



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 07:34 pm BST

PDB ID : 5TBW  
Title : Crystal structure of chlorolissoclimide bound to the yeast 80S ribosome  
Authors : Konst, Z.A.; Szklarski, A.R.; Pellegrino, S.; Michalak, S.E.; Meyer, M.; Zquette, C.; Cencic, R.; Nam, S.; Horne, D.A.; Pelletier, J.; Mobley, D.L.; Yusupova, G.; Yusupov, M.; Vanderwal, C.D.  
Deposited on : 2016-09-13  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

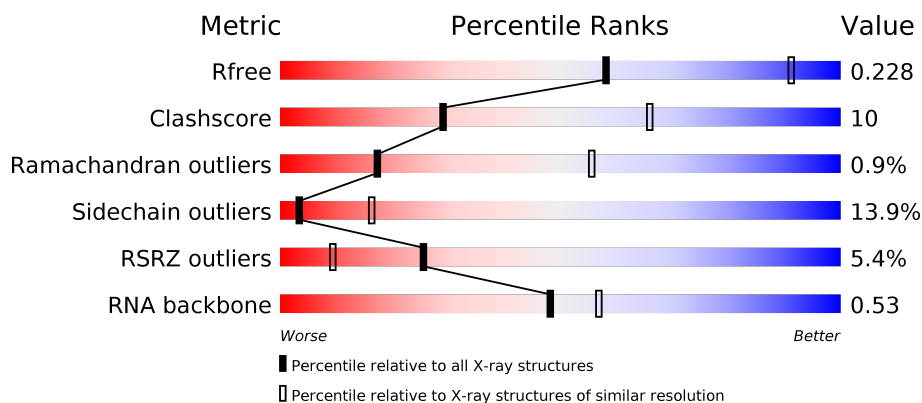
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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





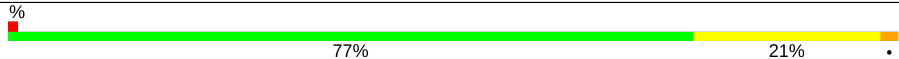
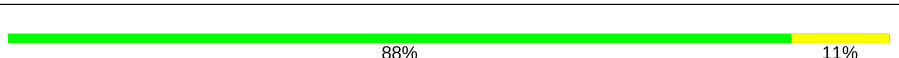
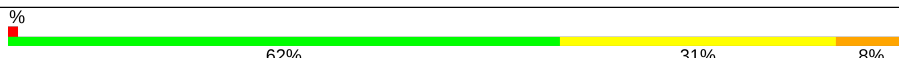
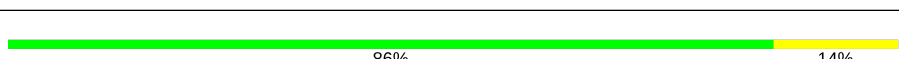
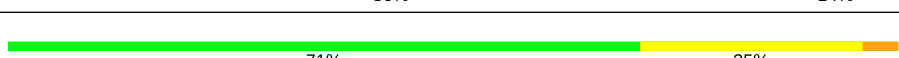
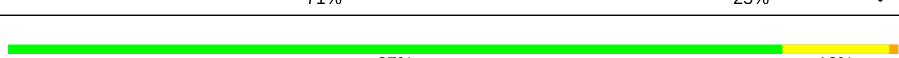
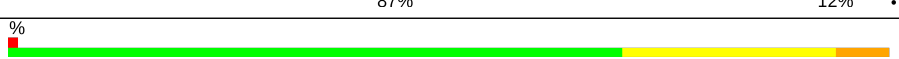

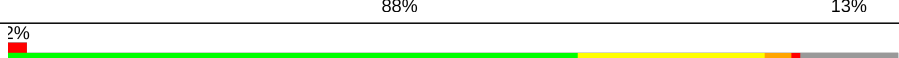



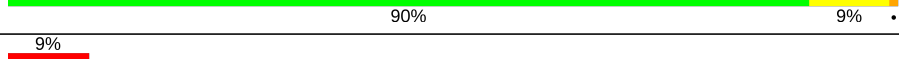



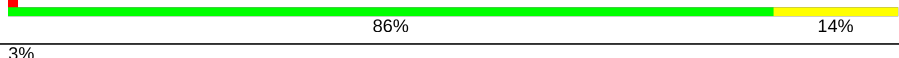
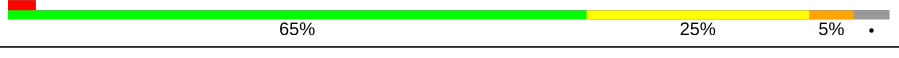

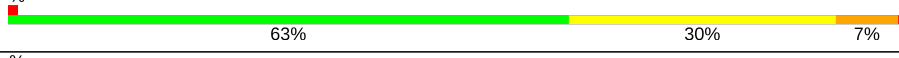



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3149	<div> <div>2%</div> <div>62% 30% 7%</div> </div>
1	AR	3149	<div> <div>3%</div> <div>60% 32% 8%</div> </div>
2	3	121	<div> <div>70% 27%</div> </div>
2	AS	121	<div> <div>66% 31%</div> </div>











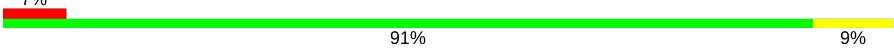


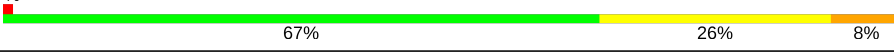
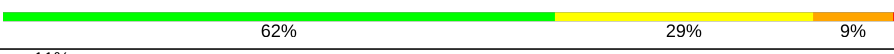
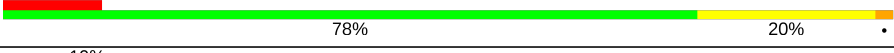

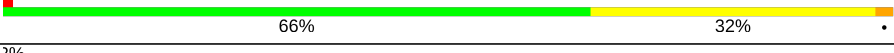







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Mol	Chain	Length	Quality of chain
3	4	158	
3	AT	158	
4	CD	252	
4	j	252	
5	CE	386	
5	k	386	
6	CF	361	
6	l	361	
7	CG	296	
7	m	296	
8	CH	175	
8	n	175	
9	CI	222	
9	o	222	
10	CJ	233	
10	p	233	
11	CK	191	
11	q	191	
12	CL	220	
12	r	220	
13	CM	169	
13	s	169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

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Mol	Chain	Length	Quality of chain
15	u	136	
16	CP	203	
16	v	203	
17	CQ	197	
17	w	197	
18	CR	183	
18	x	183	
19	CS	185	
19	y	185	
20	CT	188	
20	z	188	
21	0	172	
21	CU	172	
22	2	159	
22	CV	159	
23	5	100	
23	CW	100	
24	6	136	
24	CX	136	
25	7	98	
25	CY	98	
26	8	121	
26	CZ	121	
27	9	126	
27	DA	126	

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Mol	Chain	Length	Quality of chain
28	AA	135	
28	DB	135	
29	AB	148	
29	DC	148	
30	AC	58	
30	DD	58	
31	AD	97	
31	DE	97	
32	AE	109	
32	DF	109	
33	AF	127	
33	DG	127	
34	AG	106	
34	DH	106	
35	AH	112	
35	DI	112	
36	AI	119	
36	DJ	119	
37	AJ	99	
37	DK	99	
38	AK	87	
38	DL	87	
39	AL	77	
39	DM	77	
40	AM	50	

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Mol	Chain	Length	Quality of chain
40	DN	50	
41	AN	52	
41	DO	52	
42	AO	25	
42	DP	25	
43	AP	105	
43	DQ	105	
44	AQ	91	
44	DR	91	
45	i	168	
46	p0	219	
47	sM	104	
48	A	1800	
48	sR	1800	
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	
54	G	206	

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Mol	Chain	Length	Quality of chain
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	143	
61	c2	143	
62	O	150	
62	c3	150	
63	P	128	
63	c4	128	
64	Q	135	
64	c5	135	
65	R	142	
65	c6	142	
66	S	125	
67	T	145	


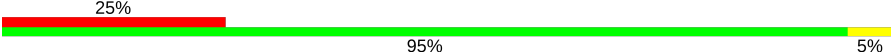
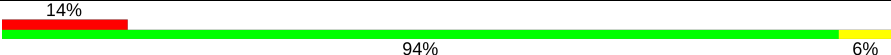
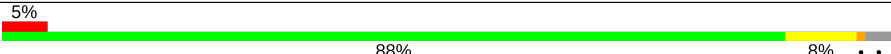
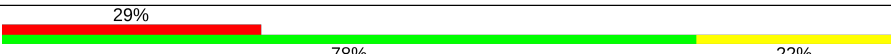
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Mol	Chain	Length	Quality of chain
67	c8	145	
68	U	143	
68	c9	143	
69	V	110	
69	d0	110	
70	W	87	
70	d1	87	
71	X	129	
71	d2	129	
72	Y	144	
72	d3	144	
73	Z	134	
73	d4	134	
74	a	70	
74	d5	70	
75	b	97	
75	d6	97	
76	c	81	
76	d7	81	
77	d	63	
77	d8	63	
78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

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Mol	Chain	Length	Quality of chain
80	g	71	
81	Rb	318	
81	h	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	3437	-	-	X	-
84	OHX	1	3474	-	-	X	-
84	OHX	1	3540	-	-	X	-
84	OHX	1	3580	-	-	X	-
84	OHX	1	3592	-	-	X	-
84	OHX	1	3673	-	-	-	X
84	OHX	1	3697	-	-	X	-
84	OHX	1	3705	-	-	X	-
84	OHX	1	3713	-	-	X	-
84	OHX	1	3718	-	-	-	X
84	OHX	1	3730	-	-	X	-
84	OHX	A	1909	-	-	X	-
84	OHX	A	2009	-	-	X	-
84	OHX	A	2024	-	-	X	-
84	OHX	A	2039	-	-	-	X
84	OHX	AP	502	-	-	X	-
84	OHX	AR	3445	-	-	X	-
84	OHX	AR	3465	-	-	X	-
84	OHX	AR	3507	-	-	X	-
84	OHX	AR	3516	-	-	X	-
84	OHX	AR	3526	-	-	X	-
84	OHX	AR	3599	-	-	X	-
84	OHX	AR	3677	-	-	X	-
84	OHX	AR	3703	-	-	X	-
84	OHX	AR	3705	-	-	X	-
84	OHX	AR	3721	-	-	X	-
84	OHX	AR	3738	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	AR	3740	-	-	-	X
84	OHX	AT	212	-	-	X	-
84	OHX	CL	301	-	-	X	-
84	OHX	sR	2040	-	-	-	X
85	MG	1	3772	-	-	-	X
85	MG	1	3787	-	-	-	X
85	MG	1	3790	-	-	-	X
85	MG	1	3802	-	-	-	X
85	MG	1	3822	-	-	-	X
85	MG	1	3834	-	-	-	X
85	MG	1	3866	-	-	-	X
85	MG	1	3878	-	-	-	X
85	MG	1	3913	-	-	-	X
85	MG	1	3985	-	-	-	X
85	MG	1	3988	-	-	-	X
85	MG	1	3994	-	-	-	X
85	MG	1	4001	-	-	-	X
85	MG	1	4003	-	-	-	X
85	MG	1	4032	-	-	-	X
85	MG	1	4104	-	-	-	X
85	MG	1	4108	-	-	-	X
85	MG	1	4116	-	-	-	X
85	MG	1	4155	-	-	-	X
85	MG	1	4162	-	-	-	X
85	MG	1	4194	-	-	-	X
85	MG	3	210	-	-	-	X
85	MG	3	216	-	-	-	X
85	MG	A	2068	-	-	-	X
85	MG	A	2102	-	-	-	X
85	MG	A	2104	-	-	-	X
85	MG	A	2113	-	-	-	X
85	MG	A	2119	-	-	-	X
85	MG	A	2134	-	-	-	X
85	MG	AR	3803	-	-	-	X
85	MG	AR	3834	-	-	-	X
85	MG	AR	3966	-	-	-	X
85	MG	AR	3972	-	-	-	X
85	MG	AR	3974	-	-	-	X
85	MG	AR	3989	-	-	-	X
85	MG	AR	4038	-	-	-	X
85	MG	AR	4055	-	-	-	X
85	MG	AR	4085	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	AR	4091	-	-	-	X
85	MG	AR	4102	-	-	-	X
85	MG	AR	4113	-	-	-	X
85	MG	AR	4126	-	-	-	X
85	MG	AR	4138	-	-	-	X
85	MG	AR	4156	-	-	-	X
85	MG	AR	4157	-	-	-	X
85	MG	AR	4169	-	-	-	X
85	MG	AR	4171	-	-	-	X
85	MG	AR	4186	-	-	-	X
85	MG	AR	4227	-	-	-	X
85	MG	AR	4233	-	-	-	X
85	MG	AR	4236	-	-	-	X
85	MG	AT	221	-	-	-	X
85	MG	AT	225	-	-	-	X
85	MG	l	403	-	-	-	X
85	MG	l	404	-	-	-	X
85	MG	l	406	-	-	-	X
85	MG	sR	2066	-	-	-	X
85	MG	sR	2082	-	-	-	X
85	MG	sR	2157	-	-	-	X
85	MG	sR	2159	-	-	-	X
85	MG	sR	2185	-	-	-	X
85	MG	sR	2187	-	-	-	X
85	MG	sR	2188	-	-	-	X
85	MG	x	206	-	-	-	X

## 2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 409612 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	6	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 protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
25	CY	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	8	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

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

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	9	126	Total	C	N	O		0	0	0
			993	625	192	176				
27	DA	126	Total	C	N	O		0	0	0
			993	625	192	176				

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L28.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

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

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

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 45 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	i	159	Total	C	N	O	0	0	0
			1104	654	221	229			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	134	LEU	ASP	conflict	UNP P39015

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 47 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	sM	104	Total	C	N	O	0	0	0
			681	404	140	137			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
sM	59	ALA	GLY	conflict	UNP P39015

- Molecule 48 is a RNA chain called 18S ribosomal RNA.

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

- 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	0	0	0
			1577	1014	278	283	2			
49	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- 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	0	0	0
			1709	1084	310	311	4			
50	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- 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	0	0	0
			1635	1047	289	297	2			
51	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- 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	0	0	0
			1734	1101	313	314	6			
52	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- 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	0	0	0
			2068	1316	389	360	3			
53	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- 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
			760	489	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			

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

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

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				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			
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	Rb	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

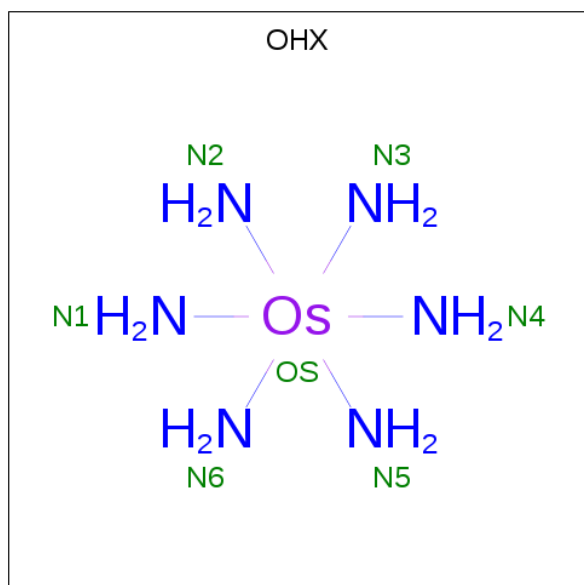
- Molecule 82 is a protein called 40S ribosomal protein S17-A.

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 (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	CX	1	Total	N	Os	0	0
			7	6	1		
84	CX	1	Total	N	Os	0	0
			7	6	1		
84	DD	1	Total	N	Os	0	0
			7	6	1		
84	DH	1	Total	N	Os	0	0
			7	6	1		
84	DL	1	Total	N	Os	0	0
			7	6	1		
84	DQ	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		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total 7	N 6	Os 1	0	0
84	H	1	Total 7	N 6	Os 1	0	0
84	J	1	Total 7	N 6	Os 1	0	0
84	M	1	Total 7	N 6	Os 1	0	0
84	O	1	Total 7	N 6	Os 1	0	0
84	Q	1	Total 7	N 6	Os 1	0	0
84	T	1	Total 7	N 6	Os 1	0	0
84	e	1	Total 7	N 6	Os 1	0	0
84	h	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	Rb	1	Total	N	Os	0	0
			7	6	1		
84	s1	1	Total	N	Os	0	0
			7	6	1		
84	s4	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	d4	1	Total	N	Os	0	0
			7	6	1		
84	d9	1	Total	N	Os	0	0
			7	6	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AP	1	Total	Mg	0	0
			1	1		
85	AK	1	Total	Mg	0	0
			1	1		
85	AB	4	Total	Mg	0	0
			4	4		
85	c6	1	Total	Mg	0	0
			1	1		
85	6	2	Total	Mg	0	0
			2	2		
85	DO	1	Total	Mg	0	0
			1	1		
85	sM	1	Total	Mg	0	0
			1	1		
85	d5	1	Total	Mg	0	0
			1	1		
85	t	3	Total	Mg	0	0
			3	3		
85	CD	2	Total	Mg	0	0
			2	2		
85	CR	6	Total	Mg	0	0
			6	6		
85	o	1	Total	Mg	0	0
			1	1		
85	DC	6	Total	Mg	0	0
			6	6		
85	AS	17	Total	Mg	0	0
			17	17		
85	DH	2	Total	Mg	0	0
			2	2		
85	J	1	Total	Mg	0	0
			1	1		
85	k	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	CU	1	Total 1	Mg 1	0	0
85	b	1	Total 1	Mg 1	0	0
85	DR	2	Total 2	Mg 2	0	0
85	w	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	A	109	Total 109	Mg 109	0	0
85	CQ	3	Total 3	Mg 3	0	0
85	n	1	Total 1	Mg 1	0	0
85	x	5	Total 5	Mg 5	0	0
85	AR	504	Total 504	Mg 504	0	0
85	d6	2	Total 2	Mg 2	0	0
85	s	1	Total 1	Mg 1	0	0
85	CG	1	Total 1	Mg 1	0	0
85	j	1	Total 1	Mg 1	0	0
85	1	485	Total 485	Mg 485	0	0
85	CN	1	Total 1	Mg 1	0	0
85	DD	1	Total 1	Mg 1	0	0
85	e	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	v	2	Total 2	Mg 2	0	0

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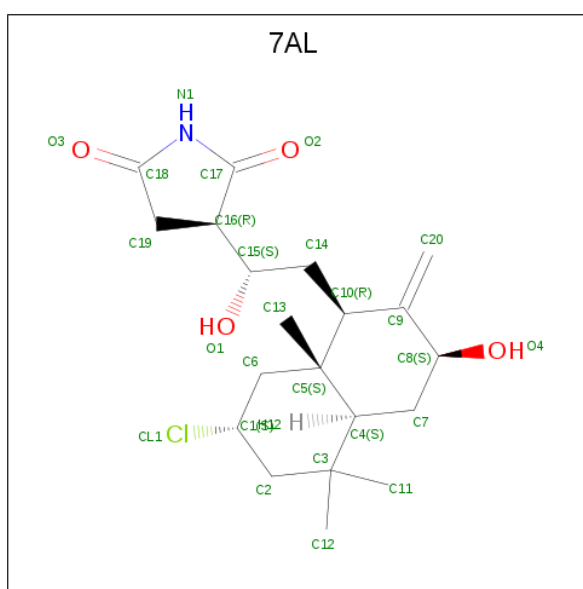
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	CJ	1	Total 1	Mg 1	0	0
85	CP	4	Total 4	Mg 4	0	0
85	4	19	Total 19	Mg 19	0	0
85	DA	1	Total 1	Mg 1	0	0
85	O	1	Total 1	Mg 1	0	0
85	r	2	Total 2	Mg 2	0	0
85	CF	1	Total 1	Mg 1	0	0
85	CX	3	Total 3	Mg 3	0	0
85	CM	2	Total 2	Mg 2	0	0
85	s1	1	Total 1	Mg 1	0	0
85	AH	1	Total 1	Mg 1	0	0
85	DP	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	D	1	Total 1	Mg 1	0	0
85	d9	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	sR	139	Total 139	Mg 139	0	0
85	z	1	Total 1	Mg 1	0	0
85	AT	13	Total 13	Mg 13	0	0
85	d4	1	Total 1	Mg 1	0	0
85	u	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	CE	2	Total	Mg	0	0
			2	2		
85	Y	1	Total	Mg	0	0
			1	1		
85	l	5	Total	Mg	0	0
			5	5		
85	3	12	Total	Mg	0	0
			12	12		

- Molecule 86 is Chlorolissoclimide (three-letter code: 7AL) (formula:  $C_{20}H_{30}ClNO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
86	1	1	Total	C	Cl	N	O	
			26	20	1	1	4	0
86	AR	1	Total	C	Cl	N	O	
			26	20	1	1	4	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	AP	1	Total	Zn	0	0
			1	1		
87	g	1	Total	Zn	0	0
			1	1		
87	AQ	1	Total	Zn	0	0
			1	1		

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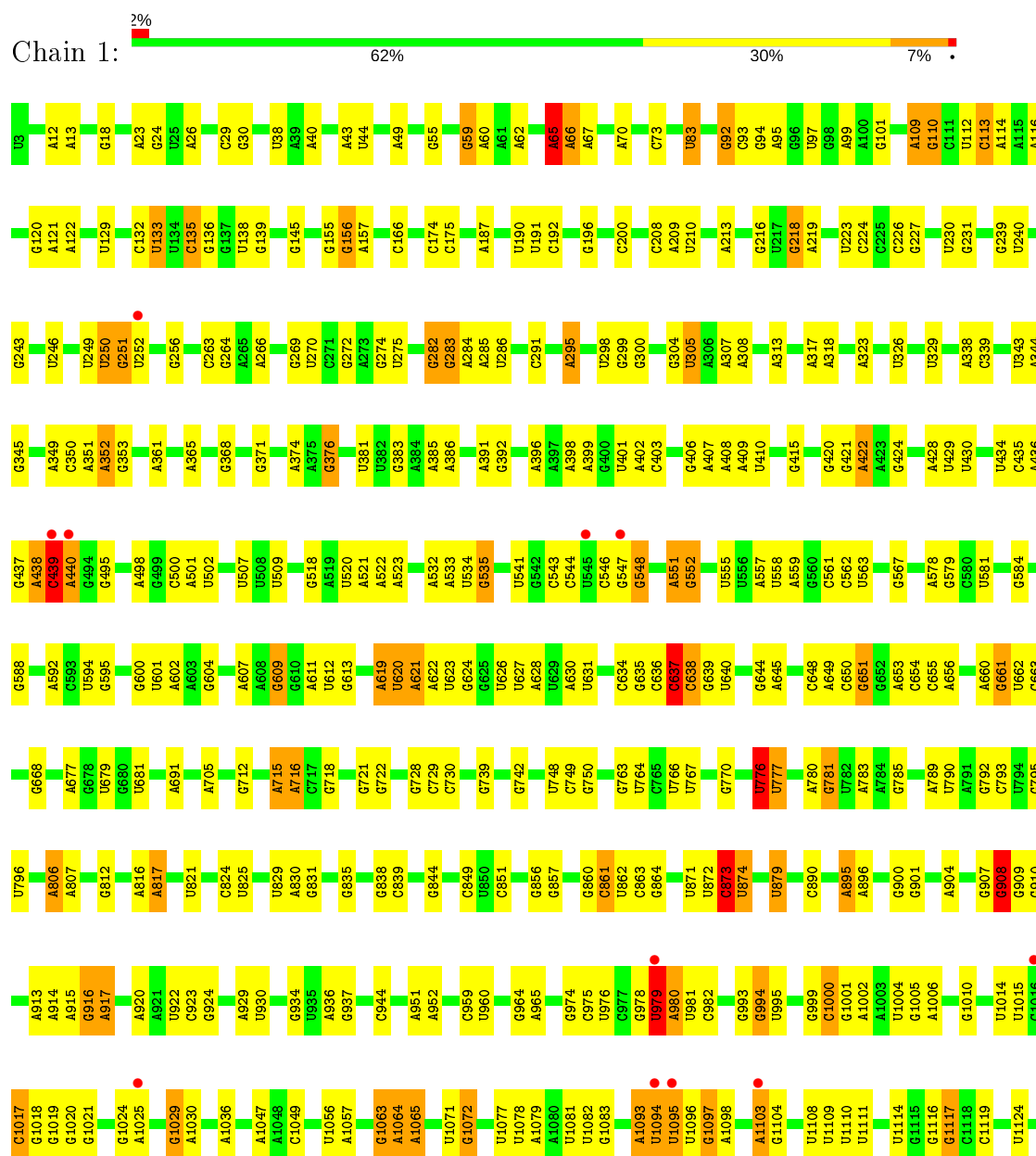
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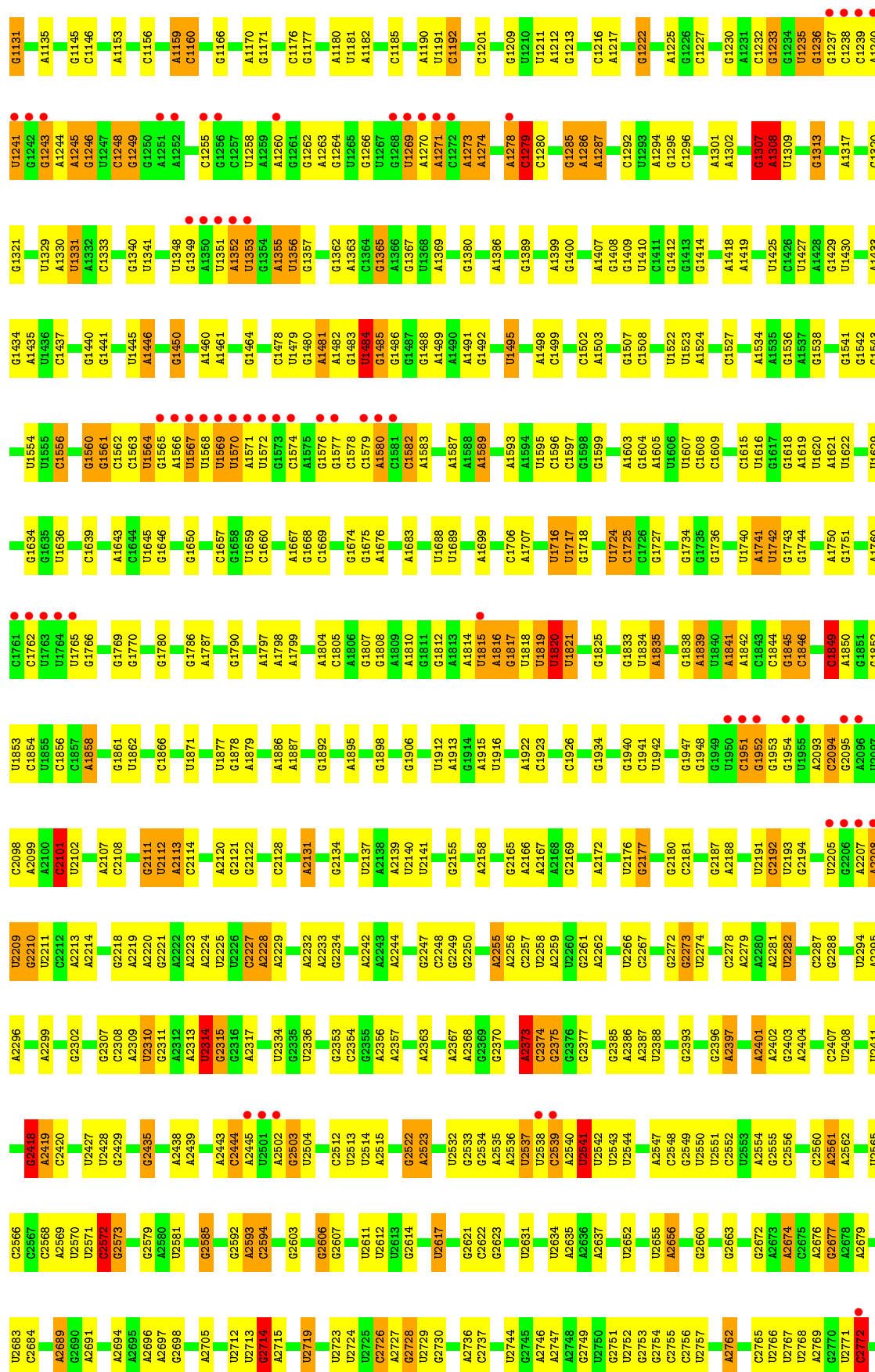
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	AK	1	Total 1	Zn 1	0	0
87	DQ	1	Total 1	Zn 1	0	0
87	e	1	Total 1	Zn 1	0	0
87	b	1	Total 1	Zn 1	0	0
87	e1	1	Total 1	Zn 1	0	0
87	c	1	Total 1	Zn 1	0	0
87	DL	1	Total 1	Zn 1	0	0
87	d9	1	Total 1	Zn 1	0	0
87	DR	1	Total 1	Zn 1	0	0
87	DO	1	Total 1	Zn 1	0	0
87	AN	1	Total 1	Zn 1	0	0
87	d7	1	Total 1	Zn 1	0	0
87	d6	1	Total 1	Zn 1	0	0

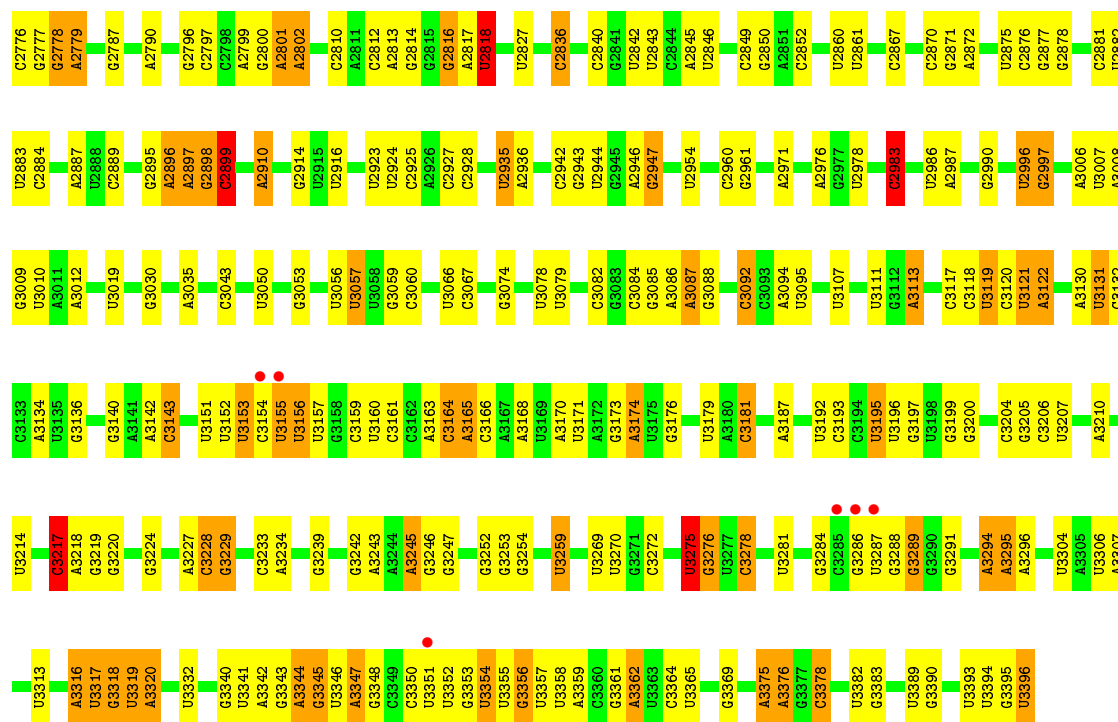
### 3 Residue-property plots

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

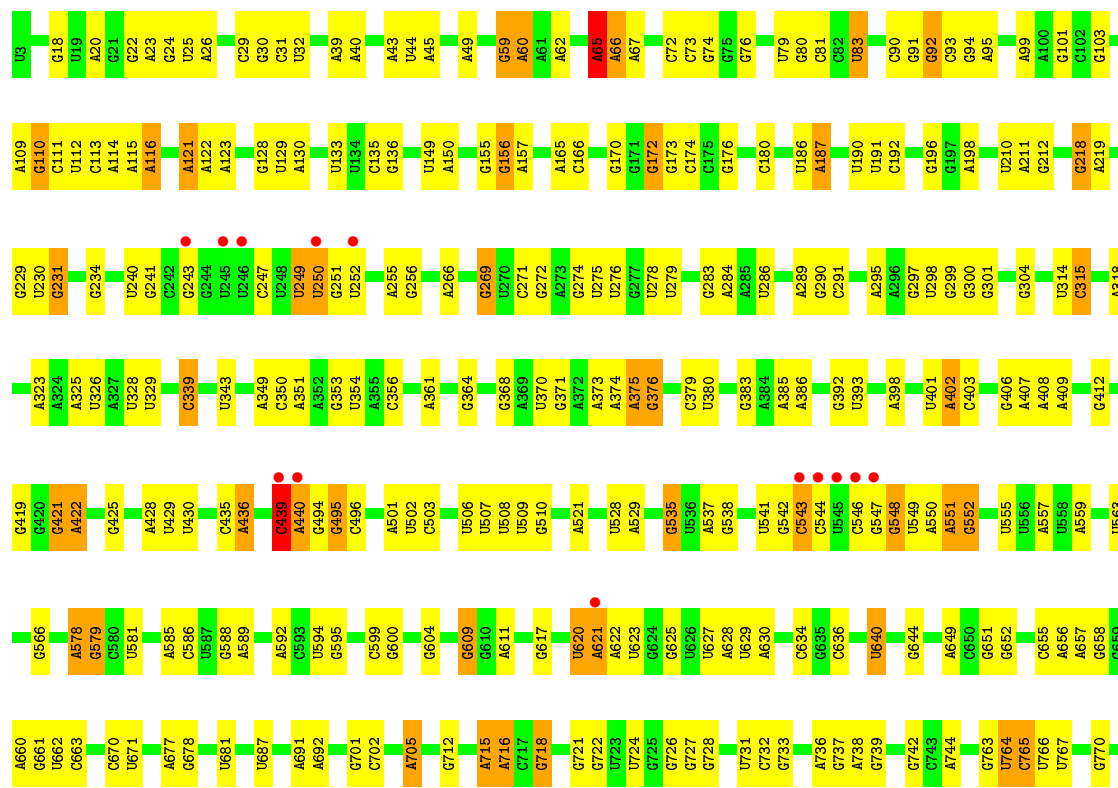
#### • Molecule 1: 25S ribosomal RNA



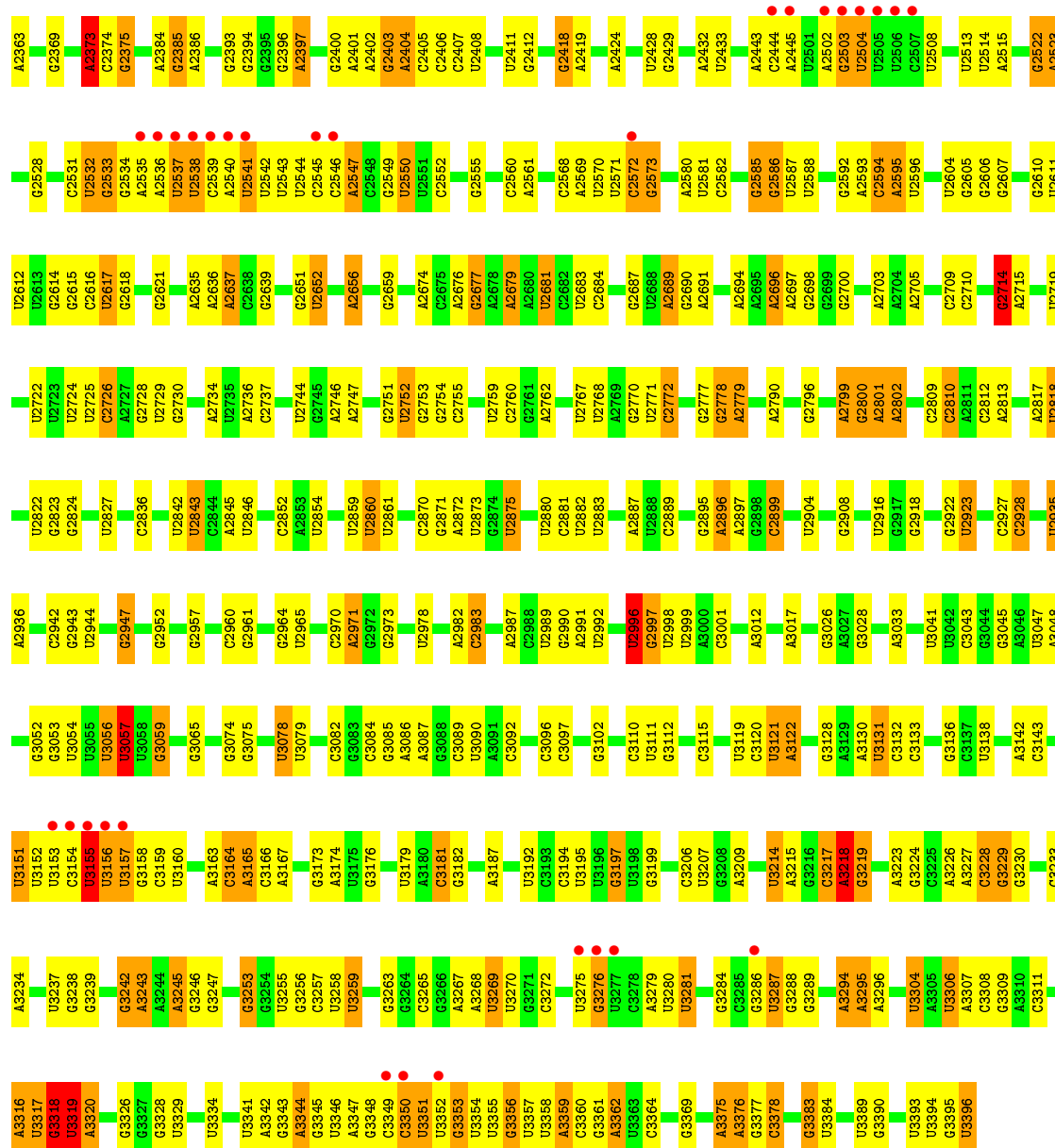




• Molecule 1: 25S ribosomal RNA

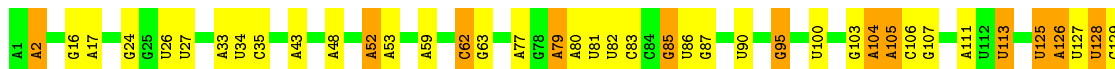








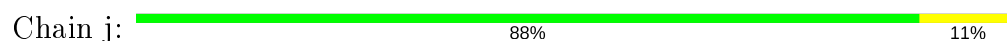
- Molecule 3: 5.8S ribosomal RNA



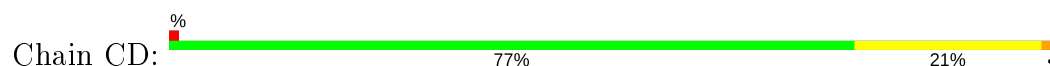
- Molecule 3: 5.8S ribosomal RNA



- Molecule 4: 60S ribosomal protein L2-A



- Molecule 4: 60S ribosomal protein L2-A

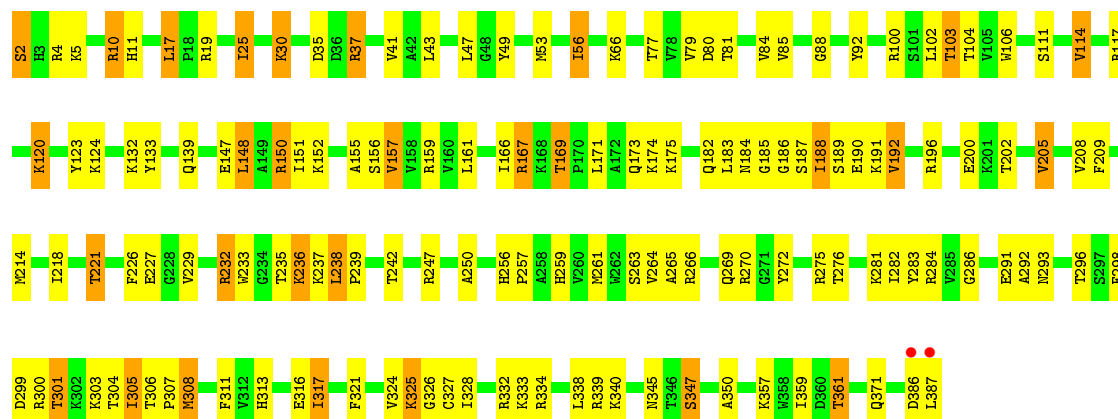


- Molecule 5: 60S ribosomal protein L3

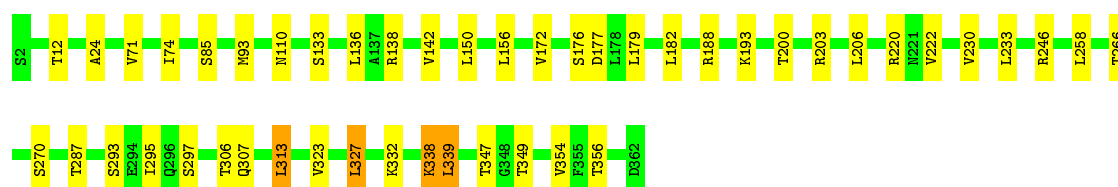
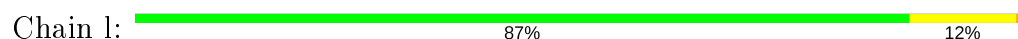




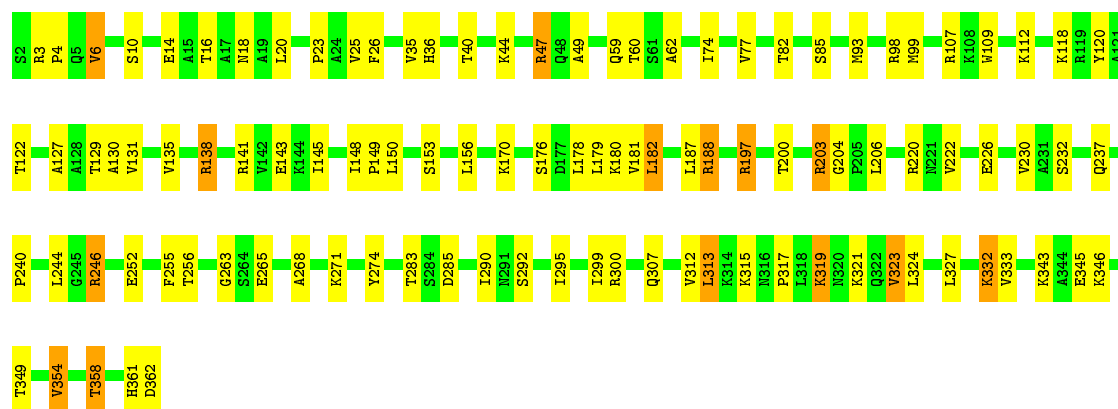
• Molecule 5: 60S ribosomal protein L3



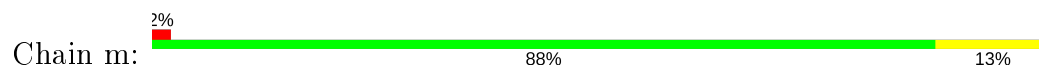
• Molecule 6: 60S ribosomal protein L4-A

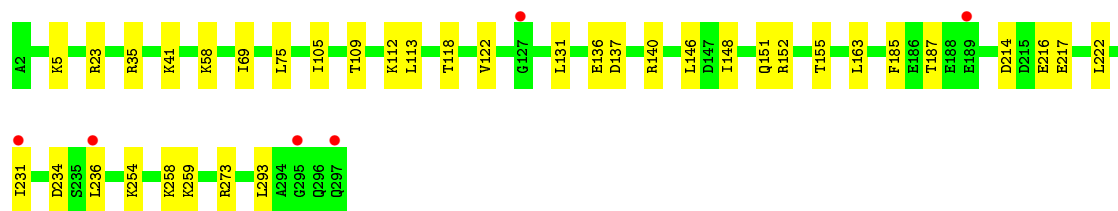


• Molecule 6: 60S ribosomal protein L4-A

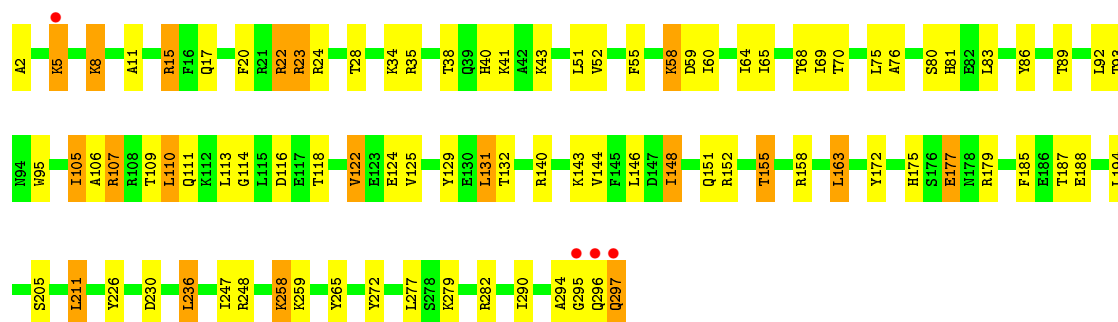
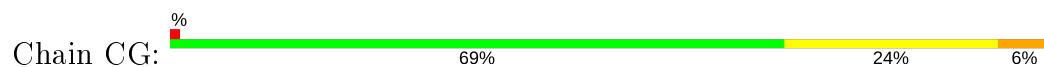


• Molecule 7: 60S ribosomal protein L5

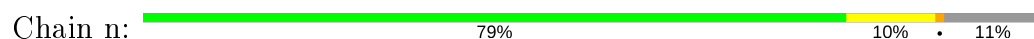




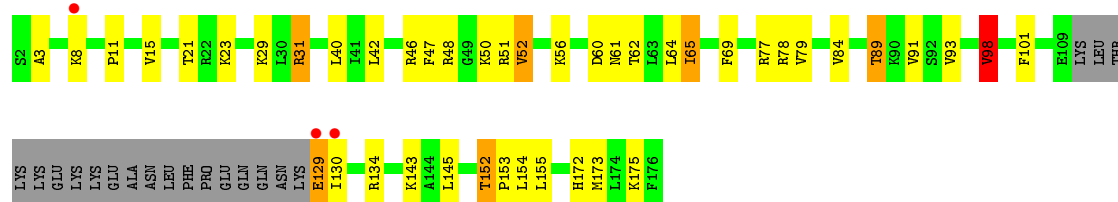
• Molecule 7: 60S ribosomal protein L5



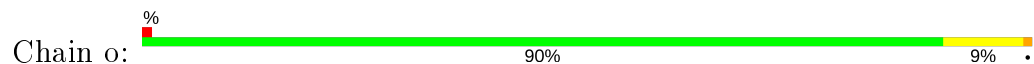
• Molecule 8: 60S ribosomal protein L6-A



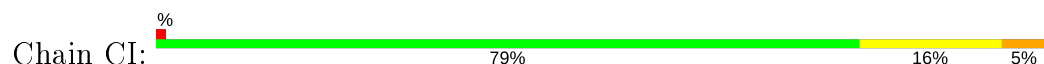
• Molecule 8: 60S ribosomal protein L6-A

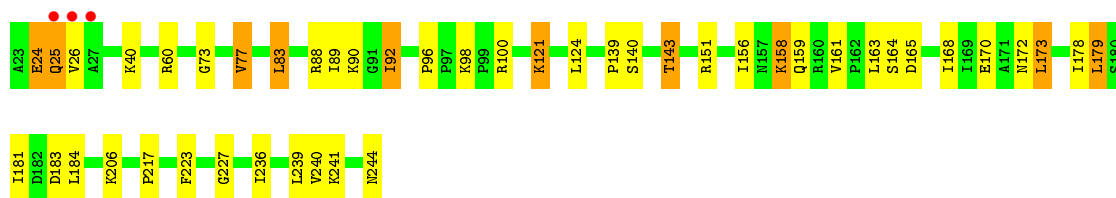


• Molecule 9: 60S ribosomal protein L7-A

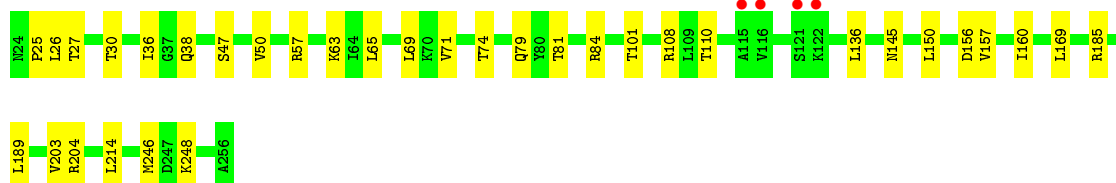
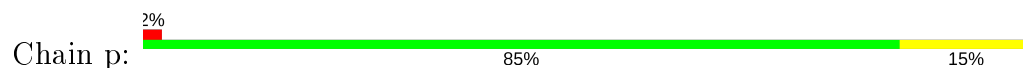


• Molecule 9: 60S ribosomal protein L7-A

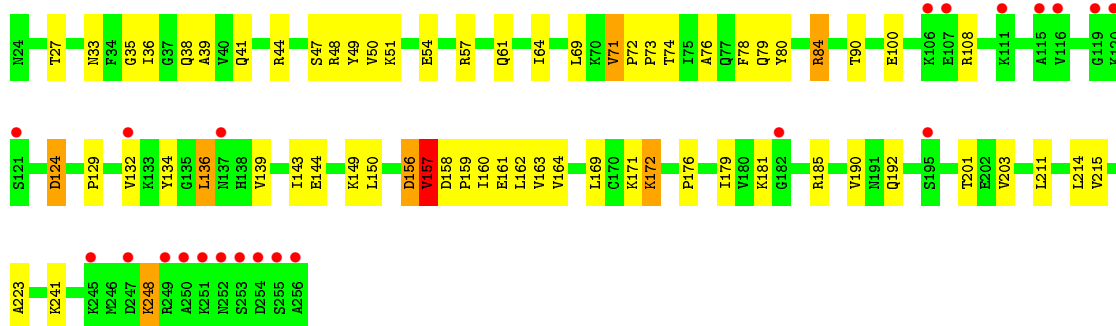
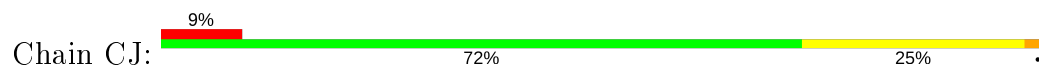




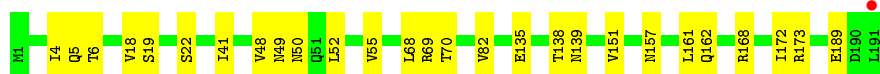
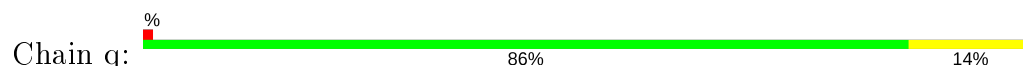
- Molecule 10: 60S ribosomal protein L8-A



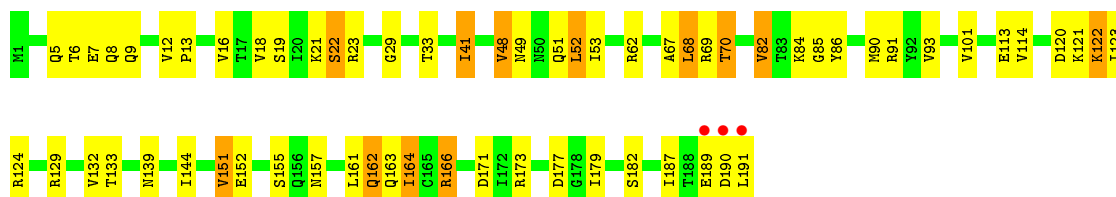
- Molecule 10: 60S ribosomal protein L8-A



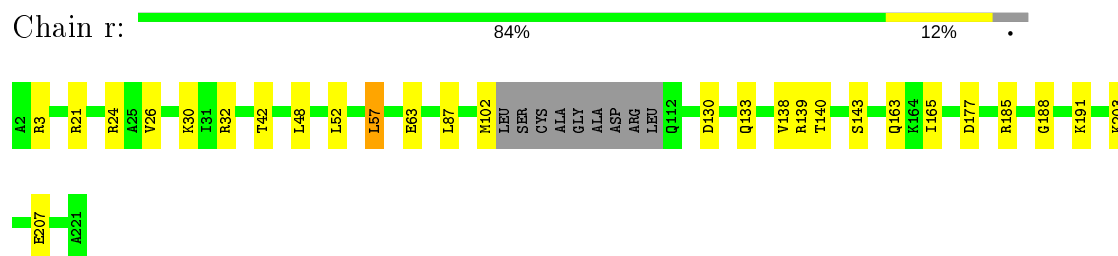
- Molecule 11: 60S ribosomal protein L9-A



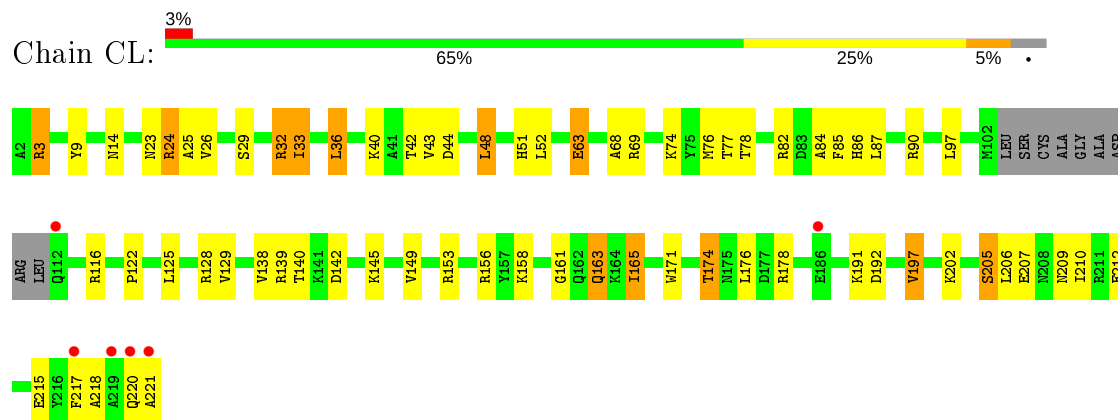
- Molecule 11: 60S ribosomal protein L9-A



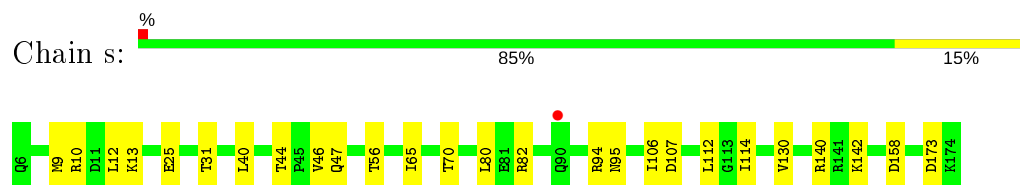
- Molecule 12: 60S ribosomal protein L10



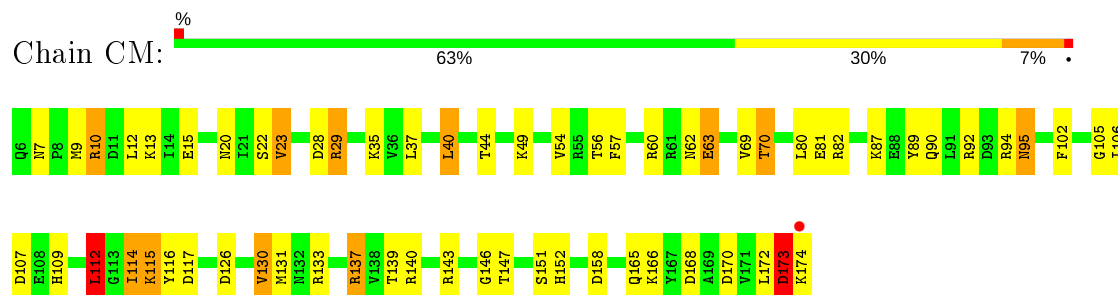
- Molecule 12: 60S ribosomal protein L10



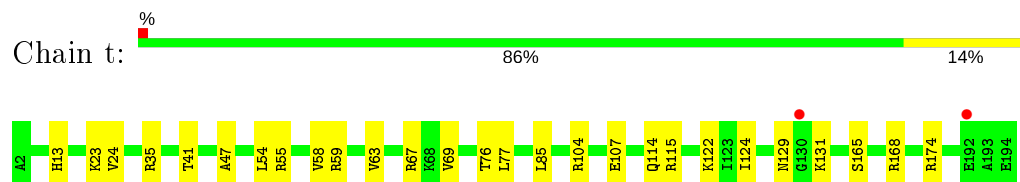
- Molecule 13: 60S ribosomal protein L11-B



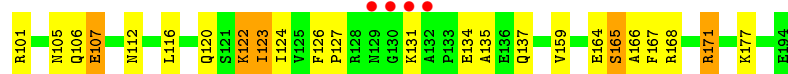
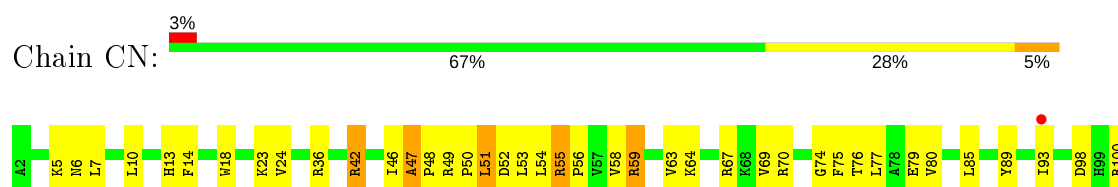
- Molecule 13: 60S ribosomal protein L11-B



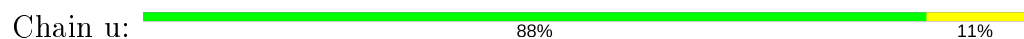
- Molecule 14: 60S ribosomal protein L13-A



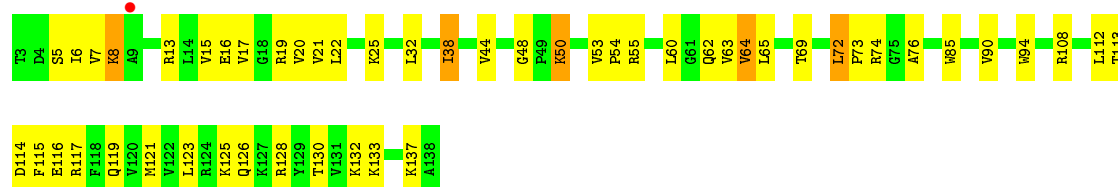
- Molecule 14: 60S ribosomal protein L13-A



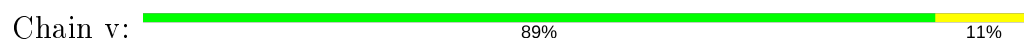
- Molecule 15: 60S ribosomal protein L14-A



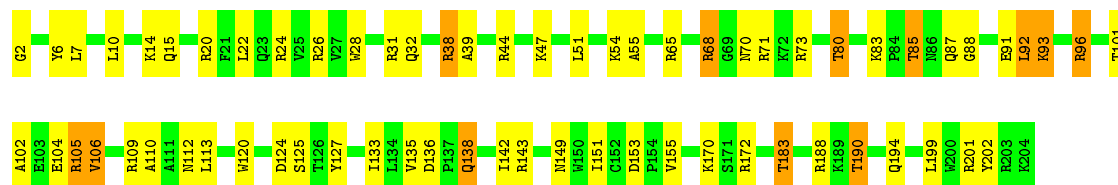
- Molecule 15: 60S ribosomal protein L14-A



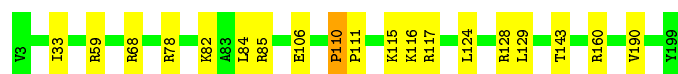
- Molecule 16: 60S ribosomal protein L15-A



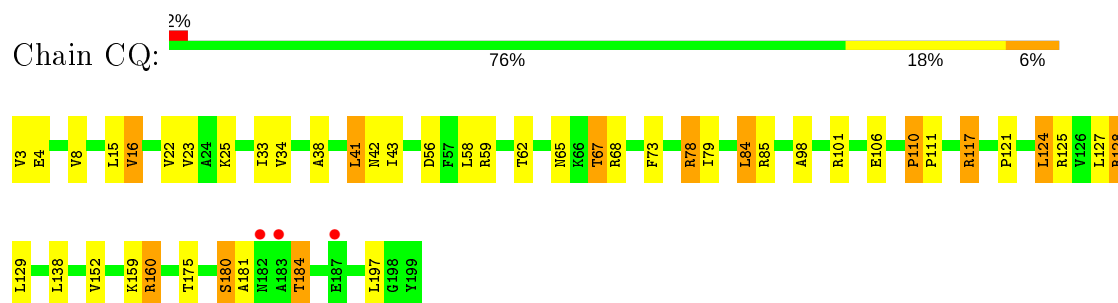
- Molecule 16: 60S ribosomal protein L15-A



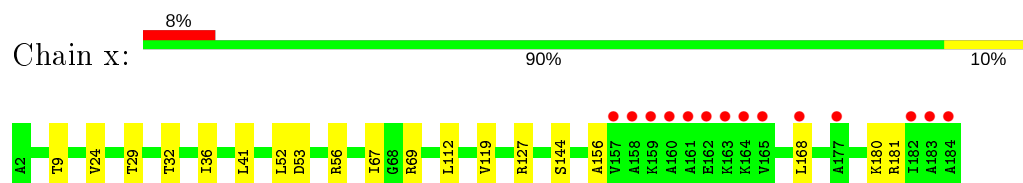
- Molecule 17: 60S ribosomal protein L16-A



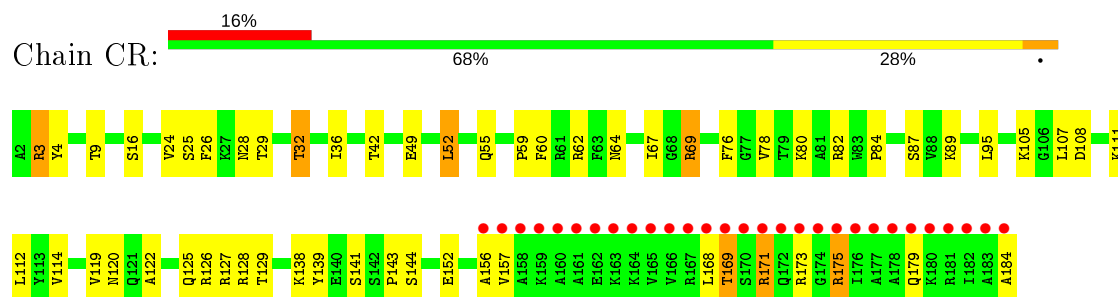
- Molecule 17: 60S ribosomal protein L16-A



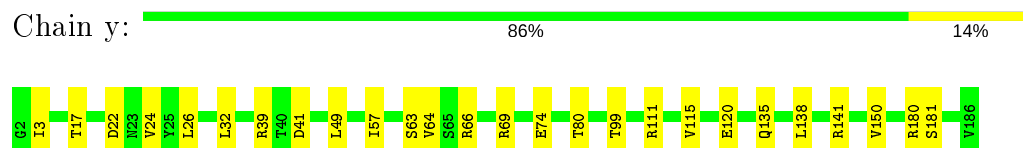
- Molecule 18: 60S ribosomal protein L17-A



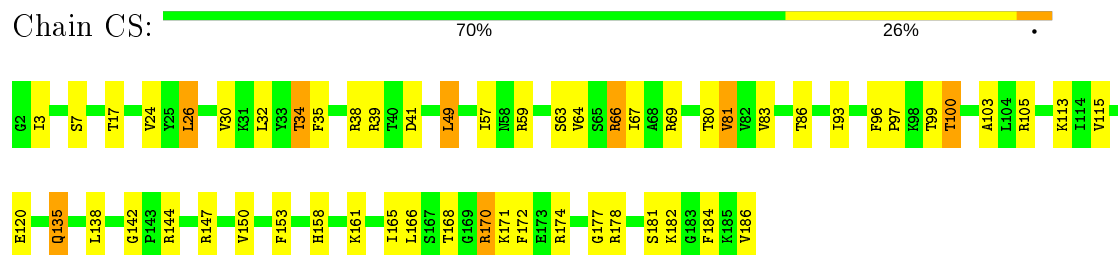
- Molecule 18: 60S ribosomal protein L17-A



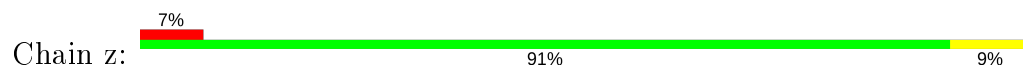
- Molecule 19: 60S ribosomal protein L18-A



- Molecule 19: 60S ribosomal protein L18-A

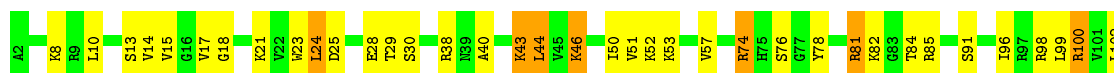


- Molecule 20: 60S ribosomal protein L19-A

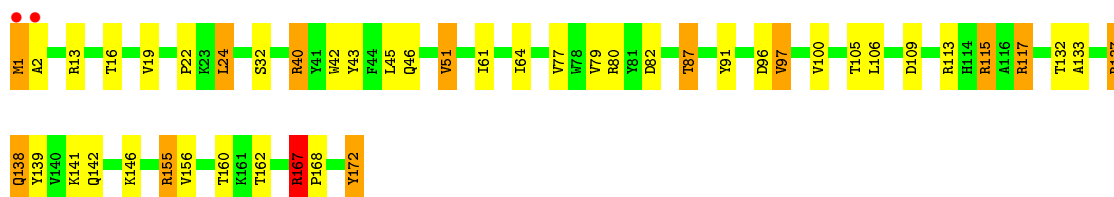
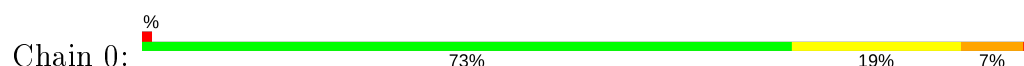




