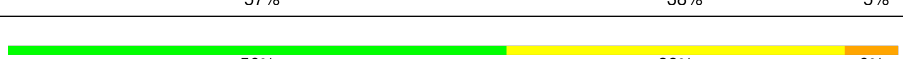
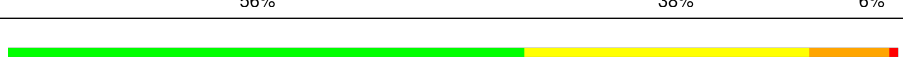
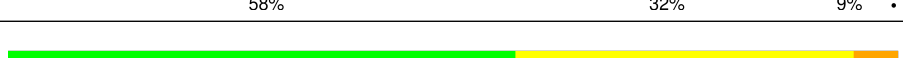
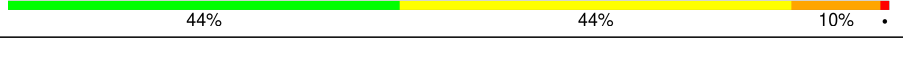
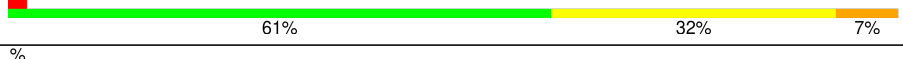
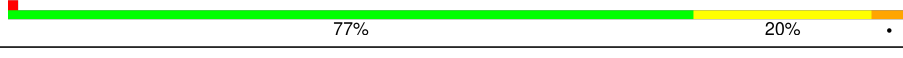
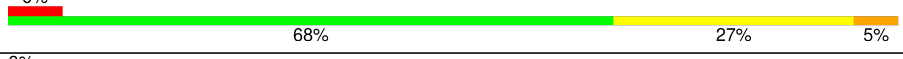
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Mol	Chain	Length	Quality of chain
54	G	206	
54	s5	206	
55	H	226	
55	s6	226	
56	I	186	
56	s7	186	
57	J	199	
57	s8	199	
58	K	185	
58	s9	185	
59	L	105	
59	c0	105	
60	M	155	
60	c1	155	
61	N	124	
61	c2	124	
62	O	150	
62	c3	150	
63	P	128	
63	c4	128	
64	Q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

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

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Mol	Chain	Length	Quality of chain
79	f	62	
80	g	71	
81	h	318	
81	sR	318	
82	c7	121	
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	3406	-	-	X	-
84	OHX	1	3471	-	-	X	-
84	OHX	1	3496	-	-	X	-
84	OHX	1	3594	-	-	X	-
84	OHX	1	3702	-	-	X	-
84	OHX	A	1954	-	-	X	-
84	OHX	AE	201	-	-	X	-
84	OHX	AR	3443	-	-	X	-
84	OHX	AR	3604	-	-	X	-
84	OHX	AR	3731	-	-	X	-
84	OHX	CG	302	-	-	X	-

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 409590 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	12	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 acidic ribosomal protein P0.

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

- Molecule 48 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein Stm1 - Mol B.

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 40S ribosomal protein S0-A.

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

- Molecule 50 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 51 is a protein called 40S ribosomal protein S2.

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

- Molecule 52 is a protein called 40S ribosomal protein S3.

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

- Molecule 53 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 54 is a protein called 40S ribosomal protein S5.

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

- Molecule 55 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 56 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 57 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 58 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 59 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	L	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
59	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- Molecule 60 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 61 is a protein called 40S ribosomal protein S12.

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

- Molecule 62 is a protein called 40S ribosomal protein S13.

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

- Molecule 63 is a protein called 40S ribosomal protein S14-B.

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

- Molecule 64 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	Q	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 65 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 66 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	S	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			

- Molecule 67 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S20.

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

- Molecule 70 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 71 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	a	70	Total	C	N	O	0	0	0
			563	360	104	99			
74	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 75 is a protein called 40S ribosomal protein S26-B.

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

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

- Molecule 76 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 77 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 78 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 79 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S31.

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

- Molecule 81 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	h	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
81	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

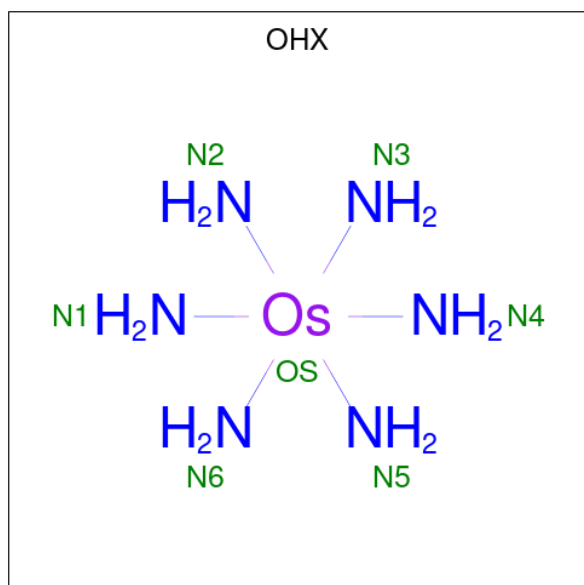
- Molecule 82 is a protein called 40S ribosomal protein S17-A.

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

- 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 (CCD ID: 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		
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		
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
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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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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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			7	6	1		
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
			7	6	1		
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
			7	6	1		
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
			7	6	1		
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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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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84	1	1	Total	N	Os	0	0
			7	6	1		
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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84	1	1	Total	N	Os	0	0
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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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84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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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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			7	6	1		
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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			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		
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			7	6	1		
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		
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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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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
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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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84	1	1	Total	N	Os	0	0
			7	6	1		
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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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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
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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
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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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84	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	3	1	Total	N	Os	0	0
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84	3	1	Total	N	Os	0	0
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84	3	1	Total	N	Os	0	0
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84	3	1	Total	N	Os	0	0
			7	6	1		
84	3	1	Total	N	Os	0	0
			7	6	1		
84	3	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	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		
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
			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		

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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
			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
			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
			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
			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
			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		

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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
			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	AS	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			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		
84	AS	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		
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		
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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	CE	1	Total	N	Os	0	0
			7	6	1		
84	CE	1	Total	N	Os	0	0
			7	6	1		
84	CF	1	Total	N	Os	0	0
			7	6	1		
84	CF	1	Total	N	Os	0	0
			7	6	1		
84	CG	1	Total	N	Os	0	0
			7	6	1		
84	CG	1	Total	N	Os	0	0
			7	6	1		
84	CG	1	Total	N	Os	0	0
			7	6	1		
84	CK	1	Total	N	Os	0	0
			7	6	1		
84	CL	1	Total	N	Os	0	0
			7	6	1		
84	CL	1	Total	N	Os	0	0
			7	6	1		
84	CM	1	Total	N	Os	0	0
			7	6	1		
84	CO	1	Total	N	Os	0	0
			7	6	1		
84	CP	1	Total	N	Os	0	0
			7	6	1		
84	CV	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	CX	1	Total	N	Os	0	0
			7	6	1		
84	CZ	1	Total	N	Os	0	0
			7	6	1		
84	DD	1	Total	N	Os	0	0
			7	6	1		
84	DG	1	Total	N	Os	0	0
			7	6	1		
84	DH	1	Total	N	Os	0	0
			7	6	1		
84	DI	1	Total	N	Os	0	0
			7	6	1		
84	DL	1	Total	N	Os	0	0
			7	6	1		
84	DL	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	H	1	Total	N	Os	0	0
			7	6	1		
84	J	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		
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	c3	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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	1	490	Total	Mg	0	0
			490	490		
85	3	12	Total	Mg	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	4	21	Total 21	Mg 21	0	0
85	j	2	Total 2	Mg 2	0	0
85	k	2	Total 2	Mg 2	0	0
85	l	2	Total 2	Mg 2	0	0
85	o	3	Total 3	Mg 3	0	0
85	r	1	Total 1	Mg 1	0	0
85	s	1	Total 1	Mg 1	0	0
85	t	2	Total 2	Mg 2	0	0
85	v	1	Total 1	Mg 1	0	0
85	w	1	Total 1	Mg 1	0	0
85	x	5	Total 5	Mg 5	0	0
85	z	2	Total 2	Mg 2	0	0
85	l2	2	Total 2	Mg 2	0	0
85	6	141	Total 141	Mg 141	0	0
85	9	1	Total 1	Mg 1	0	0
85	AB	4	Total 4	Mg 4	0	0
85	AF	2	Total 2	Mg 2	0	0
85	AH	1	Total 1	Mg 1	0	0
85	AK	1	Total 1	Mg 1	0	0
85	AP	1	Total 1	Mg 1	0	0
85	i	1	Total 1	Mg 1	0	0

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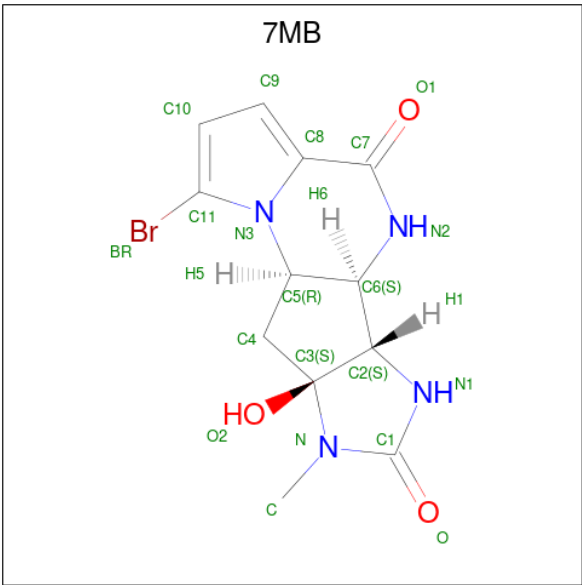
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AR	504	Total 504	Mg 504	0	0
85	AS	20	Total 20	Mg 20	0	0
85	AT	12	Total 12	Mg 12	0	0
85	CD	2	Total 2	Mg 2	0	0
85	CE	4	Total 4	Mg 4	0	0
85	CF	1	Total 1	Mg 1	0	0
85	CI	1	Total 1	Mg 1	0	0
85	CK	1	Total 1	Mg 1	0	0
85	CO	2	Total 2	Mg 2	0	0
85	CP	2	Total 2	Mg 2	0	0
85	CQ	4	Total 4	Mg 4	0	0
85	CR	6	Total 6	Mg 6	0	0
85	CU	2	Total 2	Mg 2	0	0
85	CX	2	Total 2	Mg 2	0	0
85	DA	1	Total 1	Mg 1	0	0
85	DC	4	Total 4	Mg 4	0	0
85	DD	1	Total 1	Mg 1	0	0
85	DE	1	Total 1	Mg 1	0	0
85	DF	1	Total 1	Mg 1	0	0
85	DG	1	Total 1	Mg 1	0	0
85	DH	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	DI	1	Total 1	Mg 1	0	0
85	DO	1	Total 1	Mg 1	0	0
85	DP	1	Total 1	Mg 1	0	0
85	DR	2	Total 2	Mg 2	0	0
85	sM	1	Total 1	Mg 1	0	0
85	A	111	Total 111	Mg 111	0	0
85	D	1	Total 1	Mg 1	0	0
85	F	1	Total 1	Mg 1	0	0
85	Y	1	Total 1	Mg 1	0	0
85	b	1	Total 1	Mg 1	0	0
85	s1	1	Total 1	Mg 1	0	0
85	s2	1	Total 1	Mg 1	0	0
85	s6	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	c6	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0
85	d3	3	Total 3	Mg 3	0	0
85	d5	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0
85	d9	1	Total 1	Mg 1	0	0

- Molecule 86 is Agelastatin A (CCD ID: 7MB) (formula: C₁₂H₁₃BrN₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
86	1	1	Total	Br	C	N	O	0	0
			20	1	12	4	3		
86	AR	1	Total	Br	C	N	O	0	0
			20	1	12	4	3		

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	AK	1	Total	Zn	0	0
			1	1		
87	AN	1	Total	Zn	0	0
			1	1		
87	AP	1	Total	Zn	0	0
			1	1		
87	AQ	1	Total	Zn	0	0
			1	1		
87	DL	1	Total	Zn	0	0
			1	1		
87	DO	1	Total	Zn	0	0
			1	1		
87	DQ	1	Total	Zn	0	0
			1	1		
87	DR	1	Total	Zn	0	0
			1	1		
87	b	1	Total	Zn	0	0
			1	1		
87	c	1	Total	Zn	0	0
			1	1		

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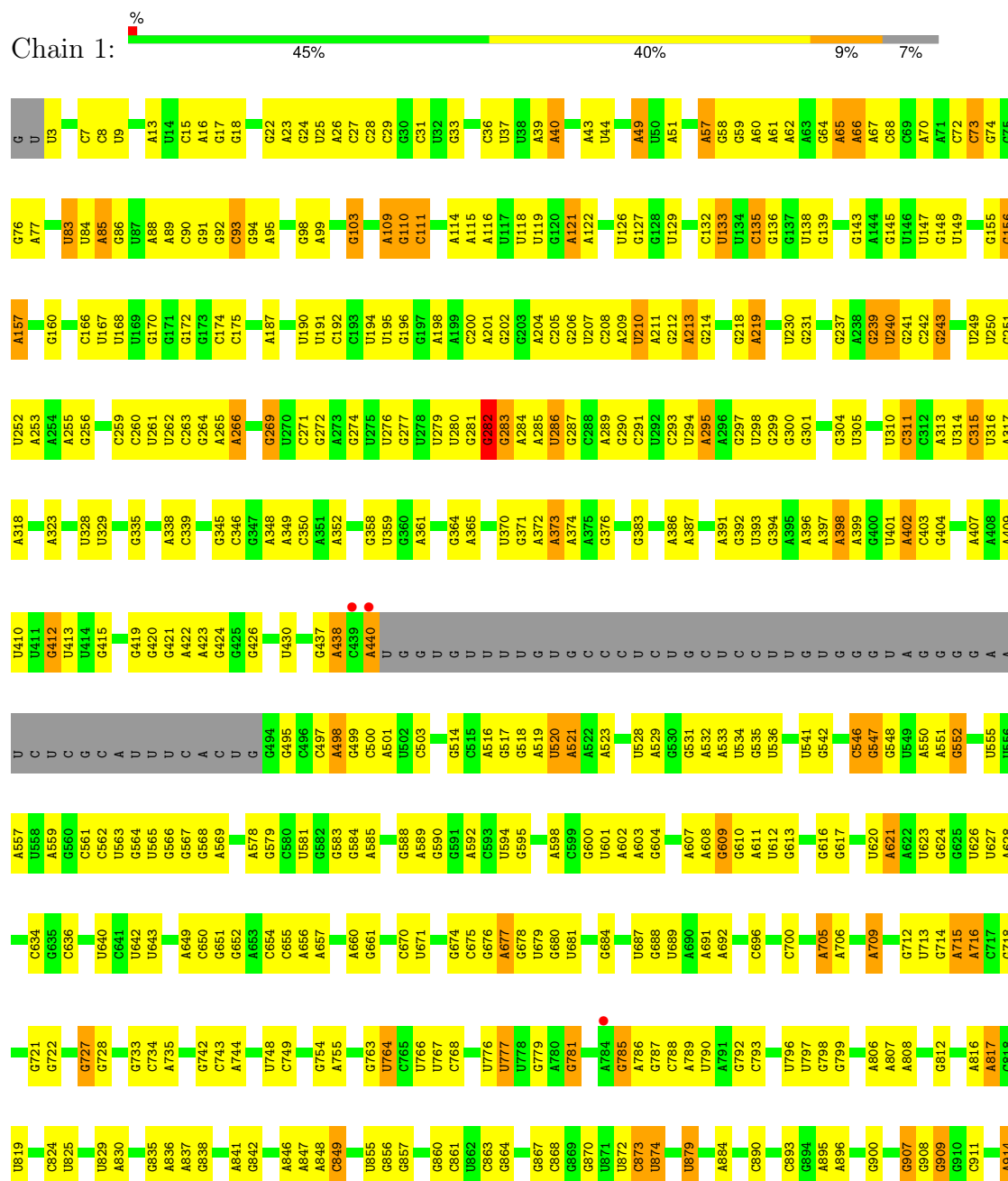
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	e	1	Total 1	Zn 1	0	0
87	g	1	Total 1	Zn 1	0	0
87	d6	1	Total 1	Zn 1	0	0
87	d7	1	Total 1	Zn 1	0	0
87	d9	1	Total 1	Zn 1	0	0
87	e1	1	Total 1	Zn 1	0	0

3 Residue-property plots

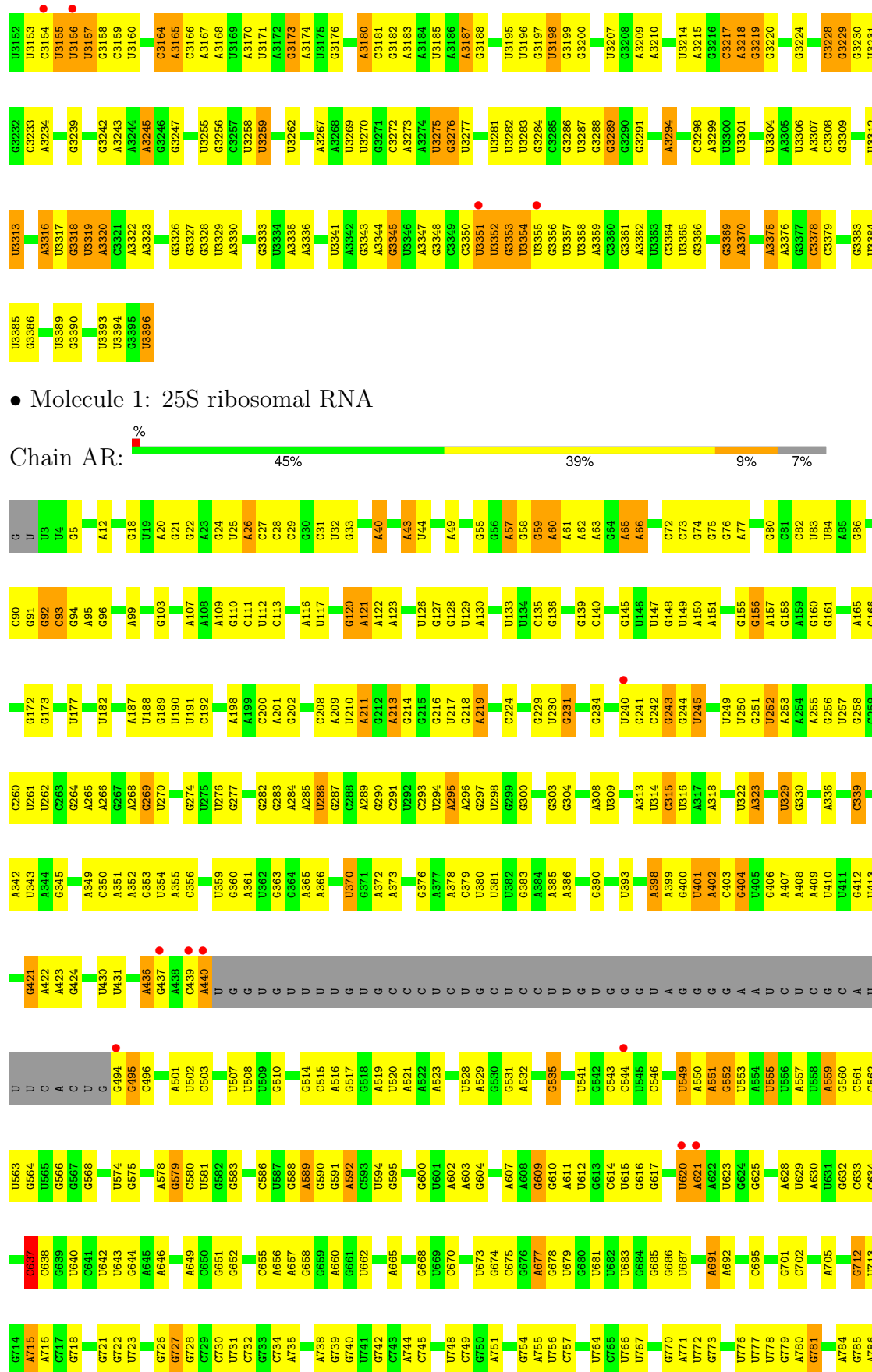
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 25S ribosomal RNA



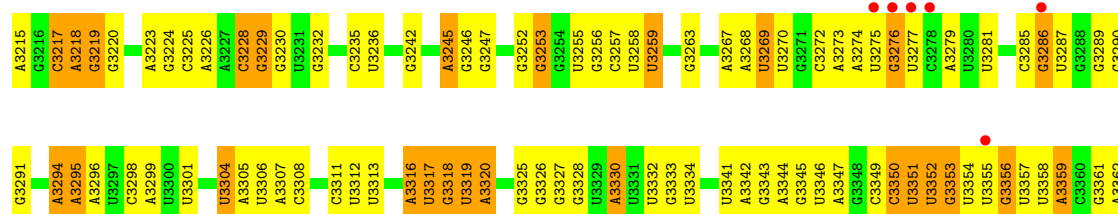
C	U1942	A1850	G1784	U1686	A1593	U1518	U1427	A1343	C1255	G1171	G1090	U1007	A915
U	C1951	G1851	U1785	U1687	A1594	U1523	A1428	G1344	G1256	C1174	A1091	U1008	G916
G	G1952	U1853	G1786	U1688	U1595	U1524	G1429	U1347	U1257	G1175	C1092	A1009	A917
U	C1953	C1854	A1787	U1689	C1597	C1527	U1430	U1348	U1258	C1176	A1093	G1010	
C	U1954	U1855	C1788	U1695	G1598	G1528	C1432	G1349	G1261	G1177	U1094	U1015	A921
U	C1955	C1856	G1789	A1696	G1599	A1529	A1433	A1350	G1262		U1095	U1016	A922
C	A	C1857	G1790	U1600	U1600	U1530	G1434	U1351	A1263		U1096	C1017	C923
G	U	A1858	U1794	A1699	A1603	C1531	A1435	U1353	G1264		A1180	G1018	G924
U	G	G1795	G1700	G1700	G1604	A1534	U1436	U1354	U1269		U1186	G1019	C928
C	U	U1796	U1701	C1709	A1605	A1535	U1437	A1355	A1270		A1190	G1020	A929
A	A	G1796	C1710	G1710	U1606	G1536	U1438	U1356	A1271		G1101	U1021	U930
G	G	A1797	U1716	U1716	U1607	A1537	G1440	G1357	C1272		A1102	G1022	
C	C	A1799	U1717	U1717	A1613	G1538	G1441	U1357	A1273		A1103	G1024	G934
G	C	C1802	U1718	U1718	C1614	G1541	A1446	C1360	A1274		A1104	A1025	U935
A	U	U	G1719	G1719	C1615	G1542	G1447	G1365	A1274		A1105	A1026	U936
C	U	C1805	U1720	U1720	U1616	G1543	U1456	U1369	A1278		U1106	A1027	G937
U	U	U1806	U1721	U1721	U1617		A1466	A1372	C1279		U1107	G1029	U939
C	G	U1807	U1722	U1722	U1620	A1546	A1467	A1373	G1285		U1109	U1033	G940
A	G	G1807	U1723	U1723	A1621	G1547	A1468	A1374	A1286		U1110	U1034	U942
U	C	A1808	U1724	U1724	U1622	U1554	A1469	A1375	A1287		U1111	U1035	U943
U	U	U1810	C1725	C1725	U1623	U1555	G1464	U1378	U1288		U1112	G1036	C944
G	G	G1811	U1729	U1729	U1630	C1556	A1465	G1379	G1289		U1113	C1037	C945
C	A	G1812	G1730	G1730	C1631	U1557	U1466	A1294			G1115	U1047	U946
G	C	A1813	U1731	U1731	G1634	A1558	G1467	G1380	A1294		G1116	A1048	
U	C	A1814	G1732	G1732	G1635	U1559	U1471	G1381	G1295		G1117	U1049	A952
C	C	U1815	U1733	U1733	G1636	G1560	U1472	G1382	C1296		U1118	A1041	G953
G	C	A1816	G1734	G1734	G1637	G1561	G1473	A1386	C1297		G1126	U1042	
C	C	U1817	U1735	U1735	A1638	C1562	U1474	G1387	U1298		U1127	G1043	C959
U	U	G1818	G1736	G1736	C1639	C1563	A1477	U1388	U1299		U1128		U960
U	G	U1819	U1740	U1740	G1640	U1564	U1478	G1389	G1300		A1129		
G	G	U1820	U1741	U1741	A1643	U1566	U1479	A1390	A1302		G1130	A1047	G964
U	C	C1822	U1742	U1742	U1643	U1567	G1480	C1391	G1307		G1132	A1048	A965
U	G	A1823	G1743	G1743	G1650	U1568	A1481	A1392	A1308		A1133	U1050	G968
U	U	U1824	U1744	U1744	U1651	U1569	A1482	A1393	U1309		G1134	C1049	C969
A	C	G1825	G1745	G1745	C1657	U1570	G1483	A1394			A1135	U1051	
G	C	C1826	U1746	U1746	U1658	A1571	U1484	A1395	G1313		G1139	A1054	G974
C	U	A1828	U1749	U1749	U1659	U1572	G1485	G1400	C1314		G1140	A1055	C975
U	U	G1830	A1750	A1750	G1660	A1573	G1486	G1401	G1315		C1141	U1056	U976
G	U	U1831	G1751	G1751	G1661	U1574	G1487	G1402	U1316		G1142	A1064	C977
C	C	G1833	U1754	U1754	G1662	G1575	G1488	G1403	A1317			A1065	U979
C	G	U1834	G1755	G1755	G1666	G1576	G1489	G1404	G1318		G1145	G1066	A980
U	A	A1835	U1756	U1756	A1667	C1577	U1490	U1410	U1319		G1146	U1067	U981
U	U	C1836	A1760	A1760	G1668	U1578	U1491	U1411	C1320		G1147	C1068	C982
G	C	U1838	G1761	G1761	G1669	C1581	U1492	G1414	G1329		A1153	G1069	A983
U	C	A1839	C1762	C1762	C1674	C1582	G1493	U1415	U1330		A1158	U1070	
U	C	U1840	U1765	U1765	G1675	A1583	A1498	G1416	G1242		A1159	U1071	G993
A	U	A1841	G1766	G1766	A1676	G1586	C1499	U1417	U1334		C1160	U1072	U994
G	G	U1842	C1767	C1767	G1677	U1587	G1500	A1418	A1244		G1161	U1073	U995
U	C	G1843	U1768	U1768	A1588	A1587	U1501	A1419	A1245		A1163	U1078	G999
C	U	C1844	G1769	G1769	U1681	U1588	C1508	C1420	U1247		G1164	U1079	C1000
U	G	G1845	G1770	G1770	A1589	A1589	G1514	G1421	C1248		A1165	A1080	G1001
C	G	C1846	G1780	G1780	U1682	G1590	U1514	U1425	G1249		G1166	U1081	A1002
U	G	U1849			U1683	G1591	G1517	U1426	C1254		A1170	G1087	A1006

G3069	G2990	A2910	U2818	C2737	G2663	U2581	G2440	G2370	U2294	A2219	A2144	G
C3072	G2983	A2912	A2819	C2741	U2664	C2582	A2441	G2371	A2296	A2220	A2145	U
A3073	G2913	C2913	A2820		C2665	G2585	A2442	A2372	U2297	G2221	C2146	A
G3074	U2996	G2914	G2824	U2744	C2666	G2586	A2443	A2373	U2298	A2222	A2147	G
G3075	G2987	U2915	G2827	U2746	G2672	U2588	A2444	C2374	U2299	A2223	U2148	A
U3078	A3000	U2916	G2828	A2747	A2673		A2445	G2375	A2149	A2224	C2149	C
U3079	C3001	U2923	G2829	A2748	G2674	G2592	U	G2376	G2150	U2225	G2150	C
G3080	C3002	U2924	A2819	A2749	A2675	A2594	A	G2377	A2151	U2226	G2151	G
G3081	G3003	G2925	G2834	C2749	C2676	A2593	G	U2380	A2152	A2227	A2152	U
G3082	A2926	A2926	U2835	U2750	A2676	U2513	A	U2381	U2153	A2228	U2153	C
G3083	C2927	C2927	C2836	G2751	G2677	U2514	G	G2382	G2155	C2230	G2155	C
G3084	U3007	C2928		U2752	A2680	A2515	U	C2383	G2156	C2231	G2157	U
G3085	A3008		G2840	G2753			G	C2384	A2158	A2232	A2158	G
G3086	A3086	A2933	G2841	C2754	U2606	G2522	U	A2385		A2233		C
G3087	A3086	A2934	U2842	G2755	G2607	A2523	U	G2386	U2162	G2234		G
G3088	U3013	U2935	C2843		A2608	A2524	A	A2387		G2240	U	U
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U3095	G3015	G2937	A2845	G2761	U2610	G2526	A	U2389		A2242		A
U3096	A3016	G2938	G2850	A2762	U2611	G2527	U	C2392		A2243		U
C3097	A3017	G2939	A2851	C2765	U2612	G2528	A	G2393		A2244		U
G3098	C3018	A2940	C2852	U2766	G2614	U2532	A	G2394	A2172	C2245	A2172	U
	U3019	A2941	A2853	U2767	G2615	G2533	G	G2395	U2173	G2246	U2173	U
	A3024	C2942		U2768	G2619	G2534	U	A2396	G2174	G2247	G2174	A
U3104		G2943	U2860	U2769	G2620	A2535	G	A2397		C2248		C2094
G3113	G3028	U2944	U2861	A2770	G2621	A2536	G	G2400	G2177	G2249	G2177	A2093
C3115	A3029	G2945	U2862	G2771	G2622	U2538	U	A2401	U2186	G2250	U2186	G2095
U3119	G3030	A2946	C2863	U2772	G2623	G2539	G	A2402	C2179	G2251	C2179	A2096
C3120	U3041	U2952	G2871	C2778	G2624	U2540	C	G2403	G2180	U2252	G2180	C2098
U3121	U3042	U2953	A2872	A2779	G2625	U2541	U	A2404	C2181	U2253	C2181	C2101
A3122	C3043	U2955	U2873	A2780	G2626	U2542	U	C2405	G2185	A2254	G2185	U2102
	G3044	A2956	C2874	U2783	A2626	U2543	C	G2406	U2187	A2255	U2187	A2107
G3128	G3045	C2960	U2875	U2784	G2627	C2630	G	C2407	U2188	U2256	U2188	C2108
A3130	U3047	G2961	C2876		U2633	U2634	C	U2411	U2189	U2257	U2189	C2108
U3131	A3048	A2969	C2881	G2787	U2712	A2637	C	C2415	U2190	G2261	U2190	G2111
C3132	U3050	C2970	U2882	U2794	U2713	C2638	C	U2416	U2191	A2262	U2191	U2112
A3133	G3051	A2971	A2887	U2795	G2714	G2639	C	U2417	C2192	G2263	C2192	A2113
C3134	G3052	U2888	U2889	G2796	A2715	A2640	G	G2418	U2193	U2264	U2193	C2114
U3135	G3053	A2890	G2800	U2716	U2716	U2641	U	U2349	G2194	G2272	G2194	A2120
G3136	U3054	A2890	A2801	U2717	A2642	A2642	A	C2422		U2273		G2121
	U3055	G2977	A2802	U2718	C2644	C2644	A	G2423	C2202	G2278	C2202	G2122
U3139	U3056	U2978	U2722	U2719	G2648		C	U2424	C2203	A2279	C2203	G2123
G3140	U3057	U2979	U2723	U2720	G2651		C	G2425	C2204	A2280	C2204	A2125
A3141	U3058	A2982	U2724	U2721	U2652		C	U2426	G2205	A2281	G2205	C2128
C3142	G3059	C2983	U2725	U2722	U2653		C	U2427	A2207	U2282	A2207	A2131
C3143	C3060	C2984	C2726	U2723	C2653		C	U2428	U2209	G2283	U2209	G2129
G3144	G3061	A2902	C2727	U2724			C	U2429	U2210	C2284	U2210	G2124
C3145	U2986	A2903	G2728	U2725	A2656		C	G2430	U2211	U2285	U2211	A2138
G3146	A2987	U2904	U2729	U2726	U2657		C	U2431	A2215	G2286	A2215	U2139
	C3067	C2988	U2730	U2727	G2658		C	U2432	G2216	U2287	G2216	U2140
U3151	U3068	C2906	U2731	U2728	G2659		U	U2433	G2217	C2288	G2217	U2141
					G2660		U	A2434	G2218	C2289	G2218	A2143



G	G1878	C1802	G1719	A1621	C1543	G1450	G1375	C1292	A1202	U1110	U1028	U956	G875	G787
A	A1879	C1803	U1720	U1622	U1549	U1455	G1380	U1293	A1203	G1113	G1029	C959	U879	C788
G	U1880	A1804	U1721	U1629	U1554	A1456	G1381	U1294	A1204	C1032	C1032	C961	U880	U790
G	A1881	C1805	U1722	U1630	C1556	G1464	G1382	G1298	G1209	G1117	U1033	C962	G881	G791
C	A1886	G1807	U1723	C1631	C1556	G1465	G1383	C1298	U1210	A1120	A1036	G963	A882	C792
C	A1887	G1808	C1725	A1632	C1560	G1466	U1384	A1302	U1211	A1121	A1036	G964	C793	C793
U	U1888	A1809	G1728	U1636	G1561	A1467	C1385	A1302	A1212	U1122	U1039	G968	G887	G795
U	G1889	A1810	A1729	A1637	C1562	A1468	C1386	U1306	U1213	U1121	A1040	C969	U888	G799
G	G1892	G1812	G1730	A1638	C1563	A1468	U1388	U1306	U1214	G1127	A1046	G968	U889	G800
U	C	A1813	G1733	C1639	U1564	G1476	U1389	G1307	U1215	U1128	A1047	A972	C890	A801
C	A1885	U1814	G1734	G1640	A1566	G1480	A1390	A1308	C1216	A1129	A1048	A975	C891	C802
A	A1901	U1815	G1735	G1643	U1567	A1481	C1391	U1309	A1217	A1130	U1050	G974	U892	C803
G	G1902	A1816	G1736	A1644	U1568	A1482	C1392	G1313	A1221	G1131	A1054	G977	G893	G803
A	U1903	U1817	U1737	U1645	U1569	G1483	A1399	C1314	G1222	U1133	U1054	G977	G894	A806
C	C	U1818	G1738	G1646	U1570	G1486	G1400	U1315	G1226	U1138	U1058	U979	A896	A807
C	G1906	U1819	U1739	A1647	U1571	G1487	G1404	C1316	G1227	U1139	U1066	U979	A896	A807
C	C	U1820	U1740	U1647	U1572	G1488	U1405	A1317	C1228	G1140	A1063	U980	A906	U811
A	G1907	U1821	U1741	A1654	U1573	G1489	U1406	A1318	G1229	G1141	A1065	U981	A907	G812
G	A1908	C1822	U1742	A1655	A1574	A1490	A1407	G1319	G1232	G1142	U1066	U982	A908	A816
C	C	U1823	G1762	G1662	A1575	A1490	G1408	A1326	C1232	G1145	U1066	U983	A909	A817
G	G	G1825	U1765	G1666	U1576	G1493	G1409	A1326	C1232	G1145	U1066	U983	A909	C818
C	C	U1826	G1766	G1667	U1577	G1494	U1410	U1329	U1235	G1148	U1070	U990	A910	G822
C	A1913	G1829	A1752	U1659	C1578	U1495	C1411	U1330	G1236	G1148	U1071	U990	A911	C823
C	G1914	U1830	A1753	C1660	C1579	U1496	G1412	U1331	G1237	G1148	U1072	U991	A912	G824
U	A1915	G1831	C1762	G1661	A1580	C1496	A1413	A1332	C1238	A1153	G1072	A992	A914	U825
U	U1916	C1832	U1765	G1662	C1581	C1497	G1414	C1333	C1239	A1153	G1072	A992	A915	G826
C	C	U1833	U1766	G1666	U1583	A1498	U1415	U1334	U1240	A1153	G1072	A992	A915	G826
U	C	U1834	G1767	G1667	U1584	A1504	U1416	U1337	U1241	C1155	A1075	A993	A916	A827
U	U1922	A1835	C1767	A1667	U1584	C1505	C1416	U1337	U1242	C1156	A1075	A993	A916	A828
G	C1923	G1838	U1768	A1668	A1587	A1506	A1419	C1339	G1243	G1157	U1077	A996	A917	U829
U	C	U1839	G1769	G1674	U1588	A1507	A1420	U1339	U1244	A1158	U1078	A997	A920	A830
U	U	U1840	G1770	G1674	A1589	C1508	G1421	U1339	U1245	A1159	A1079	A998	A921	G831
G	A1932	U1841	U1771	G1677	G1590	U1514	C1424	G1345	G1246	C1160	A1080	A999	U922	G832
A	A1933	A1842	G1779	G1678	G1591	U1514	C1424	G1346	G1249	C1161	U1081	C1000	C923	A836
C	G1934	C1846	U1780	A1679	G1592	U1520	U1425	U1347	G1250	U1162	U1082	G1001	G924	A837
U	C	C1846	U1781	G1683	A1593	U1520	U1426	U1348	G1251	U1169	U1083	A1002	A929	G838
C	U1936	U1849	U1782	A1683	C1596	U1521	U1427	G1349	A1261	A1169	A1084	A1006	U930	A847
U	U1937	C1849	U1783	U1686	C1597	U1522	A1428	A1261	A1252	A1170	U1088	A1007	U930	A848
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G	C1941	U1855	U1788	U1689	U1600	U1526	C1432	G1354	C1267	A1180	A1093	G1010	G937	U850
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G	U1944	C1857	G1790	U1691	A1602	C1527	A1434	U1356	G1262	U1096	U1096	G1014	U939	G860
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C	C	C1792	C1792	A1696	G1604	U1533	U1436	G1357	A1263	C1189	G1097	U1015	G940	C861
U	U	G1793	U1607	U1696	U1607	G1536	U1437	A1363	G1264	A1190	A1098	C1016	U943	G864
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U	C	G1795	U1607	U1696	U1607	G1536	U1437	C1365	U1266	U1191	A1099	C1017	C944	G864
C	G1952	A1867	G1700	C1701	G1611	G1538	U1438	A1366	G1266	U1191	A1099	C1017	C944	G864
C	G1953	G1868	U1702	U1702	G1612	G1541	U1442	A1366	G1266	U1191	A1099	C1017	C944	G864
U	G1954	A1797	A1797	A1714	C1613	G1542	U1443	G1367	C1284	G1194	A1102	G1020	G947	U866
C	U1955	U1871	A1798	A1714	C1614	G1543	U1443	G1368	G1285	A1195	A1103	G1021	G947	G869
U	A	A1874	A1799	U1717	C1615	A1546	U1446	G1370	G1289	A1197	G1104	G1024	G950	U872
G	G	A1874	A1800	U1717	C1615	A1546	U1446	G1370	G1289	A1197	G1104	G1024	G950	U872
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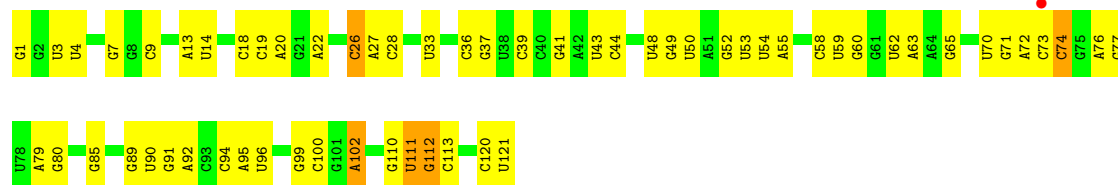




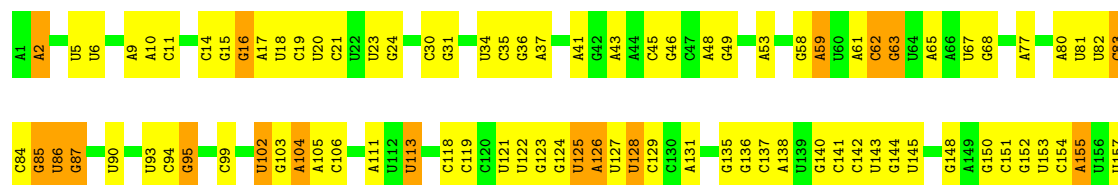
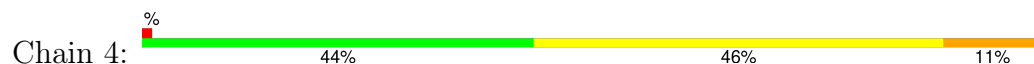
• Molecule 2: 5S ribosomal RNA



• Molecule 2: 5S ribosomal RNA

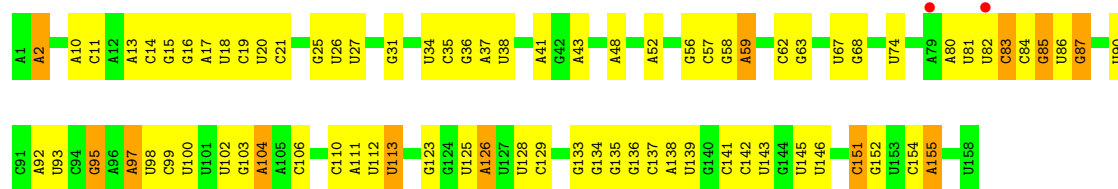


• Molecule 3: 5.8S ribosomal RNA

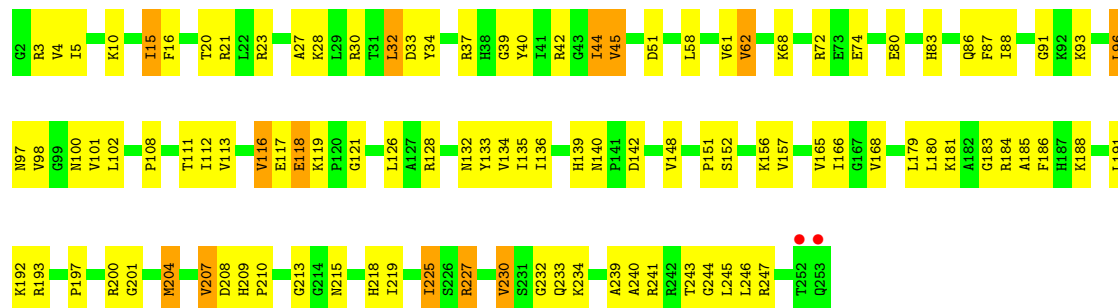


• Molecule 3: 5.8S ribosomal RNA

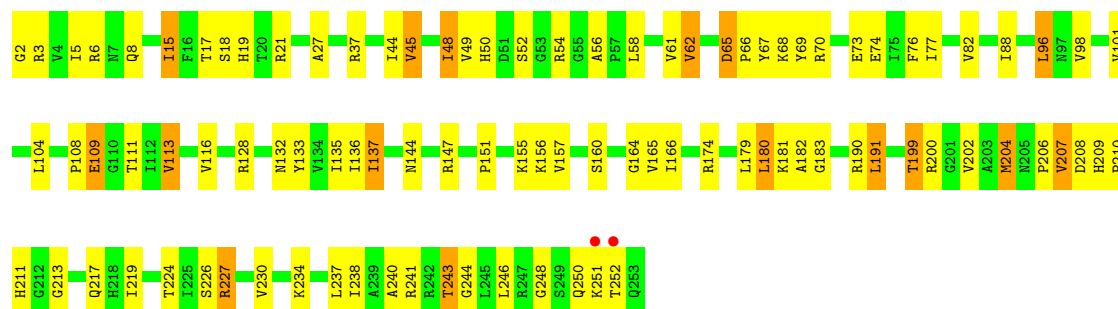




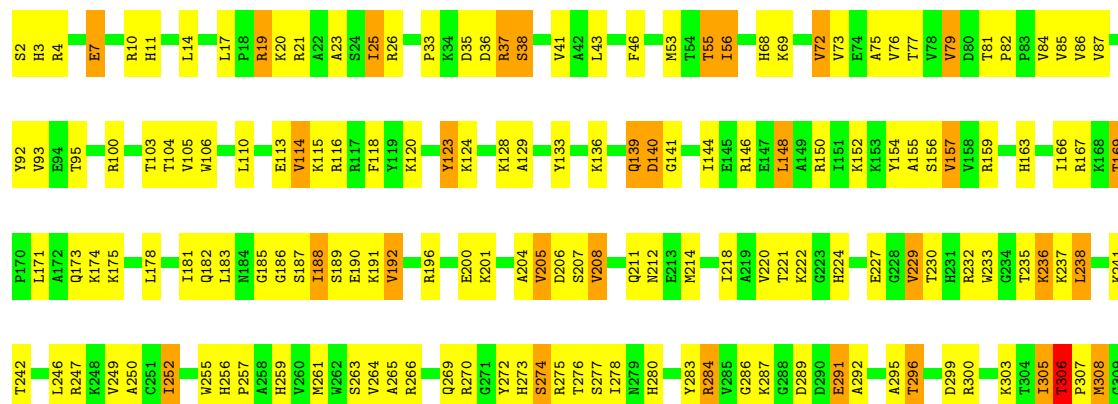
• Molecule 4: 60S ribosomal protein L2-A



• Molecule 4: 60S ribosomal protein L2-A

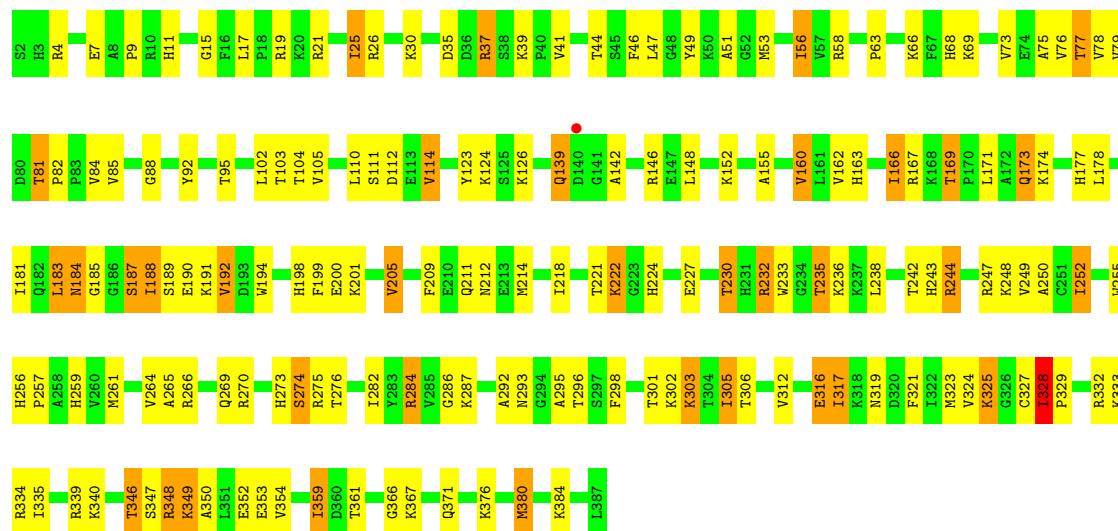


• Molecule 5: 60S ribosomal protein L3

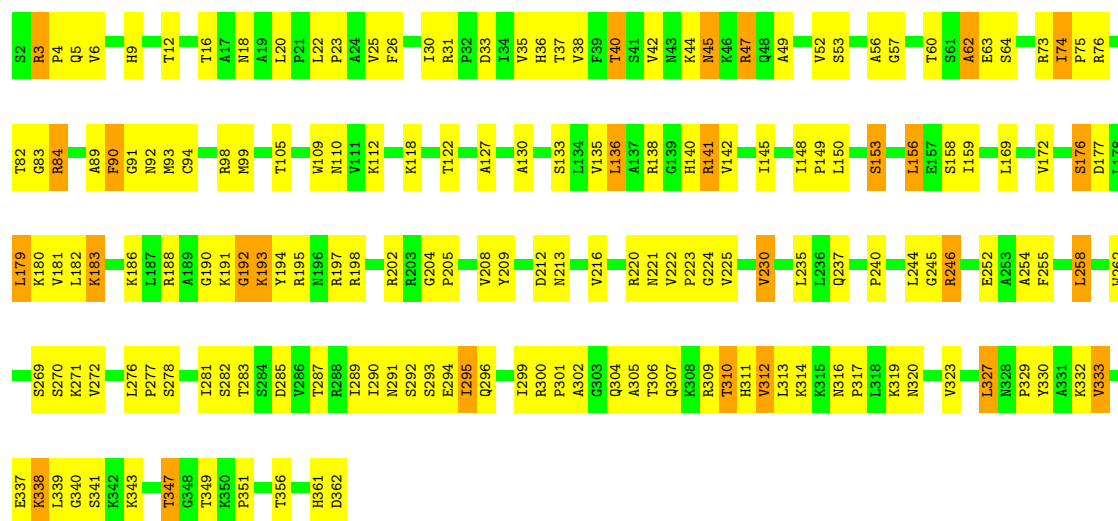




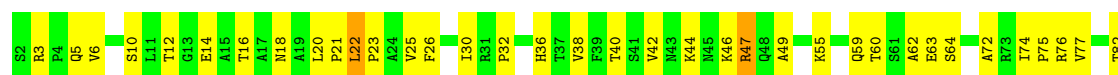
• Molecule 5: 60S ribosomal protein L3

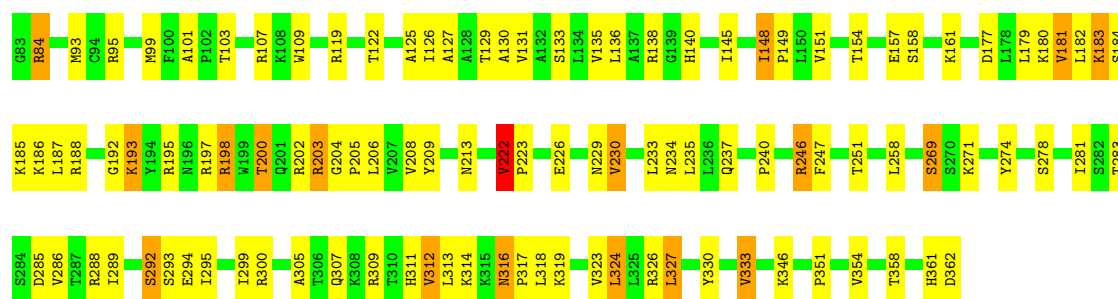


• Molecule 6: 60S ribosomal protein L4-A

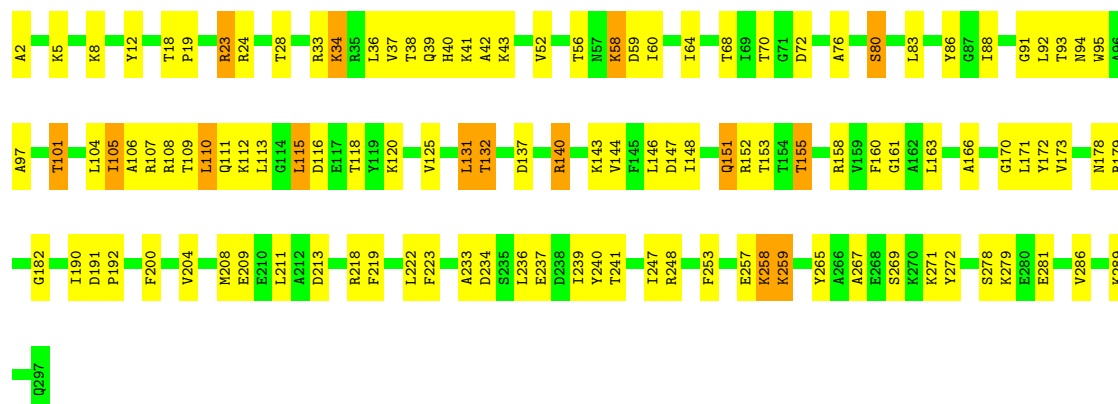


• Molecule 6: 60S ribosomal protein L4-A

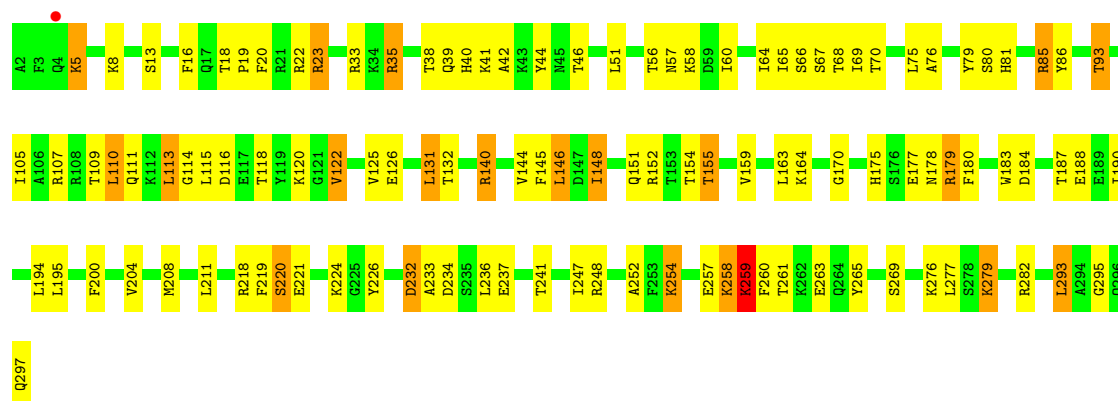




• Molecule 7: 60S ribosomal protein L5



• Molecule 7: 60S ribosomal protein L5



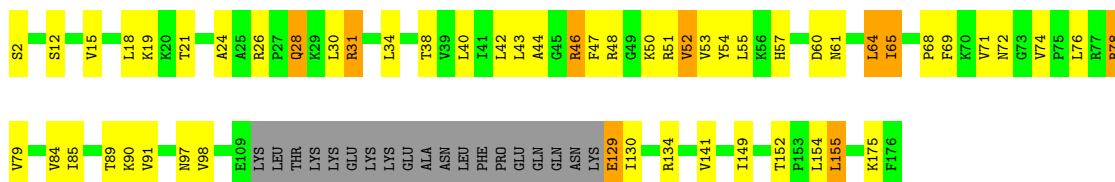
• Molecule 8: 60S ribosomal protein L6-A





• Molecule 8: 60S ribosomal protein L6-A

Chain CH: 58% 26% 5% 11%



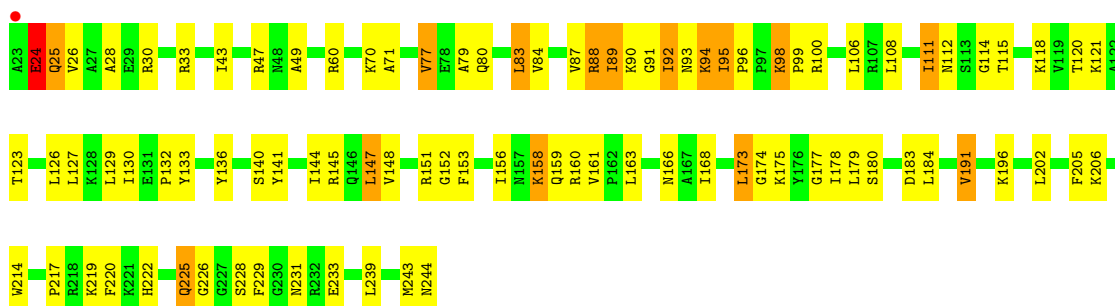
• Molecule 9: 60S ribosomal protein L7-A

Chain o: 58% 38% .



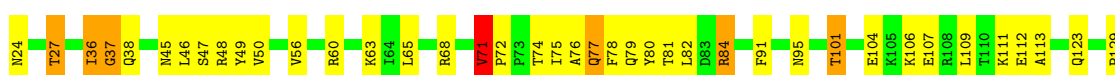
• Molecule 9: 60S ribosomal protein L7-A

Chain CI: 59% 34% 7%



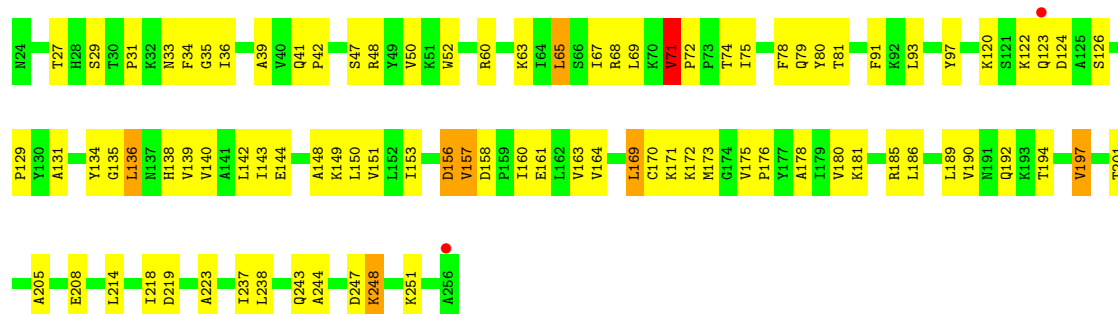
• Molecule 10: 60S ribosomal protein L8-A

Chain p: 69% 27% . .