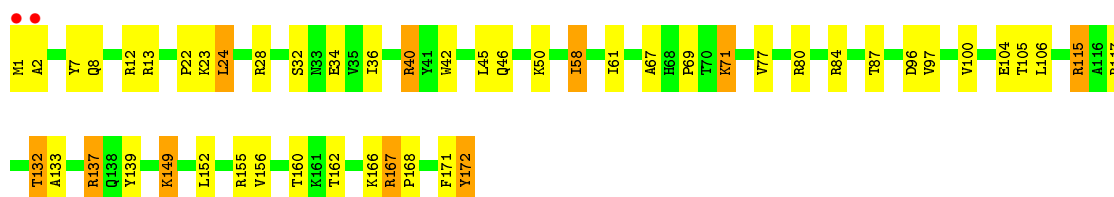
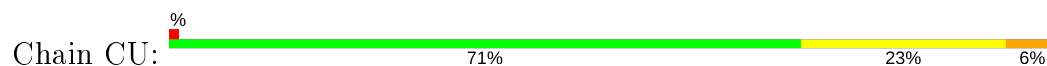
- Molecule 20: 60S ribosomal protein L19-A



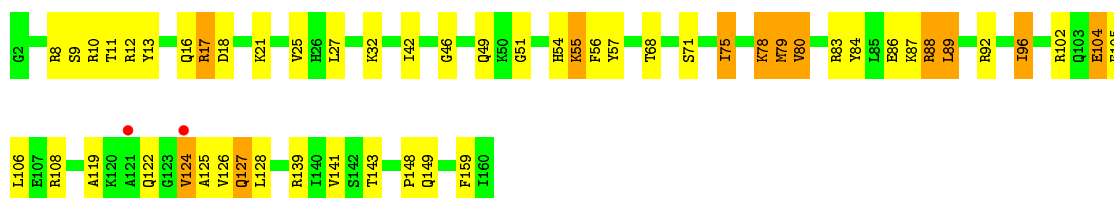
- Molecule 21: 60S ribosomal protein L20-A



- Molecule 21: 60S ribosomal protein L20-A

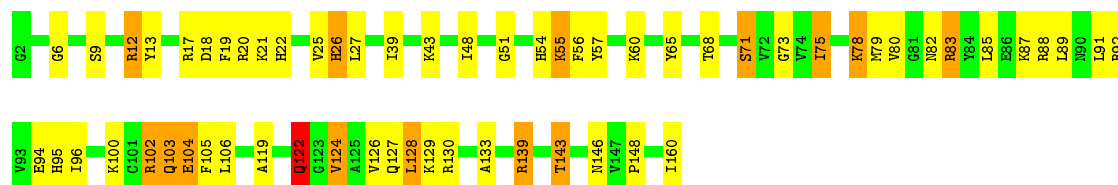


- Molecule 22: 60S ribosomal protein L21-A

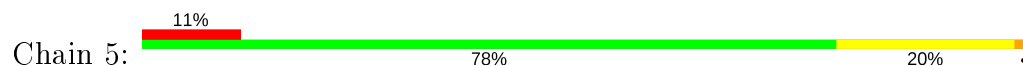


- Molecule 22: 60S ribosomal protein L21-A

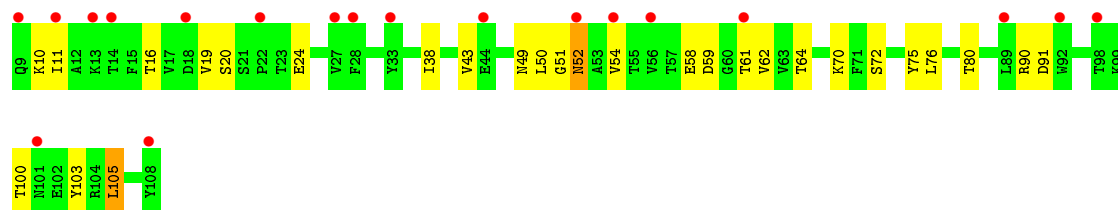
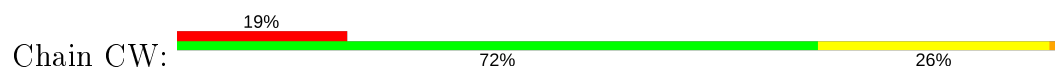




- Molecule 23: 60S ribosomal protein L22-A



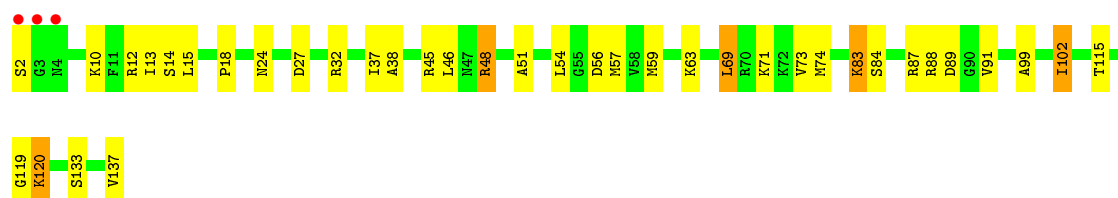
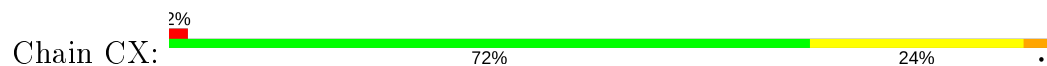
- Molecule 23: 60S ribosomal protein L22-A



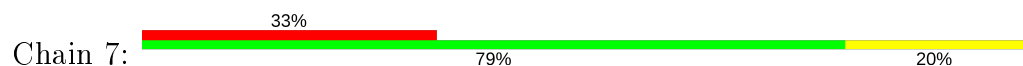
- Molecule 24: 60S ribosomal protein L23-A

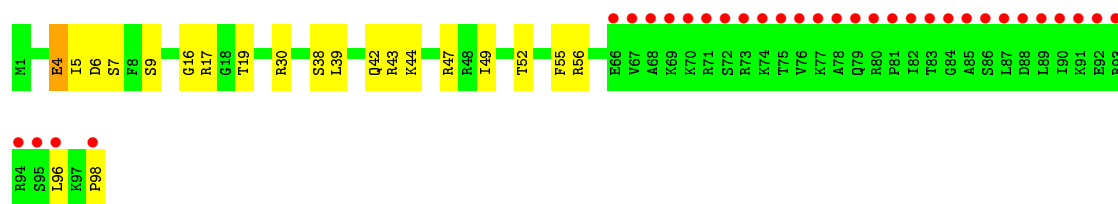


- Molecule 24: 60S ribosomal protein L23-A

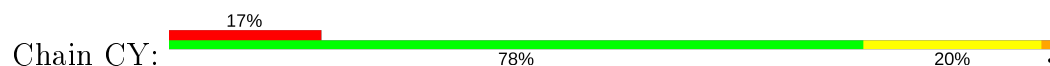


- Molecule 25: 60S ribosomal protein L24-A

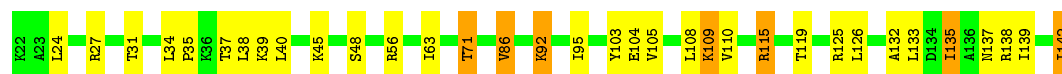




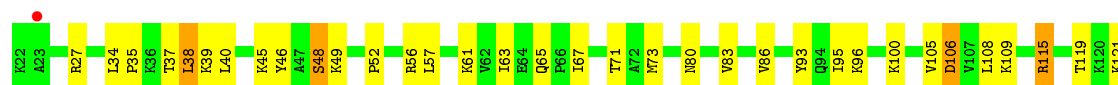
- Molecule 25: 60S ribosomal protein L24-A



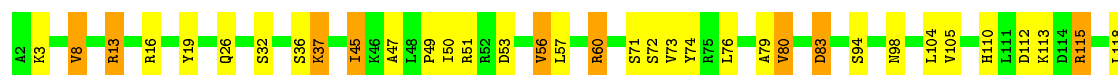
- Molecule 26: 60S ribosomal protein L25



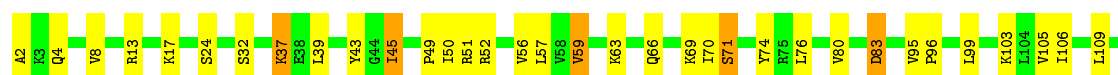
- Molecule 26: 60S ribosomal protein L25



- Molecule 27: 60S ribosomal protein L26-A

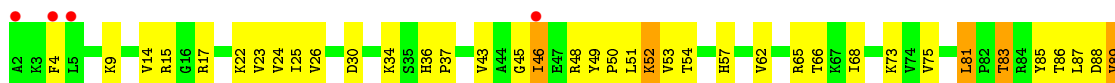


- Molecule 27: 60S ribosomal protein L26-A





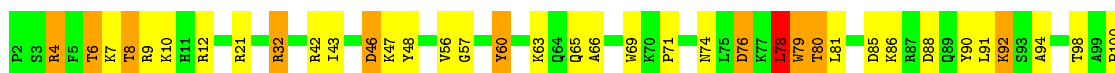
- Molecule 28: 60S ribosomal protein L27-A



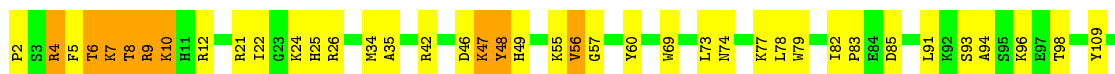
- Molecule 28: 60S ribosomal protein L27-A



- Molecule 29: 60S ribosomal protein L28



- Molecule 29: 60S ribosomal protein L28

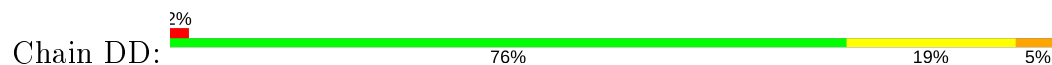


- Molecule 30: 60S ribosomal protein L29





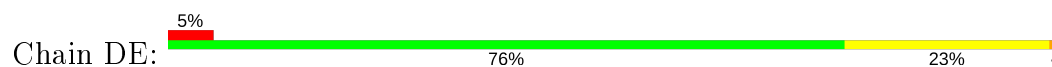
- Molecule 30: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L30



- Molecule 31: 60S ribosomal protein L30



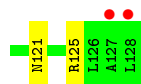
- Molecule 32: 60S ribosomal protein L31-A



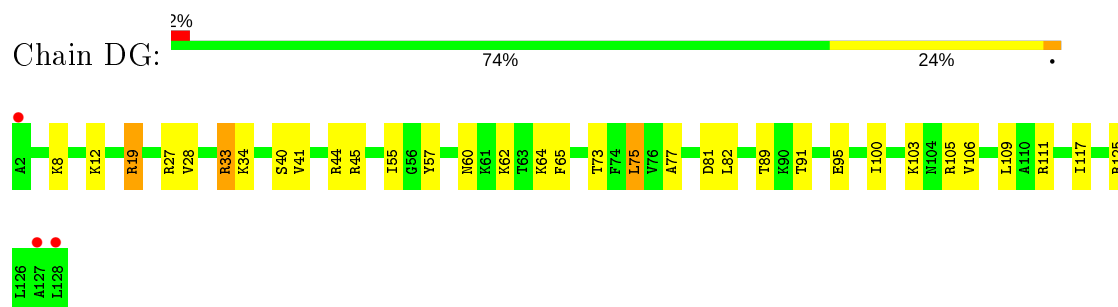
- Molecule 32: 60S ribosomal protein L31-A



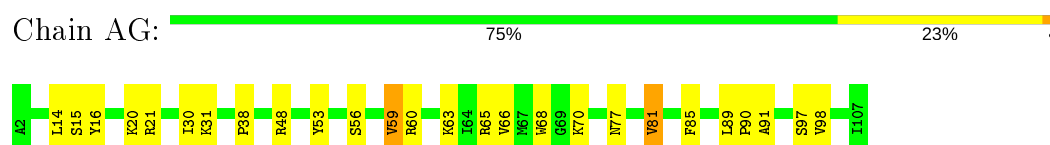
- Molecule 33: 60S ribosomal protein L32



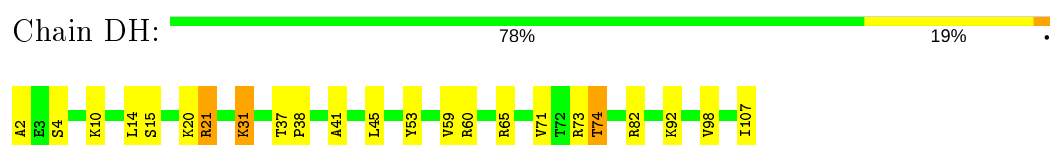
- Molecule 33: 60S ribosomal protein L32



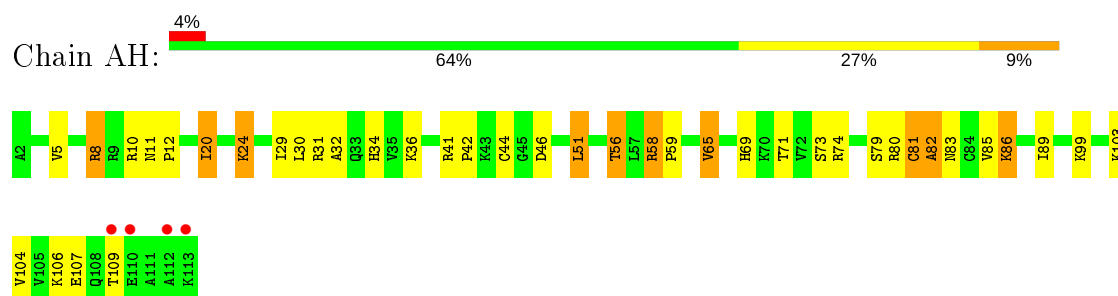
- Molecule 34: 60S ribosomal protein L33-A



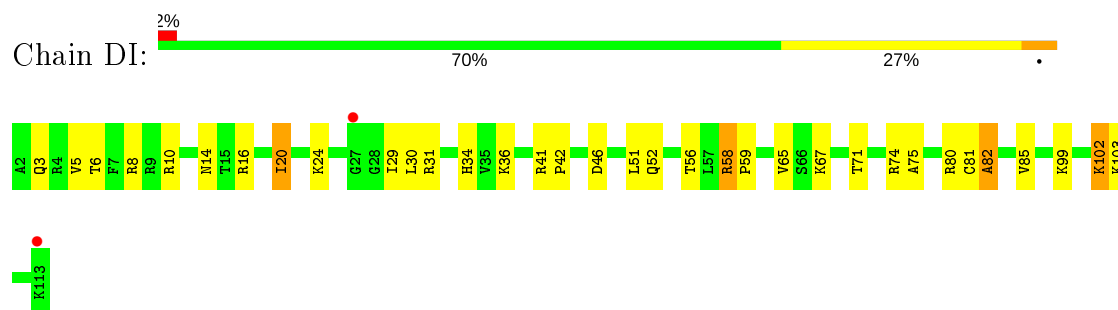
- Molecule 34: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L34-A

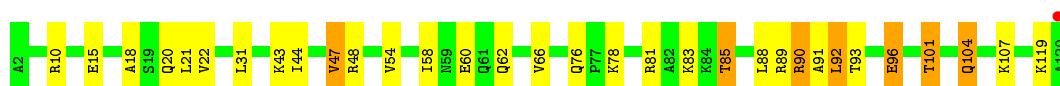


- Molecule 35: 60S ribosomal protein L34-A

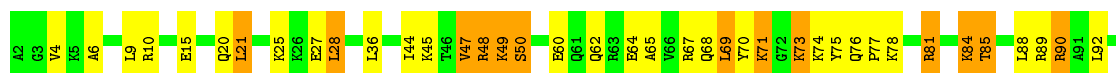


- Molecule 36: 60S ribosomal protein L35-A

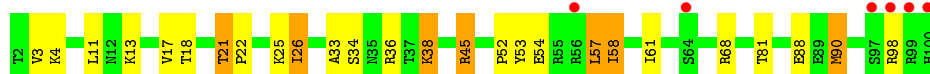
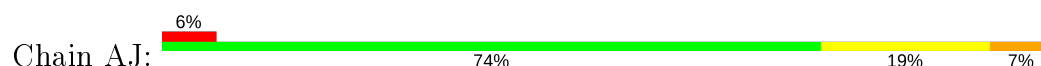




- Molecule 36: 60S ribosomal protein L35-A



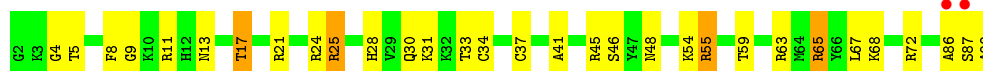
- Molecule 37: 60S ribosomal protein L36-A



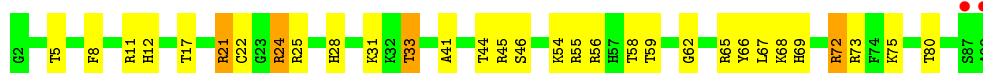
- Molecule 37: 60S ribosomal protein L36-A



- Molecule 38: 60S ribosomal protein L37-A

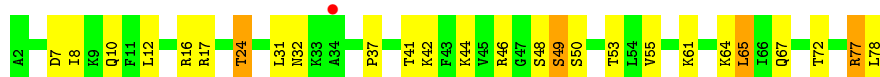


- Molecule 38: 60S ribosomal protein L37-A

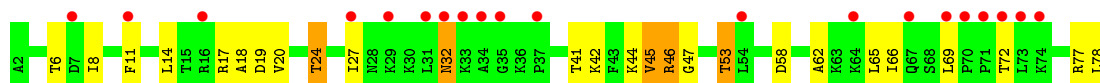


- Molecule 39: 60S ribosomal protein L38





- Molecule 39: 60S ribosomal protein L38



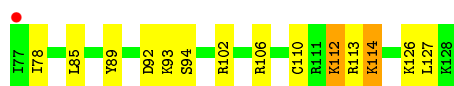
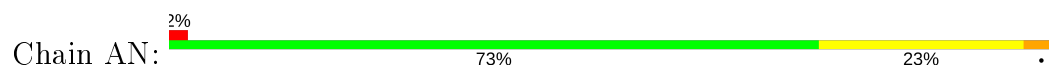
- Molecule 40: 60S ribosomal protein L39



- Molecule 40: 60S ribosomal protein L39



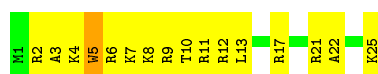
- Molecule 41: Ubiquitin-60S ribosomal protein L40



- Molecule 41: Ubiquitin-60S ribosomal protein L40



- Molecule 42: 60S ribosomal protein L41-A

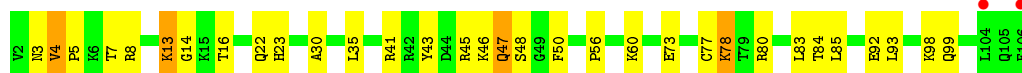
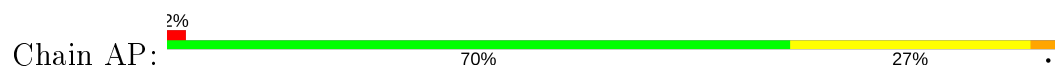


- Molecule 42: 60S ribosomal protein L41-A

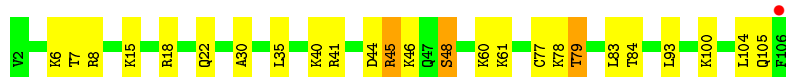
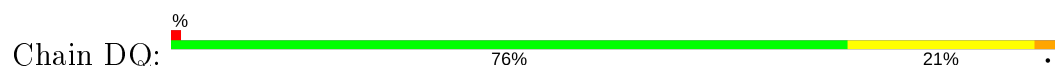




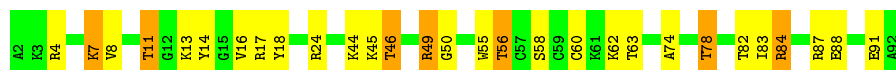
- Molecule 43: 60S ribosomal protein L42-A



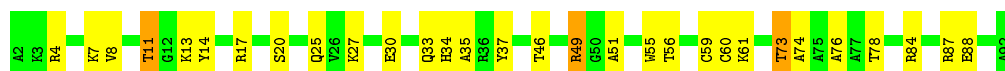
- Molecule 43: 60S ribosomal protein L42-A



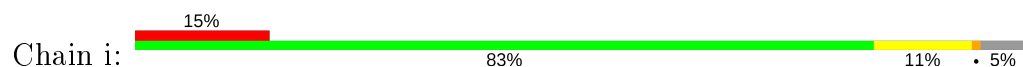
- Molecule 44: 60S ribosomal protein L43-A



- Molecule 44: 60S ribosomal protein L43-A

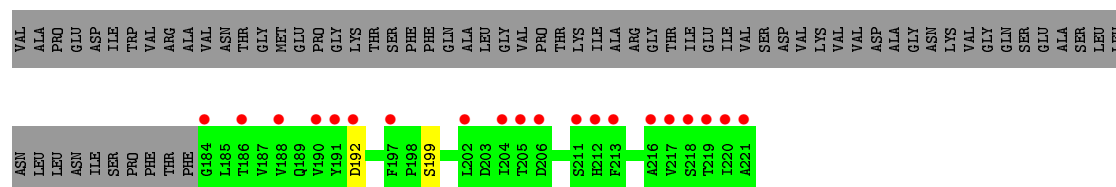


- Molecule 45: Suppressor protein STM1

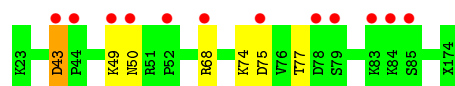


- Molecule 46: 60S acidic ribosomal protein P0

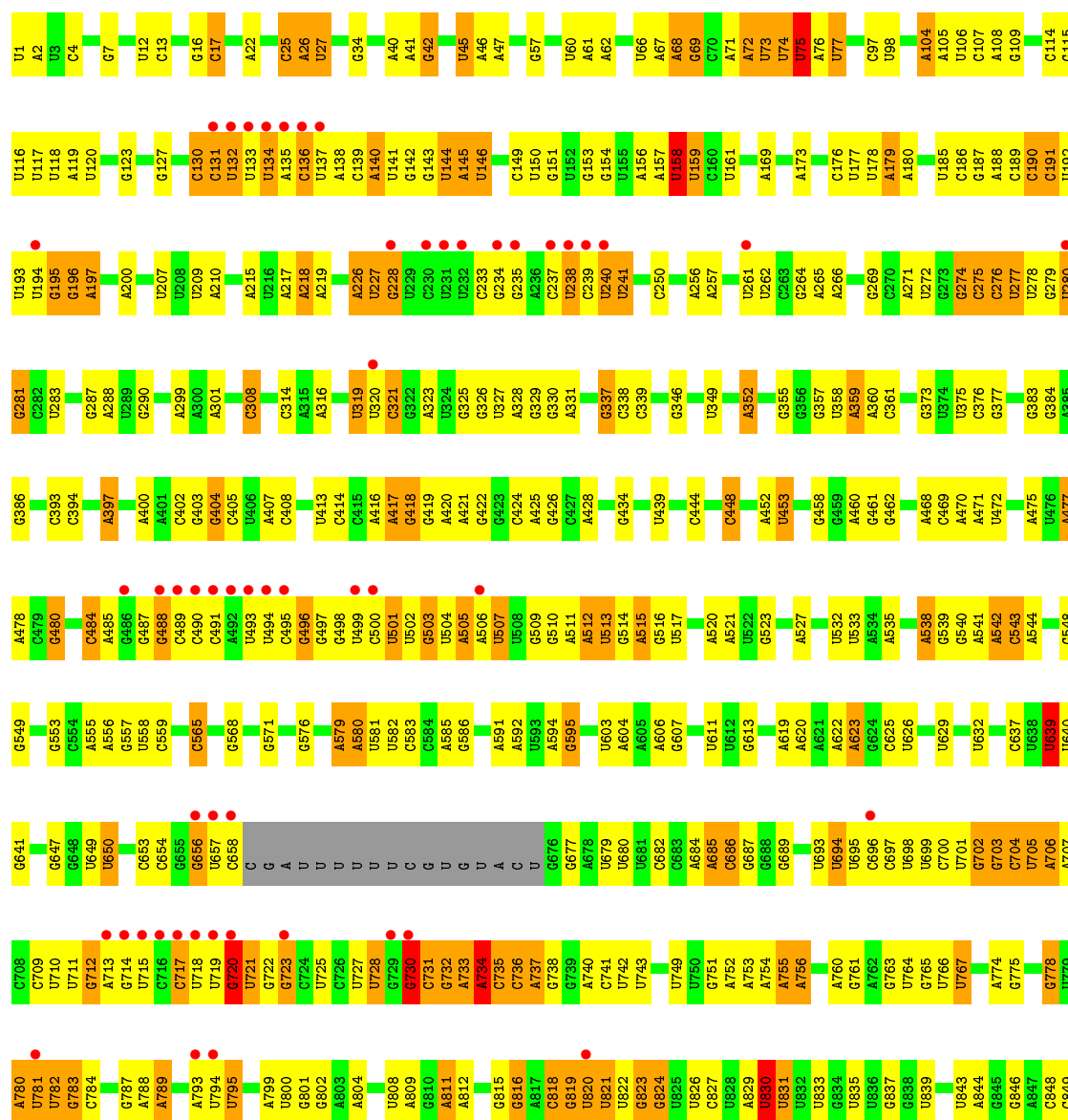


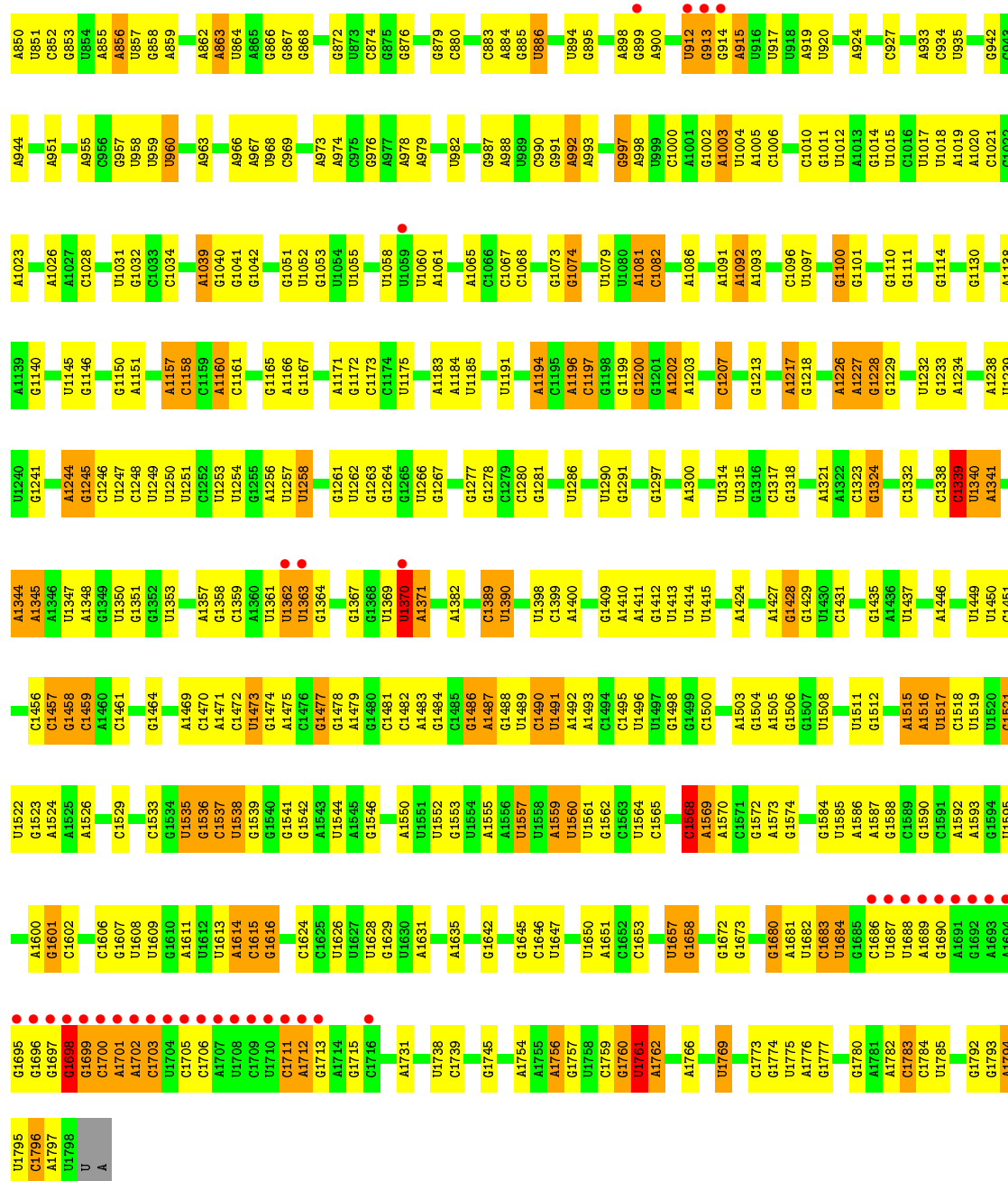


• Molecule 47: Suppressor protein STM1

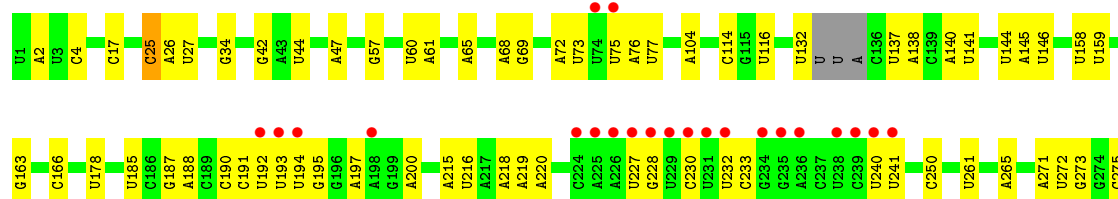
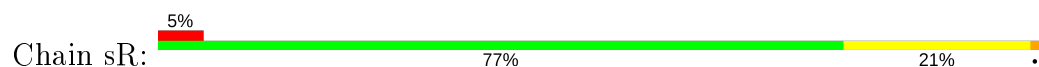


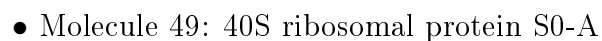
• Molecule 48: 18S ribosomal RNA



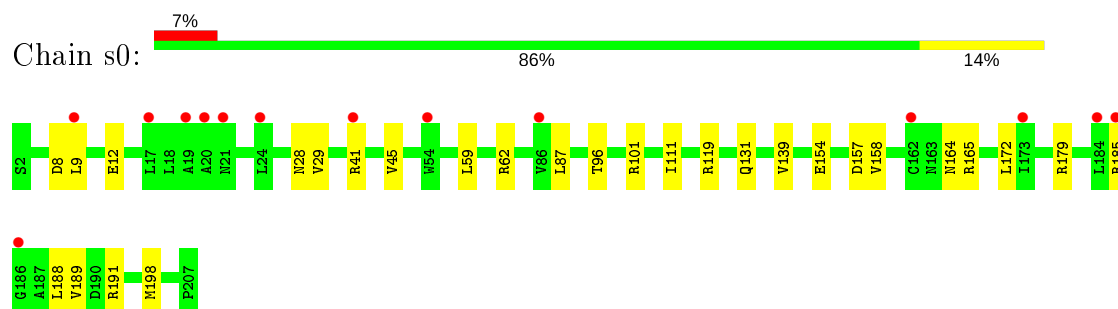


• Molecule 48: 18S ribosomal RNA

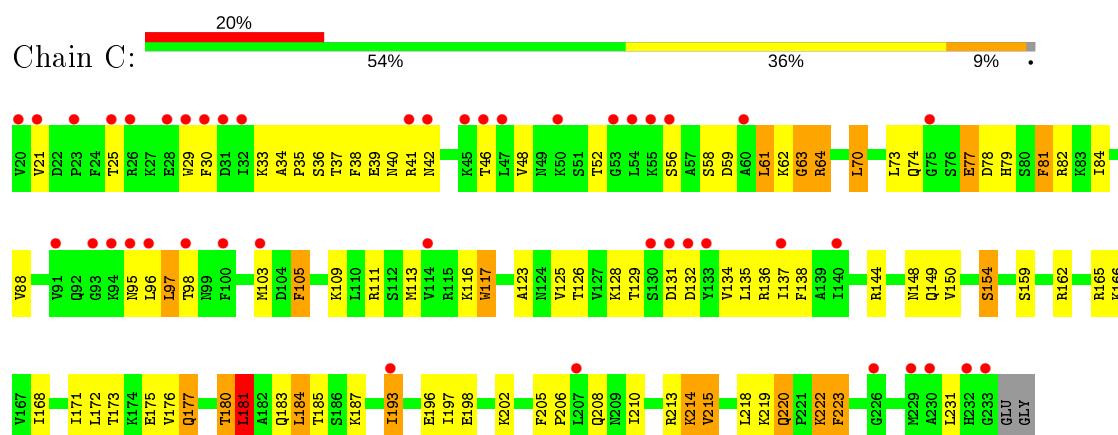




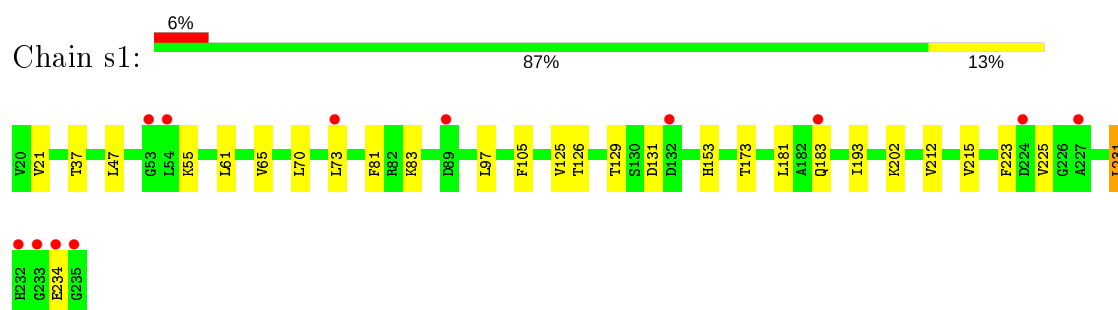
- Molecule 49: 40S ribosomal protein S0-A



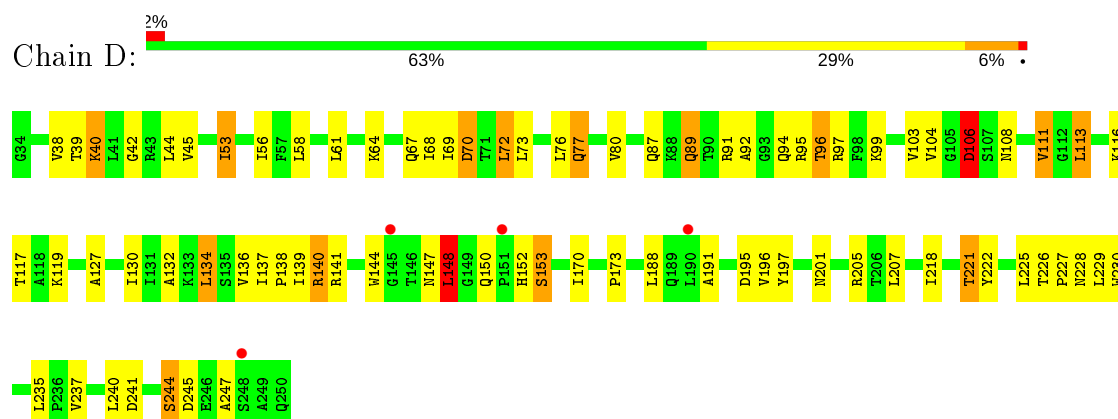
- Molecule 50: 40S ribosomal protein S1-A



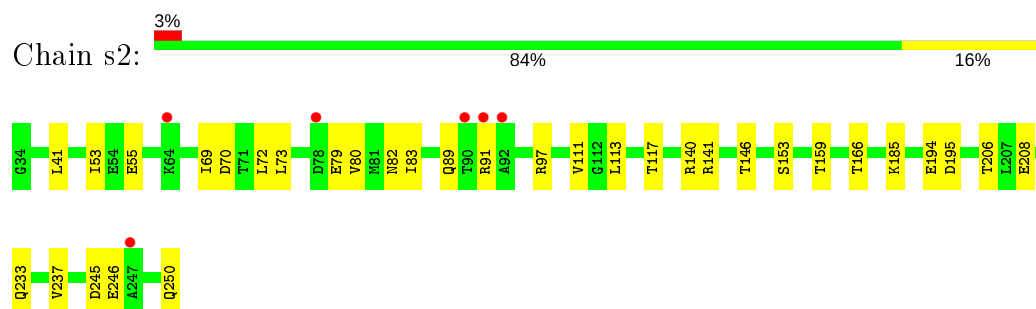
- Molecule 50: 40S ribosomal protein S1-A



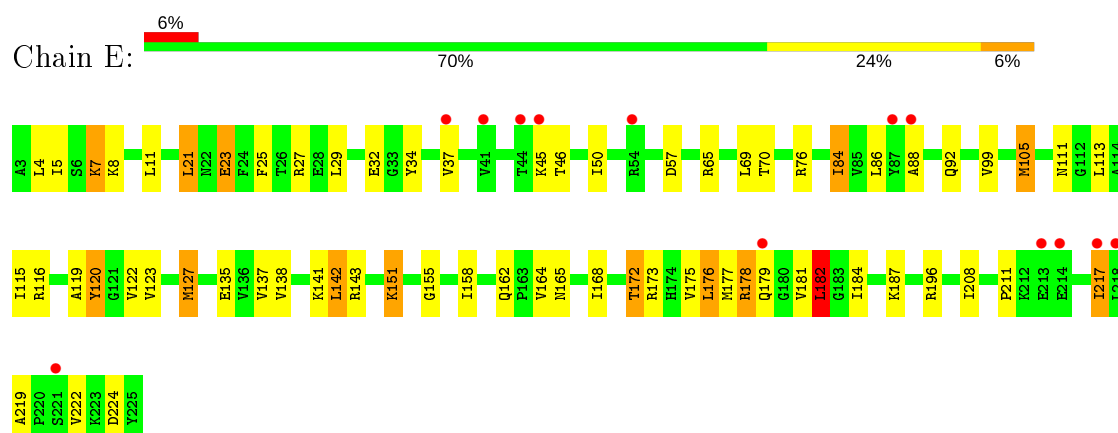
- Molecule 51: 40S ribosomal protein S2



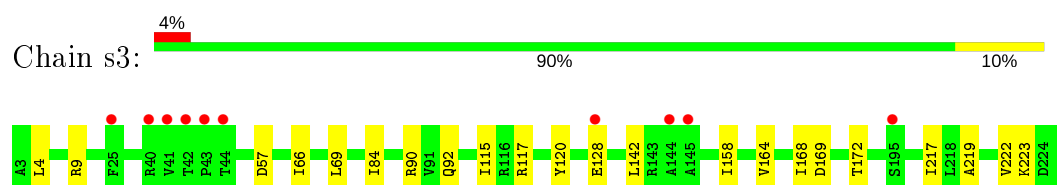
## • Molecule 51: 40S ribosomal protein S2



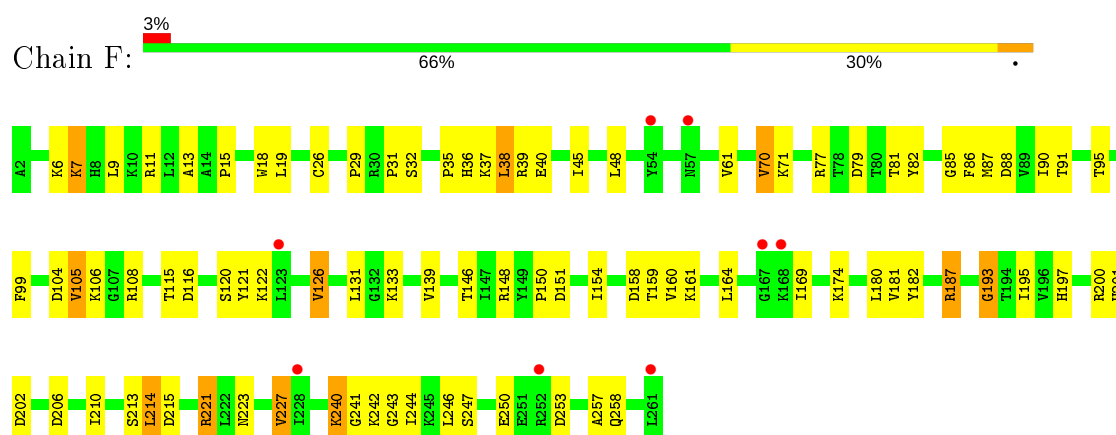
## • Molecule 52: 40S ribosomal protein S3



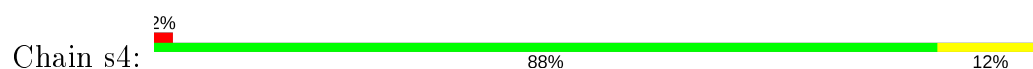
## • Molecule 52: 40S ribosomal protein S3

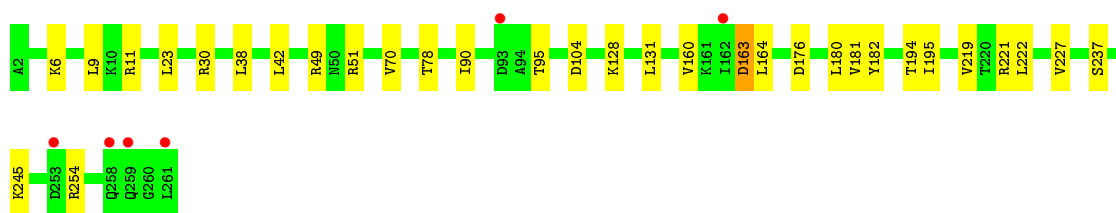


## • Molecule 53: 40S ribosomal protein S4-A

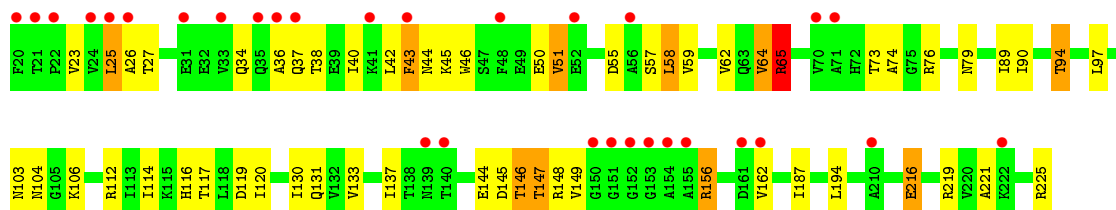
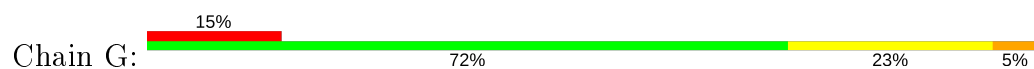


## • Molecule 53: 40S ribosomal protein S4-A

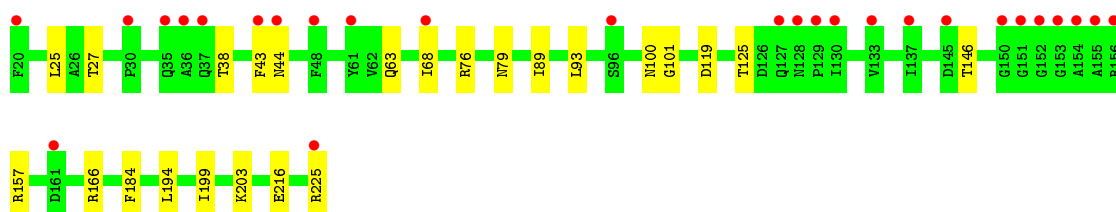
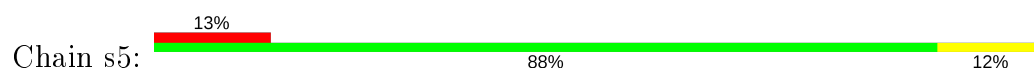




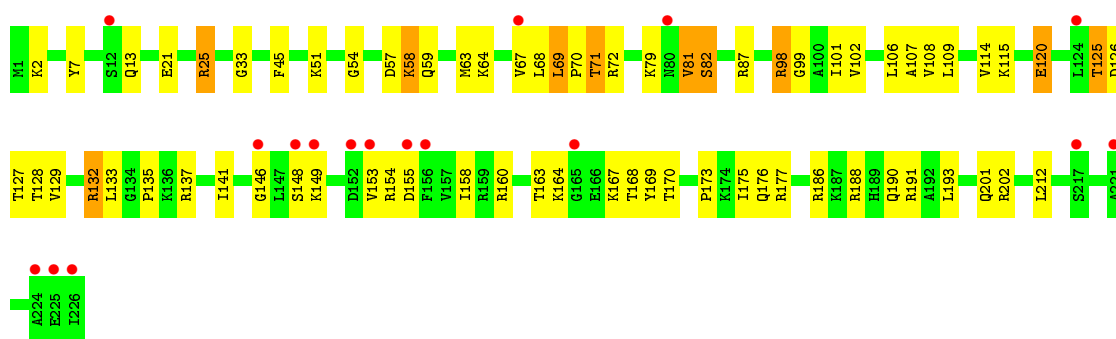
- Molecule 54: 40S ribosomal protein S5



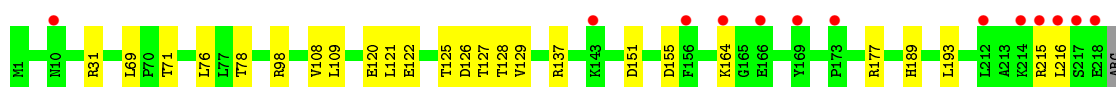
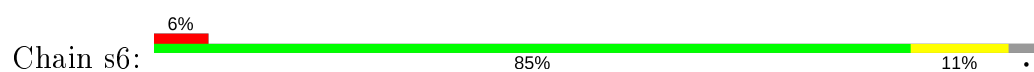
- Molecule 54: 40S ribosomal protein S5



- Molecule 55: 40S ribosomal protein S6-A

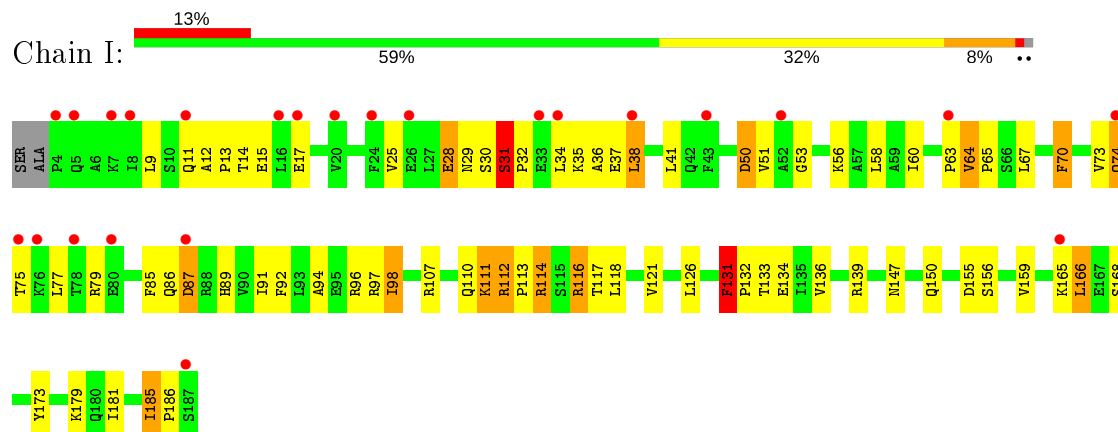


- Molecule 55: 40S ribosomal protein S6-A

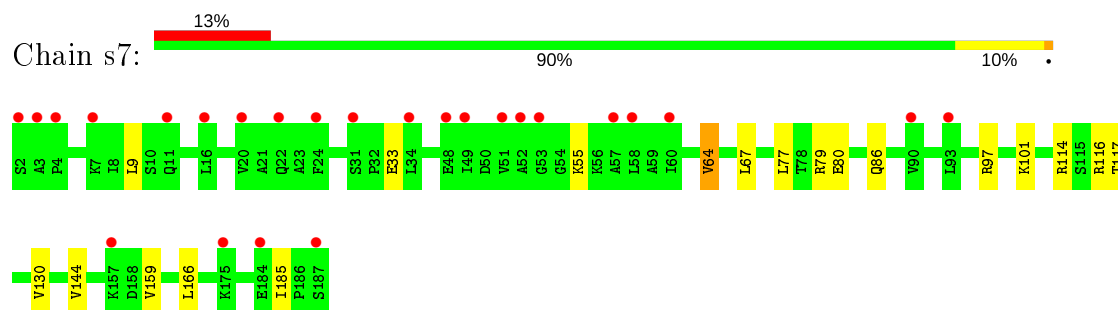


LYS  
ALA  
GLU  
LYS  
ALA  
GLU  
ILE

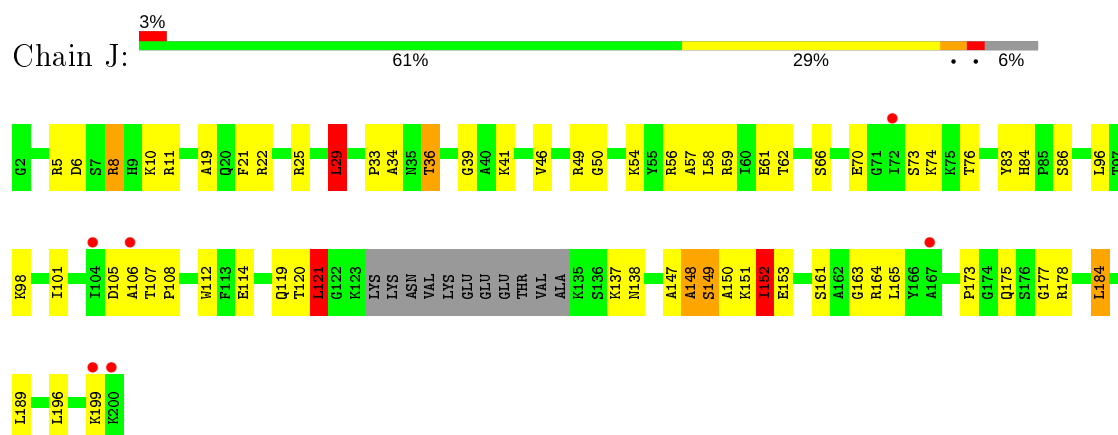
• Molecule 56: 40S ribosomal protein S7-A



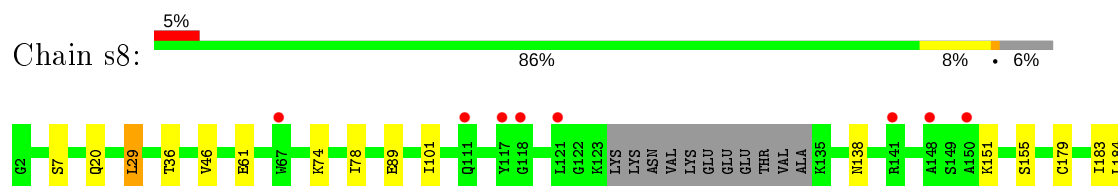
• Molecule 56: 40S ribosomal protein S7-A



• Molecule 57: 40S ribosomal protein S8-A

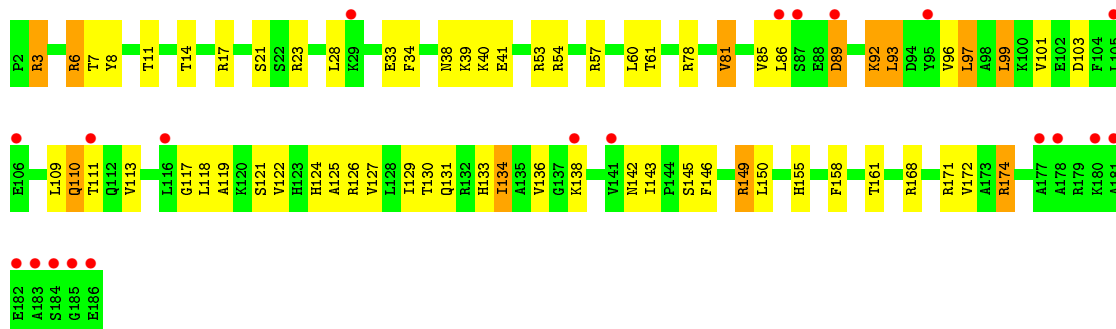


• Molecule 57: 40S ribosomal protein S8-A

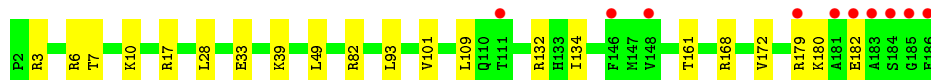
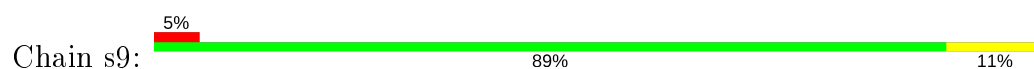




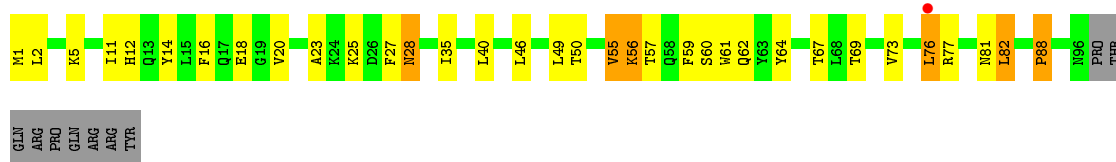
- Molecule 58: 40S ribosomal protein S9-A



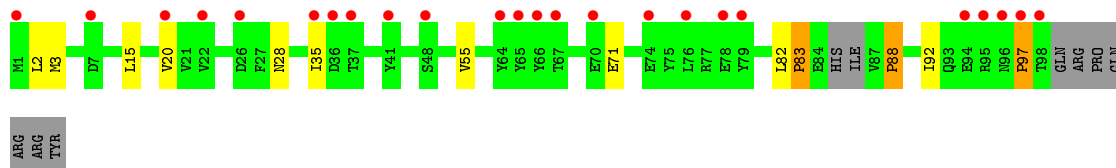
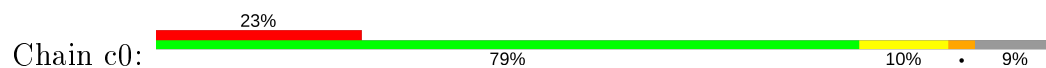
- Molecule 58: 40S ribosomal protein S9-A



- Molecule 59: 40S ribosomal protein S10-A

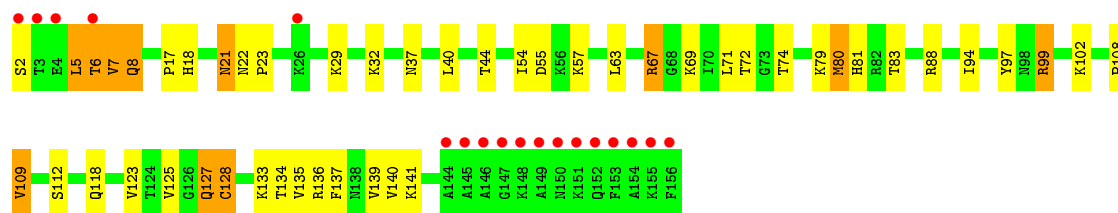


- Molecule 59: 40S ribosomal protein S10-A

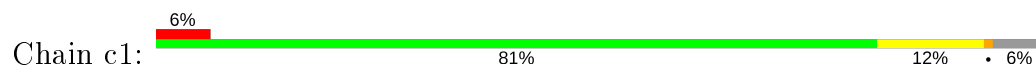


- Molecule 60: 40S ribosomal protein S11-A

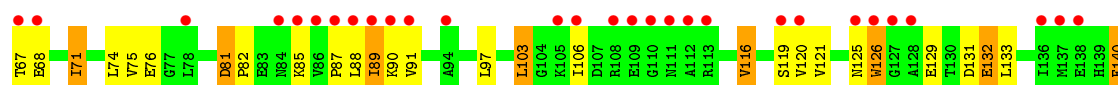
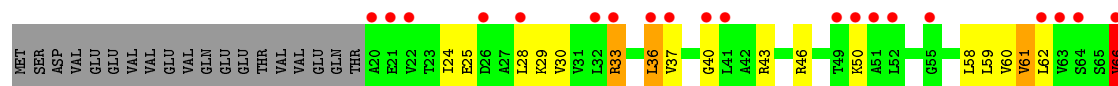




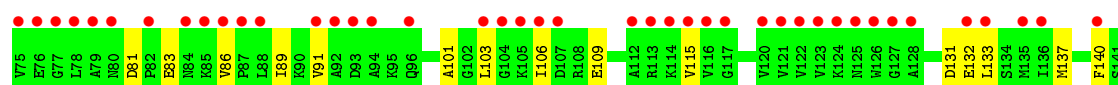
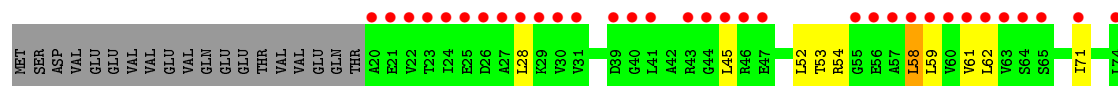
• Molecule 60: 40S ribosomal protein S11-A



• Molecule 61: 40S ribosomal protein S12



• Molecule 61: 40S ribosomal protein S12



• Molecule 62: 40S ribosomal protein S13

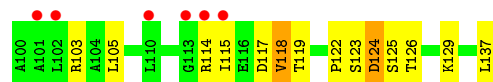
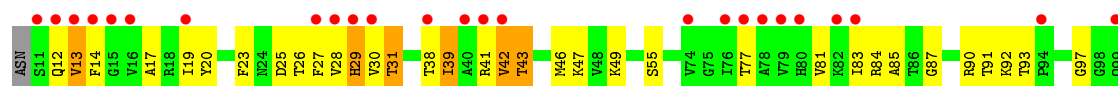




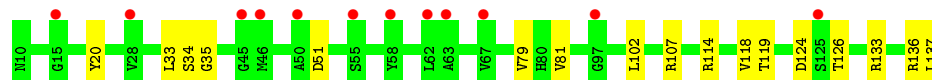
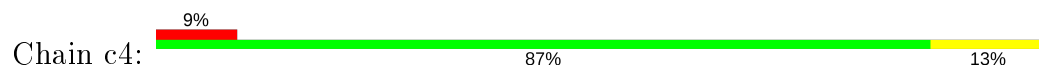
- Molecule 62: 40S ribosomal protein S13



- Molecule 63: 40S ribosomal protein S14-B



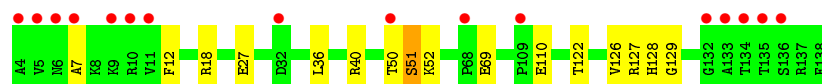
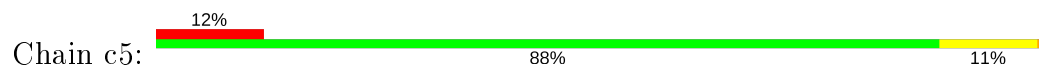
- Molecule 63: 40S ribosomal protein S14-B



- Molecule 64: 40S ribosomal protein S15

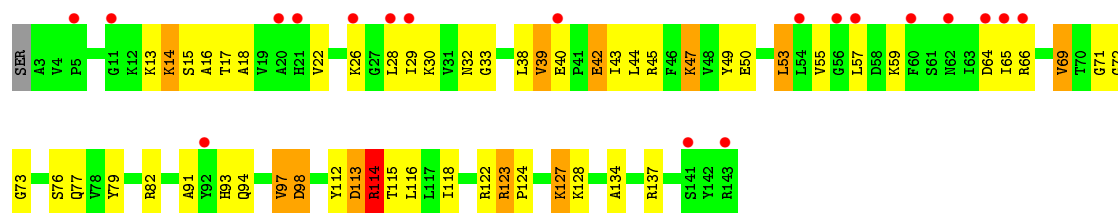


- Molecule 64: 40S ribosomal protein S15

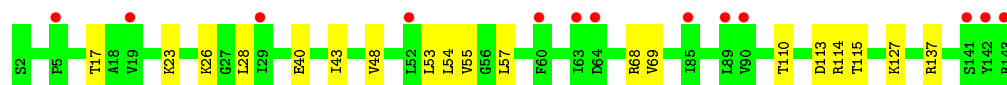
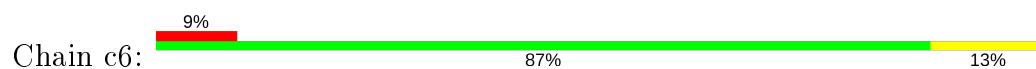


- Molecule 65: 40S ribosomal protein S16-A





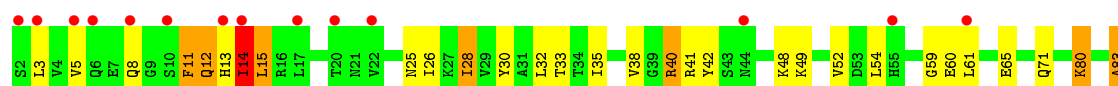
- Molecule 65: 40S ribosomal protein S16-A



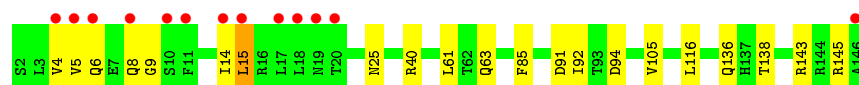
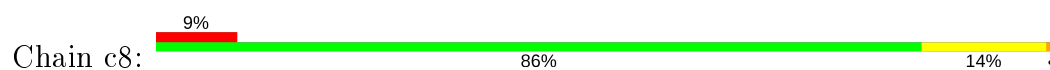
- Molecule 66: 40S ribosomal protein S17-A



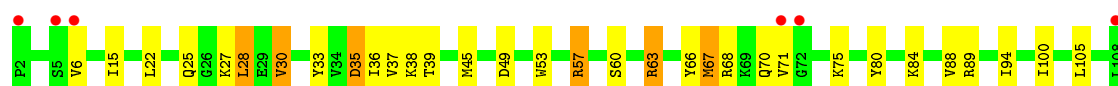
- Molecule 67: 40S ribosomal protein S18-A

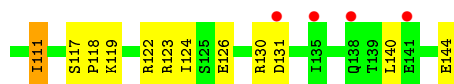


- Molecule 67: 40S ribosomal protein S18-A

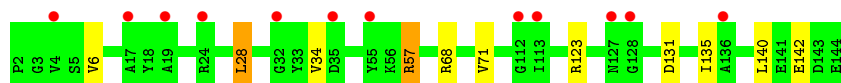


- Molecule 68: 40S ribosomal protein S19-A

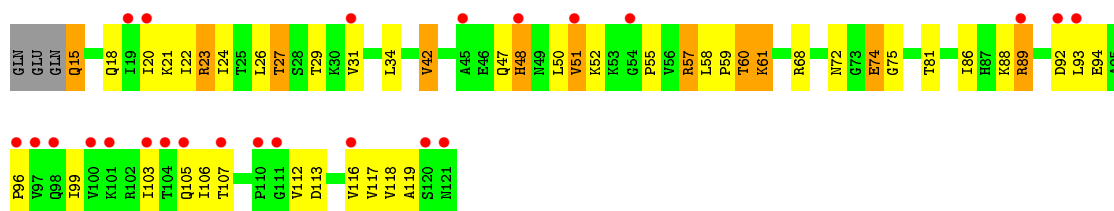




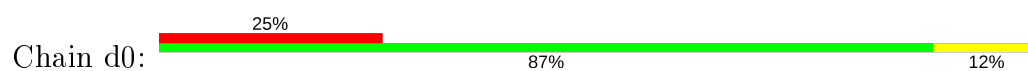
- Molecule 68: 40S ribosomal protein S19-A



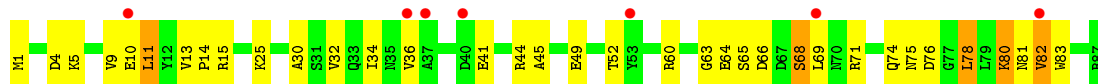
- Molecule 69: 40S ribosomal protein S20



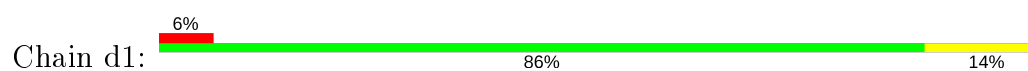
- Molecule 69: 40S ribosomal protein S20



- Molecule 70: 40S ribosomal protein S21-A

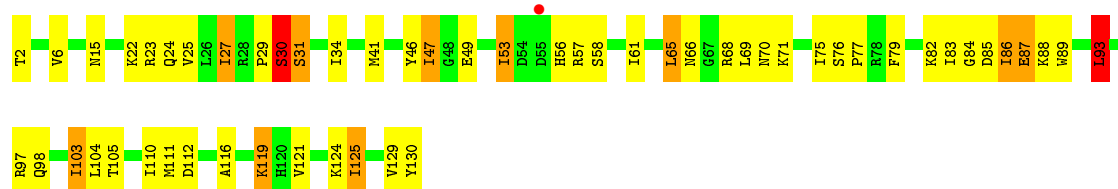


- Molecule 70: 40S ribosomal protein S21-A



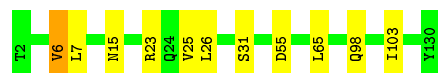
- Molecule 71: 40S ribosomal protein S22-A





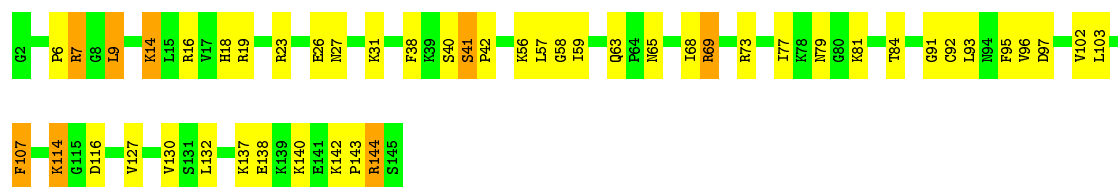
- Molecule 71: 40S ribosomal protein S22-A

Chain d2: 91% 8%



- Molecule 72: 40S ribosomal protein S23-A

Chain Y: 67% 28% 6%



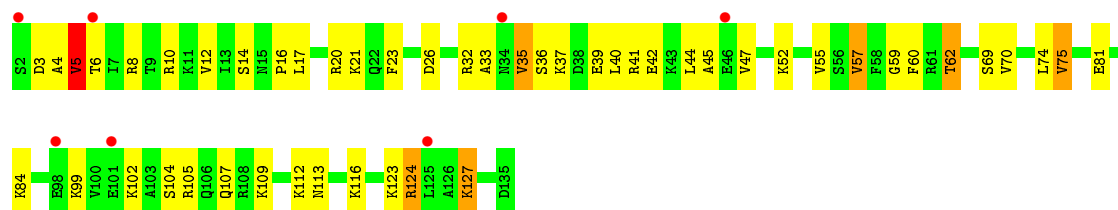
- Molecule 72: 40S ribosomal protein S23-A