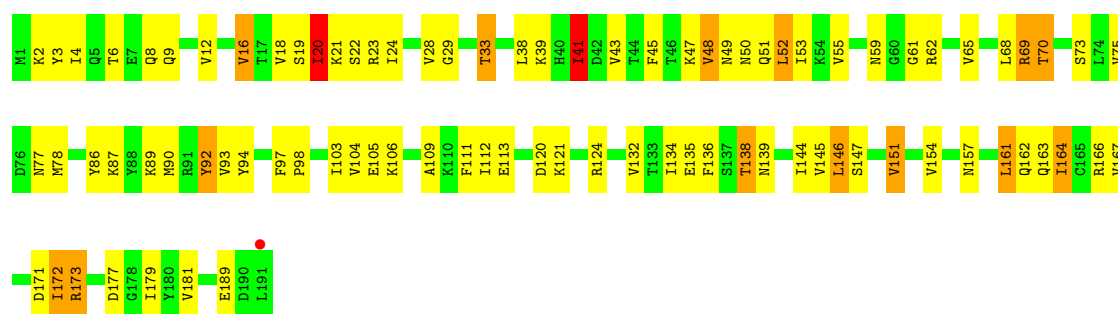




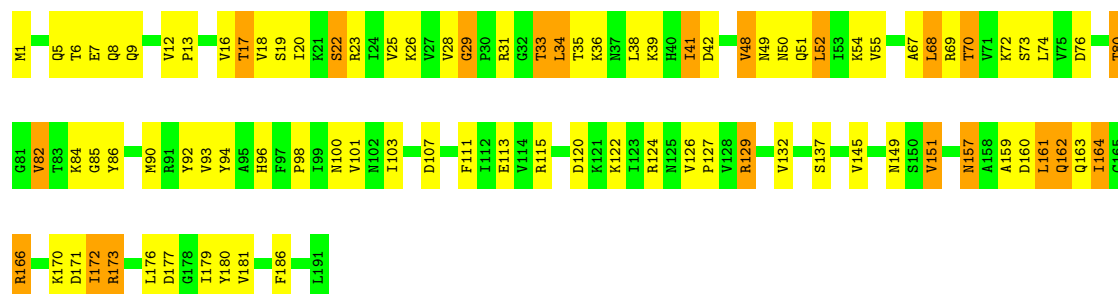
• Molecule 10: 60S ribosomal protein L8-A



• Molecule 11: 60S ribosomal protein L9-A

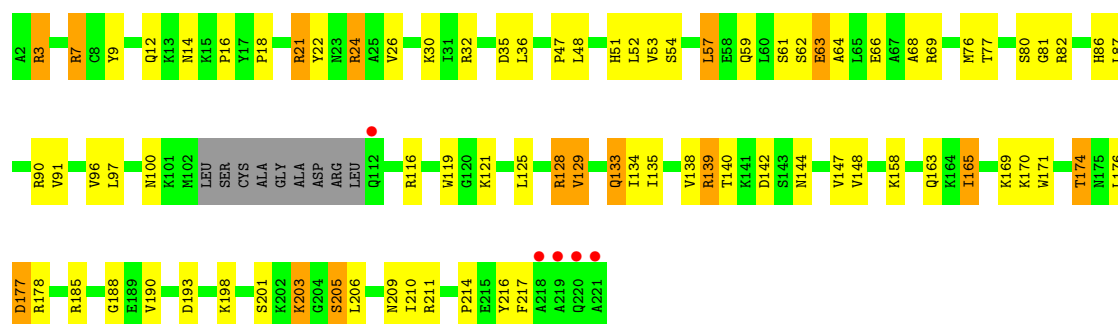


• Molecule 11: 60S ribosomal protein L9-A

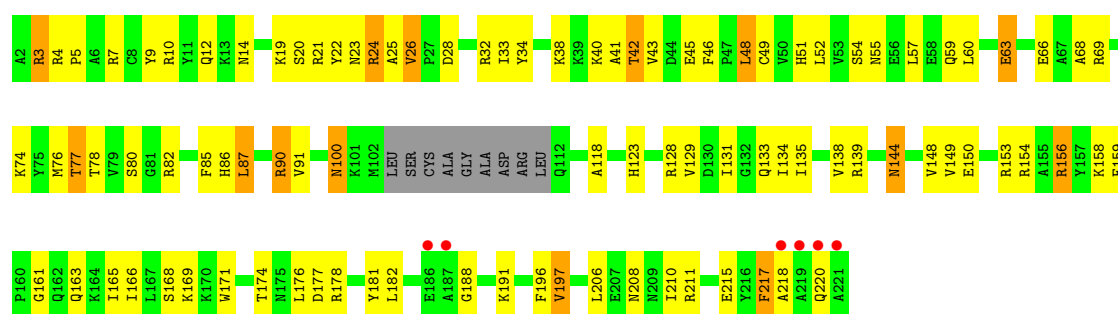


• Molecule 12: 60S ribosomal protein L10

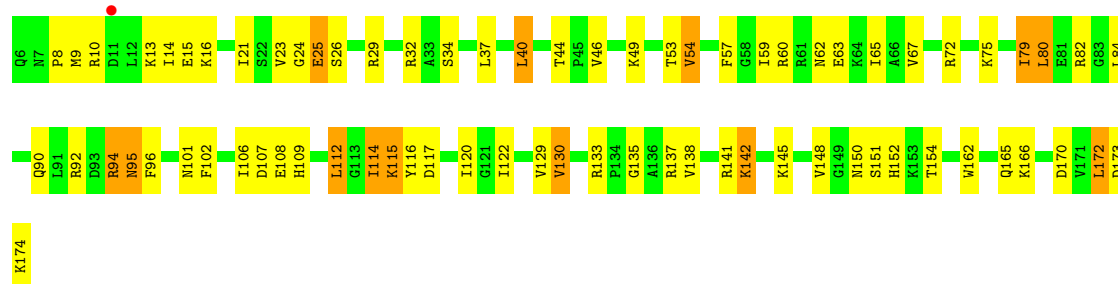




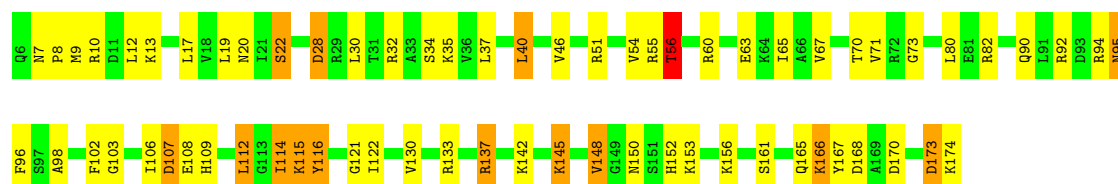
• Molecule 12: 60S ribosomal protein L10



• Molecule 13: 60S ribosomal protein L11-B

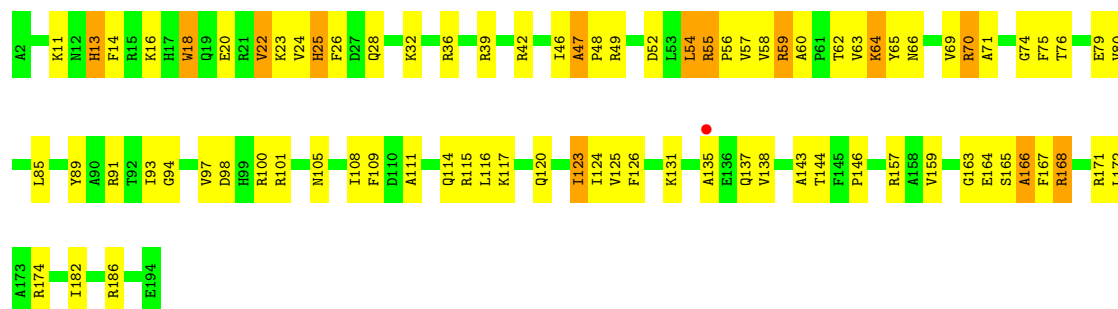


• Molecule 13: 60S ribosomal protein L11-B



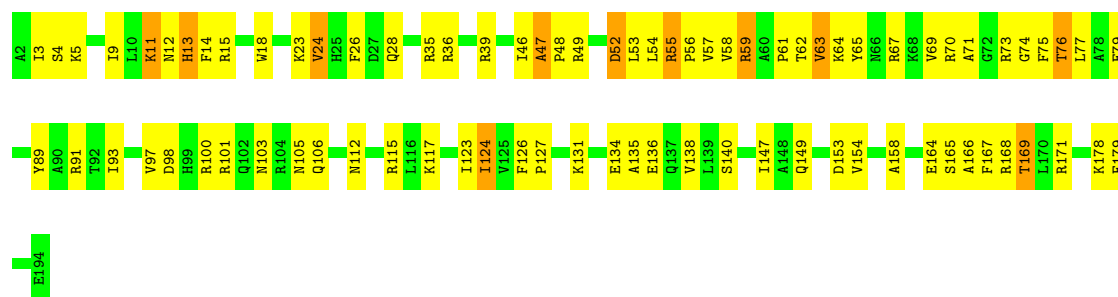
• Molecule 14: 60S ribosomal protein L13-A





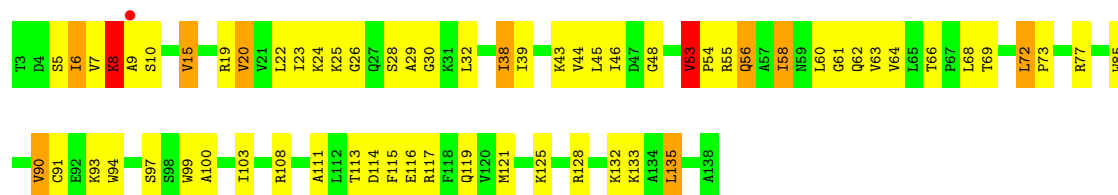
- Molecule 14: 60S ribosomal protein L13-A

Chain CN: 58% 36% 6%



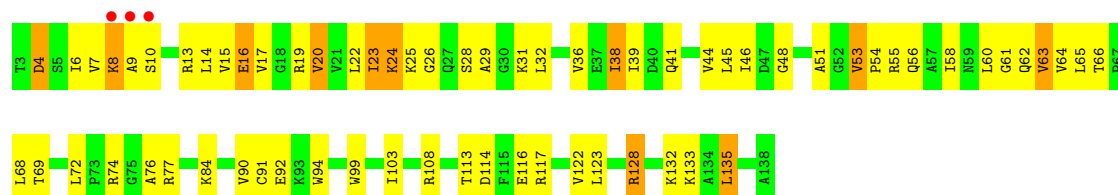
- Molecule 15: 60S ribosomal protein L14-A

Chain u: 53% 39% 7%



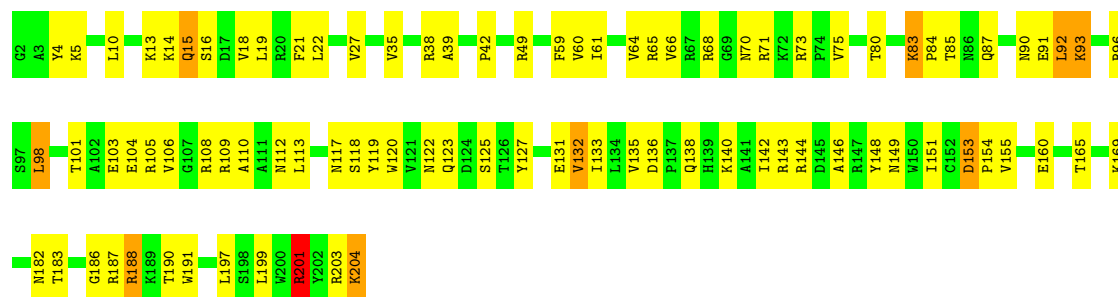
- Molecule 15: 60S ribosomal protein L14-A

Chain CO: 51% 41% 8%



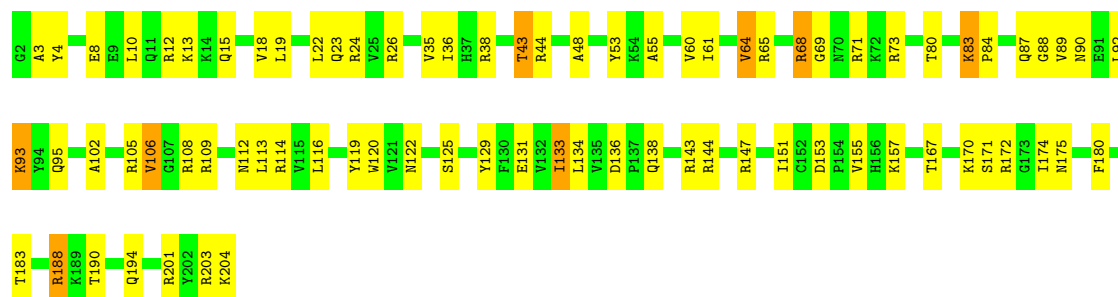
- Molecule 16: 60S ribosomal protein L15-A

Chain v: 56% 39% 5%



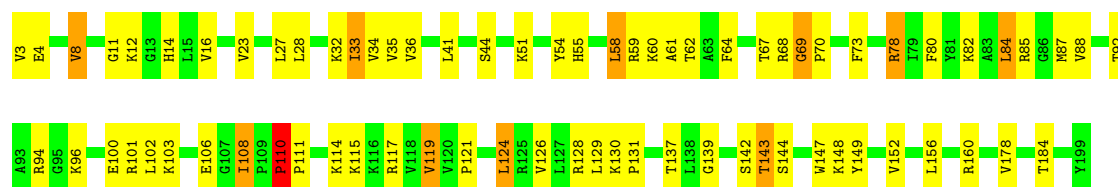
• Molecule 16: 60S ribosomal protein L15-A

Chain CP: 61% 35% •



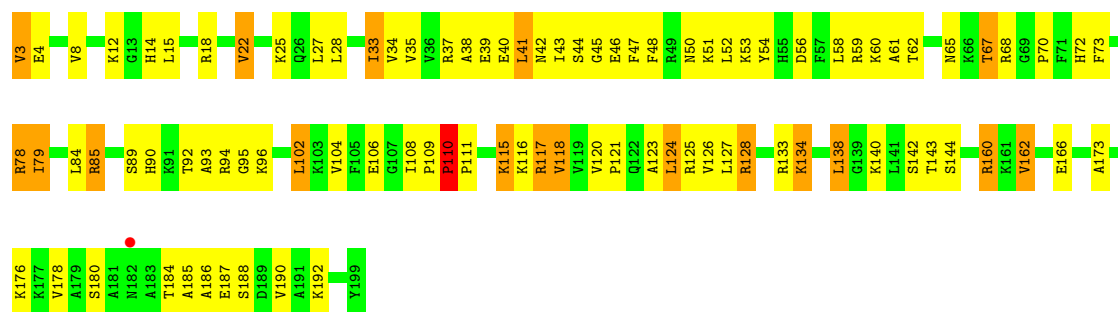
• Molecule 17: 60S ribosomal protein L16-A

Chain w: 63% 31% 5% •



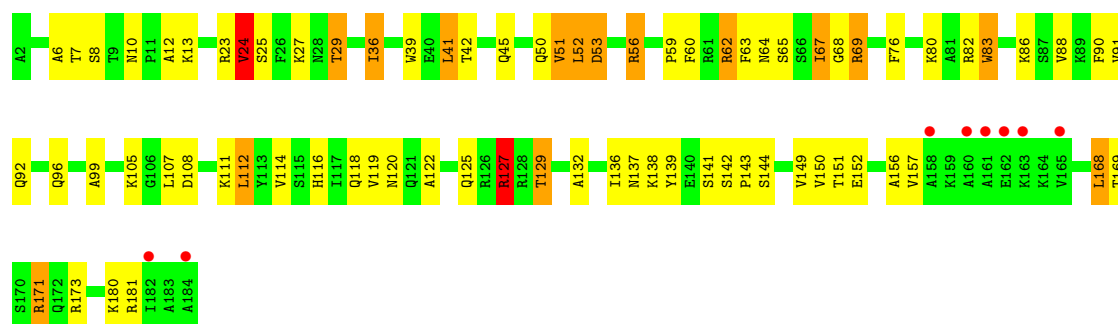
• Molecule 17: 60S ribosomal protein L16-A

Chain CQ: 52% 38% 9% •



• Molecule 18: 60S ribosomal protein L17-A

Chain x: 4% 58% 32% 8% •



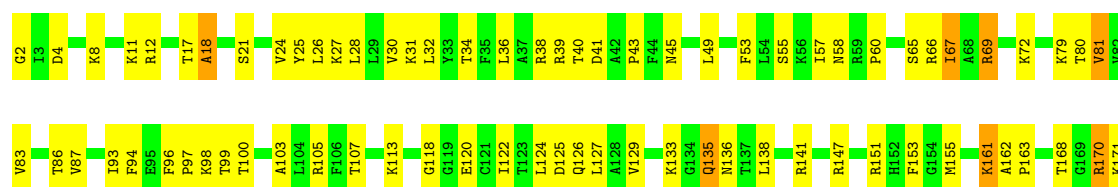
• Molecule 18: 60S ribosomal protein L17-A



• Molecule 19: 60S ribosomal protein L18-A

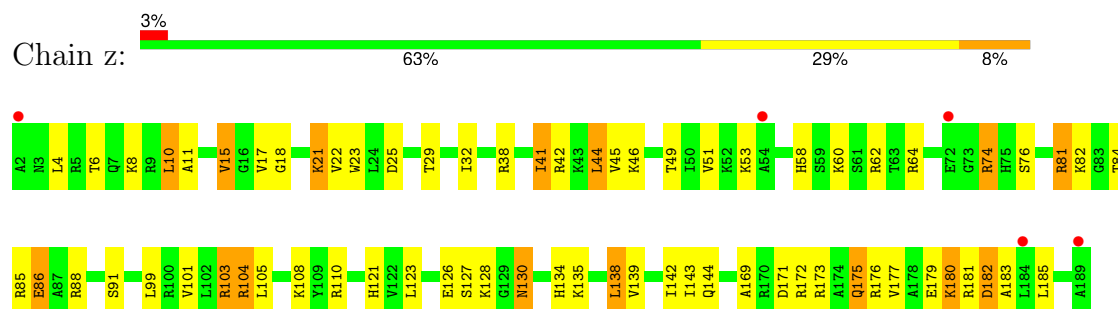


• Molecule 19: 60S ribosomal protein L18-A

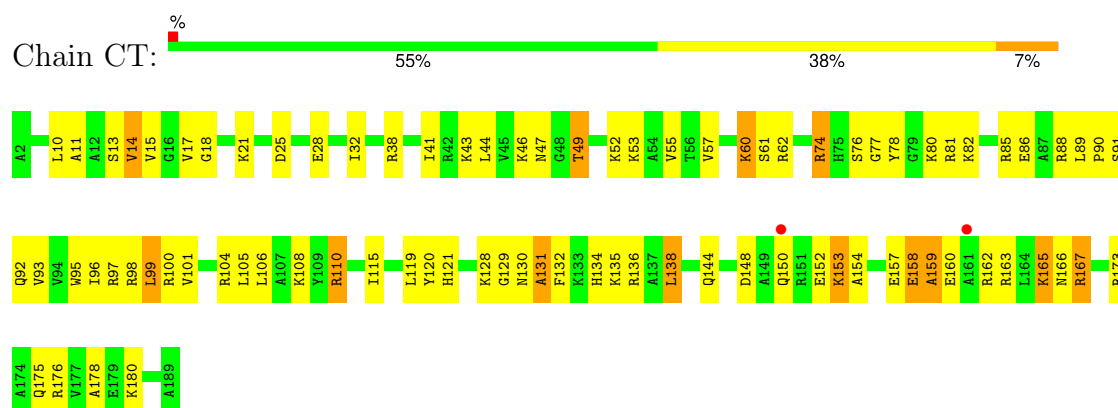




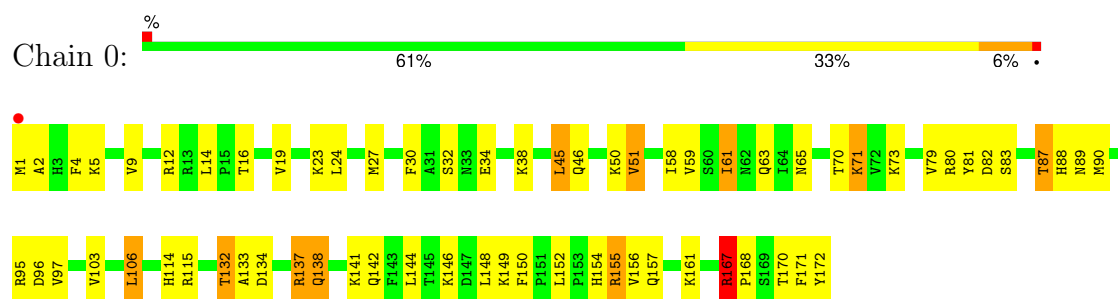
- Molecule 20: 60S ribosomal protein L19-A



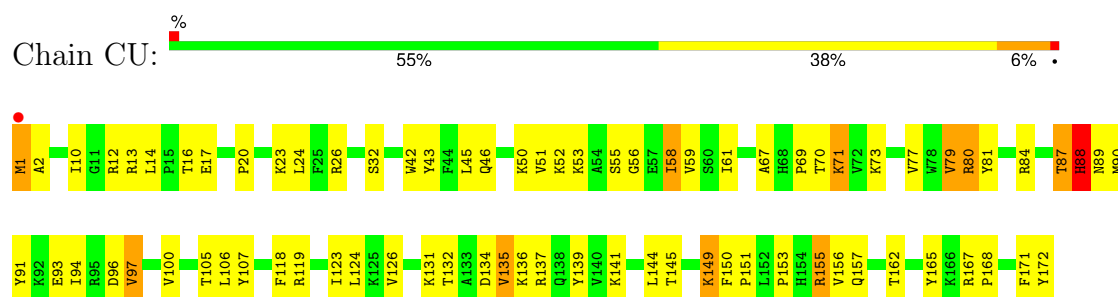
- Molecule 20: 60S ribosomal protein L19-A



- Molecule 21: 60S ribosomal protein L20-A

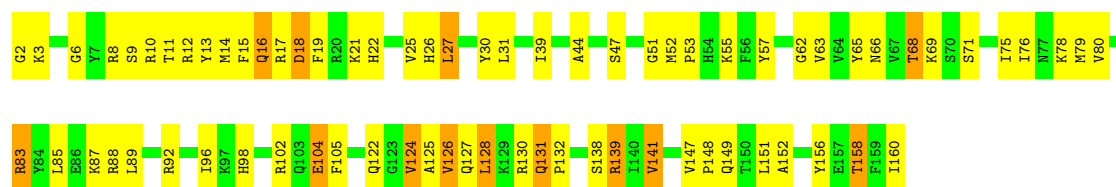


- Molecule 21: 60S ribosomal protein L20-A



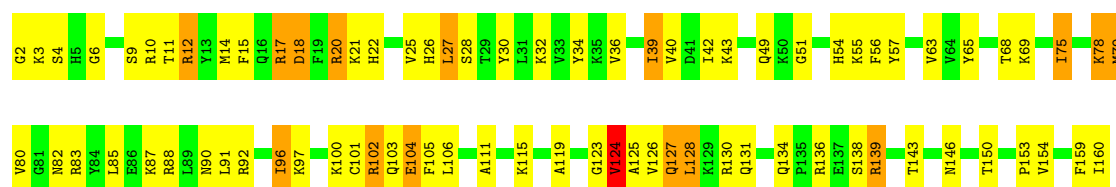
- Molecule 22: 60S ribosomal protein L21-A

Chain 2: 



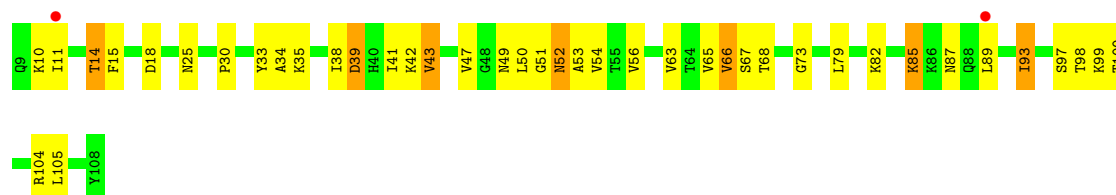
- Molecule 22: 60S ribosomal protein L21-A

Chain CV: 



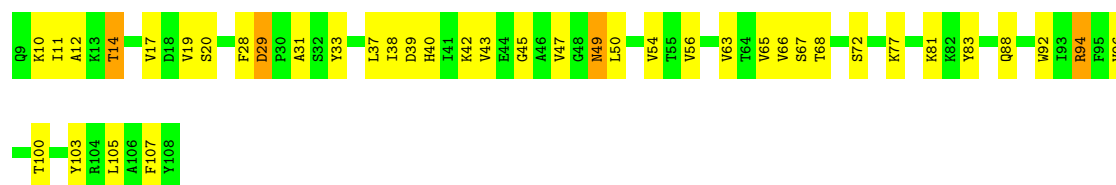
- Molecule 23: 60S ribosomal protein L22-A

Chain 5: 



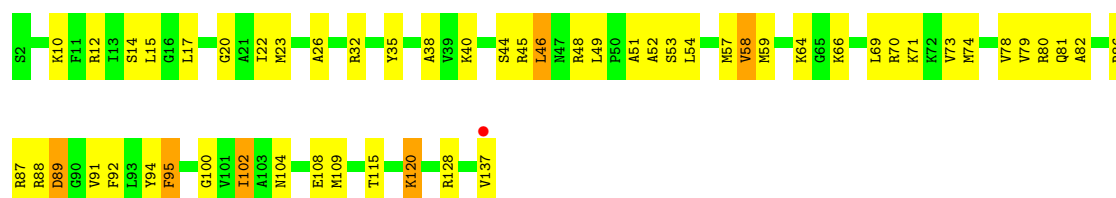
- Molecule 23: 60S ribosomal protein L22-A

Chain CW: 

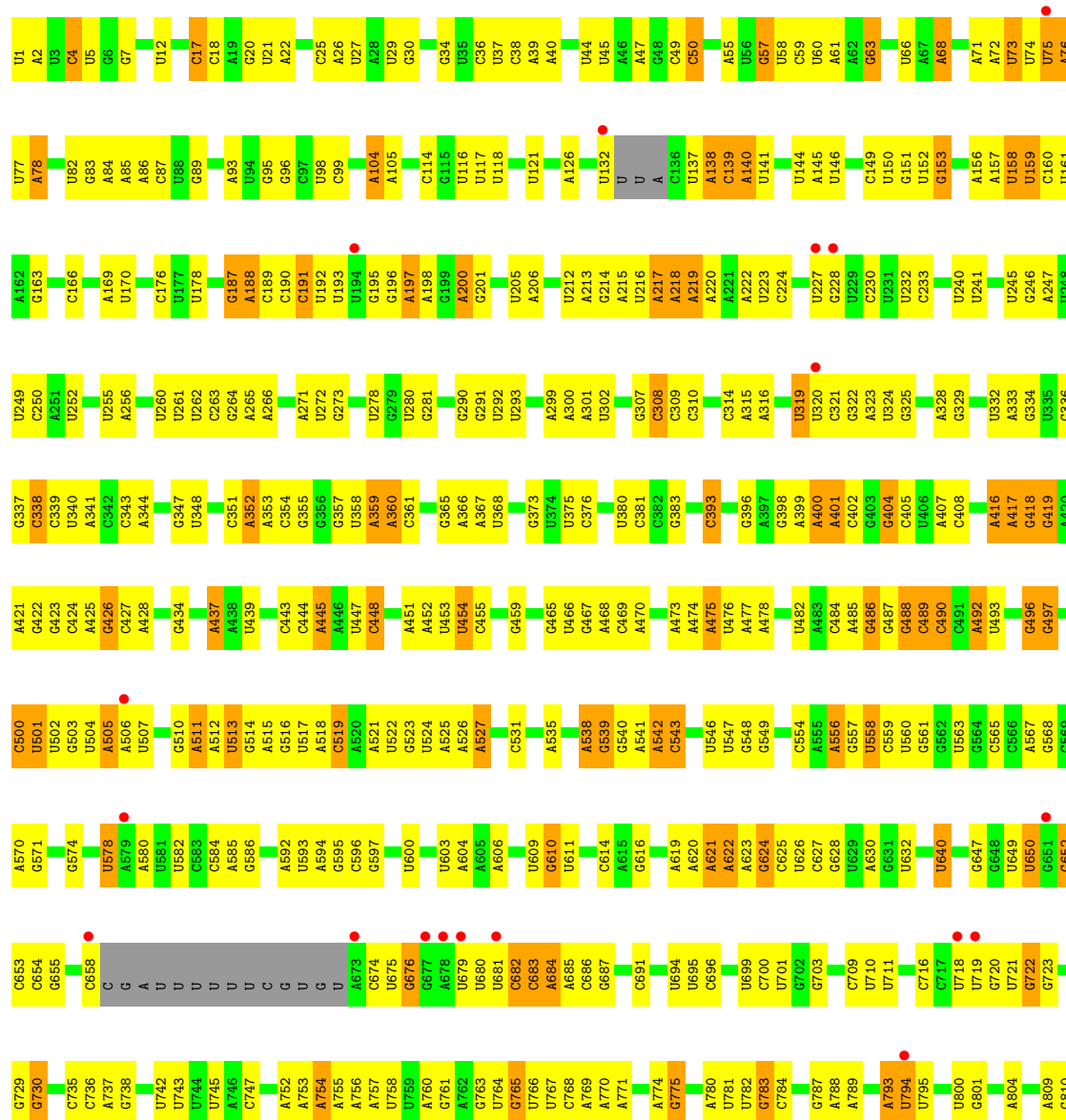


- Molecule 24: 60S ribosomal protein L23-A

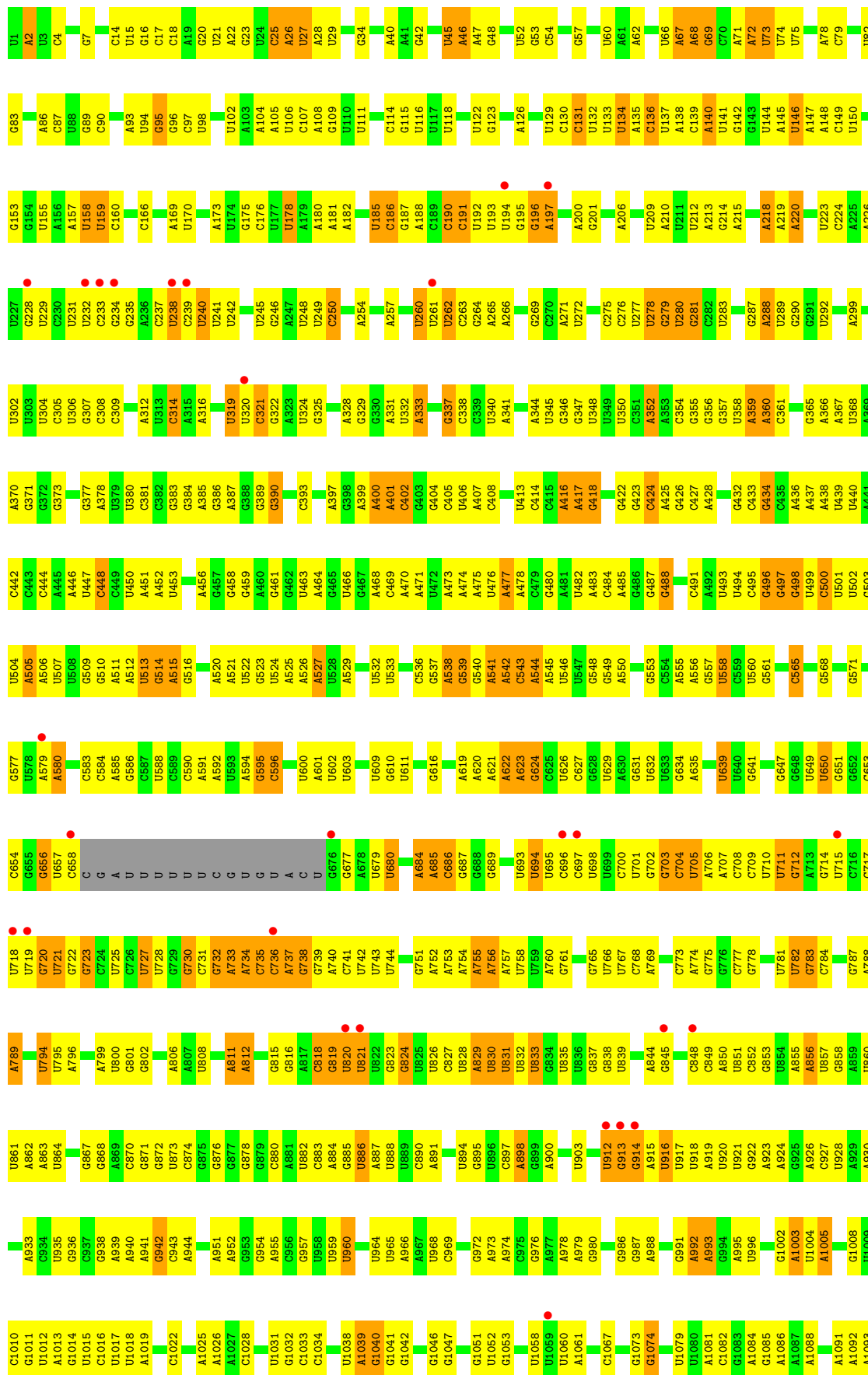
Chain I2: 

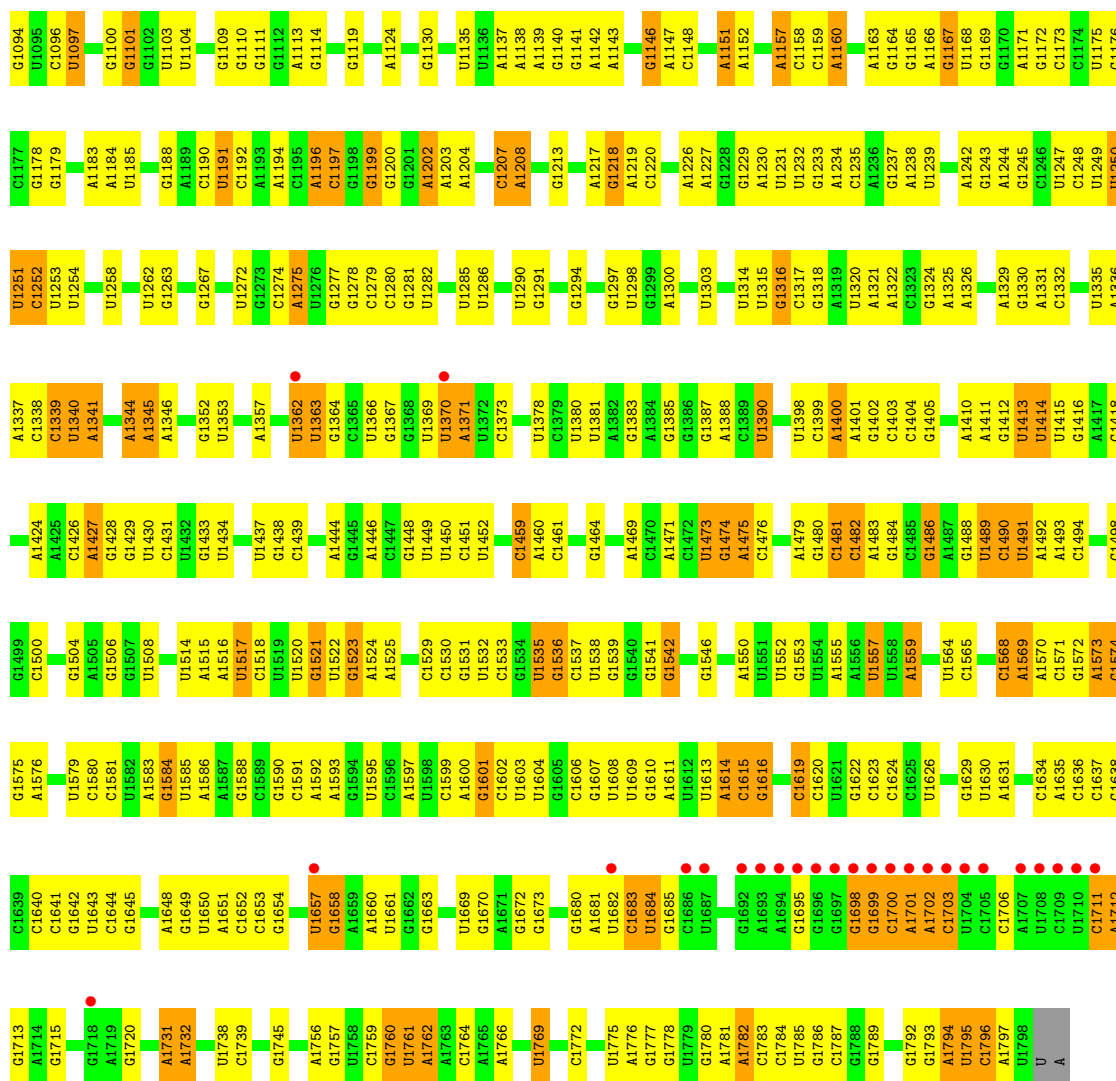


Chain CX: %

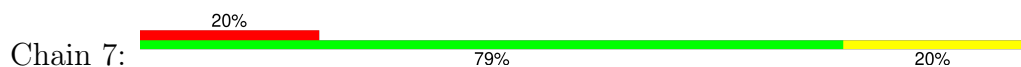




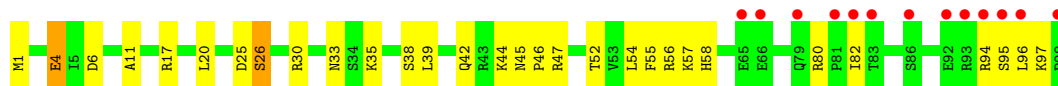




• Molecule 26: 60S ribosomal protein L24-A

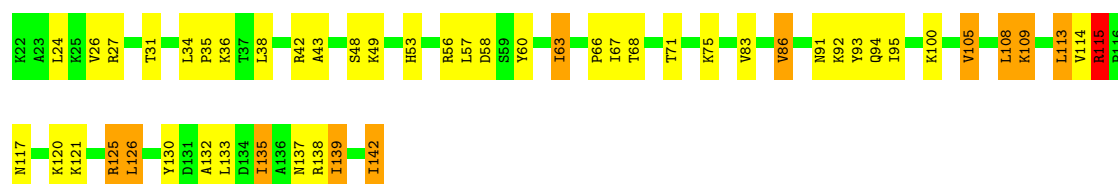


• Molecule 26: 60S ribosomal protein L24-A



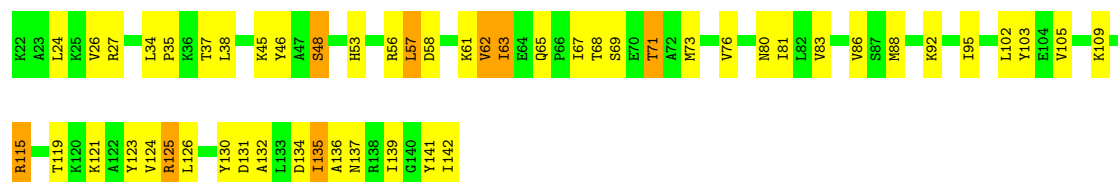
• Molecule 27: 60S ribosomal protein L25





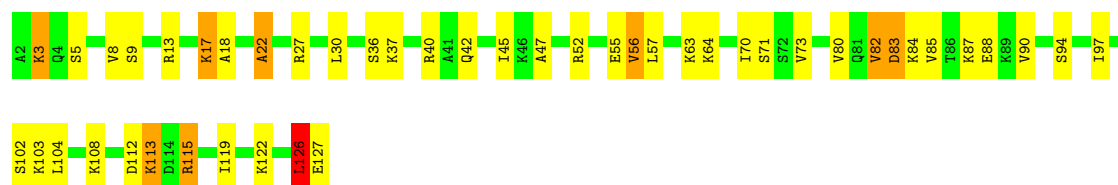
- Molecule 27: 60S ribosomal protein L25

Chain CZ: 57% 36% 7%



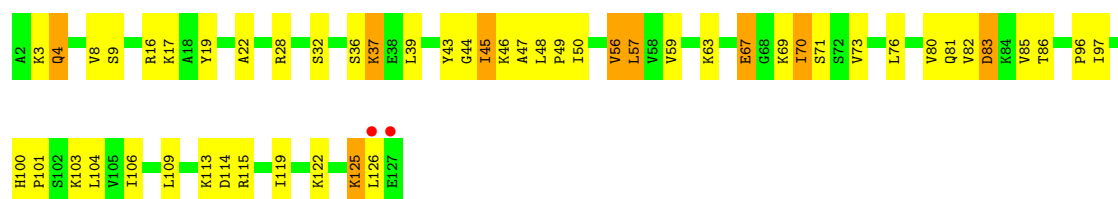
- Molecule 28: 60S ribosomal protein L26-A

Chain 9: 63% 29% 6%



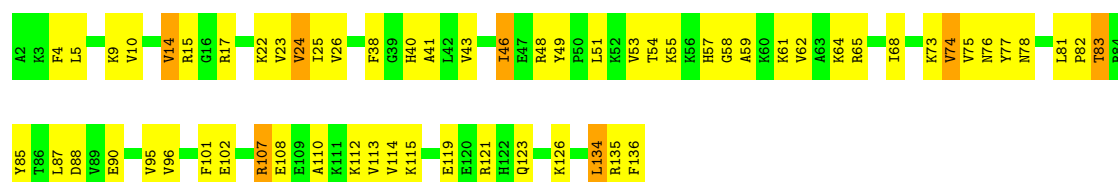
- Molecule 28: 60S ribosomal protein L26-A

Chain DA: 2% 59% 34% 7%



- Molecule 29: 60S ribosomal protein L27-A

Chain AA: 54% 41% 5%



- Molecule 29: 60S ribosomal protein L27-A

H79	A2
L80	K3
L81	F4
T82	L5
T83	
R84	K9
Y85	V10
S97	
E102	V14
Q103	R15
P104	G16
S105	R17
Q106	Y18
R107	A19
E108	
E109	V23
A110	V24
	T25
	V26
	K27
V113	R36
V114	P37
K115	
S132	A41
K133	L42
L134	V43
R135	A44
F136	G45
	L46
	E47
	R48
	Y49
	P50
	L51
	K52
	V53
	T54
	H57
	G58
	A59
	K60
	K61
	V62
	A63
	K64
	R65
	T66
	K67
	L68
	K69
	P70
	K73
	V74
	V75
	N76
	Y77
	N78

[illegible]

Y109	P2
I112	S3
L113	R4
G114	T6
K115	K7
G116	T8
R117	R9
I118	K10
P119	H11
M120	R12
V121	G13
P122	
V123	R21
I124	I22
V125	G23
K126	K24
V130	K27
L133	H28
	P29
K137	R32
E146	G33
L147	R34
I148	A35
A149	G36
	H40
	H41
	R42
	N45
	D46
	X47
	Y48
	H49
	V56
	G57
	M58
	R59
	w69
	L73
	N74
	L76
	D76
	K77
	L78
	W79
	I82
	P83
	B84
	D85
	L91

Item	Category
A2	A
K5	A
N6	A
H7	A
T8	C
A9	A
H10	A
R14	A
K15	A
A16	A
H17	B
R18	A
N19	A
G20	D
L21	A
K22	A
K23	A
P24	E
K25	A
K28	A
S31	A
D36	A
P37	A
K38	A
R41	A
L47	A
T50	A
K59	A

A2	K3	S4	K5	N6		R14	K15	A16	H17	R18		T21	K22	K23	P24	K25	T26	V27	K28	Y29			D36		H43	K44	H45	A46	L47			T50			K58	K59
----	----	----	----	----	--	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	--	-----	--	-----	-----	-----	-----	-----	--	--	-----	--	--	-----	-----

S9
I10
K13
I14
A15
L16
V17
I18
K19
I20
K22
Y23
T24
Y27
K28
S29
T30
V31
K32
S33
I34
K35
Q36
G37
K38
S39
K40
I43
T48
P49
R52
K53
S54
E55
Y59
A60
M61
E76
L77
G78
T79
A80
V87
E94
S98
D99
I100
L101
T102

L104
A105

- Molecule 32: 60S ribosomal protein L30

Chain DE: 

S9 I10 M11 Q12 Q13 L14 A15 V17 L16 I18 K19 S20 T24 T25 L25 G26 T30 L34 R35 K40 L41 T42 T43 T44 T48 K53 Y59 E76 K83 L84 P85 R86 V87 Q88 V89 V90 S91 I92 D99 T100 L101 T102 T103 L104 A105

- Molecule 33: 60S ribosomal protein L31-A

Chain AE: 

L4 K5 D6 V7 V8 E11 Y12 T13 L16 H17 K18 R19 L20 V23 S24 P25 K26 R28 A29 P30 R31 A32 E35 L42 H43 M44 G45 T46 L51 A52 P53 E54 L55 N56 Q57 A58 I59 R62 G63 V64 V67 E68 Y69 R72 L73 R74 R79 E83

K86 N87 P88 L89 F90 F92 V93 P95 V96 V98 L104 T106 E110 E111 D112

- Molecule 33: 60S ribosomal protein L31-A

Chain DF: 

L4 V7 V8 T13 L16 H17 K18 L20 S24 F25 K26 A29 P30 R31 E35 T46 D47 P53 E54 L55 H56 Q57 R62 G63 V64 K65 G66 V67 E68 Y69 R70 L71 R72 L73 R74 I75 S76 R79 K86 N87 P88 L89 E94 P95 V96 G103

L104 Q105 T106 V107 V108 V109 D112

- Molecule 34: 60S ribosomal protein L32

Chain AF: 

A2 S3 L4 P5 R19 H20 H21 S22 D23 R24 Y25 H26 R27 V28 R33 K34 Q35 S40 R44 R47 I50 S51 K54 K61 K64 P65 L66 S67 T73 F74 L75 N78 V79 L82 H88 A97 T100 S101 A102 K103 N104 R105 V106 L109

A110 R111 L115 R125 L128

- Molecule 34: 60S ribosomal protein L32

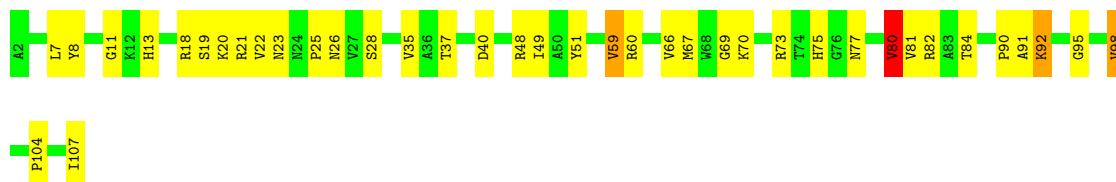
Chain DG: 

A2 S3 L4 F7 K8 T9 V10 K18 R19 H20 H21 S22 D23 R24 Y25 H26 R27 V28 A29 E30 N31 V32 R33 S40 V41 R44 R45 F46 R47 P53 K54 I55 G56 Y57 K61 K62 T63 S67 T73 F74 L75 V76 A77 R78 V79 K80 D81 L82 E83 L84 T86



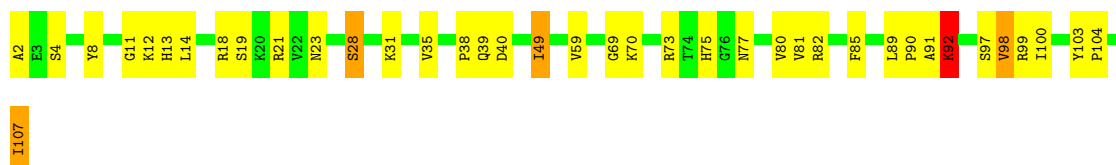
- Molecule 35: 60S ribosomal protein L33-A

Chain AG: 63% 33%



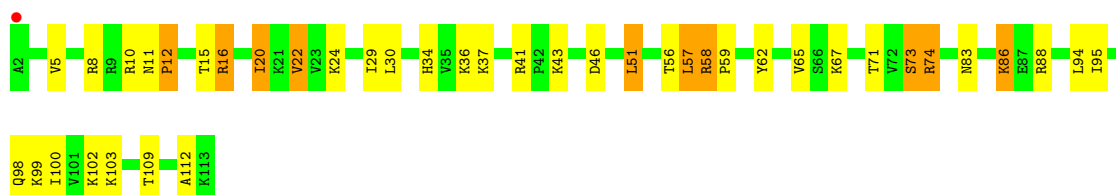
- Molecule 35: 60S ribosomal protein L33-A

Chain DH: 63% 32%



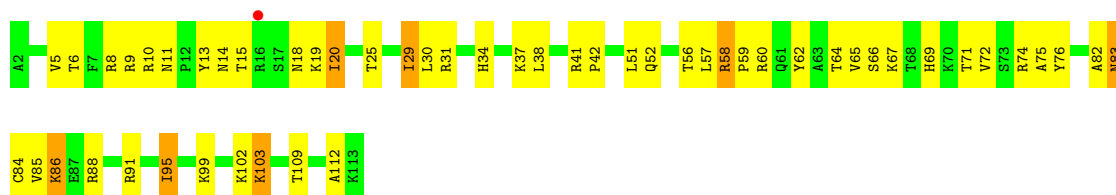
- Molecule 36: 60S ribosomal protein L34-A

Chain AH: 63% 28% 9%



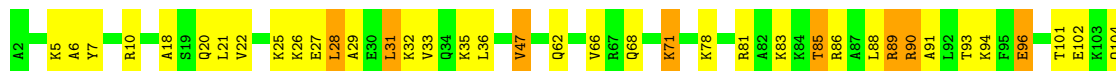
- Molecule 36: 60S ribosomal protein L34-A

Chain DI: 54% 40% 6%



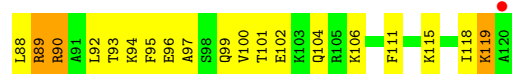
- Molecule 37: 60S ribosomal protein L35-A

Chain AI: 59% 34% 7%

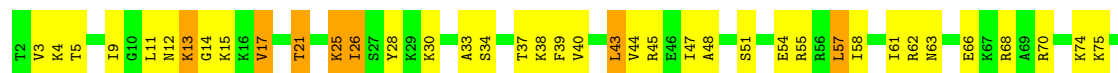




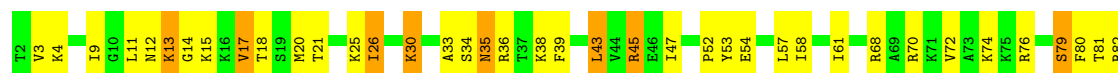
- Molecule 37: 60S ribosomal protein L35-A



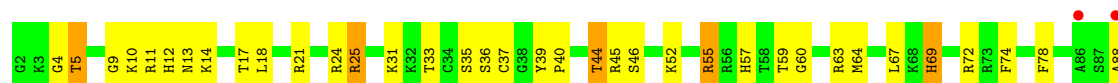
- Molecule 38: 60S ribosomal protein L36-A



- 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

Chain AL: 65% 27% 8%



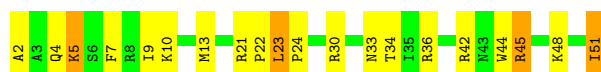
- Molecule 40: 60S ribosomal protein L38

Chain DM: 62% 29% 9%



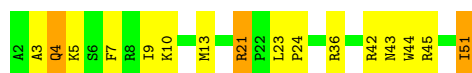
- Molecule 41: 60S ribosomal protein L39

Chain AM: 60% 32% 8%



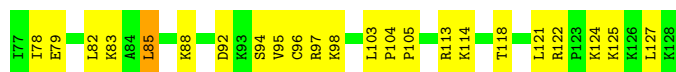
- Molecule 41: 60S ribosomal protein L39

Chain DN: 68% 26% 6%



- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain AN: 56% 42% 2%



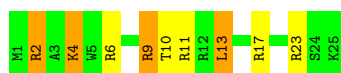
- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain DO: 2% 71% 25%

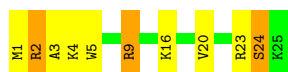


- Molecule 43: 60S ribosomal protein L41-B

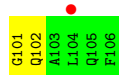
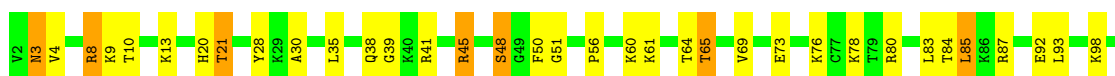
Chain AO: 64% 20% 16%



- Molecule 43: 60S ribosomal protein L41-B



- Molecule 44: 60S ribosomal protein L42-A



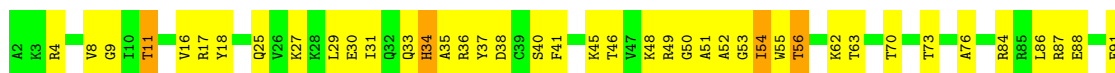
- Molecule 44: 60S ribosomal protein L42-A



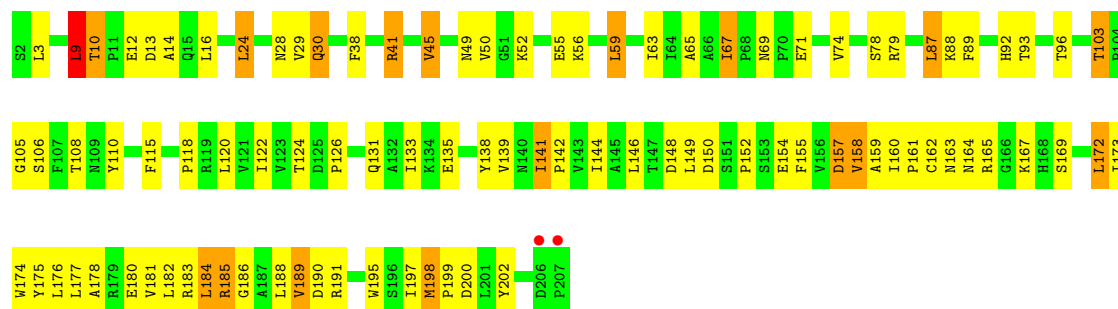
- Molecule 45: 60S ribosomal protein L43-A



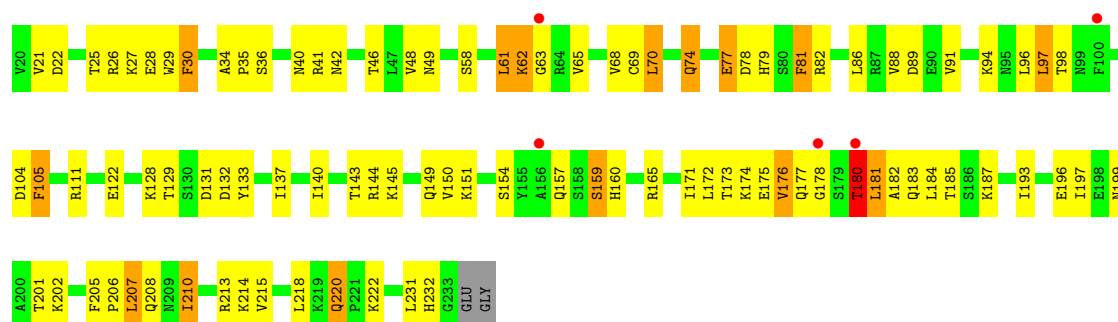
- Molecule 45: 60S ribosomal protein L43-A



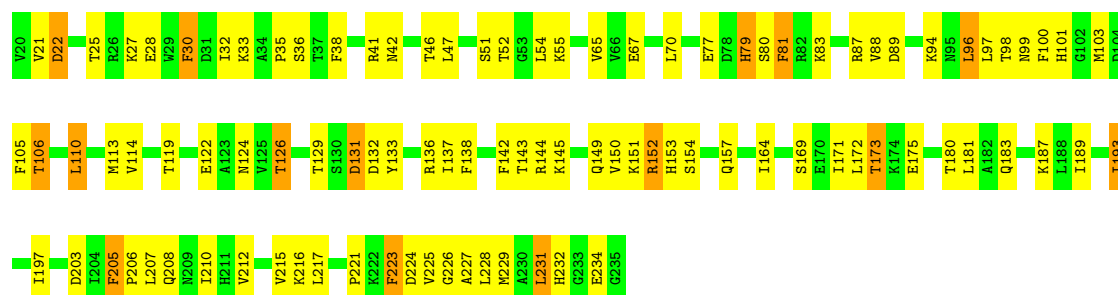
- Molecule 46: Suppressor protein STM1



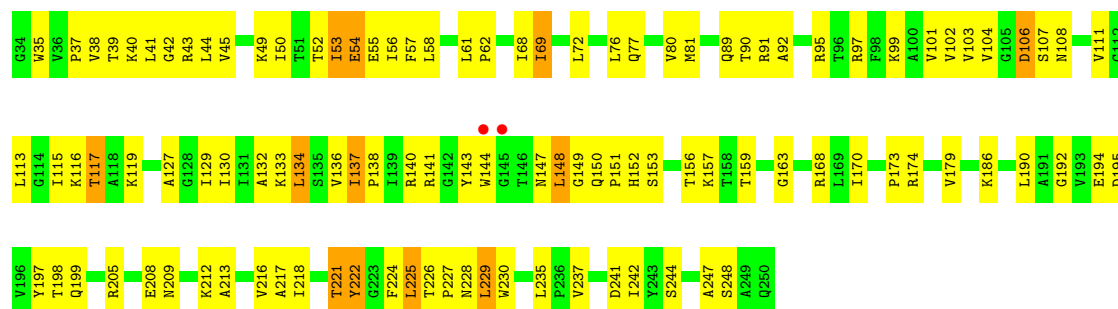
- Molecule 50: 40S ribosomal protein S1-A



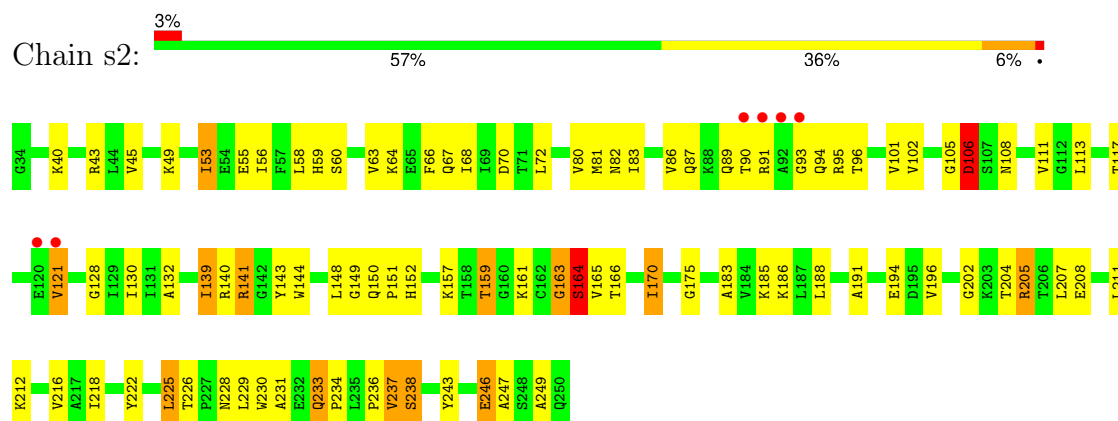
- Molecule 50: 40S ribosomal protein S1-A



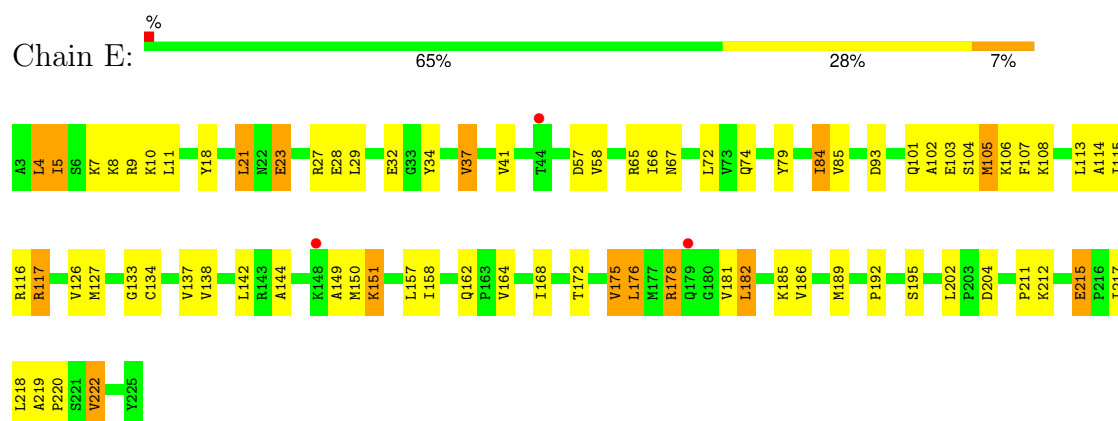
- Molecule 51: 40S ribosomal protein S2



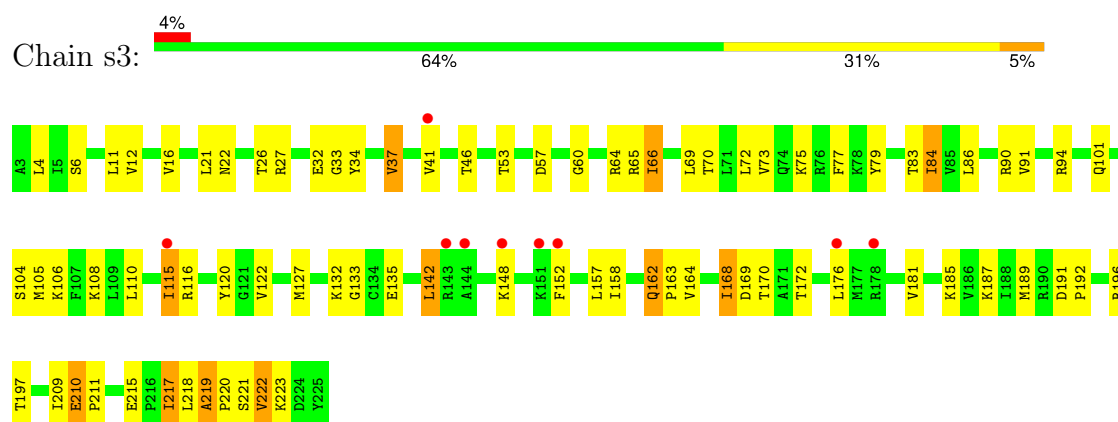
- Molecule 51: 40S ribosomal protein S2



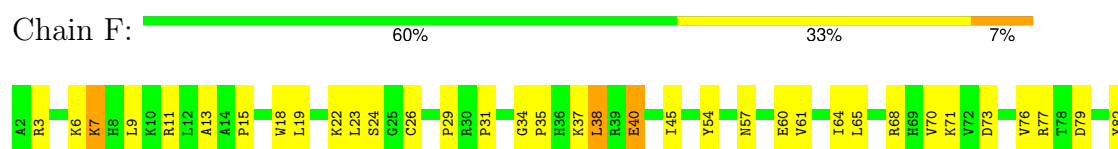
- Molecule 52: 40S ribosomal protein S3

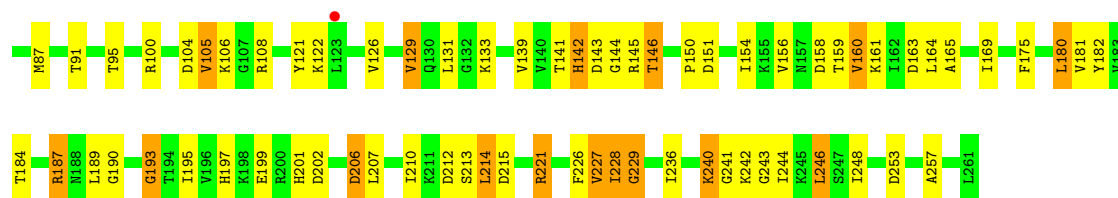


- Molecule 52: 40S ribosomal protein S3



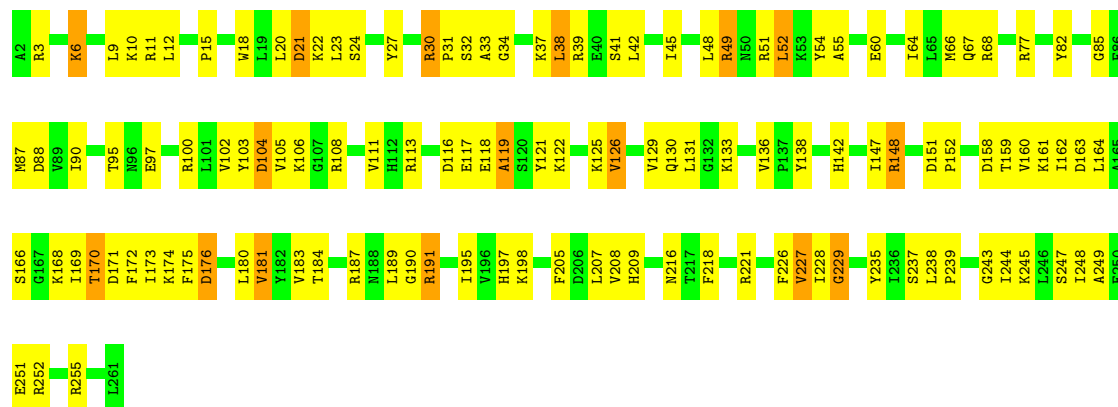
- Molecule 53: 40S ribosomal protein S4-A





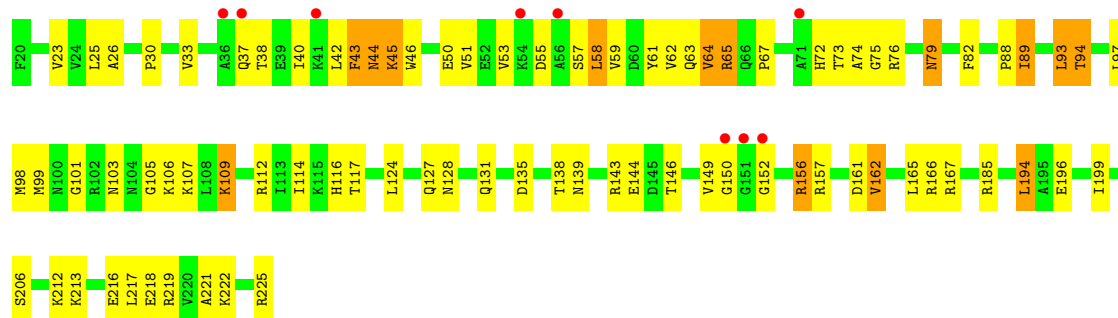
• Molecule 53: 40S ribosomal protein S4-A

Chain s4: 52% 42% 6%



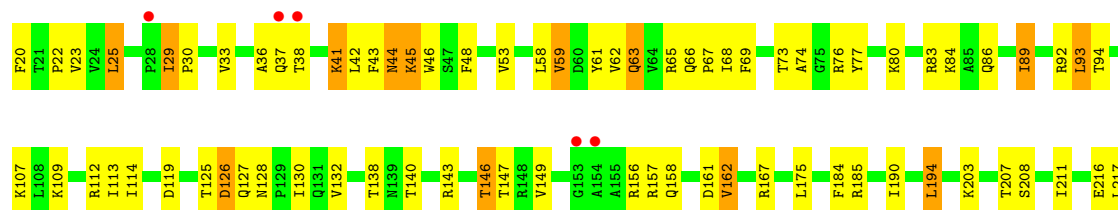
• Molecule 54: 40S ribosomal protein S5

Chain G: 4% 59% 34% 7%



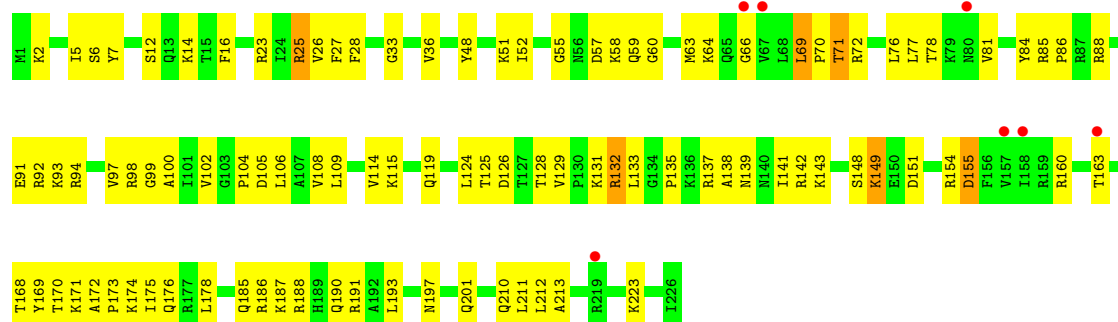
• Molecule 54: 40S ribosomal protein S5

Chain s5: 2% 62% 32% 6%

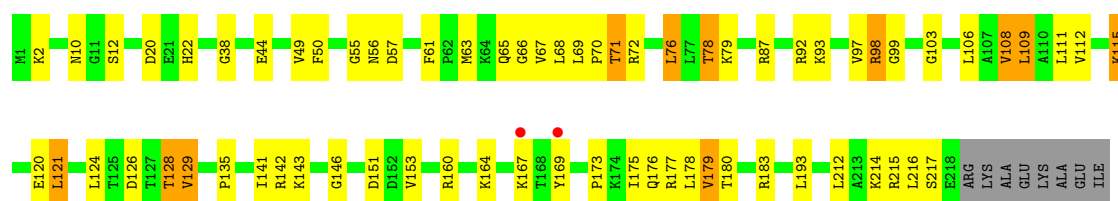




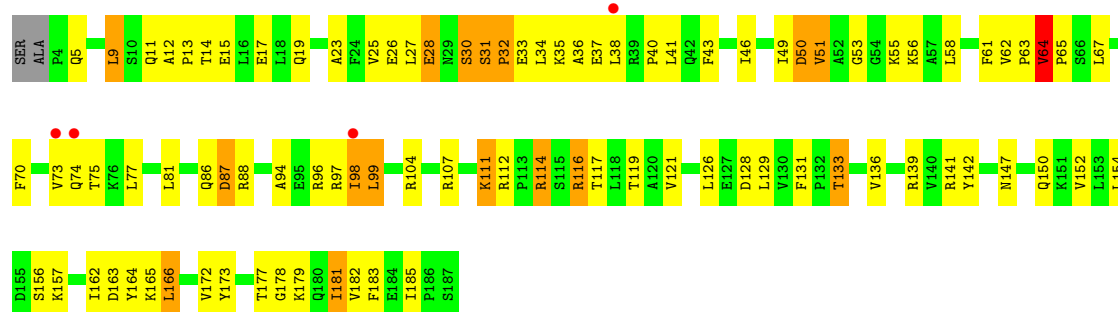
- Molecule 55: 40S ribosomal protein S6-A



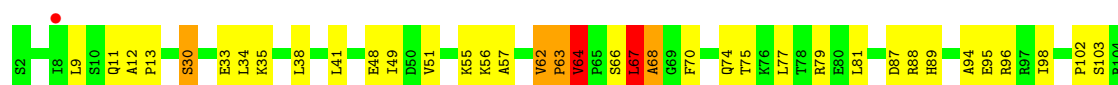
- Molecule 55: 40S ribosomal protein S6-A

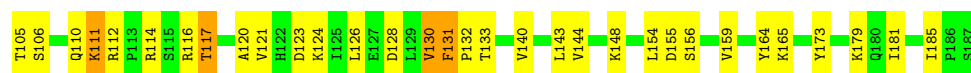


- Molecule 56: 40S ribosomal protein S7-A

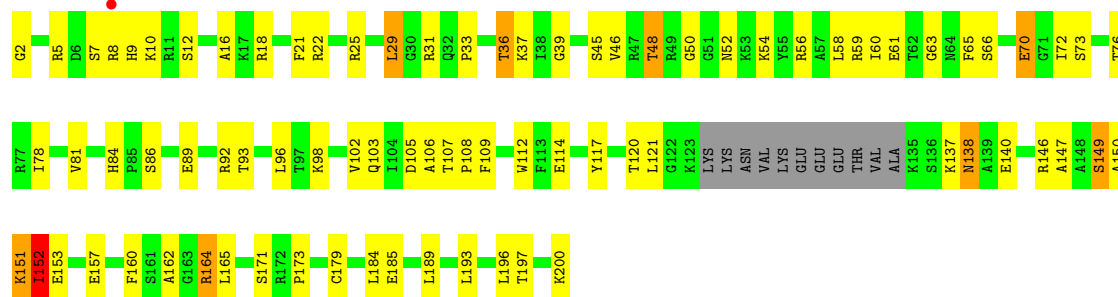


- Molecule 56: 40S ribosomal protein S7-A

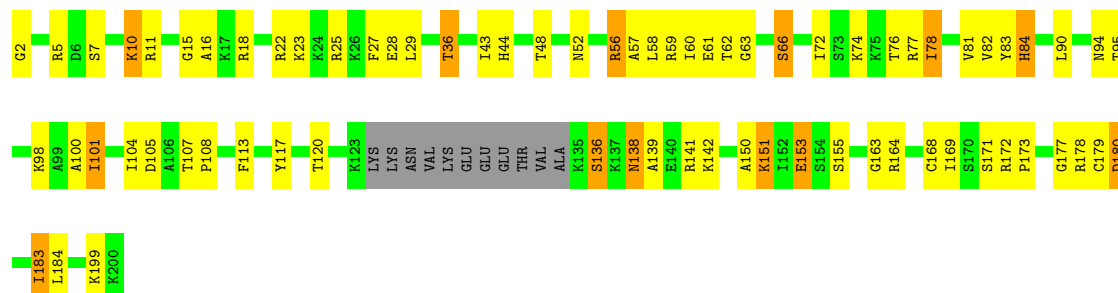




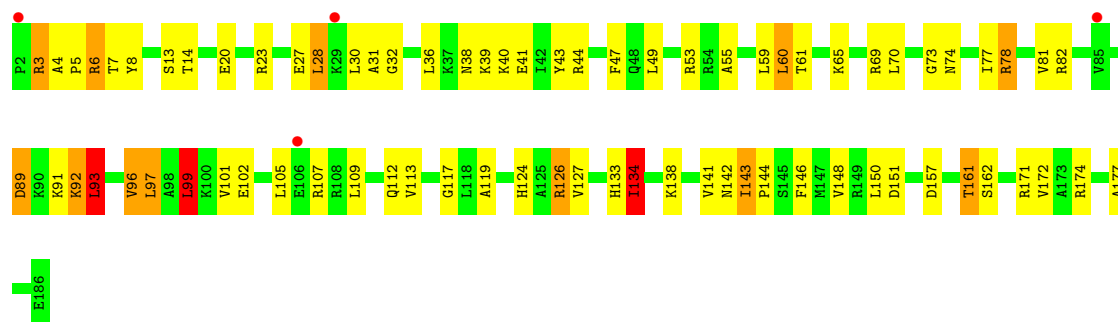
• Molecule 57: 40S ribosomal protein S8-A



• Molecule 57: 40S ribosomal protein S8-A

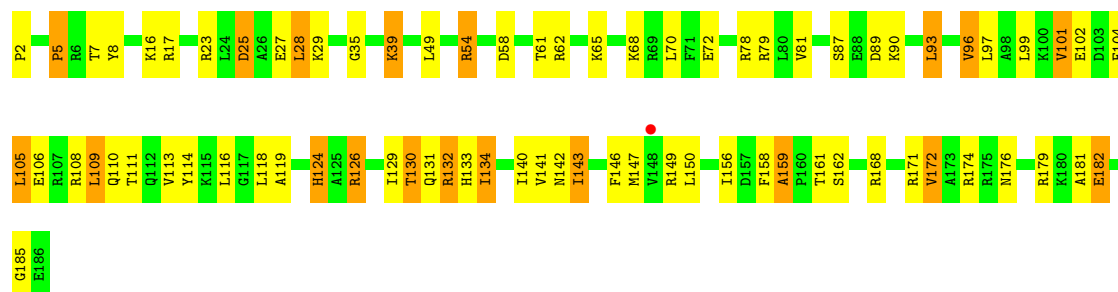


• Molecule 58: 40S ribosomal protein S9-A



• Molecule 58: 40S ribosomal protein S9-A

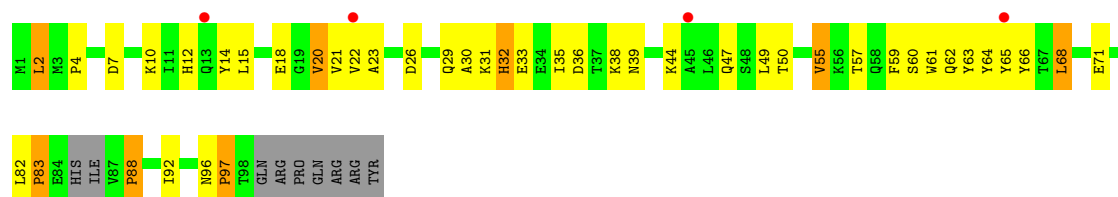




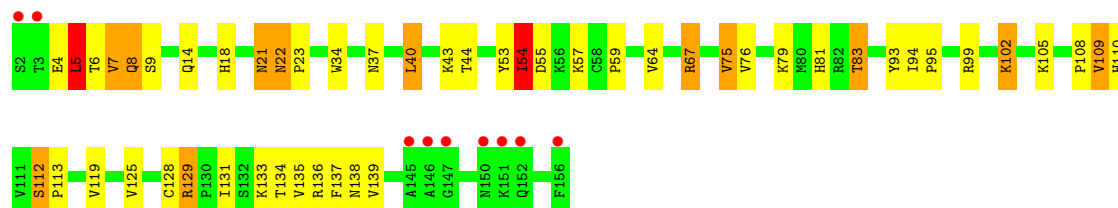
• Molecule 59: 40S ribosomal protein S10-A



• Molecule 59: 40S ribosomal protein S10-A



• Molecule 60: 40S ribosomal protein S11-A

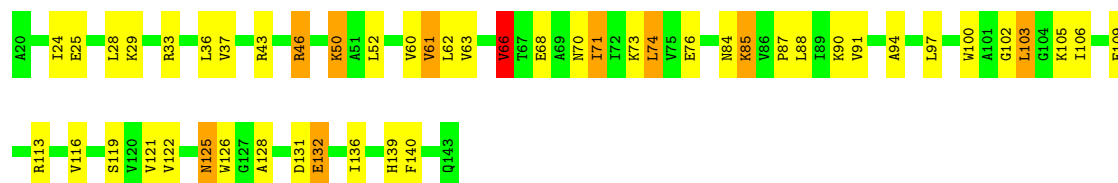


• Molecule 60: 40S ribosomal protein S11-A

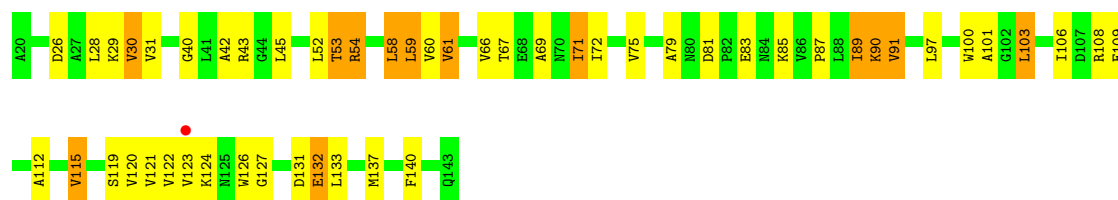




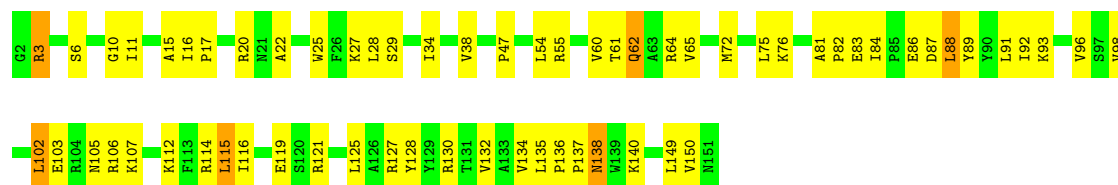
- Molecule 61: 40S ribosomal protein S12



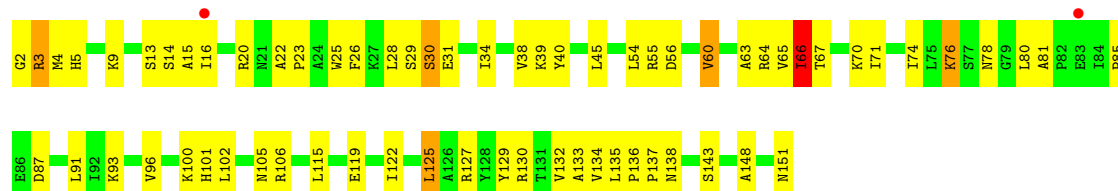
- Molecule 61: 40S ribosomal protein S12



- Molecule 62: 40S ribosomal protein S13

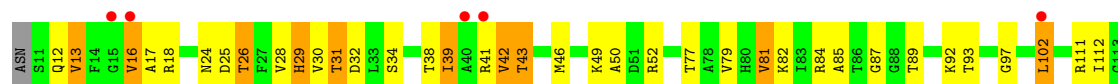


- Molecule 62: 40S ribosomal protein S13

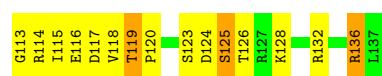
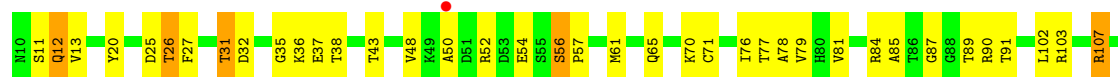


- Molecule 63: 40S ribosomal protein S14-B

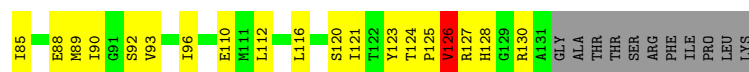
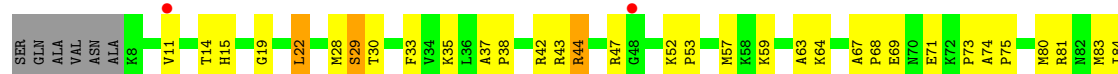




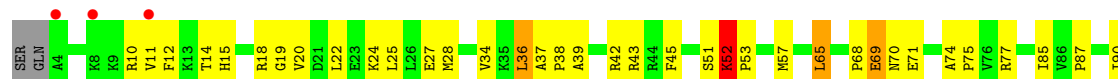
• Molecule 63: 40S ribosomal protein S14-B



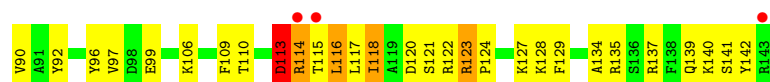
• Molecule 64: 40S ribosomal protein S15



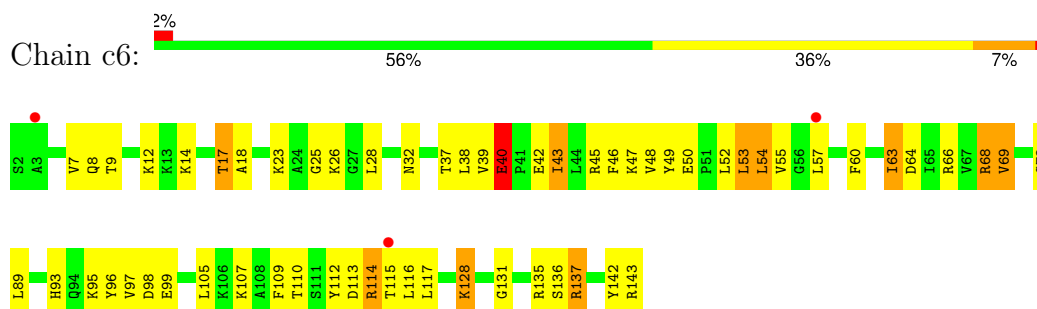
• Molecule 64: 40S ribosomal protein S15



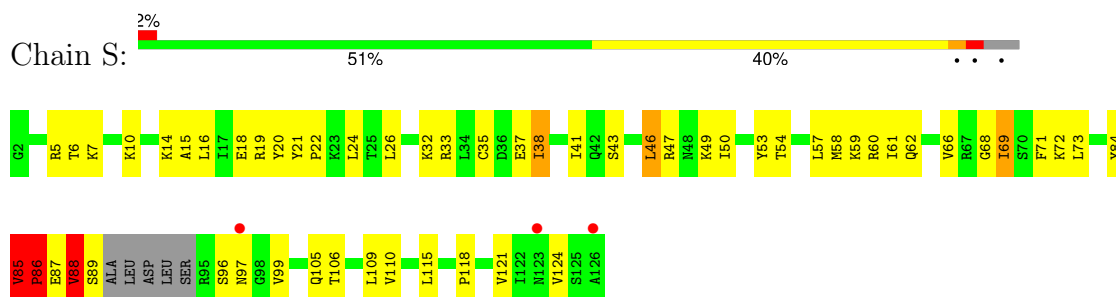
• Molecule 65: 40S ribosomal protein S16-A



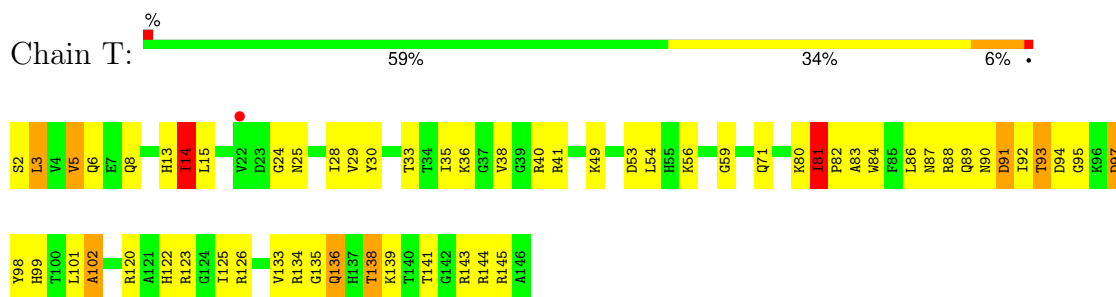
- Molecule 65: 40S ribosomal protein S16-A



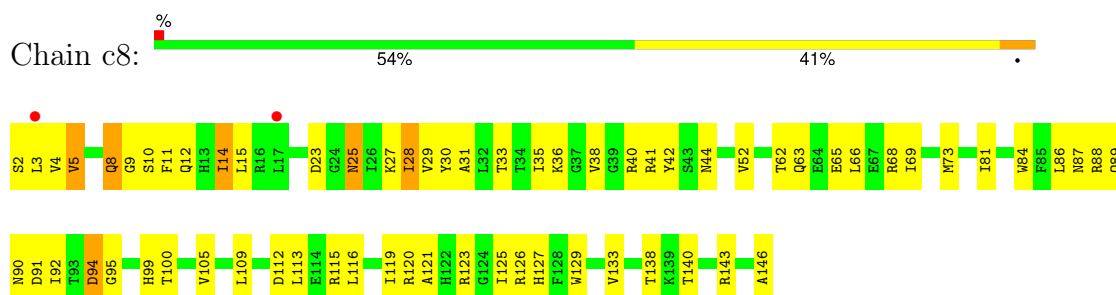
- Molecule 66: 40S ribosomal protein S17-B



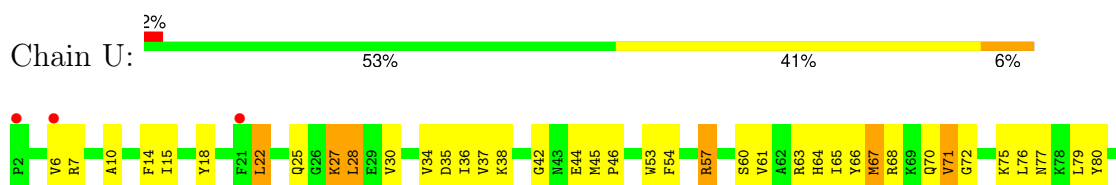
- Molecule 67: 40S ribosomal protein S18-A



- Molecule 67: 40S ribosomal protein S18-A

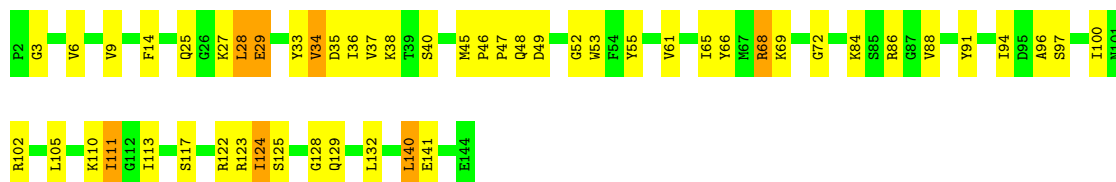


- Molecule 68: 40S ribosomal protein S19-A

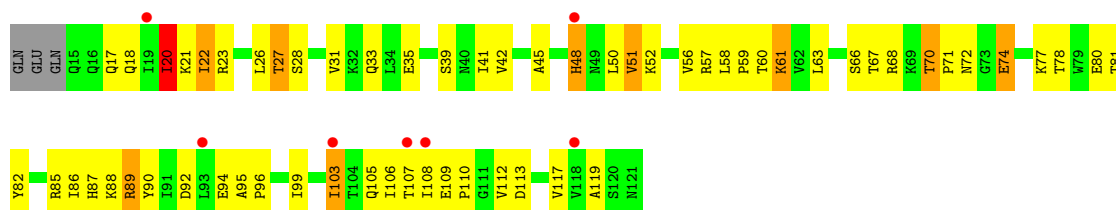




- Molecule 68: 40S ribosomal protein S19-A



- Molecule 69: 40S ribosomal protein S20



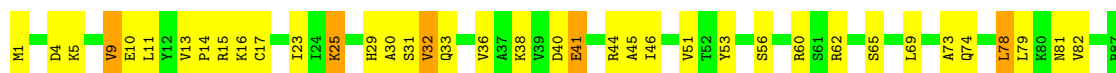
- Molecule 69: 40S ribosomal protein S20



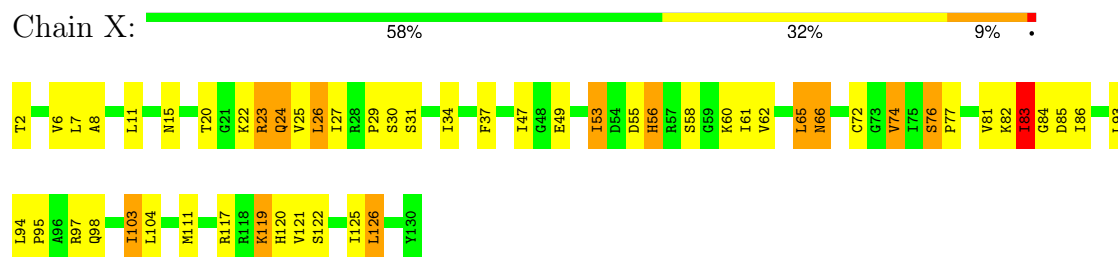
- Molecule 70: 40S ribosomal protein S21-A



- Molecule 70: 40S ribosomal protein S21-A



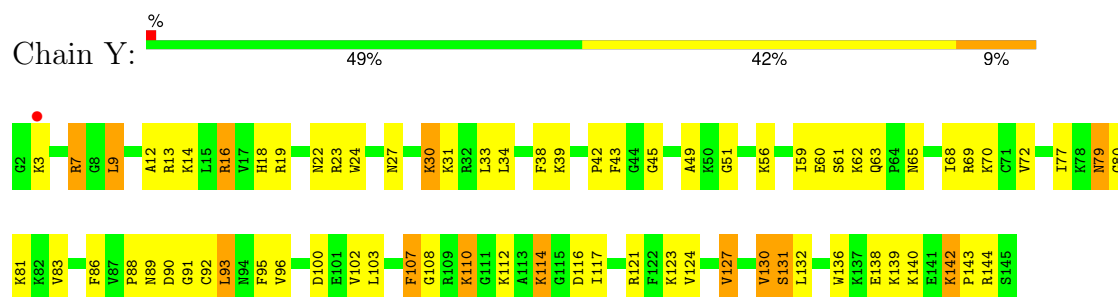
- Molecule 71: 40S ribosomal protein S22-A



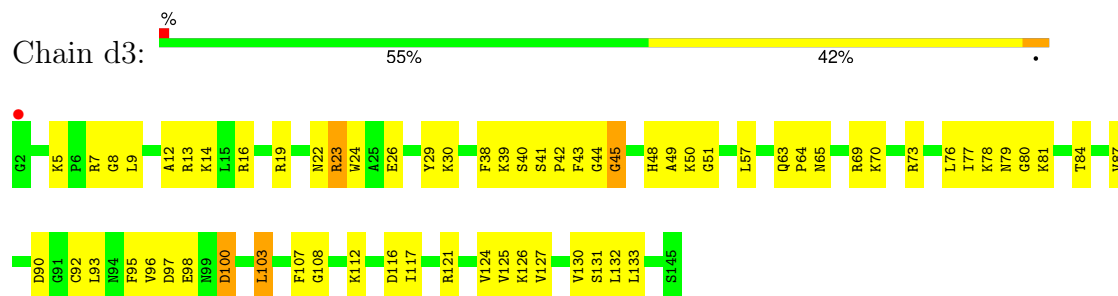
- Molecule 71: 40S ribosomal protein S22-A



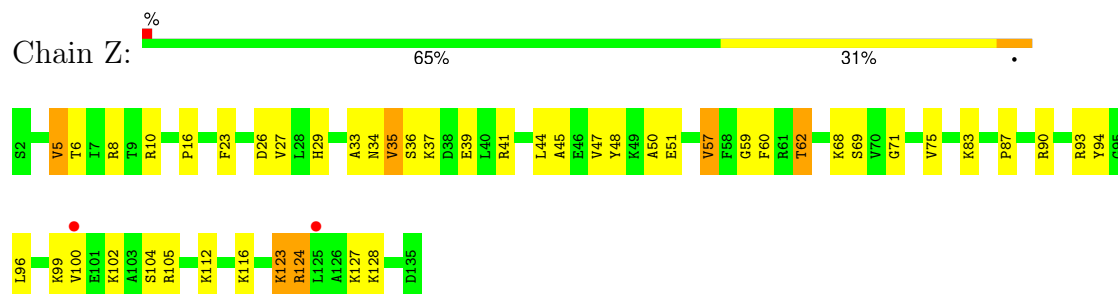
- Molecule 72: 40S ribosomal protein S23-A



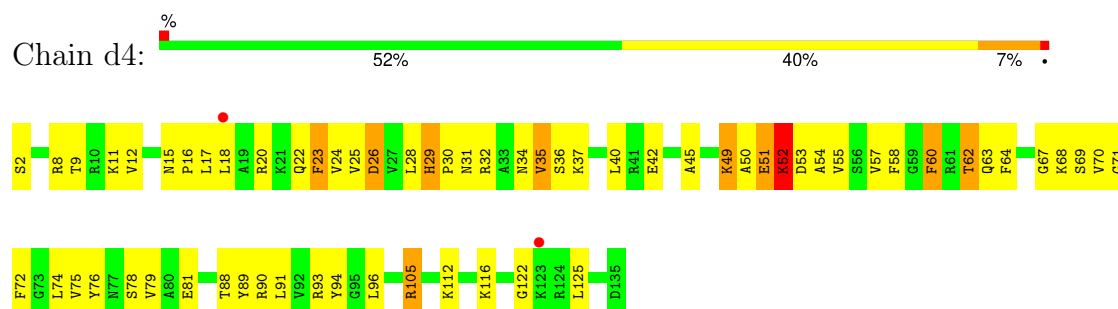
- Molecule 72: 40S ribosomal protein S23-A



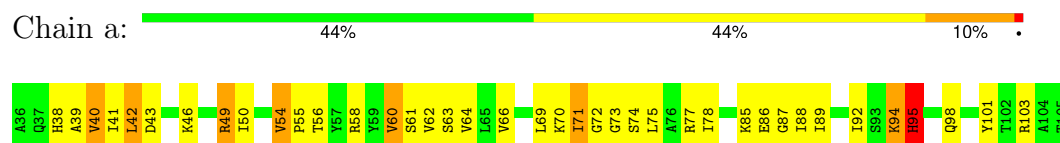
- Molecule 73: 40S ribosomal protein S24-A



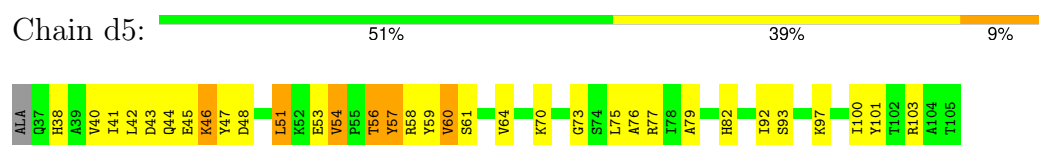
- Molecule 73: 40S ribosomal protein S24-A



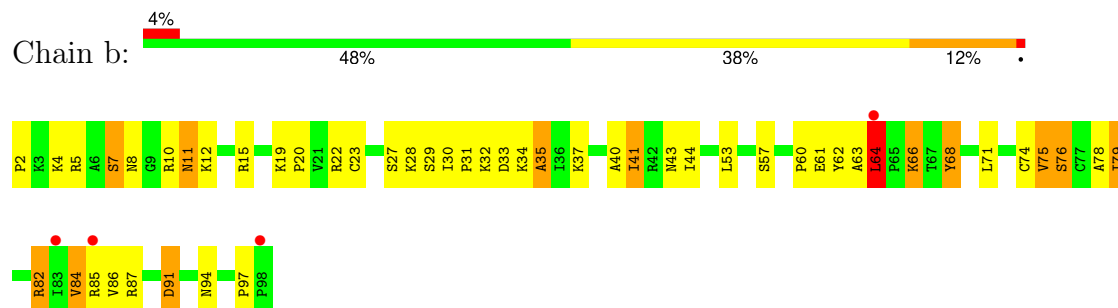
- Molecule 74: 40S ribosomal protein S25-A



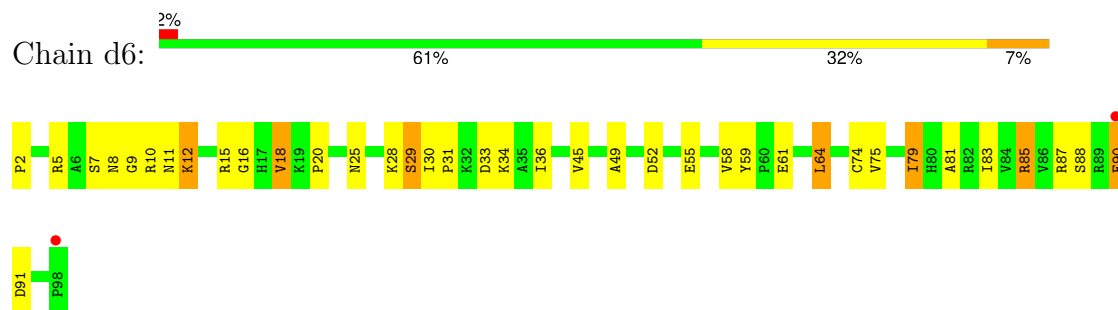
- Molecule 74: 40S ribosomal protein S25-A



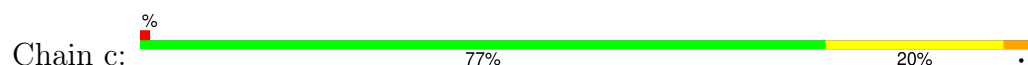
- Molecule 75: 40S ribosomal protein S26-B

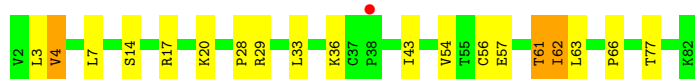


- Molecule 75: 40S ribosomal protein S26-B



- Molecule 76: 40S ribosomal protein S27-A

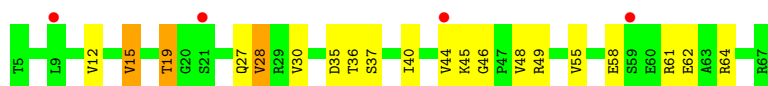




- Molecule 76: 40S ribosomal protein S27-A



- Molecule 77: 40S ribosomal protein S28-A



- Molecule 77: 40S ribosomal protein S28-A



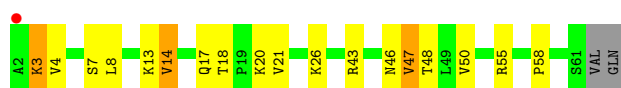
- Molecule 78: 40S ribosomal protein S29-A



- Molecule 78: 40S ribosomal protein S29-A



- Molecule 79: 40S ribosomal protein S30-A



- Molecule 79: 40S ribosomal protein S30-A

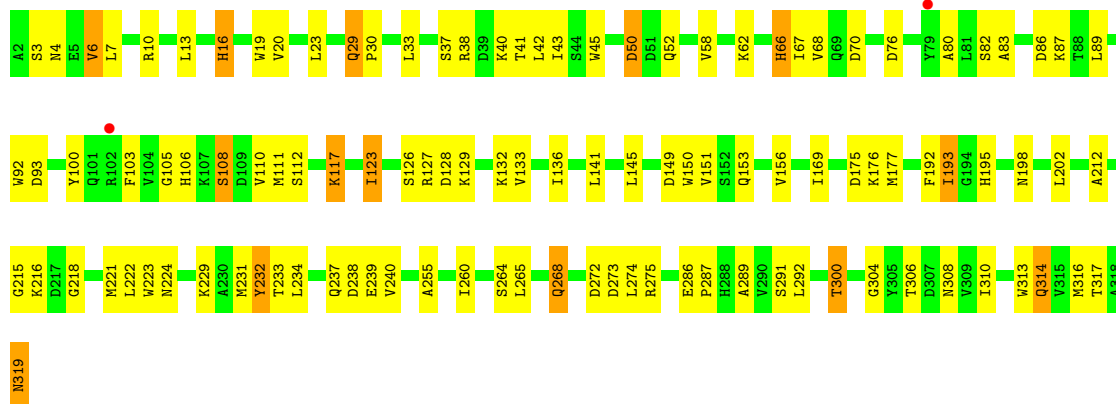




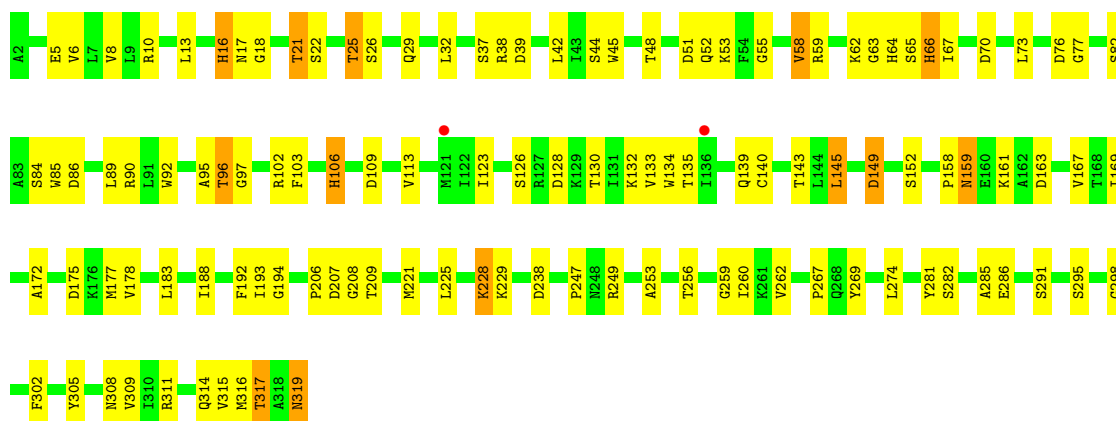
- Molecule 80: Ubiquitin-40S ribosomal protein S31



- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein

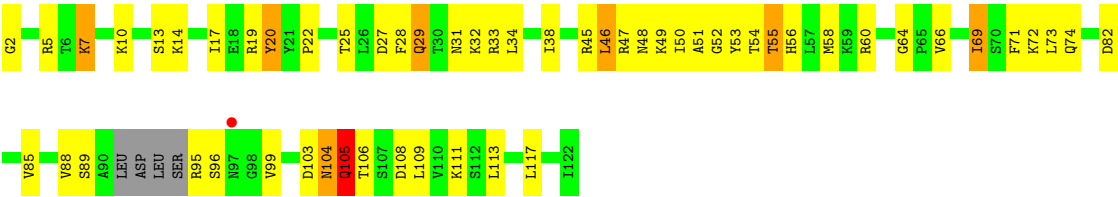


- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein

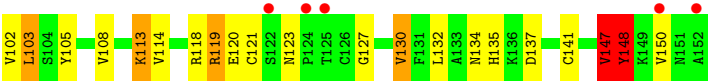


- Molecule 82: 40S ribosomal protein S17-A





● 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	304.08Å 286.55Å 436.55Å 90.00° 99.05° 90.00°	Depositor
Resolution (Å)	98.38 – 3.50 98.38 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (98.38-3.50) 100.0 (98.38-3.50)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.239 0.199 , 0.240	Depositor DCC
R_{free} test set	18298 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 83.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	409590	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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: 7MB, OHX, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.37	0/75394	0.52	1/117545 (0.0%)
1	AR	0.39	0/75394	0.53	4/117545 (0.0%)
2	3	0.35	0/2883	0.48	0/4491
2	AS	0.39	0/2883	0.52	0/4491
3	4	0.35	0/3746	0.49	0/5832
3	AT	0.34	0/3746	0.47	0/5832
4	CD	0.62	0/1948	1.00	4/2617 (0.2%)
4	j	0.61	0/1948	1.02	7/2617 (0.3%)
5	CE	0.68	0/3146	1.02	9/4228 (0.2%)
5	k	0.63	0/3146	0.98	4/4228 (0.1%)
6	CF	0.64	1/2800 (0.0%)	1.07	10/3790 (0.3%)
6	l	0.66	0/2800	1.05	12/3790 (0.3%)
7	CG	0.60	0/2425	0.96	7/3271 (0.2%)
7	m	0.49	0/2425	0.88	3/3271 (0.1%)
8	CH	0.66	0/1260	0.97	1/1694 (0.1%)
8	n	0.62	0/1260	0.92	0/1694
9	CI	0.68	0/1821	1.06	12/2451 (0.5%)
9	o	0.67	0/1821	0.99	2/2451 (0.1%)
10	CJ	0.49	0/1836	0.94	5/2481 (0.2%)
10	p	0.50	0/1836	0.96	5/2481 (0.2%)
11	CK	0.64	0/1539	0.98	3/2073 (0.1%)
11	q	0.58	0/1539	0.93	2/2073 (0.1%)
12	CL	0.63	0/1741	1.03	7/2335 (0.3%)
12	r	0.61	0/1741	0.94	0/2335
13	CM	0.61	0/1374	1.01	6/1842 (0.3%)
13	s	0.51	0/1374	0.96	4/1842 (0.2%)
14	CN	0.61	0/1568	1.06	9/2106 (0.4%)
14	t	0.64	0/1568	1.05	3/2106 (0.1%)
15	CO	0.69	0/1068	0.97	0/1438
15	u	0.64	0/1068	1.01	4/1438 (0.3%)
16	CP	0.56	0/1757	0.94	6/2354 (0.3%)
16	v	0.62	0/1757	1.01	7/2354 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CQ	0.77	0/1585	1.01	4/2128 (0.2%)
17	w	0.70	0/1585	1.00	2/2128 (0.1%)
18	CR	0.73	0/1443	1.07	6/1944 (0.3%)
18	x	0.66	0/1443	1.05	7/1944 (0.4%)
19	CS	0.63	0/1465	1.05	7/1965 (0.4%)
19	y	0.66	0/1465	1.09	6/1965 (0.3%)
20	CT	0.61	0/1538	0.97	3/2050 (0.1%)
20	z	0.50	0/1538	0.88	2/2050 (0.1%)
21	0	0.64	0/1481	1.04	5/1990 (0.3%)
21	CU	0.69	0/1481	1.05	4/1990 (0.2%)
22	2	0.61	0/1300	0.95	4/1743 (0.2%)
22	CV	0.64	0/1300	1.01	4/1743 (0.2%)
23	5	0.44	0/812	0.87	0/1099
23	CW	0.49	0/812	0.98	4/1099 (0.4%)
24	CX	0.79	0/1018	1.05	2/1369 (0.1%)
24	l2	0.61	0/1018	0.96	0/1369
25	6	0.32	0/42490	0.46	0/66207
25	A	0.26	0/42443	0.42	0/66134
26	7	0.53	0/712	0.99	2/958 (0.2%)
26	CY	0.63	0/712	1.05	3/958 (0.3%)
27	8	0.55	0/979	0.97	4/1321 (0.3%)
27	CZ	0.56	0/979	0.94	2/1321 (0.2%)
28	9	0.59	0/1004	1.05	7/1341 (0.5%)
28	DA	0.58	0/1004	1.05	3/1341 (0.2%)
29	AA	0.45	0/1118	0.83	1/1497 (0.1%)
29	DB	0.45	0/1118	0.93	2/1497 (0.1%)
30	AB	0.61	0/1204	1.09	8/1612 (0.5%)
30	DC	0.62	0/1204	1.14	8/1612 (0.5%)
31	AC	0.57	0/473	1.05	3/629 (0.5%)
31	DD	0.64	0/473	1.10	2/629 (0.3%)
32	AD	0.42	0/751	0.82	0/1008
32	DE	0.50	0/751	0.87	2/1008 (0.2%)
33	AE	0.51	0/890	0.91	1/1196 (0.1%)
33	DF	0.61	0/890	1.01	3/1196 (0.3%)
34	AF	0.69	0/1041	1.00	0/1394
34	DG	0.69	0/1041	0.96	0/1394
35	AG	0.66	0/868	1.06	3/1168 (0.3%)
35	DH	0.68	0/868	1.02	1/1168 (0.1%)
36	AH	0.50	0/890	0.94	1/1189 (0.1%)
36	DI	0.50	0/890	1.02	2/1189 (0.2%)
37	AI	0.57	0/978	0.94	0/1301
37	DJ	0.52	0/978	0.86	0/1301
38	AJ	0.56	0/778	0.96	4/1034 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DK	0.54	0/778	0.90	0/1034
39	AK	0.60	0/696	1.09	4/923 (0.4%)
39	DL	0.58	0/696	0.98	3/923 (0.3%)
40	AL	0.45	0/618	0.93	4/826 (0.5%)
40	DM	0.46	0/618	0.87	2/826 (0.2%)
41	AM	0.62	0/443	0.96	0/588
41	DN	0.56	0/443	0.89	0/588
42	AN	0.61	0/423	1.08	2/562 (0.4%)
42	DO	0.67	0/423	1.13	2/562 (0.4%)
43	AO	0.52	0/234	0.84	0/300
43	DP	0.59	0/234	0.86	0/300
44	AP	0.56	0/860	1.07	3/1136 (0.3%)
44	DQ	0.59	0/860	1.03	3/1136 (0.3%)
45	AQ	0.56	0/701	0.94	0/934
45	DR	0.62	0/701	1.08	3/934 (0.3%)
46	i	0.54	0/1113	1.05	7/1502 (0.5%)
47	p0	0.47	0/1092	0.91	3/1474 (0.2%)
48	sM	0.61	0/480	1.18	7/642 (1.1%)
49	B	0.51	0/1617	1.08	14/2215 (0.6%)
49	s0	0.54	0/1623	1.03	12/2222 (0.5%)
50	C	0.42	0/1735	0.91	5/2335 (0.2%)
50	s1	0.47	0/1748	0.95	7/2352 (0.3%)
51	D	0.49	0/1665	0.99	3/2263 (0.1%)
51	s2	0.57	0/1665	0.97	2/2263 (0.1%)
52	E	0.46	0/1759	0.90	3/2368 (0.1%)
52	s3	0.46	0/1759	0.93	7/2368 (0.3%)
53	F	0.47	0/2109	0.96	8/2839 (0.3%)
53	s4	0.52	0/2109	0.98	7/2839 (0.2%)
54	G	0.42	0/1629	0.87	2/2202 (0.1%)
54	s5	0.48	0/1629	0.89	1/2202 (0.0%)
55	H	0.42	0/1823	0.83	0/2439
55	s6	0.49	0/1779	0.89	3/2379 (0.1%)
56	I	0.44	0/1506	0.93	5/2028 (0.2%)
56	s7	0.46	0/1516	0.95	6/2043 (0.3%)
57	J	0.52	0/1514	0.89	0/2021
57	s8	0.55	0/1514	1.00	6/2021 (0.3%)
58	K	0.43	0/1519	0.90	4/2035 (0.2%)
58	s9	0.51	0/1519	0.91	5/2035 (0.2%)
59	L	0.45	0/789	1.02	4/1067 (0.4%)
59	c0	0.44	0/776	0.97	3/1047 (0.3%)
60	M	0.55	0/1239	1.02	8/1673 (0.5%)
60	c1	0.59	0/1194	0.99	2/1610 (0.1%)
61	N	0.49	0/898	0.96	1/1220 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	c2	0.46	0/898	0.95	3/1220 (0.2%)
62	O	0.47	0/1215	0.96	5/1638 (0.3%)
62	c3	0.54	0/1215	0.94	4/1638 (0.2%)
63	P	0.51	0/901	1.02	0/1217
63	c4	0.54	0/960	1.12	7/1290 (0.5%)
64	Q	0.47	0/998	0.99	0/1341
64	c5	0.52	0/1060	0.99	2/1426 (0.1%)
65	R	0.46	0/1125	0.92	5/1510 (0.3%)
65	c6	0.53	0/1131	0.98	5/1518 (0.3%)
66	S	0.54	1/935 (0.1%)	1.25	4/1254 (0.3%)
67	T	0.46	0/1211	0.90	3/1628 (0.2%)
67	c8	0.51	0/1211	0.92	2/1628 (0.1%)
68	U	0.43	0/1130	0.86	1/1517 (0.1%)
68	c9	0.46	0/1130	0.83	0/1517
69	V	0.50	0/865	0.99	5/1169 (0.4%)
69	d0	0.47	0/892	0.98	3/1205 (0.2%)
70	W	0.44	0/693	0.83	0/935
70	d1	0.49	0/693	0.94	2/935 (0.2%)
71	X	0.49	0/1038	1.05	4/1395 (0.3%)
71	d2	0.58	0/1038	0.98	2/1395 (0.1%)
72	Y	0.54	0/1139	1.00	4/1518 (0.3%)
72	d3	0.64	0/1139	1.11	5/1518 (0.3%)
73	Z	0.43	0/1087	0.86	0/1449
73	d4	0.50	0/1087	0.95	2/1449 (0.1%)
74	a	0.49	0/571	1.05	3/768 (0.4%)
74	d5	0.45	0/566	1.00	3/761 (0.4%)
75	b	0.52	0/782	0.99	4/1047 (0.4%)
75	d6	0.54	0/782	0.91	2/1047 (0.2%)
76	c	0.44	0/620	0.90	0/838
76	d7	0.46	0/620	0.91	2/838 (0.2%)
77	d	0.37	0/499	0.81	0/670
77	d8	0.43	0/499	0.90	0/670
78	d9	0.48	0/452	0.86	0/600
78	e	0.46	0/452	0.95	1/600 (0.2%)
79	e0	0.56	0/499	1.09	2/665 (0.3%)
79	f	0.51	0/483	0.93	1/643 (0.2%)
80	g	0.64	0/577	1.15	2/770 (0.3%)
81	h	0.40	0/2490	0.82	2/3389 (0.1%)
81	sR	0.42	0/2495	0.83	1/3395 (0.0%)
82	c7	0.49	0/914	1.07	5/1224 (0.4%)
83	e1	0.48	0/404	1.12	4/542 (0.7%)
All	All	0.45	2/429965 (0.0%)	0.72	520/631328 (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
7	CG	0	1
10	CJ	0	1
12	CL	0	1
15	u	0	1
17	CQ	0	1
17	w	0	1
20	CT	0	1
22	2	0	1
26	7	0	1
26	CY	0	2
28	9	0	1
28	DA	0	1
29	DB	0	1
30	AB	0	1
31	AC	0	1
48	sM	0	1
49	B	0	1
50	s1	0	1
51	D	0	1
51	s2	0	1
52	E	0	1
52	s3	0	1
53	F	0	1
54	G	0	2
54	s5	0	1
56	I	0	2
56	s7	0	4
58	K	0	1
61	c2	0	4
64	Q	0	1
64	c5	0	1
65	R	0	2
65	c6	0	1
66	S	0	2
73	d4	0	2
74	a	0	1
80	g	0	2
82	c7	0	1
All	All	0	51

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CF	77	VAL	CA-CB	-5.33	1.48	1.54
66	S	88	VAL	CA-CB	5.29	1.61	1.54

The worst 5 of 520 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	S	85	VAL	CA-C-N	20.61	145.60	119.84
66	S	85	VAL	C-N-CA	20.61	145.60	119.84
30	DC	116	GLY	N-CA-C	12.44	123.77	111.95
21	0	167	ARG	CA-C-N	12.11	134.98	119.84
21	0	167	ARG	C-N-CA	12.11	134.98	119.84

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	2	122	GLN	Peptide
26	7	94	ARG	Peptide
28	9	83	ASP	Peptide
15	u	28	SER	Peptide
17	w	110	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	67355	0	33846	1290	0
1	AR	67355	0	33843	1277	0
2	3	2579	0	1303	51	0
2	AS	2579	0	1304	50	0
3	4	3353	0	1695	71	0
3	AT	3353	0	1695	64	0
4	CD	1914	0	1981	77	0
4	j	1914	0	1981	84	0
5	CE	3075	0	3142	137	0
5	k	3075	0	3142	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	CF	2748	0	2859	94	0
6	l	2748	0	2859	124	0
7	CG	2375	0	2325	80	0
7	m	2375	0	2325	82	0
8	CH	1239	0	1326	40	0
8	n	1239	0	1326	29	0
9	CI	1784	0	1862	61	0
9	o	1784	0	1862	66	0
10	CJ	1804	0	1877	52	0
10	p	1804	0	1877	54	0
11	CK	1518	0	1587	55	0
11	q	1518	0	1587	66	0
12	CL	1705	0	1736	63	0
12	r	1705	0	1736	58	0
13	CM	1353	0	1383	38	0
13	s	1353	0	1383	49	0
14	CN	1543	0	1608	60	0
14	t	1543	0	1608	67	0
15	CO	1053	0	1149	41	0
15	u	1053	0	1149	58	0
16	CP	1720	0	1779	53	0
16	v	1720	0	1778	68	0
17	CQ	1555	0	1659	56	0
17	w	1555	0	1659	45	0
18	CR	1420	0	1437	45	0
18	x	1420	0	1437	51	0
19	CS	1441	0	1543	55	0
19	y	1441	0	1543	59	0
20	CT	1521	0	1617	57	0
20	z	1521	0	1617	52	0
21	0	1445	0	1487	49	0
21	CU	1445	0	1487	53	0
22	2	1276	0	1323	54	0
22	CV	1276	0	1323	63	0
23	5	796	0	812	24	0
23	CW	796	0	812	21	0
24	CX	1003	0	1048	37	0
24	l2	1003	0	1048	39	0
25	6	37990	0	19115	773	0
25	A	37948	0	19093	818	0
26	7	699	0	640	11	0
26	CY	699	0	640	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	8	964	0	1025	34	0
27	CZ	964	0	1025	36	0
28	9	993	0	1081	26	0
28	DA	993	0	1081	36	0
29	AA	1092	0	1155	49	0
29	DB	1092	0	1155	44	0
30	AB	1173	0	1214	64	0
30	DC	1173	0	1215	53	0
31	AC	462	0	491	10	0
31	DD	462	0	491	19	0
32	AD	743	0	797	26	0
32	DE	743	0	797	26	0
33	AE	876	0	912	28	0
33	DF	876	0	912	19	0
34	AF	1020	0	1090	22	0
34	DG	1020	0	1090	38	0
35	AG	850	0	880	27	0
35	DH	850	0	880	30	0
36	AH	880	0	945	27	0
36	DI	880	0	945	37	0
37	AI	969	0	1078	45	0
37	DJ	969	0	1078	40	0
38	AJ	771	0	849	40	0
38	DK	771	0	849	34	0
39	AK	681	0	683	25	0
39	DL	681	0	683	27	0
40	AL	612	0	682	12	0
40	DM	612	0	682	20	0
41	AM	436	0	475	21	0
41	DN	436	0	475	17	0
42	AN	417	0	455	11	0
42	DO	417	0	455	12	0
43	AO	233	0	284	8	0
43	DP	233	0	284	11	0
44	AP	847	0	917	23	0
44	DQ	847	0	918	27	0
45	AQ	694	0	736	18	0
45	DR	694	0	735	24	0
46	i	1104	0	996	32	0
47	p0	1077	0	1041	30	0
48	sM	680	0	540	24	0
49	B	1577	0	1567	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	s0	1583	0	1578	75	0
50	C	1709	0	1784	73	0
50	s1	1722	0	1793	64	0
51	D	1635	0	1723	72	0
51	s2	1635	0	1723	56	0
52	E	1734	0	1817	55	0
52	s3	1734	0	1817	55	0
53	F	2068	0	2154	71	0
53	s4	2068	0	2154	84	0
54	G	1609	0	1675	62	0
54	s5	1609	0	1675	57	0
55	H	1799	0	1879	73	0
55	s6	1755	0	1846	43	0
56	I	1481	0	1572	60	0
56	s7	1491	0	1578	41	0
57	J	1489	0	1525	60	0
57	s8	1489	0	1525	50	0
58	K	1494	0	1573	51	0
58	s9	1494	0	1573	62	0
59	L	772	0	727	27	0
59	c0	761	0	697	27	0
60	M	1213	0	1257	40	0
60	c1	1168	0	1233	41	0
61	N	890	0	887	31	0
61	c2	890	0	887	27	0
62	O	1192	0	1255	41	0
62	c3	1192	0	1255	41	0
63	P	891	0	883	45	0
63	c4	949	0	985	34	0
64	Q	977	0	1002	35	0
64	c5	1039	0	1050	44	0
65	R	1105	0	1166	42	0
65	c6	1111	0	1171	50	0
66	S	926	0	930	46	0
67	T	1192	0	1222	55	0
67	c8	1192	0	1222	55	0
68	U	1112	0	1124	45	0
68	c9	1112	0	1124	40	0
69	V	855	0	917	44	0
69	d0	882	0	939	43	0
70	W	684	0	672	28	0
70	d1	684	0	672	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	X	1021	0	1060	38	0
71	d2	1021	0	1060	43	0
72	Y	1121	0	1196	49	0
72	d3	1121	0	1196	51	0
73	Z	1073	0	1132	35	0
73	d4	1073	0	1132	51	0
74	a	563	0	603	29	0
74	d5	558	0	598	26	0
75	b	769	0	815	44	0
75	d6	769	0	814	34	0
76	c	610	0	633	12	0
76	d7	610	0	633	21	0
77	d	497	0	535	15	0
77	d8	497	0	535	23	0
78	d9	442	0	428	16	0
78	e	442	0	429	23	0
79	e0	491	0	542	23	0
79	f	475	0	525	11	0
80	g	566	0	602	25	0
81	h	2437	0	2386	65	0
81	sR	2442	0	2392	76	0
82	c7	906	0	909	43	0
83	e1	397	0	396	14	0
84	1	2317	0	0	235	0
84	2	7	0	0	0	0
84	3	56	0	0	5	0
84	4	84	0	0	7	0
84	6	1099	0	0	110	0
84	A	994	0	0	120	0
84	AC	7	0	0	1	0
84	AE	7	0	0	4	0
84	AG	7	0	0	0	0
84	AK	14	0	0	2	0
84	AP	7	0	0	3	0
84	AR	2373	0	0	242	0
84	AS	70	0	0	7	0
84	AT	133	0	0	18	0
84	CE	14	0	0	2	0
84	CF	14	0	0	1	0
84	CG	21	0	0	4	0
84	CK	7	0	0	1	0
84	CL	14	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	CM	7	0	0	1	0
84	CO	7	0	0	0	0
84	CP	7	0	0	0	0
84	CV	7	0	0	1	0
84	CX	7	0	0	0	0
84	CZ	7	0	0	0	0
84	DD	7	0	0	0	0
84	DG	7	0	0	0	0
84	DH	7	0	0	0	0
84	DI	7	0	0	1	0
84	DL	14	0	0	2	0
84	H	7	0	0	0	0
84	J	7	0	0	0	0
84	M	7	0	0	2	0
84	O	7	0	0	1	0
84	Q	7	0	0	2	0
84	T	7	0	0	1	0
84	c3	7	0	0	2	0
84	c5	7	0	0	3	0
84	c8	7	0	0	0	0
84	d9	7	0	0	0	0
84	e	7	0	0	2	0
84	h	7	0	0	0	0
84	k	14	0	0	3	0
84	l	7	0	0	2	0
84	r	7	0	0	1	0
84	s8	7	0	0	0	0
84	sR	7	0	0	0	0
84	v	7	0	0	1	0
84	x	14	0	0	3	0
84	y	7	0	0	0	0
84	z	7	0	0	0	0
85	1	490	0	0	0	0
85	3	12	0	0	0	0
85	4	21	0	0	0	0
85	6	141	0	0	0	0
85	9	1	0	0	0	0
85	A	111	0	0	0	0
85	AB	4	0	0	0	0
85	AF	2	0	0	0	0
85	AH	1	0	0	0	0
85	AK	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	AP	1	0	0	0	0
85	AR	504	0	0	0	0
85	AS	20	0	0	0	0
85	AT	12	0	0	0	0
85	CD	2	0	0	0	0
85	CE	4	0	0	0	0
85	CF	1	0	0	0	0
85	CI	1	0	0	0	0
85	CK	1	0	0	0	0
85	CO	2	0	0	0	0
85	CP	2	0	0	0	0
85	CQ	4	0	0	0	0
85	CR	6	0	0	0	0
85	CU	2	0	0	0	0
85	CX	2	0	0	0	0
85	D	1	0	0	0	0
85	DA	1	0	0	0	0
85	DC	4	0	0	0	0
85	DD	1	0	0	0	0
85	DE	1	0	0	0	0
85	DF	1	0	0	0	0
85	DG	1	0	0	0	0
85	DH	2	0	0	0	0
85	DI	1	0	0	0	0
85	DO	1	0	0	0	0
85	DP	1	0	0	0	0
85	DR	2	0	0	0	0
85	F	1	0	0	0	0
85	Y	1	0	0	0	0
85	b	1	0	0	0	0
85	c6	1	0	0	0	0
85	c9	1	0	0	0	0
85	d3	3	0	0	0	0
85	d5	1	0	0	0	0
85	d6	1	0	0	0	0
85	d9	1	0	0	0	0
85	i	1	0	0	0	0
85	j	2	0	0	0	0
85	k	2	0	0	0	0
85	l	2	0	0	0	0
85	l2	2	0	0	0	0
85	o	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	r	1	0	0	0	0
85	s	1	0	0	0	0
85	s1	1	0	0	0	0
85	s2	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	1	0	0	0	0
85	sM	1	0	0	0	0
85	t	2	0	0	0	0
85	v	1	0	0	0	0
85	w	1	0	0	0	0
85	x	5	0	0	0	0
85	z	2	0	0	0	0
86	1	20	0	0	4	0
86	AR	20	0	0	3	0
87	AK	1	0	0	0	0
87	AN	1	0	0	0	0
87	AP	1	0	0	0	0
87	AQ	1	0	0	0	0
87	DL	1	0	0	0	0
87	DO	1	0	0	0	0
87	DQ	1	0	0	0	0
87	DR	1	0	0	0	0
87	b	1	0	0	0	0
87	c	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e	1	0	0	0	0
87	e1	1	0	0	0	0
87	g	1	0	0	0	0
All	All	409590	0	296688	9415	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 9415 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)
25:6:976:G:H1	25:6:1023:A:HO2'	1.10	1.00
25:6:885:G:H21	63:c4:123:SER:HB2	1.27	0.96
1:1:1171:G:N7	84:1:3496:OHX:N2	2.13	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:1726:G:N7	84:6:2005:OHX:N2	2.12	0.95
1:AR:1481:A:O2'	1:AR:1858:A:N3	2.00	0.95

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%)	238 (95%)	12 (5%)	0	100	100
4	j	250/252 (99%)	232 (93%)	18 (7%)	0	100	100
5	CE	384/386 (100%)	355 (92%)	27 (7%)	2 (0%)	24	57
5	k	384/386 (100%)	351 (91%)	31 (8%)	2 (0%)	24	57
6	CF	359/361 (99%)	331 (92%)	28 (8%)	0	100	100
6	l	359/361 (99%)	326 (91%)	32 (9%)	1 (0%)	36	67
7	CG	294/296 (99%)	272 (92%)	22 (8%)	0	100	100
7	m	294/296 (99%)	271 (92%)	23 (8%)	0	100	100
8	CH	152/175 (87%)	144 (95%)	6 (4%)	2 (1%)	9	39
8	n	152/175 (87%)	145 (95%)	6 (4%)	1 (1%)	18	51
9	CI	220/222 (99%)	202 (92%)	15 (7%)	3 (1%)	9	38
9	o	220/222 (99%)	204 (93%)	13 (6%)	3 (1%)	9	38
10	CJ	231/233 (99%)	207 (90%)	21 (9%)	3 (1%)	9	39
10	p	231/233 (99%)	209 (90%)	18 (8%)	4 (2%)	7	35
11	CK	189/191 (99%)	178 (94%)	11 (6%)	0	100	100
11	q	189/191 (99%)	176 (93%)	12 (6%)	1 (0%)	24	57
12	CL	207/220 (94%)	195 (94%)	10 (5%)	2 (1%)	12	44
12	r	207/220 (94%)	199 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CM	167/169 (99%)	146 (87%)	18 (11%)	3 (2%)	6	34
13	s	167/169 (99%)	149 (89%)	15 (9%)	3 (2%)	6	34
14	CN	191/193 (99%)	172 (90%)	18 (9%)	1 (0%)	24	57
14	t	191/193 (99%)	173 (91%)	15 (8%)	3 (2%)	7	36
15	CO	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	8	37
15	u	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	8	37
16	CP	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
16	v	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
17	CQ	195/197 (99%)	189 (97%)	4 (2%)	2 (1%)	12	44
17	w	195/197 (99%)	188 (96%)	4 (2%)	3 (2%)	8	37
18	CR	181/183 (99%)	166 (92%)	14 (8%)	1 (1%)	21	54
18	x	181/183 (99%)	170 (94%)	10 (6%)	1 (1%)	21	54
19	CS	183/185 (99%)	171 (93%)	11 (6%)	1 (0%)	24	57
19	y	183/185 (99%)	173 (94%)	9 (5%)	1 (0%)	24	57
20	CT	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	24	57
20	z	186/188 (99%)	178 (96%)	7 (4%)	1 (0%)	24	57
21	0	170/172 (99%)	154 (91%)	15 (9%)	1 (1%)	21	54
21	CU	170/172 (99%)	158 (93%)	12 (7%)	0	100	100
22	2	157/159 (99%)	144 (92%)	12 (8%)	1 (1%)	21	54
22	CV	157/159 (99%)	147 (94%)	9 (6%)	1 (1%)	21	54
23	5	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	12	44
23	CW	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	12	44
24	CX	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
24	l2	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
26	7	96/98 (98%)	85 (88%)	10 (10%)	1 (1%)	12	44
26	CY	96/98 (98%)	83 (86%)	11 (12%)	2 (2%)	5	31
27	8	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
27	CZ	119/121 (98%)	111 (93%)	6 (5%)	2 (2%)	7	35
28	9	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
28	DA	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
29	AA	133/135 (98%)	123 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DB	133/135 (98%)	121 (91%)	10 (8%)	2 (2%)	8	37
30	AB	146/148 (99%)	127 (87%)	17 (12%)	2 (1%)	9	38
30	DC	146/148 (99%)	130 (89%)	14 (10%)	2 (1%)	9	38
31	AC	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	6	34
31	DD	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	6	34
32	AD	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
32	DE	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
33	AE	107/109 (98%)	101 (94%)	5 (5%)	1 (1%)	14	47
33	DF	107/109 (98%)	103 (96%)	3 (3%)	1 (1%)	14	47
34	AF	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
34	DG	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
35	AG	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	6	33
35	DH	104/106 (98%)	97 (93%)	6 (6%)	1 (1%)	12	44
36	AH	110/112 (98%)	104 (94%)	4 (4%)	2 (2%)	6	34
36	DI	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
37	AI	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
37	DJ	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
38	AJ	97/99 (98%)	83 (86%)	13 (13%)	1 (1%)	12	44
38	DK	97/99 (98%)	86 (89%)	10 (10%)	1 (1%)	12	44
39	AK	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
39	DL	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
40	AL	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
40	DM	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	9	39
41	AM	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
41	DN	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
42	AN	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
42	DO	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
43	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
43	DP	23/25 (92%)	23 (100%)	0	0	100	100
44	AP	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
44	DQ	103/105 (98%)	90 (87%)	12 (12%)	1 (1%)	12	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	AQ	89/91 (98%)	77 (86%)	12 (14%)	0	100	100
45	DR	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
46	i	155/168 (92%)	129 (83%)	23 (15%)	3 (2%)	6	33
47	p0	139/220 (63%)	130 (94%)	8 (6%)	1 (1%)	18	51
48	sM	61/104 (59%)	47 (77%)	13 (21%)	1 (2%)	7	36
49	B	204/206 (99%)	175 (86%)	26 (13%)	3 (2%)	8	37
49	s0	204/206 (99%)	184 (90%)	17 (8%)	3 (2%)	8	37
50	C	212/216 (98%)	175 (82%)	35 (16%)	2 (1%)	14	47
50	s1	214/216 (99%)	196 (92%)	18 (8%)	0	100	100
51	D	215/217 (99%)	196 (91%)	18 (8%)	1 (0%)	24	57
51	s2	215/217 (99%)	199 (93%)	13 (6%)	3 (1%)	9	38
52	E	221/223 (99%)	198 (90%)	21 (10%)	2 (1%)	14	47
52	s3	221/223 (99%)	198 (90%)	21 (10%)	2 (1%)	14	47
53	F	258/260 (99%)	236 (92%)	20 (8%)	2 (1%)	16	49
53	s4	258/260 (99%)	233 (90%)	24 (9%)	1 (0%)	30	62
54	G	204/206 (99%)	179 (88%)	22 (11%)	3 (2%)	8	37
54	s5	204/206 (99%)	183 (90%)	21 (10%)	0	100	100
55	H	224/226 (99%)	207 (92%)	13 (6%)	4 (2%)	6	34
55	s6	216/226 (96%)	200 (93%)	14 (6%)	2 (1%)	14	47
56	I	182/186 (98%)	160 (88%)	17 (9%)	5 (3%)	4	27
56	s7	184/186 (99%)	162 (88%)	19 (10%)	3 (2%)	7	36
57	J	184/199 (92%)	160 (87%)	23 (12%)	1 (0%)	24	57
57	s8	184/199 (92%)	167 (91%)	15 (8%)	2 (1%)	11	43
58	K	183/185 (99%)	162 (88%)	19 (10%)	2 (1%)	11	43
58	s9	183/185 (99%)	172 (94%)	11 (6%)	0	100	100
59	L	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	5	31
59	c0	92/105 (88%)	63 (68%)	20 (22%)	9 (10%)	0	6
60	M	153/155 (99%)	138 (90%)	12 (8%)	3 (2%)	6	32
60	c1	144/155 (93%)	133 (92%)	10 (7%)	1 (1%)	18	51
61	N	122/124 (98%)	86 (70%)	30 (25%)	6 (5%)	1	16
61	c2	122/124 (98%)	91 (75%)	28 (23%)	3 (2%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	O	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	18	51
62	c3	148/150 (99%)	132 (89%)	15 (10%)	1 (1%)	18	51
63	P	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16	49
63	c4	126/128 (98%)	114 (90%)	12 (10%)	0	100	100
64	Q	122/141 (86%)	107 (88%)	13 (11%)	2 (2%)	7	36
64	c5	133/141 (94%)	107 (80%)	24 (18%)	2 (2%)	8	37
65	R	139/142 (98%)	122 (88%)	14 (10%)	3 (2%)	5	30
65	c6	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
66	S	116/125 (93%)	99 (85%)	13 (11%)	4 (3%)	3	23
67	T	143/145 (99%)	127 (89%)	13 (9%)	3 (2%)	5	31
67	c8	143/145 (99%)	121 (85%)	18 (13%)	4 (3%)	4	26
68	U	141/143 (99%)	129 (92%)	12 (8%)	0	100	100
68	c9	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	18	51
69	V	105/110 (96%)	93 (89%)	12 (11%)	0	100	100
69	d0	108/110 (98%)	92 (85%)	14 (13%)	2 (2%)	6	33
70	W	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	10	41
70	d1	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
71	X	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	49
71	d2	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	16	49
72	Y	142/144 (99%)	119 (84%)	21 (15%)	2 (1%)	9	38
72	d3	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
73	Z	132/134 (98%)	121 (92%)	9 (7%)	2 (2%)	8	37
73	d4	132/134 (98%)	119 (90%)	10 (8%)	3 (2%)	5	30
74	a	68/70 (97%)	56 (82%)	10 (15%)	2 (3%)	3	26
74	d5	67/70 (96%)	59 (88%)	8 (12%)	0	100	100
75	b	95/97 (98%)	68 (72%)	24 (25%)	3 (3%)	3	24
75	d6	95/97 (98%)	76 (80%)	19 (20%)	0	100	100
76	c	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	9	39
76	d7	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	9	39
77	d	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
77	d8	61/63 (97%)	50 (82%)	11 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	d9	51/53 (96%)	46 (90%)	4 (8%)	1 (2%)	6	32
78	e	51/53 (96%)	45 (88%)	6 (12%)	0	100	100
79	e0	60/62 (97%)	50 (83%)	8 (13%)	2 (3%)	3	23
79	f	58/62 (94%)	50 (86%)	7 (12%)	1 (2%)	7	35
80	g	69/71 (97%)	44 (64%)	19 (28%)	6 (9%)	0	7
81	h	316/318 (99%)	292 (92%)	23 (7%)	1 (0%)	36	67
81	sR	316/318 (99%)	292 (92%)	24 (8%)	0	100	100
82	c7	113/121 (93%)	102 (90%)	8 (7%)	3 (3%)	4	27
83	e1	49/51 (96%)	40 (82%)	9 (18%)	0	100	100
All	All	22260/22868 (97%)	20206 (91%)	1851 (8%)	203 (1%)	14	47