Chain d3: 91% 9%



- Molecule 73: 40S ribosomal protein S24-A

Chain Z: 5% 63% 32%

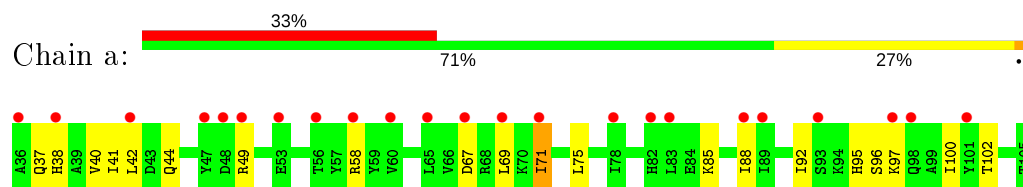


- Molecule 73: 40S ribosomal protein S24-A

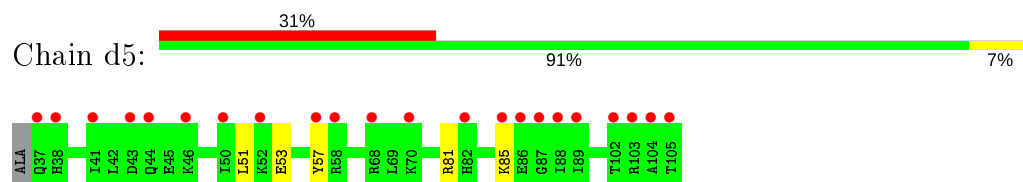
Chain d4: 4% 91% 8%



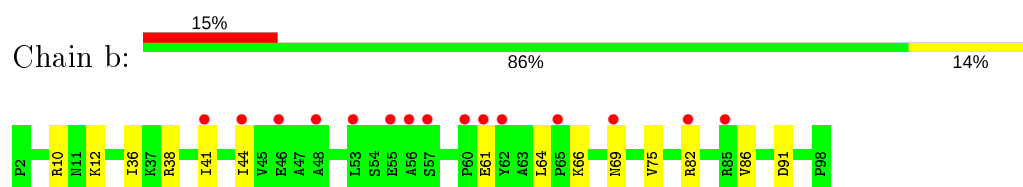
## • Molecule 74: 40S ribosomal protein S25-A



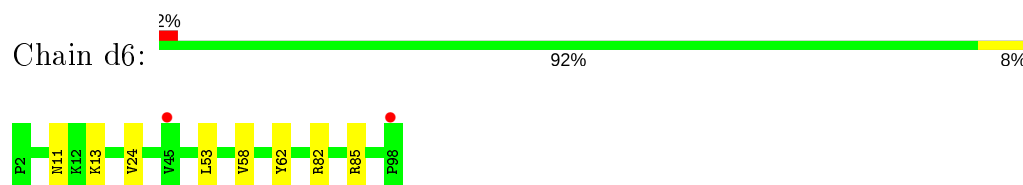
## • Molecule 74: 40S ribosomal protein S25-A



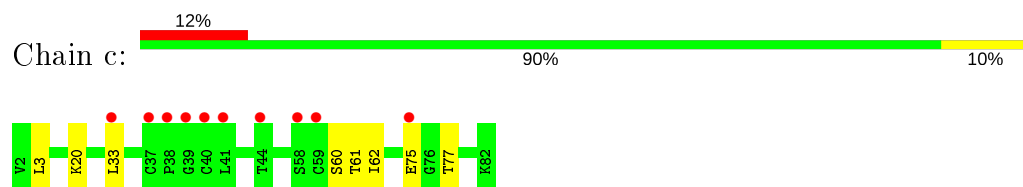
## • Molecule 75: 40S ribosomal protein S26-B



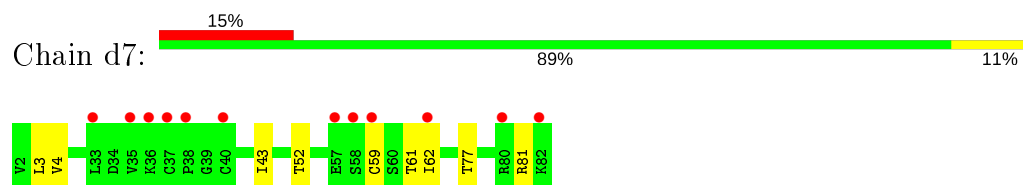
## • Molecule 75: 40S ribosomal protein S26-B



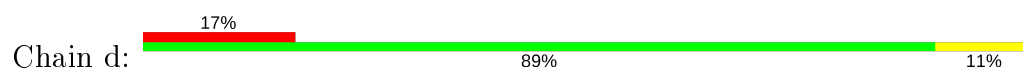
## • Molecule 76: 40S ribosomal protein S27-A

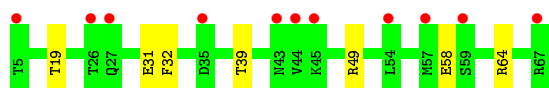


## • Molecule 76: 40S ribosomal protein S27-A

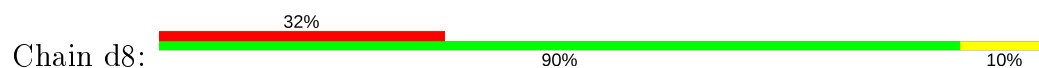


## • Molecule 77: 40S ribosomal protein S28-A

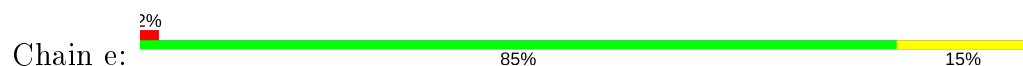




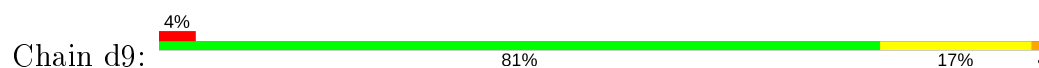
- Molecule 77: 40S ribosomal protein S28-A



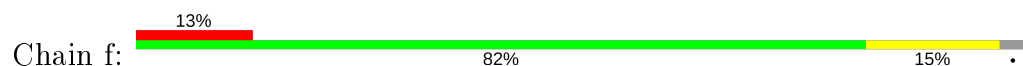
- Molecule 78: 40S ribosomal protein S29-A



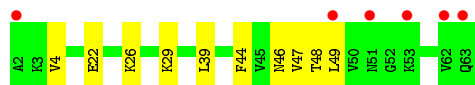
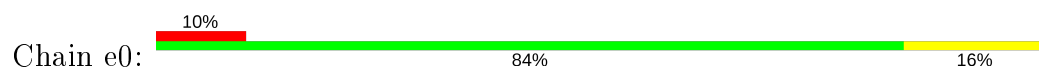
- Molecule 78: 40S ribosomal protein S29-A



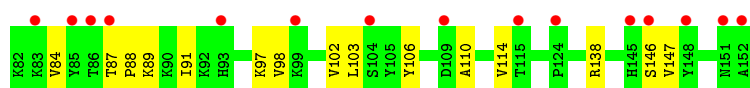
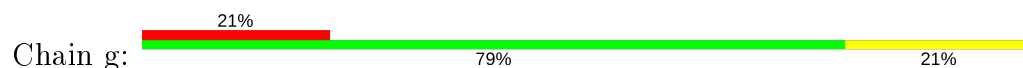
- Molecule 79: 40S ribosomal protein S30-A



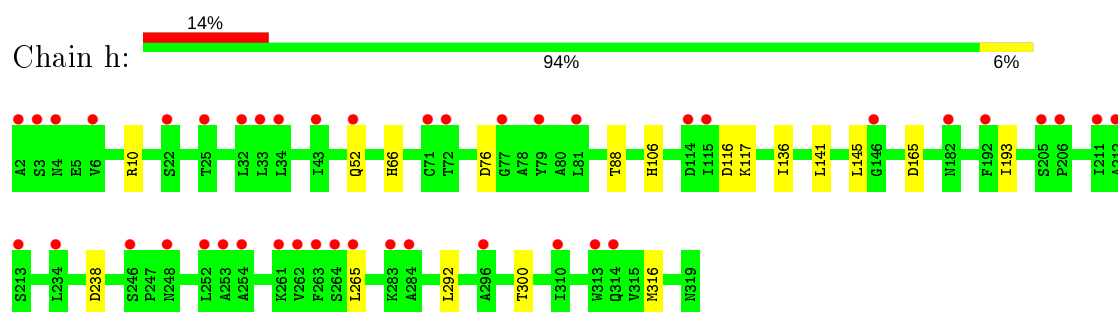
- Molecule 79: 40S ribosomal protein S30-A



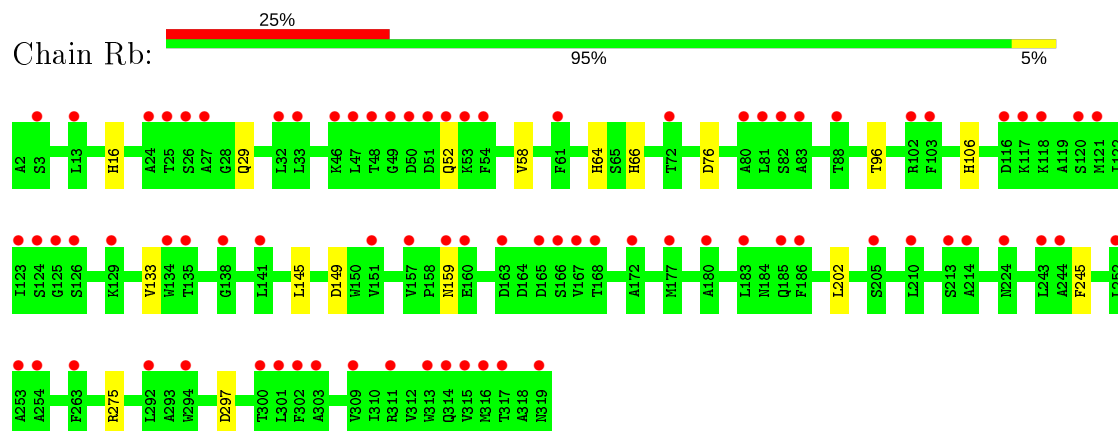
- Molecule 80: Ubiquitin-40S ribosomal protein S31



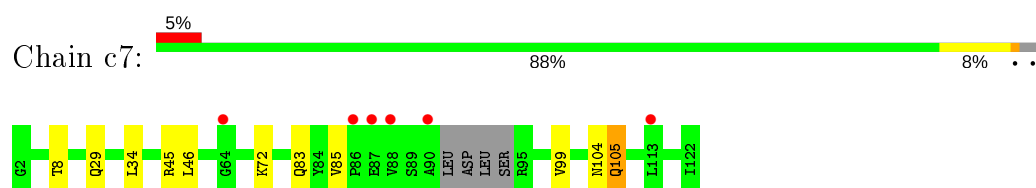
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein



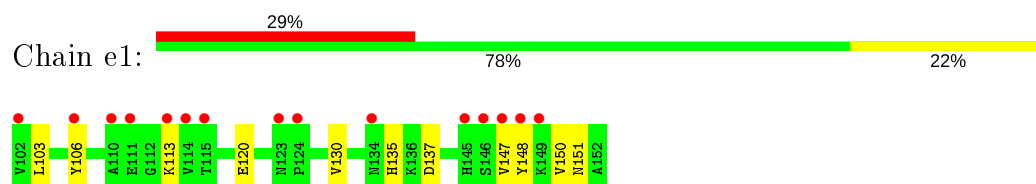
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein



- 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, $\alpha$ , $\beta$ , $\gamma$	304.80Å 288.20Å 437.68Å 90.00° 98.71° 90.00°	Depositor
Resolution (Å)	99.86 – 3.00 99.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.86-3.00) 100.0 (99.86-3.00)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.194 , 0.227 0.196 , 0.228	Depositor DCC
$R_{free}$ test set	29480 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.3	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 63.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	409612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

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

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 7AL, OHX, MG

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	0.54	0/75394	1.00	128/117545 (0.1%)
1	AR	0.54	0/75394	0.98	102/117545 (0.1%)
2	3	0.47	0/2883	0.88	0/4491
2	AS	0.52	0/2883	0.94	1/4491 (0.0%)
3	4	0.52	0/3746	0.96	1/5832 (0.0%)
3	AT	0.46	0/3746	0.91	4/5832 (0.1%)
4	CD	0.37	0/1948	0.60	0/2617
4	j	0.41	0/1948	0.65	1/2617 (0.0%)
5	CE	0.45	0/3146	0.66	1/4228 (0.0%)
5	k	0.41	0/3146	0.63	0/4228
6	CF	0.40	0/2800	0.67	2/3790 (0.1%)
6	l	0.44	0/2800	0.70	3/3790 (0.1%)
7	CG	0.39	0/2425	0.60	0/3271
7	m	0.34	0/2425	0.54	0/3271
8	CH	0.40	0/1260	0.58	0/1694
8	n	0.40	0/1260	0.58	0/1694
9	CI	0.43	0/1821	0.61	0/2451
9	o	0.43	0/1821	0.63	1/2451 (0.0%)
10	CJ	0.32	0/1836	0.54	1/2481 (0.0%)
10	p	0.34	0/1836	0.58	0/2481
11	CK	0.39	0/1539	0.58	0/2073
11	q	0.38	0/1539	0.58	0/2073
12	CL	0.40	0/1741	0.60	0/2335
12	r	0.42	0/1741	0.64	1/2335 (0.0%)
13	CM	0.39	0/1374	0.62	1/1842 (0.1%)
13	s	0.33	0/1374	0.57	0/1842
14	CN	0.39	0/1568	0.61	0/2106
14	t	0.41	0/1568	0.64	0/2106
15	CO	0.41	0/1068	0.60	0/1438
15	u	0.39	0/1068	0.59	0/1438
16	CP	0.39	0/1757	0.62	1/2354 (0.0%)
16	v	0.44	0/1757	0.66	1/2354 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	CQ	0.53	0/1585	0.63	1/2128 (0.0%)
17	w	0.47	0/1585	0.61	0/2128
18	CR	0.45	0/1443	0.66	0/1944
18	x	0.43	0/1443	0.63	0/1944
19	CS	0.41	0/1465	0.66	1/1965 (0.1%)
19	y	0.44	0/1465	0.67	0/1965
20	CT	0.34	0/1538	0.55	0/2050
20	z	0.33	0/1538	0.52	0/2050
21	0	0.40	0/1481	0.61	0/1990
21	CU	0.42	0/1481	0.60	0/1990
22	2	0.40	0/1300	0.60	0/1743
22	CV	0.43	0/1300	0.61	0/1743
23	5	0.29	0/812	0.49	0/1099
23	CW	0.32	0/812	0.54	0/1099
24	6	0.42	0/1018	0.60	0/1369
24	CX	0.44	0/1018	0.60	0/1369
25	7	0.35	0/712	0.51	0/958
25	CY	0.37	0/712	0.60	0/958
26	8	0.34	0/979	0.59	0/1321
26	CZ	0.36	0/979	0.60	1/1321 (0.1%)
27	9	0.39	0/1004	0.67	1/1341 (0.1%)
27	DA	0.39	0/1004	0.62	0/1341
28	AA	0.33	0/1118	0.52	0/1497
28	DB	0.31	0/1118	0.54	0/1497
29	AB	0.45	0/1204	0.70	1/1612 (0.1%)
29	DC	0.44	0/1204	0.65	0/1612
30	AC	0.38	0/473	0.65	1/629 (0.2%)
30	DD	0.38	0/473	0.60	0/629
31	AD	0.31	0/751	0.52	0/1008
31	DE	0.30	0/751	0.52	1/1008 (0.1%)
32	AE	0.35	0/890	0.57	0/1196
32	DF	0.39	0/890	0.57	0/1196
33	AF	0.43	0/1041	0.60	0/1394
33	DG	0.42	0/1041	0.62	0/1394
34	AG	0.48	0/868	0.62	0/1168
34	DH	0.46	0/868	0.63	0/1168
35	AH	0.37	0/890	0.60	0/1189
35	DI	0.35	0/890	0.57	0/1189
36	AI	0.39	0/978	0.57	0/1301
36	DJ	0.34	0/978	0.50	1/1301 (0.1%)
37	AJ	0.37	0/778	0.59	0/1034
37	DK	0.32	0/778	0.57	0/1034
38	AK	0.49	0/696	0.71	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DL	0.41	0/696	0.65	0/923
39	AL	0.33	0/618	0.51	0/826
39	DM	0.30	0/618	0.52	0/826
40	AM	0.42	0/443	0.67	0/588
40	DN	0.35	0/443	0.63	0/588
41	AN	0.44	0/423	0.65	0/562
41	DO	0.44	0/423	0.66	0/562
42	AO	0.36	0/234	0.57	0/300
42	DP	0.37	0/234	0.56	0/300
43	AP	0.42	0/860	0.64	0/1136
43	DQ	0.43	0/860	0.65	0/1136
44	AQ	0.40	0/701	0.64	1/934 (0.1%)
44	DR	0.37	0/701	0.63	0/934
45	i	0.33	0/1113	0.56	1/1502 (0.1%)
46	p0	0.31	0/1092	0.54	0/1474
47	sM	0.34	0/481	0.61	0/644
48	A	0.36	0/42443	0.87	45/66134 (0.1%)
48	sR	0.40	0/42490	0.88	45/66207 (0.1%)
49	B	0.29	0/1617	0.57	0/2215
49	s0	0.31	0/1623	0.55	0/2222
50	C	0.29	0/1735	0.58	1/2335 (0.0%)
50	s1	0.31	0/1748	0.59	1/2352 (0.0%)
51	D	0.30	0/1665	0.54	0/2263
51	s2	0.33	0/1665	0.60	0/2263
52	E	0.29	0/1759	0.50	1/2368 (0.0%)
52	s3	0.27	0/1759	0.47	0/2368
53	F	0.32	0/2109	0.60	1/2839 (0.0%)
53	s4	0.32	0/2109	0.60	0/2839
54	G	0.27	0/1629	0.51	0/2202
54	s5	0.28	0/1629	0.52	0/2202
55	H	0.29	0/1823	0.50	0/2439
55	s6	0.32	0/1779	0.52	0/2379
56	I	0.31	0/1506	0.54	0/2028
56	s7	0.31	0/1516	0.53	0/2043
57	J	0.33	0/1514	0.62	2/2021 (0.1%)
57	s8	0.34	0/1514	0.56	1/2021 (0.0%)
58	K	0.30	0/1519	0.56	0/2035
58	s9	0.31	0/1519	0.51	0/2035
59	L	0.32	0/789	0.64	1/1067 (0.1%)
59	c0	0.31	0/775	0.63	3/1045 (0.3%)
60	M	0.37	0/1239	0.61	0/1673
60	c1	0.35	0/1194	0.60	0/1610
61	N	0.33	0/898	0.59	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	c2	0.26	0/898	0.57	1/1220 (0.1%)
62	O	0.32	0/1215	0.52	0/1638
62	c3	0.33	0/1215	0.55	0/1638
63	P	0.29	0/901	0.59	0/1217
63	c4	0.33	0/960	0.61	0/1290
64	Q	0.31	0/998	0.56	0/1341
64	c5	0.32	0/1060	0.58	0/1426
65	R	0.29	0/1125	0.58	0/1510
65	c6	0.30	0/1131	0.54	0/1518
66	S	0.32	0/935	0.66	2/1254 (0.2%)
67	T	0.31	0/1211	0.55	0/1628
67	c8	0.30	0/1211	0.53	1/1628 (0.1%)
68	U	0.29	0/1130	0.49	0/1517
68	c9	0.29	0/1130	0.55	1/1517 (0.1%)
69	V	0.29	0/865	0.54	0/1169
69	d0	0.30	0/892	0.56	0/1205
70	W	0.29	0/693	0.51	0/935
70	d1	0.29	0/693	0.56	0/935
71	X	0.31	0/1038	0.61	1/1395 (0.1%)
71	d2	0.34	0/1038	0.57	0/1395
72	Y	0.35	0/1139	0.60	0/1518
72	d3	0.39	0/1139	0.58	0/1518
73	Z	0.30	0/1087	0.49	0/1449
73	d4	0.33	0/1087	0.58	0/1449
74	a	0.29	0/571	0.64	0/768
74	d5	0.27	0/566	0.47	0/761
75	b	0.30	0/782	0.58	0/1047
75	d6	0.33	0/782	0.55	0/1047
76	c	0.27	0/620	0.52	0/838
76	d7	0.30	0/620	0.57	0/838
77	d	0.25	0/499	0.49	0/670
77	d8	0.26	0/499	0.53	0/670
78	d9	0.32	0/452	0.52	0/600
78	e	0.37	0/452	0.61	0/600
79	e0	0.32	0/499	0.60	0/665
79	f	0.31	0/483	0.56	0/643
80	g	0.39	0/577	0.76	0/770
81	Rb	0.26	0/2495	0.47	0/3395
81	h	0.26	0/2490	0.49	0/3389
82	c7	0.29	0/914	0.50	0/1224
83	e1	0.30	0/404	0.63	0/542
All	All	0.44	0/429965	0.83	366/631328 (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
6	l	0	1
7	CG	0	2
10	p	0	1
12	r	0	1
17	CQ	0	1
17	w	0	1
21	0	0	1
22	2	0	1
22	CV	0	1
25	CY	0	1
27	9	0	1
27	DA	0	1
28	AA	0	1
28	DB	0	1
30	AC	0	1
30	DD	0	1
32	DF	0	1
36	DJ	0	1
39	AL	0	1
44	DR	0	1
51	D	0	1
52	E	0	1
52	s3	0	1
53	F	0	1
53	s4	0	1
54	G	0	2
54	s5	0	2
55	s6	0	1
56	I	0	3
56	s7	0	2
57	J	0	1
61	c2	0	1
63	P	0	1
63	c4	0	1
64	Q	0	1
64	c5	0	2
65	R	0	4
65	c6	0	2
66	S	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
67	T	0	1
70	d1	0	1
72	Y	0	1
73	d4	0	1
75	b	0	1
80	g	0	2
83	e1	0	1
All	All	0	60

There are no bond length outliers.

The worst 5 of 366 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1308	A	O5'-P-OP1	-10.26	96.47	105.70
1	1	1307	G	P-O3'-C3'	10.16	131.89	119.70
1	AR	3217	C	N1-C2-O2	9.74	124.75	118.90
1	1	406	G	O4'-C1'-N9	9.62	115.89	108.20
1	1	3278	C	N1-C2-O2	9.04	124.32	118.90

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	0	133	ALA	Peptide
6	l	338	LYS	Peptide
10	p	30	THR	Peptide
12	r	188	GLY	Peptide
17	w	110	PRO	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	67355	0	33847	742	0
1	AR	67355	0	33847	869	0
2	3	2579	0	1304	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AS	2579	0	1304	32	0
3	4	3353	0	1695	29	0
3	AT	3353	0	1695	46	0
4	CD	1914	0	1981	33	0
4	j	1914	0	1981	0	0
5	CE	3075	0	3142	107	0
5	k	3075	0	3142	0	0
6	CF	2748	0	2859	62	0
6	l	2748	0	2859	0	0
7	CG	2375	0	2325	61	0
7	m	2375	0	2325	0	0
8	CH	1239	0	1326	30	0
8	n	1239	0	1326	0	0
9	CI	1784	0	1862	26	0
9	o	1784	0	1862	0	0
10	CJ	1804	0	1877	44	0
10	p	1804	0	1877	0	0
11	CK	1518	0	1587	40	0
11	q	1518	0	1587	0	0
12	CL	1705	0	1736	52	0
12	r	1705	0	1736	0	0
13	CM	1353	0	1383	37	0
13	s	1353	0	1383	0	0
14	CN	1543	0	1608	44	0
14	t	1543	0	1608	0	0
15	CO	1053	0	1149	32	0
15	u	1053	0	1149	0	0
16	CP	1720	0	1779	47	0
16	v	1720	0	1779	0	0
17	CQ	1555	0	1659	26	0
17	w	1555	0	1659	0	0
18	CR	1420	0	1437	36	0
18	x	1420	0	1437	0	0
19	CS	1441	0	1543	32	0
19	y	1441	0	1543	0	0
20	CT	1521	0	1617	43	0
20	z	1521	0	1617	0	0
21	0	1445	0	1487	24	0
21	CU	1445	0	1487	31	0
22	2	1276	0	1323	32	0
22	CV	1276	0	1323	43	0
23	5	796	0	812	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	CW	796	0	812	11	0
24	6	1003	0	1048	23	0
24	CX	1003	0	1048	24	0
25	7	699	0	640	12	0
25	CY	699	0	640	9	0
26	8	964	0	1025	20	0
26	CZ	964	0	1025	24	0
27	9	993	0	1081	22	0
27	DA	993	0	1081	22	0
28	AA	1092	0	1155	36	0
28	DB	1092	0	1155	27	0
29	AB	1173	0	1215	37	0
29	DC	1173	0	1215	43	0
30	AC	462	0	491	14	0
30	DD	462	0	491	13	0
31	AD	743	0	797	18	0
31	DE	743	0	797	11	0
32	AE	876	0	912	20	0
32	DF	876	0	912	16	0
33	AF	1020	0	1090	20	0
33	DG	1020	0	1090	20	0
34	AG	850	0	880	16	0
34	DH	850	0	880	11	0
35	AH	880	0	945	27	0
35	DI	880	0	945	23	0
36	AI	969	0	1078	17	0
36	DJ	969	0	1078	32	0
37	AJ	771	0	849	12	0
37	DK	771	0	849	21	0
38	AK	681	0	683	22	0
38	DL	681	0	683	20	0
39	AL	612	0	682	11	0
39	DM	612	0	682	15	0
40	AM	436	0	475	16	0
40	DN	436	0	475	16	0
41	AN	417	0	455	6	0
41	DO	417	0	455	6	0
42	AO	233	0	284	11	0
42	DP	233	0	284	4	0
43	AP	847	0	914	19	0
43	DQ	847	0	914	9	0
44	AQ	694	0	734	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DR	694	0	734	17	0
45	i	1104	0	1003	0	0
46	p0	1077	0	1041	0	0
47	sM	681	0	541	0	0
48	A	37948	0	19094	565	0
48	sR	37990	0	19116	0	0
49	B	1577	0	1567	54	0
49	s0	1583	0	1578	0	0
50	C	1709	0	1784	68	0
50	s1	1722	0	1793	0	0
51	D	1635	0	1723	42	0
51	s2	1635	0	1723	0	0
52	E	1734	0	1817	42	0
52	s3	1734	0	1817	0	0
53	F	2068	0	2154	52	0
53	s4	2068	0	2154	0	0
54	G	1609	0	1675	46	0
54	s5	1609	0	1675	0	0
55	H	1799	0	1878	42	0
55	s6	1755	0	1846	0	0
56	I	1481	0	1572	55	0
56	s7	1491	0	1578	0	0
57	J	1489	0	1525	46	0
57	s8	1489	0	1525	0	0
58	K	1494	0	1573	41	0
58	s9	1494	0	1573	0	0
59	L	772	0	727	26	0
59	c0	760	0	696	0	0
60	M	1213	0	1257	31	0
60	c1	1168	0	1233	0	0
61	N	890	0	887	25	0
61	c2	890	0	887	0	0
62	O	1192	0	1255	31	0
62	c3	1192	0	1255	0	0
63	P	891	0	883	33	0
63	c4	949	0	985	0	0
64	Q	977	0	1002	25	0
64	c5	1039	0	1050	0	0
65	R	1105	0	1166	41	0
65	c6	1111	0	1171	0	0
66	S	926	0	930	33	0
67	T	1192	0	1222	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	c8	1192	0	1222	0	0
68	U	1112	0	1124	22	0
68	c9	1112	0	1124	0	0
69	V	855	0	917	35	0
69	d0	882	0	939	0	0
70	W	684	0	672	22	0
70	d1	684	0	672	0	0
71	X	1021	0	1060	40	0
71	d2	1021	0	1060	0	0
72	Y	1121	0	1196	28	0
72	d3	1121	0	1196	0	0
73	Z	1073	0	1132	38	0
73	d4	1073	0	1132	0	0
74	a	563	0	603	0	0
74	d5	558	0	598	0	0
75	b	769	0	814	0	0
75	d6	769	0	814	0	0
76	c	610	0	633	0	0
76	d7	610	0	633	0	0
77	d	497	0	535	0	0
77	d8	497	0	535	0	0
78	d9	442	0	428	0	0
78	e	442	0	428	0	0
79	e0	491	0	542	0	0
79	f	475	0	525	0	0
80	g	566	0	601	0	0
81	Rb	2442	0	2392	0	0
81	h	2437	0	2386	0	0
82	c7	906	0	909	0	0
83	e1	397	0	397	0	0
84	1	2317	0	0	252	0
84	3	56	0	0	5	0
84	4	105	0	0	8	0
84	A	994	0	0	109	0
84	AC	7	0	0	2	0
84	AG	7	0	0	1	0
84	AK	14	0	0	3	0
84	AP	7	0	0	5	0
84	AR	2422	0	0	306	0
84	AS	77	0	0	7	0
84	AT	119	0	0	20	0
84	CE	14	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	CF	14	0	0	4	0
84	CG	21	0	0	4	0
84	CK	7	0	0	0	0
84	CL	14	0	0	5	0
84	CM	7	0	0	1	0
84	CO	7	0	0	0	0
84	CP	7	0	0	1	0
84	CS	1	0	0	0	0
84	CV	7	0	0	1	0
84	CX	14	0	0	2	0
84	DD	7	0	0	1	0
84	DH	7	0	0	0	0
84	DL	7	0	0	2	0
84	DQ	7	0	0	3	0
84	H	7	0	0	0	0
84	J	7	0	0	1	0
84	M	7	0	0	1	0
84	O	7	0	0	1	0
84	Q	7	0	0	2	0
84	Rb	7	0	0	0	0
84	T	7	0	0	1	0
84	c3	7	0	0	0	0
84	c5	7	0	0	0	0
84	c8	7	0	0	0	0
84	d4	7	0	0	0	0
84	d9	7	0	0	0	0
84	e	7	0	0	0	0
84	h	7	0	0	0	0
84	k	7	0	0	0	0
84	l	7	0	0	0	0
84	r	7	0	0	0	0
84	s1	7	0	0	0	0
84	s4	7	0	0	0	0
84	s8	7	0	0	0	0
84	sR	1064	0	0	0	0
84	v	14	0	0	0	0
84	x	14	0	0	0	0
84	y	7	0	0	0	0
84	z	7	0	0	0	0
85	1	485	0	0	0	0
85	3	12	0	0	0	0
85	4	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	6	2	0	0	0	0
85	A	109	0	0	0	0
85	AB	4	0	0	0	0
85	AH	1	0	0	0	0
85	AK	1	0	0	0	0
85	AP	1	0	0	0	0
85	AR	504	0	0	0	0
85	AS	17	0	0	0	0
85	AT	13	0	0	0	0
85	CD	2	0	0	0	0
85	CE	2	0	0	0	0
85	CF	1	0	0	0	0
85	CG	1	0	0	0	0
85	CJ	1	0	0	0	0
85	CM	2	0	0	0	0
85	CN	1	0	0	0	0
85	CP	4	0	0	0	0
85	CQ	3	0	0	0	0
85	CR	6	0	0	0	0
85	CU	1	0	0	0	0
85	CX	3	0	0	0	0
85	D	1	0	0	0	0
85	DA	1	0	0	0	0
85	DC	6	0	0	0	0
85	DD	1	0	0	0	0
85	DH	2	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	J	1	0	0	0	0
85	O	1	0	0	0	0
85	Y	1	0	0	0	0
85	b	1	0	0	0	0
85	c1	1	0	0	0	0
85	c6	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	1	0	0	0	0
85	d3	2	0	0	0	0
85	d4	1	0	0	0	0
85	d5	1	0	0	0	0
85	d6	2	0	0	0	0
85	d9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	e	1	0	0	0	0
85	j	1	0	0	0	0
85	k	2	0	0	0	0
85	l	5	0	0	0	0
85	n	1	0	0	0	0
85	o	1	0	0	0	0
85	r	2	0	0	0	0
85	s	1	0	0	0	0
85	s1	1	0	0	0	0
85	s8	1	0	0	0	0
85	sM	1	0	0	0	0
85	sR	139	0	0	0	0
85	t	3	0	0	0	0
85	u	1	0	0	0	0
85	v	2	0	0	0	0
85	w	1	0	0	0	0
85	x	5	0	0	0	0
85	z	1	0	0	0	0
86	1	26	0	0	0	0
86	AR	26	0	0	1	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	409612	0	296692	4353	0

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

The worst 5 of 4353 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)
5:CE:41:VAL:HA	5:CE:185:GLY:HA3	1.34	1.05
12:CL:174:THR:HG23	12:CL:176:LEU:H	1.29	0.95
56:I:11:GLN:HG3	56:I:13:PRO:HD2	1.49	0.94
1:1:2736:A:OP1	22:2:92:ARG:NH1	2.00	0.93
48:A:1339:C:O2'	48:A:1341:A:N7	2.01	0.93

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%)	237 (95%)	13 (5%)	0	100	100
4	j	250/252 (99%)	235 (94%)	15 (6%)	0	100	100
5	CE	384/386 (100%)	357 (93%)	27 (7%)	0	100	100
5	k	384/386 (100%)	361 (94%)	22 (6%)	1 (0%)	41	76
6	CF	359/361 (99%)	333 (93%)	25 (7%)	1 (0%)	41	76
6	l	359/361 (99%)	334 (93%)	23 (6%)	2 (1%)	25	64
7	CG	294/296 (99%)	274 (93%)	19 (6%)	1 (0%)	41	76
7	m	294/296 (99%)	268 (91%)	26 (9%)	0	100	100
8	CH	152/175 (87%)	145 (95%)	6 (4%)	1 (1%)	22	60
8	n	152/175 (87%)	146 (96%)	5 (3%)	1 (1%)	22	60
9	CI	220/222 (99%)	207 (94%)	11 (5%)	2 (1%)	17	55
9	o	220/222 (99%)	208 (94%)	9 (4%)	3 (1%)	11	43
10	CJ	231/233 (99%)	208 (90%)	21 (9%)	2 (1%)	17	55
10	p	231/233 (99%)	210 (91%)	18 (8%)	3 (1%)	12	45
11	CK	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
11	q	189/191 (99%)	176 (93%)	12 (6%)	1 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	CL	207/220 (94%)	194 (94%)	12 (6%)	1 (0%)	29	68
12	r	207/220 (94%)	202 (98%)	5 (2%)	0	100	100
13	CM	167/169 (99%)	148 (89%)	16 (10%)	3 (2%)	8	37
13	s	167/169 (99%)	149 (89%)	17 (10%)	1 (1%)	25	64
14	CN	191/193 (99%)	175 (92%)	13 (7%)	3 (2%)	9	40
14	t	191/193 (99%)	174 (91%)	14 (7%)	3 (2%)	9	40
15	CO	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	10	42
15	u	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	10	42
16	CP	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
16	v	201/203 (99%)	188 (94%)	11 (6%)	2 (1%)	15	53
17	CQ	195/197 (99%)	189 (97%)	3 (2%)	3 (2%)	10	42
17	w	195/197 (99%)	190 (97%)	3 (2%)	2 (1%)	15	53
18	CR	181/183 (99%)	167 (92%)	13 (7%)	1 (1%)	25	64
18	x	181/183 (99%)	172 (95%)	8 (4%)	1 (1%)	25	64
19	CS	183/185 (99%)	172 (94%)	10 (6%)	1 (0%)	29	68
19	y	183/185 (99%)	174 (95%)	8 (4%)	1 (0%)	29	68
20	CT	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	68
20	z	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
21	0	170/172 (99%)	159 (94%)	10 (6%)	1 (1%)	25	64
21	CU	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	64
22	2	157/159 (99%)	147 (94%)	9 (6%)	1 (1%)	25	64
22	CV	157/159 (99%)	148 (94%)	8 (5%)	1 (1%)	25	64
23	5	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	15	53
23	CW	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	15	53
24	6	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
24	CX	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
25	7	96/98 (98%)	88 (92%)	7 (7%)	1 (1%)	15	53
25	CY	96/98 (98%)	89 (93%)	5 (5%)	2 (2%)	7	33
26	8	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
26	CZ	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
27	9	124/126 (98%)	118 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	DA	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
28	AA	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
28	DB	133/135 (98%)	121 (91%)	10 (8%)	2 (2%)	10	42
29	AB	146/148 (99%)	127 (87%)	17 (12%)	2 (1%)	11	43
29	DC	146/148 (99%)	133 (91%)	10 (7%)	3 (2%)	7	33
30	AC	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
30	DD	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
31	AD	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
31	DE	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
32	AE	107/109 (98%)	101 (94%)	3 (3%)	3 (3%)	5	25
32	DF	107/109 (98%)	103 (96%)	1 (1%)	3 (3%)	5	25
33	AF	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
33	DG	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
34	AG	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
34	DH	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
35	AH	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	17	55
35	DI	110/112 (98%)	103 (94%)	6 (6%)	1 (1%)	17	55
36	AI	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
36	DJ	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
37	AJ	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	15	53
37	DK	97/99 (98%)	86 (89%)	10 (10%)	1 (1%)	15	53
38	AK	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
38	DL	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
39	AL	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
39	DM	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	12	45
40	AM	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
40	DN	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
41	AN	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
41	DO	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
42	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
42	DP	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	AP	103/105 (98%)	90 (87%)	12 (12%)	1 (1%)	15	53
43	DQ	103/105 (98%)	90 (87%)	13 (13%)	0	100	100
44	AQ	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
44	DR	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	14	50
45	i	155/168 (92%)	131 (84%)	21 (14%)	3 (2%)	8	36
46	p0	139/219 (64%)	123 (88%)	14 (10%)	2 (1%)	11	43
47	sM	61/104 (59%)	50 (82%)	10 (16%)	1 (2%)	9	40
49	B	204/206 (99%)	177 (87%)	25 (12%)	2 (1%)	15	53
49	s0	204/206 (99%)	179 (88%)	23 (11%)	2 (1%)	15	53
50	C	212/216 (98%)	170 (80%)	40 (19%)	2 (1%)	17	55
50	s1	214/216 (99%)	193 (90%)	21 (10%)	0	100	100
51	D	215/217 (99%)	200 (93%)	13 (6%)	2 (1%)	17	55
51	s2	215/217 (99%)	200 (93%)	15 (7%)	0	100	100
52	E	221/223 (99%)	203 (92%)	16 (7%)	2 (1%)	17	55
52	s3	221/223 (99%)	199 (90%)	20 (9%)	2 (1%)	17	55
53	F	258/260 (99%)	236 (92%)	21 (8%)	1 (0%)	34	72
53	s4	258/260 (99%)	235 (91%)	21 (8%)	2 (1%)	19	57
54	G	204/206 (99%)	180 (88%)	21 (10%)	3 (2%)	10	42
54	s5	204/206 (99%)	181 (89%)	21 (10%)	2 (1%)	15	53
55	H	224/226 (99%)	207 (92%)	14 (6%)	3 (1%)	12	45
55	s6	216/226 (96%)	198 (92%)	16 (7%)	2 (1%)	17	55
56	I	182/186 (98%)	158 (87%)	18 (10%)	6 (3%)	4	21
56	s7	184/186 (99%)	162 (88%)	21 (11%)	1 (0%)	29	68
57	J	184/199 (92%)	162 (88%)	20 (11%)	2 (1%)	14	50
57	s8	184/199 (92%)	168 (91%)	14 (8%)	2 (1%)	14	50
58	K	183/185 (99%)	165 (90%)	17 (9%)	1 (0%)	29	68
58	s9	183/185 (99%)	168 (92%)	15 (8%)	0	100	100
59	L	94/105 (90%)	77 (82%)	16 (17%)	1 (1%)	14	50
59	c0	92/105 (88%)	64 (70%)	21 (23%)	7 (8%)	1	5
60	M	153/155 (99%)	135 (88%)	15 (10%)	3 (2%)	7	34
60	c1	144/155 (93%)	133 (92%)	9 (6%)	2 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	N	122/143 (85%)	88 (72%)	30 (25%)	4 (3%)	4	21
61	c2	122/143 (85%)	94 (77%)	24 (20%)	4 (3%)	4	21
62	O	148/150 (99%)	138 (93%)	9 (6%)	1 (1%)	22	60
62	c3	148/150 (99%)	134 (90%)	11 (7%)	3 (2%)	7	34
63	P	125/128 (98%)	112 (90%)	11 (9%)	2 (2%)	9	40
63	c4	126/128 (98%)	113 (90%)	11 (9%)	2 (2%)	9	40
64	Q	122/135 (90%)	107 (88%)	12 (10%)	3 (2%)	5	28
64	c5	133/135 (98%)	105 (79%)	22 (16%)	6 (4%)	2	14
65	R	139/142 (98%)	121 (87%)	15 (11%)	3 (2%)	6	31
65	c6	140/142 (99%)	132 (94%)	7 (5%)	1 (1%)	22	60
66	S	116/125 (93%)	97 (84%)	15 (13%)	4 (3%)	3	20
67	T	143/145 (99%)	124 (87%)	15 (10%)	4 (3%)	5	25
67	c8	143/145 (99%)	123 (86%)	16 (11%)	4 (3%)	5	25
68	U	141/143 (99%)	125 (89%)	16 (11%)	0	100	100
68	c9	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	11	43
69	V	105/110 (96%)	93 (89%)	11 (10%)	1 (1%)	15	53
69	d0	108/110 (98%)	92 (85%)	15 (14%)	1 (1%)	17	55
70	W	85/87 (98%)	73 (86%)	11 (13%)	1 (1%)	13	48
70	d1	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
71	X	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	6	29
71	d2	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	57
72	Y	142/144 (99%)	121 (85%)	20 (14%)	1 (1%)	22	60
72	d3	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
73	Z	132/134 (98%)	121 (92%)	8 (6%)	3 (2%)	6	30
73	d4	132/134 (98%)	120 (91%)	11 (8%)	1 (1%)	19	57
74	a	68/70 (97%)	55 (81%)	9 (13%)	4 (6%)	1	9
74	d5	67/70 (96%)	62 (92%)	4 (6%)	1 (2%)	10	42
75	b	95/97 (98%)	71 (75%)	21 (22%)	3 (3%)	4	22
75	d6	95/97 (98%)	78 (82%)	15 (16%)	2 (2%)	7	33
76	c	79/81 (98%)	70 (89%)	8 (10%)	1 (1%)	12	45
76	d7	79/81 (98%)	69 (87%)	8 (10%)	2 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	d	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
77	d8	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
78	d9	51/53 (96%)	44 (86%)	6 (12%)	1 (2%)	7	34
78	e	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
79	e0	60/62 (97%)	52 (87%)	7 (12%)	1 (2%)	9	39
79	f	58/62 (94%)	49 (84%)	7 (12%)	2 (3%)	3	20
80	g	69/71 (97%)	44 (64%)	19 (28%)	6 (9%)	1	3
81	Rb	316/318 (99%)	294 (93%)	22 (7%)	0	100	100
81	h	316/318 (99%)	295 (93%)	21 (7%)	0	100	100
82	c7	113/121 (93%)	101 (89%)	10 (9%)	2 (2%)	8	37
83	e1	49/51 (96%)	37 (76%)	12 (24%)	0	100	100
All	All	22260/22893 (97%)	20326 (91%)	1724 (8%)	210 (1%)	17	55

5 of 210 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	l	339	LEU
8	n	98	VAL
11	q	50	ASN
16	v	75	VAL
17	w	111	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	15
4	j	193/194 (100%)	164 (85%)	29 (15%)	3	14
5	CE	320/322 (99%)	269 (84%)	51 (16%)	2	12
5	k	320/322 (99%)	266 (83%)	54 (17%)	2	11
6	CF	288/288 (100%)	249 (86%)	39 (14%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	l	288/288 (100%)	243 (84%)	45 (16%)	2	13
7	CG	244/244 (100%)	206 (84%)	38 (16%)	2	13
7	m	244/244 (100%)	207 (85%)	37 (15%)	3	14
8	CH	134/152 (88%)	119 (89%)	15 (11%)	6	24
8	n	134/152 (88%)	116 (87%)	18 (13%)	4	17
9	CI	186/186 (100%)	169 (91%)	17 (9%)	9	34
9	o	186/186 (100%)	164 (88%)	22 (12%)	5	22
10	CJ	187/191 (98%)	169 (90%)	18 (10%)	8	32
10	p	187/191 (98%)	157 (84%)	30 (16%)	2	12
11	CK	171/171 (100%)	146 (85%)	25 (15%)	3	15
11	q	171/171 (100%)	145 (85%)	26 (15%)	3	14
12	CL	177/186 (95%)	157 (89%)	20 (11%)	6	24
12	r	177/186 (95%)	151 (85%)	26 (15%)	3	15
13	CM	147/147 (100%)	123 (84%)	24 (16%)	2	11
13	s	147/147 (100%)	122 (83%)	25 (17%)	2	10
14	CN	154/154 (100%)	135 (88%)	19 (12%)	4	21
14	t	154/154 (100%)	130 (84%)	24 (16%)	2	13
15	CO	107/107 (100%)	96 (90%)	11 (10%)	7	28
15	u	107/107 (100%)	92 (86%)	15 (14%)	3	16
16	CP	175/175 (100%)	153 (87%)	22 (13%)	4	20
16	v	175/175 (100%)	156 (89%)	19 (11%)	6	25
17	CQ	160/160 (100%)	142 (89%)	18 (11%)	6	24
17	w	160/160 (100%)	143 (89%)	17 (11%)	6	26
18	CR	140/145 (97%)	116 (83%)	24 (17%)	2	10
18	x	140/145 (97%)	122 (87%)	18 (13%)	4	19
19	CS	150/150 (100%)	125 (83%)	25 (17%)	2	11
19	y	150/150 (100%)	125 (83%)	25 (17%)	2	11
20	CT	153/153 (100%)	125 (82%)	28 (18%)	1	9
20	z	153/153 (100%)	136 (89%)	17 (11%)	6	25
21	0	156/156 (100%)	131 (84%)	25 (16%)	2	12
21	CU	156/156 (100%)	132 (85%)	24 (15%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	2	136/136 (100%)	110 (81%)	26 (19%)	1	8
22	CV	136/136 (100%)	111 (82%)	25 (18%)	1	9
23	5	87/87 (100%)	77 (88%)	10 (12%)	5	24
23	CW	87/87 (100%)	76 (87%)	11 (13%)	4	20
24	6	104/104 (100%)	88 (85%)	16 (15%)	2	13
24	CX	104/104 (100%)	91 (88%)	13 (12%)	4	20
25	7	57/86 (66%)	51 (90%)	6 (10%)	7	27
25	CY	57/86 (66%)	51 (90%)	6 (10%)	7	27
26	8	104/105 (99%)	87 (84%)	17 (16%)	2	11
26	CZ	104/105 (99%)	86 (83%)	18 (17%)	2	10
27	9	109/109 (100%)	90 (83%)	19 (17%)	2	10
27	DA	109/109 (100%)	94 (86%)	15 (14%)	3	17
28	AA	115/115 (100%)	98 (85%)	17 (15%)	3	14
28	DB	115/115 (100%)	105 (91%)	10 (9%)	10	37
29	AB	118/118 (100%)	98 (83%)	20 (17%)	2	11
29	DC	118/118 (100%)	102 (86%)	16 (14%)	3	17
30	AC	46/46 (100%)	40 (87%)	6 (13%)	4	19
30	DD	46/46 (100%)	39 (85%)	7 (15%)	3	14
31	AD	81/81 (100%)	69 (85%)	12 (15%)	3	14
31	DE	81/81 (100%)	75 (93%)	6 (7%)	13	44
32	AE	92/96 (96%)	79 (86%)	13 (14%)	3	16
32	DF	92/96 (96%)	74 (80%)	18 (20%)	1	7
33	AF	109/109 (100%)	94 (86%)	15 (14%)	3	17
33	DG	109/109 (100%)	98 (90%)	11 (10%)	7	29
34	AG	90/90 (100%)	84 (93%)	6 (7%)	16	49
34	DH	90/90 (100%)	80 (89%)	10 (11%)	6	25
35	AH	95/95 (100%)	80 (84%)	15 (16%)	2	12
35	DI	95/95 (100%)	86 (90%)	9 (10%)	8	32
36	AI	104/104 (100%)	89 (86%)	15 (14%)	3	15
36	DJ	104/104 (100%)	81 (78%)	23 (22%)	1	4
37	AJ	81/81 (100%)	66 (82%)	15 (18%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DK	81/81 (100%)	65 (80%)	16 (20%)	1	7
38	AK	70/70 (100%)	61 (87%)	9 (13%)	4	19
38	DL	70/70 (100%)	59 (84%)	11 (16%)	2	13
39	AL	68/68 (100%)	57 (84%)	11 (16%)	2	12
39	DM	68/68 (100%)	56 (82%)	12 (18%)	2	10
40	AM	45/45 (100%)	38 (84%)	7 (16%)	2	13
40	DN	45/45 (100%)	40 (89%)	5 (11%)	6	25
41	AN	47/47 (100%)	38 (81%)	9 (19%)	1	8
41	DO	47/47 (100%)	40 (85%)	7 (15%)	3	14
42	AO	23/23 (100%)	19 (83%)	4 (17%)	2	10
42	DP	23/23 (100%)	19 (83%)	4 (17%)	2	10
43	AP	90/90 (100%)	80 (89%)	10 (11%)	6	25
43	DQ	90/90 (100%)	73 (81%)	17 (19%)	1	8
44	AQ	71/71 (100%)	58 (82%)	13 (18%)	1	9
44	DR	71/71 (100%)	64 (90%)	7 (10%)	8	30
45	i	97/137 (71%)	81 (84%)	16 (16%)	2	11
46	p0	105/186 (56%)	88 (84%)	17 (16%)	2	12
47	sM	54/54 (100%)	47 (87%)	7 (13%)	4	19
49	B	164/173 (95%)	149 (91%)	15 (9%)	9	34
49	s0	165/173 (95%)	139 (84%)	26 (16%)	2	12
50	C	191/192 (100%)	160 (84%)	31 (16%)	2	12
50	s1	192/192 (100%)	164 (85%)	28 (15%)	3	15
51	D	176/176 (100%)	140 (80%)	36 (20%)	1	6
51	s2	176/176 (100%)	141 (80%)	35 (20%)	1	7
52	E	182/182 (100%)	157 (86%)	25 (14%)	3	17
52	s3	182/182 (100%)	163 (90%)	19 (10%)	7	27
53	F	221/221 (100%)	194 (88%)	27 (12%)	5	21
53	s4	221/221 (100%)	191 (86%)	30 (14%)	3	17
54	G	173/173 (100%)	158 (91%)	15 (9%)	10	37
54	s5	173/173 (100%)	153 (88%)	20 (12%)	5	23
55	H	188/193 (97%)	159 (85%)	29 (15%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	s6	187/193 (97%)	165 (88%)	22 (12%)	5	22
56	I	165/166 (99%)	144 (87%)	21 (13%)	4	19
56	s7	165/166 (99%)	148 (90%)	17 (10%)	7	28
57	J	150/160 (94%)	135 (90%)	15 (10%)	7	29
57	s8	150/160 (94%)	136 (91%)	14 (9%)	9	33
58	K	158/158 (100%)	129 (82%)	29 (18%)	1	9
58	s9	158/158 (100%)	137 (87%)	21 (13%)	4	17
59	L	77/98 (79%)	70 (91%)	7 (9%)	9	34
59	c0	73/98 (74%)	67 (92%)	6 (8%)	11	39
60	M	129/136 (95%)	108 (84%)	21 (16%)	2	11
60	c1	129/136 (95%)	110 (85%)	19 (15%)	3	15
61	N	88/119 (74%)	68 (77%)	20 (23%)	1	4
61	c2	88/119 (74%)	68 (77%)	20 (23%)	1	4
62	O	127/127 (100%)	106 (84%)	21 (16%)	2	11
62	c3	127/127 (100%)	110 (87%)	17 (13%)	4	17
63	P	81/97 (84%)	69 (85%)	12 (15%)	3	14
63	c4	97/97 (100%)	83 (86%)	14 (14%)	3	15
64	Q	101/111 (91%)	86 (85%)	15 (15%)	3	14
64	c5	103/111 (93%)	94 (91%)	9 (9%)	10	37
65	R	117/118 (99%)	100 (86%)	17 (14%)	3	15
65	c6	118/118 (100%)	102 (86%)	16 (14%)	3	17
66	S	94/113 (83%)	77 (82%)	17 (18%)	1	9
67	T	128/128 (100%)	104 (81%)	24 (19%)	1	8
67	c8	128/128 (100%)	111 (87%)	17 (13%)	4	17
68	U	115/115 (100%)	94 (82%)	21 (18%)	1	9
68	c9	115/115 (100%)	105 (91%)	10 (9%)	10	37
69	V	100/103 (97%)	84 (84%)	16 (16%)	2	12
69	d0	103/103 (100%)	89 (86%)	14 (14%)	3	17
70	W	74/74 (100%)	61 (82%)	13 (18%)	2	10
70	d1	74/74 (100%)	63 (85%)	11 (15%)	3	14
71	X	110/110 (100%)	91 (83%)	19 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	d2	110/110 (100%)	99 (90%)	11 (10%)	7	29
72	Y	119/119 (100%)	101 (85%)	18 (15%)	3	14
72	d3	119/119 (100%)	106 (89%)	13 (11%)	6	25
73	Z	112/112 (100%)	99 (88%)	13 (12%)	5	23
73	d4	112/112 (100%)	101 (90%)	11 (10%)	8	30
74	a	61/61 (100%)	44 (72%)	17 (28%)	0	2
74	d5	61/61 (100%)	57 (93%)	4 (7%)	16	49
75	b	83/83 (100%)	73 (88%)	10 (12%)	5	22
75	d6	83/83 (100%)	77 (93%)	6 (7%)	14	45
76	c	70/70 (100%)	63 (90%)	7 (10%)	7	29
76	d7	70/70 (100%)	63 (90%)	7 (10%)	7	29
77	d	56/56 (100%)	49 (88%)	7 (12%)	4	20
77	d8	56/56 (100%)	50 (89%)	6 (11%)	6	26
78	d9	47/47 (100%)	37 (79%)	10 (21%)	1	5
78	e	47/47 (100%)	39 (83%)	8 (17%)	2	10
79	e0	53/53 (100%)	44 (83%)	9 (17%)	2	10
79	f	51/53 (96%)	44 (86%)	7 (14%)	3	17
80	g	62/62 (100%)	55 (89%)	7 (11%)	6	24
81	Rb	260/261 (100%)	243 (94%)	17 (6%)	17	50
81	h	259/261 (99%)	241 (93%)	18 (7%)	15	48
82	c7	92/110 (84%)	82 (89%)	10 (11%)	6	25
83	e1	43/43 (100%)	33 (77%)	10 (23%)	1	4
All	All	18683/19203 (97%)	16080 (86%)	2603 (14%)	3	16

5 of 2603 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	CT	43	LYS
39	DM	58	ASP
62	c3	80	LEU
21	CU	97	VAL
28	DB	102	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
52	E	179	GLN
59	L	12	HIS
50	s1	149	GLN
54	G	103	ASN
58	K	110	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3149 (99%)	550 (17%)	62 (1%)
1	AR	3145/3149 (99%)	548 (17%)	63 (2%)
2	3	120/121 (99%)	14 (11%)	1 (0%)
2	AS	120/121 (99%)	14 (11%)	1 (0%)
3	4	157/158 (99%)	31 (19%)	3 (1%)
3	AT	157/158 (99%)	30 (19%)	3 (1%)
48	A	1778/1800 (98%)	417 (23%)	50 (2%)
48	sR	1780/1800 (98%)	372 (20%)	0
All	All	10402/10456 (99%)	1976 (18%)	183 (1%)

5 of 1976 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	26	A
1	1	40	A
1	1	49	A
1	1	59	G
1	1	60	A

5 of 183 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AR	1238	C
1	AR	2252	A
48	A	1226	A
1	AR	1317	A
1	AR	1589	A

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2486 ligands modelled in this entry, 1 is modelled with single atom and 1410 are monoatomic - leaving 1075 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	A	1983	-	0,6,6	0.00	-	-		
84	OHX	1	3645	-	0,6,6	0.00	-	-		
84	OHX	AR	3587	-	0,6,6	0.00	-	-		
84	OHX	1	3438	-	0,6,6	0.00	-	-		
84	OHX	1	3705	84	0,6,6	0.00	-	-		
84	OHX	1	3427	-	0,6,6	0.00	-	-		
84	OHX	A	1993	-	0,6,6	0.00	-	-		
84	OHX	sR	1965	-	0,6,6	0.00	-	-		
84	OHX	AR	3476	-	0,6,6	0.00	-	-		
84	OHX	O	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3630	-	0,6,6	0.00	-	-		
84	OHX	1	3449	-	0,6,6	0.00	-	-		
84	OHX	A	1904	-	0,6,6	0.00	-	-		
84	OHX	A	1901	-	0,6,6	0.00	-	-		
84	OHX	1	3706	-	0,6,6	0.00	-	-		
84	OHX	1	3459	-	0,6,6	0.00	-	-		
84	OHX	1	3546	-	0,6,6	0.00	-	-		
84	OHX	1	3500	-	0,6,6	0.00	-	-		
84	OHX	h	401	-	0,6,6	0.00	-	-		
84	OHX	1	3547	-	0,6,6	0.00	-	-		
84	OHX	AR	3726	-	0,6,6	0.00	-	-		
84	OHX	AR	3680	-	0,6,6	0.00	-	-		
84	OHX	A	1936	-	0,6,6	0.00	-	-		
84	OHX	1	3493	-	0,6,6	0.00	-	-		
84	OHX	1	3644	-	0,6,6	0.00	-	-		
84	OHX	1	3589	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	3	204	-	0,6,6	0.00	-	-		
84	OHX	AR	3710	-	0,6,6	0.00	-	-		
84	OHX	AR	3436	-	0,6,6	0.00	-	-		
84	OHX	AR	3558	-	0,6,6	0.00	-	-		
84	OHX	1	3447	-	0,6,6	0.00	-	-		
84	OHX	1	3620	-	0,6,6	0.00	-	-		
84	OHX	A	1922	-	0,6,6	0.00	-	-		
84	OHX	1	3628	-	0,6,6	0.00	-	-		
84	OHX	AR	3691	-	0,6,6	0.00	-	-		
84	OHX	1	3601	-	0,6,6	0.00	-	-		
84	OHX	AR	3730	-	0,6,6	0.00	-	-		
84	OHX	sR	1940	-	0,6,6	0.00	-	-		
84	OHX	sR	2040	-	0,6,6	0.00	-	-		
84	OHX	1	3487	-	0,6,6	0.00	-	-		
84	OHX	1	3498	-	0,6,6	0.00	-	-		
84	OHX	AR	3741	-	0,6,6	0.00	-	-		
84	OHX	sR	1984	-	0,6,6	0.00	-	-		
84	OHX	AR	3556	-	0,6,6	0.00	-	-		
84	OHX	1	3602	-	0,6,6	0.00	-	-		
84	OHX	AR	3422	-	0,6,6	0.00	-	-		
84	OHX	1	3503	-	0,6,6	0.00	-	-		
84	OHX	1	3456	-	0,6,6	0.00	-	-		
84	OHX	CX	202	-	0,6,6	0.00	-	-		
84	OHX	AT	206	-	0,6,6	0.00	-	-		
84	OHX	3	207	-	0,6,6	0.00	-	-		
84	OHX	1	3477	-	0,6,6	0.00	-	-		
84	OHX	1	3489	-	0,6,6	0.00	-	-		
84	OHX	1	3603	-	0,6,6	0.00	-	-		
84	OHX	A	2021	-	0,6,6	0.00	-	-		
84	OHX	AR	3543	-	0,6,6	0.00	-	-		
84	OHX	1	3414	-	0,6,6	0.00	-	-		
84	OHX	A	2020	-	0,6,6	0.00	-	-		
84	OHX	1	3436	-	0,6,6	0.00	-	-		
84	OHX	1	3615	-	0,6,6	0.00	-	-		
84	OHX	1	3709	-	0,6,6	0.00	-	-		
84	OHX	1	3692	-	0,6,6	0.00	-	-		
84	OHX	sR	2002	-	0,6,6	0.00	-	-		
84	OHX	CM	201	-	0,6,6	0.00	-	-		
84	OHX	sR	1960	-	0,6,6	0.00	-	-		
84	OHX	AR	3438	-	0,6,6	0.00	-	-		
84	OHX	1	3496	-	0,6,6	0.00	-	-		
84	OHX	AR	3504	-	0,6,6	0.00	-	-		
84	OHX	1	3418	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3452	-	0,6,6	0.00	-	-		
84	OHX	1	3529	-	0,6,6	0.00	-	-		
84	OHX	AR	3732	-	0,6,6	0.00	-	-		
84	OHX	AR	3586	-	0,6,6	0.00	-	-		
84	OHX	1	3441	-	0,6,6	0.00	-	-		
84	OHX	AR	3549	-	0,6,6	0.00	-	-		
84	OHX	AR	3490	-	0,6,6	0.00	-	-		
84	OHX	A	1985	-	0,6,6	0.00	-	-		
84	OHX	sR	1955	-	0,6,6	0.00	-	-		
84	OHX	AR	3624	-	0,6,6	0.00	-	-		
84	OHX	AR	3489	-	0,6,6	0.00	-	-		
84	OHX	c3	201	-	0,6,6	0.00	-	-		
84	OHX	1	3573	-	0,6,6	0.00	-	-		
84	OHX	1	3510	-	0,6,6	0.00	-	-		
84	OHX	d4	201	-	0,6,6	0.00	-	-		
84	OHX	A	1987	-	0,6,6	0.00	-	-		
84	OHX	AR	3506	-	0,6,6	0.00	-	-		
84	OHX	1	3649	-	0,6,6	0.00	-	-		
84	OHX	1	3406	-	0,6,6	0.00	-	-		
84	OHX	1	3585	-	0,6,6	0.00	-	-		
84	OHX	1	3502	-	0,6,6	0.00	-	-		
84	OHX	AR	3581	-	0,6,6	0.00	-	-		
84	OHX	AR	3406	-	0,6,6	0.00	-	-		
84	OHX	A	1931	-	0,6,6	0.00	-	-		
84	OHX	AR	3403	-	0,6,6	0.00	-	-		
84	OHX	AR	3554	-	0,6,6	0.00	-	-		
84	OHX	A	1934	-	0,6,6	0.00	-	-		
84	OHX	A	1994	-	0,6,6	0.00	-	-		
84	OHX	A	2042	-	0,6,6	0.00	-	-		
84	OHX	AR	3513	-	0,6,6	0.00	-	-		
84	OHX	AR	3725	-	0,6,6	0.00	-	-		
86	7AL	1	4210	-	28,28,28	0.38	0	35,45,45	0.68	1 (2%)
84	OHX	A	2038	-	0,6,6	0.00	-	-		
84	OHX	1	3691	-	0,6,6	0.00	-	-		
84	OHX	AR	3706	-	0,6,6	0.00	-	-		
84	OHX	A	2032	-	0,6,6	0.00	-	-		
84	OHX	1	3650	-	0,6,6	0.00	-	-		
84	OHX	sR	2046	-	0,6,6	0.00	-	-		
84	OHX	sR	1970	-	0,6,6	0.00	-	-		
84	OHX	sR	2026	-	0,6,6	0.00	-	-		
84	OHX	AR	3417	-	0,6,6	0.00	-	-		
84	OHX	AR	3656	-	0,6,6	0.00	-	-		
84	OHX	A	1933	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1958	-	0,6,6	0.00	-	-		
84	OHX	1	3671	-	0,6,6	0.00	-	-		
84	OHX	1	3533	-	0,6,6	0.00	-	-		
84	OHX	1	3539	-	0,6,6	0.00	-	-		
84	OHX	A	1925	-	0,6,6	0.00	-	-		
84	OHX	1	3614	-	0,6,6	0.00	-	-		
84	OHX	AR	3488	-	0,6,6	0.00	-	-		
84	OHX	1	3558	-	0,6,6	0.00	-	-		
84	OHX	AR	3475	-	0,6,6	0.00	-	-		
84	OHX	AR	3548	-	0,6,6	0.00	-	-		
84	OHX	AT	205	-	0,6,6	0.00	-	-		
84	OHX	1	3636	-	0,6,6	0.00	-	-		
84	OHX	AR	3687	-	0,6,6	0.00	-	-		
84	OHX	1	3731	-	0,6,6	0.00	-	-		
84	OHX	CG	301	-	0,6,6	0.00	-	-		
84	OHX	4	211	-	0,6,6	0.00	-	-		
84	OHX	AR	3482	-	0,6,6	0.00	-	-		
84	OHX	sR	2042	-	0,6,6	0.00	-	-		
84	OHX	AR	3651	-	0,6,6	0.00	-	-		
84	OHX	AR	3605	-	0,6,6	0.00	-	-		
84	OHX	1	3504	-	0,6,6	0.00	-	-		
84	OHX	AR	3470	-	0,6,6	0.00	-	-		
84	OHX	sR	1985	-	0,6,6	0.00	-	-		
84	OHX	1	3422	-	0,6,6	0.00	-	-		
84	OHX	AR	3448	-	0,6,6	0.00	-	-		
84	OHX	AR	3493	-	0,6,6	0.00	-	-		
84	OHX	1	3566	-	0,6,6	0.00	-	-		
84	OHX	AR	3647	-	0,6,6	0.00	-	-		
84	OHX	AR	3509	-	0,6,6	0.00	-	-		
84	OHX	AR	3690	-	0,6,6	0.00	-	-		
84	OHX	1	3491	-	0,6,6	0.00	-	-		
84	OHX	v	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3451	-	0,6,6	0.00	-	-		
84	OHX	1	3506	-	0,6,6	0.00	-	-		
84	OHX	1	3658	-	0,6,6	0.00	-	-		
84	OHX	AT	211	-	0,6,6	0.00	-	-		
84	OHX	sR	2025	-	0,6,6	0.00	-	-		
84	OHX	A	1945	-	0,6,6	0.00	-	-		
84	OHX	AR	3542	-	0,6,6	0.00	-	-		
84	OHX	sR	1903	-	0,6,6	0.00	-	-		
84	OHX	AR	3519	-	0,6,6	0.00	-	-		
84	OHX	1	3647	-	0,6,6	0.00	-	-		
84	OHX	DQ	201	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1950	-	0,6,6	0.00	-	-		
84	OHX	AR	3697	-	0,6,6	0.00	-	-		
84	OHX	AS	209	-	0,6,6	0.00	-	-		
84	OHX	A	2015	-	0,6,6	0.00	-	-		
84	OHX	1	3424	-	0,6,6	0.00	-	-		
84	OHX	1	3638	-	0,6,6	0.00	-	-		
84	OHX	sR	1939	-	0,6,6	0.00	-	-		
84	OHX	AR	3574	-	0,6,6	0.00	-	-		
84	OHX	AR	3477	-	0,6,6	0.00	-	-		
84	OHX	1	3722	-	0,6,6	0.00	-	-		
84	OHX	sR	1968	-	0,6,6	0.00	-	-		
84	OHX	sR	1983	-	0,6,6	0.00	-	-		
84	OHX	AR	3430	-	0,6,6	0.00	-	-		
84	OHX	CE	402	-	0,6,6	0.00	-	-		
84	OHX	1	3440	-	0,6,6	0.00	-	-		
84	OHX	AR	3402	-	0,6,6	0.00	-	-		
84	OHX	1	3444	-	0,6,6	0.00	-	-		
84	OHX	AR	3627	-	0,6,6	0.00	-	-		
84	OHX	AR	3539	-	0,6,6	0.00	-	-		
84	OHX	AT	204	-	0,6,6	0.00	-	-		
84	OHX	1	3531	-	0,6,6	0.00	-	-		
84	OHX	AR	3456	-	0,6,6	0.00	-	-		
84	OHX	AR	3593	-	0,6,6	0.00	-	-		
84	OHX	AR	3600	-	0,6,6	0.00	-	-		
84	OHX	A	2030	-	0,6,6	0.00	-	-		
84	OHX	A	1955	-	0,6,6	0.00	-	-		
84	OHX	1	3624	-	0,6,6	0.00	-	-		
84	OHX	AR	3560	-	0,6,6	0.00	-	-		
84	OHX	AR	3469	-	0,6,6	0.00	-	-		
84	OHX	AR	3607	-	0,6,6	0.00	-	-		
84	OHX	AR	3474	-	0,6,6	0.00	-	-		
84	OHX	sR	1956	-	0,6,6	0.00	-	-		
84	OHX	AR	3502	-	0,6,6	0.00	-	-		
84	OHX	A	1969	-	0,6,6	0.00	-	-		
84	OHX	AR	3705	-	0,6,6	0.00	-	-		
84	OHX	1	3557	-	0,6,6	0.00	-	-		
84	OHX	sR	1981	-	0,6,6	0.00	-	-		
84	OHX	A	1974	-	0,6,6	0.00	-	-		
84	OHX	1	3619	-	0,6,6	0.00	-	-		
84	OHX	AR	3668	-	0,6,6	0.00	-	-		
84	OHX	A	2006	-	0,6,6	0.00	-	-		
84	OHX	1	3634	-	0,6,6	0.00	-	-		
84	OHX	1	3714	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3743	-	0,6,6	0.00	-	-		
84	OHX	1	3642	-	0,6,6	0.00	-	-		
84	OHX	1	3643	-	0,6,6	0.00	-	-		
84	OHX	1	3445	-	0,6,6	0.00	-	-		
84	OHX	sR	1963	-	0,6,6	0.00	-	-		
84	OHX	1	3659	-	0,6,6	0.00	-	-		
84	OHX	sR	1991	-	0,6,6	0.00	-	-		
84	OHX	A	1963	-	0,6,6	0.00	-	-		
84	OHX	AR	3455	-	0,6,6	0.00	-	-		
84	OHX	3	208	-	0,6,6	0.00	-	-		
84	OHX	A	1910	-	0,6,6	0.00	-	-		
84	OHX	1	3702	-	0,6,6	0.00	-	-		
84	OHX	1	3521	-	0,6,6	0.00	-	-		
84	OHX	sR	2012	-	0,6,6	0.00	-	-		
84	OHX	AR	3515	-	0,6,6	0.00	-	-		
84	OHX	1	3607	-	0,6,6	0.00	-	-		
84	OHX	A	1908	-	0,6,6	0.00	-	-		
84	OHX	sR	1973	-	0,6,6	0.00	-	-		
84	OHX	1	3556	-	0,6,6	0.00	-	-		
84	OHX	AR	3570	-	0,6,6	0.00	-	-		
84	OHX	sR	1982	-	0,6,6	0.00	-	-		
84	OHX	1	3666	-	0,6,6	0.00	-	-		
84	OHX	1	3417	-	0,6,6	0.00	-	-		
84	OHX	1	3419	-	0,6,6	0.00	-	-		
84	OHX	sR	2029	-	0,6,6	0.00	-	-		
84	OHX	AR	3584	-	0,6,6	0.00	-	-		
84	OHX	sR	1997	-	0,6,6	0.00	-	-		
84	OHX	AR	3487	-	0,6,6	0.00	-	-		
84	OHX	1	3609	-	0,6,6	0.00	-	-		
84	OHX	AR	3692	-	0,6,6	0.00	-	-		
84	OHX	A	1916	-	0,6,6	0.00	-	-		
84	OHX	1	3446	-	0,6,6	0.00	-	-		
84	OHX	AR	3625	-	0,6,6	0.00	-	-		
84	OHX	sR	1901	-	0,6,6	0.00	-	-		
84	OHX	AT	203	-	0,6,6	0.00	-	-		
84	OHX	sR	1930	-	0,6,6	0.00	-	-		
84	OHX	sR	2048	-	0,6,6	0.00	-	-		
84	OHX	1	3678	-	0,6,6	0.00	-	-		
84	OHX	sR	2021	-	0,6,6	0.00	-	-		
84	OHX	1	3411	-	0,6,6	0.00	-	-		
84	OHX	AR	3685	-	0,6,6	0.00	-	-		
84	OHX	1	3711	-	0,6,6	0.00	-	-		
84	OHX	AR	3623	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3671	-	0,6,6	0.00	-	-		
84	OHX	AR	3738	-	0,6,6	0.00	-	-		
84	OHX	1	3622	-	0,6,6	0.00	-	-		
84	OHX	AR	3678	-	0,6,6	0.00	-	-		
84	OHX	A	1928	-	0,6,6	0.00	-	-		
84	OHX	A	1918	-	0,6,6	0.00	-	-		
84	OHX	AR	3640	-	0,6,6	0.00	-	-		
84	OHX	1	3518	-	0,6,6	0.00	-	-		
84	OHX	s8	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3717	-	0,6,6	0.00	-	-		
84	OHX	AR	3650	-	0,6,6	0.00	-	-		
84	OHX	4	215	-	0,6,6	0.00	-	-		
84	OHX	sR	2019	-	0,6,6	0.00	-	-		
84	OHX	sR	2044	-	0,6,6	0.00	-	-		
84	OHX	3	203	-	0,6,6	0.00	-	-		
84	OHX	A	2031	-	0,6,6	0.00	-	-		
84	OHX	1	3707	-	0,6,6	0.00	-	-		
84	OHX	1	3693	-	0,6,6	0.00	-	-		
84	OHX	1	3429	-	0,6,6	0.00	-	-		
84	OHX	sR	2031	-	0,6,6	0.00	-	-		
84	OHX	1	3534	-	0,6,6	0.00	-	-		
84	OHX	sR	2000	-	0,6,6	0.00	-	-		
84	OHX	AR	3527	-	0,6,6	0.00	-	-		
84	OHX	AR	3446	-	0,6,6	0.00	-	-		
84	OHX	sR	1924	-	0,6,6	0.00	-	-		
84	OHX	1	3724	-	0,6,6	0.00	-	-		
84	OHX	1	3584	-	0,6,6	0.00	-	-		
84	OHX	1	3681	-	0,6,6	0.00	-	-		
84	OHX	sR	2037	-	0,6,6	0.00	-	-		
84	OHX	1	3468	-	0,6,6	0.00	-	-		
84	OHX	A	1926	-	0,6,6	0.00	-	-		
84	OHX	AR	3592	-	0,6,6	0.00	-	-		
84	OHX	AR	3562	-	0,6,6	0.00	-	-		
84	OHX	x	202	-	0,6,6	0.00	-	-		
84	OHX	AR	3708	-	0,6,6	0.00	-	-		
84	OHX	1	3604	-	0,6,6	0.00	-	-		
84	OHX	AT	208	-	0,6,6	0.00	-	-		
84	OHX	A	1956	-	0,6,6	0.00	-	-		
84	OHX	1	3530	-	0,6,6	0.00	-	-		
84	OHX	1	3434	-	0,6,6	0.00	-	-		
84	OHX	1	3431	-	0,6,6	0.00	-	-		
84	OHX	AR	3525	-	0,6,6	0.00	-	-		
84	OHX	1	3616	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	2019	-	0,6,6	0.00	-	-		
84	OHX	AR	3672	-	0,6,6	0.00	-	-		
84	OHX	x	201	-	0,6,6	0.00	-	-		
84	OHX	AT	216	-	0,6,6	0.00	-	-		
84	OHX	A	2022	-	0,6,6	0.00	-	-		
84	OHX	4	201	-	0,6,6	0.00	-	-		
84	OHX	A	1978	-	0,6,6	0.00	-	-		
84	OHX	AR	3480	-	0,6,6	0.00	-	-		
84	OHX	AR	3521	-	0,6,6	0.00	-	-		
84	OHX	AR	3485	-	0,6,6	0.00	-	-		
84	OHX	A	1988	-	0,6,6	0.00	-	-		
84	OHX	A	1919	-	0,6,6	0.00	-	-		
84	OHX	sR	1962	-	0,6,6	0.00	-	-		
84	OHX	AR	3551	-	0,6,6	0.00	-	-		
84	OHX	A	1902	-	0,6,6	0.00	-	-		
84	OHX	AR	3628	-	0,6,6	0.00	-	-		
84	OHX	AR	3435	-	0,6,6	0.00	-	-		
84	OHX	AR	3411	-	0,6,6	0.00	-	-		
84	OHX	1	3717	-	0,6,6	0.00	-	-		
84	OHX	A	1976	-	0,6,6	0.00	-	-		
84	OHX	1	3652	-	0,6,6	0.00	-	-		
84	OHX	sR	1994	-	0,6,6	0.00	-	-		
84	OHX	sR	1957	-	0,6,6	0.00	-	-		
84	OHX	1	3527	-	0,6,6	0.00	-	-		
84	OHX	1	3698	-	0,6,6	0.00	-	-		
84	OHX	1	3723	-	0,6,6	0.00	-	-		
84	OHX	sR	2028	-	0,6,6	0.00	-	-		
84	OHX	1	3687	-	0,6,6	0.00	-	-		
84	OHX	AR	3416	-	0,6,6	0.00	-	-		
84	OHX	AR	3679	-	0,6,6	0.00	-	-		
84	OHX	sR	1980	-	0,6,6	0.00	-	-		
84	OHX	1	3490	-	0,6,6	0.00	-	-		
84	OHX	1	3472	-	0,6,6	0.00	-	-		
84	OHX	AR	3491	-	0,6,6	0.00	-	-		
84	OHX	A	1930	-	0,6,6	0.00	-	-		
84	OHX	AR	3563	-	0,6,6	0.00	-	-		
84	OHX	1	3592	-	0,6,6	0.00	-	-		
84	OHX	1	3721	-	0,6,6	0.00	-	-		
84	OHX	1	3720	-	0,6,6	0.00	-	-		
84	OHX	1	3689	-	0,6,6	0.00	-	-		
84	OHX	sR	2039	-	0,6,6	0.00	-	-		
84	OHX	AR	3606	-	0,6,6	0.00	-	-		
84	OHX	AR	3580	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	sR	1954	-	0,6,6	0.00	-	-		
84	OHX	AR	3405	-	0,6,6	0.00	-	-		
84	OHX	CF	402	-	0,6,6	0.00	-	-		
84	OHX	1	3669	-	0,6,6	0.00	-	-		
84	OHX	1	3480	-	0,6,6	0.00	-	-		
84	OHX	1	3648	-	0,6,6	0.00	-	-		
84	OHX	1	3660	-	0,6,6	0.00	-	-		
84	OHX	AR	3572	-	0,6,6	0.00	-	-		
84	OHX	AR	3505	-	0,6,6	0.00	-	-		
84	OHX	AR	3520	-	0,6,6	0.00	-	-		
84	OHX	1	3495	-	0,6,6	0.00	-	-		
84	OHX	1	3588	-	0,6,6	0.00	-	-		
84	OHX	1	3475	-	0,6,6	0.00	-	-		
84	OHX	CL	302	-	0,6,6	0.00	-	-		
84	OHX	A	2002	-	0,6,6	0.00	-	-		
84	OHX	A	1980	-	0,6,6	0.00	-	-		
84	OHX	AR	3616	-	0,6,6	0.00	-	-		
84	OHX	sR	1975	-	0,6,6	0.00	-	-		
84	OHX	sR	2045	-	0,6,6	0.00	-	-		
84	OHX	AR	3582	-	0,6,6	0.00	-	-		
84	OHX	AR	3457	-	0,6,6	0.00	-	-		
86	7AL	AR	4246	-	28,28,28	0.37	0	35,45,45	0.36	0
84	OHX	A	2033	-	0,6,6	0.00	-	-		
84	OHX	1	3464	-	0,6,6	0.00	-	-		
84	OHX	1	3483	-	0,6,6	0.00	-	-		
84	OHX	1	3581	-	0,6,6	0.00	-	-		
84	OHX	1	3416	-	0,6,6	0.00	-	-		
84	OHX	1	3486	-	0,6,6	0.00	-	-		
84	OHX	AR	3718	-	0,6,6	0.00	-	-		
84	OHX	1	3651	-	0,6,6	0.00	-	-		
84	OHX	AR	3589	-	0,6,6	0.00	-	-		
84	OHX	AR	3742	-	0,6,6	0.00	-	-		
84	OHX	1	3608	-	0,6,6	0.00	-	-		
84	OHX	AR	3569	-	0,6,6	0.00	-	-		
84	OHX	AR	3466	-	0,6,6	0.00	-	-		
84	OHX	1	3471	-	0,6,6	0.00	-	-		
84	OHX	AR	3429	-	0,6,6	0.00	-	-		
84	OHX	1	3515	-	0,6,6	0.00	-	-		
84	OHX	1	3525	-	0,6,6	0.00	-	-		
84	OHX	sR	2024	-	0,6,6	0.00	-	-		
84	OHX	AR	3734	-	0,6,6	0.00	-	-		
84	OHX	1	3586	-	0,6,6	0.00	-	-		
84	OHX	A	1913	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3557	-	0,6,6	0.00	-	-		
84	OHX	A	1998	48	0,6,6	0.00	-	-		
84	OHX	AR	3688	-	0,6,6	0.00	-	-		
84	OHX	sR	1935	-	0,6,6	0.00	-	-		
84	OHX	c5	201	-	0,6,6	0.00	-	-		
84	OHX	sR	2043	-	0,6,6	0.00	-	-		
84	OHX	AR	3443	-	0,6,6	0.00	-	-		
84	OHX	3	202	-	0,6,6	0.00	-	-		
84	OHX	A	2040	-	0,6,6	0.00	-	-		
84	OHX	AR	3673	-	0,6,6	0.00	-	-		
84	OHX	AR	3409	-	0,6,6	0.00	-	-		
84	OHX	A	1921	-	0,6,6	0.00	-	-		
84	OHX	sR	2005	-	0,6,6	0.00	-	-		
84	OHX	1	3465	-	0,6,6	0.00	-	-		
84	OHX	AR	3613	-	0,6,6	0.00	-	-		
84	OHX	4	209	-	0,6,6	0.00	-	-		
84	OHX	AR	3496	-	0,6,6	0.00	-	-		
84	OHX	CX	201	-	0,6,6	0.00	-	-		
84	OHX	A	1920	-	0,6,6	0.00	-	-		
84	OHX	A	1903	-	0,6,6	0.00	-	-		
84	OHX	1	3403	-	0,6,6	0.00	-	-		
84	OHX	sR	1925	-	0,6,6	0.00	-	-		
84	OHX	AR	3615	-	0,6,6	0.00	-	-		
84	OHX	AR	3514	-	0,6,6	0.00	-	-		
84	OHX	1	3467	-	0,6,6	0.00	-	-		
84	OHX	A	1986	-	0,6,6	0.00	-	-		
84	OHX	A	2010	-	0,6,6	0.00	-	-		
84	OHX	AR	3686	-	0,6,6	0.00	-	-		
84	OHX	sR	1904	-	0,6,6	0.00	-	-		
84	OHX	sR	1999	-	0,6,6	0.00	-	-		
84	OHX	AR	3571	-	0,6,6	0.00	-	-		
84	OHX	AR	3652	-	0,6,6	0.00	-	-		
84	OHX	AR	3675	-	0,6,6	0.00	-	-		
84	OHX	A	2024	-	0,6,6	0.00	-	-		
84	OHX	4	203	-	0,6,6	0.00	-	-		
84	OHX	sR	1978	-	0,6,6	0.00	-	-		
84	OHX	1	3686	-	0,6,6	0.00	-	-		
84	OHX	sR	1907	-	0,6,6	0.00	-	-		
84	OHX	AS	208	-	0,6,6	0.00	-	-		
84	OHX	AR	3703	84	0,6,6	0.00	-	-		
84	OHX	1	3599	-	0,6,6	0.00	-	-		
84	OHX	AR	3626	-	0,6,6	0.00	-	-		
84	OHX	A	1992	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3623	-	0,6,6	0.00	-	-		
84	OHX	e	101	-	0,6,6	0.00	-	-		
84	OHX	1	3564	-	0,6,6	0.00	-	-		
84	OHX	1	3420	-	0,6,6	0.00	-	-		
84	OHX	1	3404	-	0,6,6	0.00	-	-		
84	OHX	sR	1986	-	0,6,6	0.00	-	-		
84	OHX	sR	2033	-	0,6,6	0.00	-	-		
84	OHX	A	2025	-	0,6,6	0.00	-	-		
84	OHX	1	3492	-	0,6,6	0.00	-	-		
84	OHX	sR	1944	-	0,6,6	0.00	-	-		
84	OHX	AR	3664	-	0,6,6	0.00	-	-		
84	OHX	AR	3609	-	0,6,6	0.00	-	-		
84	OHX	AR	3479	-	0,6,6	0.00	-	-		
84	OHX	T	201	-	0,6,6	0.00	-	-		
84	OHX	sR	1908	-	0,6,6	0.00	-	-		
84	OHX	1	3591	-	0,6,6	0.00	-	-		
84	OHX	AR	3414	-	0,6,6	0.00	-	-		
84	OHX	AR	3428	-	0,6,6	0.00	-	-		
84	OHX	sR	1953	-	0,6,6	0.00	-	-		
84	OHX	AR	3500	-	0,6,6	0.00	-	-		
84	OHX	AR	3677	-	0,6,6	0.00	-	-		
84	OHX	1	3461	-	0,6,6	0.00	-	-		
84	OHX	sR	2015	-	0,6,6	0.00	-	-		
84	OHX	AR	3541	-	0,6,6	0.00	-	-		
84	OHX	A	2007	-	0,6,6	0.00	-	-		
84	OHX	1	3540	84	0,6,6	0.00	-	-		
84	OHX	1	3672	-	0,6,6	0.00	-	-		
84	OHX	1	3526	-	0,6,6	0.00	-	-		
84	OHX	1	3631	-	0,6,6	0.00	-	-		
84	OHX	AR	3603	-	0,6,6	0.00	-	-		
84	OHX	1	3683	-	0,6,6	0.00	-	-		
84	OHX	AR	3632	-	0,6,6	0.00	-	-		
84	OHX	AR	3659	-	0,6,6	0.00	-	-		
84	OHX	AR	3585	-	0,6,6	0.00	-	-		
84	OHX	sR	2008	-	0,6,6	0.00	-	-		
84	OHX	AS	202	-	0,6,6	0.00	-	-		
84	OHX	1	3715	-	0,6,6	0.00	-	-		
84	OHX	A	2026	-	0,6,6	0.00	-	-		
84	OHX	1	3675	-	0,6,6	0.00	-	-		
84	OHX	AR	3468	-	0,6,6	0.00	-	-		
84	OHX	1	3725	-	0,6,6	0.00	-	-		
84	OHX	1	3443	-	0,6,6	0.00	-	-		
84	OHX	1	3679	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3611	-	0,6,6	0.00	-	-		
84	OHX	sR	2013	-	0,6,6	0.00	-	-		
84	OHX	AR	3649	-	0,6,6	0.00	-	-		
84	OHX	1	3598	-	0,6,6	0.00	-	-		
84	OHX	A	1935	-	0,6,6	0.00	-	-		
84	OHX	1	3621	-	0,6,6	0.00	-	-		
84	OHX	AR	3674	-	0,6,6	0.00	-	-		
84	OHX	AS	210	-	0,6,6	0.00	-	-		
84	OHX	A	1941	-	0,6,6	0.00	-	-		
84	OHX	Q	201	-	0,6,6	0.00	-	-		
84	OHX	1	3653	-	0,6,6	0.00	-	-		
84	OHX	sR	1996	-	0,6,6	0.00	-	-		
84	OHX	1	3505	-	0,6,6	0.00	-	-		
84	OHX	AR	3526	-	0,6,6	0.00	-	-		
84	OHX	AR	3667	-	0,6,6	0.00	-	-		
84	OHX	AS	204	-	0,6,6	0.00	-	-		
84	OHX	AR	3552	-	0,6,6	0.00	-	-		
84	OHX	v	302	-	0,6,6	0.00	-	-		
84	OHX	sR	2007	-	0,6,6	0.00	-	-		
84	OHX	sR	1920	-	0,6,6	0.00	-	-		
84	OHX	sR	1946	-	0,6,6	0.00	-	-		
84	OHX	1	3680	-	0,6,6	0.00	-	-		
84	OHX	1	3519	-	0,6,6	0.00	-	-		
84	OHX	1	3655	-	0,6,6	0.00	-	-		
84	OHX	1	3513	-	0,6,6	0.00	-	-		
84	OHX	sR	2049	-	0,6,6	0.00	-	-		
84	OHX	A	1917	-	0,6,6	0.00	-	-		
84	OHX	1	3451	-	0,6,6	0.00	-	-		
84	OHX	1	3629	-	0,6,6	0.00	-	-		
84	OHX	sR	1951	-	0,6,6	0.00	-	-		
84	OHX	AR	3465	-	0,6,6	0.00	-	-		
84	OHX	AR	3660	-	0,6,6	0.00	-	-		
84	OHX	sR	1937	-	0,6,6	0.00	-	-		
84	OHX	z	201	-	0,6,6	0.00	-	-		
84	OHX	1	3432	-	0,6,6	0.00	-	-		
84	OHX	sR	2050	-	0,6,6	0.00	-	-		
84	OHX	1	3514	-	0,6,6	0.00	-	-		
84	OHX	AR	3739	-	0,6,6	0.00	-	-		
84	OHX	sR	1947	-	0,6,6	0.00	-	-		
84	OHX	AR	3698	-	0,6,6	0.00	-	-		
84	OHX	r	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3720	-	0,6,6	0.00	-	-		
84	OHX	AR	3669	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1927	-	0,6,6	0.00	-	-		
84	OHX	4	202	-	0,6,6	0.00	-	-		
84	OHX	AR	3704	-	0,6,6	0.00	-	-		
84	OHX	AR	3683	-	0,6,6	0.00	-	-		
84	OHX	A	2037	-	0,6,6	0.00	-	-		
84	OHX	AR	3617	-	0,6,6	0.00	-	-		
84	OHX	AR	3531	-	0,6,6	0.00	-	-		
84	OHX	AR	3736	-	0,6,6	0.00	-	-		
84	OHX	AR	3415	-	0,6,6	0.00	-	-		
84	OHX	A	2041	-	0,6,6	0.00	-	-		
84	OHX	1	3448	-	0,6,6	0.00	-	-		
84	OHX	AR	3631	-	0,6,6	0.00	-	-		
84	OHX	sR	1931	-	0,6,6	0.00	-	-		
84	OHX	AR	3681	-	0,6,6	0.00	-	-		
84	OHX	AR	3629	-	0,6,6	0.00	-	-		
84	OHX	1	3703	-	0,6,6	0.00	-	-		
84	OHX	AR	3716	-	0,6,6	0.00	-	-		
84	OHX	sR	1989	-	0,6,6	0.00	-	-		
84	OHX	A	2009	-	0,6,6	0.00	-	-		
84	OHX	A	1966	-	0,6,6	0.00	-	-		
84	OHX	AR	3467	-	0,6,6	0.00	-	-		
84	OHX	A	1909	-	0,6,6	0.00	-	-		
84	OHX	3	205	-	0,6,6	0.00	-	-		
84	OHX	sR	1915	-	0,6,6	0.00	-	-		
84	OHX	A	1915	-	0,6,6	0.00	-	-		
84	OHX	1	3524	-	0,6,6	0.00	-	-		
84	OHX	AR	3534	-	0,6,6	0.00	-	-		
84	OHX	1	3469	-	0,6,6	0.00	-	-		
84	OHX	1	3606	-	0,6,6	0.00	-	-		
84	OHX	A	1937	-	0,6,6	0.00	-	-		
84	OHX	1	3415	-	0,6,6	0.00	-	-		
84	OHX	sR	1990	-	0,6,6	0.00	-	-		
84	OHX	1	3479	-	0,6,6	0.00	-	-		
84	OHX	A	1947	-	0,6,6	0.00	-	-		
84	OHX	AR	3431	-	0,6,6	0.00	-	-		
84	OHX	AR	3594	-	0,6,6	0.00	-	-		
84	OHX	A	1911	-	0,6,6	0.00	-	-		
84	OHX	1	3641	-	0,6,6	0.00	-	-		
84	OHX	AS	211	-	0,6,6	0.00	-	-		
84	OHX	A	1995	-	0,6,6	0.00	-	-		
84	OHX	sR	2047	-	0,6,6	0.00	-	-		
84	OHX	1	3562	-	0,6,6	0.00	-	-		
84	OHX	1	3730	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AK	102	-	0,6,6	0.00	-	-		
84	OHX	sR	1992	-	0,6,6	0.00	-	-		
84	OHX	A	1964	-	0,6,6	0.00	-	-		
84	OHX	AR	3578	-	0,6,6	0.00	-	-		
84	OHX	A	2018	-	0,6,6	0.00	-	-		
84	OHX	1	3553	-	0,6,6	0.00	-	-		
84	OHX	A	1939	-	0,6,6	0.00	-	-		
84	OHX	AR	3432	-	0,6,6	0.00	-	-		
84	OHX	AR	3715	-	0,6,6	0.00	-	-		
84	OHX	1	3538	-	0,6,6	0.00	-	-		
84	OHX	sR	2051	-	0,6,6	0.00	-	-		
84	OHX	1	3523	-	0,6,6	0.00	-	-		
84	OHX	1	3632	-	0,6,6	0.00	-	-		
84	OHX	AR	3481	84	0,6,6	0.00	-	-		
84	OHX	sR	1941	-	0,6,6	0.00	-	-		
84	OHX	AR	3433	-	0,6,6	0.00	-	-		
84	OHX	AR	3658	-	0,6,6	0.00	-	-		
84	OHX	1	3537	-	0,6,6	0.00	-	-		
84	OHX	1	3667	-	0,6,6	0.00	-	-		
84	OHX	1	3637	-	0,6,6	0.00	-	-		
84	OHX	H	301	-	0,6,6	0.00	-	-		
84	OHX	AT	212	84	0,6,6	0.00	-	-		
84	OHX	A	2039	-	0,6,6	0.00	-	-		
84	OHX	AR	3425	-	0,6,6	0.00	-	-		
84	OHX	AR	3684	-	0,6,6	0.00	-	-		
84	OHX	AR	3724	-	0,6,6	0.00	-	-		
84	OHX	AR	3483	-	0,6,6	0.00	-	-		
84	OHX	AR	3410	-	0,6,6	0.00	-	-		
84	OHX	A	1912	-	0,6,6	0.00	-	-		
84	OHX	1	3719	-	0,6,6	0.00	-	-		
84	OHX	sR	1910	-	0,6,6	0.00	-	-		
84	OHX	1	3712	-	0,6,6	0.00	-	-		
84	OHX	AR	3641	-	0,6,6	0.00	-	-		
84	OHX	AS	207	-	0,6,6	0.00	-	-		
84	OHX	1	3590	-	0,6,6	0.00	-	-		
84	OHX	AR	3622	-	0,6,6	0.00	-	-		
84	OHX	A	1997	-	0,6,6	0.00	-	-		
84	OHX	A	2028	-	0,6,6	0.00	-	-		
84	OHX	AR	3540	-	0,6,6	0.00	-	-		
84	OHX	AR	3655	-	0,6,6	0.00	-	-		
84	OHX	AR	3419	-	0,6,6	0.00	-	-		
84	OHX	AR	3676	-	0,6,6	0.00	-	-		
84	OHX	1	3462	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3702	-	0,6,6	0.00	-	-		
84	OHX	1	3611	-	0,6,6	0.00	-	-		
84	OHX	AR	3566	-	0,6,6	0.00	-	-		
84	OHX	1	3454	-	0,6,6	0.00	-	-		
84	OHX	1	3576	-	0,6,6	0.00	-	-		
84	OHX	AR	3637	-	0,6,6	0.00	-	-		
84	OHX	4	212	-	0,6,6	0.00	-	-		
84	OHX	1	3565	-	0,6,6	0.00	-	-		
84	OHX	A	1971	-	0,6,6	0.00	-	-		
84	OHX	4	208	-	0,6,6	0.00	-	-		
84	OHX	1	3688	-	0,6,6	0.00	-	-		
84	OHX	AR	3700	-	0,6,6	0.00	-	-		
84	OHX	1	3593	-	0,6,6	0.00	-	-		
84	OHX	AR	3619	-	0,6,6	0.00	-	-		
84	OHX	1	3701	-	0,6,6	0.00	-	-		
84	OHX	1	3450	-	0,6,6	0.00	-	-		
84	OHX	AR	3714	-	0,6,6	0.00	-	-		
84	OHX	AR	3727	-	0,6,6	0.00	-	-		
84	OHX	1	3549	-	0,6,6	0.00	-	-		
84	OHX	A	1961	-	0,6,6	0.00	-	-		
84	OHX	sR	1972	-	0,6,6	0.00	-	-		
84	OHX	1	3460	-	0,6,6	0.00	-	-		
84	OHX	sR	1977	-	0,6,6	0.00	-	-		
84	OHX	A	2036	-	0,6,6	0.00	-	-		
84	OHX	1	3704	-	0,6,6	0.00	-	-		
84	OHX	AR	3731	-	0,6,6	0.00	-	-		
84	OHX	sR	1969	-	0,6,6	0.00	-	-		
84	OHX	1	3661	-	0,6,6	0.00	-	-		
84	OHX	AR	3598	-	0,6,6	0.00	-	-		
84	OHX	sR	2038	-	0,6,6	0.00	-	-		
84	OHX	AR	3595	-	0,6,6	0.00	-	-		
84	OHX	1	3517	-	0,6,6	0.00	-	-		
84	OHX	1	3499	-	0,6,6	0.00	-	-		
84	OHX	AR	3709	-	0,6,6	0.00	-	-		
84	OHX	A	1981	-	0,6,6	0.00	-	-		
84	OHX	sR	1909	-	0,6,6	0.00	-	-		
84	OHX	1	3428	-	0,6,6	0.00	-	-		
84	OHX	1	3664	-	0,6,6	0.00	-	-		
84	OHX	sR	2036	-	0,6,6	0.00	-	-		
84	OHX	1	3555	-	0,6,6	0.00	-	-		
84	OHX	AR	3666	-	0,6,6	0.00	-	-		
84	OHX	AR	3404	-	0,6,6	0.00	-	-		
84	OHX	1	3405	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3746	-	0,6,6	0.00	-	-		
84	OHX	sR	1967	-	0,6,6	0.00	-	-		
84	OHX	sR	1932	-	0,6,6	0.00	-	-		
84	OHX	1	3674	-	0,6,6	0.00	-	-		
84	OHX	sR	1988	-	0,6,6	0.00	-	-		
84	OHX	sR	1902	-	0,6,6	0.00	-	-		
84	OHX	AR	3565	-	0,6,6	0.00	-	-		
84	OHX	A	1989	-	0,6,6	0.00	-	-		
84	OHX	AR	3546	-	0,6,6	0.00	-	-		
84	OHX	1	3696	-	0,6,6	0.00	-	-		
84	OHX	CV	201	-	0,6,6	0.00	-	-		
84	OHX	sR	1950	-	0,6,6	0.00	-	-		
84	OHX	1	3577	-	0,6,6	0.00	-	-		
84	OHX	1	3618	-	0,6,6	0.00	-	-		
84	OHX	AR	3661	-	0,6,6	0.00	-	-		
84	OHX	1	3663	-	0,6,6	0.00	-	-		
84	OHX	AR	3427	-	0,6,6	0.00	-	-		
84	OHX	AR	3682	-	0,6,6	0.00	-	-		
84	OHX	A	1932	-	0,6,6	0.00	-	-		
84	OHX	A	1951	-	0,6,6	0.00	-	-		
84	OHX	sR	1995	-	0,6,6	0.00	-	-		
84	OHX	AR	3529	84	0,6,6	0.00	-	-		
84	OHX	1	3474	-	0,6,6	0.00	-	-		
84	OHX	1	3435	-	0,6,6	0.00	-	-		
84	OHX	AR	3499	-	0,6,6	0.00	-	-		
84	OHX	sR	2034	-	0,6,6	0.00	-	-		
84	OHX	sR	2052	-	0,6,6	0.00	-	-		
84	OHX	AR	3612	-	0,6,6	0.00	-	-		
84	OHX	1	3630	-	0,6,6	0.00	-	-		
84	OHX	1	3567	-	0,6,6	0.00	-	-		
84	OHX	1	3716	-	0,6,6	0.00	-	-		
84	OHX	1	3494	-	0,6,6	0.00	-	-		
84	OHX	4	213	-	0,6,6	0.00	-	-		
84	OHX	1	3673	-	0,6,6	0.00	-	-		
84	OHX	AR	3463	-	0,6,6	0.00	-	-		
84	OHX	AR	3723	-	0,6,6	0.00	-	-		
84	OHX	AR	3665	-	0,6,6	0.00	-	-		
84	OHX	AR	3590	-	0,6,6	0.00	-	-		
84	OHX	A	2005	-	0,6,6	0.00	-	-		
84	OHX	AT	202	84	0,6,6	0.00	-	-		
84	OHX	1	3662	-	0,6,6	0.00	-	-		
84	OHX	sR	2027	-	0,6,6	0.00	-	-		
84	OHX	A	1959	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3727	-	0,6,6	0.00	-	-		
84	OHX	AR	3464	-	0,6,6	0.00	-	-		
84	OHX	AR	3596	-	0,6,6	0.00	-	-		
84	OHX	AR	3573	-	0,6,6	0.00	-	-		
84	OHX	1	3568	-	0,6,6	0.00	-	-		
84	OHX	A	2003	-	0,6,6	0.00	-	-		
84	OHX	AR	3614	-	0,6,6	0.00	-	-		
84	OHX	AR	3440	-	0,6,6	0.00	-	-		
84	OHX	1	3635	-	0,6,6	0.00	-	-		
84	OHX	A	1957	-	0,6,6	0.00	-	-		
84	OHX	A	1943	-	0,6,6	0.00	-	-		
84	OHX	1	3481	-	0,6,6	0.00	-	-		
84	OHX	1	3509	-	0,6,6	0.00	-	-		
84	OHX	AR	3421	-	0,6,6	0.00	-	-		
84	OHX	AT	215	-	0,6,6	0.00	-	-		
84	OHX	1	3600	-	0,6,6	0.00	-	-		
84	OHX	Rb	401	-	0,6,6	0.00	-	-		
84	OHX	AR	3642	-	0,6,6	0.00	-	-		
84	OHX	A	2029	-	0,6,6	0.00	-	-		
84	OHX	AP	502	-	0,6,6	0.00	-	-		
84	OHX	1	3507	-	0,6,6	0.00	-	-		
84	OHX	DD	102	-	0,6,6	0.00	-	-		
84	OHX	sR	1976	-	0,6,6	0.00	-	-		
84	OHX	sR	1979	-	0,6,6	0.00	-	-		
84	OHX	1	3457	-	0,6,6	0.00	-	-		
84	OHX	AK	103	-	0,6,6	0.00	-	-		
84	OHX	AR	3699	-	0,6,6	0.00	-	-		
84	OHX	1	3488	-	0,6,6	0.00	-	-		
84	OHX	1	3626	-	0,6,6	0.00	-	-		
84	OHX	sR	1916	-	0,6,6	0.00	-	-		
84	OHX	A	2035	-	0,6,6	0.00	-	-		
84	OHX	4	205	-	0,6,6	0.00	-	-		
84	OHX	1	3430	-	0,6,6	0.00	-	-		
84	OHX	A	1944	-	0,6,6	0.00	-	-		
84	OHX	1	3437	-	0,6,6	0.00	-	-		
84	OHX	AR	3670	-	0,6,6	0.00	-	-		
84	OHX	AR	3576	-	0,6,6	0.00	-	-		
84	OHX	A	1970	-	0,6,6	0.00	-	-		
84	OHX	AR	3454	-	0,6,6	0.00	-	-		
84	OHX	1	3657	-	0,6,6	0.00	-	-		
84	OHX	A	1929	-	0,6,6	0.00	-	-		
84	OHX	AT	207	-	0,6,6	0.00	-	-		
84	OHX	1	3710	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3466	-	0,6,6	0.00	-	-		
84	OHX	A	2017	-	0,6,6	0.00	-	-		
84	OHX	AR	3461	-	0,6,6	0.00	-	-		
84	OHX	AR	3657	-	0,6,6	0.00	-	-		
84	OHX	AR	3472	-	0,6,6	0.00	-	-		
84	OHX	A	1973	-	0,6,6	0.00	-	-		
84	OHX	1	3482	-	0,6,6	0.00	-	-		
84	OHX	1	3612	-	0,6,6	0.00	-	-		
84	OHX	AR	3547	-	0,6,6	0.00	-	-		
84	OHX	1	3594	-	0,6,6	0.00	-	-		
84	OHX	AR	3722	-	0,6,6	0.00	-	-		
84	OHX	A	1982	-	0,6,6	0.00	-	-		
84	OHX	4	207	-	0,6,6	0.00	-	-		
84	OHX	A	2023	-	0,6,6	0.00	-	-		
84	OHX	AR	3745	-	0,6,6	0.00	-	-		
84	OHX	1	3640	-	0,6,6	0.00	-	-		
84	OHX	1	3516	-	0,6,6	0.00	-	-		
84	OHX	CO	201	-	0,6,6	0.00	-	-		
84	OHX	sR	1943	-	0,6,6	0.00	-	-		
84	OHX	AR	3733	-	0,6,6	0.00	-	-		
84	OHX	1	3541	-	0,6,6	0.00	-	-		
84	OHX	sR	1993	-	0,6,6	0.00	-	-		
84	OHX	sR	1938	-	0,6,6	0.00	-	-		
84	OHX	sR	1919	-	0,6,6	0.00	-	-		
84	OHX	1	3551	-	0,6,6	0.00	-	-		
84	OHX	AR	3460	-	0,6,6	0.00	-	-		
84	OHX	AR	3511	-	0,6,6	0.00	-	-		
84	OHX	1	3485	-	0,6,6	0.00	-	-		
84	OHX	1	3560	-	0,6,6	0.00	-	-		
84	OHX	1	3408	-	0,6,6	0.00	-	-		
84	OHX	1	3544	-	0,6,6	0.00	-	-		
84	OHX	s4	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3728	-	0,6,6	0.00	-	-		
84	OHX	1	3625	-	0,6,6	0.00	-	-		
84	OHX	1	3708	-	0,6,6	0.00	-	-		
84	OHX	AR	3424	-	0,6,6	0.00	-	-		
84	OHX	1	3685	-	0,6,6	0.00	-	-		
84	OHX	sR	2041	-	0,6,6	0.00	-	-		
84	OHX	AR	3437	-	0,6,6	0.00	-	-		
84	OHX	AR	3413	-	0,6,6	0.00	-	-		
84	OHX	J	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3634	-	0,6,6	0.00	-	-		
84	OHX	1	3442	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3426	-	0,6,6	0.00	-	-		
84	OHX	sR	2009	-	0,6,6	0.00	-	-		
84	OHX	M	201	-	0,6,6	0.00	-	-		
84	OHX	A	1905	-	0,6,6	0.00	-	-		
84	OHX	AR	3471	-	0,6,6	0.00	-	-		
84	OHX	AR	3524	-	0,6,6	0.00	-	-		
84	OHX	y	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3694	-	0,6,6	0.00	-	-		
84	OHX	sR	1952	-	0,6,6	0.00	-	-		
84	OHX	1	3670	-	0,6,6	0.00	-	-		
84	OHX	AS	205	-	0,6,6	0.00	-	-		
84	OHX	AS	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3662	-	0,6,6	0.00	-	-		
84	OHX	A	1967	-	0,6,6	0.00	-	-		
84	OHX	AR	3646	-	0,6,6	0.00	-	-		
84	OHX	A	2014	-	0,6,6	0.00	-	-		
84	OHX	sR	1998	-	0,6,6	0.00	-	-		
84	OHX	CG	303	-	0,6,6	0.00	-	-		
84	OHX	1	3578	-	0,6,6	0.00	-	-		
84	OHX	AR	3654	-	0,6,6	0.00	-	-		
84	OHX	AR	3439	-	0,6,6	0.00	-	-		
84	OHX	A	2004	-	0,6,6	0.00	-	-		
84	OHX	AR	3407	-	0,6,6	0.00	-	-		
84	OHX	1	3484	-	0,6,6	0.00	-	-		
84	OHX	1	3690	-	0,6,6	0.00	-	-		
84	OHX	1	3455	-	0,6,6	0.00	-	-		
84	OHX	AR	3523	-	0,6,6	0.00	-	-		
84	OHX	AR	3530	-	0,6,6	0.00	-	-		
84	OHX	1	3522	-	0,6,6	0.00	-	-		
84	OHX	sR	1945	-	0,6,6	0.00	-	-		
84	OHX	sR	1918	-	0,6,6	0.00	-	-		
84	OHX	AR	3693	-	0,6,6	0.00	-	-		
84	OHX	AR	3740	-	0,6,6	0.00	-	-		
84	OHX	1	3410	-	0,6,6	0.00	-	-		
84	OHX	1	3478	-	0,6,6	0.00	-	-		
84	OHX	4	204	-	0,6,6	0.00	-	-		
84	OHX	AR	3533	-	0,6,6	0.00	-	-		
84	OHX	A	2013	-	0,6,6	0.00	-	-		
84	OHX	AR	3507	-	0,6,6	0.00	-	-		
84	OHX	1	3402	-	0,6,6	0.00	-	-		
84	OHX	1	3453	-	0,6,6	0.00	-	-		
84	OHX	1	3697	-	0,6,6	0.00	-	-		
84	OHX	AR	3695	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3537	-	0,6,6	0.00	-	-		
84	OHX	AR	3452	-	0,6,6	0.00	-	-		
84	OHX	AR	3561	-	0,6,6	0.00	-	-		
84	OHX	1	3579	-	0,6,6	0.00	-	-		
84	OHX	AR	3478	-	0,6,6	0.00	-	-		
84	OHX	AR	3445	-	0,6,6	0.00	-	-		
84	OHX	A	1979	-	0,6,6	0.00	-	-		
84	OHX	1	3570	-	0,6,6	0.00	-	-		
84	OHX	1	3548	-	0,6,6	0.00	-	-		
84	OHX	AR	3553	-	0,6,6	0.00	-	-		
84	OHX	sR	1949	-	0,6,6	0.00	-	-		
84	OHX	1	3501	-	0,6,6	0.00	-	-		
84	OHX	AR	3567	-	0,6,6	0.00	-	-		
84	OHX	AR	3633	-	0,6,6	0.00	-	-		
84	OHX	sR	2018	-	0,6,6	0.00	-	-		
84	OHX	AR	3545	-	0,6,6	0.00	-	-		
84	OHX	AR	3447	-	0,6,6	0.00	-	-		
84	OHX	AR	3532	-	0,6,6	0.00	-	-		
84	OHX	1	3677	-	0,6,6	0.00	-	-		
84	OHX	1	3726	-	0,6,6	0.00	-	-		
84	OHX	A	2000	-	0,6,6	0.00	-	-		
84	OHX	AR	3719	-	0,6,6	0.00	-	-		
84	OHX	A	2001	-	0,6,6	0.00	-	-		
84	OHX	sR	2003	-	0,6,6	0.00	-	-		
84	OHX	1	3554	-	0,6,6	0.00	-	-		
84	OHX	1	3476	-	0,6,6	0.00	-	-		
84	OHX	4	206	-	0,6,6	0.00	-	-		
84	OHX	AR	3555	-	0,6,6	0.00	-	-		
84	OHX	sR	2016	-	0,6,6	0.00	-	-		
84	OHX	AR	3494	-	0,6,6	0.00	-	-		
84	OHX	AS	203	-	0,6,6	0.00	-	-		
84	OHX	AR	3711	-	0,6,6	0.00	-	-		
84	OHX	sR	2023	-	0,6,6	0.00	-	-		
84	OHX	A	2008	-	0,6,6	0.00	-	-		
84	OHX	1	3473	-	0,6,6	0.00	-	-		
84	OHX	AR	3712	-	0,6,6	0.00	-	-		
84	OHX	AR	3434	-	0,6,6	0.00	-	-		
84	OHX	AR	3575	-	0,6,6	0.00	-	-		
84	OHX	1	3656	-	0,6,6	0.00	-	-		
84	OHX	AR	3644	-	0,6,6	0.00	-	-		
84	OHX	AR	3459	-	0,6,6	0.00	-	-		
84	OHX	AR	3721	84	0,6,6	0.00	-	-		
84	OHX	AR	3604	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3684	-	0,6,6	0.00	-	-		
84	OHX	A	1948	-	0,6,6	0.00	-	-		
84	OHX	AR	3601	-	0,6,6	0.00	-	-		
84	OHX	sR	2020	-	0,6,6	0.00	-	-		
84	OHX	1	3676	-	0,6,6	0.00	-	-		
84	OHX	sR	2001	-	0,6,6	0.00	-	-		
84	OHX	k	401	-	0,6,6	0.00	-	-		
84	OHX	1	3575	-	0,6,6	0.00	-	-		
84	OHX	sR	2004	-	0,6,6	0.00	-	-		
84	OHX	1	3729	-	0,6,6	0.00	-	-		
84	OHX	AR	3544	-	0,6,6	0.00	-	-		
84	OHX	A	1990	-	0,6,6	0.00	-	-		
84	OHX	AT	210	-	0,6,6	0.00	-	-		
84	OHX	AR	3412	-	0,6,6	0.00	-	-		
84	OHX	1	3668	-	0,6,6	0.00	-	-		
84	OHX	sR	1958	-	0,6,6	0.00	-	-		
84	OHX	AR	3689	-	0,6,6	0.00	-	-		
84	OHX	1	3654	-	0,6,6	0.00	-	-		
84	OHX	1	3536	-	0,6,6	0.00	-	-		
84	OHX	1	3596	-	0,6,6	0.00	-	-		
84	OHX	sR	1936	-	0,6,6	0.00	-	-		
84	OHX	1	3511	-	0,6,6	0.00	-	-		
84	OHX	AR	3518	-	0,6,6	0.00	-	-		
84	OHX	1	3552	-	0,6,6	0.00	-	-		
84	OHX	1	3572	-	0,6,6	0.00	-	-		
84	OHX	1	3605	-	0,6,6	0.00	-	-		
84	OHX	sR	1912	-	0,6,6	0.00	-	-		
84	OHX	sR	1961	-	0,6,6	0.00	-	-		
84	OHX	AR	3517	-	0,6,6	0.00	-	-		
84	OHX	AR	3501	-	0,6,6	0.00	-	-		
84	OHX	AR	3441	-	0,6,6	0.00	-	-		
84	OHX	1	3613	-	0,6,6	0.00	-	-		
84	OHX	1	3700	-	0,6,6	0.00	-	-		
84	OHX	CL	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3663	-	0,6,6	0.00	-	-		
84	OHX	sR	2010	-	0,6,6	0.00	-	-		
84	OHX	sR	1917	-	0,6,6	0.00	-	-		
84	OHX	l	401	-	0,6,6	0.00	-	-		
84	OHX	AR	3462	-	0,6,6	0.00	-	-		
84	OHX	AR	3618	-	0,6,6	0.00	-	-		
84	OHX	1	3463	-	0,6,6	0.00	-	-		
84	OHX	1	3583	-	0,6,6	0.00	-	-		
84	OHX	1	3401	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	c8	201	-	0,6,6	0.00	-	-		
84	OHX	A	2027	-	0,6,6	0.00	-	-		
84	OHX	1	3508	-	0,6,6	0.00	-	-		
84	OHX	1	3610	-	0,6,6	0.00	-	-		
84	OHX	sR	1971	-	0,6,6	0.00	-	-		
84	OHX	1	3407	-	0,6,6	0.00	-	-		
84	OHX	1	3633	-	0,6,6	0.00	-	-		
84	OHX	AR	3550	-	0,6,6	0.00	-	-		
84	OHX	3	201	-	0,6,6	0.00	-	-		
84	OHX	sR	1906	-	0,6,6	0.00	-	-		
84	OHX	AR	3735	-	0,6,6	0.00	-	-		
84	OHX	AR	3559	-	0,6,6	0.00	-	-		
84	OHX	sR	2006	-	0,6,6	0.00	-	-		
84	OHX	1	3532	-	0,6,6	0.00	-	-		
84	OHX	1	3563	-	0,6,6	0.00	-	-		
84	OHX	AR	3713	-	0,6,6	0.00	-	-		
84	OHX	1	3713	-	0,6,6	0.00	-	-		
84	OHX	1	3458	-	0,6,6	0.00	-	-		
84	OHX	AR	3648	-	0,6,6	0.00	-	-		
84	OHX	sR	1913	-	0,6,6	0.00	-	-		
84	OHX	1	3582	-	0,6,6	0.00	-	-		
84	OHX	AC	101	-	0,6,6	0.00	-	-		
84	OHX	1	3587	-	0,6,6	0.00	-	-		
84	OHX	AT	209	-	0,6,6	0.00	-	-		
84	OHX	AR	3653	-	0,6,6	0.00	-	-		
84	OHX	CF	401	-	0,6,6	0.00	-	-		
84	OHX	AR	3707	-	0,6,6	0.00	-	-		
84	OHX	1	3426	-	0,6,6	0.00	-	-		
84	OHX	1	3694	-	0,6,6	0.00	-	-		
84	OHX	AR	3401	-	0,6,6	0.00	-	-		
84	OHX	1	3512	-	0,6,6	0.00	-	-		
84	OHX	d9	101	-	0,6,6	0.00	-	-		
84	OHX	1	3627	-	0,6,6	0.00	-	-		
84	OHX	sR	1905	-	0,6,6	0.00	-	-		
84	OHX	AR	3579	-	0,6,6	0.00	-	-		
84	OHX	sR	2030	-	0,6,6	0.00	-	-		
84	OHX	sR	1974	-	0,6,6	0.00	-	-		
84	OHX	1	3569	-	0,6,6	0.00	-	-		
84	OHX	AR	3583	-	0,6,6	0.00	-	-		
84	OHX	sR	2022	-	0,6,6	0.00	-	-		
84	OHX	AR	3538	-	0,6,6	0.00	-	-		
84	OHX	3	206	-	0,6,6	0.00	-	-		
84	OHX	AR	3588	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3580	-	0,6,6	0.00	-	-		
84	OHX	A	1907	-	0,6,6	0.00	-	-		
84	OHX	AR	3535	-	0,6,6	0.00	-	-		
84	OHX	1	3597	-	0,6,6	0.00	-	-		
84	OHX	AR	3744	-	0,6,6	0.00	-	-		
84	OHX	A	1991	-	0,6,6	0.00	-	-		
84	OHX	A	2012	-	0,6,6	0.00	-	-		
84	OHX	A	1938	-	0,6,6	0.00	-	-		
84	OHX	AR	3444	-	0,6,6	0.00	-	-		
84	OHX	AR	3473	-	0,6,6	0.00	-	-		
84	OHX	AR	3458	-	0,6,6	0.00	-	-		
84	OHX	AS	206	-	0,6,6	0.00	-	-		
84	OHX	A	1968	-	0,6,6	0.00	-	-		
84	OHX	A	1923	-	0,6,6	0.00	-	-		
84	OHX	AR	3591	-	0,6,6	0.00	-	-		
84	OHX	A	1977	-	0,6,6	0.00	-	-		
84	OHX	AR	3450	-	0,6,6	0.00	-	-		
84	OHX	AT	218	-	0,6,6	0.00	-	-		
84	OHX	AR	3635	-	0,6,6	0.00	-	-		
84	OHX	AR	3568	-	0,6,6	0.00	-	-		
84	OHX	AR	3484	-	0,6,6	0.00	-	-		
84	OHX	A	2016	-	0,6,6	0.00	-	-		
84	OHX	AR	3497	-	0,6,6	0.00	-	-		
84	OHX	1	3423	-	0,6,6	0.00	-	-		
84	OHX	1	3543	-	0,6,6	0.00	-	-		
84	OHX	1	3412	-	0,6,6	0.00	-	-		
84	OHX	sR	2035	-	0,6,6	0.00	-	-		
84	OHX	AR	3645	-	0,6,6	0.00	-	-		
84	OHX	sR	1922	-	0,6,6	0.00	-	-		
84	OHX	sR	1959	-	0,6,6	0.00	-	-		
84	OHX	AR	3639	-	0,6,6	0.00	-	-		
84	OHX	4	214	-	0,6,6	0.00	-	-		
84	OHX	1	3409	-	0,6,6	0.00	-	-		
84	OHX	1	3425	-	0,6,6	0.00	-	-		
84	OHX	AR	3423	-	0,6,6	0.00	-	-		
84	OHX	AR	3599	-	0,6,6	0.00	-	-		
84	OHX	AR	3701	-	0,6,6	0.00	-	-		
84	OHX	AR	3597	-	0,6,6	0.00	-	-		
84	OHX	A	1946	-	0,6,6	0.00	-	-		
84	OHX	A	1952	-	0,6,6	0.00	-	-		
84	OHX	1	3528	-	0,6,6	0.00	-	-		
84	OHX	AR	3729	-	0,6,6	0.00	-	-		
84	OHX	sR	1966	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	sR	2011	-	0,6,6	0.00	-	-		
84	OHX	1	3571	-	0,6,6	0.00	-	-		
84	OHX	A	1984	-	0,6,6	0.00	-	-		
84	OHX	1	3574	-	0,6,6	0.00	-	-		
84	OHX	AR	3643	-	0,6,6	0.00	-	-		
84	OHX	AT	217	-	0,6,6	0.00	-	-		
84	OHX	sR	1934	-	0,6,6	0.00	-	-		
84	OHX	AR	3492	-	0,6,6	0.00	-	-		
84	OHX	AR	3737	-	0,6,6	0.00	-	-		
84	OHX	AR	3453	-	0,6,6	0.00	-	-		
84	OHX	AR	3516	-	0,6,6	0.00	-	-		
84	OHX	AR	3608	-	0,6,6	0.00	-	-		
84	OHX	AR	3610	-	0,6,6	0.00	-	-		
84	OHX	CE	401	-	0,6,6	0.00	-	-		
84	OHX	1	3550	-	0,6,6	0.00	-	-		
84	OHX	A	2034	-	0,6,6	0.00	-	-		
84	OHX	AR	3510	-	0,6,6	0.00	-	-		
84	OHX	sR	1914	-	0,6,6	0.00	-	-		
84	OHX	sR	2032	-	0,6,6	0.00	-	-		
84	OHX	A	1924	-	0,6,6	0.00	-	-		
84	OHX	sR	1942	-	0,6,6	0.00	-	-		
84	OHX	1	3439	-	0,6,6	0.00	-	-		
84	OHX	A	1953	-	0,6,6	0.00	-	-		
84	OHX	A	1972	-	0,6,6	0.00	-	-		
84	OHX	sR	1964	-	0,6,6	0.00	-	-		
84	OHX	A	1906	-	0,6,6	0.00	-	-		
84	OHX	1	3617	-	0,6,6	0.00	-	-		
84	OHX	1	3470	-	0,6,6	0.00	-	-		
84	OHX	AR	3528	-	0,6,6	0.00	-	-		
84	OHX	s1	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3418	-	0,6,6	0.00	-	-		
84	OHX	AR	3508	-	0,6,6	0.00	-	-		
84	OHX	1	3695	-	0,6,6	0.00	-	-		
84	OHX	1	3682	-	0,6,6	0.00	-	-		
84	OHX	A	1999	-	0,6,6	0.00	-	-		
84	OHX	sR	1911	-	0,6,6	0.00	-	-		
84	OHX	DL	101	-	0,6,6	0.00	-	-		
84	OHX	A	1949	-	0,6,6	0.00	-	-		
84	OHX	1	3718	-	0,6,6	0.00	-	-		
84	OHX	CK	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3449	-	0,6,6	0.00	-	-		
84	OHX	1	3433	-	0,6,6	0.00	-	-		
84	OHX	1	3646	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	sR	2014	-	0,6,6	0.00	-	-		
84	OHX	1	3639	-	0,6,6	0.00	-	-		
84	OHX	1	3413	-	0,6,6	0.00	-	-		
84	OHX	1	3535	-	0,6,6	0.00	-	-		
84	OHX	1	3561	-	0,6,6	0.00	-	-		
84	OHX	A	1940	-	0,6,6	0.00	-	-		
84	OHX	AR	3503	-	0,6,6	0.00	-	-		
84	OHX	AR	3522	-	0,6,6	0.00	-	-		
84	OHX	1	3520	-	0,6,6	0.00	-	-		
84	OHX	AR	3564	-	0,6,6	0.00	-	-		
84	OHX	A	1996	-	0,6,6	0.00	-	-		
84	OHX	sR	1933	-	0,6,6	0.00	-	-		
84	OHX	AR	3696	-	0,6,6	0.00	-	-		
84	OHX	A	1954	-	0,6,6	0.00	-	-		
84	OHX	1	3421	-	0,6,6	0.00	-	-		
84	OHX	1	3545	-	0,6,6	0.00	-	-		
84	OHX	sR	1928	-	0,6,6	0.00	-	-		
84	OHX	AR	3638	-	0,6,6	0.00	-	-		
84	OHX	1	3595	-	0,6,6	0.00	-	-		
84	OHX	4	210	-	0,6,6	0.00	-	-		
84	OHX	A	1960	-	0,6,6	0.00	-	-		
84	OHX	sR	1923	-	0,6,6	0.00	-	-		
84	OHX	A	1965	-	0,6,6	0.00	-	-		
84	OHX	sR	1929	-	0,6,6	0.00	-	-		
84	OHX	sR	1926	-	0,6,6	0.00	-	-		
84	OHX	AR	3442	-	0,6,6	0.00	-	-		
84	OHX	1	3665	-	0,6,6	0.00	-	-		
84	OHX	DH	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3495	-	0,6,6	0.00	-	-		
84	OHX	CG	302	-	0,6,6	0.00	-	-		
84	OHX	AR	3498	-	0,6,6	0.00	-	-		
84	OHX	A	2011	-	0,6,6	0.00	-	-		
84	OHX	AR	3408	-	0,6,6	0.00	-	-		
84	OHX	AR	3512	-	0,6,6	0.00	-	-		
84	OHX	A	1942	-	0,6,6	0.00	-	-		
84	OHX	sR	1927	-	0,6,6	0.00	-	-		
84	OHX	AR	3486	-	0,6,6	0.00	-	-		
84	OHX	AR	3636	-	0,6,6	0.00	-	-		
84	OHX	AT	213	-	0,6,6	0.00	-	-		
84	OHX	1	3542	-	0,6,6	0.00	-	-		
84	OHX	sR	2017	-	0,6,6	0.00	-	-		
84	OHX	AR	3620	-	0,6,6	0.00	-	-		
84	OHX	AR	3536	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1962	-	0,6,6	0.00	-	-		
84	OHX	1	3728	-	0,6,6	0.00	-	-		
84	OHX	AR	3621	-	0,6,6	0.00	-	-		
84	OHX	A	1975	-	0,6,6	0.00	-	-		
84	OHX	AR	3420	-	0,6,6	0.00	-	-		
84	OHX	sR	1921	-	0,6,6	0.00	-	-		
84	OHX	A	1914	-	0,6,6	0.00	-	-		
84	OHX	CP	501	-	0,6,6	0.00	-	-		
84	OHX	AT	214	-	0,6,6	0.00	-	-		
84	OHX	1	3497	-	0,6,6	0.00	-	-		
84	OHX	1	3559	-	0,6,6	0.00	-	-		
84	OHX	sR	1948	-	0,6,6	0.00	-	-		
84	OHX	AR	3602	-	0,6,6	0.00	-	-		
84	OHX	1	3699	-	0,6,6	0.00	-	-		
84	OHX	sR	1987	-	0,6,6	0.00	-	-		
84	OHX	AG	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3577	-	0,6,6	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	7AL	AR	4246	-	-	2/8/60/60	0/3/3/3
86	7AL	1	4210	-	-	2/8/60/60	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	4210	7AL	O4-C8-C7	2.33	114.89	109.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	1	4210	7AL	C10-C14-C15-C16
86	AR	4246	7AL	C10-C14-C15-C16
86	1	4210	7AL	C10-C14-C15-O1
86	AR	4246	7AL	C10-C14-C15-O1

There are no ring outliers.