5 of 203 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	n	98	VAL
10	p	36	ILE
11	q	50	ASN
30	AB	48	TYR
46	i	167	PRO

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%)	165 (86%)	28 (14%)	3	17
4	j	193/194 (100%)	170 (88%)	23 (12%)	5	23
5	CE	319/322 (99%)	263 (82%)	56 (18%)	2	11
5	k	319/322 (99%)	256 (80%)	63 (20%)	1	8
6	CF	288/288 (100%)	252 (88%)	36 (12%)	4	22
6	l	288/288 (100%)	249 (86%)	39 (14%)	4	20
7	CG	244/244 (100%)	206 (84%)	38 (16%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	m	244/244 (100%)	215 (88%)	29 (12%)	5	23
8	CH	134/152 (88%)	117 (87%)	17 (13%)	4	21
8	n	134/152 (88%)	118 (88%)	16 (12%)	5	23
9	CI	186/186 (100%)	164 (88%)	22 (12%)	5	23
9	o	186/186 (100%)	166 (89%)	20 (11%)	6	26
10	CJ	187/191 (98%)	170 (91%)	17 (9%)	9	32
10	p	187/191 (98%)	169 (90%)	18 (10%)	8	30
11	CK	171/171 (100%)	137 (80%)	34 (20%)	1	7
11	q	171/171 (100%)	143 (84%)	28 (16%)	2	14
12	CL	177/186 (95%)	154 (87%)	23 (13%)	4	21
12	r	177/186 (95%)	150 (85%)	27 (15%)	3	16
13	CM	147/147 (100%)	121 (82%)	26 (18%)	2	10
13	s	147/147 (100%)	128 (87%)	19 (13%)	4	21
14	CN	154/154 (100%)	131 (85%)	23 (15%)	3	17
14	t	154/154 (100%)	133 (86%)	21 (14%)	3	19
15	CO	107/107 (100%)	87 (81%)	20 (19%)	1	9
15	u	107/107 (100%)	92 (86%)	15 (14%)	3	19
16	CP	175/175 (100%)	154 (88%)	21 (12%)	5	23
16	v	175/175 (100%)	151 (86%)	24 (14%)	3	19
17	CQ	160/160 (100%)	129 (81%)	31 (19%)	1	8
17	w	160/160 (100%)	135 (84%)	25 (16%)	2	15
18	CR	140/145 (97%)	112 (80%)	28 (20%)	1	7
18	x	140/145 (97%)	112 (80%)	28 (20%)	1	7
19	CS	150/150 (100%)	135 (90%)	15 (10%)	7	28
19	y	150/150 (100%)	130 (87%)	20 (13%)	4	20
20	CT	153/153 (100%)	130 (85%)	23 (15%)	3	17
20	z	153/153 (100%)	131 (86%)	22 (14%)	3	18
21	0	156/156 (100%)	138 (88%)	18 (12%)	5	24
21	CU	156/156 (100%)	130 (83%)	26 (17%)	2	13
22	2	136/136 (100%)	114 (84%)	22 (16%)	2	14
22	CV	136/136 (100%)	106 (78%)	30 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	5	87/87 (100%)	76 (87%)	11 (13%)	4	21
23	CW	87/87 (100%)	79 (91%)	8 (9%)	8	32
24	CX	104/104 (100%)	91 (88%)	13 (12%)	4	22
24	l2	104/104 (100%)	91 (88%)	13 (12%)	4	22
26	7	57/86 (66%)	52 (91%)	5 (9%)	9	32
26	CY	57/86 (66%)	53 (93%)	4 (7%)	14	39
27	8	104/105 (99%)	82 (79%)	22 (21%)	1	6
27	CZ	104/105 (99%)	88 (85%)	16 (15%)	2	16
28	9	109/109 (100%)	97 (89%)	12 (11%)	6	26
28	DA	109/109 (100%)	96 (88%)	13 (12%)	5	23
29	AA	115/115 (100%)	104 (90%)	11 (10%)	8	30
29	DB	115/115 (100%)	102 (89%)	13 (11%)	5	25
30	AB	118/118 (100%)	107 (91%)	11 (9%)	8	31
30	DC	118/118 (100%)	106 (90%)	12 (10%)	7	28
31	AC	46/46 (100%)	40 (87%)	6 (13%)	4	21
31	DD	46/46 (100%)	40 (87%)	6 (13%)	4	21
32	AD	81/81 (100%)	71 (88%)	10 (12%)	4	22
32	DE	81/81 (100%)	75 (93%)	6 (7%)	13	37
33	AE	92/96 (96%)	80 (87%)	12 (13%)	4	21
33	DF	92/96 (96%)	73 (79%)	19 (21%)	1	6
34	AF	109/109 (100%)	92 (84%)	17 (16%)	2	15
34	DG	109/109 (100%)	94 (86%)	15 (14%)	3	19
35	AG	90/90 (100%)	81 (90%)	9 (10%)	7	28
35	DH	90/90 (100%)	81 (90%)	9 (10%)	7	28
36	AH	95/95 (100%)	79 (83%)	16 (17%)	2	13
36	DI	95/95 (100%)	78 (82%)	17 (18%)	2	10
37	AI	104/104 (100%)	90 (86%)	14 (14%)	4	20
37	DJ	104/104 (100%)	86 (83%)	18 (17%)	2	11
38	AJ	81/81 (100%)	68 (84%)	13 (16%)	2	14
38	DK	81/81 (100%)	66 (82%)	15 (18%)	1	9
39	AK	70/70 (100%)	61 (87%)	9 (13%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DL	70/70 (100%)	60 (86%)	10 (14%)	3	18
40	AL	68/68 (100%)	57 (84%)	11 (16%)	2	14
40	DM	68/68 (100%)	59 (87%)	9 (13%)	4	20
41	AM	45/45 (100%)	39 (87%)	6 (13%)	4	20
41	DN	45/45 (100%)	42 (93%)	3 (7%)	15	41
42	AN	47/47 (100%)	40 (85%)	7 (15%)	3	17
42	DO	47/47 (100%)	43 (92%)	4 (8%)	10	34
43	AO	23/23 (100%)	17 (74%)	6 (26%)	0	3
43	DP	23/23 (100%)	19 (83%)	4 (17%)	2	11
44	AP	90/90 (100%)	75 (83%)	15 (17%)	2	13
44	DQ	90/90 (100%)	77 (86%)	13 (14%)	3	18
45	AQ	71/71 (100%)	60 (84%)	11 (16%)	2	15
45	DR	71/71 (100%)	60 (84%)	11 (16%)	2	15
46	i	97/137 (71%)	82 (84%)	15 (16%)	2	15
47	p0	105/186 (56%)	91 (87%)	14 (13%)	4	20
48	sM	54/54 (100%)	47 (87%)	7 (13%)	4	21
49	B	164/173 (95%)	149 (91%)	15 (9%)	9	32
49	s0	165/173 (95%)	145 (88%)	20 (12%)	5	22
50	C	191/192 (100%)	168 (88%)	23 (12%)	5	23
50	s1	192/192 (100%)	165 (86%)	27 (14%)	3	18
51	D	176/176 (100%)	149 (85%)	27 (15%)	3	16
51	s2	176/176 (100%)	140 (80%)	36 (20%)	1	7
52	E	182/182 (100%)	158 (87%)	24 (13%)	4	20
52	s3	182/182 (100%)	167 (92%)	15 (8%)	10	34
53	F	221/221 (100%)	192 (87%)	29 (13%)	4	20
53	s4	221/221 (100%)	186 (84%)	35 (16%)	2	15
54	G	173/173 (100%)	156 (90%)	17 (10%)	7	30
54	s5	173/173 (100%)	152 (88%)	21 (12%)	5	22
55	H	188/193 (97%)	171 (91%)	17 (9%)	9	32
55	s6	187/193 (97%)	160 (86%)	27 (14%)	3	18
56	I	165/166 (99%)	142 (86%)	23 (14%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	s7	165/166 (99%)	152 (92%)	13 (8%)	11	36
57	J	150/160 (94%)	130 (87%)	20 (13%)	4	20
57	s8	150/160 (94%)	130 (87%)	20 (13%)	4	20
58	K	158/158 (100%)	135 (85%)	23 (15%)	3	17
58	s9	158/158 (100%)	136 (86%)	22 (14%)	3	19
59	L	77/98 (79%)	68 (88%)	9 (12%)	5	24
59	c0	73/98 (74%)	66 (90%)	7 (10%)	8	30
60	M	129/136 (95%)	115 (89%)	14 (11%)	6	26
60	c1	129/136 (95%)	111 (86%)	18 (14%)	3	19
61	N	88/100 (88%)	74 (84%)	14 (16%)	2	14
61	c2	88/100 (88%)	70 (80%)	18 (20%)	1	7
62	O	127/127 (100%)	114 (90%)	13 (10%)	7	28
62	c3	127/127 (100%)	111 (87%)	16 (13%)	4	21
63	P	81/97 (84%)	62 (76%)	19 (24%)	1	4
63	c4	97/97 (100%)	84 (87%)	13 (13%)	4	20
64	Q	101/117 (86%)	90 (89%)	11 (11%)	6	26
64	c5	103/117 (88%)	91 (88%)	12 (12%)	5	24
65	R	117/118 (99%)	100 (86%)	17 (14%)	3	17
65	c6	118/118 (100%)	104 (88%)	14 (12%)	5	23
66	S	94/113 (83%)	85 (90%)	9 (10%)	8	30
67	T	128/128 (100%)	115 (90%)	13 (10%)	7	28
67	c8	128/128 (100%)	120 (94%)	8 (6%)	16	42
68	U	115/115 (100%)	95 (83%)	20 (17%)	2	11
68	c9	115/115 (100%)	106 (92%)	9 (8%)	11	36
69	V	100/103 (97%)	82 (82%)	18 (18%)	2	10
69	d0	103/103 (100%)	92 (89%)	11 (11%)	6	27
70	W	74/74 (100%)	63 (85%)	11 (15%)	3	17
70	d1	74/74 (100%)	65 (88%)	9 (12%)	5	22
71	X	110/110 (100%)	92 (84%)	18 (16%)	2	14
71	d2	110/110 (100%)	100 (91%)	10 (9%)	9	32
72	Y	119/119 (100%)	100 (84%)	19 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	d3	119/119 (100%)	105 (88%)	14 (12%)	5	23
73	Z	112/112 (100%)	103 (92%)	9 (8%)	11	35
73	d4	112/112 (100%)	104 (93%)	8 (7%)	13	38
74	a	61/61 (100%)	50 (82%)	11 (18%)	2	10
74	d5	61/61 (100%)	55 (90%)	6 (10%)	7	30
75	b	83/83 (100%)	68 (82%)	15 (18%)	2	10
75	d6	83/83 (100%)	73 (88%)	10 (12%)	5	23
76	c	70/70 (100%)	65 (93%)	5 (7%)	13	38
76	d7	70/70 (100%)	63 (90%)	7 (10%)	7	28
77	d	56/56 (100%)	50 (89%)	6 (11%)	6	27
77	d8	56/56 (100%)	48 (86%)	8 (14%)	3	18
78	d9	47/47 (100%)	41 (87%)	6 (13%)	4	21
78	e	47/47 (100%)	43 (92%)	4 (8%)	10	34
79	e0	53/53 (100%)	41 (77%)	12 (23%)	1	5
79	f	51/53 (96%)	46 (90%)	5 (10%)	7	30
80	g	62/62 (100%)	57 (92%)	5 (8%)	11	35
81	h	259/261 (99%)	236 (91%)	23 (9%)	9	32
81	sR	260/261 (100%)	240 (92%)	20 (8%)	12	37
82	c7	92/110 (84%)	80 (87%)	12 (13%)	4	21
83	e1	43/43 (100%)	33 (77%)	10 (23%)	1	5
All	All	18681/19177 (97%)	16169 (87%)	2512 (13%)	4	20

5 of 2512 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	U	28	LEU
61	c2	91	VAL
71	X	83	ILE
68	U	22	LEU
51	s2	117	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 178 such sidechains are listed below:

Mol	Chain	Res	Type
51	D	150	GLN
49	s0	69	ASN
55	H	65	GLN
68	U	101	ASN
54	s5	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3396 (92%)	564 (17%)	51 (1%)
1	AR	3145/3396 (92%)	583 (18%)	51 (1%)
2	3	120/121 (99%)	16 (13%)	0
2	AS	120/121 (99%)	15 (12%)	2 (1%)
25	6	1780/1800 (98%)	383 (21%)	30 (1%)
25	A	1778/1800 (98%)	409 (23%)	47 (2%)
3	4	157/158 (99%)	32 (20%)	2 (1%)
3	AT	157/158 (99%)	28 (17%)	3 (1%)
All	All	10402/10950 (94%)	2030 (19%)	186 (1%)

5 of 2030 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	26	A
1	1	40	A
1	1	49	A
1	1	57	A
1	1	59	G

5 of 186 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AR	2209	U
25	A	130	C
1	AR	2269	U
1	AR	3276	G
25	A	278	U

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2494 ligands modelled in this entry, 1422 are monoatomic - leaving 1072 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	DL	102	-	0,6,6	-	-	-		
84	OHX	AR	3702	-	0,6,6	-	-	-		
84	OHX	AR	3435	-	0,6,6	-	-	-		
84	OHX	1	3455	-	0,6,6	-	-	-		
84	OHX	6	2024	-	0,6,6	-	-	-		
84	OHX	AR	3650	-	0,6,6	-	-	-		
84	OHX	AS	205	-	0,6,6	-	-	-		
84	OHX	A	1952	-	0,6,6	-	-	-		
84	OHX	A	1969	-	0,6,6	-	-	-		
84	OHX	AR	3545	-	0,6,6	-	-	-		
84	OHX	1	3422	-	0,6,6	-	-	-		
84	OHX	AR	3534	-	0,6,6	-	-	-		
84	OHX	6	2007	-	0,6,6	-	-	-		
84	OHX	1	3679	-	0,6,6	-	-	-		
84	OHX	1	3555	-	0,6,6	-	-	-		
84	OHX	1	3458	-	0,6,6	-	-	-		
84	OHX	1	3618	-	0,6,6	-	-	-		
84	OHX	6	2032	-	0,6,6	-	-	-		
84	OHX	AR	3487	-	0,6,6	-	-	-		
84	OHX	AR	3522	-	0,6,6	-	-	-		
84	OHX	6	1965	-	0,6,6	-	-	-		
84	OHX	AR	3544	-	0,6,6	-	-	-		
84	OHX	AS	206	-	0,6,6	-	-	-		
84	OHX	1	3547	-	0,6,6	-	-	-		
84	OHX	1	3428	-	0,6,6	-	-	-		
84	OHX	1	401	-	0,6,6	-	-	-		
84	OHX	6	1968	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3406	-	0,6,6	-	-	-		
84	OHX	AR	3456	-	0,6,6	-	-	-		
84	OHX	AR	3641	-	0,6,6	-	-	-		
84	OHX	AR	3659	-	0,6,6	-	-	-		
84	OHX	6	2034	-	0,6,6	-	-	-		
84	OHX	AT	220	-	0,6,6	-	-	-		
84	OHX	AR	3454	-	0,6,6	-	-	-		
84	OHX	A	2014	-	0,6,6	-	-	-		
84	OHX	1	3475	-	0,6,6	-	-	-		
84	OHX	A	2030	-	0,6,6	-	-	-		
84	OHX	1	3570	-	0,6,6	-	-	-		
84	OHX	A	2008	-	0,6,6	-	-	-		
84	OHX	1	3731	-	0,6,6	-	-	-		
84	OHX	AR	3617	-	0,6,6	-	-	-		
84	OHX	AR	3424	-	0,6,6	-	-	-		
84	OHX	A	1950	-	0,6,6	-	-	-		
84	OHX	DL	101	-	0,6,6	-	-	-		
84	OHX	1	3626	-	0,6,6	-	-	-		
84	OHX	AR	3661	-	0,6,6	-	-	-		
84	OHX	1	3631	-	0,6,6	-	-	-		
84	OHX	1	3688	-	0,6,6	-	-	-		
84	OHX	1	3706	-	0,6,6	-	-	-		
84	OHX	AR	3508	-	0,6,6	-	-	-		
84	OHX	AR	3515	-	0,6,6	-	-	-		
84	OHX	1	3417	-	0,6,6	-	-	-		
84	OHX	1	3659	-	0,6,6	-	-	-		
84	OHX	6	1919	-	0,6,6	-	-	-		
84	OHX	6	2026	-	0,6,6	-	-	-		
84	OHX	AR	3401	-	0,6,6	-	-	-		
84	OHX	AR	3575	-	0,6,6	-	-	-		
84	OHX	A	1986	-	0,6,6	-	-	-		
84	OHX	AR	3568	-	0,6,6	-	-	-		
84	OHX	AT	204	-	0,6,6	-	-	-		
84	OHX	1	3465	-	0,6,6	-	-	-		
84	OHX	1	3634	-	0,6,6	-	-	-		
84	OHX	AR	3643	-	0,6,6	-	-	-		
84	OHX	AR	3517	-	0,6,6	-	-	-		
84	OHX	1	3670	-	0,6,6	-	-	-		
84	OHX	AR	3738	-	0,6,6	-	-	-		
84	OHX	AR	3529	-	0,6,6	-	-	-		
84	OHX	1	3729	-	0,6,6	-	-	-		
84	OHX	AR	3586	-	0,6,6	-	-	-		
84	OHX	A	2040	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	1959	-	0,6,6	-	-	-		
84	OHX	1	3527	-	0,6,6	-	-	-		
84	OHX	1	3516	-	0,6,6	-	-	-		
84	OHX	1	3540	-	0,6,6	-	-	-		
84	OHX	1	3620	-	0,6,6	-	-	-		
84	OHX	AR	3491	-	0,6,6	-	-	-		
84	OHX	AR	3635	-	0,6,6	-	-	-		
84	OHX	A	2032	-	0,6,6	-	-	-		
84	OHX	AR	3612	-	0,6,6	-	-	-		
84	OHX	CL	302	-	0,6,6	-	-	-		
84	OHX	6	1912	-	0,6,6	-	-	-		
84	OHX	6	1937	-	0,6,6	-	-	-		
84	OHX	6	1972	-	0,6,6	-	-	-		
84	OHX	1	3551	-	0,6,6	-	-	-		
84	OHX	AR	3601	-	0,6,6	-	-	-		
84	OHX	A	2021	-	0,6,6	-	-	-		
84	OHX	1	3528	-	0,6,6	-	-	-		
84	OHX	AR	3689	-	0,6,6	-	-	-		
84	OHX	A	1919	-	0,6,6	-	-	-		
84	OHX	6	1905	-	0,6,6	-	-	-		
84	OHX	k	401	-	0,6,6	-	-	-		
84	OHX	6	2005	-	0,6,6	-	-	-		
84	OHX	A	2035	-	0,6,6	-	-	-		
84	OHX	AR	3664	-	0,6,6	-	-	-		
84	OHX	6	2002	-	0,6,6	-	-	-		
84	OHX	1	3657	-	0,6,6	-	-	-		
84	OHX	6	1955	-	0,6,6	-	-	-		
84	OHX	6	1958	-	0,6,6	-	-	-		
84	OHX	1	3449	-	0,6,6	-	-	-		
84	OHX	A	2018	-	0,6,6	-	-	-		
84	OHX	A	1970	-	0,6,6	-	-	-		
84	OHX	A	1971	-	0,6,6	-	-	-		
84	OHX	CO	201	-	0,6,6	-	-	-		
84	OHX	A	1929	-	0,6,6	-	-	-		
84	OHX	AR	3505	-	0,6,6	-	-	-		
84	OHX	1	3593	-	0,6,6	-	-	-		
84	OHX	AR	3503	-	0,6,6	-	-	-		
84	OHX	AR	3599	-	0,6,6	-	-	-		
84	OHX	1	3606	-	0,6,6	-	-	-		
84	OHX	1	3645	-	0,6,6	-	-	-		
84	OHX	1	3635	-	0,6,6	-	-	-		
84	OHX	A	2009	-	0,6,6	-	-	-		
84	OHX	AR	3651	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	A	2002	-	0,6,6	-	-	-		
84	OHX	1	3492	-	0,6,6	-	-	-		
84	OHX	AR	3520	-	0,6,6	-	-	-		
84	OHX	6	1918	-	0,6,6	-	-	-		
84	OHX	AR	3518	-	0,6,6	-	-	-		
84	OHX	6	1913	-	0,6,6	-	-	-		
84	OHX	6	1952	-	0,6,6	-	-	-		
84	OHX	AR	3475	-	0,6,6	-	-	-		
84	OHX	AR	3592	-	0,6,6	-	-	-		
84	OHX	AR	3567	-	0,6,6	-	-	-		
84	OHX	4	204	-	0,6,6	-	-	-		
84	OHX	x	202	-	0,6,6	-	-	-		
84	OHX	1	3407	-	0,6,6	-	-	-		
84	OHX	AR	3469	-	0,6,6	-	-	-		
84	OHX	1	3487	-	0,6,6	-	-	-		
84	OHX	A	1994	-	0,6,6	-	-	-		
84	OHX	AR	3691	-	0,6,6	-	-	-		
84	OHX	1	3537	-	0,6,6	-	-	-		
84	OHX	3	207	-	0,6,6	-	-	-		
84	OHX	CG	301	-	0,6,6	-	-	-		
84	OHX	1	3406	-	0,6,6	-	-	-		
84	OHX	AT	218	-	0,6,6	-	-	-		
84	OHX	A	1960	-	0,6,6	-	-	-		
84	OHX	AR	3642	-	0,6,6	-	-	-		
84	OHX	4	210	-	0,6,6	-	-	-		
84	OHX	1	3510	-	0,6,6	-	-	-		
84	OHX	AR	3447	-	0,6,6	-	-	-		
84	OHX	CK	201	-	0,6,6	-	-	-		
84	OHX	6	1924	-	0,6,6	-	-	-		
84	OHX	6	1923	-	0,6,6	-	-	-		
84	OHX	AR	3657	-	0,6,6	-	-	-		
84	OHX	1	3617	-	0,6,6	-	-	-		
84	OHX	AR	3605	-	0,6,6	-	-	-		
84	OHX	1	3489	-	0,6,6	-	-	-		
84	OHX	AT	217	-	0,6,6	-	-	-		
84	OHX	6	1970	-	0,6,6	-	-	-		
84	OHX	6	2044	-	0,6,6	-	-	-		
84	OHX	A	2011	-	0,6,6	-	-	-		
84	OHX	1	3401	-	0,6,6	-	-	-		
84	OHX	AR	3587	-	0,6,6	-	-	-		
84	OHX	CG	303	-	0,6,6	-	-	-		
84	OHX	1	3597	-	0,6,6	-	-	-		
84	OHX	1	3517	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3713	-	0,6,6	-	-	-		
84	OHX	6	1997	-	0,6,6	-	-	-		
84	OHX	AR	3620	-	0,6,6	-	-	-		
84	OHX	1	3543	-	0,6,6	-	-	-		
84	OHX	AT	212	-	0,6,6	-	-	-		
84	OHX	A	1909	-	0,6,6	-	-	-		
84	OHX	A	1967	-	0,6,6	-	-	-		
84	OHX	AR	3490	-	0,6,6	-	-	-		
84	OHX	AR	3701	-	0,6,6	-	-	-		
84	OHX	1	3578	-	0,6,6	-	-	-		
84	OHX	1	3611	-	0,6,6	-	-	-		
84	OHX	AR	3486	-	0,6,6	-	-	-		
84	OHX	AR	3551	-	0,6,6	-	-	-		
84	OHX	1	3410	-	0,6,6	-	-	-		
84	OHX	M	201	-	0,6,6	-	-	-		
84	OHX	AR	3637	-	0,6,6	-	-	-		
84	OHX	1	3535	-	0,6,6	-	-	-		
84	OHX	1	3587	-	0,6,6	-	-	-		
84	OHX	AR	3704	-	0,6,6	-	-	-		
84	OHX	A	2023	-	0,6,6	-	-	-		
84	OHX	AR	3675	-	0,6,6	-	-	-		
84	OHX	AR	3715	-	0,6,6	-	-	-		
84	OHX	6	1963	-	0,6,6	-	-	-		
84	OHX	1	3411	-	0,6,6	-	-	-		
84	OHX	A	2027	-	0,6,6	-	-	-		
84	OHX	AR	3604	-	0,6,6	-	-	-		
84	OHX	AR	3495	-	0,6,6	-	-	-		
84	OHX	6	1993	-	0,6,6	-	-	-		
84	OHX	AR	3553	-	0,6,6	-	-	-		
84	OHX	AR	3693	-	0,6,6	-	-	-		
84	OHX	1	3711	-	0,6,6	-	-	-		
84	OHX	1	3452	-	0,6,6	-	-	-		
84	OHX	6	1977	-	0,6,6	-	-	-		
84	OHX	A	1916	-	0,6,6	-	-	-		
84	OHX	1	3408	-	0,6,6	-	-	-		
84	OHX	1	3501	-	0,6,6	-	-	-		
84	OHX	3	208	-	0,6,6	-	-	-		
84	OHX	AR	3532	-	0,6,6	-	-	-		
84	OHX	A	1937	-	0,6,6	-	-	-		
84	OHX	1	3601	-	0,6,6	-	-	-		
84	OHX	A	1927	-	0,6,6	-	-	-		
84	OHX	AR	3677	-	0,6,6	-	-	-		
84	OHX	6	2041	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3607	-	0,6,6	-	-	-		
84	OHX	AR	3471	-	0,6,6	-	-	-		
84	OHX	1	3718	-	0,6,6	-	-	-		
84	OHX	AR	3441	-	0,6,6	-	-	-		
84	OHX	6	2016	-	0,6,6	-	-	-		
84	OHX	A	1918	-	0,6,6	-	-	-		
84	OHX	6	2028	-	0,6,6	-	-	-		
84	OHX	6	2000	-	0,6,6	-	-	-		
84	OHX	AR	3493	-	0,6,6	-	-	-		
84	OHX	AR	3533	-	0,6,6	-	-	-		
84	OHX	1	3651	-	0,6,6	-	-	-		
84	OHX	AT	215	-	0,6,6	-	-	-		
84	OHX	A	1972	-	0,6,6	-	-	-		
84	OHX	1	3512	-	0,6,6	-	-	-		
84	OHX	DD	102	-	0,6,6	-	-	-		
84	OHX	6	1976	-	0,6,6	-	-	-		
84	OHX	1	3539	-	0,6,6	-	-	-		
84	OHX	1	3667	-	0,6,6	-	-	-		
84	OHX	AR	3496	-	0,6,6	-	-	-		
84	OHX	A	2037	-	0,6,6	-	-	-		
84	OHX	AR	3432	-	0,6,6	-	-	-		
84	OHX	A	1907	-	0,6,6	-	-	-		
84	OHX	1	3462	-	0,6,6	-	-	-		
84	OHX	AR	3685	-	0,6,6	-	-	-		
84	OHX	1	3723	-	0,6,6	-	-	-		
84	OHX	e	101	-	0,6,6	-	-	-		
84	OHX	AR	3713	-	0,6,6	-	-	-		
84	OHX	AR	3681	-	0,6,6	-	-	-		
84	OHX	AR	3541	-	0,6,6	-	-	-		
84	OHX	AR	3442	-	0,6,6	-	-	-		
84	OHX	AR	3410	-	0,6,6	-	-	-		
84	OHX	6	2052	-	0,6,6	-	-	-		
84	OHX	AR	3548	-	0,6,6	-	-	-		
84	OHX	AR	3610	-	0,6,6	-	-	-		
84	OHX	AR	3678	-	0,6,6	-	-	-		
84	OHX	A	2029	-	0,6,6	-	-	-		
84	OHX	6	1907	-	0,6,6	-	-	-		
84	OHX	AR	3418	-	0,6,6	-	-	-		
84	OHX	AR	3555	-	0,6,6	-	-	-		
84	OHX	AR	3700	-	0,6,6	-	-	-		
84	OHX	1	3557	-	0,6,6	-	-	-		
84	OHX	AR	3670	-	0,6,6	-	-	-		
84	OHX	A	2042	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	4	207	-	0,6,6	-	-	-		
84	OHX	AR	3481	-	0,6,6	-	-	-		
84	OHX	1	3473	-	0,6,6	-	-	-		
84	OHX	AR	3513	-	0,6,6	-	-	-		
84	OHX	A	1961	-	0,6,6	-	-	-		
84	OHX	AS	210	-	0,6,6	-	-	-		
84	OHX	A	1939	-	0,6,6	-	-	-		
84	OHX	AR	3429	-	0,6,6	-	-	-		
84	OHX	1	3443	-	0,6,6	-	-	-		
84	OHX	1	3678	-	0,6,6	-	-	-		
84	OHX	1	3579	-	0,6,6	-	-	-		
84	OHX	6	1979	-	0,6,6	-	-	-		
84	OHX	6	2057	-	0,6,6	-	-	-		
84	OHX	c3	201	-	0,6,6	-	-	-		
84	OHX	AR	3708	-	0,6,6	-	-	-		
84	OHX	4	211	-	0,6,6	-	-	-		
84	OHX	1	3700	-	0,6,6	-	-	-		
84	OHX	AR	3559	-	0,6,6	-	-	-		
84	OHX	AR	3656	-	0,6,6	-	-	-		
84	OHX	1	3569	-	0,6,6	-	-	-		
84	OHX	1	3402	-	0,6,6	-	-	-		
84	OHX	1	3495	-	0,6,6	-	-	-		
84	OHX	1	3439	-	0,6,6	-	-	-		
84	OHX	1	3553	-	0,6,6	-	-	-		
84	OHX	1	3701	-	0,6,6	-	-	-		
84	OHX	1	3426	-	0,6,6	-	-	-		
84	OHX	A	1955	-	0,6,6	-	-	-		
84	OHX	1	3519	-	0,6,6	-	-	-		
84	OHX	AR	3733	-	0,6,6	-	-	-		
84	OHX	AR	3683	-	0,6,6	-	-	-		
84	OHX	A	1912	-	0,6,6	-	-	-		
84	OHX	1	3404	-	0,6,6	-	-	-		
84	OHX	6	1930	-	0,6,6	-	-	-		
84	OHX	AR	3506	-	0,6,6	-	-	-		
84	OHX	1	3675	-	0,6,6	-	-	-		
84	OHX	AR	3590	-	0,6,6	-	-	-		
84	OHX	AS	208	-	0,6,6	-	-	-		
84	OHX	1	3677	-	0,6,6	-	-	-		
84	OHX	1	3660	-	0,6,6	-	-	-		
84	OHX	A	1944	-	0,6,6	-	-	-		
84	OHX	6	1921	-	0,6,6	-	-	-		
84	OHX	AR	3627	-	0,6,6	-	-	-		
84	OHX	AR	3667	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	1928	-	0,6,6	-	-	-		
84	OHX	6	1949	-	0,6,6	-	-	-		
84	OHX	AR	3542	-	0,6,6	-	-	-		
84	OHX	3	203	-	0,6,6	-	-	-		
84	OHX	1	3712	-	0,6,6	-	-	-		
84	OHX	6	1926	-	0,6,6	-	-	-		
84	OHX	6	1934	-	0,6,6	-	-	-		
84	OHX	6	1941	-	0,6,6	-	-	-		
84	OHX	AR	3547	-	0,6,6	-	-	-		
84	OHX	1	3600	-	0,6,6	-	-	-		
84	OHX	A	1913	-	0,6,6	-	-	-		
84	OHX	AT	207	-	0,6,6	-	-	-		
84	OHX	A	1925	-	0,6,6	-	-	-		
84	OHX	1	3642	-	0,6,6	-	-	-		
84	OHX	6	2048	-	0,6,6	-	-	-		
84	OHX	1	3654	-	0,6,6	-	-	-		
84	OHX	AR	3473	-	0,6,6	-	-	-		
84	OHX	1	3496	-	0,6,6	-	-	-		
84	OHX	1	3687	-	0,6,6	-	-	-		
84	OHX	6	2021	-	0,6,6	-	-	-		
84	OHX	AR	3603	-	0,6,6	-	-	-		
84	OHX	AR	3571	-	0,6,6	-	-	-		
84	OHX	3	202	-	0,6,6	-	-	-		
84	OHX	AR	3494	-	0,6,6	-	-	-		
84	OHX	6	1999	-	0,6,6	-	-	-		
84	OHX	1	3445	-	0,6,6	-	-	-		
84	OHX	4	206	-	0,6,6	-	-	-		
84	OHX	6	2013	-	0,6,6	-	-	-		
84	OHX	6	2019	-	0,6,6	-	-	-		
84	OHX	6	1909	-	0,6,6	-	-	-		
84	OHX	AR	3561	-	0,6,6	-	-	-		
84	OHX	1	3414	-	0,6,6	-	-	-		
84	OHX	AR	3609	-	0,6,6	-	-	-		
84	OHX	1	3653	-	0,6,6	-	-	-		
84	OHX	6	1946	-	0,6,6	-	-	-		
84	OHX	6	2018	-	0,6,6	-	-	-		
84	OHX	6	2054	-	0,6,6	-	-	-		
84	OHX	1	3610	-	0,6,6	-	-	-		
84	OHX	A	1943	-	0,6,6	-	-	-		
84	OHX	4	203	-	0,6,6	-	-	-		
84	OHX	6	1974	-	0,6,6	-	-	-		
84	OHX	AT	208	-	0,6,6	-	-	-		
84	OHX	1	3488	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3721	-	0,6,6	-	-	-		
84	OHX	1	3409	-	0,6,6	-	-	-		
84	OHX	1	3572	-	0,6,6	-	-	-		
84	OHX	AR	3611	-	0,6,6	-	-	-		
84	OHX	1	3454	-	0,6,6	-	-	-		
84	OHX	1	3566	-	0,6,6	-	-	-		
84	OHX	AR	3676	-	0,6,6	-	-	-		
84	OHX	1	3429	-	0,6,6	-	-	-		
84	OHX	AR	3438	-	0,6,6	-	-	-		
84	OHX	1	3532	-	0,6,6	-	-	-		
84	OHX	A	1984	-	0,6,6	-	-	-		
84	OHX	AR	3549	-	0,6,6	-	-	-		
84	OHX	AR	3638	-	0,6,6	-	-	-		
84	OHX	AR	3476	-	0,6,6	-	-	-		
84	OHX	AR	3562	-	0,6,6	-	-	-		
84	OHX	1	3534	-	0,6,6	-	-	-		
84	OHX	6	1901	-	0,6,6	-	-	-		
84	OHX	AT	205	-	0,6,6	-	-	-		
84	OHX	AR	3420	-	0,6,6	-	-	-		
84	OHX	1	3514	-	0,6,6	-	-	-		
84	OHX	A	1965	-	0,6,6	-	-	-		
84	OHX	6	1954	-	0,6,6	-	-	-		
84	OHX	AR	3581	-	0,6,6	-	-	-		
84	OHX	1	3683	-	0,6,6	-	-	-		
84	OHX	AR	3573	-	0,6,6	-	-	-		
84	OHX	A	1936	-	0,6,6	-	-	-		
84	OHX	1	3638	-	0,6,6	-	-	-		
84	OHX	AR	3600	-	0,6,6	-	-	-		
84	OHX	AR	3616	-	0,6,6	-	-	-		
84	OHX	1	3663	-	0,6,6	-	-	-		
84	OHX	AR	3720	-	0,6,6	-	-	-		
84	OHX	CM	201	-	0,6,6	-	-	-		
84	OHX	AR	3582	-	0,6,6	-	-	-		
84	OHX	A	1981	-	0,6,6	-	-	-		
84	OHX	AR	3613	-	0,6,6	-	-	-		
84	OHX	6	2049	-	0,6,6	-	-	-		
84	OHX	AR	3628	-	0,6,6	-	-	-		
84	OHX	1	3692	-	0,6,6	-	-	-		
84	OHX	1	3661	-	0,6,6	-	-	-		
84	OHX	6	1902	-	0,6,6	-	-	-		
84	OHX	1	3556	-	0,6,6	-	-	-		
84	OHX	A	1978	-	0,6,6	-	-	-		
84	OHX	AR	3563	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3427	-	0,6,6	-	-	-		
84	OHX	AR	3734	-	0,6,6	-	-	-		
84	OHX	1	3705	-	0,6,6	-	-	-		
84	OHX	1	3531	-	0,6,6	-	-	-		
84	OHX	A	2015	-	0,6,6	-	-	-		
84	OHX	1	3530	-	0,6,6	-	-	-		
84	OHX	AR	3709	-	0,6,6	-	-	-		
84	OHX	AR	3624	-	0,6,6	-	-	-		
84	OHX	AR	3445	-	0,6,6	-	-	-		
84	OHX	6	2023	-	0,6,6	-	-	-		
84	OHX	1	3655	-	0,6,6	-	-	-		
84	OHX	1	3668	-	0,6,6	-	-	-		
84	OHX	AR	3510	-	0,6,6	-	-	-		
84	OHX	1	3479	-	0,6,6	-	-	-		
84	OHX	AC	101	-	0,6,6	-	-	-		
84	OHX	A	1979	-	0,6,6	-	-	-		
84	OHX	1	3576	-	0,6,6	-	-	-		
84	OHX	AR	3723	-	0,6,6	-	-	-		
84	OHX	1	3571	-	0,6,6	-	-	-		
84	OHX	AR	3632	-	0,6,6	-	-	-		
84	OHX	A	2038	-	0,6,6	-	-	-		
84	OHX	1	3469	-	0,6,6	-	-	-		
84	OHX	1	3494	-	0,6,6	-	-	-		
84	OHX	AR	3431	-	0,6,6	-	-	-		
84	OHX	1	3726	-	0,6,6	-	-	-		
84	OHX	1	3558	-	0,6,6	-	-	-		
84	OHX	A	1954	-	0,6,6	-	-	-		
84	OHX	A	1962	-	0,6,6	-	-	-		
84	OHX	1	3451	-	0,6,6	-	-	-		
84	OHX	1	3609	-	0,6,6	-	-	-		
84	OHX	1	3584	-	0,6,6	-	-	-		
84	OHX	AR	3478	-	0,6,6	-	-	-		
84	OHX	AR	3669	-	0,6,6	-	-	-		
84	OHX	AR	3614	-	0,6,6	-	-	-		
84	OHX	AR	3598	-	0,6,6	-	-	-		
84	OHX	AT	210	-	0,6,6	-	-	-		
84	OHX	AR	3483	-	0,6,6	-	-	-		
84	OHX	6	1973	-	0,6,6	-	-	-		
84	OHX	AR	3426	-	0,6,6	-	-	-		
84	OHX	1	3691	-	0,6,6	-	-	-		
84	OHX	AR	3519	-	0,6,6	-	-	-		
84	OHX	1	3505	-	0,6,6	-	-	-		
84	OHX	1	3599	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3482	-	0,6,6	-	-	-		
84	OHX	6	1904	-	0,6,6	-	-	-		
84	OHX	6	1956	-	0,6,6	-	-	-		
84	OHX	6	2051	-	0,6,6	-	-	-		
84	OHX	AR	3497	-	0,6,6	-	-	-		
84	OHX	AR	3591	-	0,6,6	-	-	-		
84	OHX	AR	3452	-	0,6,6	-	-	-		
84	OHX	A	1951	-	0,6,6	-	-	-		
84	OHX	A	2017	-	0,6,6	-	-	-		
84	OHX	6	2014	-	0,6,6	-	-	-		
84	OHX	AR	3615	-	0,6,6	-	-	-		
84	OHX	A	1934	-	0,6,6	-	-	-		
84	OHX	1	3676	-	0,6,6	-	-	-		
84	OHX	A	2006	-	0,6,6	-	-	-		
84	OHX	6	1985	-	0,6,6	-	-	-		
84	OHX	DI	201	-	0,6,6	-	-	-		
84	OHX	AR	3402	-	0,6,6	-	-	-		
84	OHX	A	1957	-	0,6,6	-	-	-		
84	OHX	A	2041	-	0,6,6	-	-	-		
84	OHX	1	3484	-	0,6,6	-	-	-		
84	OHX	AR	3595	-	0,6,6	-	-	-		
84	OHX	1	3549	-	0,6,6	-	-	-		
84	OHX	6	2056	-	0,6,6	-	-	-		
84	OHX	A	1902	-	0,6,6	-	-	-		
84	OHX	AR	3710	-	0,6,6	-	-	-		
84	OHX	AR	3477	-	0,6,6	-	-	-		
84	OHX	A	1910	-	0,6,6	-	-	-		
84	OHX	AR	3466	-	0,6,6	-	-	-		
84	OHX	1	3515	-	0,6,6	-	-	-		
84	OHX	1	3420	-	0,6,6	-	-	-		
84	OHX	AT	203	-	0,6,6	-	-	-		
84	OHX	AR	3474	-	0,6,6	-	-	-		
84	OHX	AR	3589	-	0,6,6	-	-	-		
84	OHX	AR	3434	-	0,6,6	-	-	-		
84	OHX	AR	3721	-	0,6,6	-	-	-		
84	OHX	1	3450	-	0,6,6	-	-	-		
84	OHX	AR	3660	-	0,6,6	-	-	-		
84	OHX	A	1911	-	0,6,6	-	-	-		
84	OHX	1	3694	-	0,6,6	-	-	-		
84	OHX	6	2029	-	0,6,6	-	-	-		
84	OHX	6	1989	-	0,6,6	-	-	-		
84	OHX	1	3503	-	0,6,6	-	-	-		
84	OHX	AR	3739	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3504	-	0,6,6	-	-	-		
84	OHX	1	3628	-	0,6,6	-	-	-		
84	OHX	6	2001	-	0,6,6	-	-	-		
84	OHX	AR	3479	-	0,6,6	-	-	-		
84	OHX	1	3563	-	0,6,6	-	-	-		
84	OHX	1	3690	-	0,6,6	-	-	-		
84	OHX	A	1997	-	0,6,6	-	-	-		
84	OHX	AR	3417	-	0,6,6	-	-	-		
84	OHX	A	2022	-	0,6,6	-	-	-		
84	OHX	A	1932	-	0,6,6	-	-	-		
84	OHX	A	1982	-	0,6,6	-	-	-		
84	OHX	1	3582	-	0,6,6	-	-	-		
84	OHX	A	1938	-	0,6,6	-	-	-		
84	OHX	1	3459	-	0,6,6	-	-	-		
84	OHX	A	2012	-	0,6,6	-	-	-		
84	OHX	AR	3703	-	0,6,6	-	-	-		
84	OHX	1	3639	-	0,6,6	-	-	-		
84	OHX	A	1985	-	0,6,6	-	-	-		
84	OHX	A	1988	-	0,6,6	-	-	-		
84	OHX	AR	3716	-	0,6,6	-	-	-		
84	OHX	z	201	-	0,6,6	-	-	-		
84	OHX	AR	3409	-	0,6,6	-	-	-		
84	OHX	AR	3682	-	0,6,6	-	-	-		
84	OHX	AR	3467	-	0,6,6	-	-	-		
84	OHX	1	3431	-	0,6,6	-	-	-		
84	OHX	1	3596	-	0,6,6	-	-	-		
84	OHX	r	301	-	0,6,6	-	-	-		
84	OHX	AR	3465	-	0,6,6	-	-	-		
84	OHX	AR	3543	-	0,6,6	-	-	-		
84	OHX	3	206	-	0,6,6	-	-	-		
84	OHX	A	2005	-	0,6,6	-	-	-		
84	OHX	AR	3446	-	0,6,6	-	-	-		
84	OHX	AR	3552	-	0,6,6	-	-	-		
84	OHX	AR	3482	-	0,6,6	-	-	-		
84	OHX	AR	3509	-	0,6,6	-	-	-		
84	OHX	AR	3602	-	0,6,6	-	-	-		
84	OHX	AR	3644	-	0,6,6	-	-	-		
84	OHX	A	2016	-	0,6,6	-	-	-		
84	OHX	AS	204	-	0,6,6	-	-	-		
84	OHX	A	2039	-	0,6,6	-	-	-		
84	OHX	AR	3648	-	0,6,6	-	-	-		
84	OHX	1	3614	-	0,6,6	-	-	-		
84	OHX	1	3491	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3598	-	0,6,6	-	-	-		
84	OHX	6	1994	-	0,6,6	-	-	-		
84	OHX	1	3483	-	0,6,6	-	-	-		
84	OHX	1	3575	-	0,6,6	-	-	-		
84	OHX	AR	3499	-	0,6,6	-	-	-		
84	OHX	1	3568	-	0,6,6	-	-	-		
84	OHX	1	3509	-	0,6,6	-	-	-		
84	OHX	6	1984	-	0,6,6	-	-	-		
84	OHX	AR	3718	-	0,6,6	-	-	-		
84	OHX	6	1982	-	0,6,6	-	-	-		
84	OHX	AR	3455	-	0,6,6	-	-	-		
84	OHX	6	1908	-	0,6,6	-	-	-		
84	OHX	AK	102	-	0,6,6	-	-	-		
84	OHX	1	3615	-	0,6,6	-	-	-		
84	OHX	A	1930	-	0,6,6	-	-	-		
84	OHX	1	3673	-	0,6,6	-	-	-		
84	OHX	y	201	-	0,6,6	-	-	-		
84	OHX	6	2045	-	0,6,6	-	-	-		
84	OHX	1	3493	-	0,6,6	-	-	-		
84	OHX	1	3590	-	0,6,6	-	-	-		
84	OHX	1	3511	-	0,6,6	-	-	-		
84	OHX	AR	3492	-	0,6,6	-	-	-		
84	OHX	A	1935	-	0,6,6	-	-	-		
84	OHX	A	1948	-	0,6,6	-	-	-		
84	OHX	d9	101	-	0,6,6	-	-	-		
84	OHX	AR	3680	-	0,6,6	-	-	-		
84	OHX	AR	3525	-	0,6,6	-	-	-		
84	OHX	AR	3649	-	0,6,6	-	-	-		
84	OHX	c8	201	-	0,6,6	-	-	-		
84	OHX	1	3466	-	0,6,6	-	-	-		
84	OHX	1	3619	-	0,6,6	-	-	-		
84	OHX	AR	3722	-	0,6,6	-	-	-		
84	OHX	1	3434	-	0,6,6	-	-	-		
84	OHX	k	402	-	0,6,6	-	-	-		
84	OHX	AR	3697	-	0,6,6	-	-	-		
84	OHX	A	1995	-	0,6,6	-	-	-		
84	OHX	AR	3658	-	0,6,6	-	-	-		
84	OHX	AR	3566	-	0,6,6	-	-	-		
84	OHX	1	3525	-	0,6,6	-	-	-		
84	OHX	6	2004	-	0,6,6	-	-	-		
84	OHX	1	3486	-	0,6,6	-	-	-		
84	OHX	1	3508	-	0,6,6	-	-	-		
84	OHX	1	3650	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	2011	-	0,6,6	-	-	-		
84	OHX	AR	3459	-	0,6,6	-	-	-		
84	OHX	1	3559	-	0,6,6	-	-	-		
84	OHX	4	201	-	0,6,6	-	-	-		
84	OHX	1	3637	-	0,6,6	-	-	-		
84	OHX	6	1948	-	0,6,6	-	-	-		
84	OHX	AR	3498	-	0,6,6	-	-	-		
84	OHX	AR	3558	-	0,6,6	-	-	-		
84	OHX	AR	3699	-	0,6,6	-	-	-		
84	OHX	1	3442	-	0,6,6	-	-	-		
84	OHX	CF	401	-	0,6,6	-	-	-		
84	OHX	6	1920	-	0,6,6	-	-	-		
84	OHX	1	3684	-	0,6,6	-	-	-		
84	OHX	A	1964	-	0,6,6	-	-	-		
84	OHX	A	1966	-	0,6,6	-	-	-		
84	OHX	A	1922	-	0,6,6	-	-	-		
84	OHX	6	2038	-	0,6,6	-	-	-		
84	OHX	1	3463	-	0,6,6	-	-	-		
84	OHX	AR	3666	-	0,6,6	-	-	-		
84	OHX	4	205	-	0,6,6	-	-	-		
84	OHX	1	3586	-	0,6,6	-	-	-		
84	OHX	1	3522	-	0,6,6	-	-	-		
84	OHX	1	3460	-	0,6,6	-	-	-		
84	OHX	6	1962	-	0,6,6	-	-	-		
84	OHX	AR	3737	-	0,6,6	-	-	-		
84	OHX	6	2043	-	0,6,6	-	-	-		
84	OHX	1	3467	-	0,6,6	-	-	-		
84	OHX	AR	3437	-	0,6,6	-	-	-		
84	OHX	1	3521	-	0,6,6	-	-	-		
84	OHX	4	212	-	0,6,6	-	-	-		
84	OHX	AR	3535	-	0,6,6	-	-	-		
84	OHX	AR	3636	-	0,6,6	-	-	-		
84	OHX	AR	3717	-	0,6,6	-	-	-		
84	OHX	1	3714	-	0,6,6	-	-	-		
84	OHX	1	3471	-	0,6,6	-	-	-		
84	OHX	1	3703	-	0,6,6	-	-	-		
84	OHX	AR	3411	-	0,6,6	-	-	-		
84	OHX	1	3447	-	0,6,6	-	-	-		
84	OHX	AR	3608	-	0,6,6	-	-	-		
84	OHX	AR	3735	-	0,6,6	-	-	-		
84	OHX	1	3446	-	0,6,6	-	-	-		
84	OHX	1	3552	-	0,6,6	-	-	-		
84	OHX	6	1980	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3602	-	0,6,6	-	-	-		
84	OHX	1	3506	-	0,6,6	-	-	-		
84	OHX	AR	3403	-	0,6,6	-	-	-		
84	OHX	1	3629	-	0,6,6	-	-	-		
84	OHX	1	3648	-	0,6,6	-	-	-		
84	OHX	AR	3463	-	0,6,6	-	-	-		
84	OHX	AR	3606	-	0,6,6	-	-	-		
84	OHX	6	1933	-	0,6,6	-	-	-		
84	OHX	6	1987	-	0,6,6	-	-	-		
84	OHX	1	3603	-	0,6,6	-	-	-		
84	OHX	1	3481	-	0,6,6	-	-	-		
84	OHX	AR	3569	-	0,6,6	-	-	-		
84	OHX	A	2028	-	0,6,6	-	-	-		
84	OHX	1	3627	-	0,6,6	-	-	-		
84	OHX	A	2001	-	0,6,6	-	-	-		
84	OHX	6	2040	-	0,6,6	-	-	-		
84	OHX	AR	3580	-	0,6,6	-	-	-		
84	OHX	AR	3665	-	0,6,6	-	-	-		
84	OHX	A	2034	-	0,6,6	-	-	-		
84	OHX	AK	103	-	0,6,6	-	-	-		
84	OHX	AR	3416	-	0,6,6	-	-	-		
84	OHX	1	3636	-	0,6,6	-	-	-		
84	OHX	1	3715	-	0,6,6	-	-	-		
84	OHX	AR	3448	-	0,6,6	-	-	-		
84	OHX	CV	201	-	0,6,6	-	-	-		
84	OHX	A	1924	-	0,6,6	-	-	-		
84	OHX	1	3490	-	0,6,6	-	-	-		
84	OHX	6	1992	-	0,6,6	-	-	-		
84	OHX	6	1917	-	0,6,6	-	-	-		
84	OHX	A	1905	-	0,6,6	-	-	-		
84	OHX	A	1973	-	0,6,6	-	-	-		
84	OHX	1	3546	-	0,6,6	-	-	-		
84	OHX	1	3604	-	0,6,6	-	-	-		
84	OHX	1	3696	-	0,6,6	-	-	-		
84	OHX	1	3441	-	0,6,6	-	-	-		
84	OHX	AR	3698	-	0,6,6	-	-	-		
84	OHX	CP	501	-	0,6,6	-	-	-		
84	OHX	6	2003	-	0,6,6	-	-	-		
84	OHX	1	3649	-	0,6,6	-	-	-		
84	OHX	6	1906	-	0,6,6	-	-	-		
84	OHX	A	1921	-	0,6,6	-	-	-		
84	OHX	1	3722	-	0,6,6	-	-	-		
84	OHX	A	1999	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	2031	-	0,6,6	-	-	-		
84	OHX	AR	3521	-	0,6,6	-	-	-		
84	OHX	CE	402	-	0,6,6	-	-	-		
84	OHX	AR	3623	-	0,6,6	-	-	-		
84	OHX	6	2030	-	0,6,6	-	-	-		
84	OHX	6	1929	-	0,6,6	-	-	-		
84	OHX	A	1974	-	0,6,6	-	-	-		
84	OHX	1	3444	-	0,6,6	-	-	-		
84	OHX	AR	3583	-	0,6,6	-	-	-		
84	OHX	AR	3618	-	0,6,6	-	-	-		
84	OHX	AR	3516	-	0,6,6	-	-	-		
84	OHX	1	3405	-	0,6,6	-	-	-		
84	OHX	1	3656	-	0,6,6	-	-	-		
84	OHX	DG	201	-	0,6,6	-	-	-		
84	OHX	A	1993	-	0,6,6	-	-	-		
84	OHX	1	3607	-	0,6,6	-	-	-		
84	OHX	1	3565	-	0,6,6	-	-	-		
84	OHX	AR	3647	-	0,6,6	-	-	-		
84	OHX	AR	3705	-	0,6,6	-	-	-		
84	OHX	AR	3639	-	0,6,6	-	-	-		
84	OHX	6	2042	-	0,6,6	-	-	-		
84	OHX	h	401	-	0,6,6	-	-	-		
84	OHX	6	1940	-	0,6,6	-	-	-		
84	OHX	AR	3619	-	0,6,6	-	-	-		
84	OHX	AR	3502	-	0,6,6	-	-	-		
84	OHX	1	3573	-	0,6,6	-	-	-		
84	OHX	AR	3500	-	0,6,6	-	-	-		
84	OHX	AR	3588	-	0,6,6	-	-	-		
84	OHX	A	1987	-	0,6,6	-	-	-		
84	OHX	AR	3443	-	0,6,6	-	-	-		
84	OHX	1	3577	-	0,6,6	-	-	-		
84	OHX	AR	3671	-	0,6,6	-	-	-		
84	OHX	AT	206	-	0,6,6	-	-	-		
84	OHX	6	1960	-	0,6,6	-	-	-		
84	OHX	AR	3695	-	0,6,6	-	-	-		
84	OHX	AR	3640	-	0,6,6	-	-	-		
84	OHX	1	3591	-	0,6,6	-	-	-		
84	OHX	AR	3673	-	0,6,6	-	-	-		
84	OHX	T	201	-	0,6,6	-	-	-		
84	OHX	DH	201	-	0,6,6	-	-	-		
84	OHX	AR	3423	-	0,6,6	-	-	-		
84	OHX	1	3681	-	0,6,6	-	-	-		
84	OHX	1	3702	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3570	-	0,6,6	-	-	-		
84	OHX	1	3624	-	0,6,6	-	-	-		
84	OHX	v	301	-	0,6,6	-	-	-		
84	OHX	1	3403	-	0,6,6	-	-	-		
84	OHX	A	1996	-	0,6,6	-	-	-		
84	OHX	6	1998	-	0,6,6	-	-	-		
84	OHX	A	2024	-	0,6,6	-	-	-		
84	OHX	1	3710	-	0,6,6	-	-	-		
84	OHX	A	2003	-	0,6,6	-	-	-		
84	OHX	1	3544	-	0,6,6	-	-	-		
84	OHX	AR	3436	-	0,6,6	-	-	-		
84	OHX	6	2022	-	0,6,6	-	-	-		
84	OHX	AR	3631	-	0,6,6	-	-	-		
84	OHX	AR	3546	-	0,6,6	-	-	-		
84	OHX	1	3513	-	0,6,6	-	-	-		
84	OHX	6	1938	-	0,6,6	-	-	-		
84	OHX	AR	3527	-	0,6,6	-	-	-		
84	OHX	AR	3696	-	0,6,6	-	-	-		
84	OHX	1	3415	-	0,6,6	-	-	-		
84	OHX	A	1915	-	0,6,6	-	-	-		
84	OHX	1	3456	-	0,6,6	-	-	-		
84	OHX	1	3632	-	0,6,6	-	-	-		
84	OHX	Q	201	-	0,6,6	-	-	-		
84	OHX	A	1917	-	0,6,6	-	-	-		
84	OHX	A	1901	-	0,6,6	-	-	-		
84	OHX	AR	3622	-	0,6,6	-	-	-		
84	OHX	1	3658	-	0,6,6	-	-	-		
84	OHX	1	3437	-	0,6,6	-	-	-		
84	OHX	1	3507	-	0,6,6	-	-	-		
84	OHX	AR	3528	-	0,6,6	-	-	-		
84	OHX	1	3697	-	0,6,6	-	-	-		
84	OHX	6	1995	-	0,6,6	-	-	-		
84	OHX	AR	3565	-	0,6,6	-	-	-		
84	OHX	AR	3593	-	0,6,6	-	-	-		
84	OHX	A	1923	-	0,6,6	-	-	-		
84	OHX	AR	3412	-	0,6,6	-	-	-		
84	OHX	1	3698	-	0,6,6	-	-	-		
84	OHX	AR	3421	-	0,6,6	-	-	-		
84	OHX	AR	3679	-	0,6,6	-	-	-		
84	OHX	AR	3504	-	0,6,6	-	-	-		
84	OHX	A	2013	-	0,6,6	-	-	-		
84	OHX	1	3622	-	0,6,6	-	-	-		
84	OHX	AR	3577	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3562	-	0,6,6	-	-	-		
84	OHX	AR	3449	-	0,6,6	-	-	-		
84	OHX	1	3605	-	0,6,6	-	-	-		
84	OHX	AR	3433	-	0,6,6	-	-	-		
84	OHX	1	3623	-	0,6,6	-	-	-		
84	OHX	AR	3407	-	0,6,6	-	-	-		
84	OHX	A	1956	-	0,6,6	-	-	-		
84	OHX	6	2046	-	0,6,6	-	-	-		
84	OHX	AE	201	-	0,6,6	-	-	-		
84	OHX	AR	3728	-	0,6,6	-	-	-		
84	OHX	6	2010	-	0,6,6	-	-	-		
84	OHX	1	3595	-	0,6,6	-	-	-		
84	OHX	J	301	-	0,6,6	-	-	-		
84	OHX	1	3621	-	0,6,6	-	-	-		
84	OHX	1	3685	-	0,6,6	-	-	-		
84	OHX	1	3730	-	0,6,6	-	-	-		
84	OHX	6	1975	-	0,6,6	-	-	-		
84	OHX	1	3561	-	0,6,6	-	-	-		
84	OHX	6	2053	-	0,6,6	-	-	-		
84	OHX	A	1947	-	0,6,6	-	-	-		
84	OHX	A	1998	-	0,6,6	-	-	-		
84	OHX	AR	3458	-	0,6,6	-	-	-		
84	OHX	AR	3550	-	0,6,6	-	-	-		
84	OHX	A	1903	-	0,6,6	-	-	-		
84	OHX	1	3499	-	0,6,6	-	-	-		
84	OHX	s8	301	-	0,6,6	-	-	-		
84	OHX	1	3616	-	0,6,6	-	-	-		
84	OHX	1	3695	-	0,6,6	-	-	-		
84	OHX	1	3640	-	0,6,6	-	-	-		
84	OHX	6	1964	-	0,6,6	-	-	-		
84	OHX	AR	3413	-	0,6,6	-	-	-		
84	OHX	6	2020	-	0,6,6	-	-	-		
84	OHX	AR	3430	-	0,6,6	-	-	-		
84	OHX	6	1922	-	0,6,6	-	-	-		
84	OHX	6	2035	-	0,6,6	-	-	-		
84	OHX	AR	3501	-	0,6,6	-	-	-		
84	OHX	AR	3686	-	0,6,6	-	-	-		
84	OHX	AR	3707	-	0,6,6	-	-	-		
84	OHX	AR	3419	-	0,6,6	-	-	-		
84	OHX	1	3470	-	0,6,6	-	-	-		
84	OHX	1	3477	-	0,6,6	-	-	-		
84	OHX	A	1977	-	0,6,6	-	-	-		
84	OHX	A	1941	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3625	-	0,6,6	-	-	-		
84	OHX	AR	3652	-	0,6,6	-	-	-		
84	OHX	AR	3727	-	0,6,6	-	-	-		
84	OHX	6	2055	-	0,6,6	-	-	-		
84	OHX	AT	209	-	0,6,6	-	-	-		
84	OHX	6	1916	-	0,6,6	-	-	-		
84	OHX	1	3425	-	0,6,6	-	-	-		
84	OHX	1	3592	-	0,6,6	-	-	-		
84	OHX	sR	401	-	0,6,6	-	-	-		
84	OHX	6	1927	-	0,6,6	-	-	-		
84	OHX	6	1966	-	0,6,6	-	-	-		
84	OHX	A	1992	-	0,6,6	-	-	-		
84	OHX	6	2047	-	0,6,6	-	-	-		
84	OHX	1	3533	-	0,6,6	-	-	-		
84	OHX	AR	3507	-	0,6,6	-	-	-		
84	OHX	1	3478	-	0,6,6	-	-	-		
84	OHX	AR	3596	-	0,6,6	-	-	-		
84	OHX	A	2033	-	0,6,6	-	-	-		
84	OHX	AR	3453	-	0,6,6	-	-	-		
84	OHX	AT	219	-	0,6,6	-	-	-		
84	OHX	A	1976	-	0,6,6	-	-	-		
84	OHX	A	1945	-	0,6,6	-	-	-		
84	OHX	6	1932	-	0,6,6	-	-	-		
84	OHX	6	1939	-	0,6,6	-	-	-		
84	OHX	AR	3461	-	0,6,6	-	-	-		
84	OHX	AR	3468	-	0,6,6	-	-	-		
84	OHX	AR	3472	-	0,6,6	-	-	-		
84	OHX	1	3438	-	0,6,6	-	-	-		
84	OHX	AR	3530	-	0,6,6	-	-	-		
84	OHX	AR	3594	-	0,6,6	-	-	-		
84	OHX	AR	3630	-	0,6,6	-	-	-		
84	OHX	AR	3736	-	0,6,6	-	-	-		
84	OHX	1	3613	-	0,6,6	-	-	-		
84	OHX	AR	3574	-	0,6,6	-	-	-		
84	OHX	1	3625	-	0,6,6	-	-	-		
84	OHX	AR	3578	-	0,6,6	-	-	-		
84	OHX	AR	3706	-	0,6,6	-	-	-		
84	OHX	3	204	-	0,6,6	-	-	-		
84	OHX	AR	3524	-	0,6,6	-	-	-		
84	OHX	AR	3694	-	0,6,6	-	-	-		
84	OHX	A	1920	-	0,6,6	-	-	-		
84	OHX	AR	3422	-	0,6,6	-	-	-		
84	OHX	1	3474	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3537	-	0,6,6	-	-	-		
84	OHX	AS	207	-	0,6,6	-	-	-		
84	OHX	AR	3439	-	0,6,6	-	-	-		
84	OHX	AR	3690	-	0,6,6	-	-	-		
84	OHX	A	2031	-	0,6,6	-	-	-		
84	OHX	6	1957	-	0,6,6	-	-	-		
84	OHX	AR	3538	-	0,6,6	-	-	-		
84	OHX	A	2000	-	0,6,6	-	-	-		
84	OHX	H	301	-	0,6,6	-	-	-		
84	OHX	AT	211	-	0,6,6	-	-	-		
84	OHX	6	1931	-	0,6,6	-	-	-		
84	OHX	A	1990	-	0,6,6	-	-	-		
84	OHX	1	3560	-	0,6,6	-	-	-		
84	OHX	AR	3554	-	0,6,6	-	-	-		
84	OHX	1	3674	-	0,6,6	-	-	-		
84	OHX	6	2050	-	0,6,6	-	-	-		
84	OHX	6	1953	-	0,6,6	-	-	-		
84	OHX	AR	3714	-	0,6,6	-	-	-		
84	OHX	AR	3634	-	0,6,6	-	-	-		
84	OHX	1	3585	-	0,6,6	-	-	-		
84	OHX	1	3423	-	0,6,6	-	-	-		
84	OHX	AR	3646	-	0,6,6	-	-	-		
84	OHX	A	1991	-	0,6,6	-	-	-		
84	OHX	CE	403	-	0,6,6	-	-	-		
84	OHX	1	3709	-	0,6,6	-	-	-		
84	OHX	AS	202	-	0,6,6	-	-	-		
84	OHX	1	3720	-	0,6,6	-	-	-		
84	OHX	AR	3536	-	0,6,6	-	-	-		
84	OHX	AR	3692	-	0,6,6	-	-	-		
84	OHX	1	3413	-	0,6,6	-	-	-		
84	OHX	1	3686	-	0,6,6	-	-	-		
84	OHX	1	3707	-	0,6,6	-	-	-		
84	OHX	6	1969	-	0,6,6	-	-	-		
84	OHX	AR	3621	-	0,6,6	-	-	-		
84	OHX	AR	3719	-	0,6,6	-	-	-		
84	OHX	AR	3732	-	0,6,6	-	-	-		
84	OHX	AR	3672	-	0,6,6	-	-	-		
84	OHX	A	1940	-	0,6,6	-	-	-		
84	OHX	A	1949	-	0,6,6	-	-	-		
84	OHX	A	1968	-	0,6,6	-	-	-		
84	OHX	2	201	-	0,6,6	-	-	-		
84	OHX	AR	3662	-	0,6,6	-	-	-		
84	OHX	A	2036	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	A	1908	-	0,6,6	-	-	-		
84	OHX	AR	3645	-	0,6,6	-	-	-		
84	OHX	AR	3511	-	0,6,6	-	-	-		
84	OHX	AR	3450	-	0,6,6	-	-	-		
84	OHX	6	1914	-	0,6,6	-	-	-		
84	OHX	AR	3556	-	0,6,6	-	-	-		
84	OHX	1	3464	-	0,6,6	-	-	-		
84	OHX	1	3542	-	0,6,6	-	-	-		
84	OHX	1	3672	-	0,6,6	-	-	-		
84	OHX	CZ	201	-	0,6,6	-	-	-		
84	OHX	1	3424	-	0,6,6	-	-	-		
84	OHX	1	3541	-	0,6,6	-	-	-		
84	OHX	A	1983	-	0,6,6	-	-	-		
84	OHX	AR	3560	-	0,6,6	-	-	-		
84	OHX	A	1906	-	0,6,6	-	-	-		
84	OHX	1	3662	-	0,6,6	-	-	-		
84	OHX	1	3724	-	0,6,6	-	-	-		
84	OHX	6	1942	-	0,6,6	-	-	-		
84	OHX	A	1904	-	0,6,6	-	-	-		
84	OHX	AR	3404	-	0,6,6	-	-	-		
84	OHX	1	3476	-	0,6,6	-	-	-		
84	OHX	AR	3688	-	0,6,6	-	-	-		
84	OHX	AR	3405	-	0,6,6	-	-	-		
84	OHX	AR	3512	-	0,6,6	-	-	-		
84	OHX	1	3497	-	0,6,6	-	-	-		
84	OHX	AR	3485	-	0,6,6	-	-	-		
84	OHX	1	3472	-	0,6,6	-	-	-		
84	OHX	A	1959	-	0,6,6	-	-	-		
84	OHX	1	3630	-	0,6,6	-	-	-		
84	OHX	1	3574	-	0,6,6	-	-	-		
84	OHX	1	3524	-	0,6,6	-	-	-		
84	OHX	1	3523	-	0,6,6	-	-	-		
84	OHX	1	3728	-	0,6,6	-	-	-		
84	OHX	1	3538	-	0,6,6	-	-	-		
84	OHX	1	3480	-	0,6,6	-	-	-		
84	OHX	A	1980	-	0,6,6	-	-	-		
84	OHX	AT	214	-	0,6,6	-	-	-		
84	OHX	1	3669	-	0,6,6	-	-	-		
84	OHX	1	3708	-	0,6,6	-	-	-		
84	OHX	1	3589	-	0,6,6	-	-	-		
84	OHX	AR	3415	-	0,6,6	-	-	-		
84	OHX	AR	3585	-	0,6,6	-	-	-		
84	OHX	6	1903	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	1943	-	0,6,6	-	-	-		
84	OHX	1	3440	-	0,6,6	-	-	-		
84	OHX	6	2015	-	0,6,6	-	-	-		
84	OHX	6	1915	-	0,6,6	-	-	-		
84	OHX	1	3435	-	0,6,6	-	-	-		
84	OHX	AR	3557	-	0,6,6	-	-	-		
84	OHX	AR	3427	-	0,6,6	-	-	-		
84	OHX	1	3545	-	0,6,6	-	-	-		
84	OHX	AR	3597	-	0,6,6	-	-	-		
84	OHX	A	2025	-	0,6,6	-	-	-		
84	OHX	1	3689	-	0,6,6	-	-	-		
84	OHX	6	1971	-	0,6,6	-	-	-		
84	OHX	1	3526	-	0,6,6	-	-	-		
84	OHX	AR	3712	-	0,6,6	-	-	-		
84	OHX	1	3633	-	0,6,6	-	-	-		
84	OHX	1	3646	-	0,6,6	-	-	-		
84	OHX	6	1986	-	0,6,6	-	-	-		
84	OHX	AR	3579	-	0,6,6	-	-	-		
84	OHX	1	3520	-	0,6,6	-	-	-		
84	OHX	AR	3655	-	0,6,6	-	-	-		
84	OHX	AG	201	-	0,6,6	-	-	-		
84	OHX	1	3725	-	0,6,6	-	-	-		
84	OHX	1	3719	-	0,6,6	-	-	-		
84	OHX	1	3567	-	0,6,6	-	-	-		
84	OHX	AR	3464	-	0,6,6	-	-	-		
84	OHX	6	1996	-	0,6,6	-	-	-		
84	OHX	CG	302	-	0,6,6	-	-	-		
84	OHX	1	3433	-	0,6,6	-	-	-		
84	OHX	AR	3687	-	0,6,6	-	-	-		
84	OHX	AR	3653	-	0,6,6	-	-	-		
84	OHX	1	3716	-	0,6,6	-	-	-		
84	OHX	AS	209	-	0,6,6	-	-	-		
84	OHX	1	3682	-	0,6,6	-	-	-		
84	OHX	6	1910	-	0,6,6	-	-	-		
84	OHX	1	3644	-	0,6,6	-	-	-		
84	OHX	1	3453	-	0,6,6	-	-	-		
84	OHX	1	3583	-	0,6,6	-	-	-		
84	OHX	AR	3425	-	0,6,6	-	-	-		
84	OHX	A	1958	-	0,6,6	-	-	-		
84	OHX	CF	402	-	0,6,6	-	-	-		
84	OHX	1	3536	-	0,6,6	-	-	-		
84	OHX	3	201	-	0,6,6	-	-	-		
84	OHX	AR	3488	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	1936	-	0,6,6	-	-	-		
84	OHX	6	1945	-	0,6,6	-	-	-		
84	OHX	4	202	-	0,6,6	-	-	-		
84	OHX	AR	3451	-	0,6,6	-	-	-		
84	OHX	AT	213	-	0,6,6	-	-	-		
84	OHX	1	3412	-	0,6,6	-	-	-		
84	OHX	A	2020	-	0,6,6	-	-	-		
84	OHX	1	3680	-	0,6,6	-	-	-		
84	OHX	1	3704	-	0,6,6	-	-	-		
84	OHX	AR	3539	-	0,6,6	-	-	-		
84	OHX	AR	3462	-	0,6,6	-	-	-		
86	7MB	AR	4239	-	20,23,23	0.90	1 (5%)	18,38,38	0.79	1 (5%)
84	OHX	AR	3489	-	0,6,6	-	-	-		
84	OHX	1	3548	-	0,6,6	-	-	-		
84	OHX	AS	203	-	0,6,6	-	-	-		
84	OHX	6	1978	-	0,6,6	-	-	-		
84	OHX	6	1947	-	0,6,6	-	-	-		
84	OHX	AR	3480	-	0,6,6	-	-	-		
84	OHX	AR	3523	-	0,6,6	-	-	-		
84	OHX	6	1983	-	0,6,6	-	-	-		
84	OHX	AR	3440	-	0,6,6	-	-	-		
84	OHX	AR	3684	-	0,6,6	-	-	-		
84	OHX	A	1989	-	0,6,6	-	-	-		
84	OHX	1	3432	-	0,6,6	-	-	-		
84	OHX	1	3485	-	0,6,6	-	-	-		
84	OHX	AR	3726	-	0,6,6	-	-	-		
84	OHX	AR	3572	-	0,6,6	-	-	-		
84	OHX	1	3581	-	0,6,6	-	-	-		
84	OHX	A	1928	-	0,6,6	-	-	-		
84	OHX	1	3652	-	0,6,6	-	-	-		
84	OHX	A	1963	-	0,6,6	-	-	-		
84	OHX	A	1926	-	0,6,6	-	-	-		
84	OHX	A	2010	-	0,6,6	-	-	-		
84	OHX	1	3699	-	0,6,6	-	-	-		
84	OHX	1	3457	-	0,6,6	-	-	-		
84	OHX	1	3448	-	0,6,6	-	-	-		
84	OHX	1	3436	-	0,6,6	-	-	-		
84	OHX	AR	3663	-	0,6,6	-	-	-		
84	OHX	4	208	-	0,6,6	-	-	-		
84	OHX	1	3529	-	0,6,6	-	-	-		
84	OHX	AR	3526	-	0,6,6	-	-	-		
84	OHX	6	1961	-	0,6,6	-	-	-		
84	OHX	A	1975	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3554	-	0,6,6	-	-	-		
84	OHX	6	2027	-	0,6,6	-	-	-		
84	OHX	AR	3730	-	0,6,6	-	-	-		
84	OHX	A	1942	-	0,6,6	-	-	-		
84	OHX	AR	3668	-	0,6,6	-	-	-		
84	OHX	AR	3711	-	0,6,6	-	-	-		
84	OHX	A	2019	-	0,6,6	-	-	-		
84	OHX	1	3612	-	0,6,6	-	-	-		
84	OHX	A	1931	-	0,6,6	-	-	-		
84	OHX	A	1933	-	0,6,6	-	-	-		
84	OHX	1	3498	-	0,6,6	-	-	-		
84	OHX	6	1991	-	0,6,6	-	-	-		
84	OHX	AT	216	-	0,6,6	-	-	-		
84	OHX	c5	201	-	0,6,6	-	-	-		
84	OHX	AR	3633	-	0,6,6	-	-	-		
84	OHX	AR	3408	-	0,6,6	-	-	-		
84	OHX	A	1914	-	0,6,6	-	-	-		
84	OHX	AR	3674	-	0,6,6	-	-	-		
84	OHX	6	2033	-	0,6,6	-	-	-		
84	OHX	6	2012	-	0,6,6	-	-	-		
84	OHX	AS	201	-	0,6,6	-	-	-		
84	OHX	1	3717	-	0,6,6	-	-	-		
84	OHX	1	3518	-	0,6,6	-	-	-		
84	OHX	6	2025	-	0,6,6	-	-	-		
84	OHX	1	3666	-	0,6,6	-	-	-		
84	OHX	6	2017	-	0,6,6	-	-	-		
84	OHX	6	1988	-	0,6,6	-	-	-		
84	OHX	AR	3470	-	0,6,6	-	-	-		
84	OHX	AR	3564	-	0,6,6	-	-	-		
84	OHX	O	201	-	0,6,6	-	-	-		
84	OHX	4	209	-	0,6,6	-	-	-		
86	7MB	1	4216	-	20,23,23	1.61	3 (15%)	18,38,38	1.18	1 (5%)
84	OHX	AR	3629	-	0,6,6	-	-	-		
84	OHX	6	2006	-	0,6,6	-	-	-		
84	OHX	AR	3724	-	0,6,6	-	-	-		
84	OHX	6	1967	-	0,6,6	-	-	-		
84	OHX	A	2026	-	0,6,6	-	-	-		
84	OHX	AT	202	-	0,6,6	-	-	-		
84	OHX	1	3421	-	0,6,6	-	-	-		
84	OHX	6	1935	-	0,6,6	-	-	-		
84	OHX	6	1944	-	0,6,6	-	-	-		
84	OHX	1	3564	-	0,6,6	-	-	-		
84	OHX	1	3588	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3626	-	0,6,6	-	-	-		
84	OHX	AR	3731	-	0,6,6	-	-	-		
84	OHX	A	1953	-	0,6,6	-	-	-		
84	OHX	6	2039	-	0,6,6	-	-	-		
84	OHX	1	3580	-	0,6,6	-	-	-		
84	OHX	1	3641	-	0,6,6	-	-	-		
84	OHX	6	1951	-	0,6,6	-	-	-		
84	OHX	6	1925	-	0,6,6	-	-	-		
84	OHX	6	2037	-	0,6,6	-	-	-		
84	OHX	1	3461	-	0,6,6	-	-	-		
84	OHX	3	205	-	0,6,6	-	-	-		
84	OHX	1	3468	-	0,6,6	-	-	-		
84	OHX	AP	502	-	0,6,6	-	-	-		
84	OHX	1	3608	-	0,6,6	-	-	-		
84	OHX	6	1990	-	0,6,6	-	-	-		
84	OHX	AR	3576	-	0,6,6	-	-	-		
84	OHX	1	3727	-	0,6,6	-	-	-		
84	OHX	6	1911	-	0,6,6	-	-	-		
84	OHX	AR	3654	-	0,6,6	-	-	-		
84	OHX	AR	3729	-	0,6,6	-	-	-		
84	OHX	1	3430	-	0,6,6	-	-	-		
84	OHX	6	2008	-	0,6,6	-	-	-		
84	OHX	AR	3540	-	0,6,6	-	-	-		
84	OHX	6	1950	-	0,6,6	-	-	-		
84	OHX	6	2009	-	0,6,6	-	-	-		
84	OHX	AR	3584	-	0,6,6	-	-	-		
84	OHX	AR	3457	-	0,6,6	-	-	-		
84	OHX	1	3665	-	0,6,6	-	-	-		
84	OHX	AR	3444	-	0,6,6	-	-	-		
84	OHX	1	3643	-	0,6,6	-	-	-		
84	OHX	AR	3460	-	0,6,6	-	-	-		
84	OHX	1	3416	-	0,6,6	-	-	-		
84	OHX	AR	3531	-	0,6,6	-	-	-		
84	OHX	A	2004	-	0,6,6	-	-	-		
84	OHX	A	1946	-	0,6,6	-	-	-		
84	OHX	1	3693	-	0,6,6	-	-	-		
84	OHX	1	3550	-	0,6,6	-	-	-		
84	OHX	AR	3414	-	0,6,6	-	-	-		
84	OHX	AR	3514	-	0,6,6	-	-	-		
84	OHX	AR	3428	-	0,6,6	-	-	-		
84	OHX	1	3419	-	0,6,6	-	-	-		
84	OHX	6	2036	-	0,6,6	-	-	-		
84	OHX	1	3418	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3647	-	0,6,6	-	-	-		
84	OHX	AR	3484	-	0,6,6	-	-	-		
84	OHX	x	201	-	0,6,6	-	-	-		
84	OHX	CX	201	-	0,6,6	-	-	-		
84	OHX	1	3502	-	0,6,6	-	-	-		
84	OHX	1	3500	-	0,6,6	-	-	-		
84	OHX	CL	301	-	0,6,6	-	-	-		
84	OHX	1	3664	-	0,6,6	-	-	-		
84	OHX	AR	3725	-	0,6,6	-	-	-		
84	OHX	1	3594	-	0,6,6	-	-	-		
84	OHX	A	2007	-	0,6,6	-	-	-		
84	OHX	6	1981	-	0,6,6	-	-	-		
84	OHX	1	3671	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	7MB	AR	4239	-	-	-	0/4/4/4
86	7MB	1	4216	-	-	-	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	4216	7MB	C8-C7	-4.55	1.37	1.47
86	1	4216	7MB	C9-C8	-2.98	1.35	1.42
86	1	4216	7MB	O-C1	-2.30	1.19	1.23
86	AR	4239	7MB	C8-C7	-2.17	1.42	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	4216	7MB	C6-C2-N1	-2.99	108.36	113.28
86	AR	4239	7MB	C-N-C1	2.63	126.13	122.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