514 monomers are involved in 753 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3587	OHX	2	0
84	1	3705	OHX	5	0
84	1	3427	OHX	3	0
84	O	201	OHX	1	0
84	A	1904	OHX	1	0
84	A	1901	OHX	2	0
84	1	3459	OHX	1	0
84	1	3546	OHX	1	0
84	1	3500	OHX	2	0
84	AR	3726	OHX	1	0
84	A	1936	OHX	1	0
84	1	3493	OHX	3	0
84	1	3644	OHX	1	0
84	3	204	OHX	1	0
84	1	3620	OHX	1	0
84	A	1922	OHX	2	0
84	AR	3691	OHX	1	0
84	1	3601	OHX	1	0
84	AR	3730	OHX	2	0
84	AR	3741	OHX	1	0
84	AR	3556	OHX	1	0
84	1	3503	OHX	2	0
84	CX	202	OHX	2	0
84	AT	206	OHX	2	0
84	1	3489	OHX	1	0
84	1	3603	OHX	1	0
84	A	2021	OHX	1	0
84	1	3414	OHX	2	0
84	1	3436	OHX	2	0
84	1	3692	OHX	1	0
84	CM	201	OHX	1	0
84	AR	3504	OHX	1	0
84	1	3418	OHX	2	0
84	AR	3732	OHX	1	0
84	AR	3586	OHX	2	0
84	1	3441	OHX	1	0
84	AR	3490	OHX	1	0
84	A	1985	OHX	1	0
84	AR	3624	OHX	1	0
84	AR	3489	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3510	OHX	1	0
84	A	1987	OHX	1	0
84	AR	3506	OHX	2	0
84	1	3406	OHX	4	0
84	1	3502	OHX	2	0
84	AR	3406	OHX	1	0
84	A	1931	OHX	1	0
84	AR	3403	OHX	1	0
84	AR	3554	OHX	1	0
84	A	2042	OHX	1	0
84	AR	3513	OHX	3	0
84	A	2038	OHX	1	0
84	AR	3706	OHX	2	0
84	A	2032	OHX	1	0
84	AR	3417	OHX	1	0
84	AR	3656	OHX	2	0
84	1	3671	OHX	2	0
84	1	3539	OHX	2	0
84	A	1925	OHX	2	0
84	1	3614	OHX	1	0
84	AR	3488	OHX	1	0
84	AR	3475	OHX	2	0
84	AR	3548	OHX	1	0
84	AR	3687	OHX	1	0
84	AR	3605	OHX	1	0
84	1	3504	OHX	1	0
84	AR	3470	OHX	1	0
84	1	3422	OHX	1	0
84	AR	3448	OHX	1	0
84	AR	3647	OHX	2	0
84	AR	3690	OHX	1	0
84	AR	3451	OHX	1	0
84	AT	211	OHX	1	0
84	AR	3519	OHX	1	0
84	DQ	201	OHX	3	0
84	AR	3697	OHX	2	0
84	1	3424	OHX	1	0
84	AR	3574	OHX	1	0
84	AR	3477	OHX	1	0
84	1	3722	OHX	1	0
84	CE	402	OHX	1	0
84	AR	3402	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3444	OHX	1	0
84	AR	3627	OHX	1	0
84	AR	3539	OHX	2	0
84	AT	204	OHX	1	0
84	AR	3456	OHX	1	0
84	AR	3593	OHX	1	0
84	AR	3600	OHX	1	0
84	A	2030	OHX	3	0
84	1	3624	OHX	1	0
84	AR	3469	OHX	1	0
84	AR	3502	OHX	1	0
84	AR	3705	OHX	4	0
84	AR	3743	OHX	1	0
84	1	3642	OHX	1	0
84	1	3445	OHX	1	0
84	A	1963	OHX	2	0
84	AR	3455	OHX	1	0
84	A	1910	OHX	1	0
84	1	3556	OHX	2	0
84	AR	3570	OHX	1	0
84	1	3666	OHX	1	0
84	1	3417	OHX	2	0
84	1	3419	OHX	2	0
84	AR	3584	OHX	1	0
84	1	3609	OHX	1	0
84	AR	3692	OHX	1	0
84	A	1916	OHX	2	0
84	1	3446	OHX	1	0
84	AR	3625	OHX	1	0
84	AT	203	OHX	1	0
84	1	3411	OHX	1	0
84	AR	3685	OHX	1	0
84	1	3711	OHX	3	0
84	AR	3623	OHX	1	0
84	AR	3738	OHX	7	0
84	1	3622	OHX	1	0
84	AR	3678	OHX	1	0
84	A	1928	OHX	2	0
84	A	1918	OHX	1	0
84	AR	3640	OHX	1	0
84	1	3518	OHX	1	0
84	4	215	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	3	203	OHX	1	0
84	1	3429	OHX	1	0
84	1	3534	OHX	1	0
84	AR	3446	OHX	1	0
84	1	3724	OHX	1	0
84	1	3584	OHX	1	0
84	1	3468	OHX	3	0
84	AR	3592	OHX	1	0
84	AR	3562	OHX	2	0
84	1	3604	OHX	1	0
84	A	1956	OHX	1	0
84	1	3616	OHX	1	0
84	A	2019	OHX	1	0
84	AT	216	OHX	2	0
84	A	2022	OHX	1	0
84	4	201	OHX	1	0
84	AR	3521	OHX	1	0
84	A	1988	OHX	2	0
84	A	1919	OHX	1	0
84	AR	3551	OHX	1	0
84	A	1902	OHX	1	0
84	AR	3435	OHX	1	0
84	AR	3411	OHX	1	0
84	1	3652	OHX	2	0
84	1	3687	OHX	1	0
84	AR	3416	OHX	1	0
84	1	3490	OHX	1	0
84	1	3592	OHX	4	0
84	1	3721	OHX	1	0
84	1	3689	OHX	1	0
84	AR	3606	OHX	1	0
84	AR	3580	OHX	1	0
84	AR	3405	OHX	1	0
84	CF	402	OHX	1	0
84	1	3648	OHX	1	0
84	AR	3572	OHX	1	0
84	AR	3520	OHX	1	0
84	1	3588	OHX	1	0
84	AR	3582	OHX	1	0
84	AR	3457	OHX	1	0
86	AR	4246	7AL	1	0
84	1	3483	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3581	OHX	1	0
84	AR	3718	OHX	2	0
84	AR	3569	OHX	1	0
84	1	3471	OHX	1	0
84	1	3515	OHX	1	0
84	AR	3734	OHX	2	0
84	1	3586	OHX	1	0
84	A	1913	OHX	2	0
84	A	1998	OHX	2	0
84	AR	3688	OHX	2	0
84	AR	3443	OHX	1	0
84	3	202	OHX	1	0
84	AR	3409	OHX	1	0
84	1	3465	OHX	1	0
84	AR	3613	OHX	2	0
84	AR	3496	OHX	1	0
84	A	1920	OHX	1	0
84	A	1903	OHX	1	0
84	1	3403	OHX	1	0
84	AR	3615	OHX	1	0
84	AR	3514	OHX	1	0
84	A	1986	OHX	1	0
84	AR	3686	OHX	1	0
84	AR	3571	OHX	2	0
84	A	2024	OHX	6	0
84	1	3686	OHX	1	0
84	AS	208	OHX	1	0
84	AR	3703	OHX	5	0
84	1	3420	OHX	2	0
84	1	3404	OHX	1	0
84	1	3492	OHX	2	0
84	AR	3664	OHX	2	0
84	T	201	OHX	1	0
84	1	3591	OHX	2	0
84	AR	3677	OHX	4	0
84	1	3461	OHX	2	0
84	AR	3541	OHX	1	0
84	A	2007	OHX	2	0
84	1	3540	OHX	5	0
84	1	3526	OHX	1	0
84	AR	3603	OHX	1	0
84	1	3683	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3659	OHX	1	0
84	AR	3585	OHX	1	0
84	AS	202	OHX	2	0
84	1	3675	OHX	1	0
84	AR	3468	OHX	1	0
84	1	3725	OHX	2	0
84	1	3679	OHX	2	0
84	AR	3611	OHX	2	0
84	AR	3649	OHX	2	0
84	1	3598	OHX	1	0
84	AR	3674	OHX	1	0
84	AS	210	OHX	1	0
84	Q	201	OHX	2	0
84	1	3653	OHX	1	0
84	AR	3526	OHX	6	0
84	AR	3667	OHX	2	0
84	AS	204	OHX	1	0
84	AR	3552	OHX	2	0
84	1	3680	OHX	1	0
84	1	3519	OHX	2	0
84	1	3513	OHX	1	0
84	A	1917	OHX	1	0
84	1	3451	OHX	1	0
84	1	3629	OHX	1	0
84	AR	3465	OHX	4	0
84	AR	3660	OHX	2	0
84	AR	3720	OHX	1	0
84	4	202	OHX	1	0
84	A	2037	OHX	1	0
84	AR	3736	OHX	1	0
84	AR	3415	OHX	2	0
84	1	3448	OHX	1	0
84	AR	3629	OHX	1	0
84	AR	3716	OHX	1	0
84	A	2009	OHX	4	0
84	A	1966	OHX	1	0
84	AR	3467	OHX	1	0
84	A	1909	OHX	8	0
84	3	205	OHX	1	0
84	A	1915	OHX	2	0
84	1	3524	OHX	1	0
84	1	3469	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3606	OHX	1	0
84	A	1937	OHX	1	0
84	1	3479	OHX	1	0
84	A	1947	OHX	1	0
84	AR	3594	OHX	1	0
84	A	1911	OHX	2	0
84	1	3562	OHX	1	0
84	1	3730	OHX	5	0
84	AK	102	OHX	3	0
84	A	1964	OHX	2	0
84	A	1939	OHX	2	0
84	AR	3715	OHX	1	0
84	1	3538	OHX	3	0
84	1	3632	OHX	1	0
84	AR	3481	OHX	3	0
84	1	3667	OHX	1	0
84	1	3637	OHX	1	0
84	AT	212	OHX	4	0
84	AR	3684	OHX	1	0
84	AR	3483	OHX	1	0
84	AR	3410	OHX	3	0
84	A	1912	OHX	1	0
84	1	3719	OHX	1	0
84	1	3712	OHX	1	0
84	A	1997	OHX	1	0
84	AR	3655	OHX	1	0
84	AR	3419	OHX	2	0
84	1	3462	OHX	1	0
84	AR	3702	OHX	2	0
84	1	3611	OHX	1	0
84	4	208	OHX	1	0
84	1	3688	OHX	2	0
84	1	3593	OHX	1	0
84	AR	3619	OHX	1	0
84	1	3701	OHX	2	0
84	1	3450	OHX	1	0
84	1	3460	OHX	2	0
84	1	3661	OHX	2	0
84	AR	3598	OHX	1	0
84	1	3517	OHX	1	0
84	AR	3709	OHX	1	0
84	1	3428	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3664	OHX	3	0
84	1	3405	OHX	1	0
84	CV	201	OHX	1	0
84	1	3577	OHX	1	0
84	AR	3661	OHX	1	0
84	AR	3427	OHX	2	0
84	AR	3682	OHX	1	0
84	A	1932	OHX	2	0
84	A	1951	OHX	2	0
84	AR	3529	OHX	2	0
84	1	3474	OHX	4	0
84	AR	3612	OHX	3	0
84	1	3630	OHX	1	0
84	1	3567	OHX	1	0
84	1	3716	OHX	2	0
84	1	3494	OHX	3	0
84	4	213	OHX	1	0
84	AR	3463	OHX	1	0
84	AR	3590	OHX	1	0
84	A	2005	OHX	1	0
84	AT	202	OHX	1	0
84	AR	3464	OHX	2	0
84	AR	3573	OHX	1	0
84	A	2003	OHX	1	0
84	1	3635	OHX	1	0
84	A	1943	OHX	3	0
84	1	3509	OHX	1	0
84	AR	3421	OHX	1	0
84	1	3600	OHX	1	0
84	AR	3642	OHX	1	0
84	A	2029	OHX	1	0
84	AP	502	OHX	5	0
84	1	3507	OHX	1	0
84	DD	102	OHX	1	0
84	1	3457	OHX	1	0
84	1	3626	OHX	1	0
84	A	2035	OHX	1	0
84	1	3430	OHX	1	0
84	A	1944	OHX	1	0
84	1	3437	OHX	4	0
84	A	1970	OHX	1	0
84	AR	3454	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AT	207	OHX	2	0
84	1	3466	OHX	1	0
84	AR	3461	OHX	1	0
84	AR	3472	OHX	2	0
84	A	1973	OHX	2	0
84	1	3482	OHX	1	0
84	1	3612	OHX	1	0
84	1	3594	OHX	1	0
84	4	207	OHX	1	0
84	A	2023	OHX	1	0
84	1	3640	OHX	1	0
84	AR	3733	OHX	1	0
84	AR	3460	OHX	2	0
84	AR	3511	OHX	1	0
84	1	3485	OHX	1	0
84	1	3408	OHX	2	0
84	1	3544	OHX	1	0
84	AR	3728	OHX	1	0
84	AR	3424	OHX	1	0
84	AR	3437	OHX	2	0
84	AR	3413	OHX	1	0
84	J	301	OHX	1	0
84	1	3442	OHX	1	0
84	AR	3426	OHX	1	0
84	M	201	OHX	1	0
84	AR	3524	OHX	2	0
84	AR	3694	OHX	2	0
84	1	3670	OHX	1	0
84	AS	205	OHX	1	0
84	AS	201	OHX	1	0
84	CG	303	OHX	1	0
84	1	3578	OHX	1	0
84	AR	3439	OHX	1	0
84	A	2004	OHX	1	0
84	AR	3407	OHX	2	0
84	1	3690	OHX	1	0
84	AR	3530	OHX	1	0
84	1	3522	OHX	1	0
84	4	204	OHX	1	0
84	AR	3533	OHX	2	0
84	A	2013	OHX	1	0
84	AR	3507	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3402	OHX	1	0
84	1	3453	OHX	1	0
84	1	3697	OHX	4	0
84	AR	3695	OHX	3	0
84	AR	3537	OHX	1	0
84	AR	3561	OHX	2	0
84	AR	3445	OHX	8	0
84	1	3570	OHX	2	0
84	AR	3553	OHX	1	0
84	1	3501	OHX	1	0
84	AR	3567	OHX	1	0
84	AR	3633	OHX	1	0
84	AR	3545	OHX	3	0
84	AR	3447	OHX	1	0
84	AR	3532	OHX	2	0
84	1	3554	OHX	2	0
84	1	3476	OHX	1	0
84	4	206	OHX	1	0
84	AR	3711	OHX	1	0
84	A	2008	OHX	2	0
84	1	3473	OHX	1	0
84	AR	3434	OHX	1	0
84	AR	3575	OHX	1	0
84	1	3656	OHX	1	0
84	AR	3459	OHX	2	0
84	AR	3721	OHX	7	0
84	1	3684	OHX	1	0
84	1	3575	OHX	1	0
84	AT	210	OHX	1	0
84	AR	3412	OHX	1	0
84	1	3668	OHX	1	0
84	AR	3689	OHX	2	0
84	1	3654	OHX	1	0
84	1	3536	OHX	1	0
84	1	3596	OHX	1	0
84	1	3511	OHX	2	0
84	AR	3518	OHX	1	0
84	1	3552	OHX	1	0
84	AR	3517	OHX	1	0
84	AR	3441	OHX	1	0
84	CL	301	OHX	5	0
84	AR	3663	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3462	OHX	1	0
84	AR	3618	OHX	1	0
84	1	3463	OHX	1	0
84	1	3401	OHX	1	0
84	A	2027	OHX	1	0
84	1	3508	OHX	1	0
84	1	3610	OHX	1	0
84	AR	3735	OHX	1	0
84	1	3532	OHX	1	0
84	1	3563	OHX	1	0
84	AR	3713	OHX	2	0
84	1	3713	OHX	4	0
84	AC	101	OHX	2	0
84	AT	209	OHX	2	0
84	AR	3653	OHX	1	0
84	CF	401	OHX	3	0
84	1	3426	OHX	1	0
84	1	3694	OHX	1	0
84	AR	3401	OHX	1	0
84	1	3627	OHX	1	0
84	1	3569	OHX	2	0
84	AR	3583	OHX	1	0
84	3	206	OHX	1	0
84	1	3580	OHX	4	0
84	A	1907	OHX	1	0
84	AR	3535	OHX	1	0
84	AR	3744	OHX	1	0
84	A	2012	OHX	1	0
84	A	1938	OHX	1	0
84	AR	3444	OHX	2	0
84	AR	3473	OHX	1	0
84	AR	3458	OHX	2	0
84	A	1968	OHX	3	0
84	A	1923	OHX	1	0
84	AR	3450	OHX	1	0
84	AT	218	OHX	1	0
84	AR	3635	OHX	2	0
84	AR	3568	OHX	1	0
84	AR	3497	OHX	1	0
84	1	3543	OHX	1	0
84	1	3409	OHX	1	0
84	1	3425	OHX	1	0

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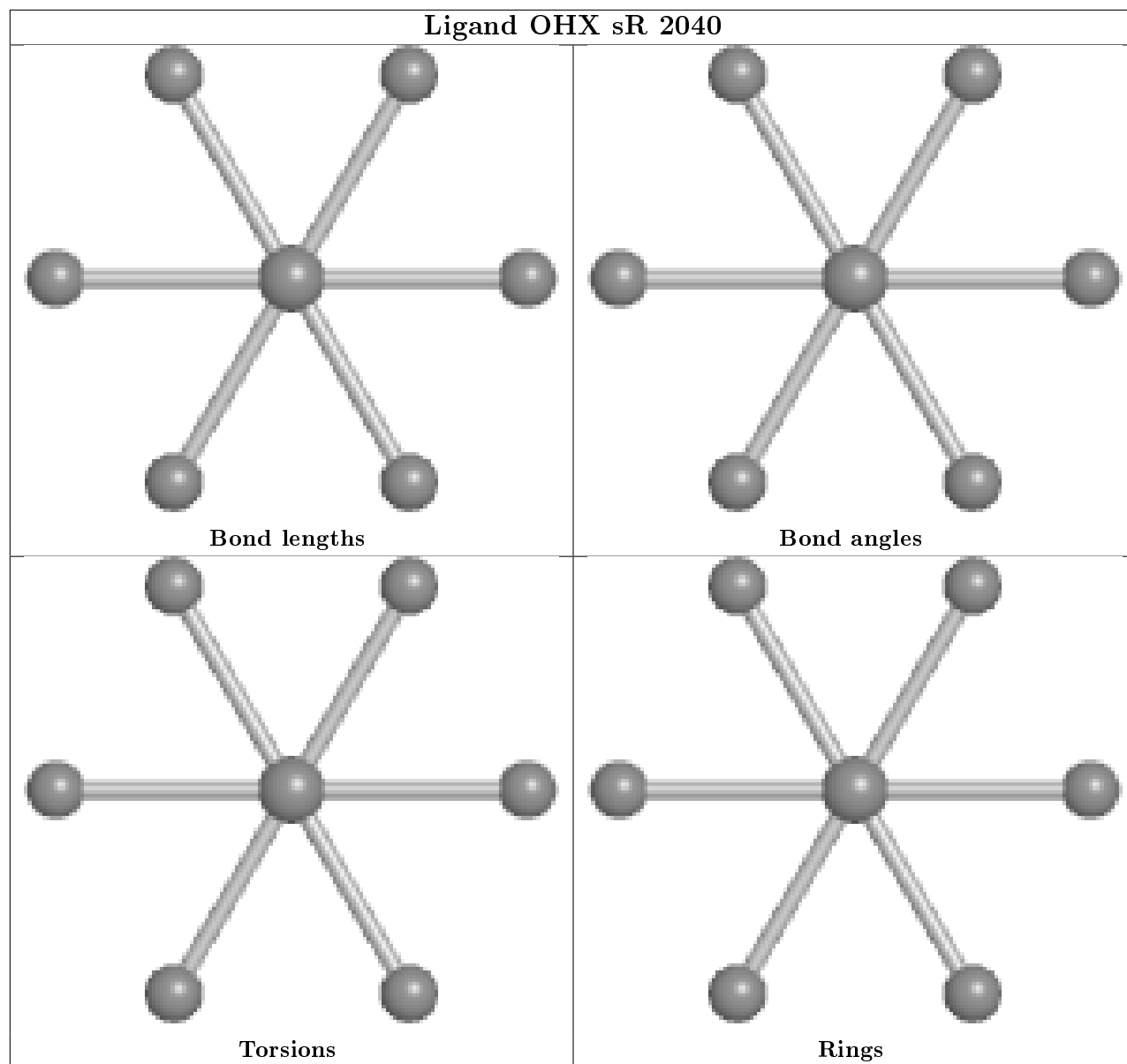
Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3599	OHX	5	0
84	AR	3597	OHX	3	0
84	A	1952	OHX	1	0
84	A	1984	OHX	1	0
84	AR	3643	OHX	1	0
84	AT	217	OHX	1	0
84	AR	3492	OHX	2	0
84	AR	3453	OHX	1	0
84	AR	3516	OHX	5	0
84	AR	3608	OHX	3	0
84	CE	401	OHX	3	0
84	AR	3510	OHX	2	0
84	A	1953	OHX	1	0
84	A	1972	OHX	1	0
84	AR	3528	OHX	2	0
84	AR	3418	OHX	1	0
84	AR	3508	OHX	2	0
84	1	3695	OHX	1	0
84	1	3682	OHX	3	0
84	A	1999	OHX	1	0
84	DL	101	OHX	2	0
84	AR	3449	OHX	1	0
84	1	3646	OHX	1	0
84	1	3639	OHX	1	0
84	1	3535	OHX	2	0
84	1	3561	OHX	2	0
84	A	1940	OHX	1	0
84	AR	3503	OHX	1	0
84	1	3520	OHX	2	0
84	AR	3564	OHX	1	0
84	AR	3696	OHX	2	0
84	A	1954	OHX	3	0
84	1	3545	OHX	1	0
84	AR	3638	OHX	2	0
84	1	3595	OHX	1	0
84	1	3665	OHX	3	0
84	AR	3495	OHX	3	0
84	CG	302	OHX	3	0
84	AR	3408	OHX	2	0
84	AR	3512	OHX	1	0
84	A	1942	OHX	1	0
84	AR	3486	OHX	2	0

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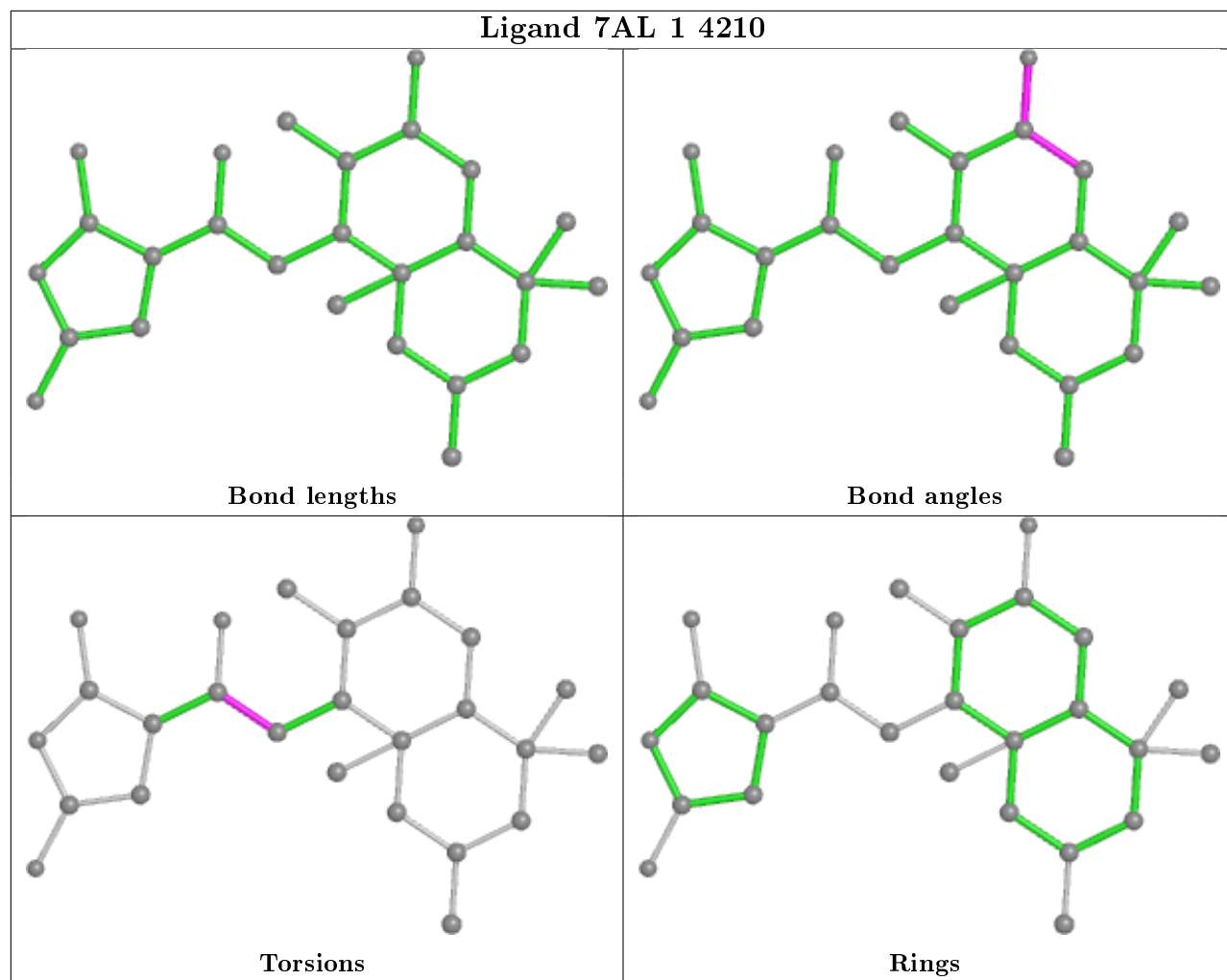
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3636	OHX	1	0
84	1	3542	OHX	1	0
84	AR	3620	OHX	1	0
84	AR	3536	OHX	1	0
84	A	1962	OHX	3	0
84	AR	3420	OHX	1	0
84	A	1914	OHX	1	0
84	CP	501	OHX	1	0
84	AT	214	OHX	2	0
84	AR	3602	OHX	1	0
84	AG	201	OHX	1	0
84	AR	3577	OHX	1	0

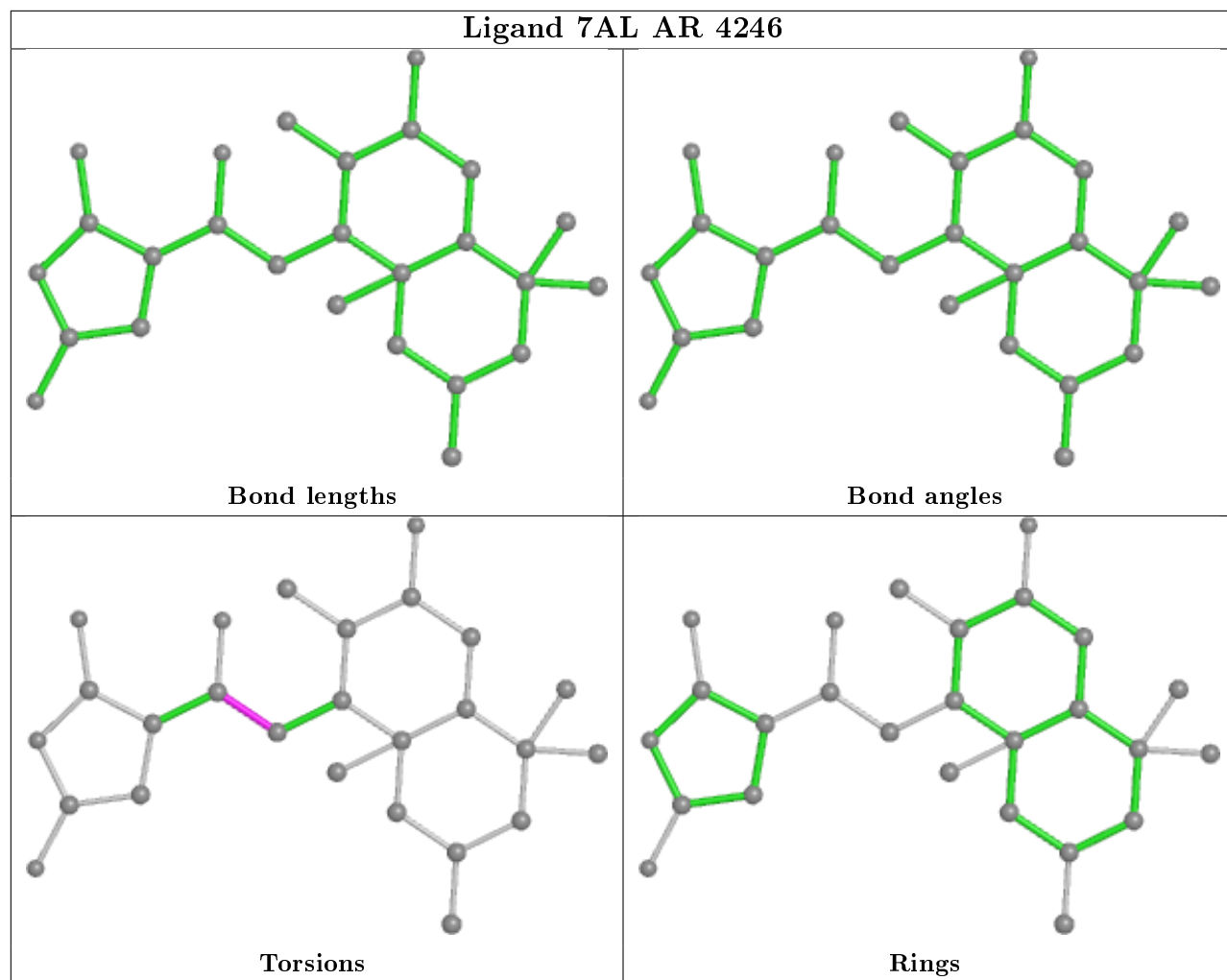
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

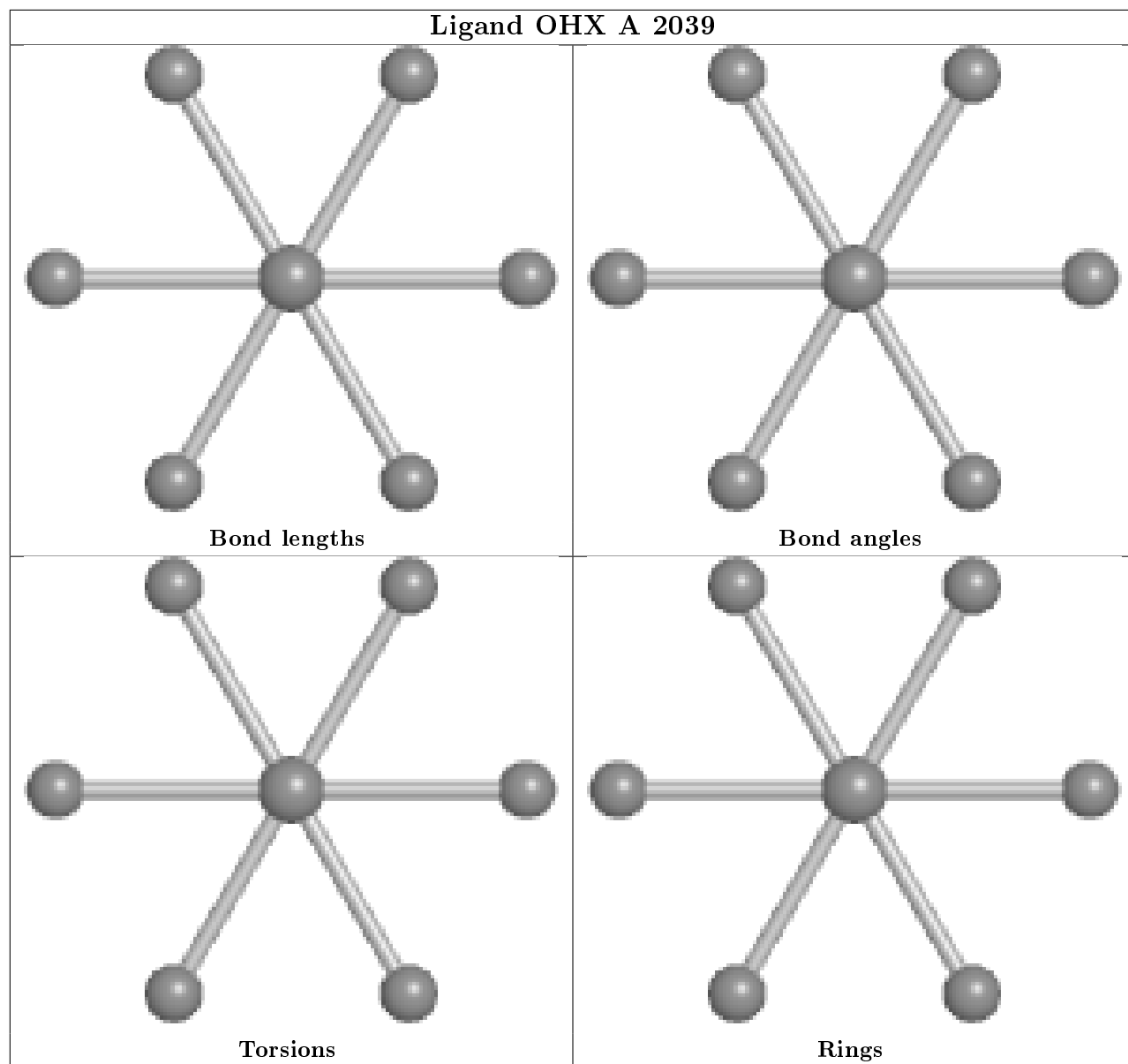


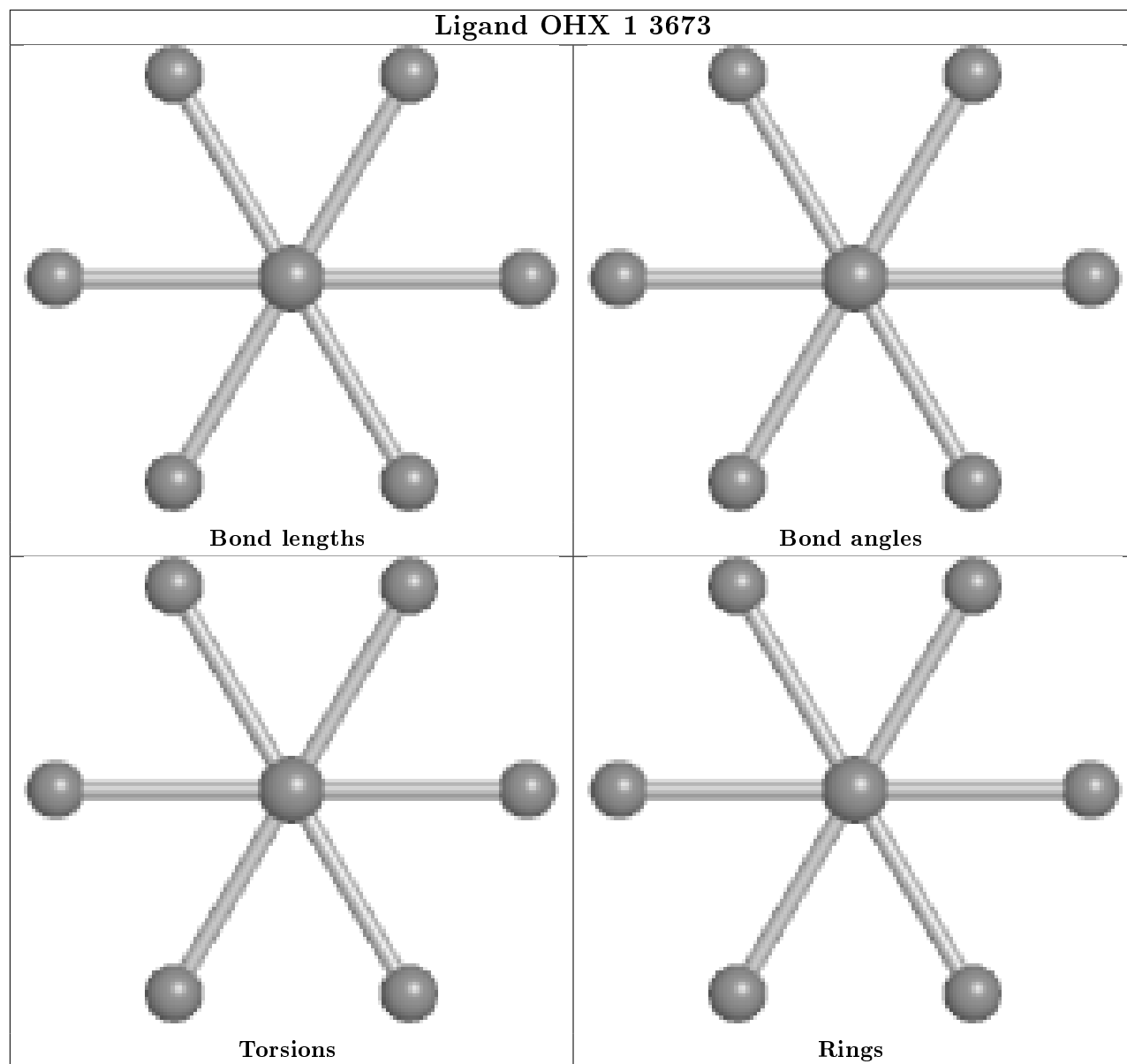
## Ligand 7AL 1 4210

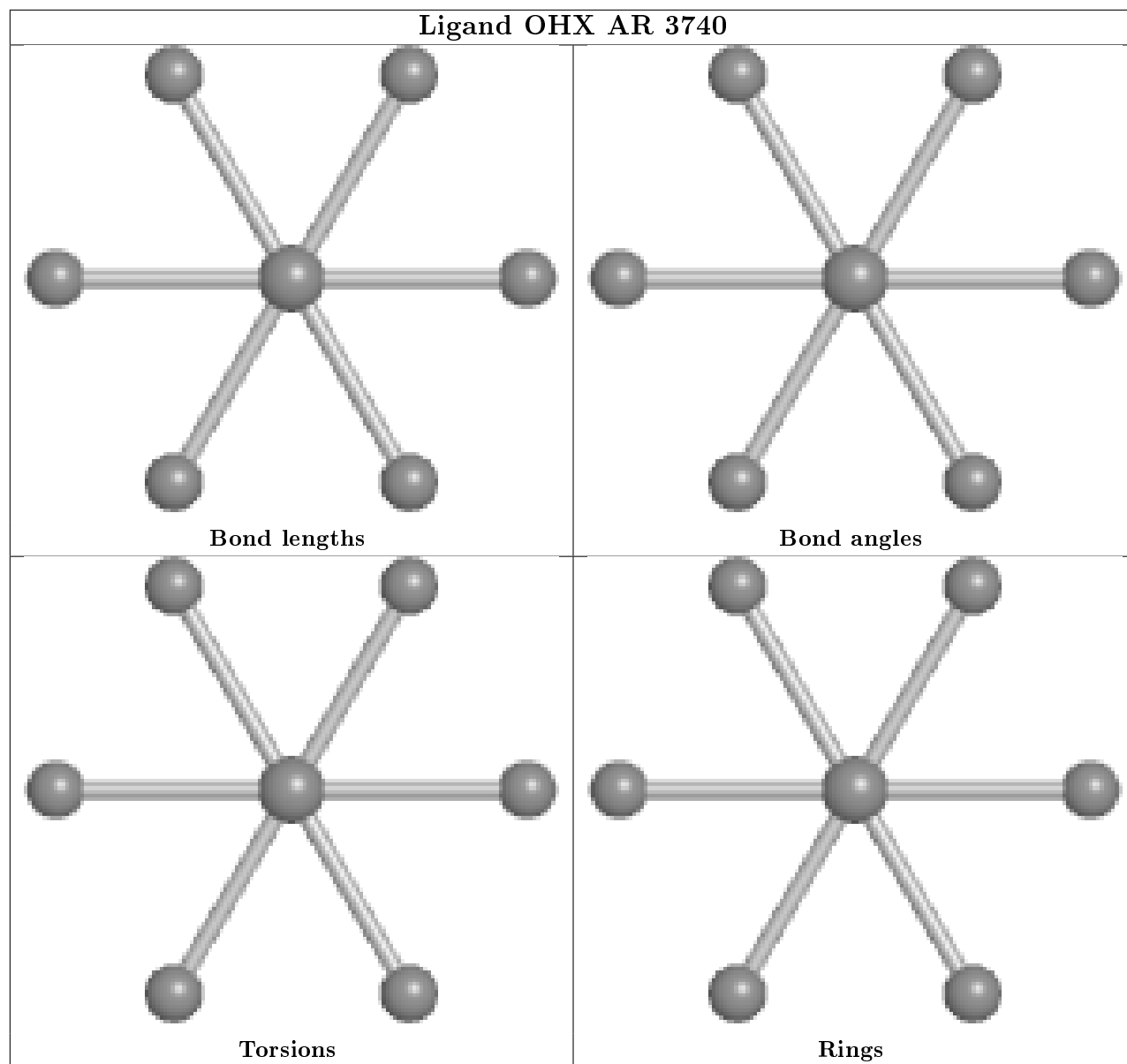


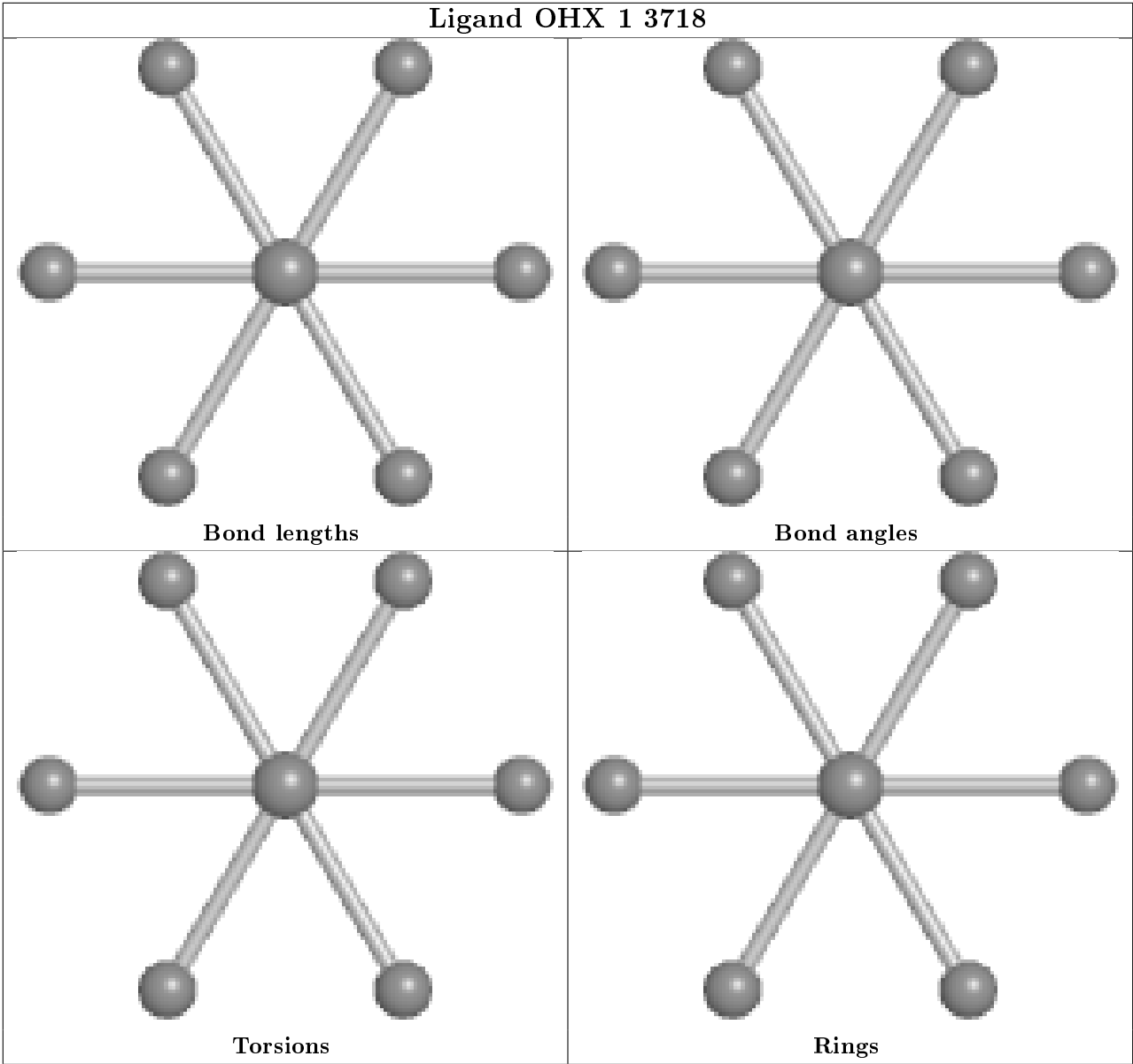
## Ligand 7AL AR 4246











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AR	3
1	1	3
47	sM	2

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Mol	Chain	Number of breaks
48	A	1

The worst 5 of 9 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	43.91
1	sM	139:UNK	C	155:UNK	N	37.53
1	1	1955:U	O3'	2093:A	P	25.84
1	AR	1955:U	O3'	2093:A	P	24.08
1	1	2445:A	O3'	2501:U	P	15.80

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	1	3149/3149 (100%)	-0.02	78 (2%)	57	29	23, 45, 148, 258	0
1	AR	3149/3149 (100%)	-0.00	87 (2%)	53	25	24, 48, 147, 276	0
2	3	121/121 (100%)	-0.34	0	100	100	33, 61, 76, 92	0
2	AS	121/121 (100%)	-0.33	0	100	100	30, 54, 69, 103	0
3	4	158/158 (100%)	-0.10	1 (0%)	89	72	28, 46, 98, 165	0
3	AT	158/158 (100%)	-0.06	2 (1%)	77	51	35, 57, 112, 166	0
4	CD	252/252 (100%)	-0.27	2 (0%)	86	65	31, 51, 76, 131	0
4	j	252/252 (100%)	-0.27	0	100	100	26, 45, 64, 113	0
5	CE	386/386 (100%)	-0.35	2 (0%)	91	75	24, 42, 66, 121	0
5	k	386/386 (100%)	-0.36	1 (0%)	94	84	26, 49, 69, 116	0
6	CF	361/361 (100%)	-0.33	0	100	100	28, 48, 75, 107	0
6	l	361/361 (100%)	-0.34	0	100	100	24, 43, 72, 92	0
7	CG	296/296 (100%)	-0.14	4 (1%)	75	49	40, 56, 94, 133	0
7	m	296/296 (100%)	0.09	6 (2%)	65	36	42, 70, 104, 152	0
8	CH	156/175 (89%)	-0.25	3 (1%)	66	37	36, 47, 85, 108	0
8	n	156/175 (89%)	-0.34	0	100	100	33, 44, 74, 119	0
9	CI	222/222 (100%)	-0.30	3 (1%)	75	49	28, 38, 86, 165	0
9	o	222/222 (100%)	-0.33	2 (0%)	84	63	28, 38, 75, 155	0
10	CJ	233/233 (100%)	0.73	22 (9%)	8	3	65, 82, 141, 172	0
10	p	233/233 (100%)	0.18	4 (1%)	70	41	50, 68, 138, 161	0
11	CK	191/191 (100%)	-0.22	3 (1%)	72	44	36, 47, 78, 142	0
11	q	191/191 (100%)	-0.31	1 (0%)	91	75	41, 56, 75, 141	0
12	CL	211/220 (95%)	0.02	6 (2%)	53	25	29, 55, 91, 155	0
12	r	211/220 (95%)	-0.24	0	100	100	28, 48, 95, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	CM	169/169 (100%)	-0.21	1 (0%) 89 72	42, 62, 82, 103	0
13	s	169/169 (100%)	-0.04	1 (0%) 89 72	50, 73, 91, 114	0
14	CN	193/193 (100%)	0.10	5 (2%) 56 27	31, 61, 121, 150	0
14	t	193/193 (100%)	-0.16	2 (1%) 82 59	25, 51, 110, 138	0
15	CO	136/136 (100%)	-0.42	1 (0%) 87 69	35, 43, 72, 91	0
15	u	136/136 (100%)	-0.42	0 100 100	38, 46, 70, 86	0
16	CP	203/203 (100%)	-0.22	0 100 100	34, 52, 67, 70	0
16	v	203/203 (100%)	-0.36	0 100 100	26, 42, 54, 71	0
17	CQ	197/197 (100%)	-0.26	3 (1%) 73 46	24, 35, 75, 89	0
17	w	197/197 (100%)	-0.37	0 100 100	27, 38, 65, 71	0
18	CR	183/183 (100%)	1.09	29 (15%) 2 1	27, 40, 169, 211	0
18	x	183/183 (100%)	0.18	14 (7%) 13 4	30, 39, 137, 171	0
19	CS	185/185 (100%)	-0.35	0 100 100	31, 45, 60, 78	0
19	y	185/185 (100%)	-0.29	0 100 100	30, 42, 79, 117	0
20	CT	188/188 (100%)	0.12	11 (5%) 22 7	44, 63, 165, 184	0
20	z	188/188 (100%)	0.19	13 (6%) 16 5	44, 60, 163, 180	0
21	0	172/172 (100%)	-0.30	2 (1%) 79 54	33, 43, 64, 89	0
21	CU	172/172 (100%)	-0.38	2 (1%) 79 54	29, 40, 62, 77	0
22	2	159/159 (100%)	-0.20	2 (1%) 77 51	29, 44, 105, 121	0
22	CV	159/159 (100%)	-0.21	0 100 100	29, 42, 100, 120	0
23	5	100/100 (100%)	0.72	11 (11%) 5 2	76, 99, 124, 160	0
23	CW	100/100 (100%)	1.19	19 (19%) 1 0	74, 95, 120, 141	0
24	6	136/136 (100%)	-0.15	1 (0%) 87 69	33, 46, 73, 108	0
24	CX	136/136 (100%)	0.02	3 (2%) 62 33	28, 42, 67, 92	0
25	7	98/98 (100%)	1.70	32 (32%) 0 0	42, 58, 175, 180	0
25	CY	98/98 (100%)	1.01	17 (17%) 1 0	39, 54, 177, 215	0
26	8	121/121 (100%)	-0.14	0 100 100	40, 57, 79, 136	0
26	CZ	121/121 (100%)	-0.01	2 (1%) 70 41	46, 63, 89, 142	0
27	9	126/126 (100%)	-0.15	1 (0%) 86 65	33, 50, 69, 92	0
27	DA	126/126 (100%)	-0.02	2 (1%) 72 44	37, 55, 79, 96	0
28	AA	135/135 (100%)	0.66	6 (4%) 34 13	65, 80, 103, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DB	135/135 (100%)	0.65	9 (6%) 17 5	75, 97, 119, 125	0
29	AB	148/148 (100%)	-0.22	0 100 100	24, 42, 79, 92	0
29	DC	148/148 (100%)	-0.15	0 100 100	26, 49, 78, 89	0
30	AC	58/58 (100%)	-0.20	0 100 100	27, 47, 111, 141	0
30	DD	58/58 (100%)	-0.21	1 (1%) 70 41	30, 53, 92, 108	0
31	AD	97/97 (100%)	0.27	3 (3%) 49 21	62, 75, 101, 127	0
31	DE	97/97 (100%)	0.35	5 (5%) 27 10	69, 84, 117, 131	0
32	AE	109/109 (100%)	-0.06	3 (2%) 53 25	40, 58, 116, 136	0
32	DF	109/109 (100%)	-0.02	5 (4%) 32 12	39, 53, 120, 142	0
33	AF	127/127 (100%)	-0.14	2 (1%) 72 44	24, 37, 56, 121	0
33	DG	127/127 (100%)	-0.05	3 (2%) 59 30	25, 41, 59, 125	0
34	AG	106/106 (100%)	-0.42	0 100 100	28, 36, 62, 95	0
34	DH	106/106 (100%)	-0.34	0 100 100	28, 36, 68, 120	0
35	AH	112/112 (100%)	-0.01	4 (3%) 42 17	39, 59, 119, 136	0
35	DI	112/112 (100%)	-0.00	2 (1%) 68 40	44, 67, 126, 145	0
36	AI	119/119 (100%)	-0.06	1 (0%) 86 65	36, 59, 75, 83	0
36	DJ	119/119 (100%)	-0.06	2 (1%) 70 41	45, 68, 84, 91	0
37	AJ	99/99 (100%)	0.07	6 (6%) 21 7	46, 60, 108, 143	0
37	DK	99/99 (100%)	0.41	6 (6%) 21 7	59, 72, 112, 151	0
38	AK	87/87 (100%)	-0.11	2 (2%) 60 31	29, 36, 59, 115	0
38	DL	87/87 (100%)	0.05	2 (2%) 60 31	34, 43, 74, 156	0
39	AL	77/77 (100%)	0.43	1 (1%) 77 51	64, 84, 120, 132	0
39	DM	77/77 (100%)	1.47	20 (25%) 0 0	67, 91, 127, 132	0
40	AM	50/50 (100%)	-0.25	1 (2%) 65 36	33, 47, 58, 65	0
40	DN	50/50 (100%)	-0.26	0 100 100	42, 52, 65, 77	0
41	AN	52/52 (100%)	-0.22	1 (1%) 66 37	36, 45, 69, 100	0
41	DO	52/52 (100%)	-0.37	0 100 100	30, 36, 59, 92	0
42	AO	25/25 (100%)	-0.14	0 100 100	50, 55, 64, 71	0
42	DP	25/25 (100%)	-0.17	0 100 100	45, 53, 65, 76	0
43	AP	105/105 (100%)	0.04	2 (1%) 66 37	28, 49, 81, 150	0
43	DQ	105/105 (100%)	-0.10	1 (0%) 82 59	33, 50, 81, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
44	AQ	91/91 (100%)	-0.31	0	100	100	36, 49, 81, 96	0
44	DR	91/91 (100%)	-0.31	0	100	100	36, 54, 76, 84	0
45	i	159/168 (94%)	0.90	25 (15%)	2	1	49, 98, 163, 168	0
46	p0	143/219 (65%)	1.32	37 (25%)	0	0	85, 106, 174, 178	0
47	sM	63/104 (60%)	0.89	12 (19%)	1	0	55, 105, 131, 138	0
48	A	1781/1800 (98%)	0.16	89 (4%)	28	10	45, 85, 220, 289	0
48	sR	1783/1800 (99%)	0.14	88 (4%)	29	11	39, 76, 187, 269	0
49	B	206/206 (100%)	0.73	24 (11%)	4	1	90, 114, 140, 174	0
49	s0	206/206 (100%)	0.47	14 (6%)	17	5	76, 100, 125, 142	0
50	C	214/216 (99%)	1.23	44 (20%)	1	0	93, 128, 163, 175	0
50	s1	216/216 (100%)	0.54	12 (5%)	24	8	66, 85, 121, 152	0
51	D	217/217 (100%)	0.13	4 (1%)	68	40	71, 90, 113, 136	0
51	s2	217/217 (100%)	0.16	6 (2%)	53	25	59, 79, 101, 128	0
52	E	223/223 (100%)	0.48	13 (5%)	23	7	74, 93, 131, 173	0
52	s3	223/223 (100%)	0.42	10 (4%)	33	12	73, 106, 139, 159	0
53	F	260/260 (100%)	0.41	8 (3%)	49	21	65, 85, 104, 157	0
53	s4	260/260 (100%)	0.19	6 (2%)	60	31	54, 80, 100, 152	0
54	G	206/206 (100%)	0.96	30 (14%)	2	1	89, 114, 139, 171	0
54	s5	206/206 (100%)	0.94	27 (13%)	3	1	78, 106, 139, 163	0
55	H	226/226 (100%)	0.50	17 (7%)	14	4	61, 95, 135, 168	0
55	s6	218/226 (96%)	0.29	13 (5%)	21	7	49, 80, 118, 141	0
56	I	184/186 (98%)	0.85	24 (13%)	3	1	81, 117, 151, 173	0
56	s7	186/186 (100%)	0.91	25 (13%)	3	1	74, 111, 152, 173	0
57	J	188/199 (94%)	0.17	6 (3%)	47	20	47, 65, 105, 130	0
57	s8	188/199 (94%)	0.35	9 (4%)	30	11	43, 71, 119, 137	0
58	K	185/185 (100%)	0.79	20 (10%)	5	2	81, 98, 138, 175	0
58	s9	185/185 (100%)	0.49	10 (5%)	25	9	67, 83, 126, 178	0
59	L	96/105 (91%)	0.55	1 (1%)	82	59	74, 102, 139, 163	0
59	c0	96/105 (91%)	1.48	24 (25%)	0	0	92, 127, 157, 175	0
60	M	155/155 (100%)	0.57	18 (11%)	4	1	52, 65, 151, 176	0
60	c1	146/155 (94%)	0.35	10 (6%)	17	5	49, 68, 116, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
61	N	124/143 (86%)	1.78	50 (40%) 0 0	124, 148, 177, 187	0
61	c2	124/143 (86%)	2.68	77 (62%) 0 0	167, 178, 203, 219	0
62	O	150/150 (100%)	0.20	4 (2%) 54 26	58, 84, 107, 127	0
62	c3	150/150 (100%)	-0.07	0 100 100	56, 77, 102, 126	0
63	P	127/128 (99%)	1.28	31 (24%) 0 0	67, 131, 155, 163	0
63	c4	128/128 (100%)	0.66	12 (9%) 8 3	53, 87, 102, 110	0
64	Q	124/135 (91%)	0.49	6 (4%) 30 11	69, 86, 147, 175	0
64	c5	135/135 (100%)	0.75	16 (11%) 4 1	77, 100, 139, 149	0
65	R	141/142 (99%)	0.80	19 (13%) 3 1	76, 104, 114, 121	0
65	c6	142/142 (100%)	0.66	13 (9%) 9 3	65, 99, 118, 149	0
66	S	120/125 (96%)	0.40	11 (9%) 9 3	83, 111, 155, 165	0
67	T	145/145 (100%)	0.56	15 (10%) 6 2	66, 100, 134, 148	0
67	c8	145/145 (100%)	0.50	13 (8%) 9 3	78, 95, 133, 156	0
68	U	143/143 (100%)	0.53	10 (6%) 16 5	78, 99, 125, 149	0
68	c9	143/143 (100%)	0.53	12 (8%) 11 3	71, 93, 120, 146	0
69	V	107/110 (97%)	1.02	24 (22%) 0 0	66, 107, 159, 169	0
69	d0	110/110 (100%)	1.34	28 (25%) 0 0	68, 113, 164, 172	0
70	W	87/87 (100%)	0.56	7 (8%) 12 4	89, 98, 123, 140	0
70	d1	87/87 (100%)	0.29	5 (5%) 23 8	70, 83, 115, 137	0
71	X	129/129 (100%)	0.20	1 (0%) 86 65	64, 80, 92, 97	0
71	d2	129/129 (100%)	-0.19	0 100 100	54, 68, 77, 86	0
72	Y	144/144 (100%)	-0.06	0 100 100	52, 62, 77, 113	0
72	d3	144/144 (100%)	-0.11	1 (0%) 87 69	43, 52, 71, 108	0
73	Z	134/134 (100%)	0.58	7 (5%) 27 10	63, 97, 136, 156	0
73	d4	134/134 (100%)	0.18	5 (3%) 41 17	58, 86, 117, 146	0
74	a	70/70 (100%)	1.49	23 (32%) 0 0	110, 129, 149, 159	0
74	d5	69/70 (98%)	1.45	22 (31%) 0 0	90, 122, 141, 152	0
75	b	97/97 (100%)	0.86	15 (15%) 2 1	73, 101, 162, 171	0
75	d6	97/97 (100%)	0.15	2 (2%) 63 34	55, 76, 112, 124	0
76	c	81/81 (100%)	0.86	10 (12%) 4 1	77, 96, 147, 155	0
76	d7	81/81 (100%)	0.69	12 (14%) 2 1	68, 84, 146, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
77	d	63/63 (100%)	1.22	11 (17%) 1 0	106, 124, 145, 152	0
77	d8	63/63 (100%)	1.59	20 (31%) 0 0	94, 117, 146, 163	0
78	d9	53/53 (100%)	0.40	2 (3%) 40 16	68, 80, 127, 157	0
78	e	53/53 (100%)	-0.08	1 (1%) 66 37	68, 75, 95, 120	0
79	e0	62/62 (100%)	0.71	6 (9%) 7 2	55, 83, 146, 149	0
79	f	60/62 (96%)	1.21	8 (13%) 3 1	55, 92, 162, 167	0
80	g	71/71 (100%)	1.15	15 (21%) 1 0	100, 130, 157, 167	0
81	Rb	318/318 (100%)	1.31	80 (25%) 0 0	103, 125, 145, 164	0
81	h	318/318 (100%)	0.89	43 (13%) 3 1	92, 114, 155, 188	0
82	c7	117/121 (96%)	0.32	6 (5%) 28 10	76, 101, 137, 150	0
83	e1	51/51 (100%)	1.49	15 (29%) 0 0	145, 158, 171, 177	0
All	All	33004/33349 (98%)	0.19	1773 (5%) 25 9	23, 66, 144, 289	0

The worst 5 of 1773 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	CR	161	ALA	21.9
18	CR	160	ALA	18.7
25	7	76	VAL	16.1
25	7	75	THR	15.5
18	CR	162	GLU	15.3