551 monomers are involved in 797 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	DL	102	OHX	1	0
84	AR	3435	OHX	1	0
84	AR	3650	OHX	2	0
84	AR	3545	OHX	1	0
84	1	3422	OHX	2	0
84	AR	3534	OHX	1	0
84	6	2007	OHX	1	0
84	1	3618	OHX	3	0
84	AR	3522	OHX	1	0
84	6	1965	OHX	1	0
84	1	3547	OHX	1	0
84	1	3428	OHX	2	0
84	1	401	OHX	2	0
84	6	1968	OHX	1	0
84	AR	3456	OHX	3	0
84	AR	3641	OHX	1	0
84	AT	220	OHX	1	0
84	AR	3454	OHX	2	0
84	A	2030	OHX	3	0
84	A	2008	OHX	2	0
84	DL	101	OHX	1	0
84	AR	3661	OHX	2	0
84	1	3631	OHX	1	0
84	1	3688	OHX	1	0
84	AR	3508	OHX	1	0
84	AR	3515	OHX	2	0
84	AR	3401	OHX	1	0
84	AR	3575	OHX	1	0
84	A	1986	OHX	1	0
84	AR	3568	OHX	3	0
84	1	3465	OHX	1	0
84	1	3634	OHX	1	0
84	AR	3643	OHX	3	0
84	AR	3517	OHX	1	0
84	AR	3586	OHX	1	0
84	1	3527	OHX	1	0
84	1	3516	OHX	1	0
84	1	3540	OHX	2	0
84	AR	3635	OHX	1	0
84	6	1912	OHX	1	0
84	AR	3601	OHX	2	0
84	A	2021	OHX	2	0
84	AR	3689	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	A	1919	OHX	1	0
84	k	401	OHX	1	0
84	6	2005	OHX	2	0
84	A	2035	OHX	2	0
84	1	3657	OHX	1	0
84	6	1955	OHX	1	0
84	6	1958	OHX	1	0
84	A	1970	OHX	3	0
84	A	1971	OHX	1	0
84	AR	3505	OHX	1	0
84	A	2009	OHX	2	0
84	6	1918	OHX	1	0
84	AR	3518	OHX	2	0
84	6	1913	OHX	1	0
84	6	1952	OHX	2	0
84	AR	3592	OHX	1	0
84	AR	3567	OHX	2	0
84	4	204	OHX	1	0
84	x	202	OHX	1	0
84	AR	3469	OHX	3	0
84	AR	3691	OHX	1	0
84	1	3537	OHX	1	0
84	1	3406	OHX	5	0
84	AT	218	OHX	1	0
84	CK	201	OHX	1	0
84	6	1924	OHX	1	0
84	AR	3657	OHX	1	0
84	1	3617	OHX	1	0
84	6	1970	OHX	1	0
84	6	2044	OHX	1	0
84	1	3401	OHX	1	0
84	1	3597	OHX	1	0
84	1	3713	OHX	1	0
84	6	1997	OHX	1	0
84	AR	3620	OHX	1	0
84	AT	212	OHX	1	0
84	A	1909	OHX	3	0
84	AR	3490	OHX	2	0
84	AR	3701	OHX	2	0
84	1	3578	OHX	1	0
84	1	3410	OHX	2	0
84	M	201	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3535	OHX	2	0
84	1	3587	OHX	1	0
84	A	2023	OHX	1	0
84	AR	3715	OHX	2	0
84	6	1963	OHX	1	0
84	A	2027	OHX	1	0
84	AR	3604	OHX	4	0
84	6	1993	OHX	2	0
84	6	1977	OHX	1	0
84	A	1916	OHX	1	0
84	1	3408	OHX	2	0
84	AR	3532	OHX	1	0
84	A	1937	OHX	1	0
84	AR	3607	OHX	1	0
84	AR	3441	OHX	1	0
84	A	1918	OHX	1	0
84	6	2028	OHX	1	0
84	6	2000	OHX	2	0
84	AR	3493	OHX	1	0
84	6	1976	OHX	2	0
84	1	3539	OHX	1	0
84	1	3667	OHX	1	0
84	A	2037	OHX	1	0
84	AR	3432	OHX	2	0
84	A	1907	OHX	1	0
84	AR	3685	OHX	1	0
84	e	101	OHX	2	0
84	AR	3713	OHX	1	0
84	AR	3442	OHX	2	0
84	AR	3410	OHX	2	0
84	AR	3548	OHX	2	0
84	AR	3678	OHX	1	0
84	A	2029	OHX	1	0
84	AR	3418	OHX	2	0
84	AR	3700	OHX	2	0
84	AR	3481	OHX	1	0
84	A	1961	OHX	1	0
84	A	1939	OHX	3	0
84	AR	3429	OHX	1	0
84	1	3579	OHX	1	0
84	6	1979	OHX	1	0
84	c3	201	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3708	OHX	1	0
84	4	211	OHX	1	0
84	AR	3656	OHX	1	0
84	1	3402	OHX	1	0
84	1	3495	OHX	1	0
84	1	3553	OHX	1	0
84	A	1955	OHX	2	0
84	AR	3683	OHX	3	0
84	A	1912	OHX	2	0
84	1	3404	OHX	1	0
84	6	1930	OHX	1	0
84	1	3677	OHX	1	0
84	A	1944	OHX	3	0
84	6	1921	OHX	1	0
84	AR	3542	OHX	2	0
84	3	203	OHX	1	0
84	1	3712	OHX	2	0
84	6	1926	OHX	1	0
84	6	1934	OHX	1	0
84	A	1913	OHX	1	0
84	A	1925	OHX	3	0
84	1	3654	OHX	2	0
84	AR	3473	OHX	1	0
84	1	3496	OHX	6	0
84	1	3687	OHX	1	0
84	6	2021	OHX	1	0
84	AR	3603	OHX	2	0
84	AR	3571	OHX	1	0
84	3	202	OHX	1	0
84	6	1999	OHX	2	0
84	4	206	OHX	1	0
84	6	2013	OHX	1	0
84	1	3414	OHX	2	0
84	6	2018	OHX	1	0
84	1	3610	OHX	1	0
84	A	1943	OHX	2	0
84	4	203	OHX	1	0
84	AT	208	OHX	1	0
84	1	3409	OHX	1	0
84	1	3572	OHX	3	0
84	AR	3611	OHX	1	0
84	1	3454	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	A	1984	OHX	1	0
84	AR	3549	OHX	1	0
84	AR	3476	OHX	1	0
84	1	3534	OHX	2	0
84	6	1901	OHX	1	0
84	AT	205	OHX	2	0
84	AR	3420	OHX	1	0
84	1	3514	OHX	2	0
84	A	1965	OHX	1	0
84	AR	3573	OHX	1	0
84	1	3663	OHX	1	0
84	AR	3720	OHX	1	0
84	CM	201	OHX	1	0
84	AR	3582	OHX	2	0
84	A	1981	OHX	1	0
84	AR	3613	OHX	1	0
84	AR	3628	OHX	1	0
84	1	3661	OHX	1	0
84	6	1902	OHX	1	0
84	1	3556	OHX	1	0
84	AR	3563	OHX	1	0
84	1	3427	OHX	1	0
84	1	3530	OHX	1	0
84	AR	3709	OHX	1	0
84	AR	3624	OHX	1	0
84	1	3668	OHX	2	0
84	AC	101	OHX	1	0
84	AR	3723	OHX	1	0
84	A	2038	OHX	2	0
84	1	3494	OHX	1	0
84	1	3558	OHX	2	0
84	A	1954	OHX	4	0
84	A	1962	OHX	1	0
84	AR	3478	OHX	2	0
84	AR	3614	OHX	1	0
84	AR	3598	OHX	1	0
84	AT	210	OHX	1	0
84	AR	3483	OHX	1	0
84	6	1973	OHX	3	0
84	1	3691	OHX	1	0
84	AR	3519	OHX	1	0
84	1	3505	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3482	OHX	2	0
84	6	1904	OHX	1	0
84	6	1956	OHX	3	0
84	AR	3591	OHX	1	0
84	A	1951	OHX	1	0
84	AR	3615	OHX	1	0
84	1	3676	OHX	2	0
84	6	1985	OHX	1	0
84	DI	201	OHX	1	0
84	A	2041	OHX	1	0
84	AR	3595	OHX	2	0
84	A	1902	OHX	1	0
84	A	1910	OHX	2	0
84	AR	3466	OHX	1	0
84	1	3515	OHX	1	0
84	1	3420	OHX	2	0
84	AT	203	OHX	3	0
84	AR	3474	OHX	1	0
84	AR	3589	OHX	1	0
84	AR	3721	OHX	2	0
84	1	3450	OHX	2	0
84	A	1911	OHX	1	0
84	1	3503	OHX	1	0
84	AR	3739	OHX	2	0
84	1	3504	OHX	2	0
84	1	3628	OHX	1	0
84	1	3563	OHX	1	0
84	1	3690	OHX	1	0
84	A	1997	OHX	1	0
84	AR	3417	OHX	2	0
84	A	2022	OHX	1	0
84	A	1932	OHX	2	0
84	1	3582	OHX	3	0
84	A	1938	OHX	2	0
84	1	3459	OHX	1	0
84	A	2012	OHX	1	0
84	1	3639	OHX	1	0
84	A	1985	OHX	1	0
84	A	1988	OHX	3	0
84	AR	3409	OHX	1	0
84	AR	3682	OHX	1	0
84	1	3596	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	r	301	OHX	1	0
84	3	206	OHX	2	0
84	A	2005	OHX	1	0
84	AR	3552	OHX	1	0
84	AR	3509	OHX	2	0
84	AS	204	OHX	1	0
84	1	3614	OHX	1	0
84	1	3491	OHX	1	0
84	1	3598	OHX	1	0
84	6	1994	OHX	3	0
84	AR	3499	OHX	1	0
84	1	3568	OHX	1	0
84	6	1982	OHX	3	0
84	AR	3455	OHX	1	0
84	6	1908	OHX	1	0
84	AK	102	OHX	2	0
84	6	2045	OHX	2	0
84	1	3493	OHX	1	0
84	1	3511	OHX	1	0
84	AR	3492	OHX	1	0
84	A	1948	OHX	1	0
84	AR	3649	OHX	1	0
84	1	3466	OHX	1	0
84	1	3619	OHX	1	0
84	k	402	OHX	2	0
84	AR	3697	OHX	3	0
84	AR	3658	OHX	1	0
84	1	3486	OHX	1	0
84	1	3650	OHX	1	0
84	6	2011	OHX	1	0
84	AR	3459	OHX	1	0
84	1	3637	OHX	1	0
84	1	3442	OHX	1	0
84	CF	401	OHX	1	0
84	1	3684	OHX	1	0
84	A	1964	OHX	3	0
84	A	1922	OHX	1	0
84	6	2038	OHX	1	0
84	1	3463	OHX	1	0
84	1	3586	OHX	2	0
84	1	3522	OHX	1	0
84	AR	3737	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	6	2043	OHX	3	0
84	AR	3437	OHX	2	0
84	1	3521	OHX	1	0
84	4	212	OHX	1	0
84	1	3714	OHX	1	0
84	1	3471	OHX	4	0
84	1	3447	OHX	2	0
84	AR	3608	OHX	1	0
84	AR	3735	OHX	1	0
84	1	3446	OHX	1	0
84	1	3552	OHX	1	0
84	6	1980	OHX	1	0
84	1	3506	OHX	1	0
84	AR	3403	OHX	1	0
84	1	3629	OHX	1	0
84	AR	3606	OHX	3	0
84	1	3603	OHX	2	0
84	6	2040	OHX	1	0
84	AR	3580	OHX	2	0
84	A	2034	OHX	1	0
84	AR	3416	OHX	2	0
84	AR	3448	OHX	1	0
84	CV	201	OHX	1	0
84	6	1992	OHX	1	0
84	A	1905	OHX	1	0
84	A	1973	OHX	2	0
84	1	3546	OHX	1	0
84	1	3604	OHX	1	0
84	1	3696	OHX	1	0
84	1	3441	OHX	1	0
84	6	1906	OHX	1	0
84	1	3722	OHX	1	0
84	A	1999	OHX	1	0
84	AR	3521	OHX	1	0
84	CE	402	OHX	2	0
84	AR	3623	OHX	1	0
84	6	2030	OHX	1	0
84	A	1974	OHX	2	0
84	1	3444	OHX	1	0
84	AR	3516	OHX	1	0
84	1	3405	OHX	2	0
84	1	3656	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	A	1993	OHX	1	0
84	1	3565	OHX	1	0
84	AR	3647	OHX	1	0
84	AR	3619	OHX	2	0
84	AR	3500	OHX	2	0
84	A	1987	OHX	1	0
84	AR	3443	OHX	7	0
84	1	3577	OHX	2	0
84	AR	3671	OHX	2	0
84	AT	206	OHX	1	0
84	AR	3640	OHX	1	0
84	T	201	OHX	1	0
84	AR	3423	OHX	1	0
84	1	3681	OHX	1	0
84	1	3702	OHX	4	0
84	AR	3570	OHX	1	0
84	1	3624	OHX	1	0
84	v	301	OHX	1	0
84	1	3403	OHX	1	0
84	A	2024	OHX	2	0
84	A	2003	OHX	1	0
84	1	3544	OHX	1	0
84	AR	3631	OHX	1	0
84	1	3513	OHX	1	0
84	AR	3527	OHX	2	0
84	AR	3696	OHX	3	0
84	1	3415	OHX	2	0
84	A	1915	OHX	2	0
84	1	3632	OHX	1	0
84	Q	201	OHX	2	0
84	A	1917	OHX	1	0
84	A	1901	OHX	1	0
84	1	3437	OHX	2	0
84	1	3507	OHX	1	0
84	6	1995	OHX	1	0
84	A	1923	OHX	1	0
84	1	3698	OHX	2	0
84	AR	3421	OHX	1	0
84	AR	3504	OHX	3	0
84	AR	3449	OHX	1	0
84	1	3605	OHX	1	0
84	AR	3407	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	A	1956	OHX	1	0
84	AE	201	OHX	4	0
84	AR	3728	OHX	1	0
84	1	3595	OHX	1	0
84	1	3730	OHX	3	0
84	A	1947	OHX	1	0
84	A	1998	OHX	2	0
84	AR	3550	OHX	2	0
84	1	3616	OHX	1	0
84	AR	3413	OHX	1	0
84	6	1922	OHX	1	0
84	6	2035	OHX	1	0
84	AR	3707	OHX	1	0
84	AR	3652	OHX	1	0
84	AR	3727	OHX	1	0
84	6	2055	OHX	1	0
84	6	1927	OHX	3	0
84	A	1992	OHX	3	0
84	6	2047	OHX	1	0
84	AR	3507	OHX	2	0
84	1	3478	OHX	2	0
84	AR	3596	OHX	1	0
84	AR	3453	OHX	1	0
84	AT	219	OHX	1	0
84	6	1932	OHX	1	0
84	6	1939	OHX	1	0
84	AR	3461	OHX	1	0
84	AR	3468	OHX	1	0
84	AR	3472	OHX	1	0
84	1	3438	OHX	2	0
84	AR	3530	OHX	1	0
84	AR	3594	OHX	1	0
84	AR	3630	OHX	2	0
84	AR	3736	OHX	1	0
84	1	3613	OHX	1	0
84	AR	3574	OHX	1	0
84	AR	3578	OHX	1	0
84	AR	3706	OHX	1	0
84	AR	3524	OHX	3	0
84	A	1920	OHX	1	0
84	1	3474	OHX	1	0
84	AR	3439	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3690	OHX	2	0
84	6	1957	OHX	1	0
84	AR	3538	OHX	1	0
84	A	2000	OHX	1	0
84	AT	211	OHX	2	0
84	A	1990	OHX	1	0
84	1	3674	OHX	1	0
84	6	2050	OHX	3	0
84	6	1953	OHX	2	0
84	1	3585	OHX	1	0
84	AR	3646	OHX	1	0
84	1	3709	OHX	1	0
84	AS	202	OHX	2	0
84	1	3720	OHX	1	0
84	AR	3536	OHX	2	0
84	1	3413	OHX	2	0
84	6	1969	OHX	1	0
84	A	1968	OHX	1	0
84	AR	3645	OHX	1	0
84	AR	3511	OHX	2	0
84	6	1914	OHX	1	0
84	AR	3556	OHX	1	0
84	1	3542	OHX	2	0
84	1	3672	OHX	2	0
84	1	3541	OHX	1	0
84	A	1983	OHX	1	0
84	AR	3560	OHX	1	0
84	1	3662	OHX	1	0
84	1	3724	OHX	1	0
84	6	1942	OHX	2	0
84	A	1904	OHX	1	0
84	AR	3512	OHX	2	0
84	1	3497	OHX	1	0
84	AR	3485	OHX	1	0
84	1	3472	OHX	1	0
84	A	1959	OHX	1	0
84	1	3524	OHX	1	0
84	1	3523	OHX	1	0
84	1	3538	OHX	2	0
84	AT	214	OHX	2	0
84	1	3669	OHX	1	0
84	1	3440	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	6	1915	OHX	3	0
84	AR	3427	OHX	1	0
84	A	2025	OHX	1	0
84	1	3689	OHX	2	0
84	AR	3712	OHX	1	0
84	1	3646	OHX	1	0
84	6	1986	OHX	3	0
84	1	3725	OHX	3	0
84	1	3567	OHX	1	0
84	CG	302	OHX	4	0
84	1	3433	OHX	2	0
84	AS	209	OHX	2	0
84	1	3682	OHX	2	0
84	6	1910	OHX	2	0
84	1	3644	OHX	1	0
84	1	3453	OHX	1	0
84	AR	3425	OHX	2	0
84	1	3536	OHX	1	0
84	3	201	OHX	1	0
84	6	1945	OHX	3	0
84	4	202	OHX	1	0
84	AT	213	OHX	1	0
84	AR	3462	OHX	1	0
86	AR	4239	7MB	3	0
84	1	3548	OHX	1	0
84	AS	203	OHX	1	0
84	6	1978	OHX	1	0
84	AR	3480	OHX	1	0
84	AR	3440	OHX	2	0
84	AR	3684	OHX	1	0
84	1	3485	OHX	1	0
84	A	1928	OHX	2	0
84	A	1963	OHX	1	0
84	A	2010	OHX	1	0
84	1	3448	OHX	2	0
84	1	3529	OHX	1	0
84	AR	3526	OHX	2	0
84	6	1961	OHX	1	0
84	1	3554	OHX	1	0
84	A	2019	OHX	1	0
84	1	3612	OHX	1	0
84	A	1931	OHX	1	0

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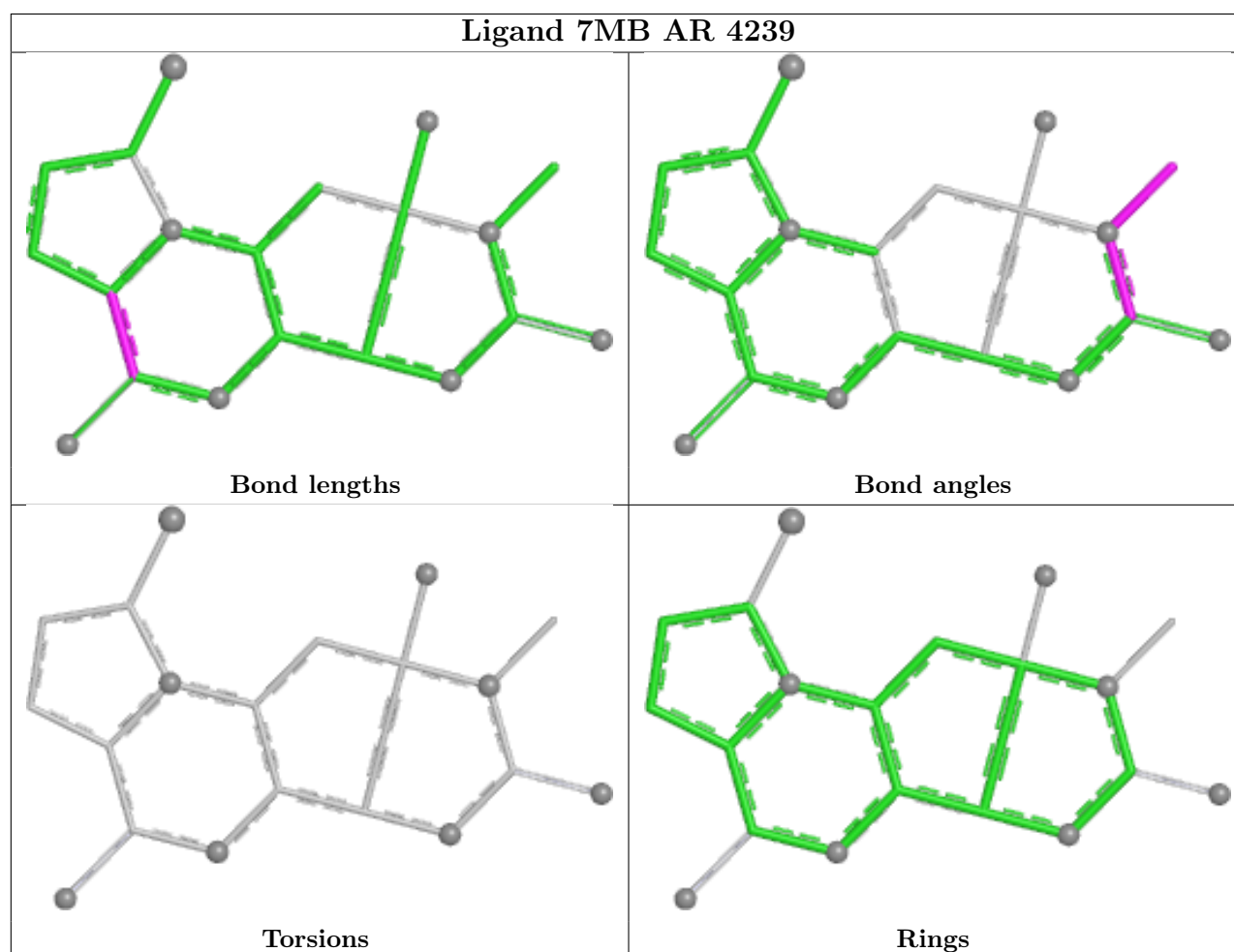
Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	A	1933	OHX	1	0
84	6	1991	OHX	1	0
84	c5	201	OHX	3	0
84	AR	3408	OHX	2	0
84	A	1914	OHX	2	0
84	AR	3674	OHX	1	0
84	6	2033	OHX	1	0
84	6	2012	OHX	1	0
84	AS	201	OHX	1	0
84	1	3717	OHX	1	0
84	1	3666	OHX	2	0
84	6	2017	OHX	1	0
84	AR	3470	OHX	1	0
84	O	201	OHX	1	0
84	4	209	OHX	1	0
86	1	4216	7MB	4	0
84	6	2006	OHX	1	0
84	A	2026	OHX	2	0
84	AT	202	OHX	1	0
84	1	3588	OHX	1	0
84	AR	3731	OHX	6	0
84	6	2039	OHX	1	0
84	1	3641	OHX	1	0
84	6	2037	OHX	2	0
84	1	3461	OHX	1	0
84	AP	502	OHX	3	0
84	6	1911	OHX	2	0
84	1	3430	OHX	2	0
84	6	2008	OHX	2	0
84	6	2009	OHX	1	0
84	AR	3457	OHX	2	0
84	1	3665	OHX	2	0
84	AR	3444	OHX	1	0
84	AR	3460	OHX	1	0
84	1	3416	OHX	2	0
84	AR	3531	OHX	1	0
84	A	2004	OHX	1	0
84	AR	3514	OHX	1	0
84	1	3419	OHX	2	0
84	AR	3484	OHX	2	0
84	x	201	OHX	2	0
84	1	3502	OHX	3	0

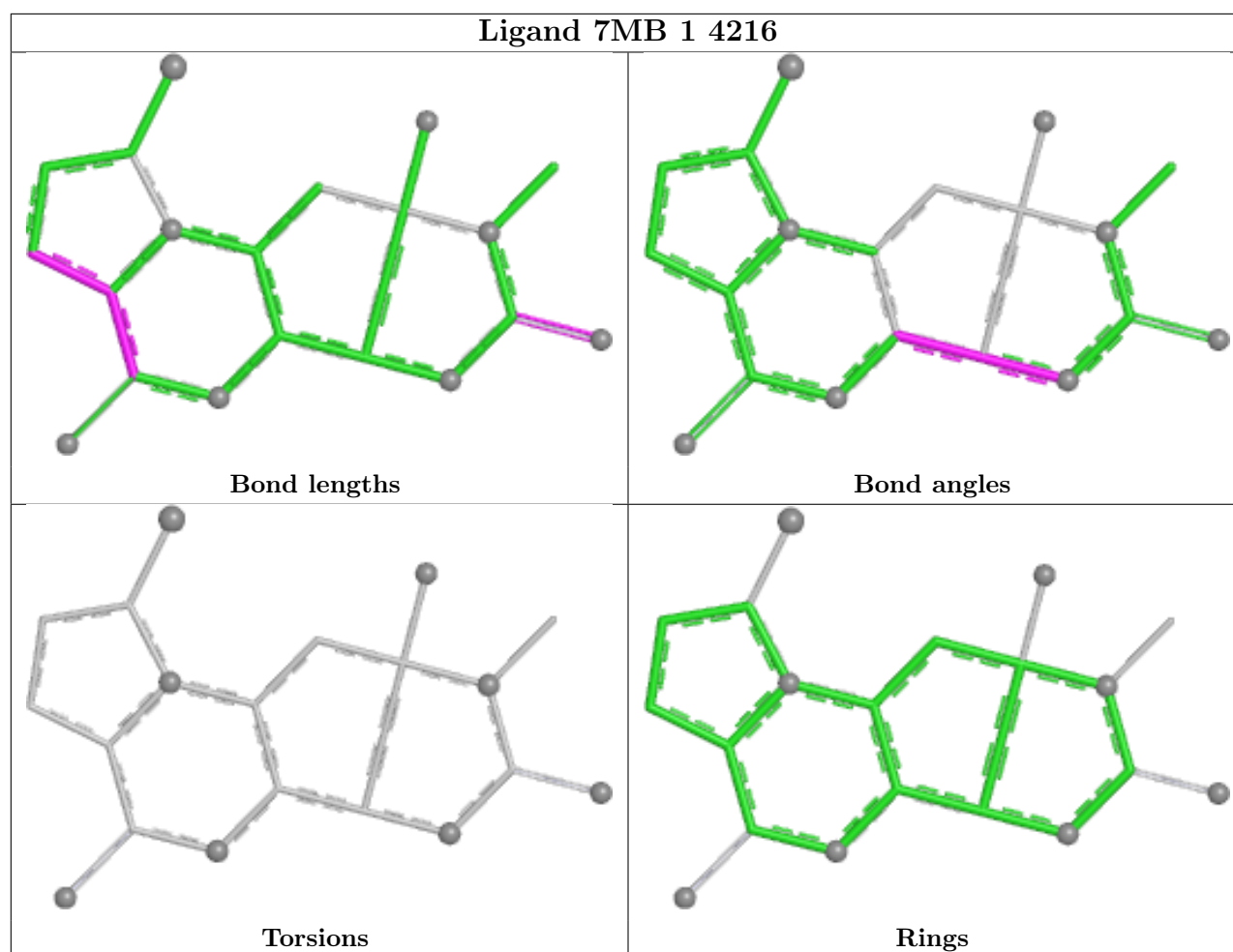
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3500	OHX	1	0
84	CL	301	OHX	2	0
84	1	3594	OHX	4	0
84	6	1981	OHX	1	0

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
25	A	1

All 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	44.36
1	sM	139:UNK	C	155:UNK	N	36.85
1	A	1716:C	O3'	1717:G	P	4.45

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%)	-0.15	31 (0%) 79 56	22, 53, 169, 269	0
1	AR	3149/3396 (92%)	-0.14	46 (1%) 72 47	22, 51, 152, 280	0
2	3	121/121 (100%)	-0.27	1 (0%) 82 60	33, 69, 92, 108	0
2	AS	121/121 (100%)	-0.34	1 (0%) 82 60	28, 56, 73, 112	0
3	4	158/158 (100%)	-0.14	1 (0%) 85 65	34, 58, 115, 203	0
3	AT	158/158 (100%)	-0.15	2 (1%) 75 50	35, 62, 125, 189	0
4	CD	252/252 (100%)	0.03	2 (0%) 82 60	30, 51, 83, 119	0
4	j	252/252 (100%)	0.06	2 (0%) 82 60	29, 54, 76, 118	0
5	CE	386/386 (100%)	-0.23	1 (0%) 90 76	21, 40, 65, 139	0
5	k	386/386 (100%)	-0.19	0 100 100	28, 54, 77, 122	0
6	CF	361/361 (100%)	-0.16	0 100 100	30, 50, 79, 110	0
6	l	361/361 (100%)	-0.14	0 100 100	28, 49, 82, 101	0
7	CG	296/296 (100%)	-0.16	1 (0%) 90 76	36, 58, 99, 128	0
7	m	296/296 (100%)	-0.06	0 100 100	46, 78, 115, 168	0
8	CH	156/175 (89%)	-0.19	0 100 100	35, 49, 88, 129	0
8	n	156/175 (89%)	-0.28	0 100 100	35, 46, 79, 132	0
9	CI	222/222 (100%)	-0.33	1 (0%) 87 68	25, 37, 91, 176	0
9	o	222/222 (100%)	-0.34	1 (0%) 87 68	28, 40, 80, 161	0
10	CJ	233/233 (100%)	0.20	2 (0%) 81 58	64, 87, 146, 191	0
10	p	233/233 (100%)	0.19	1 (0%) 88 72	54, 82, 138, 160	0
11	CK	191/191 (100%)	-0.19	0 100 100	33, 46, 77, 143	0
11	q	191/191 (100%)	-0.06	1 (0%) 87 68	46, 62, 84, 149	0
12	CL	211/220 (95%)	0.04	6 (2%) 55 32	32, 57, 100, 169	0
12	r	211/220 (95%)	-0.11	5 (2%) 59 35	35, 53, 108, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CM	169/169 (100%)	-0.15	0 100 100	45, 61, 83, 105	0
13	s	169/169 (100%)	0.12	1 (0%) 85 65	61, 80, 102, 115	0
14	CN	193/193 (100%)	-0.09	0 100 100	33, 67, 131, 148	0
14	t	193/193 (100%)	-0.09	1 (0%) 87 68	30, 60, 113, 144	0
15	CO	136/136 (100%)	-0.26	3 (2%) 62 37	30, 44, 72, 97	0
15	u	136/136 (100%)	-0.19	1 (0%) 84 63	42, 52, 77, 105	0
16	CP	203/203 (100%)	-0.12	0 100 100	37, 55, 71, 75	0
16	v	203/203 (100%)	-0.08	0 100 100	30, 51, 64, 74	0
17	CQ	197/197 (100%)	-0.27	1 (0%) 87 68	22, 33, 79, 88	0
17	w	197/197 (100%)	-0.19	0 100 100	27, 41, 75, 85	0
18	CR	183/183 (100%)	0.11	19 (10%) 11 8	25, 40, 181, 234	0
18	x	183/183 (100%)	-0.03	8 (4%) 39 21	33, 42, 124, 165	0
19	CS	185/185 (100%)	-0.13	0 100 100	36, 50, 65, 84	0
19	y	185/185 (100%)	-0.03	2 (1%) 78 54	36, 48, 84, 123	0
20	CT	188/188 (100%)	0.14	2 (1%) 78 54	42, 61, 148, 170	0
20	z	188/188 (100%)	0.17	5 (2%) 56 33	53, 73, 158, 171	0
21	0	172/172 (100%)	-0.16	1 (0%) 85 65	37, 46, 72, 91	0
21	CU	172/172 (100%)	-0.33	1 (0%) 85 65	28, 38, 66, 86	0
22	2	159/159 (100%)	-0.09	0 100 100	31, 48, 111, 126	0
22	CV	159/159 (100%)	-0.24	0 100 100	25, 42, 94, 108	0
23	5	100/100 (100%)	0.36	2 (2%) 65 39	86, 108, 135, 159	0
23	CW	100/100 (100%)	0.23	0 100 100	70, 94, 120, 162	0
24	CX	136/136 (100%)	-0.14	1 (0%) 84 63	21, 37, 66, 96	0
24	l2	136/136 (100%)	-0.08	1 (0%) 84 63	37, 51, 78, 114	0
25	6	1783/1800 (99%)	0.11	37 (2%) 63 38	34, 76, 201, 266	0
25	A	1781/1800 (98%)	0.26	53 (2%) 52 30	49, 93, 235, 311	0
26	7	98/98 (100%)	0.84	20 (20%) 3 3	52, 69, 199, 216	0
26	CY	98/98 (100%)	0.53	13 (13%) 7 6	35, 52, 188, 226	0
27	8	121/121 (100%)	0.02	0 100 100	48, 67, 91, 130	0
27	CZ	121/121 (100%)	0.04	0 100 100	48, 67, 91, 132	0
28	9	126/126 (100%)	-0.27	0 100 100	42, 58, 80, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DA	126/126 (100%)	-0.04	2 (1%) 70 45	43, 61, 87, 103	0
29	AA	135/135 (100%)	-0.11	0 100 100	76, 100, 124, 133	0
29	DB	135/135 (100%)	-0.02	0 100 100	77, 99, 124, 136	0
30	AB	148/148 (100%)	-0.11	0 100 100	25, 48, 89, 106	0
30	DC	148/148 (100%)	-0.18	0 100 100	26, 52, 87, 95	0
31	AC	58/58 (100%)	0.13	1 (1%) 69 43	31, 55, 111, 132	0
31	DD	58/58 (100%)	-0.01	0 100 100	30, 56, 92, 112	0
32	AD	97/97 (100%)	-0.00	0 100 100	77, 92, 122, 140	0
32	DE	97/97 (100%)	0.14	1 (1%) 79 56	66, 82, 112, 135	0
33	AE	109/109 (100%)	0.08	0 100 100	46, 67, 123, 146	0
33	DF	109/109 (100%)	-0.04	1 (0%) 81 58	35, 52, 119, 142	0
34	AF	127/127 (100%)	-0.19	1 (0%) 82 60	24, 40, 59, 133	0
34	DG	127/127 (100%)	-0.25	0 100 100	24, 46, 66, 132	0
35	AG	106/106 (100%)	-0.35	0 100 100	28, 37, 62, 89	0
35	DH	106/106 (100%)	-0.27	0 100 100	27, 36, 82, 124	0
36	AH	112/112 (100%)	0.27	1 (0%) 81 58	53, 73, 130, 149	0
36	DI	112/112 (100%)	0.10	1 (0%) 81 58	48, 70, 134, 155	0
37	AI	119/119 (100%)	0.04	1 (0%) 82 60	45, 68, 85, 92	0
37	DJ	119/119 (100%)	0.08	3 (2%) 58 35	51, 75, 94, 113	0
38	AJ	99/99 (100%)	0.03	0 100 100	50, 69, 116, 148	0
38	DK	99/99 (100%)	0.01	1 (1%) 79 56	59, 74, 118, 154	0
39	AK	87/87 (100%)	0.13	2 (2%) 61 37	34, 44, 77, 128	0
39	DL	87/87 (100%)	0.04	1 (1%) 78 54	33, 47, 88, 167	0
40	AL	77/77 (100%)	0.12	0 100 100	78, 94, 120, 130	0
40	DM	77/77 (100%)	0.13	0 100 100	75, 94, 120, 129	0
41	AM	50/50 (100%)	0.08	0 100 100	44, 53, 64, 76	0
41	DN	50/50 (100%)	0.07	0 100 100	48, 56, 69, 89	0
42	AN	52/52 (100%)	-0.31	0 100 100	43, 53, 80, 108	0
42	DO	52/52 (100%)	-0.32	1 (1%) 66 41	32, 39, 54, 81	0
43	AO	25/25 (100%)	0.11	0 100 100	54, 61, 69, 75	0
43	DP	25/25 (100%)	-0.07	0 100 100	42, 50, 62, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AP	105/105 (100%)	-0.02	1 (0%) 79 56	36, 58, 96, 156	0
44	DQ	105/105 (100%)	-0.01	0 100 100	42, 59, 96, 138	0
45	AQ	91/91 (100%)	0.16	1 (1%) 78 54	38, 62, 91, 121	0
45	DR	91/91 (100%)	0.05	0 100 100	32, 55, 78, 88	0
46	i	159/168 (94%)	0.59	13 (8%) 17 11	56, 101, 165, 178	0
47	p0	143/220 (65%)	0.54	2 (1%) 73 48	100, 113, 177, 185	0
48	sM	63/104 (60%)	0.55	4 (6%) 26 15	54, 106, 129, 136	0
49	B	206/206 (100%)	0.32	5 (2%) 59 35	92, 115, 139, 176	0
49	s0	206/206 (100%)	-0.01	2 (0%) 79 56	72, 95, 124, 136	0
50	C	214/216 (99%)	0.53	5 (2%) 61 37	101, 141, 172, 181	0
50	s1	216/216 (100%)	-0.03	0 100 100	68, 87, 117, 144	0
51	D	217/217 (100%)	0.37	2 (0%) 81 58	69, 91, 118, 142	0
51	s2	217/217 (100%)	0.22	6 (2%) 55 32	55, 75, 97, 121	0
52	E	223/223 (100%)	0.33	3 (1%) 75 50	78, 95, 131, 155	0
52	s3	223/223 (100%)	0.50	9 (4%) 42 23	74, 111, 145, 158	0
53	F	260/260 (100%)	0.24	1 (0%) 88 72	73, 95, 113, 153	0
53	s4	260/260 (100%)	-0.05	0 100 100	51, 79, 100, 150	0
54	G	206/206 (100%)	0.56	9 (4%) 39 21	98, 121, 152, 179	0
54	s5	206/206 (100%)	0.40	5 (2%) 59 35	71, 92, 124, 157	0
55	H	226/226 (100%)	0.50	7 (3%) 51 29	66, 105, 142, 160	0
55	s6	218/226 (96%)	0.21	2 (0%) 81 58	51, 83, 123, 148	0
56	I	184/186 (98%)	0.47	4 (2%) 62 37	85, 126, 160, 187	0
56	s7	186/186 (100%)	0.07	1 (0%) 87 68	69, 105, 156, 173	0
57	J	188/199 (94%)	0.19	1 (0%) 87 68	58, 77, 128, 150	0
57	s8	188/199 (94%)	0.07	0 100 100	43, 68, 121, 138	0
58	K	185/185 (100%)	0.42	4 (2%) 62 37	87, 107, 149, 185	0
58	s9	185/185 (100%)	0.13	1 (0%) 87 68	63, 80, 128, 169	0
59	L	96/105 (91%)	0.32	0 100 100	80, 111, 141, 172	0
59	c0	96/105 (91%)	0.68	4 (4%) 40 22	104, 137, 155, 185	0
60	M	155/155 (100%)	0.48	9 (5%) 29 17	60, 76, 162, 194	0
60	c1	146/155 (94%)	0.23	7 (4%) 35 19	42, 64, 118, 151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
61	N	124/124 (100%)	0.56	0 100 100	140, 159, 203, 214	0
61	c2	124/124 (100%)	0.60	1 (0%) 82 60	159, 186, 216, 234	0
62	O	150/150 (100%)	0.19	0 100 100	60, 90, 112, 129	0
62	c3	150/150 (100%)	0.18	2 (1%) 75 50	53, 76, 100, 121	0
63	P	127/128 (99%)	0.63	5 (3%) 43 23	65, 128, 158, 165	0
63	c4	128/128 (100%)	0.18	1 (0%) 82 60	55, 84, 100, 130	0
64	Q	124/141 (87%)	0.25	2 (1%) 70 45	80, 103, 150, 165	0
64	c5	135/141 (95%)	0.54	7 (5%) 33 19	75, 102, 144, 168	0
65	R	141/142 (99%)	0.65	6 (4%) 40 21	83, 110, 129, 132	0
65	c6	142/142 (100%)	0.43	3 (2%) 63 38	62, 88, 109, 141	0
66	S	120/125 (96%)	0.34	3 (2%) 58 35	77, 111, 159, 170	0
67	T	145/145 (100%)	0.19	1 (0%) 84 63	71, 111, 145, 160	0
67	c8	145/145 (100%)	0.01	2 (1%) 73 48	71, 88, 121, 137	0
68	U	143/143 (100%)	0.41	3 (2%) 63 38	89, 112, 136, 148	0
68	c9	143/143 (100%)	-0.00	0 100 100	66, 85, 109, 139	0
69	V	107/110 (97%)	0.78	7 (6%) 25 15	75, 110, 157, 169	0
69	d0	110/110 (100%)	0.52	1 (0%) 81 58	70, 113, 170, 190	0
70	W	87/87 (100%)	0.36	2 (2%) 61 37	91, 105, 126, 148	0
70	d1	87/87 (100%)	-0.10	0 100 100	68, 83, 119, 146	0
71	X	129/129 (100%)	0.24	0 100 100	68, 84, 96, 102	0
71	d2	129/129 (100%)	-0.04	0 100 100	50, 64, 77, 88	0
72	Y	144/144 (100%)	0.25	1 (0%) 84 63	57, 67, 88, 124	0
72	d3	144/144 (100%)	0.01	1 (0%) 84 63	40, 49, 73, 108	0
73	Z	134/134 (100%)	0.35	2 (1%) 72 47	82, 111, 137, 155	0
73	d4	134/134 (100%)	0.17	2 (1%) 72 47	59, 89, 117, 159	0
74	a	70/70 (100%)	0.36	0 100 100	117, 134, 148, 160	0
74	d5	69/70 (98%)	0.14	0 100 100	84, 111, 136, 147	0
75	b	97/97 (100%)	0.59	4 (4%) 41 22	69, 95, 165, 171	0
75	d6	97/97 (100%)	0.27	2 (2%) 63 38	54, 68, 110, 126	0
76	c	81/81 (100%)	0.45	1 (1%) 76 52	84, 107, 161, 171	0
76	d7	81/81 (100%)	0.10	0 100 100	67, 88, 144, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
77	d	63/63 (100%)	0.72	4 (6%)	26	15	103, 124, 146, 159	0
77	d8	63/63 (100%)	0.55	2 (3%)	50	29	82, 104, 132, 141	0
78	d9	53/53 (100%)	0.33	0	100	100	73, 84, 133, 153	0
78	e	53/53 (100%)	0.20	0	100	100	72, 82, 116, 137	0
79	e0	62/62 (100%)	0.30	2 (3%)	50	29	58, 81, 140, 161	0
79	f	60/62 (96%)	0.42	1 (1%)	69	43	65, 98, 158, 164	0
80	g	71/71 (100%)	0.84	5 (7%)	22	14	96, 149, 167, 187	0
81	h	318/318 (100%)	0.09	2 (0%)	85	65	100, 124, 161, 200	0
81	sR	318/318 (100%)	0.28	2 (0%)	85	65	92, 119, 148, 191	0
82	c7	117/121 (96%)	0.16	1 (0%)	81	58	72, 93, 130, 139	0
83	e1	51/51 (100%)	0.94	5 (9%)	13	9	143, 176, 188, 200	0
All	All	33004/33818 (97%)	0.06	485 (1%)	72	47	21, 72, 152, 311	0

The worst 5 of 485 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	7	88	ASP	8.1
18	CR	177	ALA	6.2
26	7	86	SER	6.0
1	AR	1103	A	5.4
17	CQ	182	ASN	5.3

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
85	MG	A	2110	1/1	0.00	0.24	108,108,108,108	0
85	MG	A	2104	1/1	0.16	0.19	131,131,131,131	0
85	MG	AR	4152	1/1	0.41	0.13	152,152,152,152	0
85	MG	A	2139	1/1	0.51	0.25	86,86,86,86	0
85	MG	AR	4059	1/1	0.54	0.19	67,67,67,67	0
85	MG	6	2097	1/1	0.55	0.24	79,79,79,79	0
85	MG	1	3751	1/1	0.56	0.24	50,50,50,50	0
85	MG	AH	201	1/1	0.59	0.38	60,60,60,60	0
85	MG	A	2147	1/1	0.59	0.17	106,106,106,106	0
85	MG	AR	3812	1/1	0.60	0.19	46,46,46,46	0
85	MG	AR	3773	1/1	0.61	0.23	113,113,113,113	0
84	OHX	6	2029	7/7	0.64	0.16	246,248,249,250	0
84	OHX	AR	3716	7/7	0.65	0.16	292,293,293,294	0
85	MG	c9	201	1/1	0.65	0.16	73,73,73,73	0
85	MG	A	2118	1/1	0.66	0.35	75,75,75,75	0
84	OHX	AR	3737	7/7	0.66	0.15	260,261,262,262	0
85	MG	A	2129	1/1	0.67	0.11	58,58,58,58	0
85	MG	1	4079	1/1	0.68	0.19	47,47,47,47	0
85	MG	6	2148	1/1	0.68	0.16	69,69,69,69	0
85	MG	6	2160	1/1	0.68	0.16	121,121,121,121	0
85	MG	A	2094	1/1	0.69	0.21	110,110,110,110	0
85	MG	1	3824	1/1	0.69	0.22	77,77,77,77	0
85	MG	6	2081	1/1	0.70	0.21	94,94,94,94	0
85	MG	1	3775	1/1	0.71	0.23	59,59,59,59	0
84	OHX	CO	201	7/7	0.71	0.13	281,282,283,284	0
85	MG	AR	4072	1/1	0.71	0.12	71,71,71,71	0
84	OHX	AR	3733	7/7	0.71	0.13	289,291,292,292	0
85	MG	A	2095	1/1	0.72	0.20	94,94,94,94	0
84	OHX	4	210	7/7	0.72	0.15	236,236,236,236	0
85	MG	1	4175	1/1	0.72	0.26	91,91,91,91	0
84	OHX	1	3719	7/7	0.72	0.15	264,264,265,265	0
84	OHX	A	2002	7/7	0.72	0.21	242,245,246,247	0
85	MG	1	3966	1/1	0.72	0.13	62,62,62,62	0
85	MG	1	3982	1/1	0.72	0.23	98,98,98,98	0
85	MG	6	2180	1/1	0.72	0.14	94,94,94,94	0
84	OHX	AS	210	7/7	0.73	0.16	235,237,238,238	0
84	OHX	AR	3717	7/7	0.73	0.17	281,282,283,283	0
85	MG	AR	4170	1/1	0.73	0.12	128,128,128,128	0
85	MG	AR	4183	1/1	0.73	0.20	93,93,93,93	0
85	MG	A	2091	1/1	0.73	0.23	60,60,60,60	0
85	MG	AR	4036	1/1	0.73	0.14	68,68,68,68	0
85	MG	1	3759	1/1	0.73	0.24	69,69,69,69	0
84	OHX	6	2042	7/7	0.74	0.14	246,246,248,248	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	4220	1/1	0.74	0.18	54,54,54,54	0
85	MG	A	2073	1/1	0.74	0.26	65,65,65,65	0
85	MG	AR	3746	1/1	0.74	0.15	39,39,39,39	0
84	OHX	CZ	201	7/7	0.74	0.15	303,304,305,305	0
84	OHX	A	1993	7/7	0.74	0.15	236,237,239,240	0
84	OHX	6	2047	7/7	0.74	0.16	237,239,240,241	0
85	MG	6	2143	1/1	0.74	0.20	90,90,90,90	0
85	MG	1	3968	1/1	0.74	0.13	50,50,50,50	0
85	MG	AR	4122	1/1	0.74	0.14	70,70,70,70	0
84	OHX	AR	3732	7/7	0.74	0.16	245,246,247,247	0
85	MG	AR	4156	1/1	0.74	0.17	71,71,71,71	0
85	MG	1	4044	1/1	0.74	0.21	40,40,40,40	0
84	OHX	1	3661	7/7	0.75	0.15	251,252,253,253	0
84	OHX	1	3703	7/7	0.75	0.12	259,259,260,261	0
85	MG	1	4132	1/1	0.75	0.23	42,42,42,42	0
84	OHX	1	3709	7/7	0.75	0.15	229,231,231,232	0
84	OHX	1	3638	7/7	0.75	0.13	245,246,247,248	0
84	OHX	AR	3680	7/7	0.75	0.15	220,222,222,223	0
84	OHX	A	2039	7/7	0.75	0.14	264,266,268,268	0
85	MG	CR	203	1/1	0.75	0.29	74,74,74,74	0
85	MG	A	2057	1/1	0.75	0.24	50,50,50,50	0
85	MG	1	3736	1/1	0.75	0.10	82,82,82,82	0
85	MG	6	2152	1/1	0.76	0.18	57,57,57,57	0
85	MG	A	2098	1/1	0.76	0.15	72,72,72,72	0
85	MG	AR	4128	1/1	0.76	0.17	54,54,54,54	0
85	MG	1	4100	1/1	0.76	0.15	87,87,87,87	0
85	MG	A	2072	1/1	0.76	0.27	44,44,44,44	0
85	MG	A	2121	1/1	0.76	0.21	66,66,66,66	0
84	OHX	A	2031	7/7	0.76	0.12	244,246,248,248	0
85	MG	A	2135	1/1	0.76	0.19	50,50,50,50	0
84	OHX	1	3648	7/7	0.76	0.17	258,259,260,260	0
85	MG	A	2092	1/1	0.76	0.28	87,87,87,87	0
85	MG	z	202	1/1	0.76	0.17	62,62,62,62	0
84	OHX	AR	3730	7/7	0.77	0.11	271,272,273,273	0
84	OHX	CE	403	7/7	0.77	0.14	237,238,239,240	0
85	MG	6	2080	1/1	0.77	0.23	53,53,53,53	0
84	OHX	1	3726	7/7	0.77	0.14	231,232,233,233	0
84	OHX	AR	3687	7/7	0.77	0.14	244,245,246,247	0
85	MG	A	2148	1/1	0.77	0.27	103,103,103,103	0
85	MG	A	2153	1/1	0.77	0.29	66,66,66,66	0
84	OHX	AR	3727	7/7	0.77	0.11	277,279,280,280	0
85	MG	d5	201	1/1	0.77	0.14	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	AR	3695	7/7	0.78	0.17	225,226,227,227	0
85	MG	1	3829	1/1	0.78	0.30	25,25,25,25	0
84	OHX	AR	3702	7/7	0.78	0.15	218,219,220,220	0
84	OHX	6	2053	7/7	0.78	0.15	250,252,253,254	0
84	OHX	AR	3641	7/7	0.78	0.15	218,219,219,220	0
85	MG	AR	3819	1/1	0.78	0.28	53,53,53,53	0
85	MG	AR	4026	1/1	0.78	0.28	62,62,62,62	0
84	OHX	AR	3664	7/7	0.78	0.20	287,287,288,288	0
85	MG	A	2142	1/1	0.78	0.12	90,90,90,90	0
84	OHX	1	3656	7/7	0.78	0.14	229,230,231,231	0
85	MG	1	3769	1/1	0.78	0.22	61,61,61,61	0
84	OHX	6	2052	7/7	0.78	0.16	244,244,246,246	0
85	MG	6	2162	1/1	0.78	0.16	69,69,69,69	0
85	MG	AR	4141	1/1	0.78	0.18	53,53,53,53	0
85	MG	A	2099	1/1	0.79	0.26	64,64,64,64	0
85	MG	A	2102	1/1	0.79	0.23	52,52,52,52	0
85	MG	A	2103	1/1	0.79	0.32	64,64,64,64	0
85	MG	AR	3803	1/1	0.79	0.10	54,54,54,54	0
84	OHX	AR	3728	7/7	0.79	0.15	238,238,239,239	0
85	MG	6	2121	1/1	0.79	0.17	71,71,71,71	0
84	OHX	1	3696	7/7	0.79	0.15	240,240,241,242	0
85	MG	A	2127	1/1	0.79	0.12	55,55,55,55	0
85	MG	A	2054	1/1	0.79	0.24	59,59,59,59	0
85	MG	A	2131	1/1	0.79	0.27	88,88,88,88	0
85	MG	1	4064	1/1	0.79	0.14	59,59,59,59	0
84	OHX	A	1985	7/7	0.79	0.16	221,222,223,224	0
84	OHX	6	1976	7/7	0.79	0.17	182,182,183,184	0
84	OHX	6	2006	7/7	0.79	0.18	199,199,201,201	0
84	OHX	6	2028	7/7	0.79	0.13	248,250,252,252	0
85	MG	1	3955	1/1	0.79	0.14	52,52,52,52	0
84	OHX	1	3722	7/7	0.79	0.23	268,268,269,269	0
84	OHX	1	3711	7/7	0.79	0.09	301,302,304,304	0
84	OHX	AR	3711	7/7	0.80	0.15	227,227,228,228	0
85	MG	3	217	1/1	0.80	0.17	48,48,48,48	0
84	OHX	CF	401	7/7	0.80	0.12	245,246,247,247	0
85	MG	AR	4215	1/1	0.80	0.19	72,72,72,72	0
85	MG	6	2066	1/1	0.80	0.26	87,87,87,87	0
84	OHX	CF	402	7/7	0.80	0.13	254,255,256,256	0
85	MG	1	3976	1/1	0.80	0.31	61,61,61,61	0
84	OHX	1	3693	7/7	0.80	0.10	264,265,266,266	0
84	OHX	6	2010	7/7	0.80	0.17	213,214,215,216	0
85	MG	6	2125	1/1	0.80	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	A	2083	1/1	0.80	0.24	62,62,62,62	0
84	OHX	A	1977	7/7	0.80	0.16	202,205,207,207	0
84	OHX	1	3731	7/7	0.80	0.17	201,202,205,205	0
84	OHX	AR	3738	7/7	0.80	0.16	270,271,272,272	0
85	MG	6	2158	1/1	0.80	0.25	64,64,64,64	0
85	MG	1	4130	1/1	0.80	0.17	68,68,68,68	0
84	OHX	6	2048	7/7	0.80	0.15	224,224,225,226	0
84	OHX	x	202	7/7	0.81	0.14	223,224,225,225	0
84	OHX	6	2054	7/7	0.81	0.12	253,254,256,256	0
85	MG	1	3801	1/1	0.81	0.12	38,38,38,38	0
85	MG	1	4090	1/1	0.81	0.09	54,54,54,54	0
85	MG	AR	3826	1/1	0.81	0.25	42,42,42,42	0
85	MG	6	2126	1/1	0.81	0.20	39,39,39,39	0
85	MG	A	2122	1/1	0.81	0.24	42,42,42,42	0
85	MG	A	2068	1/1	0.81	0.24	68,68,68,68	0
84	OHX	6	2046	7/7	0.81	0.10	244,245,247,248	0
84	OHX	6	2015	7/7	0.81	0.16	230,231,232,233	0
85	MG	A	2080	1/1	0.81	0.27	45,45,45,45	0
84	OHX	CG	303	7/7	0.81	0.14	212,213,214,214	0
84	OHX	A	2040	7/7	0.81	0.11	246,248,249,250	0
84	OHX	1	3645	7/7	0.81	0.14	220,221,221,221	0
84	OHX	1	3675	7/7	0.81	0.24	229,229,230,230	0
85	MG	6	2064	1/1	0.81	0.21	62,62,62,62	0
84	OHX	AS	208	7/7	0.81	0.19	226,226,228,228	0
85	MG	1	3998	1/1	0.81	0.28	65,65,65,65	0
85	MG	DR	502	1/1	0.82	0.15	76,76,76,76	0
85	MG	1	4056	1/1	0.82	0.13	82,82,82,82	0
84	OHX	Q	201	7/7	0.82	0.12	245,246,248,249	0
84	OHX	c3	201	7/7	0.82	0.13	212,213,214,215	0
84	OHX	4	209	7/7	0.82	0.19	194,194,195,195	0
84	OHX	CM	201	7/7	0.82	0.11	247,248,249,250	0
85	MG	A	2079	1/1	0.82	0.30	46,46,46,46	0
85	MG	6	2195	1/1	0.82	0.16	64,64,64,64	0
85	MG	1	4101	1/1	0.82	0.12	37,37,37,37	0
85	MG	1	4102	1/1	0.82	0.12	40,40,40,40	0
85	MG	AR	3753	1/1	0.82	0.21	51,51,51,51	0
84	OHX	1	3664	7/7	0.82	0.13	232,233,234,235	0
84	OHX	6	2051	7/7	0.82	0.16	228,229,230,231	0
84	OHX	1	3694	7/7	0.82	0.12	251,252,254,254	0
84	OHX	z	201	7/7	0.82	0.10	257,258,259,259	0
84	OHX	6	2037	7/7	0.82	0.17	203,204,206,206	0
85	MG	AR	3887	1/1	0.82	0.35	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	3970	1/1	0.82	0.18	53,53,53,53	0
85	MG	AR	4016	1/1	0.82	0.12	104,104,104,104	0
84	OHX	1	3710	7/7	0.82	0.13	247,248,248,249	0
85	MG	1	3907	1/1	0.82	0.31	13,13,13,13	0
85	MG	6	2068	1/1	0.82	0.25	76,76,76,76	0
85	MG	A	2123	1/1	0.82	0.24	40,40,40,40	0
85	MG	A	2125	1/1	0.82	0.30	51,51,51,51	0
85	MG	6	2071	1/1	0.82	0.12	73,73,73,73	0
84	OHX	A	2025	7/7	0.82	0.11	249,252,253,253	0
84	OHX	A	2027	7/7	0.82	0.12	236,239,240,241	0
84	OHX	A	2029	7/7	0.82	0.12	261,263,265,265	0
85	MG	6	2111	1/1	0.82	0.15	42,42,42,42	0
84	OHX	AR	3726	7/7	0.82	0.22	220,220,221,221	0
85	MG	A	2144	1/1	0.82	0.29	49,49,49,49	0
85	MG	6	2124	1/1	0.82	0.23	62,62,62,62	0
84	OHX	1	3663	7/7	0.82	0.13	214,216,217,217	0
84	OHX	AR	3678	7/7	0.82	0.14	238,238,239,239	0
85	MG	1	4042	1/1	0.82	0.11	65,65,65,65	0
84	OHX	J	301	7/7	0.82	0.11	244,245,247,247	0
84	OHX	AR	3670	7/7	0.83	0.16	229,230,230,231	0
85	MG	AR	4218	1/1	0.83	0.12	31,31,31,31	0
85	MG	1	4073	1/1	0.83	0.14	79,79,79,79	0
85	MG	AT	227	1/1	0.83	0.12	73,73,73,73	0
85	MG	6	2150	1/1	0.83	0.12	51,51,51,51	0
85	MG	6	2151	1/1	0.83	0.29	87,87,87,87	0
85	MG	1	4076	1/1	0.83	0.14	71,71,71,71	0
84	OHX	6	2038	7/7	0.83	0.12	213,215,217,217	0
84	OHX	A	1997	7/7	0.83	0.16	211,214,214,215	0
84	OHX	AR	3719	7/7	0.83	0.14	220,220,221,221	0
85	MG	6	2179	1/1	0.83	0.15	52,52,52,52	0
84	OHX	A	2005	7/7	0.83	0.15	204,206,207,207	0
85	MG	6	2189	1/1	0.83	0.19	67,67,67,67	0
85	MG	6	2193	1/1	0.83	0.21	76,76,76,76	0
84	OHX	A	2015	7/7	0.83	0.14	248,250,254,254	0
85	MG	1	4109	1/1	0.83	0.09	37,37,37,37	0
85	MG	AR	3742	1/1	0.83	0.13	29,29,29,29	0
85	MG	1	3804	1/1	0.83	0.30	18,18,18,18	0
84	OHX	AR	3720	7/7	0.83	0.13	267,269,269,270	0
85	MG	1	4172	1/1	0.83	0.17	76,76,76,76	0
84	OHX	AR	3725	7/7	0.83	0.12	261,263,264,264	0
85	MG	AR	3806	1/1	0.83	0.18	68,68,68,68	0
85	MG	1	3834	1/1	0.83	0.27	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	s	300	1/1	0.83	0.16	53,53,53,53	0
85	MG	1	3879	1/1	0.83	0.12	47,47,47,47	0
84	OHX	1	3713	7/7	0.83	0.15	217,217,218,218	0
85	MG	AR	3891	1/1	0.83	0.27	36,36,36,36	0
85	MG	AR	3892	1/1	0.83	0.30	19,19,19,19	0
84	OHX	6	2044	7/7	0.83	0.13	238,238,239,240	0
84	OHX	A	2037	7/7	0.83	0.13	238,240,241,241	0
84	OHX	A	2038	7/7	0.83	0.16	217,217,220,220	0
85	MG	6	2074	1/1	0.83	0.26	37,37,37,37	0
84	OHX	6	1993	7/7	0.83	0.15	191,192,193,194	0
84	OHX	AR	3729	7/7	0.83	0.16	214,215,216,216	0
84	OHX	1	3676	7/7	0.83	0.11	223,223,225,225	0
85	MG	1	4032	1/1	0.83	0.16	49,49,49,49	0
85	MG	1	4034	1/1	0.83	0.24	33,33,33,33	0
84	OHX	O	201	7/7	0.83	0.11	249,252,253,253	0
84	OHX	AR	3705	7/7	0.83	0.19	212,213,213,214	0
84	OHX	1	3712	7/7	0.83	0.14	215,215,216,217	0
85	MG	6	2129	1/1	0.83	0.17	53,53,53,53	0
85	MG	AR	3838	1/1	0.84	0.24	21,21,21,21	0
85	MG	1	4136	1/1	0.84	0.17	49,49,49,49	0
85	MG	1	3746	1/1	0.84	0.13	59,59,59,59	0
85	MG	A	2075	1/1	0.84	0.14	48,48,48,48	0
84	OHX	1	3671	7/7	0.84	0.14	212,213,214,214	0
84	OHX	6	2045	7/7	0.84	0.16	196,197,198,199	0
85	MG	AR	4002	1/1	0.84	0.27	42,42,42,42	0
85	MG	l	402	1/1	0.84	0.17	32,32,32,32	0
85	MG	AR	4024	1/1	0.84	0.18	33,33,33,33	0
84	OHX	1	3727	7/7	0.84	0.11	253,254,255,256	0
85	MG	1	3774	1/1	0.84	0.12	84,84,84,84	0
84	OHX	1	3728	7/7	0.84	0.12	233,233,233,234	0
85	MG	AR	4067	1/1	0.84	0.12	98,98,98,98	0
85	MG	6	2163	1/1	0.84	0.19	60,60,60,60	0
85	MG	AR	4116	1/1	0.84	0.21	105,105,105,105	0
84	OHX	AR	3685	7/7	0.84	0.18	187,187,188,188	0
84	OHX	1	3715	7/7	0.84	0.14	219,220,222,222	0
85	MG	A	2114	1/1	0.84	0.20	41,41,41,41	0
84	OHX	1	3717	7/7	0.84	0.18	217,218,219,219	0
84	OHX	1	3718	7/7	0.84	0.15	220,221,221,222	0
85	MG	6	2075	1/1	0.84	0.19	49,49,49,49	0
85	MG	AR	4167	1/1	0.84	0.22	72,72,72,72	0
84	OHX	A	1969	7/7	0.84	0.15	220,222,223,223	0
84	OHX	A	1971	7/7	0.84	0.14	216,218,220,221	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	1	3704	7/7	0.84	0.18	277,278,278,278	0
85	MG	A	2130	1/1	0.84	0.24	49,49,49,49	0
85	MG	AR	4217	1/1	0.84	0.08	65,65,65,65	0
85	MG	1	3918	1/1	0.84	0.33	26,26,26,26	0
84	OHX	1	3600	7/7	0.84	0.11	258,258,259,259	0
85	MG	1	4107	1/1	0.84	0.24	66,66,66,66	0
85	MG	A	2143	1/1	0.84	0.18	151,151,151,151	0
84	OHX	AR	3609	7/7	0.84	0.18	201,201,202,202	0
85	MG	CX	203	1/1	0.84	0.20	45,45,45,45	0
84	OHX	1	3724	7/7	0.84	0.10	243,244,245,246	0
85	MG	A	2149	1/1	0.84	0.21	49,49,49,49	0
85	MG	A	2050	1/1	0.84	0.25	68,68,68,68	0
85	MG	6	2128	1/1	0.84	0.17	53,53,53,53	0
84	OHX	AR	3718	7/7	0.84	0.10	255,256,257,257	0
87	ZN	c	101	1/1	0.84	0.08	197,197,197,197	0
85	MG	1	4033	1/1	0.85	0.16	57,57,57,57	0
84	OHX	c5	201	7/7	0.85	0.12	228,229,230,231	0
84	OHX	A	1996	7/7	0.85	0.12	208,209,211,212	0
85	MG	AR	3813	1/1	0.85	0.14	54,54,54,54	0
84	OHX	6	2026	7/7	0.85	0.14	218,219,220,222	0
85	MG	6	2098	1/1	0.85	0.26	38,38,38,38	0
85	MG	6	2107	1/1	0.85	0.27	24,24,24,24	0
85	MG	AR	3849	1/1	0.85	0.32	18,18,18,18	0
84	OHX	1	3633	7/7	0.85	0.13	193,194,195,197	0
84	OHX	1	3619	7/7	0.85	0.14	190,191,192,193	0
84	OHX	A	2006	7/7	0.85	0.11	215,218,219,219	0
85	MG	AR	3930	1/1	0.85	0.29	14,14,14,14	0
84	OHX	6	2032	7/7	0.85	0.12	236,237,238,239	0
84	OHX	A	2023	7/7	0.85	0.13	202,204,206,206	0
85	MG	1	3786	1/1	0.85	0.26	37,37,37,37	0
85	MG	AR	4020	1/1	0.85	0.18	69,69,69,69	0
85	MG	1	4092	1/1	0.85	0.20	53,53,53,53	0
84	OHX	A	2024	7/7	0.85	0.18	219,222,223,223	0
84	OHX	AR	3724	7/7	0.85	0.15	203,204,205,205	0
84	OHX	1	3720	7/7	0.85	0.14	197,197,199,199	0
84	OHX	6	2001	7/7	0.85	0.14	211,211,212,213	0
84	OHX	CL	302	7/7	0.85	0.17	200,201,201,202	0
85	MG	AR	4084	1/1	0.85	0.13	31,31,31,31	0
85	MG	AR	4087	1/1	0.85	0.17	31,31,31,31	0
85	MG	1	3853	1/1	0.85	0.24	61,61,61,61	0
84	OHX	A	2034	7/7	0.85	0.10	277,279,281,282	0
85	MG	AR	4127	1/1	0.85	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	OHX	AR	3694	7/7	0.85	0.21	212,212,213,213	0
84	OHX	1	3707	7/7	0.85	0.11	237,237,239,239	0
85	MG	1	3928	1/1	0.85	0.18	32,32,32,32	0
85	MG	1	3934	1/1	0.85	0.10	61,61,61,61	0
84	OHX	1	3667	7/7	0.85	0.17	189,189,190,191	0
85	MG	A	2134	1/1	0.85	0.25	34,34,34,34	0
84	OHX	1	3702	7/7	0.85	0.18	179,180,181,182	0
85	MG	AR	4180	1/1	0.85	0.14	93,93,93,93	0
84	OHX	H	301	7/7	0.85	0.13	231,233,235,235	0
85	MG	AR	4185	1/1	0.85	0.20	40,40,40,40	0
84	OHX	AR	3708	7/7	0.85	0.14	228,228,229,229	0
84	OHX	AR	3651	7/7	0.85	0.16	229,230,231,231	0
84	OHX	AR	3734	7/7	0.85	0.16	223,224,224,225	0
85	MG	1	4008	1/1	0.85	0.16	76,76,76,76	0
85	MG	AS	228	1/1	0.85	0.14	48,48,48,48	0
85	MG	AR	3759	1/1	0.85	0.11	103,103,103,103	0
85	MG	CO	202	1/1	0.85	0.21	57,57,57,57	0
85	MG	d9	102	1/1	0.85	0.19	106,106,106,106	0
84	OHX	AR	3657	7/7	0.85	0.15	207,207,209,209	0
85	MG	CR	205	1/1	0.86	0.14	29,29,29,29	0
84	OHX	A	2003	7/7	0.86	0.14	196,198,199,199	0
84	OHX	1	3625	7/7	0.86	0.18	186,186,187,187	0
84	OHX	1	3674	7/7	0.86	0.20	212,212,213,213	0
85	MG	AR	3889	1/1	0.86	0.26	42,42,42,42	0
84	OHX	A	2013	7/7	0.86	0.14	203,205,206,206	0
85	MG	A	2063	1/1	0.86	0.27	36,36,36,36	0
84	OHX	AR	3682	7/7	0.86	0.12	213,214,214,215	0
84	OHX	6	2008	7/7	0.86	0.12	211,213,214,216	0
84	OHX	1	3632	7/7	0.86	0.13	202,202,204,204	0
84	OHX	6	2014	7/7	0.86	0.14	219,220,221,221	0
84	OHX	6	2049	7/7	0.86	0.13	218,219,220,221	0
84	OHX	AT	219	7/7	0.86	0.15	190,190,190,191	0
84	OHX	1	3705	7/7	0.86	0.18	222,222,223,223	0
84	OHX	6	2025	7/7	0.86	0.09	248,249,250,252	0
84	OHX	1	3621	7/7	0.86	0.14	221,223,224,224	0
85	MG	A	2093	1/1	0.86	0.20	93,93,93,93	0
85	MG	AR	4055	1/1	0.86	0.19	47,47,47,47	0
85	MG	1	4163	1/1	0.86	0.12	68,68,68,68	0
84	OHX	4	211	7/7	0.86	0.13	225,225,226,226	0
84	OHX	6	2055	7/7	0.86	0.12	234,235,236,236	0
85	MG	6	2164	1/1	0.86	0.08	63,63,63,63	0
84	OHX	AR	3602	7/7	0.86	0.14	192,193,194,194	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	l	401	7/7	0.86	0.11	208,209,210,210	0
85	MG	A	2107	1/1	0.86	0.16	69,69,69,69	0
85	MG	6	2184	1/1	0.86	0.18	43,43,43,43	0
84	OHX	AR	3624	7/7	0.86	0.13	210,211,212,212	0
84	OHX	DL	102	7/7	0.86	0.20	212,212,213,213	0
85	MG	A	2119	1/1	0.86	0.23	55,55,55,55	0
85	MG	6	2061	1/1	0.86	0.19	64,64,64,64	0
85	MG	6	2197	1/1	0.86	0.14	57,57,57,57	0
85	MG	1	3988	1/1	0.86	0.17	46,46,46,46	0
85	MG	AR	4164	1/1	0.86	0.09	30,30,30,30	0
85	MG	AP	503	1/1	0.86	0.16	61,61,61,61	0
84	OHX	AR	3640	7/7	0.86	0.18	197,198,199,199	0
84	OHX	1	3653	7/7	0.86	0.13	193,195,196,196	0
85	MG	1	4010	1/1	0.86	0.19	44,44,44,44	0
84	OHX	1	3666	7/7	0.86	0.16	186,187,188,188	0
85	MG	AR	4214	1/1	0.86	0.12	61,61,61,61	0
84	OHX	1	3654	7/7	0.86	0.20	192,194,194,194	0
84	OHX	AR	3663	7/7	0.86	0.14	208,209,210,210	0
85	MG	1	3749	1/1	0.86	0.07	38,38,38,38	0
84	OHX	6	2039	7/7	0.86	0.12	204,204,206,206	0
85	MG	AR	4241	1/1	0.86	0.19	59,59,59,59	0
85	MG	AS	214	1/1	0.86	0.15	68,68,68,68	0
84	OHX	AR	3668	7/7	0.86	0.13	216,216,217,218	0
85	MG	AT	223	1/1	0.86	0.21	55,55,55,55	0
85	MG	Y	201	1/1	0.86	0.13	51,51,51,51	0
85	MG	s6	301	1/1	0.86	0.21	64,64,64,64	0
84	OHX	1	3699	7/7	0.86	0.08	304,306,307,308	0
85	MG	CE	405	1/1	0.86	0.24	34,34,34,34	0
85	MG	6	2110	1/1	0.86	0.28	40,40,40,40	0
85	MG	AR	3830	1/1	0.86	0.11	30,30,30,30	0
87	ZN	d7	101	1/1	0.86	0.11	176,176,176,176	0
85	MG	1	3761	1/1	0.87	0.21	44,44,44,44	0
84	OHX	A	1980	7/7	0.87	0.14	194,196,197,197	0
85	MG	6	2174	1/1	0.87	0.15	66,66,66,66	0
84	OHX	AR	3634	7/7	0.87	0.15	213,214,215,216	0
84	OHX	A	1989	7/7	0.87	0.10	253,254,256,256	0
84	OHX	AR	3638	7/7	0.87	0.19	208,208,209,209	0
84	OHX	6	2041	7/7	0.87	0.19	209,209,210,211	0
84	OHX	1	3655	7/7	0.87	0.18	203,204,205,205	0
84	OHX	AR	3647	7/7	0.87	0.15	203,204,205,205	0
85	MG	AS	229	1/1	0.87	0.18	68,68,68,68	0
85	MG	1	4169	1/1	0.87	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	6	2043	7/7	0.87	0.15	196,196,198,198	0
84	OHX	AR	3652	7/7	0.87	0.21	196,196,197,197	0
85	MG	1	4183	1/1	0.87	0.27	41,41,41,41	0
85	MG	1	4202	1/1	0.87	0.22	27,27,27,27	0
84	OHX	1	3617	7/7	0.87	0.15	201,202,203,204	0
85	MG	AR	3757	1/1	0.87	0.16	32,32,32,32	0
85	MG	3	219	1/1	0.87	0.11	77,77,77,77	0
85	MG	AR	3760	1/1	0.87	0.26	21,21,21,21	0
85	MG	4	230	1/1	0.87	0.11	54,54,54,54	0
84	OHX	AR	3660	7/7	0.87	0.15	167,168,169,170	0
84	OHX	A	2014	7/7	0.87	0.14	198,199,200,200	0
84	OHX	AR	3661	7/7	0.87	0.15	176,177,178,178	0
85	MG	6	2058	1/1	0.87	0.25	33,33,33,33	0
84	OHX	1	3658	7/7	0.87	0.13	211,212,212,213	0
85	MG	AR	3820	1/1	0.87	0.20	55,55,55,55	0
84	OHX	6	2021	7/7	0.87	0.13	210,210,212,213	0
85	MG	1	3950	1/1	0.87	0.12	70,70,70,70	0
85	MG	6	2067	1/1	0.87	0.24	41,41,41,41	0
85	MG	A	2084	1/1	0.87	0.12	53,53,53,53	0
85	MG	A	2086	1/1	0.87	0.16	50,50,50,50	0
85	MG	A	2089	1/1	0.87	0.26	65,65,65,65	0
84	OHX	AR	3666	7/7	0.87	0.14	217,218,218,219	0
85	MG	AR	3850	1/1	0.87	0.25	11,11,11,11	0
85	MG	AR	3858	1/1	0.87	0.25	22,22,22,22	0
84	OHX	6	2023	7/7	0.87	0.12	201,203,204,205	0
84	OHX	1	3682	7/7	0.87	0.11	204,206,207,207	0
85	MG	1	3970	1/1	0.87	0.23	59,59,59,59	0
85	MG	6	2079	1/1	0.87	0.28	37,37,37,37	0
84	OHX	6	1962	7/7	0.87	0.16	187,188,189,190	0
85	MG	AR	3958	1/1	0.87	0.12	90,90,90,90	0
85	MG	AR	3969	1/1	0.87	0.14	38,38,38,38	0
84	OHX	6	2050	7/7	0.87	0.14	190,191,192,193	0
85	MG	AR	3996	1/1	0.87	0.16	38,38,38,38	0
85	MG	A	2112	1/1	0.87	0.11	77,77,77,77	0
85	MG	AR	3999	1/1	0.87	0.17	28,28,28,28	0
85	MG	A	2117	1/1	0.87	0.13	52,52,52,52	0
85	MG	6	2091	1/1	0.87	0.23	54,54,54,54	0
84	OHX	A	2036	7/7	0.87	0.09	274,277,278,279	0
84	OHX	AT	215	7/7	0.87	0.14	212,213,213,213	0
84	OHX	AT	218	7/7	0.87	0.15	223,224,224,224	0
84	OHX	1	3692	7/7	0.87	0.14	189,190,191,191	0
84	OHX	1	3660	7/7	0.87	0.12	208,209,210,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	4053	1/1	0.87	0.20	50,50,50,50	0
84	OHX	A	2041	7/7	0.87	0.15	201,203,204,204	0
84	OHX	AR	3686	7/7	0.87	0.16	186,187,187,187	0
85	MG	1	4035	1/1	0.87	0.09	131,131,131,131	0
85	MG	A	2133	1/1	0.87	0.16	54,54,54,54	0
84	OHX	6	2000	7/7	0.87	0.12	210,211,212,213	0
85	MG	AR	4075	1/1	0.87	0.16	35,35,35,35	0
84	OHX	6	2035	7/7	0.87	0.18	157,158,159,159	0
84	OHX	3	208	7/7	0.87	0.13	230,231,232,233	0
85	MG	AR	4092	1/1	0.87	0.25	25,25,25,25	0
85	MG	6	2137	1/1	0.87	0.26	82,82,82,82	0
85	MG	1	4063	1/1	0.87	0.14	55,55,55,55	0
85	MG	6	2147	1/1	0.87	0.20	75,75,75,75	0
84	OHX	AR	3696	7/7	0.87	0.15	176,176,177,178	0
85	MG	A	2151	1/1	0.87	0.23	72,72,72,72	0
85	MG	6	2149	1/1	0.87	0.24	75,75,75,75	0
84	OHX	AR	3601	7/7	0.87	0.17	171,172,173,173	0
84	OHX	1	3670	7/7	0.87	0.16	215,215,217,217	0
84	OHX	1	3649	7/7	0.87	0.10	247,248,249,250	0
85	MG	6	2153	1/1	0.87	0.18	39,39,39,39	0
84	OHX	6	2040	7/7	0.87	0.16	199,200,201,202	0
84	OHX	AR	3629	7/7	0.87	0.11	209,210,211,212	0
84	OHX	AR	3632	7/7	0.87	0.12	227,227,228,228	0
84	OHX	AR	3669	7/7	0.88	0.10	245,246,247,248	0
84	OHX	AR	3628	7/7	0.88	0.15	209,210,211,211	0
84	OHX	AR	3675	7/7	0.88	0.15	210,211,212,212	0
85	MG	AS	221	1/1	0.88	0.11	36,36,36,36	0
84	OHX	A	1952	7/7	0.88	0.15	181,183,185,185	0
84	OHX	AR	3676	7/7	0.88	0.16	196,197,198,198	0
85	MG	AR	3789	1/1	0.88	0.14	36,36,36,36	0
84	OHX	AR	3677	7/7	0.88	0.20	180,180,181,181	0
84	OHX	1	3680	7/7	0.88	0.13	212,212,213,213	0
84	OHX	6	2019	7/7	0.88	0.13	191,192,193,194	0
85	MG	1	3989	1/1	0.88	0.28	20,20,20,20	0
85	MG	AR	3816	1/1	0.88	0.31	27,27,27,27	0
84	OHX	AR	3633	7/7	0.88	0.16	173,173,174,174	0
84	OHX	6	1990	7/7	0.88	0.15	238,238,239,240	0
85	MG	A	2046	1/1	0.88	0.15	56,56,56,56	0
84	OHX	1	3595	7/7	0.88	0.15	190,191,192,192	0
85	MG	A	2051	1/1	0.88	0.20	62,62,62,62	0
85	MG	1	4017	1/1	0.88	0.14	59,59,59,59	0
84	OHX	1	3544	7/7	0.88	0.13	187,188,190,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	c8	201	7/7	0.88	0.12	198,199,200,201	0
85	MG	A	2064	1/1	0.88	0.23	49,49,49,49	0
84	OHX	AR	3735	7/7	0.88	0.13	246,247,248,248	0
85	MG	A	2069	1/1	0.88	0.13	36,36,36,36	0
85	MG	A	2070	1/1	0.88	0.34	59,59,59,59	0
85	MG	A	2071	1/1	0.88	0.25	45,45,45,45	0
85	MG	AR	3856	1/1	0.88	0.33	10,10,10,10	0
85	MG	6	2096	1/1	0.88	0.24	48,48,48,48	0
85	MG	A	2074	1/1	0.88	0.33	38,38,38,38	0
85	MG	AR	3880	1/1	0.88	0.28	20,20,20,20	0
84	OHX	A	1999	7/7	0.88	0.11	214,215,217,217	0
84	OHX	4	212	7/7	0.88	0.17	201,202,202,202	0
84	OHX	1	3602	7/7	0.88	0.14	228,229,229,230	0
84	OHX	6	2057	7/7	0.88	0.09	247,247,250,250	0
85	MG	AR	3911	1/1	0.88	0.32	16,16,16,16	0
85	MG	AR	3923	1/1	0.88	0.22	32,32,32,32	0
84	OHX	AR	3701	7/7	0.88	0.11	207,208,208,208	0
85	MG	AR	3952	1/1	0.88	0.19	28,28,28,28	0
85	MG	AR	3955	1/1	0.88	0.09	32,32,32,32	0
85	MG	AR	3957	1/1	0.88	0.35	37,37,37,37	0
84	OHX	A	2012	7/7	0.88	0.12	218,220,220,222	0
85	MG	1	3773	1/1	0.88	0.27	15,15,15,15	0
84	OHX	AR	3564	7/7	0.88	0.17	189,190,190,190	0
84	OHX	AR	3599	7/7	0.88	0.17	201,202,203,203	0
84	OHX	1	3729	7/7	0.88	0.13	206,207,207,208	0
85	MG	AR	4001	1/1	0.88	0.25	41,41,41,41	0
84	OHX	A	2016	7/7	0.88	0.11	207,209,210,211	0
85	MG	A	2109	1/1	0.88	0.13	50,50,50,50	0
85	MG	6	2133	1/1	0.88	0.20	51,51,51,51	0
85	MG	1	3803	1/1	0.88	0.19	22,22,22,22	0
84	OHX	A	2022	7/7	0.88	0.09	229,230,232,233	0
85	MG	A	2115	1/1	0.88	0.15	85,85,85,85	0
85	MG	1	3810	1/1	0.88	0.15	86,86,86,86	0
85	MG	1	4103	1/1	0.88	0.11	60,60,60,60	0
85	MG	1	3818	1/1	0.88	0.31	19,19,19,19	0
85	MG	A	2120	1/1	0.88	0.17	74,74,74,74	0
85	MG	1	4108	1/1	0.88	0.12	33,33,33,33	0
84	OHX	AT	220	7/7	0.88	0.15	197,197,198,198	0
85	MG	AR	4062	1/1	0.88	0.17	54,54,54,54	0
85	MG	1	4117	1/1	0.88	0.26	26,26,26,26	0
84	OHX	AR	3710	7/7	0.88	0.12	213,215,216,216	0
85	MG	AR	4074	1/1	0.88	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3833	1/1	0.88	0.20	41,41,41,41	0
85	MG	6	2159	1/1	0.88	0.22	39,39,39,39	0
84	OHX	1	3635	7/7	0.88	0.10	219,220,221,222	0
85	MG	1	4142	1/1	0.88	0.46	47,47,47,47	0
85	MG	1	4144	1/1	0.88	0.11	59,59,59,59	0
85	MG	1	4150	1/1	0.88	0.23	73,73,73,73	0
85	MG	1	4159	1/1	0.88	0.07	42,42,42,42	0
84	OHX	6	2012	7/7	0.88	0.13	188,189,190,191	0
85	MG	1	3861	1/1	0.88	0.14	65,65,65,65	0
85	MG	6	2181	1/1	0.88	0.12	78,78,78,78	0
85	MG	6	2182	1/1	0.88	0.14	53,53,53,53	0
84	OHX	A	2028	7/7	0.88	0.10	252,254,254,256	0
84	OHX	AR	3612	7/7	0.88	0.17	182,183,184,184	0
85	MG	A	2152	1/1	0.88	0.25	78,78,78,78	0
85	MG	6	2190	1/1	0.88	0.10	84,84,84,84	0
85	MG	1	4180	1/1	0.88	0.30	55,55,55,55	0
84	OHX	AR	3616	7/7	0.88	0.11	210,210,211,212	0
85	MG	1	3919	1/1	0.88	0.18	30,30,30,30	0
85	MG	3	216	1/1	0.88	0.09	35,35,35,35	0
85	MG	1	3922	1/1	0.88	0.23	15,15,15,15	0
84	OHX	A	2032	7/7	0.88	0.09	234,236,237,239	0
84	OHX	1	3695	7/7	0.88	0.15	200,201,202,202	0
85	MG	6	2156	1/1	0.89	0.07	50,50,50,50	0
84	OHX	AR	3703	7/7	0.89	0.12	214,214,214,214	0
84	OHX	6	2036	7/7	0.89	0.15	172,174,175,176	0
84	OHX	AR	3706	7/7	0.89	0.11	209,210,211,212	0
85	MG	1	3770	1/1	0.89	0.19	11,11,11,11	0
84	OHX	1	3642	7/7	0.89	0.15	193,193,195,195	0
84	OHX	6	1972	7/7	0.89	0.12	196,197,198,199	0
85	MG	6	2167	1/1	0.89	0.13	52,52,52,52	0
84	OHX	A	1991	7/7	0.89	0.13	218,220,221,221	0
84	OHX	1	3605	7/7	0.89	0.15	171,171,172,172	0
85	MG	AR	4209	1/1	0.89	0.09	48,48,48,48	0
84	OHX	AR	3712	7/7	0.89	0.22	183,183,184,184	0
84	OHX	AR	3713	7/7	0.89	0.09	247,247,248,249	0
85	MG	1	4113	1/1	0.89	0.20	54,54,54,54	0
84	OHX	6	1980	7/7	0.89	0.12	206,206,208,208	0
84	OHX	6	1982	7/7	0.89	0.21	171,172,173,174	0
85	MG	1	3813	1/1	0.89	0.19	24,24,24,24	0
85	MG	6	2191	1/1	0.89	0.13	47,47,47,47	0
85	MG	AS	220	1/1	0.89	0.13	42,42,42,42	0
85	MG	1	4134	1/1	0.89	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3817	1/1	0.89	0.26	32,32,32,32	0
84	OHX	AR	3639	7/7	0.89	0.10	211,212,213,213	0
84	OHX	1	3647	7/7	0.89	0.11	203,204,205,206	0
84	OHX	1	3721	7/7	0.89	0.13	191,192,193,193	0
85	MG	1	4154	1/1	0.89	0.10	92,92,92,92	0
85	MG	CE	406	1/1	0.89	0.24	48,48,48,48	0
85	MG	1	4157	1/1	0.89	0.11	37,37,37,37	0
84	OHX	A	2007	7/7	0.89	0.09	275,277,278,279	0
84	OHX	AR	3723	7/7	0.89	0.10	240,241,242,242	0
85	MG	1	3838	1/1	0.89	0.25	20,20,20,20	0
85	MG	1	3840	1/1	0.89	0.07	39,39,39,39	0
85	MG	AR	3772	1/1	0.89	0.12	81,81,81,81	0
84	OHX	6	1998	7/7	0.89	0.10	239,240,243,244	0
85	MG	AR	3788	1/1	0.89	0.16	45,45,45,45	0
85	MG	1	3855	1/1	0.89	0.26	26,26,26,26	0
85	MG	A	2055	1/1	0.89	0.19	48,48,48,48	0
85	MG	AR	3791	1/1	0.89	0.25	32,32,32,32	0
84	OHX	1	3606	7/7	0.89	0.15	193,194,194,195	0
85	MG	1	3867	1/1	0.89	0.20	26,26,26,26	0
85	MG	A	2066	1/1	0.89	0.37	62,62,62,62	0
85	MG	1	4206	1/1	0.89	0.18	28,28,28,28	0
84	OHX	1	3630	7/7	0.89	0.11	199,200,200,201	0
85	MG	1	3900	1/1	0.89	0.35	34,34,34,34	0
85	MG	3	218	1/1	0.89	0.09	49,49,49,49	0
84	OHX	6	2002	7/7	0.89	0.10	218,220,221,221	0
85	MG	AR	3824	1/1	0.89	0.14	62,62,62,62	0
85	MG	1	3913	1/1	0.89	0.22	38,38,38,38	0
85	MG	AR	3828	1/1	0.89	0.15	47,47,47,47	0
85	MG	A	2078	1/1	0.89	0.28	28,28,28,28	0
84	OHX	1	3668	7/7	0.89	0.15	179,179,180,181	0
84	OHX	1	3651	7/7	0.89	0.11	207,208,209,209	0
85	MG	AR	3842	1/1	0.89	0.27	10,10,10,10	0
84	OHX	1	3601	7/7	0.89	0.14	200,200,201,202	0
85	MG	1	3926	1/1	0.89	0.29	21,21,21,21	0
85	MG	A	2087	1/1	0.89	0.16	57,57,57,57	0
85	MG	AR	3851	1/1	0.89	0.20	29,29,29,29	0
84	OHX	1	3618	7/7	0.89	0.14	189,190,191,192	0
85	MG	1	3933	1/1	0.89	0.24	37,37,37,37	0
84	OHX	A	2026	7/7	0.89	0.15	191,192,194,194	0
85	MG	1	3941	1/1	0.89	0.13	36,36,36,36	0
84	OHX	1	3556	7/7	0.89	0.13	180,181,182,183	0
84	OHX	1	3620	7/7	0.89	0.17	208,208,209,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3960	1/1	0.89	0.07	27,27,27,27	0
84	OHX	1	3679	7/7	0.89	0.11	230,231,232,232	0
84	OHX	1	3657	7/7	0.89	0.18	170,171,171,171	0
84	OHX	1	3640	7/7	0.89	0.14	194,195,196,196	0
84	OHX	AG	201	7/7	0.89	0.15	186,187,188,188	0
85	MG	6	2087	1/1	0.89	0.20	28,28,28,28	0
84	OHX	1	3683	7/7	0.89	0.11	197,198,199,199	0
85	MG	6	2093	1/1	0.89	0.17	47,47,47,47	0
85	MG	AR	3963	1/1	0.89	0.26	23,23,23,23	0
85	MG	AR	3967	1/1	0.89	0.22	64,64,64,64	0
84	OHX	AR	3577	7/7	0.89	0.17	201,201,202,202	0
84	OHX	AT	216	7/7	0.89	0.12	193,193,193,193	0
85	MG	1	3990	1/1	0.89	0.20	36,36,36,36	0
85	MG	6	2103	1/1	0.89	0.29	40,40,40,40	0
84	OHX	AR	3581	7/7	0.89	0.18	205,205,205,205	0
85	MG	1	4005	1/1	0.89	0.20	37,37,37,37	0
85	MG	1	4006	1/1	0.89	0.13	33,33,33,33	0
85	MG	6	2115	1/1	0.89	0.25	36,36,36,36	0
84	OHX	AR	3589	7/7	0.89	0.12	186,187,188,189	0
84	OHX	AR	3683	7/7	0.89	0.13	178,179,179,180	0
84	OHX	A	2042	7/7	0.89	0.10	240,242,244,245	0
85	MG	1	4026	1/1	0.89	0.22	44,44,44,44	0
85	MG	1	4031	1/1	0.89	0.09	38,38,38,38	0
85	MG	AR	4056	1/1	0.89	0.18	44,44,44,44	0
84	OHX	AR	3684	7/7	0.89	0.13	181,182,183,183	0
84	OHX	1	3687	7/7	0.89	0.18	196,196,197,197	0
85	MG	AR	4065	1/1	0.89	0.19	54,54,54,54	0
84	OHX	r	301	7/7	0.89	0.17	167,168,168,169	0
85	MG	AR	4070	1/1	0.89	0.11	42,42,42,42	0
85	MG	A	2146	1/1	0.89	0.17	29,29,29,29	0
84	OHX	x	201	7/7	0.89	0.22	169,169,170,170	0
84	OHX	AR	3688	7/7	0.89	0.12	199,200,201,201	0
84	OHX	AR	3692	7/7	0.89	0.14	184,186,186,187	0
85	MG	AR	4077	1/1	0.89	0.22	49,49,49,49	0
84	OHX	6	2031	7/7	0.89	0.12	210,211,213,213	0
84	OHX	1	3716	7/7	0.89	0.11	205,206,208,209	0
85	MG	AR	4091	1/1	0.89	0.17	53,53,53,53	0
84	OHX	6	2034	7/7	0.89	0.10	236,238,239,240	0
85	MG	AR	4093	1/1	0.89	0.19	46,46,46,46	0
85	MG	AR	4096	1/1	0.89	0.19	53,53,53,53	0
84	OHX	AR	3620	7/7	0.89	0.11	180,182,183,184	0
84	OHX	1	3641	7/7	0.89	0.12	195,196,197,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	2155	1/1	0.89	0.14	61,61,61,61	0
85	MG	AR	4100	1/1	0.90	0.28	67,67,67,67	0
85	MG	AR	4106	1/1	0.90	0.22	55,55,55,55	0
85	MG	AR	4109	1/1	0.90	0.21	42,42,42,42	0
85	MG	1	3881	1/1	0.90	0.24	35,35,35,35	0
85	MG	1	3887	1/1	0.90	0.17	49,49,49,49	0
85	MG	AR	4125	1/1	0.90	0.24	62,62,62,62	0
84	OHX	6	1991	7/7	0.90	0.13	184,185,187,187	0
84	OHX	A	2033	7/7	0.90	0.13	210,212,214,214	0
85	MG	1	4168	1/1	0.90	0.24	51,51,51,51	0
85	MG	1	3909	1/1	0.90	0.22	24,24,24,24	0
84	OHX	AR	3644	7/7	0.90	0.14	197,197,198,199	0
84	OHX	AR	3646	7/7	0.90	0.15	167,168,169,169	0
84	OHX	CG	302	7/7	0.90	0.10	210,211,212,213	0
84	OHX	AR	3704	7/7	0.90	0.13	223,224,225,225	0
85	MG	AR	4179	1/1	0.90	0.11	58,58,58,58	0
84	OHX	1	3697	7/7	0.90	0.10	238,240,241,241	0
84	OHX	6	1997	7/7	0.90	0.11	198,199,201,201	0
84	OHX	AR	3554	7/7	0.90	0.14	159,160,161,161	0
84	OHX	1	3698	7/7	0.90	0.14	177,178,178,179	0
85	MG	AR	4211	1/1	0.90	0.16	86,86,86,86	0
84	OHX	AR	3659	7/7	0.90	0.16	195,196,196,197	0
85	MG	AR	3764	1/1	0.90	0.12	27,27,27,27	0
85	MG	AR	3769	1/1	0.90	0.09	35,35,35,35	0
84	OHX	A	1941	7/7	0.90	0.10	195,197,198,198	0
84	OHX	A	1946	7/7	0.90	0.13	212,214,216,217	0
85	MG	AR	4230	1/1	0.90	0.20	68,68,68,68	0
85	MG	AR	3783	1/1	0.90	0.22	15,15,15,15	0
85	MG	AR	4243	1/1	0.90	0.23	22,22,22,22	0
85	MG	AR	4244	1/1	0.90	0.14	44,44,44,44	0
84	OHX	1	3559	7/7	0.90	0.15	182,183,184,184	0
85	MG	1	3963	1/1	0.90	0.13	69,69,69,69	0
85	MG	x	204	1/1	0.90	0.11	18,18,18,18	0
84	OHX	A	1959	7/7	0.90	0.12	180,182,183,184	0
85	MG	AR	3804	1/1	0.90	0.14	36,36,36,36	0
85	MG	AR	3805	1/1	0.90	0.16	39,39,39,39	0
84	OHX	1	3701	7/7	0.90	0.13	181,182,182,182	0
85	MG	AT	231	1/1	0.90	0.12	46,46,46,46	0
85	MG	AR	3807	1/1	0.90	0.12	27,27,27,27	0
85	MG	AR	3809	1/1	0.90	0.14	86,86,86,86	0
85	MG	CK	202	1/1	0.90	0.18	52,52,52,52	0
85	MG	6	2060	1/1	0.90	0.24	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	CP	502	1/1	0.90	0.14	25,25,25,25	0
84	OHX	1	3681	7/7	0.90	0.11	210,211,212,212	0
85	MG	1	3732	1/1	0.90	0.22	27,27,27,27	0
84	OHX	AR	3598	7/7	0.90	0.10	205,206,207,208	0
85	MG	DI	202	1/1	0.90	0.24	32,32,32,32	0
85	MG	1	3738	1/1	0.90	0.19	57,57,57,57	0
84	OHX	1	3608	7/7	0.90	0.14	177,177,179,179	0
84	OHX	1	3650	7/7	0.90	0.12	179,181,181,182	0
84	OHX	1	3686	7/7	0.90	0.12	207,208,209,209	0
85	MG	1	4001	1/1	0.90	0.10	65,65,65,65	0
85	MG	1	4002	1/1	0.90	0.14	104,104,104,104	0
85	MG	1	3753	1/1	0.90	0.16	28,28,28,28	0
85	MG	AR	3845	1/1	0.90	0.28	32,32,32,32	0
84	OHX	A	1990	7/7	0.90	0.11	212,215,216,216	0
84	OHX	AR	3722	7/7	0.90	0.13	200,201,201,202	0
84	OHX	AR	3606	7/7	0.90	0.16	155,156,157,157	0
84	OHX	A	1995	7/7	0.90	0.12	206,207,208,209	0
84	OHX	AR	3673	7/7	0.90	0.19	179,180,180,180	0
85	MG	AR	3864	1/1	0.90	0.24	21,21,21,21	0
85	MG	AR	3875	1/1	0.90	0.12	48,48,48,48	0
85	MG	1	4027	1/1	0.90	0.10	51,51,51,51	0
84	OHX	AR	3674	7/7	0.90	0.14	215,215,216,216	0
85	MG	6	2100	1/1	0.90	0.25	16,16,16,16	0
85	MG	A	2076	1/1	0.90	0.25	50,50,50,50	0
85	MG	AR	3890	1/1	0.90	0.30	33,33,33,33	0
84	OHX	6	2011	7/7	0.90	0.12	205,205,207,207	0
85	MG	1	3781	1/1	0.90	0.14	24,24,24,24	0
85	MG	AR	3905	1/1	0.90	0.25	24,24,24,24	0
85	MG	6	2109	1/1	0.90	0.17	39,39,39,39	0
84	OHX	1	3723	7/7	0.90	0.12	201,202,203,204	0
85	MG	1	3788	1/1	0.90	0.25	34,34,34,34	0
85	MG	AR	3941	1/1	0.90	0.13	46,46,46,46	0
85	MG	AR	3942	1/1	0.90	0.10	45,45,45,45	0
85	MG	1	4040	1/1	0.90	0.20	42,42,42,42	0
85	MG	6	2116	1/1	0.90	0.30	41,41,41,41	0
85	MG	6	2118	1/1	0.90	0.23	54,54,54,54	0
85	MG	6	2120	1/1	0.90	0.27	61,61,61,61	0
85	MG	1	3790	1/1	0.90	0.29	15,15,15,15	0
85	MG	AR	3965	1/1	0.90	0.14	54,54,54,54	0
85	MG	AR	3966	1/1	0.90	0.09	24,24,24,24	0
84	OHX	y	201	7/7	0.90	0.12	204,205,207,208	0
85	MG	AR	3968	1/1	0.90	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	AR	3618	7/7	0.90	0.15	195,196,196,196	0
84	OHX	1	3659	7/7	0.90	0.15	208,210,211,211	0
85	MG	AR	3972	1/1	0.90	0.20	38,38,38,38	0
85	MG	AR	3983	1/1	0.90	0.19	24,24,24,24	0
85	MG	AR	3994	1/1	0.90	0.22	44,44,44,44	0
85	MG	AR	3995	1/1	0.90	0.07	38,38,38,38	0
85	MG	1	3809	1/1	0.90	0.23	23,23,23,23	0
84	OHX	AR	3731	7/7	0.90	0.16	175,176,177,178	0
84	OHX	AR	3681	7/7	0.90	0.10	198,199,200,201	0
85	MG	1	4077	1/1	0.90	0.11	42,42,42,42	0
84	OHX	6	2016	7/7	0.90	0.12	194,194,196,196	0
85	MG	1	4081	1/1	0.90	0.10	35,35,35,35	0
84	OHX	6	1955	7/7	0.90	0.14	191,193,195,196	0
85	MG	1	3821	1/1	0.90	0.14	37,37,37,37	0
85	MG	AR	4032	1/1	0.90	0.17	47,47,47,47	0
84	OHX	1	3564	7/7	0.90	0.11	173,175,175,175	0
85	MG	AR	4037	1/1	0.90	0.23	33,33,33,33	0
84	OHX	1	3566	7/7	0.90	0.17	182,182,183,183	0
84	OHX	6	2024	7/7	0.90	0.11	207,208,210,211	0
84	OHX	1	3570	7/7	0.90	0.13	202,203,204,205	0
84	OHX	AR	3635	7/7	0.90	0.12	173,175,175,175	0
85	MG	A	2136	1/1	0.90	0.10	110,110,110,110	0
84	OHX	AT	211	7/7	0.90	0.17	179,179,180,180	0
85	MG	AR	4063	1/1	0.90	0.12	39,39,39,39	0
85	MG	1	3847	1/1	0.90	0.28	23,23,23,23	0
85	MG	1	4111	1/1	0.90	0.19	62,62,62,62	0
85	MG	AR	4068	1/1	0.90	0.25	25,25,25,25	0
85	MG	AR	4069	1/1	0.90	0.20	53,53,53,53	0
85	MG	1	3852	1/1	0.90	0.28	22,22,22,22	0
84	OHX	AR	3637	7/7	0.90	0.10	204,205,205,205	0
85	MG	1	4119	1/1	0.90	0.09	35,35,35,35	0
84	OHX	1	3575	7/7	0.90	0.15	187,188,189,189	0
85	MG	1	3859	1/1	0.90	0.25	33,33,33,33	0
85	MG	F	301	1/1	0.90	0.18	71,71,71,71	0
85	MG	6	2170	1/1	0.90	0.18	46,46,46,46	0
85	MG	b	101	1/1	0.90	0.11	57,57,57,57	0
84	OHX	1	3665	7/7	0.90	0.10	209,210,211,211	0
85	MG	1	3866	1/1	0.90	0.30	46,46,46,46	0
84	OHX	3	207	7/7	0.90	0.11	188,189,190,191	0
85	MG	1	3878	1/1	0.90	0.15	36,36,36,36	0
85	MG	AR	4094	1/1	0.90	0.18	38,38,38,38	0
84	OHX	AR	3700	7/7	0.90	0.14	174,175,175,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	4114	1/1	0.91	0.12	30,30,30,30	0
85	MG	1	4194	1/1	0.91	0.24	82,82,82,82	0
85	MG	AR	4121	1/1	0.91	0.21	42,42,42,42	0
85	MG	1	3958	1/1	0.91	0.15	54,54,54,54	0
85	MG	1	4204	1/1	0.91	0.33	12,12,12,12	0
85	MG	1	3959	1/1	0.91	0.13	54,54,54,54	0
85	MG	AR	3762	1/1	0.91	0.18	40,40,40,40	0
85	MG	AR	4130	1/1	0.91	0.08	19,19,19,19	0
85	MG	1	4211	1/1	0.91	0.21	21,21,21,21	0
84	OHX	1	3523	7/7	0.91	0.15	157,158,159,160	0
85	MG	1	3758	1/1	0.91	0.24	31,31,31,31	0
84	OHX	6	2056	7/7	0.91	0.10	214,215,217,218	0
85	MG	1	3967	1/1	0.91	0.23	47,47,47,47	0
85	MG	4	226	1/1	0.91	0.10	54,54,54,54	0
84	OHX	1	3568	7/7	0.91	0.11	195,196,196,197	0
84	OHX	AE	201	7/7	0.91	0.12	194,195,195,196	0
85	MG	o	303	1/1	0.91	0.14	38,38,38,38	0
84	OHX	1	3557	7/7	0.91	0.12	186,187,188,188	0
85	MG	t	201	1/1	0.91	0.07	37,37,37,37	0
84	OHX	A	2000	7/7	0.91	0.11	194,195,196,197	0
84	OHX	AR	3526	7/7	0.91	0.11	164,166,167,167	0
84	OHX	AR	3529	7/7	0.91	0.17	161,162,163,163	0
84	OHX	AR	3530	7/7	0.91	0.17	147,148,148,148	0
85	MG	1	3783	1/1	0.91	0.20	27,27,27,27	0
85	MG	6	2062	1/1	0.91	0.21	32,32,32,32	0
85	MG	AR	4223	1/1	0.91	0.09	54,54,54,54	0
84	OHX	AR	3736	7/7	0.91	0.12	184,185,186,187	0
84	OHX	1	3441	7/7	0.91	0.16	168,169,169,170	0
84	OHX	A	2011	7/7	0.91	0.10	208,209,211,211	0
84	OHX	AR	3693	7/7	0.91	0.09	238,239,240,240	0
85	MG	AS	213	1/1	0.91	0.15	40,40,40,40	0
84	OHX	1	3622	7/7	0.91	0.12	211,212,213,213	0
85	MG	6	2072	1/1	0.91	0.14	36,36,36,36	0
84	OHX	AR	3571	7/7	0.91	0.10	194,194,195,195	0
85	MG	1	3808	1/1	0.91	0.21	54,54,54,54	0
84	OHX	3	205	7/7	0.91	0.10	169,171,171,173	0
85	MG	AT	221	1/1	0.91	0.20	26,26,26,26	0
84	OHX	AR	3699	7/7	0.91	0.12	194,195,196,196	0
84	OHX	A	2019	7/7	0.91	0.09	252,253,255,256	0
85	MG	6	2085	1/1	0.91	0.16	40,40,40,40	0
85	MG	AR	3852	1/1	0.91	0.30	18,18,18,18	0
85	MG	6	2086	1/1	0.91	0.21	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	OHX	AR	3579	7/7	0.91	0.15	183,184,185,185	0
85	MG	6	2089	1/1	0.91	0.15	34,34,34,34	0
84	OHX	AR	3650	7/7	0.91	0.13	177,177,178,178	0
85	MG	CP	503	1/1	0.91	0.17	95,95,95,95	0
85	MG	AR	3876	1/1	0.91	0.18	30,30,30,30	0
85	MG	AR	3879	1/1	0.91	0.30	21,21,21,21	0
84	OHX	1	3678	7/7	0.91	0.09	228,228,229,230	0
85	MG	DE	201	1/1	0.91	0.13	55,55,55,55	0
84	OHX	AR	3584	7/7	0.91	0.15	169,169,170,171	0
85	MG	1	3828	1/1	0.91	0.27	29,29,29,29	0
84	OHX	AR	3585	7/7	0.91	0.14	165,166,167,167	0
85	MG	1	3830	1/1	0.91	0.22	60,60,60,60	0
85	MG	1	4050	1/1	0.91	0.20	34,34,34,34	0
85	MG	AR	3895	1/1	0.91	0.22	21,21,21,21	0
85	MG	AR	3900	1/1	0.91	0.22	29,29,29,29	0
85	MG	A	2056	1/1	0.91	0.21	39,39,39,39	0
85	MG	AR	3902	1/1	0.91	0.29	24,24,24,24	0
85	MG	6	2106	1/1	0.91	0.28	32,32,32,32	0
84	OHX	AR	3658	7/7	0.91	0.15	177,177,179,179	0
85	MG	A	2065	1/1	0.91	0.09	31,31,31,31	0
85	MG	AR	3915	1/1	0.91	0.28	20,20,20,20	0
84	OHX	1	3592	7/7	0.91	0.18	166,166,167,167	0
85	MG	AR	3926	1/1	0.91	0.28	10,10,10,10	0
84	OHX	AR	3707	7/7	0.91	0.18	207,207,207,207	0
85	MG	AR	3933	1/1	0.91	0.24	13,13,13,13	0
85	MG	AR	3935	1/1	0.91	0.20	22,22,22,22	0
85	MG	1	4070	1/1	0.91	0.09	37,37,37,37	0
85	MG	6	2112	1/1	0.91	0.27	25,25,25,25	0
84	OHX	AR	3597	7/7	0.91	0.13	176,177,178,178	0
85	MG	AR	3954	1/1	0.91	0.22	36,36,36,36	0
85	MG	1	4074	1/1	0.91	0.11	45,45,45,45	0
85	MG	AR	3956	1/1	0.91	0.12	41,41,41,41	0
84	OHX	CK	201	7/7	0.91	0.12	185,185,186,187	0
85	MG	A	2081	1/1	0.91	0.26	48,48,48,48	0
84	OHX	AR	3709	7/7	0.91	0.20	163,163,164,164	0
85	MG	1	4078	1/1	0.91	0.06	44,44,44,44	0
85	MG	A	2085	1/1	0.91	0.20	47,47,47,47	0
85	MG	6	2123	1/1	0.91	0.14	60,60,60,60	0
84	OHX	6	1988	7/7	0.91	0.10	191,193,195,195	0
84	OHX	6	2020	7/7	0.91	0.14	177,178,179,179	0
85	MG	1	3858	1/1	0.91	0.36	12,12,12,12	0
84	OHX	1	3549	7/7	0.91	0.15	190,190,191,192	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	4095	1/1	0.91	0.17	53,53,53,53	0
84	OHX	DI	201	7/7	0.91	0.14	194,195,195,196	0
85	MG	AR	3976	1/1	0.91	0.16	42,42,42,42	0
84	OHX	1	3610	7/7	0.91	0.10	212,212,212,212	0
85	MG	6	2139	1/1	0.91	0.06	75,75,75,75	0
84	OHX	A	1935	7/7	0.91	0.12	191,193,195,195	0
85	MG	1	3877	1/1	0.91	0.16	44,44,44,44	0
85	MG	AR	3998	1/1	0.91	0.22	18,18,18,18	0
85	MG	1	4105	1/1	0.91	0.28	64,64,64,64	0
85	MG	A	2108	1/1	0.91	0.15	39,39,39,39	0
84	OHX	AR	3714	7/7	0.91	0.13	192,193,193,194	0
84	OHX	A	1943	7/7	0.91	0.15	161,163,164,165	0
85	MG	A	2111	1/1	0.91	0.11	68,68,68,68	0
84	OHX	1	3613	7/7	0.91	0.13	166,166,167,168	0
85	MG	1	4110	1/1	0.91	0.23	37,37,37,37	0
85	MG	1	3884	1/1	0.91	0.27	27,27,27,27	0
84	OHX	1	3634	7/7	0.91	0.10	206,207,207,209	0
85	MG	1	4116	1/1	0.91	0.07	81,81,81,81	0
85	MG	1	3899	1/1	0.91	0.27	12,12,12,12	0
84	OHX	A	1958	7/7	0.91	0.10	206,207,210,210	0
85	MG	AR	4047	1/1	0.91	0.21	30,30,30,30	0
85	MG	AR	4048	1/1	0.91	0.11	33,33,33,33	0
85	MG	AR	4050	1/1	0.91	0.20	46,46,46,46	0
85	MG	1	4125	1/1	0.91	0.13	58,58,58,58	0
85	MG	1	3903	1/1	0.91	0.29	32,32,32,32	0
84	OHX	1	3615	7/7	0.91	0.14	185,186,186,187	0
84	OHX	A	1960	7/7	0.91	0.11	225,226,227,228	0
85	MG	AR	4061	1/1	0.91	0.18	40,40,40,40	0
85	MG	A	2132	1/1	0.91	0.14	71,71,71,71	0
85	MG	1	3910	1/1	0.91	0.18	30,30,30,30	0
84	OHX	AR	3671	7/7	0.91	0.21	166,166,167,167	0
85	MG	AR	4064	1/1	0.91	0.09	30,30,30,30	0
84	OHX	1	3596	7/7	0.91	0.14	183,184,185,185	0
85	MG	A	2137	1/1	0.91	0.15	40,40,40,40	0
84	OHX	1	3691	7/7	0.91	0.10	206,207,208,208	0
84	OHX	1	3708	7/7	0.91	0.09	210,211,211,211	0
84	OHX	AR	3621	7/7	0.91	0.12	208,209,210,211	0
85	MG	1	3745	1/1	0.91	0.27	20,20,20,20	0
85	MG	A	2145	1/1	0.91	0.14	83,83,83,83	0
85	MG	1	3929	1/1	0.91	0.26	20,20,20,20	0
84	OHX	AR	3622	7/7	0.91	0.11	203,203,204,205	0
85	MG	1	3747	1/1	0.91	0.21	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	6	2003	7/7	0.91	0.16	180,182,183,184	0
85	MG	1	3949	1/1	0.91	0.15	41,41,41,41	0
85	MG	1	4179	1/1	0.91	0.16	42,42,42,42	0
85	MG	1	3750	1/1	0.91	0.13	70,70,70,70	0
85	MG	AB	201	1/1	0.91	0.28	15,15,15,15	0
85	MG	1	4181	1/1	0.91	0.06	50,50,50,50	0
85	MG	1	4182	1/1	0.91	0.18	49,49,49,49	0
84	OHX	6	2004	7/7	0.91	0.15	193,194,195,196	0
85	MG	AR	4098	1/1	0.91	0.09	27,27,27,27	0
85	MG	1	4191	1/1	0.91	0.26	22,22,22,22	0
85	MG	AR	3748	1/1	0.91	0.17	41,41,41,41	0
85	MG	AR	4108	1/1	0.91	0.12	25,25,25,25	0
85	MG	AR	3750	1/1	0.91	0.18	19,19,19,19	0
84	OHX	1	3597	7/7	0.92	0.09	237,238,240,240	0
85	MG	1	4192	1/1	0.92	0.19	38,38,38,38	0
85	MG	AR	4112	1/1	0.92	0.14	70,70,70,70	0
84	OHX	1	3639	7/7	0.92	0.13	201,203,203,204	0
84	OHX	AR	3578	7/7	0.92	0.11	188,188,189,189	0
85	MG	AR	4117	1/1	0.92	0.14	53,53,53,53	0
85	MG	AR	4119	1/1	0.92	0.10	77,77,77,77	0
85	MG	1	4203	1/1	0.92	0.31	34,34,34,34	0
85	MG	1	3795	1/1	0.92	0.09	37,37,37,37	0
85	MG	1	3971	1/1	0.92	0.11	63,63,63,63	0
85	MG	AR	4126	1/1	0.92	0.16	73,73,73,73	0
85	MG	1	3975	1/1	0.92	0.12	43,43,43,43	0
85	MG	1	4221	1/1	0.92	0.29	22,22,22,22	0
85	MG	3	210	1/1	0.92	0.15	41,41,41,41	0
85	MG	AR	4138	1/1	0.92	0.16	44,44,44,44	0
85	MG	AR	3784	1/1	0.92	0.14	29,29,29,29	0
85	MG	AR	4145	1/1	0.92	0.17	38,38,38,38	0
85	MG	AR	4147	1/1	0.92	0.16	62,62,62,62	0
84	OHX	6	1977	7/7	0.92	0.10	193,194,196,196	0
85	MG	1	3978	1/1	0.92	0.20	32,32,32,32	0
85	MG	AR	4157	1/1	0.92	0.20	29,29,29,29	0
85	MG	1	3979	1/1	0.92	0.09	47,47,47,47	0
85	MG	AR	3797	1/1	0.92	0.26	18,18,18,18	0
85	MG	1	3981	1/1	0.92	0.27	59,59,59,59	0
85	MG	AR	4172	1/1	0.92	0.12	25,25,25,25	0
84	OHX	AR	3649	7/7	0.92	0.10	207,208,208,208	0
85	MG	4	228	1/1	0.92	0.23	42,42,42,42	0
84	OHX	A	2017	7/7	0.92	0.09	220,223,224,224	0
85	MG	4	233	1/1	0.92	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	4197	1/1	0.92	0.14	29,29,29,29	0
85	MG	AR	4201	1/1	0.92	0.15	31,31,31,31	0
85	MG	AR	3808	1/1	0.92	0.09	33,33,33,33	0
85	MG	1	3806	1/1	0.92	0.21	31,31,31,31	0
84	OHX	1	3609	7/7	0.92	0.11	191,193,194,195	0
84	OHX	AR	3582	7/7	0.92	0.12	166,167,167,168	0
84	OHX	6	2018	7/7	0.92	0.13	186,187,188,189	0
85	MG	t	202	1/1	0.92	0.17	64,64,64,64	0
85	MG	v	302	1/1	0.92	0.20	43,43,43,43	0
85	MG	w	201	1/1	0.92	0.09	33,33,33,33	0
85	MG	AR	4224	1/1	0.92	0.24	26,26,26,26	0
84	OHX	AR	3655	7/7	0.92	0.10	216,218,218,219	0
84	OHX	AR	3656	7/7	0.92	0.10	187,187,189,189	0
84	OHX	1	3587	7/7	0.92	0.15	188,189,189,190	0
84	OHX	AR	3587	7/7	0.92	0.11	175,176,177,177	0
85	MG	AR	3841	1/1	0.92	0.21	25,25,25,25	0
84	OHX	4	206	7/7	0.92	0.16	179,179,180,180	0
85	MG	AS	219	1/1	0.92	0.08	35,35,35,35	0
85	MG	1	4013	1/1	0.92	0.12	56,56,56,56	0
84	OHX	AR	3591	7/7	0.92	0.15	168,169,169,169	0
85	MG	AS	225	1/1	0.92	0.07	67,67,67,67	0
85	MG	AS	227	1/1	0.92	0.20	43,43,43,43	0
85	MG	6	2065	1/1	0.92	0.20	32,32,32,32	0
85	MG	1	4021	1/1	0.92	0.12	29,29,29,29	0
84	OHX	A	2030	7/7	0.92	0.10	208,209,211,212	0
84	OHX	1	3612	7/7	0.92	0.10	173,174,175,175	0
85	MG	AT	226	1/1	0.92	0.19	44,44,44,44	0
85	MG	AR	3857	1/1	0.92	0.16	46,46,46,46	0
85	MG	1	4029	1/1	0.92	0.15	42,42,42,42	0
85	MG	CD	302	1/1	0.92	0.35	39,39,39,39	0
85	MG	AR	3862	1/1	0.92	0.24	20,20,20,20	0
84	OHX	6	2022	7/7	0.92	0.10	235,235,238,239	0
84	OHX	A	1934	7/7	0.92	0.12	176,177,179,179	0
84	OHX	1	3643	7/7	0.92	0.10	192,193,194,194	0
85	MG	6	2077	1/1	0.92	0.27	51,51,51,51	0
84	OHX	A	2035	7/7	0.92	0.15	177,178,180,181	0
85	MG	CQ	203	1/1	0.92	0.17	28,28,28,28	0
85	MG	CQ	204	1/1	0.92	0.14	48,48,48,48	0
85	MG	1	3842	1/1	0.92	0.24	27,27,27,27	0
85	MG	AR	3888	1/1	0.92	0.30	33,33,33,33	0
84	OHX	AR	3665	7/7	0.92	0.13	189,189,189,189	0
85	MG	DD	101	1/1	0.92	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	2082	1/1	0.92	0.29	25,25,25,25	0
85	MG	6	2083	1/1	0.92	0.25	35,35,35,35	0
85	MG	1	4041	1/1	0.92	0.15	38,38,38,38	0
84	OHX	1	3628	7/7	0.92	0.08	234,235,236,237	0
85	MG	A	2047	1/1	0.92	0.18	55,55,55,55	0
85	MG	A	2048	1/1	0.92	0.14	42,42,42,42	0
84	OHX	6	1996	7/7	0.92	0.11	190,191,192,193	0
85	MG	1	4045	1/1	0.92	0.06	62,62,62,62	0
85	MG	1	4047	1/1	0.92	0.34	39,39,39,39	0
85	MG	AR	3908	1/1	0.92	0.27	18,18,18,18	0
84	OHX	A	1951	7/7	0.92	0.10	203,205,207,207	0
85	MG	1	4052	1/1	0.92	0.13	48,48,48,48	0
85	MG	A	2059	1/1	0.92	0.22	25,25,25,25	0
85	MG	A	2062	1/1	0.92	0.25	48,48,48,48	0
84	OHX	1	3629	7/7	0.92	0.15	161,162,162,163	0
85	MG	1	4058	1/1	0.92	0.14	37,37,37,37	0
84	OHX	6	2027	7/7	0.92	0.18	187,188,189,190	0
85	MG	AR	3932	1/1	0.92	0.23	25,25,25,25	0
85	MG	A	2067	1/1	0.92	0.27	32,32,32,32	0
84	OHX	AR	3721	7/7	0.92	0.09	212,213,213,214	0
85	MG	1	4066	1/1	0.92	0.21	66,66,66,66	0
85	MG	AR	3938	1/1	0.92	0.29	20,20,20,20	0
85	MG	1	4068	1/1	0.92	0.09	39,39,39,39	0
84	OHX	1	3589	7/7	0.92	0.13	179,180,181,181	0
85	MG	AR	3945	1/1	0.92	0.20	22,22,22,22	0
84	OHX	A	1966	7/7	0.92	0.12	194,195,196,197	0
85	MG	AR	3953	1/1	0.92	0.19	35,35,35,35	0
85	MG	1	3869	1/1	0.92	0.18	33,33,33,33	0
85	MG	1	3872	1/1	0.92	0.20	23,23,23,23	0
84	OHX	AR	3615	7/7	0.92	0.17	169,170,171,171	0
84	OHX	1	3553	7/7	0.92	0.10	184,185,186,186	0
84	OHX	1	3511	7/7	0.92	0.12	166,167,168,168	0
85	MG	1	3880	1/1	0.92	0.18	29,29,29,29	0
84	OHX	A	1978	7/7	0.92	0.09	210,212,214,214	0
85	MG	1	4091	1/1	0.92	0.14	49,49,49,49	0
84	OHX	A	1979	7/7	0.92	0.10	200,203,204,205	0
85	MG	1	3886	1/1	0.92	0.28	24,24,24,24	0
85	MG	A	2088	1/1	0.92	0.13	66,66,66,66	0
84	OHX	d9	101	7/7	0.92	0.09	234,235,236,237	0
85	MG	1	3889	1/1	0.92	0.27	19,19,19,19	0
85	MG	1	3890	1/1	0.92	0.28	23,23,23,23	0
85	MG	1	3892	1/1	0.92	0.24	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	2134	1/1	0.92	0.15	43,43,43,43	0
85	MG	AR	3988	1/1	0.92	0.06	32,32,32,32	0
85	MG	AR	3990	1/1	0.92	0.14	37,37,37,37	0
85	MG	1	3898	1/1	0.92	0.19	22,22,22,22	0
84	OHX	1	3725	7/7	0.92	0.12	203,204,205,206	0
84	OHX	A	1983	7/7	0.92	0.11	188,190,192,192	0
84	OHX	6	2033	7/7	0.92	0.15	199,200,201,202	0
85	MG	A	2105	1/1	0.92	0.14	71,71,71,71	0
85	MG	A	2106	1/1	0.92	0.16	30,30,30,30	0
85	MG	1	3744	1/1	0.92	0.26	43,43,43,43	0
84	OHX	A	1986	7/7	0.92	0.11	215,218,220,222	0
84	OHX	1	3542	7/7	0.92	0.13	156,157,158,158	0
84	OHX	AR	3623	7/7	0.92	0.11	186,187,188,188	0
85	MG	1	3914	1/1	0.92	0.27	31,31,31,31	0
85	MG	1	3915	1/1	0.92	0.25	19,19,19,19	0
85	MG	A	2113	1/1	0.92	0.07	35,35,35,35	0
85	MG	1	4120	1/1	0.92	0.12	46,46,46,46	0
85	MG	AR	4027	1/1	0.92	0.14	33,33,33,33	0
85	MG	AR	4028	1/1	0.92	0.13	44,44,44,44	0
85	MG	1	3917	1/1	0.92	0.27	18,18,18,18	0
85	MG	1	4129	1/1	0.92	0.11	51,51,51,51	0
84	OHX	AR	3495	7/7	0.92	0.12	163,165,166,166	0
85	MG	AR	4041	1/1	0.92	0.12	47,47,47,47	0
84	OHX	AR	3625	7/7	0.92	0.08	216,216,218,219	0
85	MG	6	2161	1/1	0.92	0.07	51,51,51,51	0
85	MG	AR	4049	1/1	0.92	0.12	74,74,74,74	0
85	MG	A	2126	1/1	0.92	0.09	48,48,48,48	0
84	OHX	AR	3520	7/7	0.92	0.13	175,175,176,176	0
84	OHX	1	3607	7/7	0.92	0.15	190,192,193,193	0
85	MG	1	3757	1/1	0.92	0.17	46,46,46,46	0
85	MG	6	2165	1/1	0.92	0.16	45,45,45,45	0
85	MG	6	2166	1/1	0.92	0.10	36,36,36,36	0
84	OHX	1	3636	7/7	0.92	0.14	170,171,172,172	0
84	OHX	1	3637	7/7	0.92	0.13	180,181,181,181	0
85	MG	6	2171	1/1	0.92	0.10	34,34,34,34	0
84	OHX	AR	3543	7/7	0.92	0.15	181,181,182,182	0
85	MG	1	3937	1/1	0.92	0.32	58,58,58,58	0
85	MG	1	3939	1/1	0.92	0.07	29,29,29,29	0
85	MG	1	4162	1/1	0.92	0.27	118,118,118,118	0
84	OHX	AR	3545	7/7	0.92	0.12	181,182,182,183	0
85	MG	1	3946	1/1	0.92	0.15	68,68,68,68	0
84	OHX	AR	3690	7/7	0.92	0.10	179,179,180,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	4171	1/1	0.92	0.04	26,26,26,26	0
84	OHX	A	2004	7/7	0.92	0.10	192,194,196,196	0
85	MG	1	4174	1/1	0.92	0.22	54,54,54,54	0
85	MG	1	3954	1/1	0.92	0.13	45,45,45,45	0
85	MG	AR	4086	1/1	0.92	0.12	28,28,28,28	0
84	OHX	6	1964	7/7	0.92	0.12	175,175,177,177	0
85	MG	6	2198	1/1	0.92	0.16	53,53,53,53	0
84	OHX	AR	3558	7/7	0.92	0.17	159,160,160,160	0
84	OHX	6	1971	7/7	0.92	0.11	177,178,179,180	0
85	MG	1	3782	1/1	0.92	0.25	44,44,44,44	0
84	OHX	AR	3566	7/7	0.92	0.09	205,206,207,207	0
85	MG	c6	201	1/1	0.92	0.23	67,67,67,67	0
85	MG	1	4184	1/1	0.92	0.10	55,55,55,55	0
85	MG	1	4185	1/1	0.92	0.17	48,48,48,48	0
85	MG	AR	4101	1/1	0.92	0.12	48,48,48,48	0
85	MG	AR	4102	1/1	0.92	0.14	24,24,24,24	0
85	MG	1	4189	1/1	0.92	0.21	48,48,48,48	0
85	MG	AR	3766	1/1	0.93	0.18	21,21,21,21	0
84	OHX	1	3673	7/7	0.93	0.11	192,193,194,194	0
85	MG	AR	4115	1/1	0.93	0.15	64,64,64,64	0
85	MG	1	4213	1/1	0.93	0.09	36,36,36,36	0
85	MG	1	4214	1/1	0.93	0.11	50,50,50,50	0
85	MG	1	3984	1/1	0.93	0.17	33,33,33,33	0
85	MG	1	3985	1/1	0.93	0.12	22,22,22,22	0
85	MG	AR	3787	1/1	0.93	0.09	31,31,31,31	0
85	MG	1	3986	1/1	0.93	0.22	30,30,30,30	0
85	MG	1	3805	1/1	0.93	0.15	60,60,60,60	0
84	OHX	1	3528	7/7	0.93	0.14	169,170,171,171	0
84	OHX	1	3550	7/7	0.93	0.10	196,197,198,199	0
85	MG	AR	3801	1/1	0.93	0.24	30,30,30,30	0
85	MG	4	217	1/1	0.93	0.22	44,44,44,44	0
85	MG	4	224	1/1	0.93	0.06	51,51,51,51	0
85	MG	AR	4142	1/1	0.93	0.15	55,55,55,55	0
85	MG	AR	4143	1/1	0.93	0.18	38,38,38,38	0
85	MG	1	3992	1/1	0.93	0.16	53,53,53,53	0
84	OHX	A	2010	7/7	0.93	0.10	192,195,197,197	0
84	OHX	AR	3662	7/7	0.93	0.17	168,169,169,170	0
85	MG	AR	4153	1/1	0.93	0.13	52,52,52,52	0
84	OHX	AR	3586	7/7	0.93	0.09	182,184,185,185	0
85	MG	1	3814	1/1	0.93	0.20	39,39,39,39	0
85	MG	AR	4159	1/1	0.93	0.06	64,64,64,64	0
85	MG	AR	4162	1/1	0.93	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3816	1/1	0.93	0.27	28,28,28,28	0
85	MG	AR	4166	1/1	0.93	0.10	58,58,58,58	0
84	OHX	1	3531	7/7	0.93	0.15	179,180,181,181	0
85	MG	AR	3815	1/1	0.93	0.08	75,75,75,75	0
84	OHX	AR	3588	7/7	0.93	0.12	176,177,178,178	0
85	MG	AR	4173	1/1	0.93	0.15	38,38,38,38	0
84	OHX	1	3604	7/7	0.93	0.09	204,205,206,206	0
84	OHX	1	3577	7/7	0.93	0.11	177,178,179,179	0
84	OHX	AR	3593	7/7	0.93	0.13	173,174,174,174	0
85	MG	1	4023	1/1	0.93	0.16	44,44,44,44	0
85	MG	x	205	1/1	0.93	0.25	20,20,20,20	0
85	MG	1	4025	1/1	0.93	0.15	34,34,34,34	0
85	MG	AR	4203	1/1	0.93	0.11	37,37,37,37	0
85	MG	AR	3834	1/1	0.93	0.09	30,30,30,30	0
85	MG	AR	3835	1/1	0.93	0.12	41,41,41,41	0
85	MG	z	203	1/1	0.93	0.19	45,45,45,45	0
85	MG	AR	3840	1/1	0.93	0.19	22,22,22,22	0
85	MG	AR	4216	1/1	0.93	0.10	67,67,67,67	0
85	MG	l2	202	1/1	0.93	0.10	48,48,48,48	0
84	OHX	1	3584	7/7	0.93	0.13	154,155,156,156	0
84	OHX	A	2020	7/7	0.93	0.12	188,191,192,192	0
85	MG	AR	4221	1/1	0.93	0.11	49,49,49,49	0
85	MG	1	3831	1/1	0.93	0.12	42,42,42,42	0
85	MG	1	4030	1/1	0.93	0.19	45,45,45,45	0
85	MG	AR	4225	1/1	0.93	0.19	23,23,23,23	0
85	MG	AR	4227	1/1	0.93	0.26	18,18,18,18	0
85	MG	AR	4228	1/1	0.93	0.23	12,12,12,12	0
85	MG	AR	4229	1/1	0.93	0.23	23,23,23,23	0
84	OHX	A	2021	7/7	0.93	0.11	176,177,179,179	0
85	MG	AR	4233	1/1	0.93	0.15	55,55,55,55	0
84	OHX	k	401	7/7	0.93	0.12	169,170,170,170	0
85	MG	AR	4242	1/1	0.93	0.23	56,56,56,56	0
85	MG	AR	3853	1/1	0.93	0.28	17,17,17,17	0
84	OHX	AS	209	7/7	0.93	0.14	175,176,177,177	0
85	MG	1	3839	1/1	0.93	0.34	7,7,7,7	0
84	OHX	1	3555	7/7	0.93	0.09	190,191,192,192	0
85	MG	AS	216	1/1	0.93	0.18	41,41,41,41	0
84	OHX	AT	206	7/7	0.93	0.13	155,155,156,156	0
84	OHX	AR	3600	7/7	0.93	0.11	172,173,173,174	0
85	MG	AR	3867	1/1	0.93	0.28	13,13,13,13	0
85	MG	AS	223	1/1	0.93	0.11	59,59,59,59	0
84	OHX	1	3588	7/7	0.93	0.13	168,169,170,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	1	3536	7/7	0.93	0.09	221,221,223,224	0
84	OHX	AR	3603	7/7	0.93	0.11	182,183,184,185	0
85	MG	6	2078	1/1	0.93	0.22	25,25,25,25	0
84	OHX	AR	3605	7/7	0.93	0.10	194,195,196,196	0
84	OHX	AR	3679	7/7	0.93	0.08	218,220,221,221	0
85	MG	AT	225	1/1	0.93	0.12	60,60,60,60	0
84	OHX	1	3684	7/7	0.93	0.10	170,171,172,173	0
84	OHX	AR	3608	7/7	0.93	0.10	186,187,188,188	0
85	MG	AT	229	1/1	0.93	0.11	30,30,30,30	0
84	OHX	1	3590	7/7	0.93	0.10	208,209,210,211	0
85	MG	1	4060	1/1	0.93	0.34	16,16,16,16	0
84	OHX	CG	301	7/7	0.93	0.09	191,193,193,195	0
85	MG	1	3870	1/1	0.93	0.24	11,11,11,11	0
85	MG	AR	3901	1/1	0.93	0.29	17,17,17,17	0
85	MG	6	2088	1/1	0.93	0.20	30,30,30,30	0
84	OHX	AR	3611	7/7	0.93	0.08	194,196,197,197	0
84	OHX	1	3611	7/7	0.93	0.09	184,185,185,186	0
85	MG	CQ	201	1/1	0.93	0.20	23,23,23,23	0
84	OHX	AR	3613	7/7	0.93	0.16	165,166,167,167	0
85	MG	1	4072	1/1	0.93	0.16	55,55,55,55	0
84	OHX	AR	3614	7/7	0.93	0.14	164,165,165,166	0
84	OHX	6	1941	7/7	0.93	0.14	158,159,160,161	0
85	MG	AR	3928	1/1	0.93	0.15	10,10,10,10	0
85	MG	DC	201	1/1	0.93	0.12	16,16,16,16	0
85	MG	1	4075	1/1	0.93	0.10	20,20,20,20	0
84	OHX	1	3591	7/7	0.93	0.12	185,186,187,188	0
85	MG	DG	202	1/1	0.93	0.14	21,21,21,21	0
84	OHX	AR	3689	7/7	0.93	0.09	195,197,198,198	0
85	MG	AR	3934	1/1	0.93	0.20	14,14,14,14	0
85	MG	DR	503	1/1	0.93	0.20	54,54,54,54	0
85	MG	sM	201	1/1	0.93	0.15	41,41,41,41	0
84	OHX	6	1960	7/7	0.93	0.14	155,157,157,158	0
85	MG	AR	3936	1/1	0.93	0.23	20,20,20,20	0
84	OHX	1	3539	7/7	0.93	0.13	169,169,170,170	0
85	MG	AR	3939	1/1	0.93	0.39	16,16,16,16	0
85	MG	1	3888	1/1	0.93	0.10	21,21,21,21	0
85	MG	A	2053	1/1	0.93	0.23	39,39,39,39	0
84	OHX	M	201	7/7	0.93	0.10	202,204,205,206	0
84	OHX	A	1930	7/7	0.93	0.13	164,165,166,167	0
85	MG	AR	3951	1/1	0.93	0.14	26,26,26,26	0
84	OHX	A	1932	7/7	0.93	0.11	178,180,182,182	0
85	MG	1	3893	1/1	0.93	0.26	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	A	2061	1/1	0.93	0.13	27,27,27,27	0
84	OHX	s8	301	7/7	0.93	0.09	214,216,216,218	0
84	OHX	1	3662	7/7	0.93	0.11	178,179,180,180	0
84	OHX	6	1966	7/7	0.93	0.13	164,165,166,167	0
84	OHX	AR	3477	7/7	0.93	0.18	119,119,119,120	0
84	OHX	1	3614	7/7	0.93	0.08	199,200,201,203	0
85	MG	AR	3962	1/1	0.93	0.11	43,43,43,43	0
84	OHX	sR	401	7/7	0.93	0.09	215,216,219,219	0
84	OHX	1	3594	7/7	0.93	0.14	150,150,151,151	0
85	MG	1	3735	1/1	0.93	0.13	39,39,39,39	0
84	OHX	AR	3626	7/7	0.93	0.09	204,205,205,205	0
85	MG	6	2130	1/1	0.93	0.11	42,42,42,42	0
84	OHX	AR	3627	7/7	0.93	0.11	173,173,174,174	0
85	MG	1	4112	1/1	0.93	0.09	41,41,41,41	0
85	MG	1	3743	1/1	0.93	0.19	23,23,23,23	0
85	MG	6	2138	1/1	0.93	0.19	49,49,49,49	0
85	MG	AR	3979	1/1	0.93	0.12	45,45,45,45	0
85	MG	AR	3980	1/1	0.93	0.16	32,32,32,32	0
85	MG	1	4115	1/1	0.93	0.11	97,97,97,97	0
85	MG	AR	3984	1/1	0.93	0.13	49,49,49,49	0
85	MG	A	2082	1/1	0.93	0.17	65,65,65,65	0
85	MG	AR	3986	1/1	0.93	0.27	41,41,41,41	0
85	MG	6	2141	1/1	0.93	0.11	56,56,56,56	0
84	OHX	6	1973	7/7	0.93	0.13	161,162,163,163	0
84	OHX	1	3616	7/7	0.93	0.14	177,177,178,178	0
85	MG	1	4118	1/1	0.93	0.17	87,87,87,87	0
85	MG	1	3920	1/1	0.93	0.21	29,29,29,29	0
84	OHX	1	3521	7/7	0.93	0.13	144,145,147,147	0
85	MG	1	3925	1/1	0.93	0.21	15,15,15,15	0
85	MG	1	4128	1/1	0.93	0.08	27,27,27,27	0
84	OHX	AR	3535	7/7	0.93	0.13	157,157,158,158	0
85	MG	AR	4005	1/1	0.93	0.17	24,24,24,24	0
85	MG	AR	4014	1/1	0.93	0.19	32,32,32,32	0
85	MG	AR	4015	1/1	0.93	0.23	43,43,43,43	0
84	OHX	AR	3539	7/7	0.93	0.11	169,170,172,172	0
85	MG	A	2100	1/1	0.93	0.25	60,60,60,60	0
85	MG	A	2101	1/1	0.93	0.20	64,64,64,64	0
85	MG	AR	4018	1/1	0.93	0.16	40,40,40,40	0
84	OHX	AR	3540	7/7	0.93	0.13	151,152,153,154	0
85	MG	AR	4023	1/1	0.93	0.09	36,36,36,36	0
85	MG	1	3930	1/1	0.93	0.21	19,19,19,19	0
85	MG	AR	4025	1/1	0.93	0.18	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	1	3504	7/7	0.93	0.12	154,156,157,158	0
84	OHX	1	3644	7/7	0.93	0.12	170,171,173,173	0
85	MG	1	3754	1/1	0.93	0.31	38,38,38,38	0
85	MG	AR	4029	1/1	0.93	0.07	32,32,32,32	0
85	MG	1	4146	1/1	0.93	0.06	39,39,39,39	0
84	OHX	6	1983	7/7	0.93	0.12	169,169,170,170	0
84	OHX	AR	3555	7/7	0.93	0.13	148,149,149,150	0
85	MG	AR	4039	1/1	0.93	0.17	37,37,37,37	0
85	MG	AR	4040	1/1	0.93	0.14	27,27,27,27	0
85	MG	A	2116	1/1	0.93	0.12	49,49,49,49	0
85	MG	1	4155	1/1	0.93	0.23	66,66,66,66	0
85	MG	AR	4045	1/1	0.93	0.05	33,33,33,33	0
84	OHX	1	3700	7/7	0.93	0.17	161,162,163,163	0
85	MG	1	3947	1/1	0.93	0.13	34,34,34,34	0
85	MG	1	4161	1/1	0.93	0.11	37,37,37,37	0
85	MG	1	3760	1/1	0.93	0.38	26,26,26,26	0
85	MG	AR	4051	1/1	0.93	0.12	62,62,62,62	0
84	OHX	AR	3642	7/7	0.93	0.13	189,189,191,191	0
85	MG	1	3952	1/1	0.93	0.06	34,34,34,34	0
84	OHX	AR	3559	7/7	0.93	0.11	177,178,179,179	0
85	MG	AR	4058	1/1	0.93	0.14	57,57,57,57	0
85	MG	1	4170	1/1	0.93	0.07	33,33,33,33	0
84	OHX	AR	3561	7/7	0.93	0.10	171,171,172,172	0
84	OHX	6	1989	7/7	0.93	0.13	169,170,172,172	0
85	MG	6	2185	1/1	0.93	0.10	60,60,60,60	0
85	MG	6	2188	1/1	0.93	0.24	55,55,55,55	0
84	OHX	AR	3648	7/7	0.93	0.10	196,197,198,198	0
84	OHX	1	3548	7/7	0.93	0.10	179,180,181,181	0
85	MG	1	3778	1/1	0.93	0.11	20,20,20,20	0
85	MG	6	2192	1/1	0.93	0.16	54,54,54,54	0
85	MG	1	3964	1/1	0.93	0.13	51,51,51,51	0
84	OHX	1	3598	7/7	0.93	0.13	173,173,174,175	0
85	MG	6	2196	1/1	0.93	0.05	46,46,46,46	0
84	OHX	AR	3573	7/7	0.93	0.14	178,178,179,180	0
84	OHX	AR	3574	7/7	0.93	0.12	171,172,173,173	0
85	MG	9	201	1/1	0.93	0.15	33,33,33,33	0
85	MG	1	3785	1/1	0.93	0.20	21,21,21,21	0
85	MG	AB	203	1/1	0.93	0.08	37,37,37,37	0
85	MG	A	2150	1/1	0.93	0.06	52,52,52,52	0
84	OHX	AR	3653	7/7	0.93	0.15	178,178,179,179	0
85	MG	1	4186	1/1	0.93	0.19	51,51,51,51	0
85	MG	1	4188	1/1	0.93	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3972	1/1	0.93	0.22	31,31,31,31	0
85	MG	1	3973	1/1	0.93	0.18	33,33,33,33	0
84	OHX	6	1992	7/7	0.93	0.12	185,186,187,188	0
84	OHX	A	2001	7/7	0.93	0.12	185,188,189,189	0
85	MG	1	4195	1/1	0.93	0.21	52,52,52,52	0
84	OHX	1	3672	7/7	0.93	0.14	161,162,164,164	0
85	MG	d3	202	1/1	0.93	0.25	56,56,56,56	0
84	OHX	6	1995	7/7	0.93	0.10	171,173,174,175	0
85	MG	d6	101	1/1	0.93	0.20	37,37,37,37	0
85	MG	AR	4107	1/1	0.93	0.11	79,79,79,79	0
85	MG	1	3980	1/1	0.93	0.11	19,19,19,19	0
84	OHX	3	206	7/7	0.93	0.11	176,177,179,179	0
85	MG	1	3999	1/1	0.94	0.09	38,38,38,38	0
85	MG	1	3865	1/1	0.94	0.22	13,13,13,13	0
84	OHX	A	1998	7/7	0.94	0.09	213,217,219,219	0
85	MG	AR	4204	1/1	0.94	0.04	31,31,31,31	0
85	MG	AR	3910	1/1	0.94	0.19	17,17,17,17	0
85	MG	AR	4210	1/1	0.94	0.12	33,33,33,33	0
84	OHX	AT	217	7/7	0.94	0.10	184,185,185,186	0
85	MG	AR	4213	1/1	0.94	0.09	34,34,34,34	0
85	MG	AR	3912	1/1	0.94	0.25	1,1,1,1	0
85	MG	AR	3914	1/1	0.94	0.21	13,13,13,13	0
85	MG	6	2140	1/1	0.94	0.16	46,46,46,46	0
85	MG	AR	3920	1/1	0.94	0.14	19,19,19,19	0
85	MG	AR	3922	1/1	0.94	0.23	20,20,20,20	0
85	MG	AR	4219	1/1	0.94	0.15	47,47,47,47	0
84	OHX	1	3685	7/7	0.94	0.14	173,173,175,175	0
85	MG	6	2142	1/1	0.94	0.13	72,72,72,72	0
84	OHX	1	3491	7/7	0.94	0.15	138,138,139,139	0
85	MG	AR	3929	1/1	0.94	0.18	75,75,75,75	0
85	MG	6	2146	1/1	0.94	0.12	44,44,44,44	0
84	OHX	3	202	7/7	0.94	0.13	176,177,177,178	0
85	MG	1	3874	1/1	0.94	0.23	19,19,19,19	0
85	MG	1	4016	1/1	0.94	0.04	11,11,11,11	0
85	MG	1	3875	1/1	0.94	0.17	18,18,18,18	0
85	MG	1	3748	1/1	0.94	0.16	23,23,23,23	0
85	MG	AR	4234	1/1	0.94	0.17	17,17,17,17	0
84	OHX	1	3576	7/7	0.94	0.10	189,189,191,191	0
85	MG	1	4024	1/1	0.94	0.14	15,15,15,15	0
84	OHX	1	3690	7/7	0.94	0.10	174,175,176,176	0
84	OHX	1	3512	7/7	0.94	0.10	170,172,172,173	0
85	MG	AS	212	1/1	0.94	0.16	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	OHX	6	1956	7/7	0.94	0.12	192,194,195,196	0
85	MG	AR	3949	1/1	0.94	0.17	19,19,19,19	0
85	MG	1	3883	1/1	0.94	0.26	17,17,17,17	0
85	MG	1	4200	1/1	0.94	0.24	18,18,18,18	0
84	OHX	6	1994	7/7	0.94	0.11	168,169,171,171	0
84	OHX	AR	3619	7/7	0.94	0.12	169,169,170,170	0
84	OHX	6	1958	7/7	0.94	0.12	153,153,155,156	0
84	OHX	1	3631	7/7	0.94	0.09	198,199,199,199	0
85	MG	1	4210	1/1	0.94	0.14	32,32,32,32	0
84	OHX	AR	3667	7/7	0.94	0.07	207,209,210,210	0
84	OHX	AR	3575	7/7	0.94	0.10	156,158,159,159	0
85	MG	1	3765	1/1	0.94	0.11	41,41,41,41	0
85	MG	1	4217	1/1	0.94	0.18	18,18,18,18	0
85	MG	1	4220	1/1	0.94	0.17	25,25,25,25	0
85	MG	1	3767	1/1	0.94	0.11	34,34,34,34	0
85	MG	1	3768	1/1	0.94	0.21	24,24,24,24	0
85	MG	3	214	1/1	0.94	0.26	12,12,12,12	0
84	OHX	AR	3576	7/7	0.94	0.11	168,169,169,170	0
85	MG	AR	3971	1/1	0.94	0.08	38,38,38,38	0
84	OHX	4	201	7/7	0.94	0.12	143,143,144,144	0
84	OHX	4	205	7/7	0.94	0.09	172,173,174,174	0
84	OHX	A	2018	7/7	0.94	0.08	214,215,216,217	0
85	MG	3	220	1/1	0.94	0.09	31,31,31,31	0
84	OHX	A	1927	7/7	0.94	0.12	158,160,162,162	0
85	MG	4	223	1/1	0.94	0.13	44,44,44,44	0
85	MG	1	4055	1/1	0.94	0.16	33,33,33,33	0
85	MG	4	225	1/1	0.94	0.12	43,43,43,43	0
85	MG	1	3777	1/1	0.94	0.07	40,40,40,40	0
85	MG	CR	201	1/1	0.94	0.27	14,14,14,14	0
85	MG	4	227	1/1	0.94	0.07	42,42,42,42	0
85	MG	CR	204	1/1	0.94	0.12	46,46,46,46	0
85	MG	1	3911	1/1	0.94	0.19	20,20,20,20	0
85	MG	1	3912	1/1	0.94	0.28	30,30,30,30	0
85	MG	4	231	1/1	0.94	0.10	30,30,30,30	0
85	MG	DC	204	1/1	0.94	0.12	45,45,45,45	0
84	OHX	1	3580	7/7	0.94	0.11	162,164,164,165	0
85	MG	AR	4000	1/1	0.94	0.21	30,30,30,30	0
85	MG	1	3779	1/1	0.94	0.09	29,29,29,29	0
85	MG	AF	202	1/1	0.94	0.13	32,32,32,32	0
84	OHX	6	1970	7/7	0.94	0.11	178,179,180,180	0
85	MG	AR	4009	1/1	0.94	0.19	25,25,25,25	0
85	MG	AR	4013	1/1	0.94	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	1	3581	7/7	0.94	0.14	153,153,154,154	0
85	MG	i	201	1/1	0.94	0.15	57,57,57,57	0
84	OHX	1	3552	7/7	0.94	0.12	173,174,175,175	0
85	MG	A	2049	1/1	0.94	0.14	35,35,35,35	0
85	MG	AR	3743	1/1	0.94	0.08	41,41,41,41	0
85	MG	AR	3744	1/1	0.94	0.23	20,20,20,20	0
85	MG	A	2052	1/1	0.94	0.22	27,27,27,27	0
85	MG	AR	4021	1/1	0.94	0.09	36,36,36,36	0
85	MG	AR	4022	1/1	0.94	0.09	41,41,41,41	0
85	MG	1	3784	1/1	0.94	0.13	30,30,30,30	0
84	OHX	AR	3494	7/7	0.94	0.13	144,145,146,146	0
85	MG	AR	3749	1/1	0.94	0.24	19,19,19,19	0
84	OHX	1	3517	7/7	0.94	0.15	141,142,143,143	0
85	MG	AR	3752	1/1	0.94	0.20	16,16,16,16	0
84	OHX	A	1945	7/7	0.94	0.08	201,203,204,205	0
85	MG	AR	3755	1/1	0.94	0.18	34,34,34,34	0
84	OHX	AR	3500	7/7	0.94	0.11	136,138,139,140	0
85	MG	x	206	1/1	0.94	0.14	32,32,32,32	0
85	MG	1	3792	1/1	0.94	0.15	16,16,16,16	0
84	OHX	A	1947	7/7	0.94	0.12	162,164,165,165	0
85	MG	1	3798	1/1	0.94	0.19	29,29,29,29	0
85	MG	AR	3765	1/1	0.94	0.20	23,23,23,23	0
85	MG	AR	4043	1/1	0.94	0.08	48,48,48,48	0
84	OHX	6	1974	7/7	0.94	0.13	176,176,178,178	0
85	MG	6	2059	1/1	0.94	0.19	40,40,40,40	0
84	OHX	AR	3523	7/7	0.94	0.12	175,176,176,177	0
84	OHX	A	1956	7/7	0.94	0.12	171,173,174,175	0
85	MG	AR	3778	1/1	0.94	0.23	42,42,42,42	0
85	MG	1	3938	1/1	0.94	0.08	41,41,41,41	0
84	OHX	AR	3524	7/7	0.94	0.12	152,153,154,155	0
84	OHX	AR	3592	7/7	0.94	0.14	151,152,152,153	0
85	MG	1	3807	1/1	0.94	0.11	37,37,37,37	0
84	OHX	1	3646	7/7	0.94	0.09	182,183,184,185	0
84	OHX	A	1962	7/7	0.94	0.12	175,176,177,178	0
85	MG	AR	4060	1/1	0.94	0.10	56,56,56,56	0
85	MG	AR	3794	1/1	0.94	0.13	19,19,19,19	0
85	MG	6	2070	1/1	0.94	0.27	17,17,17,17	0
85	MG	AR	3799	1/1	0.94	0.11	83,83,83,83	0
84	OHX	AR	3594	7/7	0.94	0.14	169,170,171,171	0
84	OHX	A	1967	7/7	0.94	0.11	167,168,169,170	0
85	MG	6	2073	1/1	0.94	0.27	57,57,57,57	0
85	MG	A	2090	1/1	0.94	0.16	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	6	2009	7/7	0.94	0.14	181,181,183,183	0
84	OHX	A	1970	7/7	0.94	0.15	178,180,182,182	0
85	MG	6	2076	1/1	0.94	0.22	18,18,18,18	0
85	MG	1	3956	1/1	0.94	0.16	15,15,15,15	0
84	OHX	AR	3643	7/7	0.94	0.10	157,158,159,160	0
85	MG	A	2097	1/1	0.94	0.23	55,55,55,55	0
85	MG	AR	3810	1/1	0.94	0.23	28,28,28,28	0
85	MG	AR	3811	1/1	0.94	0.14	25,25,25,25	0
85	MG	AR	4079	1/1	0.94	0.18	36,36,36,36	0
85	MG	AR	4083	1/1	0.94	0.24	23,23,23,23	0
84	OHX	A	1973	7/7	0.94	0.10	201,204,206,208	0
84	OHX	1	3573	7/7	0.94	0.10	196,196,197,197	0
85	MG	1	3961	1/1	0.94	0.14	26,26,26,26	0
85	MG	1	3822	1/1	0.94	0.17	22,22,22,22	0
84	OHX	AR	3645	7/7	0.94	0.13	174,175,176,176	0
85	MG	6	2084	1/1	0.94	0.10	35,35,35,35	0
85	MG	AR	3821	1/1	0.94	0.20	26,26,26,26	0
85	MG	AR	3823	1/1	0.94	0.19	15,15,15,15	0
85	MG	1	3826	1/1	0.94	0.16	44,44,44,44	0
84	OHX	6	1978	7/7	0.94	0.11	176,178,180,181	0
84	OHX	AR	3691	7/7	0.94	0.13	170,171,172,172	0
85	MG	1	3969	1/1	0.94	0.15	45,45,45,45	0
85	MG	1	4126	1/1	0.94	0.17	30,30,30,30	0
85	MG	1	4127	1/1	0.94	0.09	58,58,58,58	0
85	MG	AR	3836	1/1	0.94	0.24	15,15,15,15	0
85	MG	6	2092	1/1	0.94	0.13	45,45,45,45	0
84	OHX	A	1981	7/7	0.94	0.08	231,234,235,236	0
85	MG	6	2095	1/1	0.94	0.23	32,32,32,32	0
84	OHX	A	1982	7/7	0.94	0.10	164,166,167,167	0
85	MG	1	3832	1/1	0.94	0.23	13,13,13,13	0
85	MG	AR	3846	1/1	0.94	0.30	17,17,17,17	0
85	MG	1	4131	1/1	0.94	0.06	38,38,38,38	0
84	OHX	e	101	7/7	0.94	0.08	205,208,210,210	0
84	OHX	AR	3538	7/7	0.94	0.10	184,185,186,186	0
85	MG	1	4135	1/1	0.94	0.14	64,64,64,64	0
84	OHX	6	1979	7/7	0.94	0.12	165,165,166,167	0
85	MG	1	4138	1/1	0.94	0.14	37,37,37,37	0
85	MG	1	4139	1/1	0.94	0.05	29,29,29,29	0
84	OHX	1	3627	7/7	0.94	0.09	176,176,178,179	0
85	MG	AR	4131	1/1	0.94	0.27	59,59,59,59	0
85	MG	AR	4133	1/1	0.94	0.17	35,35,35,35	0
84	OHX	AR	3541	7/7	0.94	0.10	170,171,172,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	AR	3604	7/7	0.94	0.12	150,151,151,151	0
85	MG	AR	3866	1/1	0.94	0.18	20,20,20,20	0
84	OHX	AT	209	7/7	0.94	0.12	163,163,163,163	0
85	MG	1	3851	1/1	0.94	0.08	34,34,34,34	0
85	MG	1	3983	1/1	0.94	0.18	59,59,59,59	0
85	MG	AR	4151	1/1	0.94	0.08	30,30,30,30	0
84	OHX	6	1981	7/7	0.94	0.11	195,197,199,199	0
84	OHX	AT	212	7/7	0.94	0.12	160,160,161,161	0
85	MG	AR	3883	1/1	0.94	0.22	12,12,12,12	0
85	MG	AR	3884	1/1	0.94	0.20	27,27,27,27	0
85	MG	1	3854	1/1	0.94	0.19	13,13,13,13	0
85	MG	AR	4160	1/1	0.94	0.08	31,31,31,31	0
85	MG	AR	4161	1/1	0.94	0.12	56,56,56,56	0
84	OHX	AR	3544	7/7	0.94	0.11	177,178,179,179	0
84	OHX	1	3714	7/7	0.94	0.13	155,156,157,158	0
85	MG	D	301	1/1	0.94	0.22	42,42,42,42	0
85	MG	6	2127	1/1	0.94	0.16	52,52,52,52	0
85	MG	1	3739	1/1	0.94	0.22	15,15,15,15	0
85	MG	1	3991	1/1	0.94	0.11	30,30,30,30	0
85	MG	AR	3893	1/1	0.94	0.17	40,40,40,40	0
85	MG	1	3741	1/1	0.94	0.15	40,40,40,40	0
85	MG	AR	3897	1/1	0.94	0.18	18,18,18,18	0
85	MG	AR	3899	1/1	0.94	0.18	46,46,46,46	0
85	MG	6	2131	1/1	0.94	0.16	32,32,32,32	0
85	MG	1	3864	1/1	0.94	0.24	33,33,33,33	0
85	MG	AR	4186	1/1	0.94	0.16	33,33,33,33	0
87	ZN	AP	501	1/1	0.94	0.15	115,115,115,115	0
85	MG	AR	4194	1/1	0.94	0.14	47,47,47,47	0
85	MG	AR	4196	1/1	0.94	0.15	39,39,39,39	0
84	OHX	1	3540	7/7	0.95	0.14	145,146,146,148	0
85	MG	AR	4163	1/1	0.95	0.12	30,30,30,30	0
84	OHX	AR	3572	7/7	0.95	0.10	174,175,176,176	0
85	MG	AR	3882	1/1	0.95	0.24	11,11,11,11	0
84	OHX	1	3569	7/7	0.95	0.11	166,166,167,168	0
85	MG	AR	4168	1/1	0.95	0.08	45,45,45,45	0
85	MG	1	3791	1/1	0.95	0.17	21,21,21,21	0
85	MG	AR	3885	1/1	0.95	0.28	38,38,38,38	0
84	OHX	1	3466	7/7	0.95	0.15	120,121,122,123	0
85	MG	AR	4175	1/1	0.95	0.07	27,27,27,27	0
85	MG	AR	4177	1/1	0.95	0.23	18,18,18,18	0
84	OHX	1	3572	7/7	0.95	0.12	168,168,169,170	0
84	OHX	3	204	7/7	0.95	0.09	163,164,165,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	4182	1/1	0.95	0.17	48,48,48,48	0
85	MG	1	4133	1/1	0.95	0.14	28,28,28,28	0
84	OHX	A	2009	7/7	0.95	0.10	191,192,194,195	0
85	MG	1	3802	1/1	0.95	0.09	32,32,32,32	0
85	MG	AR	4192	1/1	0.95	0.10	44,44,44,44	0
84	OHX	1	3543	7/7	0.95	0.13	166,166,167,167	0
85	MG	AR	3894	1/1	0.95	0.23	24,24,24,24	0
84	OHX	1	3484	7/7	0.95	0.13	131,131,133,133	0
84	OHX	1	3545	7/7	0.95	0.12	156,157,158,159	0
85	MG	AR	4202	1/1	0.95	0.08	72,72,72,72	0
85	MG	1	4140	1/1	0.95	0.10	49,49,49,49	0
85	MG	1	4141	1/1	0.95	0.14	36,36,36,36	0
85	MG	AR	4206	1/1	0.95	0.11	31,31,31,31	0
85	MG	AR	4208	1/1	0.95	0.08	62,62,62,62	0
84	OHX	1	3546	7/7	0.95	0.09	147,148,149,150	0
84	OHX	1	3547	7/7	0.95	0.14	168,169,170,170	0
84	OHX	AT	207	7/7	0.95	0.11	162,163,164,164	0
85	MG	AR	4212	1/1	0.95	0.14	48,48,48,48	0
85	MG	AR	3906	1/1	0.95	0.24	15,15,15,15	0
85	MG	6	2135	1/1	0.95	0.14	38,38,38,38	0
84	OHX	AT	208	7/7	0.95	0.10	154,154,155,155	0
84	OHX	4	204	7/7	0.95	0.11	160,160,161,161	0
84	OHX	6	1984	7/7	0.95	0.09	198,200,201,201	0
84	OHX	6	1986	7/7	0.95	0.10	157,157,159,159	0
84	OHX	AT	214	7/7	0.95	0.10	173,173,174,174	0
85	MG	AR	3917	1/1	0.95	0.20	29,29,29,29	0
85	MG	AR	3919	1/1	0.95	0.31	11,11,11,11	0
84	OHX	6	1987	7/7	0.95	0.11	179,179,180,181	0
84	OHX	1	3516	7/7	0.95	0.24	131,132,133,133	0
85	MG	1	3819	1/1	0.95	0.20	25,25,25,25	0
85	MG	AR	3925	1/1	0.95	0.25	14,14,14,14	0
85	MG	1	4165	1/1	0.95	0.11	38,38,38,38	0
84	OHX	1	3706	7/7	0.95	0.09	144,145,146,146	0
84	OHX	AR	3590	7/7	0.95	0.13	172,173,173,173	0
84	OHX	4	207	7/7	0.95	0.10	174,175,175,176	0
85	MG	AR	3931	1/1	0.95	0.14	13,13,13,13	0
85	MG	1	3825	1/1	0.95	0.15	42,42,42,42	0
84	OHX	1	3485	7/7	0.95	0.11	151,152,153,153	0
84	OHX	1	3488	7/7	0.95	0.14	140,140,141,141	0
84	OHX	1	3551	7/7	0.95	0.10	191,192,192,193	0
85	MG	1	4178	1/1	0.95	0.16	42,42,42,42	0
84	OHX	AR	3596	7/7	0.95	0.09	208,209,210,211	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3987	1/1	0.95	0.13	32,32,32,32	0
85	MG	AR	3940	1/1	0.95	0.11	34,34,34,34	0
85	MG	AS	218	1/1	0.95	0.07	52,52,52,52	0
84	OHX	1	3677	7/7	0.95	0.14	170,171,171,171	0
84	OHX	1	3432	7/7	0.95	0.17	131,131,132,132	0
84	OHX	k	402	7/7	0.95	0.10	156,157,158,158	0
84	OHX	1	3524	7/7	0.95	0.10	164,164,166,167	0
85	MG	1	3835	1/1	0.95	0.18	19,19,19,19	0
85	MG	1	3993	1/1	0.95	0.13	27,27,27,27	0
85	MG	1	3997	1/1	0.95	0.20	37,37,37,37	0
84	OHX	1	3554	7/7	0.95	0.10	167,168,169,169	0
85	MG	6	2169	1/1	0.95	0.07	39,39,39,39	0
85	MG	AT	222	1/1	0.95	0.16	35,35,35,35	0
84	OHX	6	1999	7/7	0.95	0.08	177,179,179,181	0
85	MG	AT	224	1/1	0.95	0.18	35,35,35,35	0
85	MG	1	4000	1/1	0.95	0.18	36,36,36,36	0
84	OHX	1	3500	7/7	0.95	0.10	156,157,159,159	0
85	MG	AR	3960	1/1	0.95	0.06	17,17,17,17	0
85	MG	AT	228	1/1	0.95	0.11	34,34,34,34	0
84	OHX	CP	501	7/7	0.95	0.11	177,178,178,178	0
85	MG	1	4198	1/1	0.95	0.17	36,36,36,36	0
85	MG	CD	301	1/1	0.95	0.19	28,28,28,28	0
85	MG	1	3843	1/1	0.95	0.25	11,11,11,11	0
85	MG	1	3845	1/1	0.95	0.32	14,14,14,14	0
85	MG	1	3846	1/1	0.95	0.25	16,16,16,16	0
84	OHX	1	3461	7/7	0.95	0.15	136,137,137,138	0
84	OHX	DH	201	7/7	0.95	0.13	155,156,157,157	0
85	MG	1	4014	1/1	0.95	0.13	46,46,46,46	0
85	MG	1	4015	1/1	0.95	0.09	38,38,38,38	0
84	OHX	1	3652	7/7	0.95	0.10	173,174,174,174	0
85	MG	CQ	202	1/1	0.95	0.08	26,26,26,26	0
85	MG	AR	3974	1/1	0.95	0.16	28,28,28,28	0
85	MG	AR	3975	1/1	0.95	0.19	31,31,31,31	0
84	OHX	1	3534	7/7	0.95	0.13	148,149,149,150	0
85	MG	CR	202	1/1	0.95	0.11	20,20,20,20	0
85	MG	1	4019	1/1	0.95	0.08	31,31,31,31	0
85	MG	6	2194	1/1	0.95	0.23	34,34,34,34	0
84	OHX	AR	3607	7/7	0.95	0.11	166,166,167,167	0
84	OHX	A	1929	7/7	0.95	0.11	157,159,160,160	0
85	MG	DA	201	1/1	0.95	0.13	29,29,29,29	0
85	MG	3	209	1/1	0.95	0.17	46,46,46,46	0
85	MG	DC	202	1/1	0.95	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	DC	203	1/1	0.95	0.12	35,35,35,35	0
84	OHX	AR	3484	7/7	0.95	0.18	133,134,135,135	0
85	MG	3	211	1/1	0.95	0.15	33,33,33,33	0
85	MG	3	213	1/1	0.95	0.14	23,23,23,23	0
85	MG	DF	201	1/1	0.95	0.12	30,30,30,30	0
84	OHX	6	1914	7/7	0.95	0.12	119,120,121,123	0
85	MG	DH	202	1/1	0.95	0.20	30,30,30,30	0
85	MG	AF	201	1/1	0.95	0.11	27,27,27,27	0
85	MG	3	215	1/1	0.95	0.15	39,39,39,39	0
84	OHX	6	2005	7/7	0.95	0.12	152,153,155,155	0
85	MG	AK	104	1/1	0.95	0.14	44,44,44,44	0
84	OHX	6	1927	7/7	0.95	0.21	128,128,130,130	0
84	OHX	A	1940	7/7	0.95	0.10	174,175,177,178	0
85	MG	AR	3740	1/1	0.95	0.12	46,46,46,46	0
84	OHX	h	401	7/7	0.95	0.08	203,206,208,210	0
85	MG	AR	4012	1/1	0.95	0.05	50,50,50,50	0
84	OHX	AR	3515	7/7	0.95	0.10	159,160,161,162	0
85	MG	4	215	1/1	0.95	0.15	23,23,23,23	0
84	OHX	AR	3516	7/7	0.95	0.10	174,176,178,178	0
85	MG	4	221	1/1	0.95	0.10	52,52,52,52	0
84	OHX	AR	3518	7/7	0.95	0.10	161,162,163,163	0
85	MG	AR	4019	1/1	0.95	0.08	29,29,29,29	0
84	OHX	6	1928	7/7	0.95	0.12	150,151,152,152	0
85	MG	A	2058	1/1	0.95	0.18	27,27,27,27	0
84	OHX	AR	3617	7/7	0.95	0.14	158,158,159,159	0
85	MG	1	4036	1/1	0.95	0.19	35,35,35,35	0
85	MG	1	4037	1/1	0.95	0.11	61,61,61,61	0
84	OHX	A	1950	7/7	0.95	0.10	168,169,170,171	0
85	MG	AR	3758	1/1	0.95	0.12	81,81,81,81	0
84	OHX	AR	3698	7/7	0.95	0.10	166,167,167,168	0
84	OHX	AR	3522	7/7	0.95	0.13	134,135,136,136	0
85	MG	4	232	1/1	0.95	0.20	43,43,43,43	0
84	OHX	A	1954	7/7	0.95	0.10	172,174,175,175	0
85	MG	AR	4030	1/1	0.95	0.24	37,37,37,37	0
84	OHX	6	1931	7/7	0.95	0.13	151,152,153,153	0
85	MG	1	4046	1/1	0.95	0.06	54,54,54,54	0
85	MG	AR	3768	1/1	0.95	0.19	23,23,23,23	0
84	OHX	6	1932	7/7	0.95	0.15	129,129,131,131	0
85	MG	AR	3770	1/1	0.95	0.12	36,36,36,36	0
85	MG	1	3882	1/1	0.95	0.22	11,11,11,11	0
85	MG	1	4051	1/1	0.95	0.09	63,63,63,63	0
85	MG	AR	4044	1/1	0.95	0.22	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	3775	1/1	0.95	0.13	16,16,16,16	0
84	OHX	6	1936	7/7	0.95	0.12	145,146,146,146	0
85	MG	AR	3780	1/1	0.95	0.21	20,20,20,20	0
84	OHX	6	1940	7/7	0.95	0.14	149,151,152,153	0
85	MG	x	203	1/1	0.95	0.25	64,64,64,64	0
85	MG	AR	3785	1/1	0.95	0.18	29,29,29,29	0
85	MG	AR	4052	1/1	0.95	0.11	28,28,28,28	0
84	OHX	1	3624	7/7	0.95	0.11	171,172,173,174	0
84	OHX	A	1964	7/7	0.95	0.11	168,169,170,170	0
84	OHX	A	1965	7/7	0.95	0.10	167,169,170,171	0
85	MG	AR	3790	1/1	0.95	0.17	17,17,17,17	0
84	OHX	AR	3533	7/7	0.95	0.14	166,166,167,167	0
85	MG	AR	3793	1/1	0.95	0.22	23,23,23,23	0
84	OHX	AR	3534	7/7	0.95	0.11	162,163,164,165	0
85	MG	AR	3795	1/1	0.95	0.09	22,22,22,22	0
84	OHX	6	1947	7/7	0.95	0.12	142,144,145,145	0
84	OHX	6	1950	7/7	0.95	0.12	171,171,173,174	0
85	MG	AR	3800	1/1	0.95	0.22	22,22,22,22	0
85	MG	1	4069	1/1	0.95	0.17	39,39,39,39	0
85	MG	1	3894	1/1	0.95	0.23	26,26,26,26	0
84	OHX	6	2017	7/7	0.95	0.12	158,159,160,161	0
84	OHX	6	1952	7/7	0.95	0.09	183,184,185,186	0
85	MG	AR	4071	1/1	0.95	0.09	32,32,32,32	0
84	OHX	AR	3631	7/7	0.95	0.10	153,155,155,155	0
85	MG	1	3901	1/1	0.95	0.22	12,12,12,12	0
84	OHX	6	1953	7/7	0.95	0.12	154,155,157,158	0
85	MG	1	3905	1/1	0.95	0.22	14,14,14,14	0
84	OHX	1	3535	7/7	0.95	0.11	196,198,199,200	0
85	MG	AR	4081	1/1	0.95	0.19	52,52,52,52	0
84	OHX	1	3561	7/7	0.95	0.08	184,184,185,186	0
85	MG	1	4080	1/1	0.95	0.17	55,55,55,55	0
84	OHX	1	3688	7/7	0.95	0.10	220,221,221,222	0
85	MG	1	4082	1/1	0.95	0.12	22,22,22,22	0
85	MG	AR	4088	1/1	0.95	0.11	50,50,50,50	0
85	MG	AR	4090	1/1	0.95	0.07	62,62,62,62	0
85	MG	1	4084	1/1	0.95	0.08	44,44,44,44	0
85	MG	1	4085	1/1	0.95	0.07	43,43,43,43	0
85	MG	1	4088	1/1	0.95	0.10	28,28,28,28	0
84	OHX	AR	3548	7/7	0.95	0.10	165,166,166,166	0
85	MG	1	3763	1/1	0.95	0.16	34,34,34,34	0
85	MG	1	3764	1/1	0.95	0.31	38,38,38,38	0
85	MG	AR	4099	1/1	0.95	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	4093	1/1	0.95	0.14	16,16,16,16	0
84	OHX	AR	3549	7/7	0.95	0.14	156,157,158,158	0
85	MG	AR	3829	1/1	0.95	0.21	16,16,16,16	0
85	MG	1	4096	1/1	0.95	0.16	53,53,53,53	0
85	MG	1	3766	1/1	0.95	0.16	23,23,23,23	0
84	OHX	AR	3550	7/7	0.95	0.10	164,164,165,165	0
84	OHX	AR	3551	7/7	0.95	0.11	161,162,163,164	0
85	MG	AR	4110	1/1	0.95	0.15	45,45,45,45	0
84	OHX	A	1987	7/7	0.95	0.11	172,173,174,175	0
84	OHX	1	3562	7/7	0.95	0.07	200,200,201,202	0
85	MG	1	3772	1/1	0.95	0.25	32,32,32,32	0
84	OHX	6	1961	7/7	0.95	0.12	152,153,154,155	0
84	OHX	1	3599	7/7	0.95	0.08	190,191,192,193	0
84	OHX	1	3506	7/7	0.95	0.12	159,160,161,162	0
85	MG	AR	4120	1/1	0.95	0.07	32,32,32,32	0
85	MG	1	3776	1/1	0.95	0.16	29,29,29,29	0
84	OHX	A	1994	7/7	0.95	0.09	200,203,204,205	0
85	MG	AR	4124	1/1	0.95	0.22	54,54,54,54	0
84	OHX	AR	3560	7/7	0.95	0.10	173,174,175,175	0
84	OHX	1	3565	7/7	0.95	0.10	168,169,170,170	0
85	MG	1	3780	1/1	0.95	0.19	26,26,26,26	0
85	MG	AR	3855	1/1	0.95	0.11	37,37,37,37	0
85	MG	6	2099	1/1	0.95	0.10	19,19,19,19	0
84	OHX	AR	3563	7/7	0.95	0.13	173,173,174,174	0
85	MG	6	2101	1/1	0.95	0.16	37,37,37,37	0
85	MG	AR	4134	1/1	0.95	0.16	10,10,10,10	0
85	MG	AR	3859	1/1	0.95	0.17	28,28,28,28	0
85	MG	AR	3860	1/1	0.95	0.24	6,6,6,6	0
84	OHX	1	3507	7/7	0.95	0.14	149,149,150,150	0
85	MG	6	2104	1/1	0.95	0.12	22,22,22,22	0
84	OHX	AR	3565	7/7	0.95	0.10	161,162,163,164	0
85	MG	s2	301	1/1	0.95	0.16	46,46,46,46	0
85	MG	AR	4146	1/1	0.95	0.15	37,37,37,37	0
84	OHX	1	3603	7/7	0.95	0.14	162,162,164,164	0
85	MG	AR	3868	1/1	0.95	0.16	33,33,33,33	0
85	MG	AR	3870	1/1	0.95	0.16	14,14,14,14	0
85	MG	d3	203	1/1	0.95	0.13	29,29,29,29	0
85	MG	AR	3871	1/1	0.95	0.22	20,20,20,20	0
85	MG	AR	3873	1/1	0.95	0.14	23,23,23,23	0
85	MG	AR	3874	1/1	0.95	0.21	18,18,18,18	0
86	7MB	1	4216	20/20	0.95	0.14	48,48,48,48	0
85	MG	1	4124	1/1	0.95	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	OHX	AR	3569	7/7	0.95	0.09	182,182,183,183	0
85	MG	AR	3878	1/1	0.95	0.17	12,12,12,12	0
84	OHX	AS	207	7/7	0.96	0.09	163,165,166,166	0
84	OHX	AR	3654	7/7	0.96	0.10	161,162,163,164	0
85	MG	1	4148	1/1	0.96	0.34	35,35,35,35	0
84	OHX	AR	3570	7/7	0.96	0.10	161,162,163,163	0
85	MG	AR	4176	1/1	0.96	0.14	52,52,52,52	0
85	MG	1	4151	1/1	0.96	0.13	53,53,53,53	0
85	MG	AR	3907	1/1	0.96	0.23	20,20,20,20	0
85	MG	1	4152	1/1	0.96	0.12	40,40,40,40	0
85	MG	AR	3909	1/1	0.96	0.20	14,14,14,14	0
85	MG	1	4153	1/1	0.96	0.06	39,39,39,39	0
84	OHX	6	1954	7/7	0.96	0.08	181,182,184,185	0
85	MG	6	2145	1/1	0.96	0.05	51,51,51,51	0
85	MG	AR	4187	1/1	0.96	0.15	27,27,27,27	0
85	MG	AR	4190	1/1	0.96	0.37	107,107,107,107	0
85	MG	AR	4191	1/1	0.96	0.20	38,38,38,38	0
85	MG	AR	3913	1/1	0.96	0.21	20,20,20,20	0
85	MG	AR	4193	1/1	0.96	0.15	62,62,62,62	0
84	OHX	AT	205	7/7	0.96	0.11	151,151,151,151	0
84	OHX	1	3515	7/7	0.96	0.14	128,128,129,129	0
85	MG	1	3812	1/1	0.96	0.18	29,29,29,29	0
85	MG	AR	4199	1/1	0.96	0.23	64,64,64,64	0
85	MG	AR	3918	1/1	0.96	0.17	21,21,21,21	0
85	MG	1	4160	1/1	0.96	0.08	40,40,40,40	0
84	OHX	1	3541	7/7	0.96	0.10	154,155,156,156	0
84	OHX	1	3493	7/7	0.96	0.11	147,148,148,149	0
85	MG	1	3977	1/1	0.96	0.07	21,21,21,21	0
85	MG	AR	3924	1/1	0.96	0.18	13,13,13,13	0
85	MG	1	4164	1/1	0.96	0.09	48,48,48,48	0
84	OHX	6	2007	7/7	0.96	0.10	148,150,151,151	0
85	MG	1	4167	1/1	0.96	0.10	52,52,52,52	0
84	OHX	AT	210	7/7	0.96	0.09	164,164,165,165	0
84	OHX	1	3567	7/7	0.96	0.09	177,178,178,179	0
84	OHX	1	3495	7/7	0.96	0.13	133,134,135,135	0
84	OHX	AT	213	7/7	0.96	0.09	175,176,176,177	0
84	OHX	1	3518	7/7	0.96	0.14	134,135,135,136	0
85	MG	1	4173	1/1	0.96	0.09	33,33,33,33	0
85	MG	1	3823	1/1	0.96	0.13	51,51,51,51	0
84	OHX	AK	103	7/7	0.96	0.11	145,146,146,146	0
85	MG	1	4177	1/1	0.96	0.09	45,45,45,45	0
84	OHX	AP	502	7/7	0.96	0.15	124,124,126,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	AR	3430	7/7	0.96	0.15	137,137,138,138	0
84	OHX	AR	3583	7/7	0.96	0.12	148,149,150,150	0
84	OHX	AR	3464	7/7	0.96	0.20	117,118,118,118	0
85	MG	6	2173	1/1	0.96	0.14	69,69,69,69	0
84	OHX	AR	3466	7/7	0.96	0.12	114,115,116,116	0
85	MG	6	2175	1/1	0.96	0.10	41,41,41,41	0
85	MG	6	2177	1/1	0.96	0.15	25,25,25,25	0
85	MG	AR	4232	1/1	0.96	0.21	33,33,33,33	0
84	OHX	CE	402	7/7	0.96	0.10	142,143,144,144	0
84	OHX	AR	3467	7/7	0.96	0.13	137,138,138,139	0
85	MG	AR	4240	1/1	0.96	0.08	33,33,33,33	0
84	OHX	AR	3472	7/7	0.96	0.15	129,130,130,130	0
84	OHX	AR	3672	7/7	0.96	0.14	137,138,138,138	0
85	MG	6	2183	1/1	0.96	0.20	44,44,44,44	0
84	OHX	AR	3473	7/7	0.96	0.12	121,122,122,122	0
85	MG	AS	211	1/1	0.96	0.22	22,22,22,22	0
84	OHX	6	1963	7/7	0.96	0.10	159,159,161,161	0
85	MG	1	4190	1/1	0.96	0.16	26,26,26,26	0
84	OHX	4	203	7/7	0.96	0.09	181,182,183,184	0
85	MG	AS	215	1/1	0.96	0.27	12,12,12,12	0
85	MG	AR	3964	1/1	0.96	0.16	28,28,28,28	0
84	OHX	AR	3485	7/7	0.96	0.17	135,136,137,137	0
84	OHX	CL	301	7/7	0.96	0.11	165,166,167,168	0
84	OHX	AR	3488	7/7	0.96	0.10	129,130,130,131	0
85	MG	1	3844	1/1	0.96	0.18	9,9,9,9	0
85	MG	AS	222	1/1	0.96	0.15	13,13,13,13	0
85	MG	1	4007	1/1	0.96	0.18	16,16,16,16	0
84	OHX	AR	3489	7/7	0.96	0.11	149,150,151,152	0
85	MG	1	4009	1/1	0.96	0.10	41,41,41,41	0
84	OHX	AR	3493	7/7	0.96	0.11	137,139,139,140	0
84	OHX	6	2013	7/7	0.96	0.10	149,151,152,153	0
85	MG	AT	201	1/1	0.96	0.17	31,31,31,31	0
85	MG	1	4207	1/1	0.96	0.07	44,44,44,44	0
85	MG	1	3848	1/1	0.96	0.17	26,26,26,26	0
85	MG	1	3849	1/1	0.96	0.22	21,21,21,21	0
85	MG	AB	204	1/1	0.96	0.14	42,42,42,42	0
85	MG	AR	3982	1/1	0.96	0.09	35,35,35,35	0
84	OHX	6	1965	7/7	0.96	0.10	161,162,163,163	0
84	OHX	AR	3496	7/7	0.96	0.14	147,147,148,149	0
85	MG	AR	3985	1/1	0.96	0.16	19,19,19,19	0
84	OHX	AR	3497	7/7	0.96	0.11	140,140,141,141	0
84	OHX	1	3520	7/7	0.96	0.09	149,150,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	AR	3504	7/7	0.96	0.22	116,117,117,118	0
85	MG	AR	3993	1/1	0.96	0.12	62,62,62,62	0
85	MG	CE	404	1/1	0.96	0.24	24,24,24,24	0
85	MG	1	3856	1/1	0.96	0.20	15,15,15,15	0
85	MG	1	3857	1/1	0.96	0.19	12,12,12,12	0
85	MG	CF	403	1/1	0.96	0.10	30,30,30,30	0
85	MG	CI	301	1/1	0.96	0.16	48,48,48,48	0
84	OHX	A	1928	7/7	0.96	0.09	156,158,159,159	0
85	MG	AR	3997	1/1	0.96	0.17	45,45,45,45	0
85	MG	CO	203	1/1	0.96	0.12	46,46,46,46	0
84	OHX	AR	3505	7/7	0.96	0.11	138,140,141,141	0
85	MG	1	3860	1/1	0.96	0.22	19,19,19,19	0
84	OHX	AR	3506	7/7	0.96	0.11	158,159,159,160	0
85	MG	1	3862	1/1	0.96	0.17	18,18,18,18	0
84	OHX	T	201	7/7	0.96	0.11	133,135,137,138	0
84	OHX	A	1931	7/7	0.96	0.08	166,168,169,169	0
85	MG	AR	4006	1/1	0.96	0.07	33,33,33,33	0
85	MG	AR	4007	1/1	0.96	0.09	23,23,23,23	0
85	MG	AR	4008	1/1	0.96	0.12	33,33,33,33	0
84	OHX	AR	3508	7/7	0.96	0.13	139,139,140,140	0
85	MG	AR	4010	1/1	0.96	0.09	28,28,28,28	0
85	MG	CX	202	1/1	0.96	0.21	6,6,6,6	0
84	OHX	AR	3512	7/7	0.96	0.14	132,132,132,133	0
85	MG	AR	3754	1/1	0.96	0.11	35,35,35,35	0
84	OHX	6	1967	7/7	0.96	0.11	157,159,160,160	0
84	OHX	A	1936	7/7	0.96	0.11	160,162,163,163	0
85	MG	4	219	1/1	0.96	0.23	24,24,24,24	0
85	MG	4	220	1/1	0.96	0.10	37,37,37,37	0
85	MG	1	4039	1/1	0.96	0.26	40,40,40,40	0
85	MG	4	222	1/1	0.96	0.18	61,61,61,61	0
85	MG	AR	3763	1/1	0.96	0.12	18,18,18,18	0
84	OHX	A	1937	7/7	0.96	0.11	152,154,157,157	0
85	MG	1	3873	1/1	0.96	0.23	18,18,18,18	0
84	OHX	6	1968	7/7	0.96	0.12	145,146,147,148	0
85	MG	DP	101	1/1	0.96	0.24	43,43,43,43	0
85	MG	1	4043	1/1	0.96	0.14	40,40,40,40	0
84	OHX	AR	3517	7/7	0.96	0.12	134,135,135,136	0
84	OHX	6	1969	7/7	0.96	0.09	163,163,165,165	0
85	MG	A	2043	1/1	0.96	0.19	47,47,47,47	0
85	MG	A	2044	1/1	0.96	0.13	25,25,25,25	0
85	MG	4	229	1/1	0.96	0.07	57,57,57,57	0
85	MG	1	3733	1/1	0.96	0.16	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3734	1/1	0.96	0.25	27,27,27,27	0
85	MG	1	4048	1/1	0.96	0.24	27,27,27,27	0
85	MG	AR	4033	1/1	0.96	0.13	63,63,63,63	0
85	MG	1	4049	1/1	0.96	0.13	36,36,36,36	0
85	MG	j	301	1/1	0.96	0.05	26,26,26,26	0
84	OHX	1	3496	7/7	0.96	0.19	115,116,117,117	0
84	OHX	AR	3521	7/7	0.96	0.10	160,161,161,162	0
84	OHX	1	3522	7/7	0.96	0.11	133,134,134,135	0
85	MG	1	4053	1/1	0.96	0.08	32,32,32,32	0
84	OHX	A	1949	7/7	0.96	0.09	165,167,169,169	0
84	OHX	1	3574	7/7	0.96	0.13	138,139,140,140	0
85	MG	1	4057	1/1	0.96	0.10	30,30,30,30	0
85	MG	AR	3792	1/1	0.96	0.07	28,28,28,28	0
85	MG	1	3885	1/1	0.96	0.25	10,10,10,10	0
85	MG	1	3742	1/1	0.96	0.15	19,19,19,19	0
85	MG	1	4061	1/1	0.96	0.21	23,23,23,23	0
85	MG	1	4062	1/1	0.96	0.06	33,33,33,33	0
84	OHX	4	208	7/7	0.96	0.08	187,187,188,188	0
84	OHX	AR	3525	7/7	0.96	0.12	150,151,151,152	0
84	OHX	A	1953	7/7	0.96	0.09	180,182,184,184	0
85	MG	AR	3802	1/1	0.96	0.21	16,16,16,16	0
85	MG	1	4067	1/1	0.96	0.10	24,24,24,24	0
84	OHX	1	3478	7/7	0.96	0.13	133,134,135,135	0
84	OHX	AR	3528	7/7	0.96	0.10	147,147,148,149	0
84	OHX	A	1957	7/7	0.96	0.11	169,171,172,173	0
85	MG	1	4071	1/1	0.96	0.23	16,16,16,16	0
85	MG	6	2063	1/1	0.96	0.17	31,31,31,31	0
84	OHX	1	3503	7/7	0.96	0.10	145,146,147,148	0
85	MG	AR	4066	1/1	0.96	0.11	35,35,35,35	0
85	MG	1	3895	1/1	0.96	0.08	29,29,29,29	0
85	MG	1	3896	1/1	0.96	0.26	10,10,10,10	0
84	OHX	1	3526	7/7	0.96	0.08	167,168,169,170	0
84	OHX	1	3578	7/7	0.96	0.10	168,170,170,171	0
84	OHX	1	3579	7/7	0.96	0.08	175,175,177,177	0
84	OHX	A	1963	7/7	0.96	0.09	185,187,189,190	0
85	MG	AR	3817	1/1	0.96	0.15	20,20,20,20	0
85	MG	1	3755	1/1	0.96	0.22	41,41,41,41	0
85	MG	AR	4076	1/1	0.96	0.14	38,38,38,38	0
84	OHX	1	3527	7/7	0.96	0.09	138,139,140,140	0
84	OHX	1	3458	7/7	0.96	0.12	131,132,133,133	0
85	MG	AR	4080	1/1	0.96	0.09	16,16,16,16	0
84	OHX	1	3583	7/7	0.96	0.10	144,144,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	4082	1/1	0.96	0.05	48,48,48,48	0
84	OHX	1	3530	7/7	0.96	0.10	151,151,151,152	0
84	OHX	1	3586	7/7	0.96	0.07	182,183,185,186	0
85	MG	AR	3827	1/1	0.96	0.25	40,40,40,40	0
85	MG	1	3762	1/1	0.96	0.20	40,40,40,40	0
84	OHX	AR	3542	7/7	0.96	0.23	133,134,134,134	0
84	OHX	6	1985	7/7	0.96	0.08	191,193,194,195	0
84	OHX	A	1972	7/7	0.96	0.07	195,196,198,199	0
84	OHX	AR	3630	7/7	0.96	0.08	172,173,174,175	0
84	OHX	A	1974	7/7	0.96	0.09	196,198,200,201	0
84	OHX	A	1975	7/7	0.96	0.07	190,193,195,195	0
85	MG	1	4099	1/1	0.96	0.15	16,16,16,16	0
84	OHX	A	1976	7/7	0.96	0.09	165,166,167,168	0
85	MG	1	3921	1/1	0.96	0.20	45,45,45,45	0
84	OHX	AR	3715	7/7	0.96	0.09	144,146,147,147	0
85	MG	1	3923	1/1	0.96	0.22	7,7,7,7	0
85	MG	AR	3847	1/1	0.96	0.16	35,35,35,35	0
85	MG	AR	4103	1/1	0.96	0.07	35,35,35,35	0
85	MG	AR	4104	1/1	0.96	0.11	55,55,55,55	0
84	OHX	1	3470	7/7	0.96	0.11	141,142,143,143	0
85	MG	1	4106	1/1	0.96	0.10	30,30,30,30	0
84	OHX	1	3533	7/7	0.96	0.08	196,197,198,199	0
84	OHX	AR	3547	7/7	0.96	0.14	147,147,147,148	0
84	OHX	1	3475	7/7	0.96	0.15	128,129,130,130	0
84	OHX	1	3509	7/7	0.96	0.10	155,155,157,157	0
85	MG	AR	4113	1/1	0.96	0.08	17,17,17,17	0
84	OHX	AR	3636	7/7	0.96	0.09	187,188,188,189	0
84	OHX	1	3558	7/7	0.96	0.10	166,167,168,168	0
84	OHX	1	3623	7/7	0.96	0.08	224,225,226,226	0
84	OHX	1	3490	7/7	0.96	0.14	134,135,136,136	0
85	MG	AR	4118	1/1	0.96	0.07	29,29,29,29	0
85	MG	A	2124	1/1	0.96	0.25	57,57,57,57	0
84	OHX	1	3593	7/7	0.96	0.07	206,207,208,209	0
85	MG	AR	3861	1/1	0.96	0.14	16,16,16,16	0
85	MG	1	3940	1/1	0.96	0.04	21,21,21,21	0
85	MG	6	2105	1/1	0.96	0.17	24,24,24,24	0
84	OHX	AR	3556	7/7	0.96	0.13	138,139,140,140	0
85	MG	1	3944	1/1	0.96	0.27	33,33,33,33	0
85	MG	6	2108	1/1	0.96	0.23	44,44,44,44	0
85	MG	1	3945	1/1	0.96	0.06	17,17,17,17	0
85	MG	1	4122	1/1	0.96	0.20	45,45,45,45	0
84	OHX	6	1937	7/7	0.96	0.11	140,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	1	3626	7/7	0.96	0.20	137,137,138,138	0
85	MG	6	2114	1/1	0.96	0.22	28,28,28,28	0
84	OHX	1	3560	7/7	0.96	0.11	155,156,158,158	0
85	MG	A	2140	1/1	0.96	0.16	55,55,55,55	0
85	MG	AR	4135	1/1	0.96	0.08	66,66,66,66	0
84	OHX	6	1945	7/7	0.96	0.09	149,150,151,152	0
85	MG	AR	4139	1/1	0.96	0.18	37,37,37,37	0
85	MG	AR	4140	1/1	0.96	0.09	24,24,24,24	0
85	MG	6	2117	1/1	0.96	0.20	21,21,21,21	0
85	MG	1	3951	1/1	0.96	0.11	43,43,43,43	0
85	MG	6	2119	1/1	0.96	0.17	31,31,31,31	0
85	MG	AR	4144	1/1	0.96	0.11	35,35,35,35	0
84	OHX	AR	3562	7/7	0.96	0.09	173,174,175,176	0
85	MG	1	3953	1/1	0.96	0.20	32,32,32,32	0
85	MG	6	2122	1/1	0.96	0.15	48,48,48,48	0
85	MG	AR	4149	1/1	0.96	0.09	28,28,28,28	0
85	MG	AR	4150	1/1	0.96	0.07	49,49,49,49	0
85	MG	AR	3886	1/1	0.96	0.14	15,15,15,15	0
84	OHX	1	3537	7/7	0.96	0.10	160,161,162,162	0
84	OHX	6	1949	7/7	0.96	0.10	165,167,168,168	0
85	MG	AR	4154	1/1	0.96	0.13	50,50,50,50	0
85	MG	AR	4155	1/1	0.96	0.05	27,27,27,27	0
84	OHX	1	3476	7/7	0.96	0.15	121,121,122,123	0
85	MG	1	3957	1/1	0.96	0.16	29,29,29,29	0
85	MG	d3	201	1/1	0.96	0.21	48,48,48,48	0
84	OHX	1	3563	7/7	0.96	0.12	151,152,152,152	0
85	MG	1	3796	1/1	0.96	0.07	33,33,33,33	0
84	OHX	AR	3567	7/7	0.96	0.10	159,159,160,160	0
84	OHX	AR	3568	7/7	0.96	0.10	162,163,164,165	0
84	OHX	3	203	7/7	0.96	0.11	143,144,145,145	0
85	MG	AR	3896	1/1	0.96	0.20	37,37,37,37	0
84	OHX	AR	3739	7/7	0.96	0.15	151,152,152,152	0
85	MG	AR	3898	1/1	0.96	0.23	16,16,16,16	0
84	OHX	AS	206	7/7	0.96	0.09	146,146,148,148	0
87	ZN	e1	501	1/1	0.96	0.05	176,176,176,176	0
85	MG	AR	3796	1/1	0.97	0.20	32,32,32,32	0
84	OHX	AR	3487	7/7	0.97	0.12	116,117,117,117	0
85	MG	AR	3798	1/1	0.97	0.09	21,21,21,21	0
84	OHX	1	3473	7/7	0.97	0.10	119,120,121,121	0
85	MG	6	2094	1/1	0.97	0.18	24,24,24,24	0
84	OHX	6	2030	7/7	0.97	0.10	160,161,162,162	0
84	OHX	AR	3491	7/7	0.97	0.12	130,131,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	4004	1/1	0.97	0.11	27,27,27,27	0
84	OHX	AR	3492	7/7	0.97	0.12	134,135,135,135	0
85	MG	1	4018	1/1	0.97	0.12	26,26,26,26	0
84	OHX	6	1946	7/7	0.97	0.10	160,161,163,164	0
85	MG	1	4020	1/1	0.97	0.06	38,38,38,38	0
85	MG	1	3891	1/1	0.97	0.27	16,16,16,16	0
85	MG	AR	4235	1/1	0.97	0.11	15,15,15,15	0
85	MG	AR	4236	1/1	0.97	0.13	22,22,22,22	0
85	MG	AR	4237	1/1	0.97	0.10	26,26,26,26	0
84	OHX	CX	201	7/7	0.97	0.16	121,122,123,124	0
84	OHX	A	2008	7/7	0.97	0.08	156,158,159,159	0
84	OHX	1	3474	7/7	0.97	0.12	131,132,133,133	0
84	OHX	DG	201	7/7	0.97	0.17	132,133,133,134	0
84	OHX	1	3459	7/7	0.97	0.15	134,134,135,136	0
84	OHX	1	3497	7/7	0.97	0.11	140,141,142,142	0
85	MG	AR	3814	1/1	0.97	0.13	27,27,27,27	0
84	OHX	DL	101	7/7	0.97	0.10	144,144,144,144	0
84	OHX	6	1951	7/7	0.97	0.09	165,167,169,170	0
84	OHX	A	1913	7/7	0.97	0.14	121,122,123,124	0
85	MG	1	3902	1/1	0.97	0.21	4,4,4,4	0
84	OHX	A	1915	7/7	0.97	0.09	149,151,152,154	0
85	MG	1	4176	1/1	0.97	0.04	27,27,27,27	0
85	MG	AR	3822	1/1	0.97	0.07	52,52,52,52	0
85	MG	1	3789	1/1	0.97	0.26	51,51,51,51	0
84	OHX	A	1918	7/7	0.97	0.12	120,122,123,123	0
84	OHX	A	1920	7/7	0.97	0.10	141,142,143,144	0
84	OHX	A	1921	7/7	0.97	0.11	139,141,143,143	0
85	MG	AS	226	1/1	0.97	0.12	36,36,36,36	0
85	MG	1	3793	1/1	0.97	0.20	12,12,12,12	0
84	OHX	A	1924	7/7	0.97	0.09	153,154,155,156	0
84	OHX	A	1926	7/7	0.97	0.09	149,150,151,152	0
85	MG	AR	4034	1/1	0.97	0.15	42,42,42,42	0
85	MG	AR	4035	1/1	0.97	0.07	39,39,39,39	0
85	MG	AR	3832	1/1	0.97	0.11	46,46,46,46	0
85	MG	AR	3833	1/1	0.97	0.12	37,37,37,37	0
85	MG	AR	4038	1/1	0.97	0.11	30,30,30,30	0
84	OHX	AR	3499	7/7	0.97	0.11	130,131,133,133	0
85	MG	1	3799	1/1	0.97	0.18	28,28,28,28	0
84	OHX	1	3498	7/7	0.97	0.11	150,150,151,152	0
85	MG	AR	4042	1/1	0.97	0.08	20,20,20,20	0
85	MG	AR	3837	1/1	0.97	0.05	16,16,16,16	0
85	MG	AT	230	1/1	0.97	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	AR	3502	7/7	0.97	0.10	131,132,132,133	0
84	OHX	1	3525	7/7	0.97	0.09	151,152,153,154	0
85	MG	AR	4046	1/1	0.97	0.14	45,45,45,45	0
84	OHX	1	3669	7/7	0.97	0.12	125,126,127,127	0
84	OHX	1	3449	7/7	0.97	0.10	119,120,121,121	0
85	MG	AR	3843	1/1	0.97	0.07	13,13,13,13	0
84	OHX	A	1933	7/7	0.97	0.08	154,155,156,157	0
84	OHX	1	3477	7/7	0.97	0.10	118,119,120,120	0
85	MG	6	2132	1/1	0.97	0.07	38,38,38,38	0
84	OHX	AR	3580	7/7	0.97	0.11	139,139,140,140	0
85	MG	AR	4054	1/1	0.97	0.11	33,33,33,33	0
85	MG	1	4196	1/1	0.97	0.13	35,35,35,35	0
84	OHX	AR	3510	7/7	0.97	0.08	154,155,156,157	0
85	MG	AR	4057	1/1	0.97	0.08	46,46,46,46	0
85	MG	6	2136	1/1	0.97	0.21	29,29,29,29	0
85	MG	1	4199	1/1	0.97	0.26	25,25,25,25	0
85	MG	AR	3854	1/1	0.97	0.18	28,28,28,28	0
85	MG	1	4054	1/1	0.97	0.12	40,40,40,40	0
85	MG	1	4201	1/1	0.97	0.17	31,31,31,31	0
84	OHX	1	3462	7/7	0.97	0.13	115,116,117,118	0
85	MG	1	3811	1/1	0.97	0.09	42,42,42,42	0
84	OHX	A	1939	7/7	0.97	0.09	153,155,156,157	0
85	MG	CU	201	1/1	0.97	0.22	44,44,44,44	0
85	MG	CU	202	1/1	0.97	0.15	31,31,31,31	0
85	MG	1	3931	1/1	0.97	0.10	31,31,31,31	0
84	OHX	AR	3513	7/7	0.97	0.09	152,153,154,154	0
84	OHX	AR	3514	7/7	0.97	0.09	146,147,147,148	0
85	MG	1	3936	1/1	0.97	0.07	48,48,48,48	0
85	MG	AR	3865	1/1	0.97	0.22	23,23,23,23	0
85	MG	1	3815	1/1	0.97	0.23	40,40,40,40	0
84	OHX	A	1942	7/7	0.97	0.08	163,165,166,167	0
85	MG	1	4215	1/1	0.97	0.24	28,28,28,28	0
84	OHX	6	1959	7/7	0.97	0.08	154,155,156,157	0
85	MG	1	4218	1/1	0.97	0.05	84,84,84,84	0
85	MG	1	4219	1/1	0.97	0.17	47,47,47,47	0
85	MG	AR	4078	1/1	0.97	0.09	23,23,23,23	0
85	MG	6	2154	1/1	0.97	0.08	38,38,38,38	0
84	OHX	1	3529	7/7	0.97	0.08	143,144,145,146	0
84	OHX	1	3479	7/7	0.97	0.12	136,137,138,138	0
85	MG	AR	3877	1/1	0.97	0.22	14,14,14,14	0
85	MG	6	2157	1/1	0.97	0.18	45,45,45,45	0
84	OHX	1	3483	7/7	0.97	0.11	118,119,120,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	A	1948	7/7	0.97	0.08	166,169,170,170	0
85	MG	A	2045	1/1	0.97	0.12	35,35,35,35	0
84	OHX	AR	3519	7/7	0.97	0.15	135,135,136,136	0
84	OHX	1	3464	7/7	0.97	0.12	136,137,138,139	0
85	MG	AR	4089	1/1	0.97	0.25	15,15,15,15	0
84	OHX	v	301	7/7	0.97	0.09	155,155,156,156	0
84	OHX	1	3510	7/7	0.97	0.09	148,148,149,149	0
85	MG	1	3827	1/1	0.97	0.15	21,21,21,21	0
84	OHX	1	3453	7/7	0.97	0.09	130,132,133,133	0
84	OHX	1	3730	7/7	0.97	0.10	141,142,143,143	0
84	OHX	AR	3595	7/7	0.97	0.09	160,161,161,162	0
85	MG	AR	4097	1/1	0.97	0.08	26,26,26,26	0
85	MG	6	2168	1/1	0.97	0.19	50,50,50,50	0
84	OHX	1	3582	7/7	0.97	0.09	152,153,154,155	0
85	MG	4	213	1/1	0.97	0.14	34,34,34,34	0
85	MG	4	214	1/1	0.97	0.15	18,18,18,18	0
84	OHX	1	3486	7/7	0.97	0.11	146,146,147,147	0
85	MG	4	216	1/1	0.97	0.17	42,42,42,42	0
84	OHX	AR	3527	7/7	0.97	0.10	138,139,140,141	0
85	MG	6	2176	1/1	0.97	0.09	73,73,73,73	0
84	OHX	6	1919	7/7	0.97	0.13	112,113,114,114	0
85	MG	6	2178	1/1	0.97	0.05	26,26,26,26	0
85	MG	1	4083	1/1	0.97	0.10	34,34,34,34	0
84	OHX	A	1961	7/7	0.97	0.07	175,176,179,180	0
85	MG	AR	4111	1/1	0.97	0.14	48,48,48,48	0
84	OHX	6	1923	7/7	0.97	0.10	136,138,139,139	0
85	MG	AR	3904	1/1	0.97	0.28	11,11,11,11	0
85	MG	1	4086	1/1	0.97	0.18	16,16,16,16	0
84	OHX	1	3513	7/7	0.97	0.09	140,141,142,142	0
85	MG	1	3962	1/1	0.97	0.15	33,33,33,33	0
84	OHX	AR	3532	7/7	0.97	0.17	129,130,130,131	0
84	OHX	AS	202	7/7	0.97	0.11	122,123,124,124	0
85	MG	A	2077	1/1	0.97	0.16	25,25,25,25	0
85	MG	1	3965	1/1	0.97	0.11	32,32,32,32	0
84	OHX	AS	204	7/7	0.97	0.10	140,141,141,141	0
84	OHX	AS	205	7/7	0.97	0.09	144,146,147,147	0
85	MG	1	4097	1/1	0.97	0.15	61,61,61,61	0
85	MG	AR	4123	1/1	0.97	0.07	39,39,39,39	0
84	OHX	A	1968	7/7	0.97	0.08	168,170,171,172	0
84	OHX	1	3585	7/7	0.97	0.08	173,174,174,175	0
85	MG	1	3737	1/1	0.97	0.21	36,36,36,36	0
85	MG	k	403	1/1	0.97	0.14	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	k	404	1/1	0.97	0.15	71,71,71,71	0
85	MG	AR	4129	1/1	0.97	0.11	21,21,21,21	0
84	OHX	6	1929	7/7	0.97	0.11	147,148,151,152	0
85	MG	AR	3921	1/1	0.97	0.16	10,10,10,10	0
85	MG	o	301	1/1	0.97	0.07	39,39,39,39	0
85	MG	o	302	1/1	0.97	0.10	27,27,27,27	0
84	OHX	6	1975	7/7	0.97	0.08	160,161,162,162	0
85	MG	AR	4136	1/1	0.97	0.15	41,41,41,41	0
85	MG	AR	4137	1/1	0.97	0.11	57,57,57,57	0
85	MG	A	2096	1/1	0.97	0.17	51,51,51,51	0
85	MG	r	302	1/1	0.97	0.12	40,40,40,40	0
84	OHX	AR	3536	7/7	0.97	0.11	141,141,142,142	0
85	MG	AR	3927	1/1	0.97	0.36	11,11,11,11	0
85	MG	1	3974	1/1	0.97	0.14	43,43,43,43	0
84	OHX	1	3514	7/7	0.97	0.11	148,148,149,149	0
84	OHX	AT	204	7/7	0.97	0.08	143,143,143,143	0
84	OHX	AK	102	7/7	0.97	0.11	121,122,122,122	0
84	OHX	1	3468	7/7	0.97	0.14	104,104,104,105	0
84	OHX	AR	3610	7/7	0.97	0.12	139,140,140,140	0
84	OHX	6	1933	7/7	0.97	0.14	121,122,123,123	0
85	MG	AR	4148	1/1	0.97	0.09	36,36,36,36	0
84	OHX	6	1935	7/7	0.97	0.09	136,137,138,139	0
85	MG	x	207	1/1	0.97	0.10	17,17,17,17	0
85	MG	AR	3745	1/1	0.97	0.19	32,32,32,32	0
85	MG	1	4114	1/1	0.97	0.14	33,33,33,33	0
84	OHX	AR	3457	7/7	0.97	0.10	107,107,108,108	0
85	MG	l2	201	1/1	0.97	0.19	21,21,21,21	0
84	OHX	AR	3463	7/7	0.97	0.13	114,114,115,115	0
85	MG	AR	3943	1/1	0.97	0.08	73,73,73,73	0
85	MG	AR	3944	1/1	0.97	0.15	39,39,39,39	0
85	MG	AR	4158	1/1	0.97	0.05	21,21,21,21	0
84	OHX	1	3448	7/7	0.97	0.18	104,105,106,106	0
85	MG	AR	3947	1/1	0.97	0.13	26,26,26,26	0
85	MG	AR	3948	1/1	0.97	0.15	16,16,16,16	0
85	MG	1	3752	1/1	0.97	0.15	27,27,27,27	0
84	OHX	AR	3546	7/7	0.97	0.13	140,140,141,141	0
84	OHX	1	3472	7/7	0.97	0.12	114,115,115,116	0
85	MG	1	4121	1/1	0.97	0.07	32,32,32,32	0
84	OHX	6	1938	7/7	0.97	0.08	145,146,148,148	0
85	MG	1	4123	1/1	0.97	0.09	41,41,41,41	0
85	MG	1	3756	1/1	0.97	0.10	22,22,22,22	0
85	MG	A	2128	1/1	0.97	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	6	1939	7/7	0.97	0.10	131,133,134,135	0
84	OHX	A	1988	7/7	0.97	0.07	158,160,162,162	0
85	MG	AR	4174	1/1	0.97	0.13	23,23,23,23	0
85	MG	1	3871	1/1	0.97	0.12	27,27,27,27	0
85	MG	6	2069	1/1	0.97	0.24	26,26,26,26	0
84	OHX	1	3492	7/7	0.97	0.14	127,128,128,128	0
85	MG	AR	4178	1/1	0.97	0.08	48,48,48,48	0
85	MG	1	3994	1/1	0.97	0.10	32,32,32,32	0
85	MG	1	3995	1/1	0.97	0.12	54,54,54,54	0
85	MG	A	2138	1/1	0.97	0.11	35,35,35,35	0
85	MG	1	3996	1/1	0.97	0.19	51,51,51,51	0
85	MG	AR	3771	1/1	0.97	0.20	24,24,24,24	0
85	MG	A	2141	1/1	0.97	0.15	73,73,73,73	0
84	OHX	AR	3475	7/7	0.97	0.14	114,115,115,116	0
84	OHX	AR	3552	7/7	0.97	0.11	148,148,149,149	0
84	OHX	A	1992	7/7	0.97	0.09	167,169,170,171	0
85	MG	AR	3776	1/1	0.97	0.07	32,32,32,32	0
85	MG	1	3876	1/1	0.97	0.15	39,39,39,39	0
85	MG	AR	3973	1/1	0.97	0.11	27,27,27,27	0
85	MG	AR	3779	1/1	0.97	0.24	20,20,20,20	0
84	OHX	AR	3476	7/7	0.97	0.10	127,128,129,130	0
85	MG	AR	4195	1/1	0.97	0.08	21,21,21,21	0
85	MG	AR	3782	1/1	0.97	0.10	30,30,30,30	0
85	MG	AR	3977	1/1	0.97	0.27	26,26,26,26	0
85	MG	AR	4198	1/1	0.97	0.12	34,34,34,34	0
85	MG	AR	3978	1/1	0.97	0.10	20,20,20,20	0
85	MG	AR	4200	1/1	0.97	0.30	30,30,30,30	0
84	OHX	4	202	7/7	0.97	0.07	157,158,158,158	0
85	MG	1	4003	1/1	0.97	0.16	46,46,46,46	0
85	MG	AR	3981	1/1	0.97	0.06	17,17,17,17	0
85	MG	1	4004	1/1	0.97	0.05	31,31,31,31	0
85	MG	AR	4205	1/1	0.97	0.09	30,30,30,30	0
84	OHX	AR	3479	7/7	0.97	0.12	119,119,120,120	0
84	OHX	AR	3480	7/7	0.97	0.14	132,132,132,133	0
84	OHX	AR	3481	7/7	0.97	0.10	132,132,133,133	0
85	MG	1	4145	1/1	0.97	0.10	48,48,48,48	0
85	MG	AR	3987	1/1	0.97	0.12	50,50,50,50	0
84	OHX	AR	3482	7/7	0.97	0.14	116,117,117,117	0
85	MG	AR	3989	1/1	0.97	0.07	85,85,85,85	0
84	OHX	6	1943	7/7	0.97	0.09	147,149,150,150	0
86	7MB	AR	4239	20/20	0.97	0.10	44,44,44,44	0
85	MG	AR	3992	1/1	0.97	0.30	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	ZN	DQ	501	1/1	0.97	0.06	105,105,105,105	0
84	OHX	6	1944	7/7	0.97	0.10	154,155,157,158	0
87	ZN	g	501	1/1	0.97	0.04	143,143,143,143	0
85	MG	1	4011	1/1	0.97	0.10	38,38,38,38	0
85	MG	1	4012	1/1	0.97	0.13	26,26,26,26	0
85	MG	AR	3946	1/1	0.98	0.05	28,28,28,28	0
85	MG	1	3740	1/1	0.98	0.13	7,7,7,7	0
84	OHX	AR	3501	7/7	0.98	0.11	118,118,120,120	0
85	MG	1	4212	1/1	0.98	0.04	27,27,27,27	0
84	OHX	6	1948	7/7	0.98	0.09	145,147,148,148	0
84	OHX	AR	3503	7/7	0.98	0.09	152,153,154,154	0
84	OHX	1	3434	7/7	0.98	0.11	94,95,95,95	0
84	OHX	1	3494	7/7	0.98	0.09	141,142,144,144	0
84	OHX	1	3435	7/7	0.98	0.13	103,104,105,105	0
84	OHX	AR	3507	7/7	0.98	0.09	136,136,137,137	0
85	MG	1	4087	1/1	0.98	0.11	37,37,37,37	0
84	OHX	1	3454	7/7	0.98	0.14	111,112,113,113	0
85	MG	1	4222	1/1	0.98	0.09	30,30,30,30	0
85	MG	AR	3961	1/1	0.98	0.16	23,23,23,23	0
85	MG	1	4089	1/1	0.98	0.05	30,30,30,30	0
84	OHX	AR	3509	7/7	0.98	0.10	135,136,136,137	0
85	MG	CR	206	1/1	0.98	0.05	30,30,30,30	0
84	OHX	1	3455	7/7	0.98	0.11	104,104,105,105	0
84	OHX	1	3456	7/7	0.98	0.09	114,115,116,117	0
84	OHX	1	3499	7/7	0.98	0.13	124,125,126,126	0
84	OHX	1	3440	7/7	0.98	0.10	94,95,95,95	0
84	OHX	6	1957	7/7	0.98	0.08	144,145,146,147	0
84	OHX	1	3689	7/7	0.98	0.09	140,141,142,142	0
84	OHX	1	3501	7/7	0.98	0.10	123,124,125,125	0
84	OHX	1	3502	7/7	0.98	0.10	100,101,102,102	0
85	MG	AR	4132	1/1	0.98	0.10	36,36,36,36	0
84	OHX	1	3532	7/7	0.98	0.12	133,133,134,134	0
84	OHX	1	3407	7/7	0.98	0.17	83,83,83,83	0
85	MG	AR	3818	1/1	0.98	0.12	45,45,45,45	0
84	OHX	6	1902	7/7	0.98	0.17	102,102,102,102	0
85	MG	1	4104	1/1	0.98	0.17	32,32,32,32	0
84	OHX	6	1907	7/7	0.98	0.15	100,101,101,101	0
85	MG	DO	202	1/1	0.98	0.08	46,46,46,46	0
84	OHX	1	3460	7/7	0.98	0.10	112,114,115,116	0
85	MG	4	218	1/1	0.98	0.18	7,7,7,7	0
84	OHX	6	1917	7/7	0.98	0.09	113,114,116,117	0
85	MG	AR	3825	1/1	0.98	0.16	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	AR	3401	7/7	0.98	0.22	93,93,93,93	0
84	OHX	AR	3427	7/7	0.98	0.14	87,87,87,87	0
84	OHX	AR	3429	7/7	0.98	0.07	105,105,106,106	0
84	OHX	6	1918	7/7	0.98	0.11	103,104,105,105	0
84	OHX	AR	3433	7/7	0.98	0.12	94,94,94,95	0
85	MG	AR	3831	1/1	0.98	0.18	45,45,45,45	0
84	OHX	AR	3435	7/7	0.98	0.10	96,96,96,96	0
84	OHX	AR	3531	7/7	0.98	0.09	123,124,124,124	0
85	MG	1	3771	1/1	0.98	0.22	23,23,23,23	0
85	MG	AR	3991	1/1	0.98	0.15	15,15,15,15	0
84	OHX	AR	3438	7/7	0.98	0.11	89,89,89,90	0
84	OHX	AR	3697	7/7	0.98	0.12	115,116,116,116	0
84	OHX	AR	3441	7/7	0.98	0.12	109,110,110,111	0
84	OHX	AR	3442	7/7	0.98	0.11	110,111,111,111	0
85	MG	AR	3839	1/1	0.98	0.10	30,30,30,30	0
84	OHX	AR	3443	7/7	0.98	0.10	98,99,100,101	0
84	OHX	AR	3444	7/7	0.98	0.10	101,102,102,103	0
85	MG	A	2060	1/1	0.98	0.17	20,20,20,20	0
84	OHX	A	1909	7/7	0.98	0.10	124,125,128,129	0
85	MG	j	302	1/1	0.98	0.10	29,29,29,29	0
84	OHX	A	1911	7/7	0.98	0.10	115,117,118,120	0
84	OHX	A	1912	7/7	0.98	0.10	132,133,135,136	0
85	MG	AR	4003	1/1	0.98	0.11	73,73,73,73	0
85	MG	AR	4165	1/1	0.98	0.05	88,88,88,88	0
84	OHX	AR	3537	7/7	0.98	0.08	133,134,135,135	0
85	MG	l	403	1/1	0.98	0.06	20,20,20,20	0
84	OHX	AR	3445	7/7	0.98	0.11	94,94,94,95	0
85	MG	AR	4169	1/1	0.98	0.04	34,34,34,34	0
85	MG	6	2172	1/1	0.98	0.08	32,32,32,32	0
84	OHX	A	1916	7/7	0.98	0.08	128,130,131,131	0
84	OHX	A	1917	7/7	0.98	0.10	126,128,129,130	0
84	OHX	AR	3450	7/7	0.98	0.09	109,110,112,113	0
85	MG	AR	4011	1/1	0.98	0.20	31,31,31,31	0
84	OHX	A	1919	7/7	0.98	0.12	113,115,116,116	0
85	MG	1	3787	1/1	0.98	0.12	15,15,15,15	0
84	OHX	AR	3451	7/7	0.98	0.12	104,105,106,106	0
84	OHX	AR	3452	7/7	0.98	0.10	108,109,110,111	0
85	MG	1	3897	1/1	0.98	0.19	13,13,13,13	0
84	OHX	A	1922	7/7	0.98	0.08	138,140,141,141	0
84	OHX	A	1923	7/7	0.98	0.08	137,138,140,140	0
85	MG	AR	4184	1/1	0.98	0.05	35,35,35,35	0
85	MG	1	4137	1/1	0.98	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	3863	1/1	0.98	0.24	15,15,15,15	0
84	OHX	AR	3453	7/7	0.98	0.10	127,128,128,128	0
84	OHX	A	1925	7/7	0.98	0.07	171,172,174,175	0
85	MG	6	2186	1/1	0.98	0.05	82,82,82,82	0
85	MG	6	2187	1/1	0.98	0.12	82,82,82,82	0
85	MG	1	3794	1/1	0.98	0.06	31,31,31,31	0
85	MG	AR	3869	1/1	0.98	0.14	12,12,12,12	0
84	OHX	AR	3455	7/7	0.98	0.12	106,107,108,108	0
85	MG	1	3904	1/1	0.98	0.22	4,4,4,4	0
85	MG	AR	3872	1/1	0.98	0.22	0,0,0,0	0
85	MG	AR	4031	1/1	0.98	0.10	31,31,31,31	0
84	OHX	AR	3456	7/7	0.98	0.10	109,110,110,111	0
85	MG	1	3797	1/1	0.98	0.07	41,41,41,41	0
85	MG	1	3908	1/1	0.98	0.20	14,14,14,14	0
85	MG	1	4147	1/1	0.98	0.14	28,28,28,28	0
84	OHX	1	3505	7/7	0.98	0.09	139,139,140,140	0
85	MG	1	4149	1/1	0.98	0.18	45,45,45,45	0
84	OHX	AR	3459	7/7	0.98	0.11	97,97,98,99	0
85	MG	1	3800	1/1	0.98	0.12	37,37,37,37	0
85	MG	AR	4207	1/1	0.98	0.10	50,50,50,50	0
85	MG	AR	3881	1/1	0.98	0.17	12,12,12,12	0
85	MG	1	4028	1/1	0.98	0.06	24,24,24,24	0
84	OHX	AR	3460	7/7	0.98	0.09	109,109,110,110	0
84	OHX	AR	3461	7/7	0.98	0.09	108,109,109,110	0
84	OHX	6	1920	7/7	0.98	0.10	124,126,127,128	0
85	MG	1	4156	1/1	0.98	0.10	65,65,65,65	0
84	OHX	6	1921	7/7	0.98	0.11	121,124,124,126	0
85	MG	1	3916	1/1	0.98	0.20	14,14,14,14	0
84	OHX	6	1922	7/7	0.98	0.09	111,112,113,114	0
84	OHX	1	3442	7/7	0.98	0.10	98,99,99,100	0
84	OHX	AR	3553	7/7	0.98	0.06	160,160,161,162	0
84	OHX	AR	3469	7/7	0.98	0.08	122,124,125,125	0
85	MG	AR	3741	1/1	0.98	0.14	14,14,14,14	0
84	OHX	AR	3470	7/7	0.98	0.08	125,127,127,128	0
85	MG	AR	4222	1/1	0.98	0.05	27,27,27,27	0
84	OHX	AR	3471	7/7	0.98	0.16	127,127,128,128	0
84	OHX	AR	3557	7/7	0.98	0.07	144,145,146,146	0
84	OHX	6	1925	7/7	0.98	0.12	116,116,118,118	0
85	MG	AR	4226	1/1	0.98	0.28	16,16,16,16	0
84	OHX	6	1926	7/7	0.98	0.08	122,123,124,124	0
84	OHX	A	1944	7/7	0.98	0.08	161,163,165,165	0
84	OHX	AR	3474	7/7	0.98	0.11	119,120,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	1	3480	7/7	0.98	0.08	141,141,142,142	0
85	MG	AR	4231	1/1	0.98	0.12	9,9,9,9	0
85	MG	AR	3751	1/1	0.98	0.15	29,29,29,29	0
84	OHX	1	3538	7/7	0.98	0.10	135,135,137,137	0
84	OHX	3	201	7/7	0.98	0.10	106,107,108,108	0
84	OHX	6	1930	7/7	0.98	0.09	114,115,116,117	0
85	MG	1	3820	1/1	0.98	0.16	30,30,30,30	0
85	MG	AR	3756	1/1	0.98	0.30	11,11,11,11	0
84	OHX	1	3508	7/7	0.98	0.07	140,142,143,144	0
84	OHX	1	3571	7/7	0.98	0.07	144,145,145,146	0
85	MG	6	2090	1/1	0.98	0.23	45,45,45,45	0
84	OHX	1	3481	7/7	0.98	0.08	130,131,132,133	0
84	OHX	AR	3483	7/7	0.98	0.12	124,125,125,126	0
84	OHX	6	1934	7/7	0.98	0.08	141,141,143,144	0
85	MG	AR	4073	1/1	0.98	0.05	33,33,33,33	0
85	MG	1	3942	1/1	0.98	0.14	20,20,20,20	0
85	MG	AR	3916	1/1	0.98	0.17	3,3,3,3	0
85	MG	1	3943	1/1	0.98	0.10	22,22,22,22	0
84	OHX	A	1955	7/7	0.98	0.06	145,148,150,150	0
85	MG	1	4059	1/1	0.98	0.13	32,32,32,32	0
84	OHX	1	3482	7/7	0.98	0.09	116,116,117,117	0
84	OHX	1	3444	7/7	0.98	0.09	103,104,104,105	0
84	OHX	1	3463	7/7	0.98	0.12	108,109,109,109	0
85	MG	1	3948	1/1	0.98	0.17	46,46,46,46	0
85	MG	6	2102	1/1	0.98	0.17	14,14,14,14	0
85	MG	AS	224	1/1	0.98	0.06	55,55,55,55	0
85	MG	AR	3774	1/1	0.98	0.14	23,23,23,23	0
85	MG	AR	4085	1/1	0.98	0.07	37,37,37,37	0
84	OHX	1	3445	7/7	0.98	0.11	95,95,95,96	0
84	OHX	1	3465	7/7	0.98	0.10	113,114,114,114	0
85	MG	AR	3777	1/1	0.98	0.09	50,50,50,50	0
85	MG	AS	230	1/1	0.98	0.04	67,67,67,67	0
84	OHX	1	3487	7/7	0.98	0.09	139,140,142,142	0
85	MG	s8	302	1/1	0.98	0.13	44,44,44,44	0
84	OHX	1	3446	7/7	0.98	0.11	107,108,109,110	0
84	OHX	6	1942	7/7	0.98	0.07	142,143,144,145	0
85	MG	AR	3781	1/1	0.98	0.19	11,11,11,11	0
85	MG	1	4197	1/1	0.98	0.07	48,48,48,48	0
84	OHX	1	3489	7/7	0.98	0.10	114,115,116,117	0
85	MG	1	3836	1/1	0.98	0.18	17,17,17,17	0
85	MG	1	3837	1/1	0.98	0.22	25,25,25,25	0
85	MG	AR	3937	1/1	0.98	0.18	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	3786	1/1	0.98	0.05	16,16,16,16	0
84	OHX	1	3467	7/7	0.98	0.09	124,125,126,126	0
84	OHX	1	3519	7/7	0.98	0.13	112,112,113,113	0
84	OHX	AR	3498	7/7	0.98	0.07	143,144,145,146	0
85	MG	1	3841	1/1	0.98	0.16	19,19,19,19	0
84	OHX	1	3433	7/7	0.98	0.13	90,90,90,90	0
84	OHX	1	3469	7/7	0.98	0.11	118,118,119,120	0
85	MG	1	4208	1/1	0.98	0.26	30,30,30,30	0
84	OHX	AR	3440	7/7	0.99	0.08	98,98,98,99	0
85	MG	AR	3848	1/1	0.99	0.12	15,15,15,15	0
84	OHX	6	1911	7/7	0.99	0.10	99,100,100,100	0
84	OHX	6	1912	7/7	0.99	0.07	107,108,110,110	0
84	OHX	6	1913	7/7	0.99	0.10	105,105,106,107	0
84	OHX	1	3451	7/7	0.99	0.07	101,101,102,103	0
84	OHX	6	1915	7/7	0.99	0.09	100,101,102,102	0
84	OHX	AS	201	7/7	0.99	0.10	98,99,100,101	0
84	OHX	AR	3446	7/7	0.99	0.09	99,100,100,101	0
84	OHX	AS	203	7/7	0.99	0.08	118,119,120,120	0
84	OHX	AR	3447	7/7	0.99	0.09	88,88,89,89	0
84	OHX	AR	3448	7/7	0.99	0.09	109,110,110,110	0
84	OHX	AR	3449	7/7	0.99	0.08	98,99,99,100	0
84	OHX	6	1916	7/7	0.99	0.09	102,103,104,104	0
84	OHX	1	3452	7/7	0.99	0.10	111,111,112,113	0
85	MG	DH	203	1/1	0.99	0.09	41,41,41,41	0
84	OHX	1	3415	7/7	0.99	0.09	89,90,90,90	0
84	OHX	1	3416	7/7	0.99	0.12	86,86,86,86	0
84	OHX	AT	202	7/7	0.99	0.15	86,86,87,87	0
84	OHX	AT	203	7/7	0.99	0.15	83,83,83,83	0
84	OHX	AR	3454	7/7	0.99	0.08	120,120,121,121	0
84	OHX	1	3417	7/7	0.99	0.14	97,97,97,97	0
84	OHX	1	3418	7/7	0.99	0.09	85,85,85,85	0
85	MG	1	4143	1/1	0.99	0.07	53,53,53,53	0
84	OHX	1	3457	7/7	0.99	0.09	108,108,109,109	0
85	MG	AR	4017	1/1	0.99	0.10	27,27,27,27	0
84	OHX	AR	3458	7/7	0.99	0.08	100,101,101,102	0
84	OHX	1	3419	7/7	0.99	0.16	93,93,93,93	0
84	OHX	6	1924	7/7	0.99	0.07	123,124,126,127	0
85	MG	AB	202	1/1	0.99	0.08	34,34,34,34	0
85	MG	AR	4171	1/1	0.99	0.06	59,59,59,59	0
84	OHX	A	1984	7/7	0.99	0.06	151,152,153,154	0
84	OHX	1	3420	7/7	0.99	0.14	91,91,92,92	0
84	OHX	AR	3462	7/7	0.99	0.07	106,107,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	1	3421	7/7	0.99	0.10	84,84,84,84	0
85	MG	1	4022	1/1	0.99	0.09	24,24,24,24	0
84	OHX	1	3422	7/7	0.99	0.13	94,94,94,94	0
84	OHX	AR	3465	7/7	0.99	0.09	100,101,102,102	0
84	OHX	1	3423	7/7	0.99	0.11	91,92,92,92	0
84	OHX	1	3425	7/7	0.99	0.11	93,93,93,93	0
85	MG	AR	4181	1/1	0.99	0.06	37,37,37,37	0
84	OHX	AR	3468	7/7	0.99	0.07	111,112,113,114	0
85	MG	1	4158	1/1	0.99	0.09	29,29,29,29	0
84	OHX	1	3426	7/7	0.99	0.11	93,93,93,94	0
84	OHX	1	3427	7/7	0.99	0.11	87,87,87,87	0
84	OHX	1	3428	7/7	0.99	0.10	96,96,96,96	0
85	MG	1	3906	1/1	0.99	0.21	29,29,29,29	0
85	MG	AR	4188	1/1	0.99	0.05	35,35,35,35	0
85	MG	AR	3747	1/1	0.99	0.19	23,23,23,23	0
84	OHX	1	3429	7/7	0.99	0.09	89,89,90,90	0
84	OHX	1	3430	7/7	0.99	0.10	97,97,97,98	0
84	OHX	1	3431	7/7	0.99	0.11	95,95,95,95	0
85	MG	1	4166	1/1	0.99	0.07	30,30,30,30	0
84	OHX	1	3402	7/7	0.99	0.19	90,90,91,91	0
84	OHX	1	3471	7/7	0.99	0.11	118,118,121,121	0
84	OHX	1	3403	7/7	0.99	0.19	90,90,90,90	0
85	MG	1	4038	1/1	0.99	0.12	33,33,33,33	0
84	OHX	AR	3478	7/7	0.99	0.07	102,103,103,104	0
84	OHX	1	3404	7/7	0.99	0.15	93,93,93,93	0
84	OHX	1	3405	7/7	0.99	0.22	97,98,98,98	0
84	OHX	1	3436	7/7	0.99	0.09	101,102,104,104	0
85	MG	AR	3903	1/1	0.99	0.20	5,5,5,5	0
84	OHX	1	3437	7/7	0.99	0.10	100,101,102,102	0
85	MG	AR	3761	1/1	0.99	0.06	41,41,41,41	0
84	OHX	1	3438	7/7	0.99	0.09	91,91,92,92	0
84	OHX	CV	201	7/7	0.99	0.15	91,91,91,91	0
84	OHX	1	3439	7/7	0.99	0.09	102,103,103,104	0
84	OHX	1	3406	7/7	0.99	0.17	85,85,85,85	0
84	OHX	DD	102	7/7	0.99	0.12	88,89,89,89	0
85	MG	AR	3767	1/1	0.99	0.04	34,34,34,34	0
84	OHX	AR	3486	7/7	0.99	0.08	118,119,120,121	0
85	MG	1	3924	1/1	0.99	0.36	8,8,8,8	0
84	OHX	1	3401	7/7	0.99	0.20	89,89,90,90	0
84	OHX	1	3408	7/7	0.99	0.08	89,89,89,89	0
85	MG	1	3927	1/1	0.99	0.20	6,6,6,6	0
84	OHX	1	3443	7/7	0.99	0.11	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	OHX	AR	3490	7/7	0.99	0.06	108,108,109,110	0
84	OHX	A	1901	7/7	0.99	0.17	101,101,102,102	0
84	OHX	A	1902	7/7	0.99	0.13	96,97,97,97	0
85	MG	1	3932	1/1	0.99	0.17	24,24,24,24	0
84	OHX	A	1903	7/7	0.99	0.16	117,118,118,119	0
84	OHX	A	1904	7/7	0.99	0.10	107,107,108,108	0
85	MG	1	3935	1/1	0.99	0.17	24,24,24,24	0
84	OHX	A	1905	7/7	0.99	0.11	102,102,103,103	0
84	OHX	A	1906	7/7	0.99	0.11	112,113,113,113	0
84	OHX	A	1907	7/7	0.99	0.08	117,118,120,121	0
85	MG	6	2113	1/1	0.99	0.27	23,23,23,23	0
85	MG	1	4065	1/1	0.99	0.10	35,35,35,35	0
84	OHX	A	1908	7/7	0.99	0.10	111,111,113,114	0
84	OHX	1	3409	7/7	0.99	0.15	85,85,85,85	0
84	OHX	A	1910	7/7	0.99	0.09	123,125,127,128	0
84	OHX	1	3411	7/7	0.99	0.14	93,93,93,93	0
84	OHX	1	3412	7/7	0.99	0.16	88,88,88,88	0
85	MG	1	4205	1/1	0.99	0.20	26,26,26,26	0
84	OHX	AC	101	7/7	0.99	0.12	89,90,90,90	0
84	OHX	A	1914	7/7	0.99	0.07	109,110,111,112	0
85	MG	AR	4238	1/1	0.99	0.17	27,27,27,27	0
84	OHX	1	3447	7/7	0.99	0.08	95,95,95,95	0
85	MG	1	4209	1/1	0.99	0.29	22,22,22,22	0
84	OHX	1	3413	7/7	0.99	0.11	88,88,89,89	0
84	OHX	2	201	7/7	0.99	0.11	94,94,94,94	0
84	OHX	6	1901	7/7	0.99	0.20	92,92,92,92	0
84	OHX	1	3414	7/7	0.99	0.11	90,90,90,90	0
84	OHX	6	1903	7/7	0.99	0.16	89,89,90,90	0
84	OHX	AR	3402	7/7	0.99	0.21	89,89,89,89	0
84	OHX	AR	3403	7/7	0.99	0.15	86,86,86,86	0
84	OHX	AR	3404	7/7	0.99	0.14	88,89,89,89	0
85	MG	AR	4095	1/1	0.99	0.13	36,36,36,36	0
85	MG	AS	217	1/1	0.99	0.04	18,18,18,18	0
84	OHX	AR	3405	7/7	0.99	0.18	94,94,94,94	0
84	OHX	AR	3406	7/7	0.99	0.17	86,86,86,86	0
85	MG	AR	3950	1/1	0.99	0.15	41,41,41,41	0
84	OHX	AR	3407	7/7	0.99	0.18	88,88,88,88	0
84	OHX	AR	3408	7/7	0.99	0.14	83,83,83,83	0
84	OHX	AR	3409	7/7	0.99	0.17	92,92,92,92	0
84	OHX	AR	3410	7/7	0.99	0.08	86,86,86,86	0
84	OHX	AR	3411	7/7	0.99	0.15	83,83,83,83	0
85	MG	3	212	1/1	0.99	0.21	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	AR	4105	1/1	0.99	0.08	41,41,41,41	0
84	OHX	AR	3511	7/7	0.99	0.08	96,96,96,97	0
84	OHX	AR	3412	7/7	0.99	0.11	85,85,85,85	0
85	MG	AR	3959	1/1	0.99	0.12	32,32,32,32	0
84	OHX	AR	3413	7/7	0.99	0.13	84,84,84,84	0
85	MG	6	2144	1/1	0.99	0.08	42,42,42,42	0
84	OHX	AR	3414	7/7	0.99	0.12	90,90,90,90	0
84	OHX	AR	3415	7/7	0.99	0.16	86,86,86,87	0
85	MG	1	4094	1/1	0.99	0.04	43,43,43,43	0
84	OHX	AR	3416	7/7	0.99	0.12	88,88,88,89	0
84	OHX	AR	3418	7/7	0.99	0.09	92,92,93,93	0
84	OHX	A	1938	7/7	0.99	0.07	138,139,140,141	0
85	MG	1	4098	1/1	0.99	0.10	33,33,33,33	0
84	OHX	AR	3419	7/7	0.99	0.09	94,94,95,95	0
84	OHX	AR	3420	7/7	0.99	0.12	87,87,87,87	0
84	OHX	AR	3421	7/7	0.99	0.10	89,89,89,89	0
84	OHX	AR	3422	7/7	0.99	0.11	86,86,86,86	0
85	MG	1	3850	1/1	0.99	0.04	29,29,29,29	0
85	MG	CE	401	1/1	0.99	0.09	30,30,30,30	0
85	MG	s1	301	1/1	0.99	0.10	67,67,67,67	0
84	OHX	AR	3423	7/7	0.99	0.14	85,85,85,85	0
84	OHX	AR	3424	7/7	0.99	0.12	86,87,87,87	0
84	OHX	AR	3425	7/7	0.99	0.09	85,85,85,85	0
84	OHX	6	1905	7/7	0.99	0.14	100,100,101,101	0
84	OHX	AR	3428	7/7	0.99	0.08	97,97,98,98	0
84	OHX	6	1906	7/7	0.99	0.13	94,94,95,95	0
84	OHX	1	3450	7/7	0.99	0.10	116,117,118,118	0
84	OHX	AR	3431	7/7	0.99	0.11	86,86,86,86	0
84	OHX	AR	3432	7/7	0.99	0.10	91,91,91,91	0
84	OHX	6	1908	7/7	0.99	0.13	91,91,91,91	0
84	OHX	AR	3434	7/7	0.99	0.10	87,87,88,88	0
84	OHX	6	1909	7/7	0.99	0.11	103,104,104,104	0
85	MG	1	3863	1/1	0.99	0.22	25,25,25,25	0
84	OHX	AR	3436	7/7	0.99	0.09	87,87,87,87	0
87	ZN	AQ	501	1/1	0.99	0.03	77,77,77,77	0
84	OHX	AR	3437	7/7	0.99	0.09	89,89,89,89	0
87	ZN	DR	501	1/1	0.99	0.02	73,73,73,73	0
87	ZN	b	102	1/1	0.99	0.03	68,68,68,68	0
84	OHX	6	1910	7/7	0.99	0.12	93,93,93,93	0
85	MG	AR	3844	1/1	0.99	0.07	25,25,25,25	0
84	OHX	AR	3439	7/7	0.99	0.09	91,91,92,92	0
87	ZN	d9	103	1/1	0.99	0.04	86,86,86,86	0