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3834	1/1	0.28	0.47	61,61,61,61	0
85	MG	1	4165	1/1	0.32	0.36	153,153,153,153	0
85	MG	AR	4138	1/1	0.39	0.48	75,75,75,75	0
85	MG	AR	4055	1/1	0.40	0.54	72,72,72,72	0
85	MG	1	3970	1/1	0.41	0.29	82,82,82,82	0
85	MG	sR	2066	1/1	0.41	0.43	73,73,73,73	0
85	MG	AR	4156	1/1	0.43	0.66	56,56,56,56	0
85	MG	sR	2157	1/1	0.47	0.66	71,71,71,71	0
85	MG	4	229	1/1	0.47	0.37	55,55,55,55	0
85	MG	3	210	1/1	0.52	0.45	46,46,46,46	0
85	MG	AR	4006	1/1	0.53	0.20	54,54,54,54	0
85	MG	1	3822	1/1	0.55	0.73	69,69,69,69	0
85	MG	AR	4102	1/1	0.56	0.69	53,53,53,53	0
85	MG	AR	4126	1/1	0.57	0.79	46,46,46,46	0
85	MG	3	216	1/1	0.57	0.49	78,78,78,78	0
85	MG	AR	4230	1/1	0.58	0.40	59,59,59,59	0
85	MG	AR	4113	1/1	0.59	0.52	63,63,63,63	0
85	MG	sR	2142	1/1	0.59	0.28	65,65,65,65	0
85	MG	AR	3957	1/1	0.59	0.30	57,57,57,57	0
85	MG	A	2119	1/1	0.59	0.67	66,66,66,66	0
84	OHX	AR	3742	7/7	0.60	0.35	225,225,226,226	0
85	MG	AR	4004	1/1	0.60	0.36	68,68,68,68	0
85	MG	1	4076	1/1	0.61	0.34	82,82,82,82	0
85	MG	1	4116	1/1	0.61	0.51	52,52,52,52	0
85	MG	l	404	1/1	0.61	0.57	44,44,44,44	0
85	MG	sR	2185	1/1	0.61	0.60	68,68,68,68	0
85	MG	s	300	1/1	0.62	0.18	63,63,63,63	0
85	MG	1	4115	1/1	0.62	0.31	60,60,60,60	0
85	MG	AR	4236	1/1	0.62	0.53	58,58,58,58	0
84	OHX	CG	302	7/7	0.64	0.33	208,208,209,209	0
85	MG	AR	4091	1/1	0.64	0.49	70,70,70,70	0
85	MG	sR	2082	1/1	0.64	0.60	63,63,63,63	0
85	MG	AR	4085	1/1	0.65	0.41	73,73,73,73	0
85	MG	A	2098	1/1	0.65	0.21	96,96,96,96	0
85	MG	1	4155	1/1	0.65	0.68	71,71,71,71	0
85	MG	AR	4186	1/1	0.65	0.45	60,60,60,60	0
85	MG	AR	4038	1/1	0.65	0.47	57,57,57,57	0
85	MG	A	2068	1/1	0.65	0.44	73,73,73,73	0
85	MG	x	206	1/1	0.65	0.56	47,47,47,47	0
85	MG	sR	2151	1/1	0.66	0.40	63,63,63,63	0
85	MG	A	2113	1/1	0.66	0.41	78,78,78,78	0
85	MG	AR	4059	1/1	0.66	0.19	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3817	1/1	0.66	0.18	106,106,106,106	0
85	MG	1	3979	1/1	0.67	0.35	59,59,59,59	0
85	MG	sR	2170	1/1	0.67	0.39	59,59,59,59	0
85	MG	1	3802	1/1	0.67	0.47	52,52,52,52	0
85	MG	AR	4183	1/1	0.67	0.14	102,102,102,102	0
85	MG	AR	3777	1/1	0.67	0.25	78,78,78,78	0
85	MG	AR	4130	1/1	0.67	0.24	64,64,64,64	0
85	MG	1	3921	1/1	0.68	0.39	39,39,39,39	0
85	MG	A	2115	1/1	0.68	0.34	69,69,69,69	0
85	MG	AR	4048	1/1	0.68	0.33	68,68,68,68	0
85	MG	AR	3908	1/1	0.68	0.39	41,41,41,41	0
84	OHX	AR	3740	7/7	0.68	0.55	212,212,213,213	0
85	MG	1	4033	1/1	0.68	0.32	73,73,73,73	0
85	MG	AR	4145	1/1	0.68	0.27	48,48,48,48	0
85	MG	d3	202	1/1	0.69	0.30	59,59,59,59	0
85	MG	1	4045	1/1	0.69	0.26	58,58,58,58	0
85	MG	AR	4037	1/1	0.69	0.30	70,70,70,70	0
85	MG	AR	4027	1/1	0.70	0.12	105,105,105,105	0
85	MG	AR	4124	1/1	0.70	0.17	73,73,73,73	0
84	OHX	sR	2041	7/7	0.70	0.30	238,238,239,240	0
85	MG	A	2104	1/1	0.71	0.59	67,67,67,67	0
85	MG	sR	2121	1/1	0.71	0.32	69,69,69,69	0
85	MG	AR	4049	1/1	0.71	0.20	52,52,52,52	0
85	MG	AR	4227	1/1	0.71	0.60	78,78,78,78	0
85	MG	1	4104	1/1	0.71	0.57	47,47,47,47	0
85	MG	AR	3796	1/1	0.71	0.34	62,62,62,62	0
85	MG	1	3994	1/1	0.72	0.59	45,45,45,45	0
85	MG	1	4183	1/1	0.72	0.14	67,67,67,67	0
85	MG	AR	4169	1/1	0.72	0.99	101,101,101,101	0
85	MG	sR	2069	1/1	0.72	0.33	53,53,53,53	0
85	MG	AR	4014	1/1	0.72	0.19	53,53,53,53	0
85	MG	AR	3972	1/1	0.72	0.64	52,52,52,52	0
85	MG	A	2110	1/1	0.73	0.25	78,78,78,78	0
85	MG	AR	4110	1/1	0.73	0.30	56,56,56,56	0
85	MG	sR	2187	1/1	0.73	0.59	70,70,70,70	0
85	MG	AR	4155	1/1	0.73	0.35	46,46,46,46	0
85	MG	A	2046	1/1	0.73	0.27	55,55,55,55	0
85	MG	AR	3989	1/1	0.73	0.72	58,58,58,58	0
85	MG	DA	201	1/1	0.73	0.22	52,52,52,52	0
85	MG	A	2150	1/1	0.73	0.39	51,51,51,51	0
85	MG	1	3834	1/1	0.73	0.45	42,42,42,42	0
84	OHX	1	3673	7/7	0.74	0.47	183,183,183,183	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4176	1/1	0.74	0.22	60,60,60,60	0
85	MG	1	4138	1/1	0.74	0.35	44,44,44,44	0
85	MG	1	4125	1/1	0.74	0.38	49,49,49,49	0
85	MG	AR	3974	1/1	0.74	0.41	71,71,71,71	0
85	MG	1	4003	1/1	0.74	0.43	62,62,62,62	0
85	MG	1	3988	1/1	0.74	0.44	44,44,44,44	0
85	MG	1	4032	1/1	0.74	0.58	66,66,66,66	0
85	MG	A	2134	1/1	0.75	0.55	53,53,53,53	0
84	OHX	AR	3746	7/7	0.75	0.20	269,269,270,270	0
85	MG	1	4100	1/1	0.75	0.28	46,46,46,46	0
85	MG	AT	221	1/1	0.75	0.77	57,57,57,57	0
85	MG	sR	2074	1/1	0.75	0.37	51,51,51,51	0
85	MG	A	2138	1/1	0.76	0.33	74,74,74,74	0
85	MG	AR	3966	1/1	0.76	0.55	55,55,55,55	0
85	MG	1	4152	1/1	0.76	0.35	37,37,37,37	0
84	OHX	AR	3735	7/7	0.76	0.34	208,208,208,209	0
85	MG	A	2097	1/1	0.76	0.25	75,75,75,75	0
84	OHX	sR	2052	7/7	0.76	0.22	208,209,210,210	0
85	MG	1	4187	1/1	0.76	0.33	52,52,52,52	0
85	MG	AR	4171	1/1	0.76	0.45	50,50,50,50	0
85	MG	l	402	1/1	0.76	0.20	39,39,39,39	0
85	MG	1	3772	1/1	0.76	0.43	50,50,50,50	0
85	MG	1	3790	1/1	0.76	0.79	72,72,72,72	0
85	MG	A	2082	1/1	0.76	0.26	69,69,69,69	0
85	MG	1	4167	1/1	0.76	0.24	57,57,57,57	0
84	OHX	1	3718	7/7	0.77	0.42	254,254,255,255	0
85	MG	AR	4157	1/1	0.77	0.44	62,62,62,62	0
85	MG	AR	4161	1/1	0.77	0.27	52,52,52,52	0
85	MG	1	3824	1/1	0.77	0.34	53,53,53,53	0
85	MG	1	3875	1/1	0.77	0.28	32,32,32,32	0
85	MG	sR	2094	1/1	0.77	0.29	33,33,33,33	0
85	MG	J	302	1/1	0.77	0.30	55,55,55,55	0
85	MG	AR	4233	1/1	0.77	0.44	54,54,54,54	0
85	MG	sR	2159	1/1	0.77	0.63	58,58,58,58	0
85	MG	DC	205	1/1	0.77	0.40	34,34,34,34	0
85	MG	1	4093	1/1	0.77	0.13	68,68,68,68	0
85	MG	sR	2132	1/1	0.77	0.21	59,59,59,59	0
85	MG	CP	504	1/1	0.77	0.40	51,51,51,51	0
85	MG	1	4184	1/1	0.78	0.26	48,48,48,48	0
85	MG	e	102	1/1	0.78	0.17	81,81,81,81	0
85	MG	AR	4187	1/1	0.78	0.29	50,50,50,50	0
84	OHX	A	2039	7/7	0.78	0.40	234,235,236,236	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4162	1/1	0.78	0.49	32,32,32,32	0
85	MG	1	4088	1/1	0.78	0.28	53,53,53,53	0
85	MG	1	3866	1/1	0.78	0.41	44,44,44,44	0
85	MG	l	403	1/1	0.78	0.45	63,63,63,63	0
85	MG	1	4130	1/1	0.78	0.33	69,69,69,69	0
85	MG	1	3985	1/1	0.78	0.46	85,85,85,85	0
85	MG	w	201	1/1	0.78	0.40	54,54,54,54	0
85	MG	1	3784	1/1	0.78	0.39	54,54,54,54	0
85	MG	1	3785	1/1	0.78	0.37	30,30,30,30	0
85	MG	AR	4118	1/1	0.78	0.15	55,55,55,55	0
85	MG	6	202	1/1	0.78	0.30	67,67,67,67	0
85	MG	sR	2076	1/1	0.78	0.37	77,77,77,77	0
85	MG	A	2087	1/1	0.78	0.30	70,70,70,70	0
84	OHX	AR	3670	7/7	0.78	0.37	245,245,245,245	0
85	MG	AR	3803	1/1	0.78	0.51	43,43,43,43	0
85	MG	AR	4150	1/1	0.78	0.31	63,63,63,63	0
85	MG	l	406	1/1	0.78	0.81	72,72,72,72	0
85	MG	AT	224	1/1	0.78	0.29	70,70,70,70	0
85	MG	1	3787	1/1	0.79	0.49	63,63,63,63	0
85	MG	AR	4029	1/1	0.79	0.16	51,51,51,51	0
85	MG	A	2051	1/1	0.79	0.35	69,69,69,69	0
85	MG	AT	225	1/1	0.79	0.71	72,72,72,72	0
84	OHX	1	3698	7/7	0.79	0.29	245,245,246,246	0
84	OHX	sR	2040	7/7	0.79	0.42	165,166,166,167	0
84	OHX	AR	3693	7/7	0.79	0.30	221,222,222,223	0
85	MG	1	4004	1/1	0.79	0.13	66,66,66,66	0
85	MG	1	4094	1/1	0.79	0.32	59,59,59,59	0
85	MG	A	2124	1/1	0.79	0.25	67,67,67,67	0
85	MG	1	4001	1/1	0.79	0.58	61,61,61,61	0
85	MG	sR	2158	1/1	0.79	0.20	62,62,62,62	0
85	MG	AR	4100	1/1	0.79	0.32	63,63,63,63	0
85	MG	1	4123	1/1	0.79	0.28	53,53,53,53	0
84	OHX	AR	3725	7/7	0.79	0.37	178,178,178,178	0
85	MG	sR	2188	1/1	0.79	0.43	62,62,62,62	0
85	MG	1	3878	1/1	0.79	0.49	53,53,53,53	0
85	MG	A	2084	1/1	0.79	0.28	66,66,66,66	0
85	MG	sR	2086	1/1	0.80	0.28	81,81,81,81	0
85	MG	1	3913	1/1	0.80	0.44	40,40,40,40	0
85	MG	sR	2087	1/1	0.80	0.33	53,53,53,53	0
85	MG	A	2102	1/1	0.80	0.61	75,75,75,75	0
85	MG	4	232	1/1	0.80	0.17	52,52,52,52	0
85	MG	AR	3983	1/1	0.80	0.28	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4234	1/1	0.80	0.40	59,59,59,59	0
85	MG	1	3871	1/1	0.80	0.33	70,70,70,70	0
85	MG	1	4005	1/1	0.80	0.30	49,49,49,49	0
85	MG	AR	4182	1/1	0.80	0.28	40,40,40,40	0
85	MG	1	4194	1/1	0.80	0.41	29,29,29,29	0
85	MG	1	4108	1/1	0.80	0.51	69,69,69,69	0
85	MG	1	4110	1/1	0.80	0.34	76,76,76,76	0
84	OHX	1	3682	7/7	0.80	0.28	179,179,180,180	0
85	MG	A	2106	1/1	0.81	0.47	71,71,71,71	0
85	MG	3	219	1/1	0.81	0.16	68,68,68,68	0
84	OHX	4	215	7/7	0.81	0.27	167,168,168,168	0
85	MG	AR	4194	1/1	0.81	0.29	54,54,54,54	0
85	MG	AR	3751	1/1	0.81	0.50	33,33,33,33	0
85	MG	1	3738	1/1	0.81	0.40	36,36,36,36	0
85	MG	A	2132	1/1	0.81	0.23	68,68,68,68	0
85	MG	AR	4162	1/1	0.81	0.40	69,69,69,69	0
85	MG	AR	4043	1/1	0.81	0.39	45,45,45,45	0
85	MG	AR	3899	1/1	0.81	0.43	32,32,32,32	0
85	MG	1	4132	1/1	0.81	0.36	54,54,54,54	0
85	MG	1	4192	1/1	0.81	0.20	32,32,32,32	0
85	MG	AR	4082	1/1	0.81	0.23	37,37,37,37	0
85	MG	1	4185	1/1	0.81	0.35	42,42,42,42	0
85	MG	AT	227	1/1	0.81	0.79	75,75,75,75	0
85	MG	A	2129	1/1	0.81	0.61	65,65,65,65	0
85	MG	1	4047	1/1	0.81	0.65	63,63,63,63	0
85	MG	CE	403	1/1	0.81	0.39	31,31,31,31	0
85	MG	1	4176	1/1	0.81	0.32	66,66,66,66	0
85	MG	CF	403	1/1	0.81	0.38	37,37,37,37	0
85	MG	AR	3985	1/1	0.81	0.37	61,61,61,61	0
85	MG	1	3935	1/1	0.81	0.26	38,38,38,38	0
85	MG	A	2069	1/1	0.81	0.53	65,65,65,65	0
84	OHX	A	2015	7/7	0.81	0.46	213,214,216,216	0
85	MG	sR	2161	1/1	0.81	0.35	58,58,58,58	0
84	OHX	sR	2051	7/7	0.81	0.29	196,196,197,198	0
85	MG	1	3762	1/1	0.81	0.50	45,45,45,45	0
84	OHX	AR	3669	7/7	0.81	0.21	188,189,189,189	0
85	MG	sR	2180	1/1	0.81	0.46	68,68,68,68	0
85	MG	sR	2141	1/1	0.81	0.15	62,62,62,62	0
85	MG	AR	4235	1/1	0.81	0.37	66,66,66,66	0
85	MG	sR	2179	1/1	0.81	0.45	64,64,64,64	0
85	MG	1	3960	1/1	0.82	0.64	47,47,47,47	0
85	MG	AR	4046	1/1	0.82	0.46	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	sR	2085	1/1	0.82	0.68	64,64,64,64	0
85	MG	d6	102	1/1	0.82	0.40	59,59,59,59	0
85	MG	1	3984	1/1	0.82	0.36	54,54,54,54	0
85	MG	AR	4200	1/1	0.82	0.36	46,46,46,46	0
85	MG	AR	3876	1/1	0.82	0.20	50,50,50,50	0
85	MG	AR	3774	1/1	0.82	0.34	48,48,48,48	0
85	MG	AR	4202	1/1	0.82	0.42	50,50,50,50	0
85	MG	CM	202	1/1	0.82	0.17	60,60,60,60	0
85	MG	AR	4207	1/1	0.82	0.23	54,54,54,54	0
85	MG	x	203	1/1	0.82	0.43	65,65,65,65	0
85	MG	A	2061	1/1	0.82	0.44	68,68,68,68	0
85	MG	4	226	1/1	0.82	0.36	55,55,55,55	0
85	MG	AR	4222	1/1	0.82	0.33	73,73,73,73	0
85	MG	1	3971	1/1	0.82	0.23	41,41,41,41	0
85	MG	AR	3982	1/1	0.82	0.30	45,45,45,45	0
85	MG	1	4020	1/1	0.82	0.24	62,62,62,62	0
85	MG	sR	2110	1/1	0.82	0.48	61,61,61,61	0
84	OHX	A	2034	7/7	0.82	0.16	261,262,263,263	0
85	MG	DC	204	1/1	0.82	0.62	47,47,47,47	0
85	MG	1	3808	1/1	0.82	0.32	52,52,52,52	0
85	MG	1	3952	1/1	0.82	0.45	75,75,75,75	0
85	MG	AR	3980	1/1	0.82	0.41	66,66,66,66	0
84	OHX	1	3704	7/7	0.82	0.45	181,181,181,181	0
85	MG	1	4181	1/1	0.83	0.16	50,50,50,50	0
85	MG	AR	3778	1/1	0.83	0.39	52,52,52,52	0
85	MG	A	2053	1/1	0.83	0.50	49,49,49,49	0
85	MG	sR	2116	1/1	0.83	0.32	64,64,64,64	0
85	MG	1	4062	1/1	0.83	0.37	47,47,47,47	0
85	MG	4	230	1/1	0.83	0.50	60,60,60,60	0
85	MG	sR	2138	1/1	0.83	0.26	65,65,65,65	0
85	MG	AR	4238	1/1	0.83	0.39	54,54,54,54	0
85	MG	AR	3819	1/1	0.83	0.37	56,56,56,56	0
85	MG	sR	2183	1/1	0.83	0.58	68,68,68,68	0
85	MG	sR	2124	1/1	0.83	0.52	54,54,54,54	0
85	MG	1	4180	1/1	0.83	0.20	58,58,58,58	0
85	MG	AR	4140	1/1	0.83	0.26	64,64,64,64	0
85	MG	AR	4022	1/1	0.83	0.42	36,36,36,36	0
85	MG	1	4051	1/1	0.83	0.32	44,44,44,44	0
85	MG	sR	2191	1/1	0.83	0.16	67,67,67,67	0
85	MG	n	201	1/1	0.83	0.21	48,48,48,48	0
84	OHX	1	3719	7/7	0.83	0.28	176,176,177,177	0
84	OHX	AS	209	7/7	0.83	0.25	182,183,183,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3968	1/1	0.83	0.31	47,47,47,47	0
85	MG	1	4160	1/1	0.83	0.22	51,51,51,51	0
84	OHX	CM	201	7/7	0.83	0.31	200,200,201,201	0
85	MG	A	2088	1/1	0.83	0.28	55,55,55,55	0
85	MG	1	3981	1/1	0.83	0.25	49,49,49,49	0
85	MG	AR	4165	1/1	0.84	0.34	43,43,43,43	0
85	MG	AR	3830	1/1	0.84	0.24	47,47,47,47	0
85	MG	AR	4122	1/1	0.84	0.47	62,62,62,62	0
85	MG	1	4021	1/1	0.84	0.39	46,46,46,46	0
85	MG	1	4195	1/1	0.84	0.39	25,25,25,25	0
85	MG	AR	4197	1/1	0.84	0.17	82,82,82,82	0
85	MG	1	4122	1/1	0.84	0.24	51,51,51,51	0
85	MG	A	2070	1/1	0.84	0.41	70,70,70,70	0
84	OHX	A	2041	7/7	0.84	0.45	182,182,183,183	0
85	MG	A	2135	1/1	0.84	0.56	70,70,70,70	0
85	MG	t	203	1/1	0.84	0.66	41,41,41,41	0
84	OHX	AR	3653	7/7	0.84	0.32	167,167,168,168	0
84	OHX	A	1971	7/7	0.84	0.18	164,165,166,166	0
85	MG	sR	2122	1/1	0.84	0.23	71,71,71,71	0
84	OHX	AR	3732	7/7	0.84	0.27	227,228,228,228	0
84	OHX	AR	3711	7/7	0.84	0.29	180,181,181,181	0
85	MG	1	4109	1/1	0.84	0.36	40,40,40,40	0
85	MG	k	403	1/1	0.84	0.37	37,37,37,37	0
85	MG	AR	4087	1/1	0.84	0.28	72,72,72,72	0
85	MG	AR	4172	1/1	0.84	0.17	73,73,73,73	0
85	MG	AR	4023	1/1	0.84	0.29	73,73,73,73	0
85	MG	AR	4245	1/1	0.84	0.26	56,56,56,56	0
85	MG	AR	4149	1/1	0.84	0.29	53,53,53,53	0
85	MG	AR	4196	1/1	0.84	0.20	72,72,72,72	0
85	MG	AR	4134	1/1	0.84	0.35	46,46,46,46	0
85	MG	1	4058	1/1	0.84	0.25	45,45,45,45	0
85	MG	1	4178	1/1	0.84	0.33	39,39,39,39	0
85	MG	1	4097	1/1	0.84	0.25	55,55,55,55	0
85	MG	k	402	1/1	0.84	0.25	57,57,57,57	0
85	MG	sR	2172	1/1	0.84	0.39	101,101,101,101	0
85	MG	1	3757	1/1	0.84	0.16	63,63,63,63	0
85	MG	1	4061	1/1	0.84	0.44	55,55,55,55	0
85	MG	sR	2176	1/1	0.84	0.32	64,64,64,64	0
85	MG	d5	201	1/1	0.84	0.08	74,74,74,74	0
85	MG	1	4066	1/1	0.84	0.27	45,45,45,45	0
85	MG	AR	3828	1/1	0.84	0.74	64,64,64,64	0
85	MG	AR	3842	1/1	0.84	0.20	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3896	1/1	0.84	0.56	35,35,35,35	0
85	MG	AR	4166	1/1	0.84	0.11	91,91,91,91	0
85	MG	AR	3753	1/1	0.84	0.27	39,39,39,39	0
84	OHX	A	2040	7/7	0.84	0.27	215,216,216,216	0
84	OHX	z	201	7/7	0.84	0.39	229,229,229,230	0
85	MG	AR	4053	1/1	0.84	0.14	47,47,47,47	0
85	MG	CG	304	1/1	0.84	0.20	59,59,59,59	0
85	MG	AR	4079	1/1	0.85	0.10	57,57,57,57	0
84	OHX	AS	211	7/7	0.85	0.25	190,191,192,192	0
85	MG	1	3753	1/1	0.85	0.39	30,30,30,30	0
85	MG	A	2133	1/1	0.85	0.24	68,68,68,68	0
85	MG	AR	4247	1/1	0.85	0.30	31,31,31,31	0
85	MG	DD	101	1/1	0.85	0.47	41,41,41,41	0
85	MG	d6	101	1/1	0.85	0.62	50,50,50,50	0
85	MG	AR	4052	1/1	0.85	0.46	42,42,42,42	0
85	MG	AR	3920	1/1	0.85	0.56	27,27,27,27	0
84	OHX	sR	2022	7/7	0.85	0.22	215,216,217,218	0
85	MG	1	4154	1/1	0.85	0.31	69,69,69,69	0
85	MG	1	3954	1/1	0.85	0.32	38,38,38,38	0
85	MG	1	3880	1/1	0.85	0.59	48,48,48,48	0
85	MG	3	220	1/1	0.85	0.23	58,58,58,58	0
85	MG	1	4103	1/1	0.85	0.24	48,48,48,48	0
85	MG	AR	4104	1/1	0.85	0.26	49,49,49,49	0
85	MG	AR	3996	1/1	0.85	0.20	63,63,63,63	0
85	MG	AR	4028	1/1	0.85	0.23	48,48,48,48	0
85	MG	1	3780	1/1	0.85	0.23	43,43,43,43	0
85	MG	1	3987	1/1	0.85	0.23	51,51,51,51	0
85	MG	A	2105	1/1	0.85	0.40	58,58,58,58	0
84	OHX	A	1946	7/7	0.85	0.16	181,182,183,183	0
85	MG	AR	4081	1/1	0.85	0.15	107,107,107,107	0
85	MG	sR	2117	1/1	0.85	0.16	88,88,88,88	0
84	OHX	1	3709	7/7	0.85	0.33	189,190,190,190	0
85	MG	A	2131	1/1	0.85	0.20	90,90,90,90	0
84	OHX	4	214	7/7	0.85	0.33	187,187,187,187	0
85	MG	1	4083	1/1	0.85	0.43	56,56,56,56	0
84	OHX	1	3697	7/7	0.85	0.40	154,155,155,155	0
85	MG	CR	203	1/1	0.85	0.37	112,112,112,112	0
85	MG	AR	4089	1/1	0.85	0.31	52,52,52,52	0
85	MG	AR	4012	1/1	0.85	0.37	60,60,60,60	0
85	MG	AR	4036	1/1	0.85	0.30	61,61,61,61	0
85	MG	A	2109	1/1	0.85	0.53	60,60,60,60	0
85	MG	1	4046	1/1	0.85	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4061	1/1	0.85	0.22	56,56,56,56	0
85	MG	CE	404	1/1	0.85	0.32	31,31,31,31	0
85	MG	j	301	1/1	0.85	0.36	33,33,33,33	0
84	OHX	sR	2050	7/7	0.85	0.31	224,224,225,225	0
85	MG	A	2085	1/1	0.85	0.15	75,75,75,75	0
85	MG	AR	3835	1/1	0.85	0.63	58,58,58,58	0
85	MG	1	3855	1/1	0.85	0.26	31,31,31,31	0
85	MG	1	4029	1/1	0.85	0.36	46,46,46,46	0
85	MG	AR	3759	1/1	0.85	0.38	50,50,50,50	0
85	MG	1	3982	1/1	0.85	0.24	46,46,46,46	0
85	MG	1	4065	1/1	0.85	0.20	46,46,46,46	0
85	MG	1	3949	1/1	0.85	0.20	46,46,46,46	0
85	MG	AR	4056	1/1	0.85	0.25	55,55,55,55	0
85	MG	1	4073	1/1	0.85	0.63	47,47,47,47	0
85	MG	AR	4163	1/1	0.85	0.18	50,50,50,50	0
84	OHX	s1	301	7/7	0.85	0.41	188,189,190,190	0
85	MG	AS	228	1/1	0.85	0.07	72,72,72,72	0
85	MG	sR	2079	1/1	0.85	0.40	46,46,46,46	0
85	MG	AR	3921	1/1	0.85	0.57	31,31,31,31	0
85	MG	1	4161	1/1	0.85	0.29	54,54,54,54	0
85	MG	1	4098	1/1	0.85	0.44	50,50,50,50	0
85	MG	1	3820	1/1	0.85	0.29	51,51,51,51	0
85	MG	AB	204	1/1	0.86	0.24	35,35,35,35	0
85	MG	sR	2080	1/1	0.86	0.52	70,70,70,70	0
85	MG	AR	3789	1/1	0.86	0.38	25,25,25,25	0
85	MG	AR	3826	1/1	0.86	0.35	69,69,69,69	0
84	OHX	A	2024	7/7	0.86	0.51	164,165,166,166	0
85	MG	1	3966	1/1	0.86	0.20	70,70,70,70	0
85	MG	AR	4129	1/1	0.86	0.26	91,91,91,91	0
84	OHX	A	2029	7/7	0.86	0.18	219,220,221,221	0
85	MG	1	4027	1/1	0.86	0.43	41,41,41,41	0
85	MG	AR	3909	1/1	0.86	0.30	22,22,22,22	0
85	MG	1	4030	1/1	0.86	0.35	60,60,60,60	0
85	MG	1	4036	1/1	0.86	0.59	55,55,55,55	0
85	MG	A	2086	1/1	0.86	0.23	50,50,50,50	0
85	MG	AR	4024	1/1	0.86	0.55	48,48,48,48	0
84	OHX	AR	3726	7/7	0.86	0.33	214,215,215,216	0
85	MG	1	4163	1/1	0.86	0.22	45,45,45,45	0
85	MG	sR	2083	1/1	0.86	0.47	69,69,69,69	0
84	OHX	CO	201	7/7	0.86	0.25	244,244,245,245	0
85	MG	A	2081	1/1	0.86	0.42	61,61,61,61	0
85	MG	1	3806	1/1	0.86	0.23	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4117	1/1	0.86	0.34	60,60,60,60	0
85	MG	AR	4168	1/1	0.86	0.30	44,44,44,44	0
85	MG	AR	4008	1/1	0.86	0.43	58,58,58,58	0
85	MG	sR	2118	1/1	0.86	0.28	72,72,72,72	0
85	MG	AR	4051	1/1	0.86	0.39	43,43,43,43	0
85	MG	AR	4003	1/1	0.86	0.26	45,45,45,45	0
85	MG	sR	2070	1/1	0.86	0.41	65,65,65,65	0
85	MG	AR	4034	1/1	0.86	0.12	52,52,52,52	0
85	MG	4	231	1/1	0.86	0.28	66,66,66,66	0
84	OHX	AR	3652	7/7	0.86	0.28	140,141,141,141	0
85	MG	AR	3869	1/1	0.86	0.48	28,28,28,28	0
85	MG	AS	217	1/1	0.86	0.32	50,50,50,50	0
84	OHX	A	2042	7/7	0.86	0.19	211,213,213,214	0
85	MG	sR	2123	1/1	0.86	0.31	65,65,65,65	0
84	OHX	A	2036	7/7	0.86	0.13	277,278,279,279	0
85	MG	AR	3916	1/1	0.86	0.46	49,49,49,49	0
85	MG	AR	4131	1/1	0.86	0.13	65,65,65,65	0
85	MG	1	3859	1/1	0.86	0.33	43,43,43,43	0
85	MG	sR	2102	1/1	0.86	0.44	45,45,45,45	0
85	MG	sR	2186	1/1	0.86	0.33	86,86,86,86	0
85	MG	1	3831	1/1	0.86	0.77	66,66,66,66	0
85	MG	AR	3911	1/1	0.86	0.67	35,35,35,35	0
85	MG	sR	2160	1/1	0.86	0.30	51,51,51,51	0
85	MG	AR	3976	1/1	0.86	0.45	39,39,39,39	0
85	MG	sR	2068	1/1	0.86	0.41	60,60,60,60	0
85	MG	A	2094	1/1	0.86	0.46	62,62,62,62	0
85	MG	1	3939	1/1	0.86	0.43	55,55,55,55	0
85	MG	AR	3772	1/1	0.86	0.24	36,36,36,36	0
85	MG	A	2064	1/1	0.86	0.24	69,69,69,69	0
84	OHX	1	3727	7/7	0.87	0.38	167,168,168,168	0
85	MG	1	4172	1/1	0.87	0.26	44,44,44,44	0
85	MG	A	2089	1/1	0.87	0.43	72,72,72,72	0
84	OHX	AR	3637	7/7	0.87	0.16	213,213,213,214	0
84	OHX	1	3710	7/7	0.87	0.18	243,243,244,244	0
84	OHX	c3	201	7/7	0.87	0.21	189,190,191,191	0
85	MG	AR	3762	1/1	0.87	0.31	37,37,37,37	0
85	MG	1	3941	1/1	0.87	0.18	44,44,44,44	0
85	MG	AR	4112	1/1	0.87	0.33	54,54,54,54	0
85	MG	CX	204	1/1	0.87	0.18	57,57,57,57	0
85	MG	A	2137	1/1	0.87	0.33	60,60,60,60	0
84	OHX	AR	3607	7/7	0.87	0.19	168,169,169,169	0
85	MG	1	4050	1/1	0.87	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2076	1/1	0.87	0.50	72,72,72,72	0
85	MG	sR	2064	1/1	0.87	0.77	60,60,60,60	0
85	MG	1	3944	1/1	0.87	0.29	46,46,46,46	0
85	MG	A	2127	1/1	0.87	0.25	72,72,72,72	0
85	MG	sR	2164	1/1	0.87	0.23	107,107,107,107	0
85	MG	AR	4224	1/1	0.87	0.20	79,79,79,79	0
84	OHX	AR	3687	7/7	0.87	0.23	167,168,168,168	0
84	OHX	1	3726	7/7	0.87	0.45	182,183,183,183	0
84	OHX	1	3729	7/7	0.87	0.46	178,179,179,179	0
85	MG	1	4149	1/1	0.87	0.41	27,27,27,27	0
85	MG	1	3754	1/1	0.87	0.48	50,50,50,50	0
85	MG	AR	4042	1/1	0.87	0.36	58,58,58,58	0
84	OHX	AR	3646	7/7	0.87	0.28	162,162,163,163	0
84	OHX	AR	3744	7/7	0.87	0.51	196,196,197,197	0
85	MG	z	202	1/1	0.87	0.27	63,63,63,63	0
85	MG	1	4151	1/1	0.87	0.24	51,51,51,51	0
84	OHX	AR	3676	7/7	0.87	0.21	193,193,193,193	0
85	MG	1	4038	1/1	0.87	0.30	47,47,47,47	0
85	MG	1	4055	1/1	0.87	0.17	41,41,41,41	0
84	OHX	AS	210	7/7	0.87	0.34	153,153,154,154	0
85	MG	1	4191	1/1	0.87	0.09	52,52,52,52	0
85	MG	3	218	1/1	0.87	0.24	64,64,64,64	0
85	MG	1	3948	1/1	0.87	0.18	50,50,50,50	0
85	MG	AR	4067	1/1	0.87	0.29	51,51,51,51	0
85	MG	AR	4088	1/1	0.87	0.34	46,46,46,46	0
84	OHX	AR	3569	7/7	0.87	0.19	143,143,144,144	0
85	MG	AR	4248	1/1	0.87	0.73	45,45,45,45	0
85	MG	AR	3783	1/1	0.87	0.34	33,33,33,33	0
85	MG	1	3967	1/1	0.87	0.44	53,53,53,53	0
85	MG	c8	202	1/1	0.87	0.30	80,80,80,80	0
85	MG	1	4173	1/1	0.87	0.34	51,51,51,51	0
85	MG	AR	3768	1/1	0.87	0.38	40,40,40,40	0
85	MG	AR	3902	1/1	0.87	0.49	44,44,44,44	0
85	MG	A	2146	1/1	0.87	0.62	50,50,50,50	0
85	MG	1	4024	1/1	0.87	0.41	43,43,43,43	0
84	OHX	x	201	7/7	0.87	0.46	143,144,144,144	0
84	OHX	AR	3718	7/7	0.87	0.44	158,158,159,159	0
85	MG	sR	2140	1/1	0.87	0.23	69,69,69,69	0
85	MG	1	3884	1/1	0.87	0.25	45,45,45,45	0
85	MG	sR	2060	1/1	0.87	0.41	46,46,46,46	0
85	MG	AR	4209	1/1	0.87	0.31	58,58,58,58	0
85	MG	AR	4090	1/1	0.87	0.46	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	AR	4244	1/1	0.87	0.21	52,52,52,52	0
85	MG	CP	502	1/1	0.87	0.34	49,49,49,49	0
85	MG	O	202	1/1	0.87	0.47	55,55,55,55	0
85	MG	AR	3812	1/1	0.87	0.53	39,39,39,39	0
84	OHX	sR	1960	7/7	0.87	0.21	140,140,141,141	0
85	MG	x	204	1/1	0.87	0.37	33,33,33,33	0
84	OHX	AR	3720	7/7	0.88	0.37	169,170,170,170	0
85	MG	AR	4214	1/1	0.88	0.26	50,50,50,50	0
87	ZN	e1	501	1/1	0.88	0.03	156,156,156,156	0
84	OHX	AR	3677	7/7	0.88	0.36	146,146,147,147	0
85	MG	1	3829	1/1	0.88	0.42	41,41,41,41	0
85	MG	AR	3815	1/1	0.88	0.35	35,35,35,35	0
85	MG	sR	2071	1/1	0.88	0.43	38,38,38,38	0
85	MG	1	3852	1/1	0.88	0.43	73,73,73,73	0
85	MG	AR	3797	1/1	0.88	0.47	56,56,56,56	0
85	MG	AR	4215	1/1	0.88	0.54	38,38,38,38	0
85	MG	1	4064	1/1	0.88	0.20	57,57,57,57	0
85	MG	A	2056	1/1	0.88	0.38	47,47,47,47	0
85	MG	AT	223	1/1	0.88	0.70	58,58,58,58	0
85	MG	AR	4210	1/1	0.88	0.32	44,44,44,44	0
85	MG	v	304	1/1	0.88	0.47	46,46,46,46	0
85	MG	1	4011	1/1	0.88	0.54	53,53,53,53	0
85	MG	CJ	301	1/1	0.88	0.28	75,75,75,75	0
85	MG	A	2147	1/1	0.88	0.19	103,103,103,103	0
85	MG	1	3733	1/1	0.88	0.80	50,50,50,50	0
85	MG	AR	4075	1/1	0.88	0.23	58,58,58,58	0
85	MG	1	3786	1/1	0.88	0.40	44,44,44,44	0
85	MG	AR	4065	1/1	0.88	0.55	45,45,45,45	0
85	MG	sR	2174	1/1	0.88	0.29	53,53,53,53	0
85	MG	AR	3851	1/1	0.88	0.51	50,50,50,50	0
85	MG	1	4124	1/1	0.88	0.33	71,71,71,71	0
85	MG	AR	3977	1/1	0.88	0.23	24,24,24,24	0
85	MG	1	4182	1/1	0.88	0.55	75,75,75,75	0
85	MG	1	4015	1/1	0.88	0.21	56,56,56,56	0
85	MG	1	4010	1/1	0.88	0.57	51,51,51,51	0
85	MG	sR	2137	1/1	0.88	0.15	61,61,61,61	0
85	MG	sR	2092	1/1	0.88	0.45	77,77,77,77	0
84	OHX	1	3617	7/7	0.88	0.33	165,165,166,166	0
85	MG	1	4111	1/1	0.88	0.29	50,50,50,50	0
85	MG	AR	4181	1/1	0.88	0.47	51,51,51,51	0
85	MG	CR	202	1/1	0.88	0.35	39,39,39,39	0
84	OHX	1	3708	7/7	0.88	0.31	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	1	3888	1/1	0.88	0.10	54,54,54,54	0
85	MG	1	3877	1/1	0.88	0.25	56,56,56,56	0
85	MG	A	2052	1/1	0.88	0.51	53,53,53,53	0
85	MG	1	4146	1/1	0.88	0.24	76,76,76,76	0
85	MG	1	3775	1/1	0.88	0.18	72,72,72,72	0
85	MG	AR	4167	1/1	0.88	0.30	44,44,44,44	0
85	MG	AR	4018	1/1	0.88	0.53	50,50,50,50	0
85	MG	A	2060	1/1	0.88	0.56	45,45,45,45	0
85	MG	AR	3766	1/1	0.88	0.32	58,58,58,58	0
85	MG	AT	219	1/1	0.88	0.39	38,38,38,38	0
85	MG	AR	3953	1/1	0.88	0.58	48,48,48,48	0
85	MG	AP	503	1/1	0.88	0.14	68,68,68,68	0
85	MG	CR	206	1/1	0.88	0.29	46,46,46,46	0
85	MG	1	3978	1/1	0.88	0.38	47,47,47,47	0
85	MG	AR	4069	1/1	0.88	0.43	51,51,51,51	0
85	MG	sR	2096	1/1	0.88	0.51	60,60,60,60	0
85	MG	AR	3814	1/1	0.88	0.33	82,82,82,82	0
85	MG	1	4127	1/1	0.88	0.20	64,64,64,64	0
87	ZN	c	101	1/1	0.88	0.39	190,190,190,190	0
85	MG	1	3963	1/1	0.88	0.29	33,33,33,33	0
84	OHX	AR	3674	7/7	0.88	0.23	153,153,153,154	0
85	MG	1	4081	1/1	0.88	0.34	52,52,52,52	0
85	MG	AR	4094	1/1	0.88	0.29	56,56,56,56	0
85	MG	AR	4026	1/1	0.88	0.24	46,46,46,46	0
85	MG	s8	302	1/1	0.88	0.31	54,54,54,54	0
84	OHX	AR	3713	7/7	0.88	0.29	164,164,164,164	0
85	MG	1	4054	1/1	0.88	0.44	45,45,45,45	0
85	MG	AR	4031	1/1	0.88	0.24	73,73,73,73	0
84	OHX	AR	3743	7/7	0.88	0.16	160,161,161,162	0
85	MG	AR	3840	1/1	0.88	0.29	68,68,68,68	0
85	MG	sR	2126	1/1	0.88	0.36	58,58,58,58	0
85	MG	1	4016	1/1	0.88	0.34	51,51,51,51	0
84	OHX	CF	402	7/7	0.88	0.51	190,191,192,192	0
85	MG	1	3977	1/1	0.88	0.21	48,48,48,48	0
84	OHX	AT	218	7/7	0.88	0.34	162,162,163,163	0
85	MG	AR	4041	1/1	0.88	0.45	48,48,48,48	0
84	OHX	3	208	7/7	0.88	0.18	190,190,191,191	0
84	OHX	1	3607	7/7	0.88	0.23	152,152,153,153	0
85	MG	1	3848	1/1	0.88	0.44	43,43,43,43	0
84	OHX	1	3720	7/7	0.88	0.45	163,163,163,163	0
85	MG	AR	4057	1/1	0.88	0.12	50,50,50,50	0
85	MG	AR	4030	1/1	0.88	0.21	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	d3	201	1/1	0.88	0.30	55,55,55,55	0
84	OHX	1	3721	7/7	0.88	0.42	172,172,173,173	0
85	MG	1	4200	1/1	0.88	0.61	49,49,49,49	0
84	OHX	AR	3522	7/7	0.88	0.17	164,165,165,165	0
84	OHX	AR	3730	7/7	0.88	0.17	207,207,208,208	0
85	MG	AR	4219	1/1	0.88	0.21	40,40,40,40	0
85	MG	1	3746	1/1	0.88	0.31	46,46,46,46	0
84	OHX	1	3716	7/7	0.88	0.39	164,164,165,165	0
85	MG	AR	3905	1/1	0.88	0.56	49,49,49,49	0
85	MG	AR	4035	1/1	0.88	0.19	38,38,38,38	0
85	MG	AR	4148	1/1	0.89	0.42	50,50,50,50	0
85	MG	AR	3963	1/1	0.89	0.14	34,34,34,34	0
84	OHX	1	3713	7/7	0.89	0.27	138,139,139,139	0
85	MG	AR	4141	1/1	0.89	0.50	81,81,81,81	0
84	OHX	AT	213	7/7	0.89	0.29	187,187,187,187	0
84	OHX	AR	3729	7/7	0.89	0.31	177,177,178,178	0
85	MG	1	3749	1/1	0.89	0.54	41,41,41,41	0
84	OHX	1	3648	7/7	0.89	0.20	195,195,195,196	0
85	MG	1	4000	1/1	0.89	0.32	60,60,60,60	0
84	OHX	AR	3739	7/7	0.89	0.45	190,191,191,191	0
84	OHX	AR	3736	7/7	0.89	0.32	154,155,155,156	0
85	MG	AR	3776	1/1	0.89	0.22	31,31,31,31	0
85	MG	AR	4178	1/1	0.89	0.06	94,94,94,94	0
84	OHX	1	3730	7/7	0.89	0.36	159,160,160,160	0
85	MG	4	222	1/1	0.89	0.47	40,40,40,40	0
84	OHX	sR	2042	7/7	0.89	0.29	179,180,180,181	0
85	MG	AR	4226	1/1	0.89	0.28	38,38,38,38	0
84	OHX	AR	3602	7/7	0.89	0.27	173,174,174,175	0
84	OHX	1	3699	7/7	0.89	0.32	151,151,152,152	0
84	OHX	sR	2047	7/7	0.89	0.26	195,195,196,196	0
85	MG	AR	3927	1/1	0.89	0.48	36,36,36,36	0
85	MG	1	3938	1/1	0.89	0.45	52,52,52,52	0
84	OHX	sR	2046	7/7	0.89	0.40	178,178,178,179	0
84	OHX	AR	3702	7/7	0.89	0.33	156,156,157,157	0
84	OHX	1	3724	7/7	0.89	0.47	186,186,187,188	0
84	OHX	A	2011	7/7	0.89	0.22	182,183,183,183	0
85	MG	AR	3981	1/1	0.89	0.45	39,39,39,39	0
85	MG	1	4216	1/1	0.89	0.12	53,53,53,53	0
85	MG	AR	4107	1/1	0.89	0.28	38,38,38,38	0
84	OHX	A	2007	7/7	0.89	0.19	220,222,222,223	0
84	OHX	AR	3708	7/7	0.89	0.34	181,182,182,182	0
85	MG	AR	4137	1/1	0.89	0.33	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	sR	2136	1/1	0.89	0.33	71,71,71,71	0
85	MG	1	3773	1/1	0.89	0.44	28,28,28,28	0
85	MG	1	3943	1/1	0.89	0.36	40,40,40,40	0
85	MG	AR	4237	1/1	0.89	0.71	59,59,59,59	0
85	MG	AR	3944	1/1	0.89	0.55	41,41,41,41	0
85	MG	A	2103	1/1	0.89	0.40	89,89,89,89	0
84	OHX	sR	2003	7/7	0.89	0.21	188,188,189,189	0
85	MG	AR	4013	1/1	0.89	0.60	52,52,52,52	0
85	MG	1	4199	1/1	0.89	0.40	31,31,31,31	0
85	MG	AR	3965	1/1	0.89	0.19	46,46,46,46	0
85	MG	1	3750	1/1	0.89	0.21	57,57,57,57	0
85	MG	AR	4105	1/1	0.89	0.33	51,51,51,51	0
85	MG	1	3764	1/1	0.89	0.53	47,47,47,47	0
85	MG	c6	201	1/1	0.89	0.23	82,82,82,82	0
85	MG	AR	3893	1/1	0.89	0.39	32,32,32,32	0
85	MG	1	4107	1/1	0.89	0.19	43,43,43,43	0
85	MG	sR	2145	1/1	0.89	0.36	58,58,58,58	0
85	MG	AR	3951	1/1	0.89	0.12	39,39,39,39	0
84	OHX	1	3671	7/7	0.89	0.44	152,153,154,154	0
85	MG	1	4044	1/1	0.89	0.25	39,39,39,39	0
85	MG	1	3758	1/1	0.89	0.31	41,41,41,41	0
85	MG	sR	2133	1/1	0.89	0.30	50,50,50,50	0
85	MG	1	4140	1/1	0.89	0.44	56,56,56,56	0
84	OHX	AR	3688	7/7	0.89	0.42	182,182,182,183	0
84	OHX	A	2030	7/7	0.89	0.33	163,164,165,165	0
85	MG	AR	4211	1/1	0.89	0.41	69,69,69,69	0
84	OHX	A	2038	7/7	0.89	0.52	164,164,166,166	0
85	MG	1	3942	1/1	0.89	0.27	44,44,44,44	0
85	MG	AR	3884	1/1	0.89	0.24	46,46,46,46	0
85	MG	1	4019	1/1	0.89	0.45	53,53,53,53	0
85	MG	AT	222	1/1	0.89	0.72	48,48,48,48	0
85	MG	1	4075	1/1	0.89	0.26	75,75,75,75	0
84	OHX	sR	1991	7/7	0.89	0.31	174,175,175,176	0
85	MG	AR	4173	1/1	0.89	0.26	54,54,54,54	0
85	MG	AR	4019	1/1	0.89	0.25	35,35,35,35	0
85	MG	1	3889	1/1	0.89	0.40	52,52,52,52	0
85	MG	b	101	1/1	0.89	0.22	75,75,75,75	0
85	MG	CM	203	1/1	0.89	0.14	60,60,60,60	0
85	MG	u	201	1/1	0.89	0.19	62,62,62,62	0
85	MG	sR	2154	1/1	0.89	0.14	72,72,72,72	0
85	MG	1	3816	1/1	0.89	0.31	47,47,47,47	0
85	MG	AR	3757	1/1	0.89	0.33	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4025	1/1	0.89	0.22	36,36,36,36	0
84	OHX	AR	3733	7/7	0.89	0.38	153,153,154,154	0
85	MG	AR	4193	1/1	0.89	0.28	57,57,57,57	0
85	MG	1	4114	1/1	0.89	0.75	57,57,57,57	0
85	MG	sR	2155	1/1	0.89	0.22	67,67,67,67	0
85	MG	AR	3755	1/1	0.89	0.33	49,49,49,49	0
85	MG	1	4128	1/1	0.89	0.30	53,53,53,53	0
85	MG	AS	218	1/1	0.89	0.25	60,60,60,60	0
84	OHX	AR	3724	7/7	0.89	0.39	217,218,219,219	0
85	MG	1	3832	1/1	0.89	0.44	57,57,57,57	0
85	MG	AR	3978	1/1	0.89	0.21	55,55,55,55	0
85	MG	1	3957	1/1	0.89	0.21	56,56,56,56	0
84	OHX	AR	3737	7/7	0.89	0.26	189,189,190,190	0
85	MG	A	2054	1/1	0.89	0.31	61,61,61,61	0
85	MG	AR	4251	1/1	0.89	0.09	45,45,45,45	0
85	MG	AR	4083	1/1	0.89	0.16	57,57,57,57	0
85	MG	AR	4198	1/1	0.89	0.55	54,54,54,54	0
85	MG	1	4186	1/1	0.89	0.32	59,59,59,59	0
85	MG	1	4022	1/1	0.89	0.31	42,42,42,42	0
85	MG	1	3741	1/1	0.89	0.34	43,43,43,43	0
85	MG	AR	3818	1/1	0.89	0.33	32,32,32,32	0
85	MG	Y	201	1/1	0.89	0.17	55,55,55,55	0
84	OHX	1	3728	7/7	0.89	0.33	211,212,212,212	0
85	MG	4	216	1/1	0.89	0.62	55,55,55,55	0
84	OHX	AR	3723	7/7	0.89	0.34	168,168,168,169	0
85	MG	AR	3994	1/1	0.90	0.57	49,49,49,49	0
85	MG	AR	3780	1/1	0.90	0.35	76,76,76,76	0
85	MG	AS	220	1/1	0.90	0.24	70,70,70,70	0
84	OHX	AR	3681	7/7	0.90	0.26	165,165,166,166	0
85	MG	1	4164	1/1	0.90	0.38	34,34,34,34	0
85	MG	1	3874	1/1	0.90	0.43	36,36,36,36	0
85	MG	1	3969	1/1	0.90	0.24	66,66,66,66	0
84	OHX	1	3703	7/7	0.90	0.36	209,209,210,210	0
85	MG	1	3825	1/1	0.90	0.25	75,75,75,75	0
85	MG	AS	227	1/1	0.90	0.30	57,57,57,57	0
85	MG	1	4034	1/1	0.90	0.22	34,34,34,34	0
84	OHX	A	2022	7/7	0.90	0.29	194,195,195,196	0
85	MG	A	2128	1/1	0.90	0.35	63,63,63,63	0
85	MG	AR	3785	1/1	0.90	0.29	60,60,60,60	0
85	MG	1	3879	1/1	0.90	0.46	43,43,43,43	0
85	MG	AR	4120	1/1	0.90	0.27	45,45,45,45	0
85	MG	A	2140	1/1	0.90	0.49	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3878	1/1	0.90	0.41	51,51,51,51	0
84	OHX	A	2025	7/7	0.90	0.27	202,203,204,204	0
84	OHX	1	3696	7/7	0.90	0.39	213,214,214,214	0
85	MG	AR	3940	1/1	0.90	0.34	28,28,28,28	0
84	OHX	A	1997	7/7	0.90	0.27	179,180,180,180	0
85	MG	DC	201	1/1	0.90	0.47	44,44,44,44	0
85	MG	A	2080	1/1	0.90	0.44	59,59,59,59	0
85	MG	1	3958	1/1	0.90	0.39	71,71,71,71	0
85	MG	AR	4040	1/1	0.90	0.19	53,53,53,53	0
85	MG	1	4135	1/1	0.90	0.47	44,44,44,44	0
84	OHX	AR	3727	7/7	0.90	0.31	174,174,174,175	0
85	MG	AR	4177	1/1	0.90	0.19	45,45,45,45	0
84	OHX	sR	1969	7/7	0.90	0.17	155,155,156,156	0
85	MG	sR	2105	1/1	0.90	0.46	56,56,56,56	0
85	MG	AR	3924	1/1	0.90	0.36	35,35,35,35	0
85	MG	AR	4032	1/1	0.90	0.34	40,40,40,40	0
85	MG	AR	4044	1/1	0.90	0.17	44,44,44,44	0
84	OHX	AT	217	7/7	0.90	0.28	153,153,153,153	0
84	OHX	AR	3715	7/7	0.90	0.26	139,139,139,139	0
85	MG	1	3843	1/1	0.90	0.40	34,34,34,34	0
85	MG	AR	3988	1/1	0.90	0.31	54,54,54,54	0
84	OHX	sR	2009	7/7	0.90	0.14	175,176,176,177	0
85	MG	A	2111	1/1	0.90	0.52	86,86,86,86	0
84	OHX	AR	3614	7/7	0.90	0.32	151,152,152,152	0
85	MG	1	3821	1/1	0.90	0.25	27,27,27,27	0
85	MG	1	4159	1/1	0.90	0.34	54,54,54,54	0
85	MG	sR	2153	1/1	0.90	0.33	63,63,63,63	0
85	MG	1	4002	1/1	0.90	0.38	38,38,38,38	0
85	MG	A	2063	1/1	0.90	0.44	44,44,44,44	0
85	MG	sR	2062	1/1	0.90	0.41	47,47,47,47	0
85	MG	1	3811	1/1	0.90	0.24	77,77,77,77	0
85	MG	AR	3843	1/1	0.90	0.39	41,41,41,41	0
85	MG	AR	4174	1/1	0.90	0.21	60,60,60,60	0
84	OHX	AR	3734	7/7	0.90	0.17	240,241,242,242	0
85	MG	AR	3813	1/1	0.90	0.22	60,60,60,60	0
85	MG	CQ	201	1/1	0.90	0.34	48,48,48,48	0
85	MG	1	4072	1/1	0.90	0.23	44,44,44,44	0
85	MG	v	303	1/1	0.90	0.47	45,45,45,45	0
85	MG	AR	3771	1/1	0.90	0.47	49,49,49,49	0
85	MG	1	4060	1/1	0.90	0.23	47,47,47,47	0
84	OHX	DL	101	7/7	0.90	0.34	167,167,167,167	0
85	MG	AR	3993	1/1	0.90	0.20	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	sR	2044	7/7	0.90	0.27	194,194,195,195	0
85	MG	sR	2184	1/1	0.90	0.25	55,55,55,55	0
85	MG	AR	3795	1/1	0.90	0.24	39,39,39,39	0
85	MG	sR	2169	1/1	0.90	0.70	55,55,55,55	0
85	MG	1	4134	1/1	0.90	0.24	43,43,43,43	0
84	OHX	AR	3701	7/7	0.90	0.24	168,168,169,169	0
85	MG	AR	4011	1/1	0.90	0.41	30,30,30,30	0
85	MG	1	4179	1/1	0.90	0.19	52,52,52,52	0
85	MG	1	3965	1/1	0.90	0.37	42,42,42,42	0
85	MG	1	4126	1/1	0.90	0.41	54,54,54,54	0
84	OHX	AR	3719	7/7	0.90	0.21	227,227,228,228	0
85	MG	1	4074	1/1	0.90	0.30	53,53,53,53	0
84	OHX	1	3693	7/7	0.90	0.38	183,184,184,184	0
84	OHX	1	3654	7/7	0.90	0.22	159,159,159,159	0
85	MG	AR	4070	1/1	0.90	0.51	63,63,63,63	0
85	MG	d9	102	1/1	0.90	0.13	94,94,94,94	0
84	OHX	sR	2020	7/7	0.90	0.31	174,175,176,176	0
84	OHX	sR	2034	7/7	0.90	0.30	177,178,179,179	0
85	MG	1	3867	1/1	0.90	0.60	58,58,58,58	0
85	MG	1	3947	1/1	0.90	0.41	40,40,40,40	0
85	MG	AR	3794	1/1	0.90	0.40	43,43,43,43	0
85	MG	AR	4084	1/1	0.90	0.25	50,50,50,50	0
85	MG	sR	2059	1/1	0.90	0.42	63,63,63,63	0
85	MG	3	209	1/1	0.90	0.31	49,49,49,49	0
84	OHX	1	3725	7/7	0.90	0.11	188,189,189,189	0
85	MG	1	3991	1/1	0.90	0.62	44,44,44,44	0
85	MG	AR	4073	1/1	0.90	0.14	62,62,62,62	0
85	MG	AR	4111	1/1	0.90	0.09	41,41,41,41	0
84	OHX	sR	1998	7/7	0.90	0.21	190,191,192,192	0
84	OHX	A	2012	7/7	0.90	0.26	162,162,163,163	0
85	MG	1	4113	1/1	0.90	0.30	43,43,43,43	0
85	MG	AR	4160	1/1	0.90	0.34	52,52,52,52	0
85	MG	sR	2143	1/1	0.90	0.14	51,51,51,51	0
85	MG	AR	3992	1/1	0.90	0.22	50,50,50,50	0
85	MG	AR	4116	1/1	0.90	0.47	65,65,65,65	0
84	OHX	sR	2049	7/7	0.90	0.20	217,218,219,219	0
84	OHX	1	3631	7/7	0.90	0.23	170,170,171,172	0
85	MG	AR	3832	1/1	0.90	0.17	53,53,53,53	0
84	OHX	AR	3659	7/7	0.90	0.31	144,144,145,145	0
85	MG	1	4096	1/1	0.90	0.34	45,45,45,45	0
85	MG	AR	3809	1/1	0.90	0.49	43,43,43,43	0
85	MG	1	3929	1/1	0.90	0.67	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3895	1/1	0.90	0.58	50,50,50,50	0
84	OHX	1	3678	7/7	0.90	0.23	189,189,190,190	0
84	OHX	1	3629	7/7	0.90	0.19	163,163,163,163	0
85	MG	AT	201	1/1	0.91	0.29	57,57,57,57	0
85	MG	AR	4017	1/1	0.91	0.35	31,31,31,31	0
85	MG	AR	3754	1/1	0.91	0.29	23,23,23,23	0
85	MG	3	213	1/1	0.91	0.50	32,32,32,32	0
84	OHX	sR	2031	7/7	0.91	0.25	134,134,135,135	0
85	MG	1	4082	1/1	0.91	0.41	58,58,58,58	0
85	MG	4	217	1/1	0.91	0.55	47,47,47,47	0
85	MG	1	4141	1/1	0.91	0.42	53,53,53,53	0
85	MG	AR	3971	1/1	0.91	0.28	42,42,42,42	0
85	MG	sR	2091	1/1	0.91	0.36	56,56,56,56	0
84	OHX	A	2023	7/7	0.91	0.28	178,179,180,180	0
85	MG	AR	4109	1/1	0.91	0.53	50,50,50,50	0
85	MG	AR	3954	1/1	0.91	0.50	48,48,48,48	0
85	MG	AR	4062	1/1	0.91	0.20	64,64,64,64	0
85	MG	A	2117	1/1	0.91	0.53	69,69,69,69	0
85	MG	1	3956	1/1	0.91	0.44	53,53,53,53	0
85	MG	CU	201	1/1	0.91	0.36	48,48,48,48	0
84	OHX	1	3619	7/7	0.91	0.20	179,180,180,181	0
85	MG	DC	203	1/1	0.91	0.32	57,57,57,57	0
85	MG	sR	2067	1/1	0.91	0.33	56,56,56,56	0
85	MG	sR	2072	1/1	0.91	0.87	70,70,70,70	0
85	MG	1	4018	1/1	0.91	0.22	43,43,43,43	0
84	OHX	AR	3645	7/7	0.91	0.20	165,165,166,166	0
85	MG	AR	3833	1/1	0.91	0.32	56,56,56,56	0
85	MG	AR	4097	1/1	0.91	0.26	37,37,37,37	0
85	MG	AS	221	1/1	0.91	0.17	50,50,50,50	0
84	OHX	1	3702	7/7	0.91	0.48	192,192,193,193	0
84	OHX	sR	2007	7/7	0.91	0.20	185,186,187,187	0
84	OHX	AR	3745	7/7	0.91	0.23	208,208,209,209	0
84	OHX	A	1993	7/7	0.91	0.42	172,173,174,174	0
85	MG	1	3907	1/1	0.91	0.47	30,30,30,30	0
84	OHX	1	3598	7/7	0.91	0.39	180,180,180,180	0
85	MG	AR	3889	1/1	0.91	0.48	36,36,36,36	0
84	OHX	sR	2036	7/7	0.91	0.34	173,173,174,175	0
85	MG	AR	3847	1/1	0.91	0.50	52,52,52,52	0
85	MG	A	2095	1/1	0.91	0.37	79,79,79,79	0
85	MG	1	4201	1/1	0.91	0.71	47,47,47,47	0
84	OHX	1	3623	7/7	0.91	0.23	148,148,148,148	0
84	OHX	AR	3511	7/7	0.91	0.21	126,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	1981	7/7	0.91	0.11	215,217,217,217	0
85	MG	AR	4009	1/1	0.91	0.57	35,35,35,35	0
84	OHX	1	3555	7/7	0.91	0.19	153,153,154,154	0
84	OHX	1	3564	7/7	0.91	0.21	142,142,143,143	0
84	OHX	1	3665	7/7	0.91	0.38	150,150,151,151	0
84	OHX	1	3622	7/7	0.91	0.21	151,151,152,152	0
84	OHX	1	3731	7/7	0.91	0.20	165,166,167,168	0
85	MG	A	2114	1/1	0.91	0.31	55,55,55,55	0
85	MG	AR	3897	1/1	0.91	0.57	55,55,55,55	0
85	MG	AR	3781	1/1	0.91	0.26	72,72,72,72	0
85	MG	A	2047	1/1	0.91	0.69	55,55,55,55	0
85	MG	AR	4213	1/1	0.91	0.18	52,52,52,52	0
84	OHX	AR	3741	7/7	0.91	0.26	172,173,173,173	0
85	MG	AR	4188	1/1	0.91	0.15	46,46,46,46	0
85	MG	AR	4152	1/1	0.91	0.36	69,69,69,69	0
84	OHX	1	3692	7/7	0.91	0.50	183,183,184,184	0
84	OHX	H	301	7/7	0.91	0.35	182,183,184,184	0
85	MG	1	4166	1/1	0.91	0.23	70,70,70,70	0
85	MG	1	3794	1/1	0.91	0.42	23,23,23,23	0
84	OHX	1	3618	7/7	0.91	0.23	161,161,161,162	0
84	OHX	AR	3692	7/7	0.91	0.49	146,146,146,146	0
84	OHX	1	3606	7/7	0.91	0.35	141,142,142,143	0
85	MG	1	3946	1/1	0.91	0.56	44,44,44,44	0
85	MG	AR	3955	1/1	0.91	0.13	36,36,36,36	0
84	OHX	A	2026	7/7	0.91	0.38	150,150,151,151	0
85	MG	1	3997	1/1	0.91	0.15	52,52,52,52	0
85	MG	sR	2134	1/1	0.91	0.32	58,58,58,58	0
85	MG	1	3992	1/1	0.91	0.60	56,56,56,56	0
85	MG	A	2057	1/1	0.91	0.50	58,58,58,58	0
85	MG	A	2112	1/1	0.91	0.30	91,91,91,91	0
85	MG	1	4041	1/1	0.91	0.38	43,43,43,43	0
85	MG	1	3760	1/1	0.91	0.51	49,49,49,49	0
85	MG	AR	4010	1/1	0.91	0.38	62,62,62,62	0
85	MG	1	3774	1/1	0.91	0.27	72,72,72,72	0
85	MG	AR	4159	1/1	0.91	0.63	51,51,51,51	0
84	OHX	AR	3728	7/7	0.91	0.45	172,172,173,173	0
85	MG	AR	4095	1/1	0.91	0.39	46,46,46,46	0
85	MG	AR	3882	1/1	0.91	0.45	50,50,50,50	0
85	MG	AR	4071	1/1	0.91	0.25	46,46,46,46	0
85	MG	1	4204	1/1	0.91	0.38	42,42,42,42	0
85	MG	1	4209	1/1	0.91	0.23	42,42,42,42	0
85	MG	AR	4001	1/1	0.91	0.69	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4076	1/1	0.91	0.20	43,43,43,43	0
85	MG	AR	3865	1/1	0.91	0.27	39,39,39,39	0
84	OHX	AR	3650	7/7	0.91	0.24	157,158,158,159	0
85	MG	sR	2165	1/1	0.91	0.65	59,59,59,59	0
85	MG	sR	2144	1/1	0.91	0.93	85,85,85,85	0
85	MG	1	4057	1/1	0.91	0.31	68,68,68,68	0
85	MG	1	4023	1/1	0.91	0.83	58,58,58,58	0
84	OHX	sR	2030	7/7	0.91	0.28	190,190,191,192	0
85	MG	AR	3752	1/1	0.91	0.21	38,38,38,38	0
85	MG	1	4196	1/1	0.91	0.21	68,68,68,68	0
85	MG	1	3813	1/1	0.91	0.53	36,36,36,36	0
85	MG	AR	4058	1/1	0.91	0.25	48,48,48,48	0
85	MG	A	2048	1/1	0.91	0.28	45,45,45,45	0
85	MG	A	2101	1/1	0.91	0.64	63,63,63,63	0
85	MG	4	220	1/1	0.91	0.52	54,54,54,54	0
85	MG	A	2071	1/1	0.91	0.34	53,53,53,53	0
85	MG	AR	4133	1/1	0.91	0.14	97,97,97,97	0
84	OHX	sR	2019	7/7	0.91	0.19	222,223,224,225	0
84	OHX	AR	3722	7/7	0.91	0.23	188,188,188,189	0
85	MG	1	4067	1/1	0.91	0.21	64,64,64,64	0
84	OHX	sR	2023	7/7	0.91	0.33	153,154,155,155	0
85	MG	AR	4033	1/1	0.91	0.38	44,44,44,44	0
85	MG	t	202	1/1	0.91	0.39	86,86,86,86	0
84	OHX	1	3717	7/7	0.91	0.33	188,189,189,189	0
85	MG	1	4136	1/1	0.91	0.29	58,58,58,58	0
84	OHX	AR	3606	7/7	0.91	0.30	145,146,146,146	0
85	MG	1	4091	1/1	0.91	0.29	48,48,48,48	0
85	MG	1	3751	1/1	0.91	0.32	74,74,74,74	0
85	MG	AR	4068	1/1	0.91	0.43	57,57,57,57	0
85	MG	sR	2146	1/1	0.91	0.22	40,40,40,40	0
84	OHX	d9	101	7/7	0.91	0.39	182,183,183,184	0
85	MG	1	4153	1/1	0.91	0.30	52,52,52,52	0
85	MG	AR	3969	1/1	0.91	0.71	57,57,57,57	0
85	MG	1	4039	1/1	0.91	0.39	57,57,57,57	0
84	OHX	CG	301	7/7	0.91	0.19	174,175,176,176	0
85	MG	AR	4080	1/1	0.91	0.46	43,43,43,43	0
85	MG	DR	503	1/1	0.91	0.33	80,80,80,80	0
85	MG	DH	202	1/1	0.91	0.23	51,51,51,51	0
85	MG	CD	302	1/1	0.91	0.47	46,46,46,46	0
85	MG	1	4079	1/1	0.91	0.21	55,55,55,55	0
85	MG	AR	3973	1/1	0.91	0.34	44,44,44,44	0
85	MG	1	3788	1/1	0.91	0.39	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4154	1/1	0.91	0.34	47,47,47,47	0
84	OHX	1	3647	7/7	0.91	0.39	147,148,148,148	0
84	OHX	1	3656	7/7	0.91	0.32	137,137,137,137	0
84	OHX	AR	3604	7/7	0.91	0.19	156,157,157,157	0
85	MG	sR	2131	1/1	0.91	0.51	53,53,53,53	0
85	MG	A	2139	1/1	0.91	0.20	65,65,65,65	0
85	MG	1	4143	1/1	0.91	0.36	47,47,47,47	0
84	OHX	A	2028	7/7	0.91	0.21	186,187,187,188	0
84	OHX	AR	3621	7/7	0.91	0.31	159,159,160,160	0
85	MG	A	2072	1/1	0.91	0.29	60,60,60,60	0
85	MG	o	301	1/1	0.92	0.20	44,44,44,44	0
84	OHX	1	3560	7/7	0.92	0.16	169,169,170,170	0
85	MG	AR	3995	1/1	0.92	0.23	42,42,42,42	0
85	MG	AR	3852	1/1	0.92	0.31	45,45,45,45	0
85	MG	A	2125	1/1	0.92	0.60	52,52,52,52	0
84	OHX	AR	3699	7/7	0.92	0.28	202,202,203,203	0
84	OHX	sR	2048	7/7	0.92	0.27	188,189,190,190	0
85	MG	1	3912	1/1	0.92	0.30	39,39,39,39	0
84	OHX	AR	3658	7/7	0.92	0.34	146,146,146,146	0
84	OHX	AR	3697	7/7	0.92	0.44	157,158,158,159	0
85	MG	AR	4217	1/1	0.92	0.56	43,43,43,43	0
85	MG	AR	3888	1/1	0.92	0.61	37,37,37,37	0
85	MG	AR	3883	1/1	0.92	0.35	47,47,47,47	0
85	MG	1	3783	1/1	0.92	0.29	30,30,30,30	0
85	MG	AR	3962	1/1	0.92	0.30	46,46,46,46	0
85	MG	DR	502	1/1	0.92	0.18	61,61,61,61	0
84	OHX	A	2037	7/7	0.92	0.34	188,189,189,189	0
84	OHX	AR	3714	7/7	0.92	0.26	169,170,170,170	0
85	MG	1	3747	1/1	0.92	0.43	31,31,31,31	0
85	MG	1	3810	1/1	0.92	0.49	45,45,45,45	0
85	MG	AR	3885	1/1	0.92	0.56	41,41,41,41	0
84	OHX	1	3557	7/7	0.92	0.20	145,145,145,145	0
84	OHX	1	3668	7/7	0.92	0.26	120,121,121,121	0
85	MG	AR	4218	1/1	0.92	0.40	60,60,60,60	0
85	MG	1	4144	1/1	0.92	0.51	34,34,34,34	0
84	OHX	sR	2027	7/7	0.92	0.24	177,177,178,178	0
85	MG	AR	3930	1/1	0.92	0.36	38,38,38,38	0
84	OHX	1	3657	7/7	0.92	0.20	166,167,167,167	0
84	OHX	AR	3680	7/7	0.92	0.38	170,170,171,171	0
85	MG	1	4215	1/1	0.92	0.48	40,40,40,40	0
85	MG	1	3950	1/1	0.92	0.40	51,51,51,51	0
84	OHX	1	3663	7/7	0.92	0.22	169,169,170,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AT	216	7/7	0.92	0.39	154,155,155,155	0
85	MG	A	2121	1/1	0.92	0.25	73,73,73,73	0
84	OHX	1	3681	7/7	0.92	0.24	160,161,162,162	0
85	MG	AS	213	1/1	0.92	0.51	31,31,31,31	0
85	MG	AR	4232	1/1	0.92	0.18	41,41,41,41	0
84	OHX	sR	2039	7/7	0.92	0.41	197,198,198,198	0
85	MG	1	3796	1/1	0.92	0.47	59,59,59,59	0
85	MG	1	3891	1/1	0.92	0.41	36,36,36,36	0
84	OHX	A	2035	7/7	0.92	0.36	148,149,150,150	0
85	MG	AR	3984	1/1	0.92	0.27	48,48,48,48	0
85	MG	1	4150	1/1	0.92	0.84	36,36,36,36	0
85	MG	A	2067	1/1	0.92	0.86	73,73,73,73	0
85	MG	AR	4240	1/1	0.92	0.79	66,66,66,66	0
84	OHX	1	3679	7/7	0.92	0.38	165,166,166,166	0
85	MG	AR	3931	1/1	0.92	0.33	30,30,30,30	0
85	MG	AB	202	1/1	0.92	0.26	62,62,62,62	0
85	MG	1	3737	1/1	0.92	0.27	32,32,32,32	0
85	MG	1	4053	1/1	0.92	0.26	55,55,55,55	0
85	MG	AR	3904	1/1	0.92	0.55	29,29,29,29	0
85	MG	1	3959	1/1	0.92	0.27	29,29,29,29	0
85	MG	AR	3862	1/1	0.92	0.19	26,26,26,26	0
84	OHX	1	3652	7/7	0.92	0.42	154,155,155,155	0
85	MG	A	2149	1/1	0.92	0.20	73,73,73,73	0
85	MG	A	2130	1/1	0.92	0.36	58,58,58,58	0
85	MG	AR	3836	1/1	0.92	0.26	52,52,52,52	0
84	OHX	AR	3707	7/7	0.92	0.44	177,177,177,178	0
85	MG	AR	4050	1/1	0.92	0.25	48,48,48,48	0
85	MG	1	3953	1/1	0.92	0.07	63,63,63,63	0
85	MG	AR	4101	1/1	0.92	0.14	52,52,52,52	0
84	OHX	A	1966	7/7	0.92	0.17	146,147,147,148	0
84	OHX	sR	2014	7/7	0.92	0.33	141,141,142,142	0
84	OHX	1	3660	7/7	0.92	0.42	177,177,178,178	0
84	OHX	sR	2038	7/7	0.92	0.39	167,167,168,169	0
85	MG	1	3973	1/1	0.92	0.19	55,55,55,55	0
85	MG	1	3795	1/1	0.92	0.35	50,50,50,50	0
84	OHX	CL	302	7/7	0.92	0.16	142,142,143,143	0
84	OHX	AR	3533	7/7	0.92	0.22	114,114,114,114	0
85	MG	A	2062	1/1	0.92	0.58	58,58,58,58	0
85	MG	1	3972	1/1	0.92	0.19	42,42,42,42	0
85	MG	AR	3804	1/1	0.92	0.51	30,30,30,30	0
85	MG	AR	4098	1/1	0.92	0.25	65,65,65,65	0
84	OHX	A	1959	7/7	0.92	0.16	165,166,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4069	1/1	0.92	0.40	95,95,95,95	0
84	OHX	A	2021	7/7	0.92	0.41	158,159,160,160	0
85	MG	AR	4074	1/1	0.92	0.27	53,53,53,53	0
85	MG	AR	3756	1/1	0.92	0.32	48,48,48,48	0
85	MG	s1	302	1/1	0.92	0.13	63,63,63,63	0
85	MG	AR	4206	1/1	0.92	0.35	44,44,44,44	0
85	MG	1	3968	1/1	0.92	0.18	48,48,48,48	0
84	OHX	AR	3710	7/7	0.92	0.45	180,180,181,181	0
85	MG	AR	3868	1/1	0.92	0.65	28,28,28,28	0
85	MG	1	3789	1/1	0.92	0.34	36,36,36,36	0
85	MG	AS	219	1/1	0.92	0.39	52,52,52,52	0
85	MG	AR	3820	1/1	0.92	0.26	40,40,40,40	0
85	MG	AR	4072	1/1	0.92	0.17	73,73,73,73	0
84	OHX	A	1977	7/7	0.92	0.27	175,176,177,177	0
85	MG	AR	4225	1/1	0.92	0.10	82,82,82,82	0
84	OHX	1	3489	7/7	0.92	0.22	107,108,108,108	0
85	MG	CQ	202	1/1	0.92	0.45	40,40,40,40	0
84	OHX	1	3608	7/7	0.92	0.26	173,173,173,173	0
85	MG	D	301	1/1	0.92	0.64	72,72,72,72	0
85	MG	1	4077	1/1	0.92	0.21	58,58,58,58	0
85	MG	AR	3854	1/1	0.92	0.58	39,39,39,39	0
85	MG	A	2122	1/1	0.92	0.17	87,87,87,87	0
85	MG	A	2066	1/1	0.92	0.68	76,76,76,76	0
85	MG	AR	3769	1/1	0.92	0.16	39,39,39,39	0
85	MG	AR	3767	1/1	0.92	0.20	65,65,65,65	0
84	OHX	1	3625	7/7	0.92	0.17	156,157,158,158	0
84	OHX	AR	3609	7/7	0.92	0.15	171,171,172,172	0
84	OHX	A	2017	7/7	0.92	0.26	186,187,188,188	0
85	MG	4	233	1/1	0.92	0.34	44,44,44,44	0
84	OHX	1	3646	7/7	0.92	0.29	168,169,169,169	0
85	MG	1	4014	1/1	0.92	0.48	63,63,63,63	0
85	MG	A	2144	1/1	0.92	0.36	61,61,61,61	0
84	OHX	A	1985	7/7	0.92	0.22	146,147,148,148	0
84	OHX	A	2018	7/7	0.92	0.31	190,191,191,192	0
85	MG	1	3980	1/1	0.92	0.37	37,37,37,37	0
84	OHX	1	3649	7/7	0.92	0.26	154,155,156,156	0
85	MG	AR	3979	1/1	0.92	0.20	56,56,56,56	0
85	MG	AR	3822	1/1	0.92	0.66	55,55,55,55	0
85	MG	1	3873	1/1	0.92	0.57	33,33,33,33	0
85	MG	c1	201	1/1	0.92	0.47	69,69,69,69	0
85	MG	1	3894	1/1	0.93	0.33	45,45,45,45	0
85	MG	DC	202	1/1	0.93	0.38	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	1	4212	1/1	0.93	0.19	25,25,25,25	0
85	MG	AR	4119	1/1	0.93	0.18	47,47,47,47	0
85	MG	AR	3991	1/1	0.93	0.20	38,38,38,38	0
84	OHX	1	3630	7/7	0.93	0.28	149,149,150,150	0
85	MG	AR	3939	1/1	0.93	0.42	30,30,30,30	0
85	MG	A	2065	1/1	0.93	0.62	49,49,49,49	0
84	OHX	AR	3684	7/7	0.93	0.39	171,171,172,172	0
84	OHX	A	2009	7/7	0.93	0.35	156,157,157,158	0
84	OHX	AR	3664	7/7	0.93	0.29	143,144,144,144	0
85	MG	sR	2090	1/1	0.93	0.61	44,44,44,44	0
84	OHX	A	2001	7/7	0.93	0.20	169,170,171,171	0
85	MG	1	3778	1/1	0.93	0.32	43,43,43,43	0
84	OHX	1	3674	7/7	0.93	0.44	151,151,151,151	0
85	MG	sR	2104	1/1	0.93	0.22	68,68,68,68	0
85	MG	1	4040	1/1	0.93	0.75	61,61,61,61	0
85	MG	1	3777	1/1	0.93	0.08	38,38,38,38	0
85	MG	AR	3875	1/1	0.93	0.54	29,29,29,29	0
85	MG	AT	229	1/1	0.93	0.49	65,65,65,65	0
85	MG	1	3742	1/1	0.93	0.46	39,39,39,39	0
84	OHX	AR	3712	7/7	0.93	0.20	171,171,172,172	0
85	MG	A	2100	1/1	0.93	0.60	54,54,54,54	0
85	MG	6	201	1/1	0.93	0.44	27,27,27,27	0
84	OHX	1	3568	7/7	0.93	0.15	152,153,153,154	0
84	OHX	A	2005	7/7	0.93	0.33	157,157,158,158	0
85	MG	AR	3891	1/1	0.93	0.54	27,27,27,27	0
85	MG	AR	4212	1/1	0.93	0.24	36,36,36,36	0
85	MG	1	3803	1/1	0.93	0.51	46,46,46,46	0
84	OHX	AR	3628	7/7	0.93	0.23	163,164,164,164	0
85	MG	1	3799	1/1	0.93	0.15	37,37,37,37	0
84	OHX	AR	3717	7/7	0.93	0.29	201,201,202,202	0
85	MG	1	4059	1/1	0.93	0.23	40,40,40,40	0
85	MG	1	3798	1/1	0.93	0.14	44,44,44,44	0
84	OHX	sR	2037	7/7	0.93	0.35	174,174,175,175	0
85	MG	AR	4216	1/1	0.93	0.17	29,29,29,29	0
85	MG	AR	3792	1/1	0.93	0.29	33,33,33,33	0
85	MG	AT	226	1/1	0.93	0.17	67,67,67,67	0
85	MG	DO	202	1/1	0.93	0.15	45,45,45,45	0
84	OHX	AR	3532	7/7	0.93	0.19	129,129,130,130	0
84	OHX	1	3589	7/7	0.93	0.17	151,151,152,152	0
85	MG	AR	4021	1/1	0.93	0.46	53,53,53,53	0
85	MG	sR	2173	1/1	0.93	0.21	77,77,77,77	0
85	MG	1	3745	1/1	0.93	0.42	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	AR	4136	1/1	0.93	0.26	64,64,64,64	0
85	MG	1	3993	1/1	0.93	0.96	52,52,52,52	0
84	OHX	AR	3709	7/7	0.93	0.36	174,174,174,174	0
84	OHX	1	3638	7/7	0.93	0.16	167,167,168,168	0
85	MG	1	3732	1/1	0.93	0.47	39,39,39,39	0
85	MG	1	3781	1/1	0.93	0.26	43,43,43,43	0
84	OHX	sR	2033	7/7	0.93	0.45	154,155,155,156	0
85	MG	1	4049	1/1	0.93	0.20	38,38,38,38	0
85	MG	1	3830	1/1	0.93	0.38	32,32,32,32	0
85	MG	c7	201	1/1	0.93	0.52	71,71,71,71	0
84	OHX	1	3690	7/7	0.93	0.35	173,173,174,174	0
85	MG	1	4193	1/1	0.93	0.58	45,45,45,45	0
85	MG	1	4131	1/1	0.93	0.22	52,52,52,52	0
85	MG	A	2142	1/1	0.93	0.15	70,70,70,70	0
84	OHX	AR	3640	7/7	0.93	0.28	136,136,136,136	0
85	MG	1	3955	1/1	0.93	0.26	44,44,44,44	0
85	MG	1	3951	1/1	0.93	0.27	52,52,52,52	0
85	MG	1	3923	1/1	0.93	0.36	42,42,42,42	0
85	MG	4	228	1/1	0.93	0.18	52,52,52,52	0
84	OHX	sR	2025	7/7	0.93	0.29	173,173,174,175	0
84	OHX	AR	3662	7/7	0.93	0.27	164,164,165,165	0
84	OHX	A	1974	7/7	0.93	0.13	168,169,170,170	0
85	MG	1	4013	1/1	0.93	0.26	37,37,37,37	0
85	MG	1	4188	1/1	0.93	0.20	54,54,54,54	0
85	MG	AR	3949	1/1	0.93	0.12	31,31,31,31	0
84	OHX	1	3695	7/7	0.93	0.48	190,190,190,190	0
84	OHX	3	205	7/7	0.93	0.15	133,134,135,135	0
84	OHX	A	1964	7/7	0.93	0.28	139,139,140,140	0
84	OHX	CS	201	1/7	0.93	0.09	173,173,173,173	0
84	OHX	sR	2016	7/7	0.93	0.30	158,158,159,159	0
84	OHX	s4	301	7/7	0.93	0.18	178,179,179,180	0
84	OHX	A	1958	7/7	0.93	0.17	191,191,193,193	0
84	OHX	1	3666	7/7	0.93	0.22	134,134,134,135	0
84	OHX	sR	2002	7/7	0.93	0.37	139,140,141,141	0
84	OHX	sR	2029	7/7	0.93	0.34	157,157,157,158	0
85	MG	AR	3748	1/1	0.93	0.29	28,28,28,28	0
85	MG	AR	4099	1/1	0.93	0.27	41,41,41,41	0
85	MG	CQ	203	1/1	0.93	0.23	55,55,55,55	0
85	MG	AS	225	1/1	0.93	0.17	54,54,54,54	0
85	MG	A	2126	1/1	0.93	0.34	77,77,77,77	0
85	MG	sR	2100	1/1	0.93	0.49	35,35,35,35	0
85	MG	1	3846	1/1	0.93	0.45	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3628	7/7	0.93	0.19	163,164,164,164	0
85	MG	AR	3857	1/1	0.93	0.67	36,36,36,36	0
84	OHX	1	3715	7/7	0.93	0.24	173,173,174,174	0
85	MG	sR	2063	1/1	0.93	0.39	81,81,81,81	0
84	OHX	A	2032	7/7	0.93	0.21	185,186,186,187	0
85	MG	sR	2103	1/1	0.93	0.42	57,57,57,57	0
85	MG	AR	3802	1/1	0.93	0.22	51,51,51,51	0
85	MG	1	3827	1/1	0.93	0.46	49,49,49,49	0
84	OHX	1	3712	7/7	0.93	0.38	176,177,177,177	0
85	MG	CR	204	1/1	0.93	0.31	59,59,59,59	0
84	OHX	sR	1932	7/7	0.93	0.21	125,125,126,126	0
84	OHX	4	213	7/7	0.93	0.26	142,142,143,143	0
84	OHX	A	2033	7/7	0.93	0.22	178,179,179,179	0
85	MG	sR	2107	1/1	0.93	0.56	40,40,40,40	0
84	OHX	sR	2032	7/7	0.93	0.28	149,150,150,151	0
84	OHX	AR	3655	7/7	0.93	0.31	177,177,177,177	0
85	MG	AR	4128	1/1	0.93	0.39	46,46,46,46	0
84	OHX	1	3676	7/7	0.93	0.23	134,134,135,135	0
85	MG	1	4043	1/1	0.93	0.31	39,39,39,39	0
85	MG	sR	2129	1/1	0.93	0.32	36,36,36,36	0
85	MG	AR	3901	1/1	0.93	0.59	37,37,37,37	0
85	MG	A	2148	1/1	0.93	0.33	86,86,86,86	0
84	OHX	CE	402	7/7	0.93	0.40	187,187,188,188	0
85	MG	sR	2167	1/1	0.93	0.43	47,47,47,47	0
85	MG	1	3844	1/1	0.93	0.67	35,35,35,35	0
85	MG	AR	3903	1/1	0.93	0.82	42,42,42,42	0
84	OHX	A	2031	7/7	0.93	0.24	199,200,201,202	0
85	MG	1	4198	1/1	0.93	0.57	32,32,32,32	0
85	MG	AR	3765	1/1	0.93	0.40	31,31,31,31	0
84	OHX	AR	3683	7/7	0.93	0.35	136,136,136,137	0
84	OHX	1	3694	7/7	0.93	0.23	160,161,161,161	0
84	OHX	AR	3679	7/7	0.93	0.19	147,148,148,148	0
84	OHX	sR	2008	7/7	0.93	0.17	175,175,176,177	0
84	OHX	sR	2035	7/7	0.93	0.19	179,179,181,181	0
85	MG	AR	3827	1/1	0.93	0.52	56,56,56,56	0
85	MG	AR	4223	1/1	0.93	0.58	57,57,57,57	0
85	MG	AR	4108	1/1	0.93	0.42	52,52,52,52	0
85	MG	1	3864	1/1	0.93	0.31	32,32,32,32	0
85	MG	AR	3808	1/1	0.93	0.30	33,33,33,33	0
85	MG	AR	3970	1/1	0.93	0.15	97,97,97,97	0
85	MG	1	4101	1/1	0.93	0.31	27,27,27,27	0
84	OHX	AR	3700	7/7	0.93	0.38	183,183,184,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3756	1/1	0.93	0.27	32,32,32,32	0
84	OHX	sR	2043	7/7	0.93	0.26	197,198,198,199	0
84	OHX	AR	3666	7/7	0.93	0.31	146,146,147,147	0
85	MG	sR	2163	1/1	0.93	0.33	62,62,62,62	0
85	MG	AR	3816	1/1	0.93	0.28	37,37,37,37	0
84	OHX	sR	2024	7/7	0.93	0.28	188,189,190,191	0
84	OHX	AR	3731	7/7	0.93	0.34	162,163,163,164	0
85	MG	CD	301	1/1	0.93	0.77	52,52,52,52	0
85	MG	1	3765	1/1	0.93	0.22	33,33,33,33	0
85	MG	1	4112	1/1	0.93	0.17	52,52,52,52	0
84	OHX	A	2002	7/7	0.93	0.19	177,179,179,179	0
85	MG	sR	2101	1/1	0.93	0.55	55,55,55,55	0
85	MG	1	4006	1/1	0.93	0.77	70,70,70,70	0
84	OHX	CK	201	7/7	0.93	0.21	150,151,151,151	0
85	MG	sR	2114	1/1	0.93	0.31	77,77,77,77	0
84	OHX	1	3675	7/7	0.93	0.37	169,169,170,170	0
85	MG	1	4008	1/1	0.93	0.29	22,22,22,22	0
85	MG	sR	2148	1/1	0.93	0.20	58,58,58,58	0
85	MG	AR	3887	1/1	0.93	0.44	44,44,44,44	0
85	MG	AR	3845	1/1	0.93	0.29	31,31,31,31	0
85	MG	AR	4005	1/1	0.93	0.38	68,68,68,68	0
84	OHX	sR	2012	7/7	0.93	0.25	167,168,168,169	0
84	OHX	sR	1950	7/7	0.93	0.17	145,145,146,147	0
85	MG	AR	3749	1/1	0.93	0.40	49,49,49,49	0
85	MG	1	4007	1/1	0.93	0.33	59,59,59,59	0
85	MG	1	4208	1/1	0.93	0.24	26,26,26,26	0
85	MG	1	3776	1/1	0.93	0.44	34,34,34,34	0
85	MG	sR	2056	1/1	0.94	0.26	67,67,67,67	0
84	OHX	1	3655	7/7	0.94	0.17	165,165,166,166	0
84	OHX	AR	3675	7/7	0.94	0.12	200,201,201,201	0
85	MG	AR	3926	1/1	0.94	0.36	47,47,47,47	0
84	OHX	1	3672	7/7	0.94	0.31	154,155,155,156	0
85	MG	AR	3791	1/1	0.94	0.33	21,21,21,21	0
85	MG	AR	4086	1/1	0.94	0.36	41,41,41,41	0
84	OHX	AR	3618	7/7	0.94	0.28	128,129,129,129	0
84	OHX	1	3662	7/7	0.94	0.27	187,188,188,189	0
84	OHX	AR	3626	7/7	0.94	0.28	172,173,173,174	0
85	MG	AR	3950	1/1	0.94	0.11	39,39,39,39	0
85	MG	A	2090	1/1	0.94	0.39	55,55,55,55	0
84	OHX	1	3486	7/7	0.94	0.17	120,121,121,121	0
84	OHX	A	2020	7/7	0.94	0.15	156,157,157,157	0
84	OHX	AR	3690	7/7	0.94	0.40	145,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3545	7/7	0.94	0.15	142,143,143,143	0
85	MG	AR	3821	1/1	0.94	0.38	51,51,51,51	0
85	MG	AR	3894	1/1	0.94	0.35	61,61,61,61	0
84	OHX	AR	3526	7/7	0.94	0.28	124,125,125,126	0
84	OHX	AR	3716	7/7	0.94	0.21	162,162,163,163	0
84	OHX	1	3664	7/7	0.94	0.28	188,189,190,190	0
84	OHX	sR	2001	7/7	0.94	0.14	160,160,161,161	0
84	OHX	sR	2017	7/7	0.94	0.28	150,150,151,151	0
84	OHX	AR	3620	7/7	0.94	0.24	133,133,133,134	0
84	OHX	AR	3605	7/7	0.94	0.24	145,146,146,146	0
84	OHX	A	1915	7/7	0.94	0.17	133,134,135,135	0
85	MG	AR	4077	1/1	0.94	0.28	43,43,43,43	0
85	MG	AT	230	1/1	0.94	0.79	49,49,49,49	0
85	MG	AR	3943	1/1	0.94	0.47	30,30,30,30	0
85	MG	AR	3844	1/1	0.94	0.39	28,28,28,28	0
84	OHX	1	3707	7/7	0.94	0.41	174,175,175,175	0
85	MG	1	4197	1/1	0.94	0.42	68,68,68,68	0
85	MG	sR	2125	1/1	0.94	0.21	52,52,52,52	0
84	OHX	sR	1940	7/7	0.94	0.13	162,163,164,164	0
84	OHX	sR	2021	7/7	0.94	0.13	162,162,163,164	0
84	OHX	AK	102	7/7	0.94	0.14	114,114,114,114	0
85	MG	AR	4000	1/1	0.94	0.11	64,64,64,64	0
85	MG	1	4017	1/1	0.94	0.34	41,41,41,41	0
85	MG	sR	2135	1/1	0.94	0.12	82,82,82,82	0
85	MG	1	3734	1/1	0.94	0.40	37,37,37,37	0
84	OHX	AR	3691	7/7	0.94	0.26	149,149,150,150	0
85	MG	AR	3960	1/1	0.94	0.37	34,34,34,34	0
84	OHX	AR	3663	7/7	0.94	0.28	161,161,162,162	0
84	OHX	sR	1966	7/7	0.94	0.16	146,146,147,147	0
85	MG	1	3876	1/1	0.94	0.48	61,61,61,61	0
85	MG	sR	2130	1/1	0.94	0.12	83,83,83,83	0
85	MG	1	3853	1/1	0.94	0.61	34,34,34,34	0
85	MG	1	3999	1/1	0.94	0.43	47,47,47,47	0
85	MG	4	225	1/1	0.94	0.23	59,59,59,59	0
84	OHX	1	3446	7/7	0.94	0.25	99,99,100,100	0
85	MG	1	4071	1/1	0.94	0.25	37,37,37,37	0
84	OHX	1	3667	7/7	0.94	0.25	142,142,142,143	0
85	MG	sR	2139	1/1	0.94	0.19	54,54,54,54	0
85	MG	AR	3784	1/1	0.94	0.43	41,41,41,41	0
84	OHX	sR	2006	7/7	0.94	0.25	148,149,150,150	0
85	MG	sR	2168	1/1	0.94	0.34	47,47,47,47	0
85	MG	1	3814	1/1	0.94	0.22	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AS	223	1/1	0.94	0.30	75,75,75,75	0
84	OHX	1	3593	7/7	0.94	0.31	147,147,148,148	0
84	OHX	AT	215	7/7	0.94	0.21	157,157,157,158	0
84	OHX	AR	3641	7/7	0.94	0.20	164,164,165,165	0
84	OHX	sR	2026	7/7	0.94	0.47	143,144,144,144	0
84	OHX	AR	3639	7/7	0.94	0.17	153,154,154,154	0
85	MG	AR	3811	1/1	0.94	0.41	53,53,53,53	0
85	MG	1	4105	1/1	0.94	0.28	41,41,41,41	0
84	OHX	AR	3595	7/7	0.94	0.38	135,135,136,136	0
85	MG	1	3983	1/1	0.94	0.26	47,47,47,47	0
87	ZN	d7	101	1/1	0.94	0.45	180,180,180,180	0
85	MG	AR	4143	1/1	0.94	0.21	55,55,55,55	0
84	OHX	1	3502	7/7	0.94	0.18	123,123,124,124	0
84	OHX	A	1918	7/7	0.94	0.18	108,109,109,109	0
84	OHX	AR	3682	7/7	0.94	0.26	153,154,154,154	0
84	OHX	1	3611	7/7	0.94	0.25	141,141,141,141	0
85	MG	CP	505	1/1	0.94	0.85	106,106,106,106	0
85	MG	3	214	1/1	0.94	0.48	30,30,30,30	0
85	MG	AB	203	1/1	0.94	0.56	44,44,44,44	0
84	OHX	AR	3499	7/7	0.94	0.17	127,128,128,128	0
84	OHX	AR	3590	7/7	0.94	0.12	153,154,155,155	0
85	MG	1	3924	1/1	0.94	0.42	49,49,49,49	0
85	MG	AR	4054	1/1	0.94	0.34	35,35,35,35	0
84	OHX	AR	3665	7/7	0.94	0.29	161,162,162,162	0
85	MG	AR	4063	1/1	0.94	0.41	49,49,49,49	0
85	MG	4	234	1/1	0.94	0.66	52,52,52,52	0
84	OHX	1	3616	7/7	0.94	0.36	146,147,147,148	0
85	MG	1	3904	1/1	0.94	0.52	32,32,32,32	0
84	OHX	AR	3541	7/7	0.94	0.17	148,148,149,149	0
85	MG	AR	3947	1/1	0.94	0.55	34,34,34,34	0
84	OHX	1	3722	7/7	0.94	0.26	176,176,177,177	0
85	MG	AR	3879	1/1	0.94	0.39	30,30,30,30	0
85	MG	sR	2115	1/1	0.94	0.28	59,59,59,59	0
84	OHX	sR	1976	7/7	0.94	0.15	170,171,172,172	0
84	OHX	AR	3647	7/7	0.94	0.34	156,156,157,157	0
85	MG	AR	4096	1/1	0.94	0.34	28,28,28,28	0
85	MG	1	3976	1/1	0.94	0.43	52,52,52,52	0
85	MG	sR	2088	1/1	0.94	0.45	74,74,74,74	0
85	MG	1	3911	1/1	0.94	0.38	44,44,44,44	0
85	MG	A	2075	1/1	0.94	0.45	61,61,61,61	0
85	MG	A	2120	1/1	0.94	0.38	49,49,49,49	0
84	OHX	AR	3633	7/7	0.94	0.26	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3560	7/7	0.94	0.23	122,122,122,122	0
85	MG	A	2059	1/1	0.94	0.55	60,60,60,60	0
84	OHX	sR	1919	7/7	0.94	0.18	107,107,108,108	0
85	MG	1	4203	1/1	0.94	0.60	45,45,45,45	0
85	MG	AR	3758	1/1	0.94	0.46	42,42,42,42	0
85	MG	sR	2097	1/1	0.94	0.49	48,48,48,48	0
84	OHX	AR	3643	7/7	0.94	0.33	158,159,159,159	0
85	MG	AR	4060	1/1	0.94	0.36	47,47,47,47	0
85	MG	1	4190	1/1	0.94	0.33	18,18,18,18	0
85	MG	A	2077	1/1	0.94	0.39	53,53,53,53	0
85	MG	sR	2054	1/1	0.94	0.39	57,57,57,57	0
85	MG	sR	2156	1/1	0.94	0.27	62,62,62,62	0
84	OHX	sR	1981	7/7	0.94	0.33	127,128,129,129	0
85	MG	AR	4020	1/1	0.94	0.37	43,43,43,43	0
84	OHX	AR	3705	7/7	0.94	0.43	142,142,142,143	0
84	OHX	1	3635	7/7	0.94	0.26	142,143,143,143	0
85	MG	sR	2055	1/1	0.94	0.75	54,54,54,54	0
84	OHX	A	2013	7/7	0.94	0.27	154,155,155,155	0
85	MG	1	4070	1/1	0.94	0.28	47,47,47,47	0
84	OHX	AR	3695	7/7	0.94	0.24	160,161,161,162	0
84	OHX	1	3670	7/7	0.94	0.31	151,152,152,152	0
85	MG	1	3928	1/1	0.94	0.55	23,23,23,23	0
85	MG	1	3779	1/1	0.94	0.38	39,39,39,39	0
85	MG	AR	3958	1/1	0.94	0.40	24,24,24,24	0
84	OHX	AR	3642	7/7	0.94	0.51	153,154,154,154	0
85	MG	1	3801	1/1	0.94	0.37	49,49,49,49	0
85	MG	1	4168	1/1	0.94	0.27	34,34,34,34	0
84	OHX	AR	3613	7/7	0.94	0.33	154,155,155,155	0
85	MG	1	4148	1/1	0.94	0.19	53,53,53,53	0
84	OHX	AR	3627	7/7	0.94	0.34	164,164,165,165	0
85	MG	d4	202	1/1	0.94	0.32	60,60,60,60	0
84	OHX	sR	2045	7/7	0.94	0.38	163,164,164,165	0
85	MG	3	215	1/1	0.94	0.37	53,53,53,53	0
84	OHX	sR	1979	7/7	0.94	0.26	160,160,161,161	0
85	MG	AR	3890	1/1	0.94	0.47	25,25,25,25	0
84	OHX	AR	3601	7/7	0.94	0.18	150,150,151,151	0
85	MG	AK	104	1/1	0.94	0.83	59,59,59,59	0
84	OHX	1	3626	7/7	0.94	0.25	182,182,183,183	0
85	MG	1	3766	1/1	0.94	0.49	44,44,44,44	0
85	MG	sR	2078	1/1	0.94	0.54	48,48,48,48	0
84	OHX	s8	301	7/7	0.94	0.32	194,195,195,196	0
85	MG	A	2074	1/1	0.94	0.52	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	4177	1/1	0.94	0.48	80,80,80,80	0
85	MG	sR	2081	1/1	0.94	0.34	59,59,59,59	0
84	OHX	1	3706	7/7	0.94	0.25	194,194,195,195	0
85	MG	1	3823	1/1	0.94	0.46	29,29,29,29	0
85	MG	4	221	1/1	0.94	0.42	36,36,36,36	0
84	OHX	sR	2005	7/7	0.94	0.28	176,176,177,178	0
85	MG	CX	203	1/1	0.94	0.43	30,30,30,30	0
85	MG	AR	3941	1/1	0.94	0.59	47,47,47,47	0
85	MG	1	3763	1/1	0.94	0.43	46,46,46,46	0
84	OHX	1	3604	7/7	0.94	0.24	145,146,146,146	0
85	MG	AR	4127	1/1	0.94	0.28	43,43,43,43	0
85	MG	4	227	1/1	0.94	0.45	39,39,39,39	0
85	MG	AT	228	1/1	0.94	0.35	43,43,43,43	0
84	OHX	x	202	7/7	0.94	0.33	176,176,176,176	0
85	MG	AR	3907	1/1	0.94	0.59	30,30,30,30	0
84	OHX	A	1991	7/7	0.94	0.15	183,184,185,185	0
84	OHX	1	3659	7/7	0.94	0.28	169,169,169,169	0
85	MG	1	4087	1/1	0.94	0.25	40,40,40,40	0
84	OHX	A	2019	7/7	0.94	0.21	210,210,212,212	0
85	MG	AR	3824	1/1	0.94	0.23	24,24,24,24	0
85	MG	AR	3853	1/1	0.94	0.27	43,43,43,43	0
84	OHX	AR	3570	7/7	0.94	0.15	169,170,170,171	0
85	MG	1	3809	1/1	0.94	0.48	49,49,49,49	0
85	MG	CR	205	1/1	0.94	0.37	44,44,44,44	0
85	MG	AR	3932	1/1	0.94	0.45	34,34,34,34	0
85	MG	A	2118	1/1	0.94	0.13	67,67,67,67	0
84	OHX	AR	3657	7/7	0.94	0.21	165,165,166,166	0
84	OHX	O	201	7/7	0.94	0.15	198,199,199,199	0
84	OHX	1	3645	7/7	0.94	0.29	162,162,163,163	0
84	OHX	sR	1961	7/7	0.94	0.16	135,136,136,137	0
84	OHX	AR	3548	7/7	0.94	0.22	142,142,142,143	0
84	OHX	sR	2028	7/7	0.94	0.35	184,184,185,185	0
84	OHX	1	3511	7/7	0.94	0.21	118,118,119,119	0
84	OHX	sR	2000	7/7	0.94	0.22	162,163,163,164	0
85	MG	1	3885	1/1	0.94	0.52	36,36,36,36	0
85	MG	AH	201	1/1	0.94	0.17	47,47,47,47	0
84	OHX	AT	214	7/7	0.94	0.24	153,153,153,153	0
84	OHX	sR	1978	7/7	0.94	0.21	126,126,127,127	0
84	OHX	A	1953	7/7	0.94	0.27	164,165,166,166	0
84	OHX	AR	3508	7/7	0.94	0.15	117,118,119,119	0
85	MG	CX	205	1/1	0.94	0.19	48,48,48,48	0
85	MG	1	4080	1/1	0.94	0.19	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	sR	2120	1/1	0.94	0.40	70,70,70,70	0
84	OHX	A	1980	7/7	0.94	0.22	166,166,167,167	0
84	OHX	1	3463	7/7	0.94	0.21	104,104,105,105	0
84	OHX	sR	1971	7/7	0.94	0.19	151,151,152,152	0
84	OHX	AR	3685	7/7	0.94	0.25	182,182,183,183	0
84	OHX	AR	3611	7/7	0.94	0.27	136,136,137,137	0
84	OHX	A	2010	7/7	0.94	0.19	171,173,173,174	0
85	MG	AR	3859	1/1	0.94	0.40	39,39,39,39	0
84	OHX	AR	3623	7/7	0.94	0.28	147,148,148,148	0
85	MG	1	4084	1/1	0.94	0.29	52,52,52,52	0
84	OHX	sR	1996	7/7	0.94	0.17	184,184,185,186	0
85	MG	AR	4015	1/1	0.94	0.59	49,49,49,49	0
85	MG	sR	2190	1/1	0.94	0.38	57,57,57,57	0
85	MG	AR	3986	1/1	0.94	0.07	63,63,63,63	0
85	MG	1	3743	1/1	0.95	0.59	42,42,42,42	0
85	MG	A	2083	1/1	0.95	0.34	53,53,53,53	0
85	MG	sR	2077	1/1	0.95	0.52	41,41,41,41	0
84	OHX	AR	3558	7/7	0.95	0.25	121,121,121,122	0
84	OHX	1	3562	7/7	0.95	0.18	141,141,141,142	0
84	OHX	sR	2015	7/7	0.95	0.31	158,159,159,160	0
85	MG	AR	3871	1/1	0.95	0.78	44,44,44,44	0
84	OHX	sR	1985	7/7	0.95	0.17	137,137,138,138	0
85	MG	1	3839	1/1	0.95	0.58	28,28,28,28	0
85	MG	A	2055	1/1	0.95	0.40	61,61,61,61	0
84	OHX	AR	3518	7/7	0.95	0.11	163,164,165,165	0
85	MG	sR	2089	1/1	0.95	0.51	44,44,44,44	0
85	MG	1	3759	1/1	0.95	0.33	55,55,55,55	0
85	MG	1	4028	1/1	0.95	0.42	61,61,61,61	0
84	OHX	1	3621	7/7	0.95	0.11	200,201,201,201	0
85	MG	AR	3945	1/1	0.95	0.40	43,43,43,43	0
84	OHX	AR	3600	7/7	0.95	0.25	157,158,158,159	0
84	OHX	1	3470	7/7	0.95	0.19	108,109,109,109	0
84	OHX	AT	206	7/7	0.95	0.15	128,128,128,128	0
85	MG	1	3861	1/1	0.95	0.30	44,44,44,44	0
84	OHX	AR	3738	7/7	0.95	0.26	129,130,130,130	0
84	OHX	1	3537	7/7	0.95	0.23	127,128,128,128	0
85	MG	AR	3831	1/1	0.95	0.64	34,34,34,34	0
85	MG	4	223	1/1	0.95	0.58	50,50,50,50	0
85	MG	A	2136	1/1	0.95	0.12	96,96,96,96	0
85	MG	AR	3849	1/1	0.95	0.40	40,40,40,40	0
84	OHX	Q	201	7/7	0.95	0.19	187,187,188,188	0
84	OHX	AR	3536	7/7	0.95	0.13	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3651	7/7	0.95	0.21	149,149,150,150	0
84	OHX	A	1963	7/7	0.95	0.22	165,166,167,167	0
85	MG	1	4147	1/1	0.95	0.14	62,62,62,62	0
85	MG	AS	224	1/1	0.95	0.15	88,88,88,88	0
85	MG	1	3815	1/1	0.95	0.49	47,47,47,47	0
84	OHX	1	3701	7/7	0.95	0.33	147,148,148,148	0
84	OHX	1	3597	7/7	0.95	0.11	158,158,158,159	0
85	MG	AR	3837	1/1	0.95	0.64	25,25,25,25	0
84	OHX	1	3547	7/7	0.95	0.15	147,147,148,148	0
85	MG	AR	4201	1/1	0.95	0.66	40,40,40,40	0
85	MG	1	4142	1/1	0.95	0.19	47,47,47,47	0
84	OHX	AR	3610	7/7	0.95	0.13	155,155,156,156	0
84	OHX	sR	2018	7/7	0.95	0.27	157,158,158,159	0
84	OHX	AT	212	7/7	0.95	0.26	152,152,152,152	0
84	OHX	1	3661	7/7	0.95	0.21	145,145,146,146	0
84	OHX	1	3714	7/7	0.95	0.40	163,164,164,165	0
84	OHX	AT	211	7/7	0.95	0.15	163,163,164,164	0
85	MG	AR	4125	1/1	0.95	0.85	32,32,32,32	0
84	OHX	A	1995	7/7	0.95	0.11	177,178,179,179	0
84	OHX	1	3643	7/7	0.95	0.25	157,158,158,158	0
85	MG	AR	3918	1/1	0.95	0.42	24,24,24,24	0
85	MG	AR	4132	1/1	0.95	0.24	37,37,37,37	0
84	OHX	1	3711	7/7	0.95	0.42	157,157,158,158	0
85	MG	sR	2189	1/1	0.95	0.25	58,58,58,58	0
85	MG	AR	4229	1/1	0.95	0.64	92,92,92,92	0
84	OHX	A	1998	7/7	0.95	0.23	178,179,180,181	0
85	MG	1	3755	1/1	0.95	0.29	40,40,40,40	0
84	OHX	CX	202	7/7	0.95	0.20	131,132,132,132	0
85	MG	AR	3896	1/1	0.95	0.71	46,46,46,46	0
85	MG	AR	3823	1/1	0.95	0.12	80,80,80,80	0
84	OHX	AS	207	7/7	0.95	0.10	152,153,154,154	0
85	MG	AR	3873	1/1	0.95	0.41	47,47,47,47	0
84	OHX	A	1978	7/7	0.95	0.17	167,168,169,169	0
85	MG	A	2143	1/1	0.95	0.11	115,115,115,115	0
84	OHX	AR	3580	7/7	0.95	0.19	132,132,133,133	0
85	MG	1	3869	1/1	0.95	0.51	41,41,41,41	0
84	OHX	sR	1995	7/7	0.95	0.19	159,160,161,161	0
84	OHX	AR	3543	7/7	0.95	0.16	137,138,138,139	0
85	MG	sR	2112	1/1	0.95	0.23	62,62,62,62	0
85	MG	3	217	1/1	0.95	0.21	47,47,47,47	0
85	MG	AR	4115	1/1	0.95	0.14	53,53,53,53	0
84	OHX	sR	1973	7/7	0.95	0.17	145,145,146,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3637	7/7	0.95	0.26	143,144,144,144	0
84	OHX	1	3609	7/7	0.95	0.17	134,135,135,135	0
84	OHX	sR	1977	7/7	0.95	0.12	159,160,161,161	0
85	MG	AR	4092	1/1	0.95	0.31	41,41,41,41	0
84	OHX	AR	3667	7/7	0.95	0.41	143,143,143,143	0
85	MG	1	4171	1/1	0.95	0.37	44,44,44,44	0
84	OHX	AR	3553	7/7	0.95	0.15	136,136,137,137	0
84	OHX	AR	3625	7/7	0.95	0.26	147,148,148,149	0
84	OHX	sR	1988	7/7	0.95	0.22	173,173,174,174	0
85	MG	1	3945	1/1	0.95	0.36	34,34,34,34	0
84	OHX	AR	3706	7/7	0.95	0.29	146,146,146,147	0
84	OHX	A	2003	7/7	0.95	0.26	153,154,155,155	0
85	MG	AR	4205	1/1	0.95	0.14	36,36,36,36	0
84	OHX	AR	3656	7/7	0.95	0.37	152,152,153,153	0
85	MG	AR	4078	1/1	0.95	0.54	34,34,34,34	0
84	OHX	AR	3564	7/7	0.95	0.14	149,149,149,150	0
84	OHX	1	3600	7/7	0.95	0.27	154,154,155,155	0
84	OHX	AR	3624	7/7	0.95	0.18	139,139,140,140	0
84	OHX	1	3636	7/7	0.95	0.27	194,194,195,195	0
84	OHX	AR	3644	7/7	0.95	0.32	156,157,157,157	0
84	OHX	1	3620	7/7	0.95	0.17	148,148,149,149	0
84	OHX	AR	3573	7/7	0.95	0.12	145,145,145,145	0
85	MG	1	3961	1/1	0.95	0.37	67,67,67,67	0
84	OHX	AR	3549	7/7	0.95	0.16	137,138,138,138	0
85	MG	1	4106	1/1	0.95	0.15	37,37,37,37	0
84	OHX	AR	3458	7/7	0.95	0.18	109,110,110,110	0
85	MG	1	3857	1/1	0.95	0.48	33,33,33,33	0
84	OHX	1	3482	7/7	0.95	0.17	99,99,100,100	0
85	MG	AR	4142	1/1	0.95	0.09	69,69,69,69	0
85	MG	1	4133	1/1	0.95	0.43	74,74,74,74	0
84	OHX	1	3640	7/7	0.95	0.25	145,145,146,146	0
84	OHX	1	3680	7/7	0.95	0.29	180,180,181,181	0
85	MG	DH	203	1/1	0.95	0.38	39,39,39,39	0
85	MG	A	2045	1/1	0.95	0.56	45,45,45,45	0
84	OHX	AR	3577	7/7	0.95	0.16	156,156,157,157	0
85	MG	1	4095	1/1	0.95	0.14	57,57,57,57	0
85	MG	AR	4185	1/1	0.95	0.49	53,53,53,53	0
85	MG	1	3882	1/1	0.95	0.42	22,22,22,22	0
85	MG	1	3886	1/1	0.95	0.63	31,31,31,31	0
85	MG	A	2093	1/1	0.95	0.33	54,54,54,54	0
85	MG	AR	3999	1/1	0.95	0.23	42,42,42,42	0
85	MG	1	3986	1/1	0.95	0.29	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3612	7/7	0.95	0.17	149,150,151,151	0
84	OHX	AR	3612	7/7	0.95	0.24	139,140,140,140	0
84	OHX	1	3691	7/7	0.95	0.28	152,152,153,153	0
85	MG	1	3934	1/1	0.95	0.14	34,34,34,34	0
84	OHX	CG	303	7/7	0.95	0.35	158,159,159,160	0
84	OHX	4	211	7/7	0.95	0.16	160,160,160,160	0
84	OHX	1	3515	7/7	0.95	0.18	124,124,124,125	0
84	OHX	AR	3694	7/7	0.95	0.38	147,148,148,149	0
85	MG	AR	4189	1/1	0.95	0.34	46,46,46,46	0
84	OHX	A	2004	7/7	0.95	0.22	167,168,169,169	0
85	MG	AR	3800	1/1	0.95	0.63	48,48,48,48	0
84	OHX	A	2006	7/7	0.95	0.18	162,163,164,164	0
84	OHX	AR	3668	7/7	0.95	0.21	136,136,136,136	0
84	OHX	c5	201	7/7	0.95	0.26	179,180,181,181	0
84	OHX	1	3455	7/7	0.95	0.16	110,111,111,111	0
84	OHX	3	207	7/7	0.95	0.16	158,158,159,159	0
84	OHX	1	3685	7/7	0.95	0.26	172,172,173,173	0
84	OHX	3	203	7/7	0.95	0.16	113,114,114,114	0
85	MG	AR	3987	1/1	0.95	0.30	45,45,45,45	0
85	MG	AR	4007	1/1	0.95	0.45	52,52,52,52	0
85	MG	sR	2095	1/1	0.95	0.46	36,36,36,36	0
84	OHX	sR	1982	7/7	0.95	0.31	140,140,140,140	0
85	MG	1	3840	1/1	0.95	0.61	22,22,22,22	0
84	OHX	AR	3634	7/7	0.95	0.27	173,173,174,174	0
84	OHX	AR	3598	7/7	0.95	0.23	137,138,138,138	0
84	OHX	l	401	7/7	0.95	0.30	163,163,164,164	0
85	MG	1	3919	1/1	0.95	0.66	23,23,23,23	0
85	MG	AR	3855	1/1	0.95	0.35	56,56,56,56	0
85	MG	AS	214	1/1	0.95	0.35	57,57,57,57	0
84	OHX	A	2000	7/7	0.95	0.20	167,168,168,168	0
84	OHX	1	3519	7/7	0.95	0.17	110,110,111,111	0
85	MG	1	3793	1/1	0.95	0.47	25,25,25,25	0
85	MG	AR	4199	1/1	0.95	0.27	54,54,54,54	0
84	OHX	AR	3661	7/7	0.95	0.43	164,165,165,166	0
85	MG	1	3996	1/1	0.95	0.30	46,46,46,46	0
85	MG	1	4085	1/1	0.95	0.17	39,39,39,39	0
84	OHX	A	2014	7/7	0.95	0.37	154,155,155,155	0
85	MG	A	2116	1/1	0.95	0.45	76,76,76,76	0
85	MG	1	4207	1/1	0.95	0.42	35,35,35,35	0
85	MG	AR	3961	1/1	0.95	0.27	28,28,28,28	0
84	OHX	AR	3696	7/7	0.95	0.30	145,146,147,147	0
84	OHX	1	3615	7/7	0.95	0.22	151,151,152,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3942	1/1	0.95	0.66	34,34,34,34	0
84	OHX	sR	1999	7/7	0.95	0.25	161,161,162,162	0
84	OHX	AR	3477	7/7	0.95	0.17	120,120,121,121	0
84	OHX	AR	3689	7/7	0.95	0.34	152,153,153,153	0
85	MG	l	405	1/1	0.95	0.34	40,40,40,40	0
85	MG	sR	2099	1/1	0.95	0.38	42,42,42,42	0
84	OHX	AR	3704	7/7	0.95	0.24	136,136,136,137	0
85	MG	AS	222	1/1	0.95	0.32	34,34,34,34	0
85	MG	AR	4228	1/1	0.95	0.35	62,62,62,62	0
84	OHX	1	3686	7/7	0.95	0.24	154,154,155,155	0
85	MG	AR	4220	1/1	0.95	0.35	47,47,47,47	0
85	MG	sR	2128	1/1	0.95	0.31	38,38,38,38	0
84	OHX	1	3633	7/7	0.95	0.23	178,179,179,180	0
84	OHX	AR	3672	7/7	0.95	0.16	159,160,160,160	0
85	MG	A	2043	1/1	0.95	0.37	55,55,55,55	0
84	OHX	CF	401	7/7	0.95	0.30	165,166,166,167	0
85	MG	1	3887	1/1	0.95	0.45	31,31,31,31	0
85	MG	4	218	1/1	0.95	0.61	48,48,48,48	0
84	OHX	1	3700	7/7	0.95	0.24	149,149,150,150	0
84	OHX	A	1947	7/7	0.95	0.17	124,125,125,125	0
84	OHX	sR	2013	7/7	0.95	0.15	170,170,171,171	0
85	MG	CN	201	1/1	0.95	0.17	72,72,72,72	0
85	MG	CP	503	1/1	0.95	0.30	42,42,42,42	0
84	OHX	1	3677	7/7	0.95	0.16	196,197,197,198	0
85	MG	AR	3799	1/1	0.95	0.36	46,46,46,46	0
84	OHX	A	2027	7/7	0.95	0.20	197,198,199,199	0
84	OHX	A	1968	7/7	0.95	0.28	146,147,147,148	0
85	MG	A	2151	1/1	0.95	0.14	67,67,67,67	0
85	MG	AR	3886	1/1	0.95	0.45	28,28,28,28	0
85	MG	1	3736	1/1	0.95	0.34	53,53,53,53	0
84	OHX	AR	3559	7/7	0.95	0.17	115,116,116,116	0
85	MG	1	3768	1/1	0.95	0.30	28,28,28,28	0
85	MG	sR	2053	1/1	0.95	0.65	49,49,49,49	0
85	MG	AR	4158	1/1	0.95	0.23	52,52,52,52	0
84	OHX	1	3582	7/7	0.95	0.29	125,125,126,126	0
85	MG	sR	2181	1/1	0.95	0.13	108,108,108,108	0
85	MG	AR	3750	1/1	0.95	0.12	39,39,39,39	0
85	MG	1	3989	1/1	0.95	0.22	45,45,45,45	0
84	OHX	AR	3542	7/7	0.95	0.14	145,146,147,147	0
84	OHX	sR	1987	7/7	0.95	0.27	144,145,146,146	0
85	MG	1	4052	1/1	0.95	0.17	51,51,51,51	0
84	OHX	AR	3597	7/7	0.95	0.34	126,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3554	7/7	0.95	0.14	145,146,146,146	0
84	OHX	1	3669	7/7	0.95	0.24	150,150,151,151	0
85	MG	sR	2127	1/1	0.95	0.28	65,65,65,65	0
85	MG	1	3835	1/1	0.95	0.42	25,25,25,25	0
85	MG	1	3998	1/1	0.95	0.18	54,54,54,54	0
85	MG	AR	3938	1/1	0.95	0.54	52,52,52,52	0
87	ZN	g	501	1/1	0.95	0.05	121,121,121,121	0
84	OHX	1	3613	7/7	0.95	0.35	140,141,141,141	0
84	OHX	1	3599	7/7	0.95	0.35	146,146,146,147	0
85	MG	1	3812	1/1	0.95	0.50	60,60,60,60	0
84	OHX	A	1999	7/7	0.95	0.21	169,170,170,171	0
84	OHX	AR	3616	7/7	0.95	0.32	156,157,158,158	0
84	OHX	1	3689	7/7	0.95	0.31	131,132,132,132	0
85	MG	AR	4153	1/1	0.95	0.34	36,36,36,36	0
84	OHX	AR	3503	7/7	0.95	0.14	118,119,119,120	0
84	OHX	sR	2011	7/7	0.95	0.26	172,172,173,173	0
84	OHX	AR	3629	7/7	0.95	0.24	157,157,158,158	0
84	OHX	1	3658	7/7	0.95	0.12	173,174,174,175	0
85	MG	1	3770	1/1	0.95	0.62	42,42,42,42	0
84	OHX	AR	3686	7/7	0.95	0.32	173,174,175,175	0
85	MG	sR	2149	1/1	0.95	0.51	59,59,59,59	0
85	MG	1	4211	1/1	0.95	0.29	22,22,22,22	0
85	MG	AR	4123	1/1	0.95	0.15	40,40,40,40	0
85	MG	AR	4164	1/1	0.95	0.11	152,152,152,152	0
85	MG	AS	216	1/1	0.95	0.55	26,26,26,26	0
84	OHX	AR	3635	7/7	0.95	0.15	158,159,159,159	0
84	OHX	sR	1954	7/7	0.95	0.09	176,177,178,179	0
85	MG	AR	3838	1/1	0.95	0.28	27,27,27,27	0
85	MG	sR	2113	1/1	0.95	0.39	52,52,52,52	0
85	MG	1	4078	1/1	0.95	0.26	38,38,38,38	0
84	OHX	sR	1986	7/7	0.96	0.16	172,173,174,174	0
84	OHX	AR	3622	7/7	0.96	0.30	127,127,127,128	0
85	MG	AR	3858	1/1	0.96	0.49	29,29,29,29	0
84	OHX	sR	1992	7/7	0.96	0.29	144,144,145,145	0
84	OHX	CL	301	7/7	0.96	0.16	151,151,151,152	0
85	MG	1	3872	1/1	0.96	0.34	31,31,31,31	0
84	OHX	1	3553	7/7	0.96	0.09	170,170,171,171	0
84	OHX	1	3504	7/7	0.96	0.10	137,137,138,138	0
84	OHX	AR	3585	7/7	0.96	0.24	156,156,156,156	0
85	MG	1	3791	1/1	0.96	0.55	37,37,37,37	0
85	MG	1	4205	1/1	0.96	0.42	58,58,58,58	0
84	OHX	c8	201	7/7	0.96	0.14	166,166,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AT	220	1/1	0.96	0.58	52,52,52,52	0
85	MG	1	3863	1/1	0.96	0.49	42,42,42,42	0
84	OHX	1	3540	7/7	0.96	0.21	130,131,131,131	0
84	OHX	1	3499	7/7	0.96	0.15	106,107,107,107	0
85	MG	1	4175	1/1	0.96	0.38	54,54,54,54	0
84	OHX	1	3526	7/7	0.96	0.25	118,119,119,119	0
84	OHX	1	3650	7/7	0.96	0.18	148,149,149,149	0
85	MG	1	3932	1/1	0.96	0.43	22,22,22,22	0
85	MG	AR	3964	1/1	0.96	0.25	38,38,38,38	0
84	OHX	A	1973	7/7	0.96	0.20	167,168,169,170	0
85	MG	1	4174	1/1	0.96	0.27	60,60,60,60	0
85	MG	AR	4093	1/1	0.96	0.30	33,33,33,33	0
84	OHX	AR	3550	7/7	0.96	0.19	117,117,118,118	0
84	OHX	A	1996	7/7	0.96	0.25	162,162,163,163	0
85	MG	1	4170	1/1	0.96	0.13	50,50,50,50	0
84	OHX	1	3538	7/7	0.96	0.20	114,114,114,115	0
84	OHX	1	3539	7/7	0.96	0.13	130,131,131,132	0
84	OHX	1	3614	7/7	0.96	0.19	133,133,134,134	0
84	OHX	1	3523	7/7	0.96	0.12	131,131,132,132	0
85	MG	AR	4103	1/1	0.96	0.28	38,38,38,38	0
84	OHX	AR	3721	7/7	0.96	0.27	125,126,126,126	0
84	OHX	AT	205	7/7	0.96	0.12	136,137,137,137	0
85	MG	DP	101	1/1	0.96	0.34	52,52,52,52	0
84	OHX	A	1948	7/7	0.96	0.12	140,141,141,142	0
84	OHX	sR	1952	7/7	0.96	0.10	159,159,160,160	0
85	MG	AR	3998	1/1	0.96	0.16	48,48,48,48	0
84	OHX	y	201	7/7	0.96	0.18	151,152,153,154	0
84	OHX	1	3512	7/7	0.96	0.16	107,107,108,108	0
85	MG	1	3936	1/1	0.96	0.12	40,40,40,40	0
85	MG	1	4139	1/1	0.96	0.48	35,35,35,35	0
85	MG	AR	3790	1/1	0.96	0.41	40,40,40,40	0
84	OHX	1	3549	7/7	0.96	0.12	147,147,147,148	0
84	OHX	1	3602	7/7	0.96	0.10	168,168,169,169	0
85	MG	1	3836	1/1	0.96	0.30	36,36,36,36	0
85	MG	sR	2108	1/1	0.96	0.34	55,55,55,55	0
85	MG	1	3868	1/1	0.96	0.60	33,33,33,33	0
85	MG	1	3915	1/1	0.96	0.31	39,39,39,39	0
85	MG	3	211	1/1	0.96	0.48	33,33,33,33	0
84	OHX	1	3653	7/7	0.96	0.28	133,133,133,134	0
84	OHX	1	3605	7/7	0.96	0.13	141,142,142,142	0
84	OHX	A	1921	7/7	0.96	0.14	124,125,126,126	0
84	OHX	AR	3582	7/7	0.96	0.33	145,145,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3531	7/7	0.96	0.14	121,121,122,122	0
85	MG	1	4214	1/1	0.96	0.42	36,36,36,36	0
85	MG	sR	2057	1/1	0.96	0.50	56,56,56,56	0
84	OHX	sR	1967	7/7	0.96	0.15	142,143,144,144	0
85	MG	AR	4047	1/1	0.96	0.23	45,45,45,45	0
84	OHX	1	3603	7/7	0.96	0.25	136,136,137,137	0
86	7AL	1	4210	26/26	0.96	0.23	31,31,32,32	0
84	OHX	sR	1989	7/7	0.96	0.15	151,151,152,152	0
85	MG	1	3964	1/1	0.96	0.38	43,43,43,43	0
84	OHX	AS	208	7/7	0.96	0.24	135,135,136,136	0
84	OHX	AR	3535	7/7	0.96	0.20	107,107,108,108	0
85	MG	1	3800	1/1	0.96	0.50	62,62,62,62	0
84	OHX	AR	3476	7/7	0.96	0.21	84,84,85,85	0
84	OHX	sR	1994	7/7	0.96	0.17	157,158,159,159	0
84	OHX	A	1932	7/7	0.96	0.14	143,144,144,145	0
84	OHX	AR	3671	7/7	0.96	0.26	161,161,161,161	0
84	OHX	AR	3648	7/7	0.96	0.30	152,152,153,153	0
84	OHX	sR	1956	7/7	0.96	0.10	175,176,177,178	0
84	OHX	1	3634	7/7	0.96	0.27	128,128,129,129	0
85	MG	AR	4190	1/1	0.96	0.24	48,48,48,48	0
84	OHX	AT	209	7/7	0.96	0.20	133,133,134,134	0
84	OHX	1	3641	7/7	0.96	0.14	154,155,156,156	0
84	OHX	sR	1975	7/7	0.96	0.39	135,135,136,136	0
85	MG	A	2044	1/1	0.96	0.64	40,40,40,40	0
85	MG	1	3838	1/1	0.96	0.82	49,49,49,49	0
85	MG	sR	2162	1/1	0.96	0.40	50,50,50,50	0
84	OHX	1	3521	7/7	0.96	0.17	134,134,135,135	0
85	MG	1	3933	1/1	0.96	0.26	32,32,32,32	0
84	OHX	A	2016	7/7	0.96	0.18	161,162,162,163	0
84	OHX	1	3723	7/7	0.96	0.23	157,158,158,159	0
85	MG	AR	3910	1/1	0.96	0.49	38,38,38,38	0
85	MG	AR	4242	1/1	0.96	0.51	36,36,36,36	0
85	MG	AR	4114	1/1	0.96	0.51	37,37,37,37	0
85	MG	AR	3959	1/1	0.96	0.36	30,30,30,30	0
85	MG	1	3902	1/1	0.96	0.69	37,37,37,37	0
84	OHX	sR	1984	7/7	0.96	0.12	158,159,159,160	0
85	MG	sR	2119	1/1	0.96	0.46	67,67,67,67	0
84	OHX	1	3592	7/7	0.96	0.21	118,119,119,119	0
84	OHX	1	3528	7/7	0.96	0.15	138,139,139,139	0
85	MG	AR	3801	1/1	0.96	0.68	41,41,41,41	0
85	MG	1	3909	1/1	0.96	0.46	27,27,27,27	0
84	OHX	1	3591	7/7	0.96	0.15	169,170,171,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3481	7/7	0.96	0.13	120,120,121,121	0
85	MG	1	4120	1/1	0.96	0.35	42,42,42,42	0
84	OHX	AR	3537	7/7	0.96	0.12	142,142,143,143	0
84	OHX	AR	3592	7/7	0.96	0.20	147,148,148,149	0
84	OHX	AR	3678	7/7	0.96	0.34	123,124,124,124	0
84	OHX	Rb	401	7/7	0.96	0.16	195,195,197,197	0
84	OHX	1	3576	7/7	0.96	0.24	130,130,130,131	0
84	OHX	AR	3638	7/7	0.96	0.25	130,130,130,130	0
85	MG	A	2073	1/1	0.96	0.72	75,75,75,75	0
85	MG	1	4056	1/1	0.96	0.42	50,50,50,50	0
85	MG	1	3771	1/1	0.96	0.65	41,41,41,41	0
84	OHX	1	3488	7/7	0.96	0.15	111,112,112,112	0
85	MG	1	3937	1/1	0.96	0.15	50,50,50,50	0
84	OHX	AR	3561	7/7	0.96	0.18	122,123,123,123	0
85	MG	1	3841	1/1	0.96	0.33	40,40,40,40	0
85	MG	A	2049	1/1	0.96	0.57	48,48,48,48	0
84	OHX	AR	3563	7/7	0.96	0.12	143,144,144,144	0
84	OHX	AR	3554	7/7	0.96	0.16	125,125,125,126	0
85	MG	1	3940	1/1	0.96	0.41	52,52,52,52	0
84	OHX	1	3432	7/7	0.96	0.23	84,85,85,85	0
84	OHX	A	1960	7/7	0.96	0.13	167,168,168,169	0
85	MG	1	3962	1/1	0.96	0.22	93,93,93,93	0
84	OHX	1	3552	7/7	0.96	0.21	130,131,132,132	0
85	MG	1	3862	1/1	0.96	0.39	21,21,21,21	0
84	OHX	AT	207	7/7	0.96	0.21	135,135,135,135	0
84	OHX	AR	3587	7/7	0.96	0.20	120,121,121,121	0
85	MG	AR	3779	1/1	0.96	0.27	49,49,49,49	0
85	MG	AR	4151	1/1	0.96	0.36	49,49,49,49	0
85	MG	sR	2147	1/1	0.96	0.21	67,67,67,67	0
85	MG	AR	3906	1/1	0.96	0.78	47,47,47,47	0
84	OHX	sR	1933	7/7	0.96	0.17	106,106,107,107	0
85	MG	AR	3786	1/1	0.96	0.35	40,40,40,40	0
84	OHX	1	3596	7/7	0.96	0.14	146,147,147,147	0
85	MG	1	3899	1/1	0.96	0.32	22,22,22,22	0
85	MG	1	3865	1/1	0.96	0.67	29,29,29,29	0
85	MG	x	207	1/1	0.96	0.33	42,42,42,42	0
84	OHX	sR	2010	7/7	0.96	0.17	138,139,140,140	0
84	OHX	AR	3649	7/7	0.96	0.23	145,146,146,147	0
85	MG	AR	3956	1/1	0.96	0.32	41,41,41,41	0
84	OHX	h	401	7/7	0.96	0.12	193,195,196,196	0
84	OHX	AR	3619	7/7	0.96	0.24	138,139,139,139	0
84	OHX	1	3705	7/7	0.96	0.25	123,124,124,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3574	7/7	0.96	0.12	152,152,153,153	0
85	MG	1	4012	1/1	0.96	0.25	49,49,49,49	0
85	MG	AR	4170	1/1	0.96	0.27	55,55,55,55	0
84	OHX	1	3595	7/7	0.96	0.14	183,183,184,185	0
85	MG	1	3805	1/1	0.96	0.53	21,21,21,21	0
84	OHX	1	3627	7/7	0.96	0.18	134,135,135,135	0
85	MG	1	4026	1/1	0.96	0.67	47,47,47,47	0
85	MG	AR	3782	1/1	0.96	0.26	28,28,28,28	0
84	OHX	AR	3608	7/7	0.96	0.17	128,128,128,128	0
84	OHX	AR	3583	7/7	0.96	0.11	170,170,171,171	0
84	OHX	1	3580	7/7	0.96	0.18	117,117,118,118	0
84	OHX	AR	3581	7/7	0.96	0.25	131,132,132,132	0
85	MG	A	2096	1/1	0.96	0.17	91,91,91,91	0
84	OHX	AR	3603	7/7	0.96	0.16	142,143,143,143	0
84	OHX	AR	3698	7/7	0.96	0.31	147,148,148,148	0
85	MG	1	3990	1/1	0.96	0.31	31,31,31,31	0
85	MG	AR	3914	1/1	0.96	0.57	31,31,31,31	0
85	MG	AR	3810	1/1	0.96	0.54	25,25,25,25	0
85	MG	sM	201	1/1	0.96	0.25	44,44,44,44	0
85	MG	1	3807	1/1	0.96	0.25	33,33,33,33	0
84	OHX	AR	3547	7/7	0.96	0.11	157,157,158,158	0
84	OHX	AT	210	7/7	0.96	0.19	136,136,137,137	0
84	OHX	1	3683	7/7	0.96	0.27	135,136,136,137	0
84	OHX	AR	3632	7/7	0.96	0.23	151,151,151,151	0
85	MG	AR	3761	1/1	0.96	0.15	56,56,56,56	0
84	OHX	AR	3571	7/7	0.96	0.21	129,130,130,130	0
85	MG	AR	4239	1/1	0.96	0.29	38,38,38,38	0
84	OHX	AR	3568	7/7	0.96	0.16	147,147,148,148	0
84	OHX	AR	3519	7/7	0.96	0.17	108,108,109,109	0
84	OHX	AR	3594	7/7	0.96	0.22	137,138,138,138	0
84	OHX	AR	3576	7/7	0.96	0.21	138,139,139,140	0
84	OHX	AR	3538	7/7	0.96	0.15	124,124,124,124	0
84	OHX	1	3687	7/7	0.96	0.32	149,150,150,150	0
84	OHX	A	1965	7/7	0.96	0.12	148,149,150,150	0
84	OHX	1	3583	7/7	0.96	0.19	139,140,140,140	0
85	MG	1	3828	1/1	0.96	0.29	29,29,29,29	0
85	MG	AR	4203	1/1	0.96	0.22	40,40,40,40	0
84	OHX	sR	1943	7/7	0.96	0.12	131,132,132,132	0
84	OHX	AR	3673	7/7	0.96	0.25	179,180,181,181	0
86	7AL	AR	4246	26/26	0.96	0.20	33,33,33,33	0
84	OHX	sR	1990	7/7	0.96	0.11	159,159,160,161	0
85	MG	1	3905	1/1	0.96	0.41	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4191	1/1	0.96	0.19	26,26,26,26	0
85	MG	1	4217	1/1	0.96	0.14	36,36,36,36	0
85	MG	1	3735	1/1	0.96	0.47	50,50,50,50	0
85	MG	sR	2093	1/1	0.96	0.28	50,50,50,50	0
85	MG	AR	4192	1/1	0.96	0.49	47,47,47,47	0
84	OHX	1	3541	7/7	0.96	0.15	141,141,142,142	0
84	OHX	d4	201	7/7	0.96	0.22	171,172,172,172	0
85	MG	AB	201	1/1	0.96	0.36	26,26,26,26	0
85	MG	AR	3829	1/1	0.96	0.42	38,38,38,38	0
84	OHX	sR	1955	7/7	0.96	0.11	168,169,170,171	0
85	MG	AR	3841	1/1	0.96	0.32	53,53,53,53	0
85	MG	1	3850	1/1	0.96	0.62	40,40,40,40	0
85	MG	1	3797	1/1	0.96	0.59	54,54,54,54	0
84	OHX	sR	1929	7/7	0.96	0.15	154,154,155,156	0
85	MG	AR	3863	1/1	0.96	0.23	49,49,49,49	0
85	MG	AR	4144	1/1	0.96	0.45	30,30,30,30	0
84	OHX	AR	3617	7/7	0.96	0.15	146,146,147,147	0
85	MG	AR	3764	1/1	0.96	0.54	15,15,15,15	0
84	OHX	AR	3478	7/7	0.96	0.19	99,99,100,100	0
85	MG	sR	2058	1/1	0.96	0.36	51,51,51,51	0
84	OHX	A	1975	7/7	0.96	0.10	169,171,172,172	0
84	OHX	AR	3459	7/7	0.96	0.17	100,101,101,102	0
85	MG	AR	3825	1/1	0.96	0.39	27,27,27,27	0
84	OHX	AP	502	7/7	0.96	0.20	102,102,103,104	0
85	MG	1	3908	1/1	0.96	0.29	21,21,21,21	0
84	OHX	sR	1921	7/7	0.96	0.15	124,125,126,127	0
84	OHX	e	101	7/7	0.96	0.33	167,168,169,169	0
84	OHX	AR	3630	7/7	0.96	0.20	173,173,174,174	0
84	OHX	A	1936	7/7	0.96	0.14	127,128,128,128	0
84	OHX	AR	3447	7/7	0.97	0.16	87,87,88,88	0
84	OHX	sR	1941	7/7	0.97	0.17	110,111,111,112	0
84	OHX	sR	1963	7/7	0.97	0.12	126,126,127,127	0
84	OHX	1	3533	7/7	0.97	0.11	160,161,162,162	0
84	OHX	4	210	7/7	0.97	0.20	123,123,123,123	0
84	OHX	1	3566	7/7	0.97	0.17	143,143,143,143	0
84	OHX	1	3503	7/7	0.97	0.17	109,110,110,110	0
85	MG	1	3916	1/1	0.97	0.41	43,43,43,43	0
85	MG	AR	4139	1/1	0.97	0.13	51,51,51,51	0
84	OHX	AS	203	7/7	0.97	0.18	114,115,115,115	0
85	MG	1	3975	1/1	0.97	0.45	43,43,43,43	0
84	OHX	1	3588	7/7	0.97	0.20	152,152,153,153	0
84	OHX	v	302	7/7	0.97	0.15	121,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3898	1/1	0.97	0.29	45,45,45,45	0
85	MG	1	3818	1/1	0.97	0.49	44,44,44,44	0
84	OHX	A	1944	7/7	0.97	0.13	135,136,136,137	0
84	OHX	AR	3631	7/7	0.97	0.26	164,164,164,164	0
85	MG	AR	4175	1/1	0.97	0.28	47,47,47,47	0
85	MG	A	2092	1/1	0.97	0.19	80,80,80,80	0
85	MG	1	3826	1/1	0.97	0.22	38,38,38,38	0
85	MG	AR	3881	1/1	0.97	0.67	28,28,28,28	0
85	MG	AR	4039	1/1	0.97	0.34	47,47,47,47	0
85	MG	AR	3807	1/1	0.97	0.50	32,32,32,32	0
84	OHX	1	3578	7/7	0.97	0.19	129,130,130,131	0
85	MG	AR	3806	1/1	0.97	0.33	76,76,76,76	0
84	OHX	AR	3429	7/7	0.97	0.21	81,81,81,81	0
85	MG	AR	3763	1/1	0.97	0.17	25,25,25,25	0
85	MG	1	4129	1/1	0.97	0.46	26,26,26,26	0
85	MG	1	3767	1/1	0.97	0.28	39,39,39,39	0
84	OHX	AR	3578	7/7	0.97	0.20	132,133,133,134	0
85	MG	1	3858	1/1	0.97	0.65	37,37,37,37	0
84	OHX	AR	3589	7/7	0.97	0.15	121,122,122,122	0
84	OHX	A	1939	7/7	0.97	0.10	143,144,145,145	0
84	OHX	AR	3488	7/7	0.97	0.20	100,100,101,101	0
84	OHX	AR	3654	7/7	0.97	0.37	148,148,149,149	0
85	MG	1	3748	1/1	0.97	0.34	39,39,39,39	0
84	OHX	k	401	7/7	0.97	0.18	123,123,124,124	0
84	OHX	1	3496	7/7	0.97	0.14	115,116,116,116	0
85	MG	A	2058	1/1	0.97	0.54	49,49,49,49	0
84	OHX	AR	3540	7/7	0.97	0.15	104,104,105,105	0
85	MG	1	3739	1/1	0.97	0.45	31,31,31,31	0
85	MG	t	201	1/1	0.97	0.14	44,44,44,44	0
85	MG	1	3901	1/1	0.97	0.46	18,18,18,18	0
84	OHX	J	301	7/7	0.97	0.27	177,178,179,179	0
84	OHX	M	201	7/7	0.97	0.30	145,146,147,147	0
84	OHX	AR	3524	7/7	0.97	0.18	117,117,117,117	0
84	OHX	AR	3492	7/7	0.97	0.12	127,128,128,129	0
84	OHX	1	3449	7/7	0.97	0.19	91,91,92,92	0
85	MG	AR	3880	1/1	0.97	0.44	27,27,27,27	0
85	MG	AR	3856	1/1	0.97	0.47	34,34,34,34	0
84	OHX	4	207	7/7	0.97	0.17	130,131,131,132	0
84	OHX	1	3688	7/7	0.97	0.23	122,122,123,123	0
84	OHX	A	1910	7/7	0.97	0.20	102,103,104,104	0
84	OHX	A	1967	7/7	0.97	0.13	136,137,137,138	0
84	OHX	AR	3557	7/7	0.97	0.29	129,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3591	7/7	0.97	0.20	141,141,142,142	0
85	MG	AR	3915	1/1	0.97	0.38	28,28,28,28	0
84	OHX	sR	1972	7/7	0.97	0.33	168,169,170,170	0
84	OHX	AR	3484	7/7	0.97	0.16	105,105,106,106	0
84	OHX	1	3594	7/7	0.97	0.27	138,138,139,139	0
85	MG	A	2079	1/1	0.97	0.58	53,53,53,53	0
85	MG	4	219	1/1	0.97	0.37	43,43,43,43	0
84	OHX	A	1945	7/7	0.97	0.12	160,161,162,162	0
85	MG	AR	3948	1/1	0.97	0.50	37,37,37,37	0
84	OHX	1	3451	7/7	0.97	0.17	101,101,102,102	0
85	MG	sR	2111	1/1	0.97	0.52	43,43,43,43	0
84	OHX	1	3472	7/7	0.97	0.18	97,98,98,98	0
85	MG	sR	2175	1/1	0.97	0.25	36,36,36,36	0
85	MG	1	3761	1/1	0.97	0.58	44,44,44,44	0
84	OHX	sR	1983	7/7	0.97	0.20	155,155,156,156	0
85	MG	1	3804	1/1	0.97	0.26	21,21,21,21	0
85	MG	AR	3892	1/1	0.97	0.41	36,36,36,36	0
84	OHX	AR	3546	7/7	0.97	0.15	138,139,139,139	0
85	MG	AR	3967	1/1	0.97	0.34	38,38,38,38	0
85	MG	1	3860	1/1	0.97	0.49	31,31,31,31	0
84	OHX	1	3532	7/7	0.97	0.19	113,114,114,114	0
84	OHX	AR	3586	7/7	0.97	0.14	128,129,129,129	0
85	MG	4	224	1/1	0.97	0.24	44,44,44,44	0
85	MG	1	3927	1/1	0.97	0.61	20,20,20,20	0
84	OHX	AR	3490	7/7	0.97	0.16	95,95,96,96	0
85	MG	AR	4250	1/1	0.97	0.43	28,28,28,28	0
84	OHX	AR	3469	7/7	0.97	0.14	101,102,102,103	0
85	MG	sR	2106	1/1	0.97	0.29	41,41,41,41	0
84	OHX	1	3484	7/7	0.97	0.12	113,113,114,114	0
84	OHX	1	3544	7/7	0.97	0.23	120,121,121,121	0
85	MG	AR	3913	1/1	0.97	0.71	36,36,36,36	0
84	OHX	AR	3575	7/7	0.97	0.17	161,161,161,161	0
84	OHX	1	3624	7/7	0.97	0.18	103,103,103,103	0
84	OHX	AR	3660	7/7	0.97	0.17	131,132,133,133	0
85	MG	AS	212	1/1	0.97	0.40	40,40,40,40	0
85	MG	1	3925	1/1	0.97	0.54	27,27,27,27	0
84	OHX	A	1952	7/7	0.97	0.21	139,140,140,141	0
84	OHX	sR	1938	7/7	0.97	0.12	121,121,122,122	0
84	OHX	A	1986	7/7	0.97	0.28	169,171,172,173	0
84	OHX	A	1969	7/7	0.97	0.21	158,158,159,159	0
84	OHX	A	1970	7/7	0.97	0.19	136,136,137,137	0
84	OHX	AR	3482	7/7	0.97	0.18	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4206	1/1	0.97	0.60	25,25,25,25	0
85	MG	AR	3975	1/1	0.97	0.33	31,31,31,31	0
85	MG	AR	4002	1/1	0.97	0.35	27,27,27,27	0
84	OHX	1	3550	7/7	0.97	0.17	134,134,135,135	0
84	OHX	AR	3466	7/7	0.97	0.16	97,98,98,98	0
85	MG	AR	3872	1/1	0.97	0.42	29,29,29,29	0
85	MG	1	3856	1/1	0.97	0.40	23,23,23,23	0
85	MG	AR	3850	1/1	0.97	0.36	21,21,21,21	0
84	OHX	1	3468	7/7	0.97	0.16	109,110,110,111	0
84	OHX	1	3642	7/7	0.97	0.22	128,129,130,130	0
84	OHX	1	3567	7/7	0.97	0.26	116,117,117,118	0
85	MG	1	3917	1/1	0.97	0.51	46,46,46,46	0
84	OHX	AT	204	7/7	0.97	0.13	116,116,116,116	0
84	OHX	sR	1974	7/7	0.97	0.14	129,129,130,130	0
85	MG	AR	3922	1/1	0.97	0.59	41,41,41,41	0
84	OHX	AR	3529	7/7	0.97	0.22	127,128,128,128	0
84	OHX	AR	3544	7/7	0.97	0.12	140,140,141,142	0
85	MG	1	3918	1/1	0.97	0.50	33,33,33,33	0
84	OHX	sR	1947	7/7	0.97	0.12	124,124,125,125	0
85	MG	sR	2178	1/1	0.97	0.17	78,78,78,78	0
84	OHX	AR	3444	7/7	0.97	0.16	91,91,92,92	0
84	OHX	AS	206	7/7	0.97	0.12	114,114,115,115	0
84	OHX	1	3458	7/7	0.97	0.19	83,83,83,83	0
84	OHX	AR	3574	7/7	0.97	0.20	114,115,115,116	0
84	OHX	1	3518	7/7	0.97	0.16	109,110,110,111	0
85	MG	1	3837	1/1	0.97	0.33	33,33,33,33	0
84	OHX	AR	3443	7/7	0.97	0.14	105,105,106,106	0
84	OHX	1	3476	7/7	0.97	0.15	107,107,108,108	0
84	OHX	AT	202	7/7	0.97	0.14	134,134,134,134	0
85	MG	1	3974	1/1	0.97	0.09	59,59,59,59	0
84	OHX	1	3575	7/7	0.97	0.19	134,135,135,135	0
84	OHX	1	3522	7/7	0.97	0.13	128,129,130,130	0
84	OHX	AR	3463	7/7	0.97	0.18	85,86,86,86	0
84	OHX	A	1927	7/7	0.97	0.12	130,130,131,131	0
84	OHX	1	3473	7/7	0.97	0.18	99,99,99,100	0
84	OHX	r	301	7/7	0.97	0.17	105,105,105,106	0
85	MG	1	3870	1/1	0.97	0.56	27,27,27,27	0
84	OHX	A	1928	7/7	0.97	0.12	128,129,130,130	0
85	MG	sR	2073	1/1	0.97	0.61	58,58,58,58	0
84	OHX	1	3610	7/7	0.97	0.20	136,137,137,137	0
84	OHX	A	1933	7/7	0.97	0.16	119,120,120,120	0
85	MG	AR	4117	1/1	0.97	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3445	7/7	0.97	0.16	106,106,107,107	0
85	MG	AR	3877	1/1	0.97	0.75	36,36,36,36	0
84	OHX	1	3546	7/7	0.97	0.13	145,145,146,146	0
84	OHX	A	1979	7/7	0.97	0.17	154,155,156,157	0
84	OHX	1	3570	7/7	0.97	0.21	125,126,126,126	0
85	MG	AR	3775	1/1	0.97	0.19	38,38,38,38	0
84	OHX	A	1951	7/7	0.97	0.17	152,152,153,154	0
84	OHX	1	3563	7/7	0.97	0.12	135,135,135,136	0
84	OHX	A	1931	7/7	0.97	0.11	133,134,135,135	0
84	OHX	1	3464	7/7	0.97	0.15	108,108,109,109	0
85	MG	1	3833	1/1	0.97	0.44	23,23,23,23	0
85	MG	1	3769	1/1	0.97	0.31	50,50,50,50	0
84	OHX	1	3509	7/7	0.97	0.12	124,124,125,125	0
85	MG	1	4102	1/1	0.97	0.26	66,66,66,66	0
85	MG	1	3740	1/1	0.97	0.49	27,27,27,27	0
85	MG	1	3819	1/1	0.97	0.28	35,35,35,35	0
85	MG	AR	3997	1/1	0.97	0.34	37,37,37,37	0
84	OHX	A	1937	7/7	0.97	0.13	134,135,136,136	0
85	MG	AR	3860	1/1	0.97	0.43	26,26,26,26	0
85	MG	1	4037	1/1	0.97	0.28	55,55,55,55	0
85	MG	AR	4135	1/1	0.97	0.23	35,35,35,35	0
84	OHX	A	1956	7/7	0.97	0.12	145,146,147,147	0
85	MG	1	4048	1/1	0.97	0.58	37,37,37,37	0
84	OHX	1	3639	7/7	0.97	0.25	140,141,141,141	0
85	MG	1	3845	1/1	0.97	0.54	22,22,22,22	0
85	MG	1	4145	1/1	0.97	0.08	44,44,44,44	0
85	MG	AS	226	1/1	0.97	0.35	50,50,50,50	0
84	OHX	4	206	7/7	0.97	0.13	129,129,129,129	0
85	MG	1	3897	1/1	0.97	0.47	39,39,39,39	0
84	OHX	AR	3651	7/7	0.97	0.36	150,151,151,151	0
85	MG	1	4035	1/1	0.97	0.08	91,91,91,91	0
84	OHX	A	1943	7/7	0.97	0.15	119,120,120,121	0
85	MG	AR	3923	1/1	0.97	0.50	32,32,32,32	0
84	OHX	A	1994	7/7	0.97	0.17	158,159,160,160	0
84	OHX	1	3572	7/7	0.97	0.21	104,105,105,105	0
84	OHX	1	3585	7/7	0.97	0.19	128,128,129,129	0
85	MG	AR	3866	1/1	0.97	0.45	30,30,30,30	0
84	OHX	1	3573	7/7	0.97	0.19	144,144,145,145	0
84	OHX	A	1976	7/7	0.97	0.24	135,135,136,136	0
85	MG	1	4009	1/1	0.97	0.18	64,64,64,64	0
84	OHX	1	3542	7/7	0.97	0.18	123,124,125,125	0
84	OHX	AR	3572	7/7	0.97	0.17	130,130,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3480	7/7	0.97	0.17	103,104,104,104	0
84	OHX	AR	3636	7/7	0.97	0.14	127,127,128,128	0
84	OHX	sR	1980	7/7	0.97	0.31	161,162,163,163	0
84	OHX	1	3579	7/7	0.97	0.19	115,115,116,116	0
85	MG	1	4092	1/1	0.97	0.40	46,46,46,46	0
84	OHX	A	1988	7/7	0.97	0.18	132,133,133,134	0
84	OHX	1	3587	7/7	0.97	0.13	142,142,143,143	0
84	OHX	1	3535	7/7	0.97	0.21	126,126,126,126	0
84	OHX	1	3590	7/7	0.97	0.17	125,126,126,126	0
84	OHX	A	1982	7/7	0.97	0.28	135,136,136,137	0
84	OHX	1	3586	7/7	0.97	0.16	132,132,132,132	0
84	OHX	sR	1905	7/7	0.97	0.25	96,97,97,97	0
84	OHX	AR	3579	7/7	0.97	0.16	134,134,135,135	0
84	OHX	AR	3523	7/7	0.97	0.13	127,128,128,129	0
85	MG	AR	3788	1/1	0.97	0.57	39,39,39,39	0
84	OHX	sR	1964	7/7	0.97	0.12	137,137,138,138	0
84	OHX	AR	3588	7/7	0.97	0.28	124,124,125,125	0
84	OHX	AR	3528	7/7	0.97	0.11	115,115,115,116	0
84	OHX	1	3495	7/7	0.97	0.13	119,119,119,120	0
85	MG	A	2108	1/1	0.97	0.30	79,79,79,79	0
84	OHX	1	3498	7/7	0.97	0.12	127,128,129,129	0
84	OHX	sR	1993	7/7	0.97	0.19	141,142,142,143	0
85	MG	1	3817	1/1	0.97	0.28	39,39,39,39	0
85	MG	1	4213	1/1	0.97	0.08	72,72,72,72	0
84	OHX	4	212	7/7	0.97	0.21	144,144,145,145	0
84	OHX	1	3485	7/7	0.97	0.11	121,121,122,122	0
84	OHX	1	3684	7/7	0.97	0.10	145,145,145,146	0
84	OHX	AR	3516	7/7	0.97	0.28	114,115,115,115	0
84	OHX	A	1940	7/7	0.97	0.19	126,127,127,128	0
85	MG	AR	3874	1/1	0.97	0.43	34,34,34,34	0
85	MG	sR	2109	1/1	0.97	0.53	48,48,48,48	0
84	OHX	1	3534	7/7	0.97	0.12	161,161,162,162	0
84	OHX	sR	1939	7/7	0.97	0.11	130,131,131,132	0
84	OHX	AR	3512	7/7	0.97	0.11	133,134,134,134	0
84	OHX	4	209	7/7	0.97	0.17	129,130,130,130	0
85	MG	A	2145	1/1	0.97	0.27	89,89,89,89	0
84	OHX	AR	3517	7/7	0.97	0.17	116,116,117,117	0
84	OHX	1	3490	7/7	0.97	0.16	101,102,102,102	0
84	OHX	1	3543	7/7	0.97	0.15	113,114,114,114	0
85	MG	A	2099	1/1	0.97	0.32	50,50,50,50	0
84	OHX	1	3584	7/7	0.97	0.18	149,149,150,150	0
85	MG	AR	4106	1/1	0.97	0.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	sR	1959	7/7	0.97	0.14	141,142,143,143	0
84	OHX	1	3507	7/7	0.97	0.26	118,118,118,119	0
84	OHX	AR	3562	7/7	0.97	0.16	120,121,121,121	0
85	MG	1	4202	1/1	0.97	0.49	36,36,36,36	0
84	OHX	AR	3703	7/7	0.97	0.22	106,106,107,107	0
85	MG	AR	3805	1/1	0.97	0.60	38,38,38,38	0
84	OHX	AT	208	7/7	0.97	0.14	138,138,139,139	0
85	MG	AR	3846	1/1	0.97	0.46	40,40,40,40	0
84	OHX	AR	3551	7/7	0.97	0.19	136,136,137,137	0
84	OHX	AR	3453	7/7	0.97	0.18	86,87,87,87	0
85	MG	1	3883	1/1	0.97	0.59	30,30,30,30	0
84	OHX	sR	1965	7/7	0.97	0.21	124,125,125,125	0
85	MG	sR	2065	1/1	0.97	0.55	42,42,42,42	0
85	MG	AR	3848	1/1	0.97	0.29	29,29,29,29	0
85	MG	1	4090	1/1	0.97	0.09	43,43,43,43	0
84	OHX	AR	3500	7/7	0.97	0.24	108,109,109,109	0
84	OHX	AG	201	7/7	0.97	0.21	127,127,128,128	0
84	OHX	A	1983	7/7	0.97	0.17	161,162,163,163	0
84	OHX	1	3632	7/7	0.97	0.17	172,173,173,174	0
84	OHX	A	1909	7/7	0.97	0.17	116,116,118,118	0
85	MG	AR	3990	1/1	0.97	0.73	48,48,48,48	0
85	MG	sR	2061	1/1	0.97	0.32	84,84,84,84	0
84	OHX	AR	3539	7/7	0.97	0.20	120,120,120,120	0
85	MG	sR	2098	1/1	0.97	0.49	62,62,62,62	0
84	OHX	A	1911	7/7	0.97	0.18	110,111,112,112	0
84	OHX	AR	3593	7/7	0.97	0.14	137,137,138,138	0
84	OHX	A	1935	7/7	0.97	0.18	149,150,150,150	0
84	OHX	1	3520	7/7	0.97	0.18	113,113,114,114	0
85	MG	AR	4121	1/1	0.97	0.18	50,50,50,50	0
85	MG	AR	4016	1/1	0.97	0.29	28,28,28,28	0
84	OHX	1	3565	7/7	0.97	0.24	155,155,155,156	0
85	MG	AR	4249	1/1	0.97	0.18	38,38,38,38	0
84	OHX	1	3510	7/7	0.97	0.15	118,118,119,119	0
84	OHX	1	3508	7/7	0.97	0.13	116,116,117,117	0
84	OHX	AR	3498	7/7	0.97	0.13	146,147,147,147	0
84	OHX	A	1955	7/7	0.97	0.11	132,133,134,135	0
84	OHX	AS	204	7/7	0.97	0.13	109,110,110,110	0
84	OHX	AR	3552	7/7	0.97	0.20	109,109,109,110	0
84	OHX	1	3441	7/7	0.97	0.17	88,88,89,89	0
84	OHX	1	3474	7/7	0.97	0.17	118,119,119,119	0
85	MG	r	302	1/1	0.97	0.26	35,35,35,35	0
84	OHX	3	206	7/7	0.97	0.11	137,138,138,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3798	1/1	0.97	0.32	30,30,30,30	0
84	OHX	sR	1957	7/7	0.97	0.13	125,126,126,127	0
84	OHX	1	3493	7/7	0.97	0.12	107,107,108,108	0
84	OHX	sR	1911	7/7	0.97	0.21	98,98,98,99	0
84	OHX	sR	1946	7/7	0.97	0.10	135,136,137,137	0
84	OHX	3	202	7/7	0.97	0.12	122,122,123,123	0
84	OHX	A	1972	7/7	0.98	0.12	163,164,165,165	0
85	MG	A	2078	1/1	0.98	0.53	43,43,43,43	0
85	MG	sR	2075	1/1	0.98	0.16	63,63,63,63	0
84	OHX	A	1957	7/7	0.98	0.21	139,140,140,141	0
84	OHX	A	1941	7/7	0.98	0.15	146,146,147,147	0
85	MG	3	212	1/1	0.98	0.42	47,47,47,47	0
85	MG	AR	3937	1/1	0.98	0.38	25,25,25,25	0
85	MG	1	3893	1/1	0.98	0.55	28,28,28,28	0
84	OHX	sR	1948	7/7	0.98	0.13	118,119,119,120	0
84	OHX	sR	1918	7/7	0.98	0.14	93,94,94,94	0
84	OHX	A	1934	7/7	0.98	0.13	138,139,140,140	0
84	OHX	4	205	7/7	0.98	0.13	111,111,111,111	0
85	MG	AR	4243	1/1	0.98	0.26	27,27,27,27	0
85	MG	1	3931	1/1	0.98	0.14	29,29,29,29	0
84	OHX	AR	3449	7/7	0.98	0.17	82,82,82,82	0
85	MG	AR	3919	1/1	0.98	0.47	34,34,34,34	0
85	MG	AR	4066	1/1	0.98	0.20	71,71,71,71	0
85	MG	AR	3793	1/1	0.98	0.48	53,53,53,53	0
84	OHX	A	1929	7/7	0.98	0.16	113,113,114,114	0
84	OHX	sR	1934	7/7	0.98	0.12	123,123,124,124	0
84	OHX	1	3505	7/7	0.98	0.14	108,108,109,109	0
84	OHX	AR	3505	7/7	0.98	0.14	121,121,121,122	0
85	MG	sR	2182	1/1	0.98	0.20	60,60,60,60	0
84	OHX	AR	3525	7/7	0.98	0.20	119,120,120,120	0
84	OHX	AR	3506	7/7	0.98	0.26	117,118,118,118	0
84	OHX	AR	3596	7/7	0.98	0.14	109,110,110,110	0
85	MG	sR	2084	1/1	0.98	0.31	52,52,52,52	0
84	OHX	A	1992	7/7	0.98	0.19	142,143,143,144	0
84	OHX	AR	3474	7/7	0.98	0.14	97,97,97,97	0
84	OHX	AR	3510	7/7	0.98	0.14	117,118,118,118	0
85	MG	AR	3934	1/1	0.98	0.49	38,38,38,38	0
84	OHX	AR	3440	7/7	0.98	0.17	79,79,79,79	0
85	MG	AR	3760	1/1	0.98	0.57	33,33,33,33	0
84	OHX	4	201	7/7	0.98	0.28	79,80,80,80	0
84	OHX	1	3559	7/7	0.98	0.13	156,156,157,157	0
85	MG	AR	3900	1/1	0.98	0.42	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3515	7/7	0.98	0.12	116,116,116,117	0
85	MG	1	3892	1/1	0.98	0.68	34,34,34,34	0
85	MG	AR	3933	1/1	0.98	0.57	42,42,42,42	0
85	MG	AR	4045	1/1	0.98	0.23	74,74,74,74	0
84	OHX	AS	202	7/7	0.98	0.17	91,92,93,93	0
85	MG	AR	3787	1/1	0.98	0.55	31,31,31,31	0
84	OHX	AR	3434	7/7	0.98	0.20	85,85,85,85	0
84	OHX	1	3516	7/7	0.98	0.12	102,102,102,102	0
85	MG	sR	2166	1/1	0.98	0.09	59,59,59,59	0
84	OHX	1	3480	7/7	0.98	0.15	95,96,96,96	0
84	OHX	CE	401	7/7	0.98	0.12	110,110,111,111	0
84	OHX	1	3527	7/7	0.98	0.21	124,124,124,124	0
85	MG	1	4068	1/1	0.98	0.62	33,33,33,33	0
84	OHX	AR	3467	7/7	0.98	0.15	84,84,84,84	0
84	OHX	AR	3455	7/7	0.98	0.13	110,111,111,111	0
84	OHX	1	3551	7/7	0.98	0.15	122,123,123,123	0
84	OHX	1	3417	7/7	0.98	0.23	85,85,86,86	0
84	OHX	AR	3413	7/7	0.98	0.25	77,78,78,78	0
85	MG	AR	4025	1/1	0.98	0.19	36,36,36,36	0
85	MG	AR	3864	1/1	0.98	0.61	27,27,27,27	0
85	MG	1	3903	1/1	0.98	0.38	29,29,29,29	0
84	OHX	sR	1924	7/7	0.98	0.12	111,111,112,112	0
84	OHX	AR	3472	7/7	0.98	0.13	102,103,103,103	0
85	MG	AR	4195	1/1	0.98	0.12	81,81,81,81	0
84	OHX	3	204	7/7	0.98	0.13	119,119,120,120	0
84	OHX	AR	3565	7/7	0.98	0.19	128,128,128,128	0
84	OHX	A	1930	7/7	0.98	0.14	120,121,121,121	0
84	OHX	sR	2004	7/7	0.98	0.14	124,125,126,126	0
85	MG	1	4086	1/1	0.98	0.08	40,40,40,40	0
85	MG	1	3849	1/1	0.98	0.40	27,27,27,27	0
85	MG	AR	3936	1/1	0.98	0.71	22,22,22,22	0
85	MG	r	303	1/1	0.98	0.12	43,43,43,43	0
84	OHX	AR	3487	7/7	0.98	0.25	110,110,110,110	0
84	OHX	A	1990	7/7	0.98	0.21	150,151,152,152	0
84	OHX	1	3459	7/7	0.98	0.16	93,94,94,94	0
85	MG	AR	3952	1/1	0.98	0.13	59,59,59,59	0
84	OHX	sR	1958	7/7	0.98	0.14	119,119,120,120	0
85	MG	A	2107	1/1	0.98	0.10	147,147,147,147	0
84	OHX	4	204	7/7	0.98	0.14	103,103,103,104	0
84	OHX	1	3581	7/7	0.98	0.30	120,120,121,121	0
84	OHX	AR	3507	7/7	0.98	0.18	90,90,91,91	0
84	OHX	1	3467	7/7	0.98	0.15	102,102,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3752	1/1	0.98	0.50	36,36,36,36	0
84	OHX	AR	3485	7/7	0.98	0.14	98,98,98,98	0
85	MG	1	3782	1/1	0.98	0.47	35,35,35,35	0
85	MG	1	3898	1/1	0.98	0.39	29,29,29,29	0
84	OHX	1	3525	7/7	0.98	0.16	112,112,113,113	0
85	MG	1	3922	1/1	0.98	0.46	34,34,34,34	0
84	OHX	A	1984	7/7	0.98	0.13	130,131,131,132	0
84	OHX	1	3447	7/7	0.98	0.12	93,93,93,94	0
84	OHX	A	1913	7/7	0.98	0.15	114,114,115,115	0
84	OHX	AR	3452	7/7	0.98	0.13	107,107,108,108	0
85	MG	CR	201	1/1	0.98	0.60	35,35,35,35	0
84	OHX	AR	3545	7/7	0.98	0.21	104,105,105,105	0
84	OHX	1	3644	7/7	0.98	0.22	144,145,145,145	0
84	OHX	sR	1931	7/7	0.98	0.12	115,115,116,116	0
84	OHX	1	3601	7/7	0.98	0.28	118,118,119,119	0
85	MG	1	4119	1/1	0.98	0.10	69,69,69,69	0
84	OHX	AR	3514	7/7	0.98	0.11	110,110,110,111	0
84	OHX	sR	1949	7/7	0.98	0.12	144,145,146,146	0
84	OHX	AR	3555	7/7	0.98	0.14	116,116,117,117	0
84	OHX	1	3475	7/7	0.98	0.14	105,105,106,106	0
84	OHX	AR	3446	7/7	0.98	0.16	88,88,88,88	0
85	MG	A	2091	1/1	0.98	0.69	56,56,56,56	0
84	OHX	AR	3567	7/7	0.98	0.20	111,112,112,112	0
84	OHX	1	3448	7/7	0.98	0.14	89,89,90,90	0
84	OHX	AR	3457	7/7	0.98	0.16	100,101,101,101	0
84	OHX	1	3461	7/7	0.98	0.16	103,103,104,104	0
84	OHX	1	3487	7/7	0.98	0.14	90,91,91,92	0
84	OHX	sR	1916	7/7	0.98	0.15	93,93,94,94	0
84	OHX	1	3483	7/7	0.98	0.20	117,118,118,119	0
85	MG	1	4042	1/1	0.98	0.08	57,57,57,57	0
84	OHX	AR	3556	7/7	0.98	0.11	142,142,143,143	0
85	MG	AR	3946	1/1	0.98	0.48	21,21,21,21	0
84	OHX	sR	1937	7/7	0.98	0.13	110,110,111,111	0
84	OHX	1	3569	7/7	0.98	0.28	122,122,123,123	0
84	OHX	A	2008	7/7	0.98	0.16	132,133,133,133	0
84	OHX	AR	3479	7/7	0.98	0.13	110,111,111,112	0
84	OHX	T	201	7/7	0.98	0.15	115,116,117,117	0
84	OHX	AR	3461	7/7	0.98	0.15	95,95,95,96	0
85	MG	1	3906	1/1	0.98	0.65	23,23,23,23	0
84	OHX	A	1987	7/7	0.98	0.16	146,146,147,147	0
85	MG	1	3792	1/1	0.98	0.50	20,20,20,20	0
84	OHX	3	201	7/7	0.98	0.15	95,95,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	sR	1936	7/7	0.98	0.16	101,101,101,102	0
85	MG	AR	3925	1/1	0.98	0.53	32,32,32,32	0
84	OHX	sR	1944	7/7	0.98	0.09	145,146,147,147	0
84	OHX	A	1922	7/7	0.98	0.13	110,111,111,111	0
85	MG	AR	3917	1/1	0.98	0.62	34,34,34,34	0
84	OHX	1	3548	7/7	0.98	0.09	124,125,126,126	0
84	OHX	DH	201	7/7	0.98	0.15	119,119,120,120	0
84	OHX	sR	1997	7/7	0.98	0.19	151,152,153,153	0
85	MG	1	3881	1/1	0.98	0.31	29,29,29,29	0
84	OHX	1	3530	7/7	0.98	0.19	114,115,115,115	0
84	OHX	sR	1913	7/7	0.98	0.17	97,98,98,98	0
84	OHX	A	1926	7/7	0.98	0.12	122,123,123,123	0
84	OHX	1	3556	7/7	0.98	0.17	127,127,127,128	0
85	MG	1	4089	1/1	0.98	0.45	23,23,23,23	0
84	OHX	sR	1970	7/7	0.98	0.15	135,135,136,136	0
85	MG	AS	215	1/1	0.98	0.57	77,77,77,77	0
84	OHX	1	3452	7/7	0.98	0.16	99,99,99,100	0
84	OHX	1	3529	7/7	0.98	0.12	131,132,132,132	0
84	OHX	sR	1920	7/7	0.98	0.14	114,115,116,116	0
84	OHX	AR	3481	7/7	0.98	0.21	96,97,97,97	0
84	OHX	AR	3509	7/7	0.98	0.16	97,97,97,97	0
85	MG	AR	3861	1/1	0.98	0.53	30,30,30,30	0
84	OHX	1	3513	7/7	0.98	0.19	104,105,105,105	0
84	OHX	AK	103	7/7	0.98	0.14	100,100,101,101	0
85	MG	1	3900	1/1	0.98	0.50	25,25,25,25	0
84	OHX	sR	1942	7/7	0.98	0.13	130,131,131,132	0
84	OHX	A	1949	7/7	0.98	0.09	144,146,146,146	0
84	OHX	AR	3470	7/7	0.98	0.15	95,96,96,96	0
84	OHX	sR	1951	7/7	0.98	0.13	137,138,139,139	0
84	OHX	AR	3432	7/7	0.98	0.17	79,80,80,80	0
84	OHX	AR	3435	7/7	0.98	0.17	90,90,91,91	0
85	MG	1	3854	1/1	0.98	0.60	29,29,29,29	0
84	OHX	AR	3483	7/7	0.98	0.14	102,102,102,102	0
84	OHX	1	3477	7/7	0.98	0.14	103,103,104,104	0
84	OHX	AR	3450	7/7	0.98	0.17	92,93,93,93	0
84	OHX	1	3506	7/7	0.98	0.14	120,120,121,121	0
84	OHX	DQ	201	7/7	0.98	0.14	107,107,107,108	0
84	OHX	sR	1909	7/7	0.98	0.18	102,103,103,104	0
85	MG	AR	3895	1/1	0.98	0.31	25,25,25,25	0
84	OHX	1	3514	7/7	0.98	0.12	116,117,117,117	0
84	OHX	AR	3491	7/7	0.98	0.16	103,103,104,104	0
84	OHX	sR	1907	7/7	0.98	0.24	98,99,99,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3914	1/1	0.98	0.56	31,31,31,31	0
85	MG	1	3847	1/1	0.98	0.55	38,38,38,38	0
84	OHX	sR	1968	7/7	0.98	0.22	132,133,134,134	0
87	ZN	AQ	501	1/1	0.98	0.11	60,60,60,60	0
85	MG	AR	3747	1/1	0.98	0.19	46,46,46,46	0
84	OHX	4	208	7/7	0.98	0.23	126,126,126,126	0
84	OHX	AR	3527	7/7	0.98	0.11	120,121,121,122	0
84	OHX	A	1989	7/7	0.98	0.27	183,183,184,184	0
84	OHX	1	3536	7/7	0.98	0.16	100,100,101,101	0
84	OHX	AR	3584	7/7	0.98	0.14	109,109,110,110	0
84	OHX	AR	3520	7/7	0.98	0.15	112,112,113,113	0
84	OHX	1	3501	7/7	0.98	0.14	106,107,107,108	0
85	MG	AR	3935	1/1	0.98	0.60	35,35,35,35	0
85	MG	DC	206	1/1	0.98	0.15	38,38,38,38	0
85	MG	sR	2171	1/1	0.98	0.15	101,101,101,101	0
84	OHX	1	3426	7/7	0.98	0.19	79,79,80,80	0
84	OHX	AR	3475	7/7	0.98	0.15	90,91,91,91	0
84	OHX	AR	3454	7/7	0.98	0.15	109,110,110,110	0
84	OHX	AR	3451	7/7	0.98	0.13	103,103,104,104	0
84	OHX	1	3531	7/7	0.98	0.11	124,125,126,126	0
84	OHX	AR	3496	7/7	0.98	0.14	106,107,107,107	0
84	OHX	A	1903	7/7	0.98	0.26	107,108,108,108	0
85	MG	1	3920	1/1	0.98	0.38	25,25,25,25	0
84	OHX	AR	3501	7/7	0.98	0.09	133,134,134,135	0
84	OHX	AR	3504	7/7	0.98	0.19	106,106,106,107	0
84	OHX	A	1923	7/7	0.98	0.14	115,116,116,116	0
84	OHX	AR	3495	7/7	0.98	0.13	99,100,100,100	0
84	OHX	A	1912	7/7	0.98	0.13	105,105,106,106	0
85	MG	1	4137	1/1	0.98	0.13	62,62,62,62	0
85	MG	1	3890	1/1	0.98	0.43	27,27,27,27	0
84	OHX	AR	3497	7/7	0.98	0.20	104,104,105,105	0
84	OHX	A	1906	7/7	0.98	0.17	102,103,104,104	0
84	OHX	A	1942	7/7	0.98	0.17	127,128,128,129	0
84	OHX	A	1938	7/7	0.98	0.15	121,122,122,123	0
84	OHX	1	3577	7/7	0.98	0.14	146,147,147,148	0
84	OHX	1	3462	7/7	0.98	0.13	92,92,93,93	0
84	OHX	AR	3521	7/7	0.98	0.14	112,112,113,113	0
84	OHX	sR	1930	7/7	0.98	0.16	98,99,99,100	0
84	OHX	1	3561	7/7	0.98	0.15	116,116,116,116	0
85	MG	AR	3839	1/1	0.98	0.54	45,45,45,45	0
84	OHX	1	3436	7/7	0.98	0.18	87,88,88,88	0
85	MG	A	2050	1/1	0.98	0.45	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AS	205	7/7	0.98	0.11	112,113,113,113	0
84	OHX	sR	1953	7/7	0.98	0.12	132,133,134,134	0
84	OHX	AR	3599	7/7	0.98	0.19	130,130,131,131	0
84	OHX	1	3571	7/7	0.98	0.09	155,155,155,155	0
84	OHX	sR	1926	7/7	0.98	0.12	114,115,115,116	0
85	MG	1	4031	1/1	0.98	0.19	33,33,33,33	0
84	OHX	1	3558	7/7	0.98	0.19	127,127,128,128	0
84	OHX	1	3456	7/7	0.98	0.14	96,97,97,97	0
84	OHX	AR	3462	7/7	0.98	0.21	83,83,83,84	0
84	OHX	A	1961	7/7	0.98	0.11	154,155,156,157	0
84	OHX	sR	1962	7/7	0.98	0.20	148,148,149,149	0
85	MG	1	4157	1/1	0.98	0.10	57,57,57,57	0
84	OHX	AR	3566	7/7	0.98	0.09	156,156,157,157	0
84	OHX	AR	3534	7/7	0.98	0.13	104,104,105,105	0
84	OHX	sR	1928	7/7	0.98	0.12	126,127,127,127	0
87	ZN	DQ	202	1/1	0.98	0.04	82,82,82,82	0
85	MG	AR	3870	1/1	0.98	0.35	35,35,35,35	0
84	OHX	A	1962	7/7	0.98	0.15	133,134,135,135	0
85	MG	A	2123	1/1	0.98	0.46	50,50,50,50	0
84	OHX	1	3453	7/7	0.98	0.13	101,102,102,102	0
84	OHX	CP	501	7/7	0.98	0.18	137,137,138,138	0
85	MG	1	3995	1/1	0.98	0.12	29,29,29,29	0
85	MG	AR	4147	1/1	0.98	0.08	55,55,55,55	0
84	OHX	1	3497	7/7	0.98	0.14	104,105,105,105	0
84	OHX	DD	102	7/7	0.99	0.23	82,82,83,83	0
84	OHX	AC	101	7/7	0.99	0.24	84,84,84,85	0
84	OHX	AR	3402	7/7	0.99	0.31	82,82,82,82	0
84	OHX	1	3439	7/7	0.99	0.18	86,86,86,86	0
85	MG	sR	2152	1/1	0.99	0.08	110,110,110,110	0
84	OHX	AR	3464	7/7	0.99	0.11	98,98,98,99	0
84	OHX	A	1905	7/7	0.99	0.18	93,94,94,94	0
84	OHX	AR	3420	7/7	0.99	0.23	84,84,84,84	0
84	OHX	1	3437	7/7	0.99	0.20	85,85,85,85	0
84	OHX	AR	3473	7/7	0.99	0.13	103,103,104,104	0
84	OHX	AR	3428	7/7	0.99	0.20	81,81,81,81	0
84	OHX	AR	3427	7/7	0.99	0.17	77,77,77,77	0
84	OHX	1	3471	7/7	0.99	0.12	98,99,99,99	0
84	OHX	A	1950	7/7	0.99	0.14	116,117,117,118	0
84	OHX	A	1914	7/7	0.99	0.15	101,102,103,103	0
84	OHX	1	3440	7/7	0.99	0.17	82,83,83,83	0
84	OHX	1	3442	7/7	0.99	0.15	88,89,89,89	0
84	OHX	AR	3513	7/7	0.99	0.15	81,81,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3443	7/7	0.99	0.15	89,90,90,91	0
84	OHX	sR	1927	7/7	0.99	0.15	100,100,101,101	0
84	OHX	1	3410	7/7	0.99	0.24	82,83,83,83	0
84	OHX	A	1954	7/7	0.99	0.15	129,130,130,130	0
85	MG	1	3744	1/1	0.99	0.76	52,52,52,52	0
84	OHX	AR	3401	7/7	0.99	0.34	88,88,88,88	0
84	OHX	1	3444	7/7	0.99	0.18	90,90,91,91	0
84	OHX	sR	1904	7/7	0.99	0.19	90,90,90,91	0
84	OHX	1	3402	7/7	0.99	0.30	84,84,84,84	0
84	OHX	AR	3422	7/7	0.99	0.22	83,84,84,84	0
84	OHX	sR	1901	7/7	0.99	0.27	87,87,87,87	0
84	OHX	1	3416	7/7	0.99	0.18	80,80,80,80	0
84	OHX	AR	3493	7/7	0.99	0.19	83,83,83,83	0
87	ZN	AP	501	1/1	0.99	0.03	75,75,75,75	0
84	OHX	AR	3530	7/7	0.99	0.07	128,129,129,130	0
84	OHX	1	3450	7/7	0.99	0.14	97,98,99,99	0
84	OHX	1	3478	7/7	0.99	0.15	93,93,93,94	0
84	OHX	AR	3486	7/7	0.99	0.16	87,87,88,88	0
84	OHX	A	1901	7/7	0.99	0.21	92,93,93,93	0
85	MG	AR	3867	1/1	0.99	0.34	37,37,37,37	0
84	OHX	AR	3433	7/7	0.99	0.19	80,80,80,80	0
84	OHX	1	3454	7/7	0.99	0.13	90,91,91,91	0
84	OHX	sR	1925	7/7	0.99	0.16	101,101,102,102	0
85	MG	AR	3929	1/1	0.99	0.49	31,31,31,31	0
84	OHX	AR	3412	7/7	0.99	0.26	80,80,80,80	0
84	OHX	AR	3441	7/7	0.99	0.16	87,87,87,88	0
85	MG	1	4121	1/1	0.99	0.18	66,66,66,66	0
84	OHX	1	3435	7/7	0.99	0.20	92,92,93,93	0
84	OHX	A	1904	7/7	0.99	0.17	97,97,97,97	0
84	OHX	AR	3426	7/7	0.99	0.20	82,82,83,83	0
84	OHX	AR	3410	7/7	0.99	0.24	78,79,79,79	0
84	OHX	sR	1910	7/7	0.99	0.20	87,88,88,88	0
84	OHX	1	3419	7/7	0.99	0.20	79,79,79,79	0
84	OHX	AR	3407	7/7	0.99	0.25	80,80,80,80	0
84	OHX	1	3438	7/7	0.99	0.18	85,86,86,86	0
84	OHX	sR	1922	7/7	0.99	0.16	103,103,104,104	0
84	OHX	AR	3409	7/7	0.99	0.24	82,82,83,83	0
84	OHX	1	3427	7/7	0.99	0.20	88,88,89,89	0
85	MG	1	4189	1/1	0.99	0.14	46,46,46,46	0
85	MG	1	4156	1/1	0.99	0.12	83,83,83,83	0
84	OHX	1	3445	7/7	0.99	0.17	85,85,85,85	0
84	OHX	A	1920	7/7	0.99	0.12	102,102,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	1924	7/7	0.99	0.08	121,121,122,123	0
85	MG	AR	3773	1/1	0.99	0.59	43,43,43,43	0
84	OHX	sR	1915	7/7	0.99	0.16	92,93,93,94	0
84	OHX	1	3500	7/7	0.99	0.13	81,82,82,82	0
84	OHX	1	3469	7/7	0.99	0.23	85,85,85,86	0
84	OHX	AR	3442	7/7	0.99	0.12	95,96,96,97	0
84	OHX	1	3403	7/7	0.99	0.30	83,83,83,83	0
84	OHX	1	3492	7/7	0.99	0.11	106,106,107,107	0
84	OHX	AR	3431	7/7	0.99	0.17	81,81,82,82	0
84	OHX	AR	3615	7/7	0.99	0.18	107,107,107,107	0
85	MG	1	3851	1/1	0.99	0.17	38,38,38,38	0
84	OHX	A	1908	7/7	0.99	0.17	103,104,105,105	0
84	OHX	AR	3439	7/7	0.99	0.17	79,79,79,79	0
85	MG	A	2141	1/1	0.99	0.28	78,78,78,78	0
85	MG	AR	4231	1/1	0.99	0.14	80,80,80,80	0
84	OHX	AR	3468	7/7	0.99	0.11	101,101,102,102	0
84	OHX	sR	1935	7/7	0.99	0.13	109,109,110,110	0
84	OHX	1	3517	7/7	0.99	0.11	117,117,118,118	0
84	OHX	1	3429	7/7	0.99	0.20	93,93,94,94	0
84	OHX	CX	201	7/7	0.99	0.15	93,94,94,94	0
84	OHX	1	3405	7/7	0.99	0.28	91,91,91,91	0
84	OHX	1	3460	7/7	0.99	0.13	82,82,83,83	0
85	MG	x	205	1/1	0.99	0.63	31,31,31,31	0
84	OHX	1	3479	7/7	0.99	0.11	108,108,109,109	0
84	OHX	1	3433	7/7	0.99	0.18	86,86,87,87	0
84	OHX	sR	1906	7/7	0.99	0.20	90,90,90,90	0
84	OHX	AR	3425	7/7	0.99	0.21	81,81,81,82	0
87	ZN	DR	501	1/1	0.99	0.11	62,62,62,62	0
84	OHX	4	202	7/7	0.99	0.24	83,83,83,83	0
84	OHX	CV	201	7/7	0.99	0.26	85,85,85,85	0
84	OHX	1	3420	7/7	0.99	0.21	86,86,86,87	0
84	OHX	1	3466	7/7	0.99	0.13	94,95,95,95	0
84	OHX	sR	1902	7/7	0.99	0.24	98,99,99,99	0
84	OHX	AR	3424	7/7	0.99	0.23	82,82,82,82	0
85	MG	AR	4184	1/1	0.99	0.14	43,43,43,43	0
85	MG	AR	4146	1/1	0.99	0.07	42,42,42,42	0
87	ZN	DL	102	1/1	0.99	0.18	44,44,44,44	0
84	OHX	1	3434	7/7	0.99	0.18	86,87,87,87	0
84	OHX	1	3414	7/7	0.99	0.20	80,81,81,81	0
87	ZN	AK	101	1/1	0.99	0.16	39,39,39,39	0
84	OHX	1	3401	7/7	0.99	0.30	84,84,84,85	0
84	OHX	1	3465	7/7	0.99	0.14	93,93,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3489	7/7	0.99	0.15	95,95,95,96	0
85	MG	1	3930	1/1	0.99	0.52	26,26,26,26	0
84	OHX	1	3418	7/7	0.99	0.21	84,84,84,84	0
84	OHX	A	1902	7/7	0.99	0.18	88,89,89,89	0
87	ZN	b	102	1/1	0.99	0.10	84,84,84,84	0
85	MG	sR	2177	1/1	0.99	0.15	84,84,84,84	0
85	MG	1	3910	1/1	0.99	0.44	31,31,31,31	0
85	MG	1	3842	1/1	0.99	0.44	27,27,27,27	0
84	OHX	1	3494	7/7	0.99	0.14	89,90,90,90	0
85	MG	1	3926	1/1	0.99	0.63	23,23,23,23	0
84	OHX	sR	1917	7/7	0.99	0.13	98,99,100,100	0
84	OHX	AR	3456	7/7	0.99	0.15	83,83,83,83	0
85	MG	AR	4221	1/1	0.99	0.15	40,40,40,40	0
84	OHX	AR	3421	7/7	0.99	0.20	89,89,89,89	0
84	OHX	AR	3494	7/7	0.99	0.10	106,107,107,107	0
85	MG	1	4118	1/1	0.99	0.16	100,100,100,100	0
84	OHX	AR	3423	7/7	0.99	0.20	82,82,82,82	0
84	OHX	1	3524	7/7	0.99	0.14	107,107,108,108	0
84	OHX	AR	3406	7/7	0.99	0.26	82,82,82,82	0
84	OHX	AR	3404	7/7	0.99	0.29	81,81,82,82	0
84	OHX	AS	201	7/7	0.99	0.17	88,88,88,89	0
84	OHX	1	3412	7/7	0.99	0.24	83,83,84,84	0
84	OHX	AR	3403	7/7	0.99	0.29	80,80,80,80	0
84	OHX	1	3428	7/7	0.99	0.18	83,83,83,83	0
85	MG	AR	4179	1/1	0.99	0.14	70,70,70,70	0
87	ZN	e	103	1/1	0.99	0.09	82,82,82,82	0
84	OHX	1	3406	7/7	0.99	0.26	79,79,79,79	0
84	OHX	A	1917	7/7	0.99	0.12	105,106,106,107	0
84	OHX	1	3407	7/7	0.99	0.23	78,78,78,78	0
84	OHX	1	3415	7/7	0.99	0.24	90,90,91,91	0
84	OHX	AR	3419	7/7	0.99	0.20	81,82,82,82	0
84	OHX	1	3408	7/7	0.99	0.27	83,83,83,83	0
85	MG	AR	4180	1/1	0.99	0.15	66,66,66,66	0
85	MG	AR	4241	1/1	0.99	0.67	41,41,41,41	0
84	OHX	A	1907	7/7	0.99	0.15	99,100,100,101	0
84	OHX	AR	3460	7/7	0.99	0.12	90,91,91,91	0
84	OHX	AR	3418	7/7	0.99	0.17	84,84,84,84	0
84	OHX	sR	1945	7/7	0.99	0.12	118,119,119,120	0
84	OHX	4	203	7/7	0.99	0.14	83,83,84,84	0
84	OHX	AR	3416	7/7	0.99	0.21	82,82,82,82	0
84	OHX	AR	3448	7/7	0.99	0.16	86,86,86,87	0
84	OHX	1	3431	7/7	0.99	0.15	81,81,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3430	7/7	0.99	0.13	86,86,86,86	0
84	OHX	AR	3417	7/7	0.99	0.22	79,80,80,80	0
84	OHX	AR	3471	7/7	0.99	0.14	90,91,91,92	0
85	MG	AR	3770	1/1	0.99	0.29	55,55,55,55	0
85	MG	1	4169	1/1	0.99	0.16	39,39,39,39	0
84	OHX	AR	3408	7/7	0.99	0.24	77,77,77,77	0
84	OHX	1	3423	7/7	0.99	0.18	88,88,88,88	0
84	OHX	A	1925	7/7	0.99	0.11	135,135,136,136	0
84	OHX	AR	3465	7/7	0.99	0.11	102,103,103,103	0
84	OHX	1	3413	7/7	0.99	0.24	82,83,83,83	0
84	OHX	1	3457	7/7	0.99	0.14	94,95,95,95	0
85	MG	AR	4064	1/1	0.99	0.12	84,84,84,84	0
84	OHX	AT	203	7/7	0.99	0.13	104,104,104,104	0
85	MG	1	4063	1/1	0.99	0.52	35,35,35,35	0
84	OHX	1	3425	7/7	0.99	0.21	87,88,88,88	0
84	OHX	A	1919	7/7	0.99	0.13	100,100,101,101	0
84	OHX	1	3422	7/7	0.99	0.20	85,86,86,86	0
84	OHX	sR	1923	7/7	0.99	0.14	92,93,93,94	0
84	OHX	AR	3502	7/7	0.99	0.12	112,112,113,113	0
84	OHX	sR	1912	7/7	0.99	0.16	89,89,90,90	0
85	MG	AR	3928	1/1	0.99	0.67	42,42,42,42	0
84	OHX	AR	3405	7/7	0.99	0.27	86,86,87,87	0
85	MG	sR	2150	1/1	0.99	0.09	76,76,76,76	0
84	OHX	AR	3414	7/7	0.99	0.24	80,80,80,80	0
84	OHX	1	3409	7/7	0.99	0.25	85,86,86,86	0
84	OHX	sR	1903	7/7	0.99	0.21	86,86,86,87	0
84	OHX	AR	3415	7/7	0.99	0.21	78,78,79,79	0
84	OHX	sR	1908	7/7	0.99	0.18	87,88,88,88	0
84	OHX	AR	3438	7/7	0.99	0.14	84,84,85,85	0
84	OHX	AR	3411	7/7	0.99	0.26	87,87,88,88	0
84	OHX	A	1916	7/7	0.99	0.13	106,107,108,108	0
84	OHX	1	3424	7/7	0.99	0.16	84,84,84,84	0
84	OHX	AR	3436	7/7	0.99	0.15	80,81,81,81	0
84	OHX	1	3491	7/7	0.99	0.14	97,97,98,98	0
84	OHX	v	301	7/7	0.99	0.15	92,92,92,93	0
84	OHX	AR	3437	7/7	0.99	0.14	83,83,83,84	0
84	OHX	AR	3430	7/7	0.99	0.15	84,84,85,85	0
84	OHX	1	3404	7/7	0.99	0.29	89,89,89,89	0
84	OHX	sR	1914	7/7	0.99	0.15	104,104,105,106	0
87	ZN	AN	500	1/1	1.00	0.15	43,43,43,43	0
85	MG	AR	4208	1/1	1.00	0.17	73,73,73,73	0
87	ZN	d6	103	1/1	1.00	0.12	68,68,68,68	0

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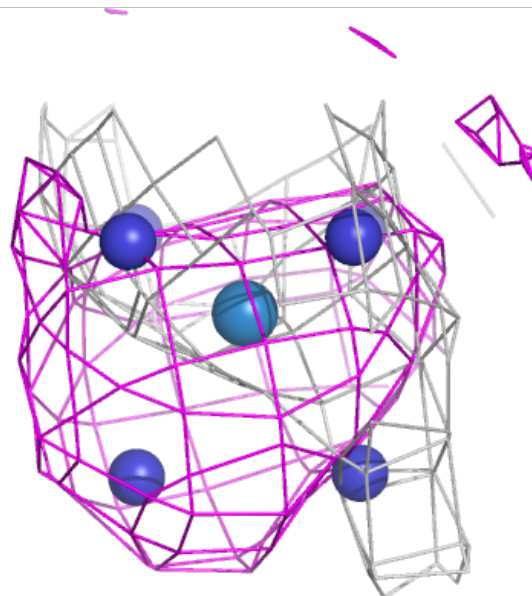
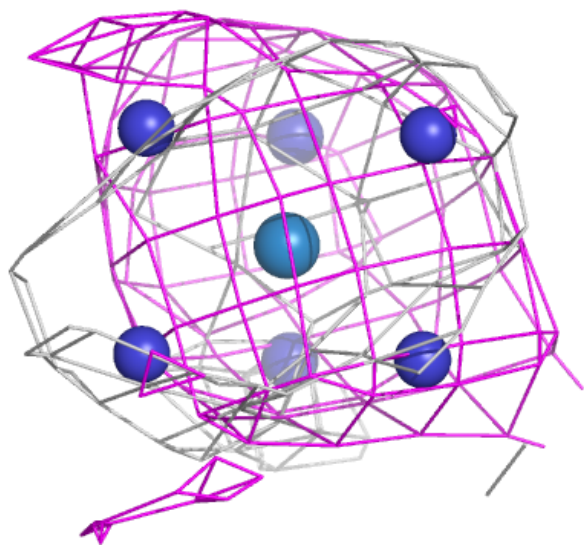
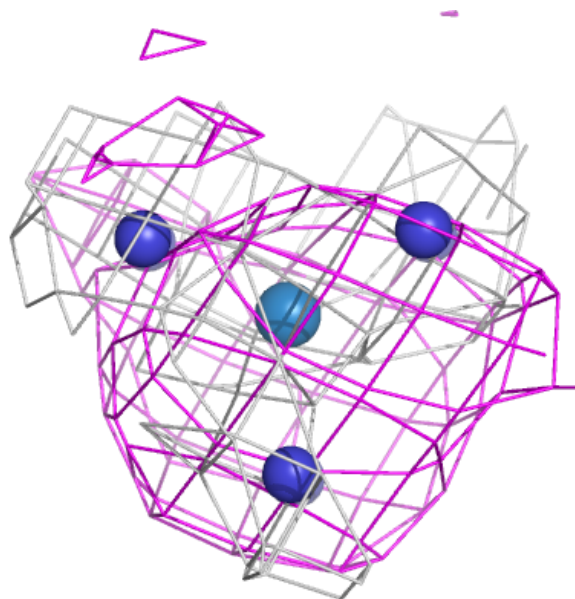
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	ZN	d9	103	1/1	1.00	0.12	81,81,81,81	0
85	MG	1	4099	1/1	1.00	0.17	68,68,68,68	0
87	ZN	DO	201	1/1	1.00	0.16	29,29,29,29	0
85	MG	AR	3912	1/1	1.00	0.58	29,29,29,29	0
85	MG	1	4158	1/1	1.00	0.15	57,57,57,57	0
84	OHX	1	3411	7/7	1.00	0.22	81,82,82,82	0
84	OHX	1	3421	7/7	1.00	0.21	84,84,85,85	0
85	MG	AR	4204	1/1	1.00	0.17	63,63,63,63	0