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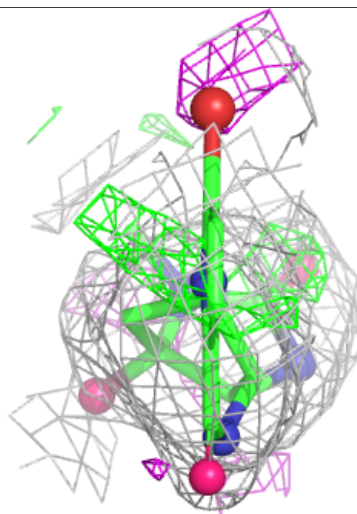
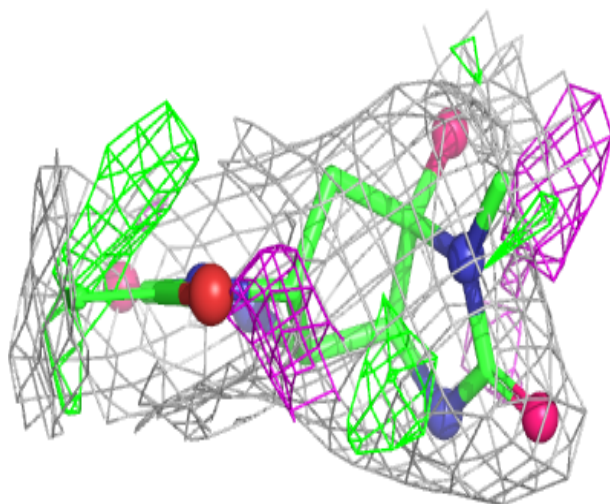
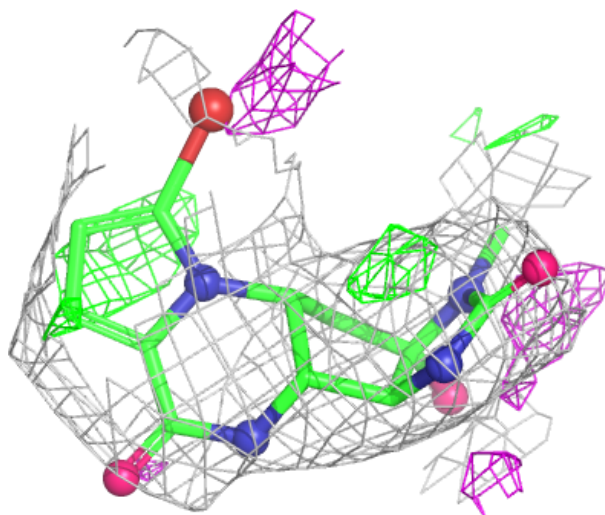
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3868	1/1	0.99	0.29	9,9,9,9	0
84	OHX	1	3410	7/7	1.00	0.13	88,88,88,88	0
84	OHX	AR	3417	7/7	1.00	0.11	86,86,86,86	0
87	ZN	DL	103	1/1	1.00	0.01	37,37,37,37	0
87	ZN	DO	201	1/1	1.00	0.02	31,31,31,31	0
84	OHX	AR	3426	7/7	1.00	0.08	88,88,88,89	0
85	MG	1	4193	1/1	1.00	0.19	9,9,9,9	0
85	MG	AR	4189	1/1	1.00	0.04	32,32,32,32	0
85	MG	1	4187	1/1	1.00	0.05	55,55,55,55	0
87	ZN	e	102	1/1	1.00	0.03	74,74,74,74	0
84	OHX	1	3424	7/7	1.00	0.13	92,93,93,93	0
87	ZN	d6	102	1/1	1.00	0.02	59,59,59,59	0
84	OHX	6	1904	7/7	1.00	0.12	96,96,96,96	0
87	ZN	AK	101	1/1	1.00	0.01	38,38,38,38	0
87	ZN	AN	500	1/1	1.00	0.02	43,43,43,43	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.