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

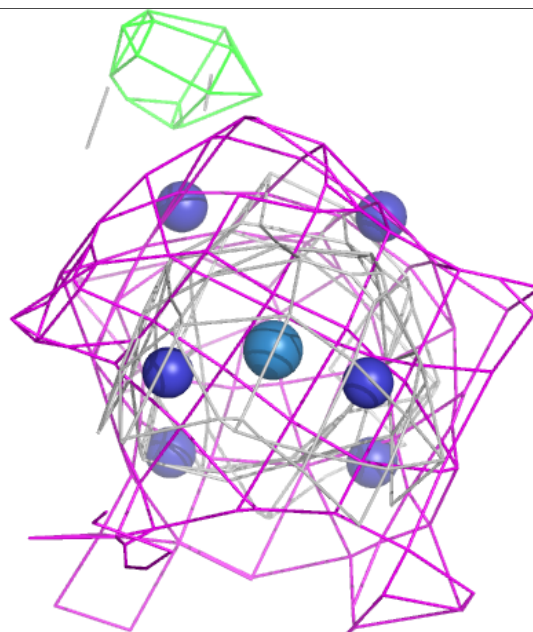
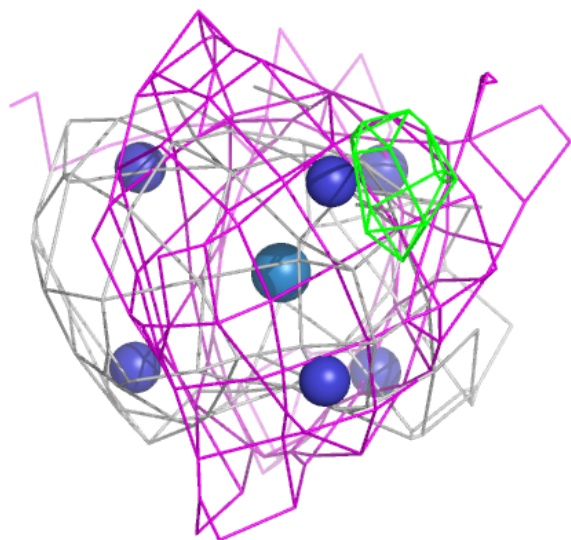
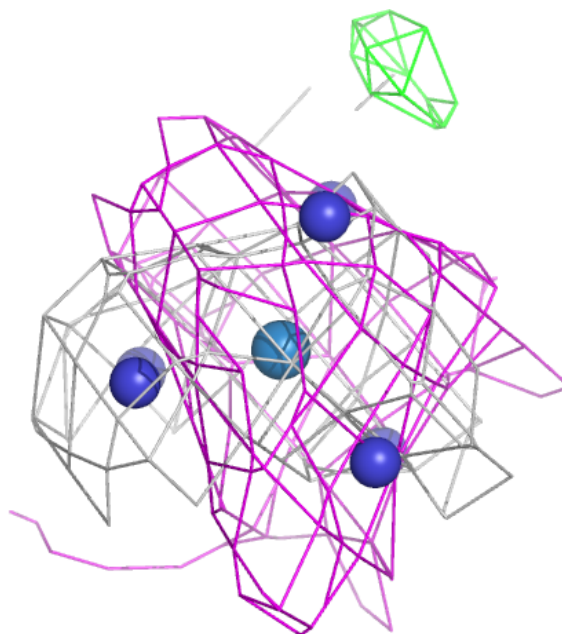
**Electron density around OHX AR 3740:**

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



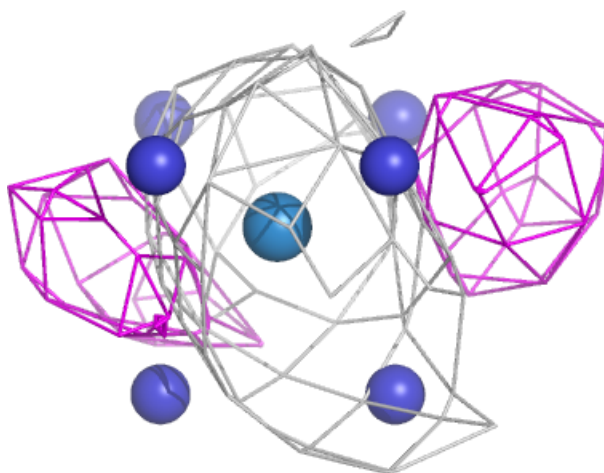
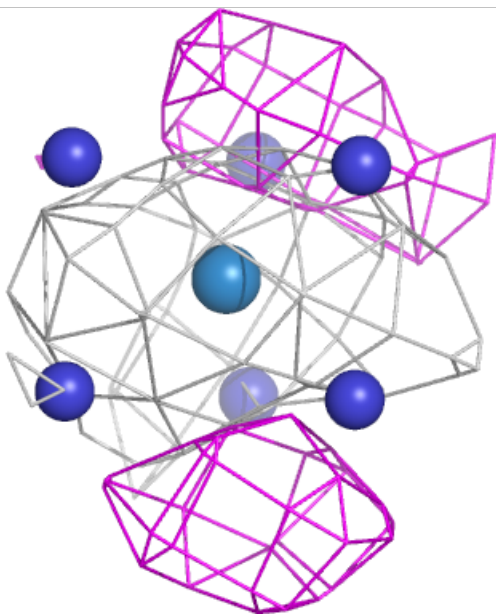
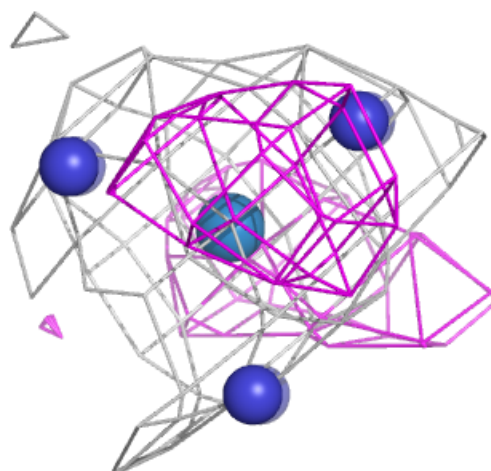
**Electron density around OHX 1 3673:**

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



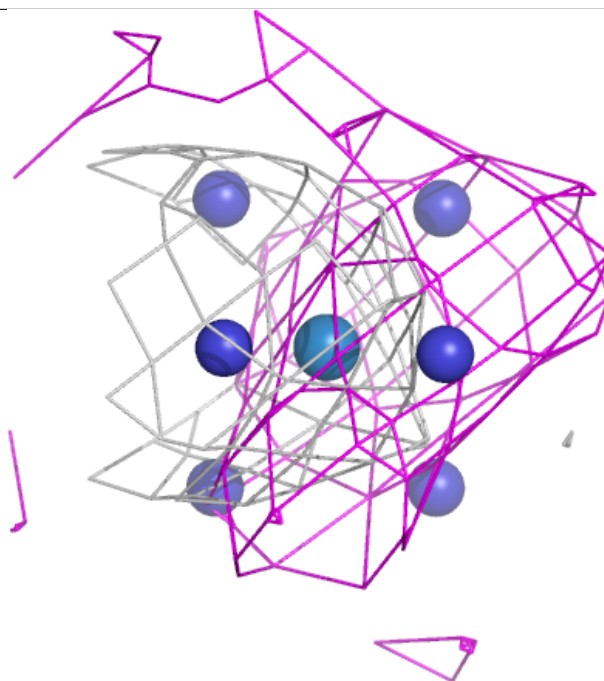
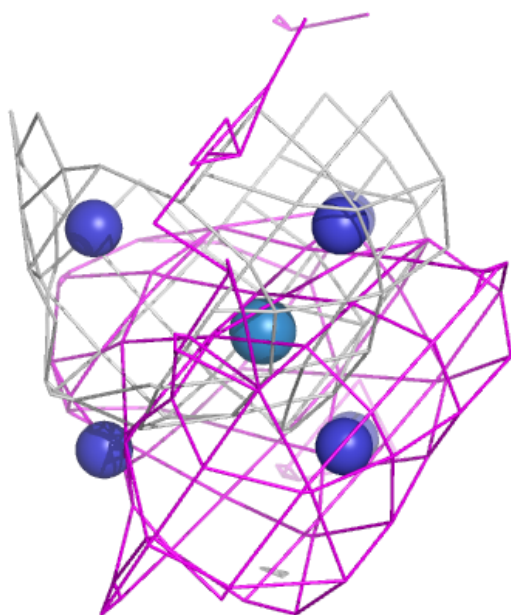
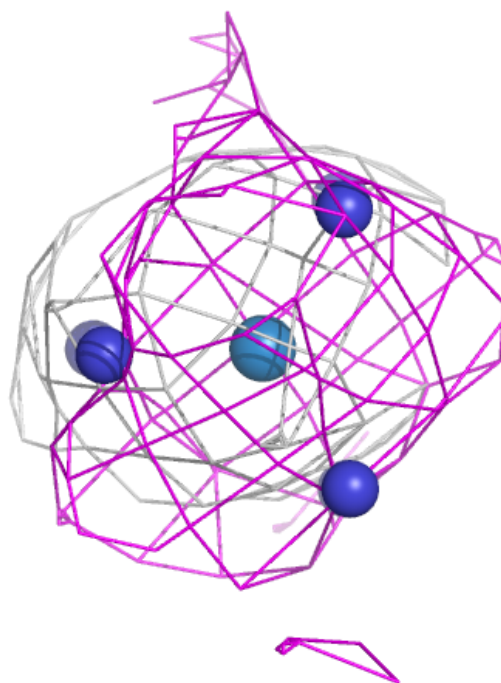
**Electron density around OHX 1 3718:**

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



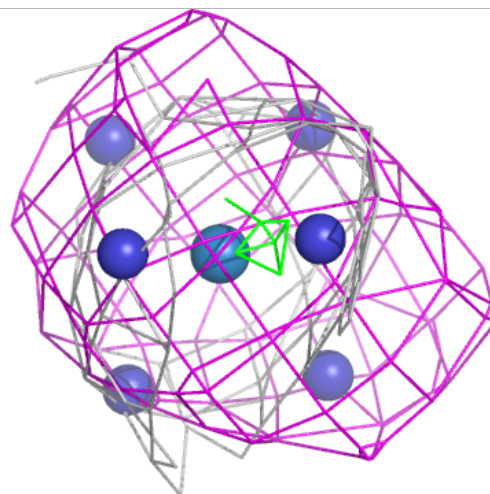
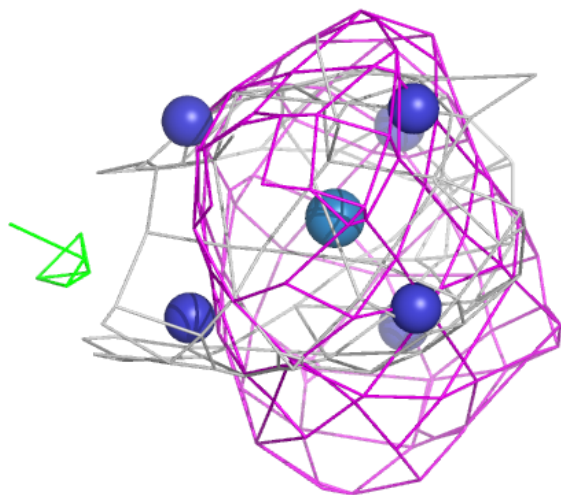
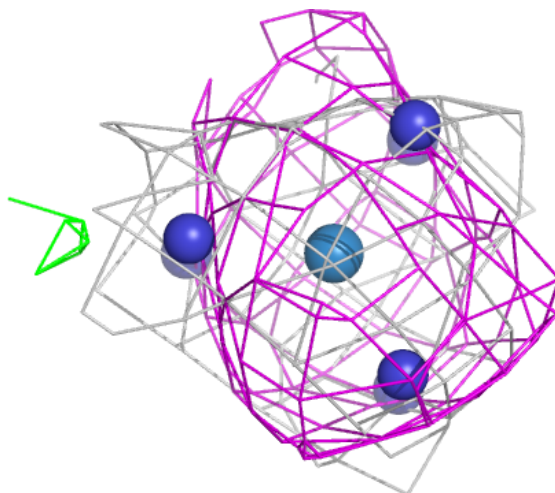
**Electron density around OHX A 2039:**

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



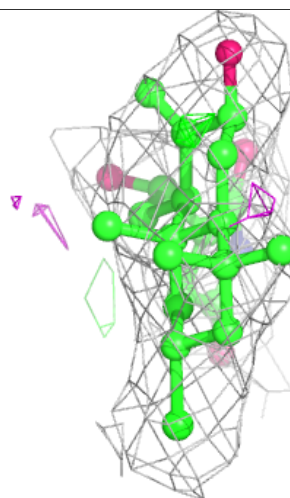
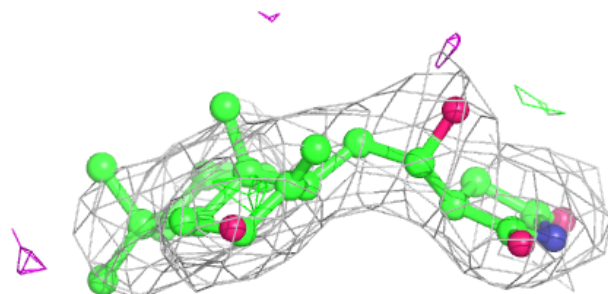
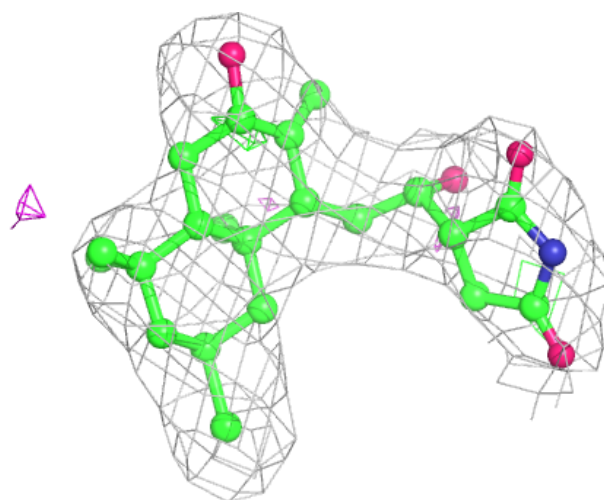
**Electron density around OHX sR 2040:**

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



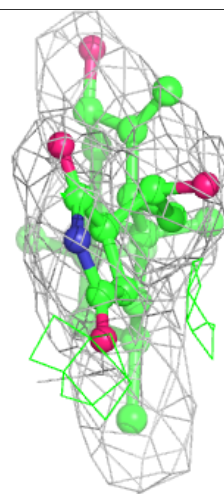
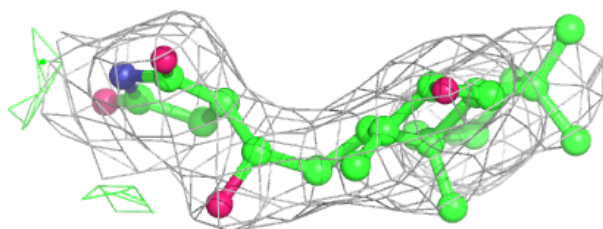
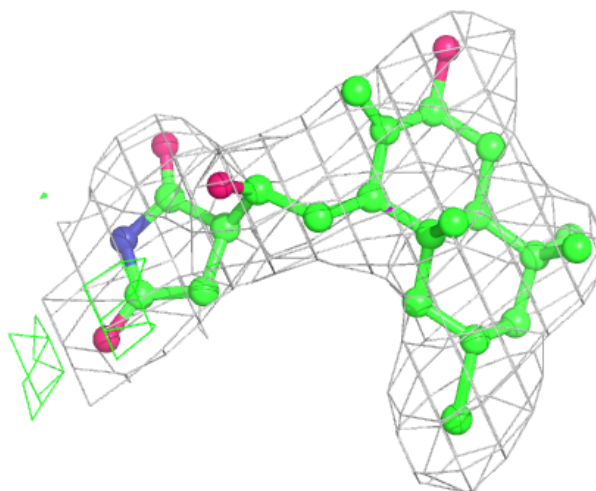
**Electron density around 7AL 1 4210:**

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



**Electron density around 7AL AR 4246:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.