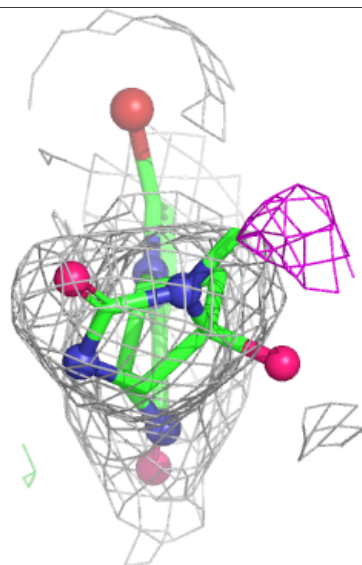
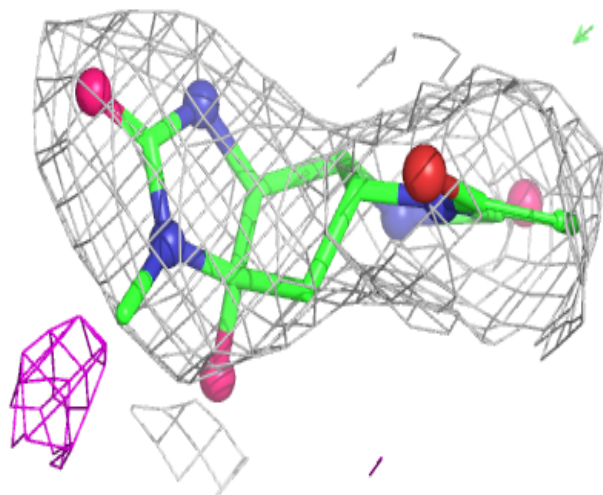
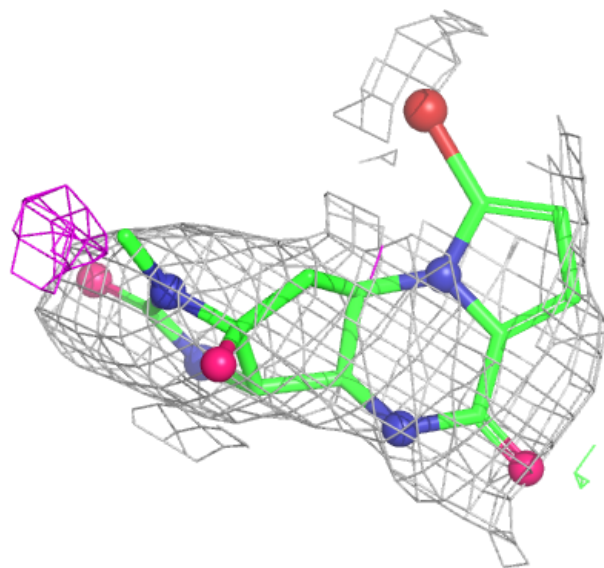
Electron density around 7MB 1 4216:

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



Electron density around 7MB AR 4239:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.