



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2020 – 01:29 pm BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

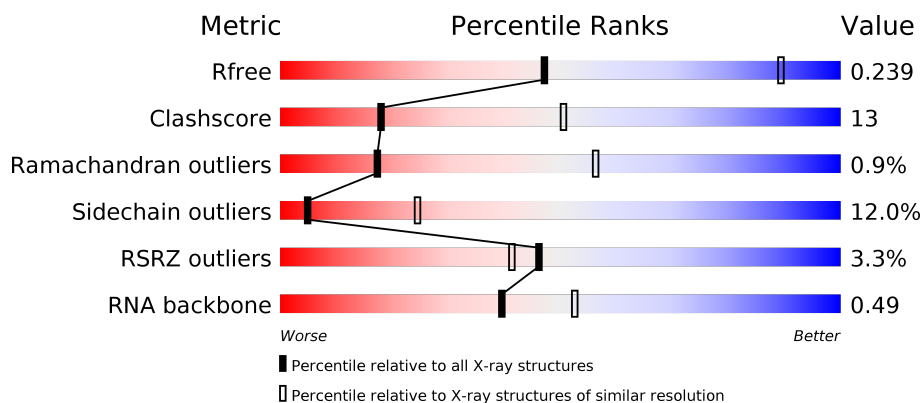
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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






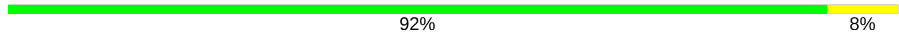








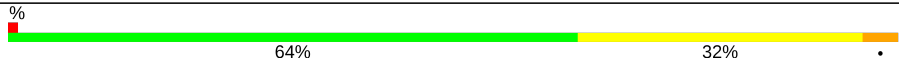


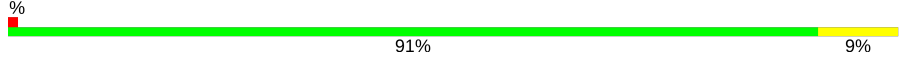







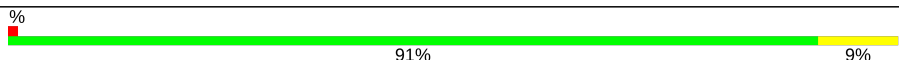

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	1	3396	<div> <div>2%</div> <div>45% 37% 10% 7%</div> </div>
1	AR	3396	<div> <div>2%</div> <div>42% 39% 11% 7%</div> </div>
2	3	121	<div> <div>59% 36% 6%</div> </div>
2	AS	121	<div> <div>% 50% 46%</div> </div>




















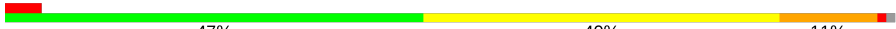
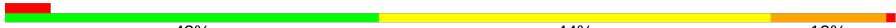




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Mol	Chain	Length	Quality of chain
3	4	158	
3	AT	158	
4	CD	252	
4	j	252	
5	CE	386	
5	k	386	
6	CF	361	
6	l	361	
7	CG	296	
7	m	296	
8	CH	175	
8	n	175	
9	CI	222	
9	o	222	
10	CJ	233	
10	p	233	
11	CK	191	
11	q	191	
12	CL	220	
12	r	220	
13	CM	169	
13	s	169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

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Mol	Chain	Length	Quality of chain
15	u	136	
16	CP	203	
16	v	203	
17	CQ	197	
17	w	197	
18	CR	183	
18	x	183	
19	CS	185	
19	y	185	
20	CT	188	
20	z	188	
21	0	172	
21	CU	172	
22	2	159	
22	CV	159	
23	5	100	
23	CW	100	
24	CX	136	
24	12	136	
25	6	1800	
25	A	1800	
26	7	98	
26	CY	98	
27	8	121	
27	CZ	121	

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

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Mol	Chain	Length	Quality of chain
40	DM	77	
41	AM	50	
41	DN	50	
42	AN	52	
42	DO	52	
43	AO	25	
43	DP	25	
44	AP	105	
44	DQ	105	
45	AQ	91	
45	DR	91	
46	i	168	
47	p0	220	
48	sM	104	
49	B	206	
49	s0	206	
50	C	216	
50	s1	216	
51	D	217	
51	s2	217	
52	E	223	
52	s3	223	
53	F	260	
53	s4	260	
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	124	
61	c2	124	
62	O	150	
62	c3	150	
63	P	128	
63	c4	128	
64	Q	141	
64	c5	141	
65	R	142	
65	c6	142	
66	S	125	
67	T	145	



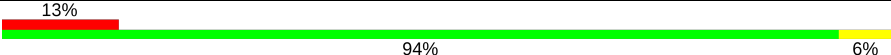
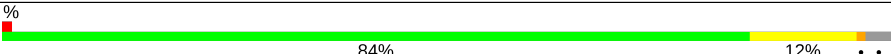
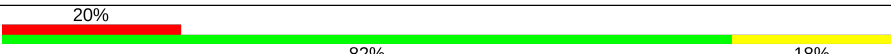
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Mol	Chain	Length	Quality of chain
67	c8	145	
68	U	143	
68	c9	143	
69	V	110	
69	d0	110	
70	W	87	
70	d1	87	
71	X	129	
71	d2	129	
72	Y	144	
72	d3	144	
73	Z	134	
73	d4	134	
74	a	70	
74	d5	70	
75	b	97	
75	d6	97	
76	c	81	
76	d7	81	
77	d	63	
77	d8	63	
78	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	h	318	
81	sR	318	
82	c7	121	
83	e1	51	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	1	3406	-	-	X	-
84	OHX	1	3471	-	-	X	-
84	OHX	1	3496	-	-	X	-
84	OHX	1	3594	-	-	X	-
84	OHX	1	3675	-	-	-	X
84	OHX	1	3702	-	-	X	-
84	OHX	1	3722	-	-	-	X
84	OHX	A	1954	-	-	X	-
84	OHX	AE	201	-	-	X	-
84	OHX	AR	3443	-	-	X	-
84	OHX	AR	3604	-	-	X	-
84	OHX	AR	3731	-	-	X	-
84	OHX	CG	302	-	-	X	-
85	MG	1	3758	-	-	-	X
85	MG	1	3789	-	-	-	X
85	MG	1	3801	-	-	-	X
85	MG	1	3830	-	-	-	X
85	MG	1	3949	-	-	-	X
85	MG	1	4008	-	-	-	X
85	MG	1	4010	-	-	-	X
85	MG	1	4063	-	-	-	X
85	MG	1	4140	-	-	-	X
85	MG	1	4175	-	-	-	X
85	MG	1	4183	-	-	-	X
85	MG	1	4192	-	-	-	X
85	MG	1	4206	-	-	-	X
85	MG	4	217	-	-	-	X
85	MG	6	2065	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	6	2170	-	-	-	X
85	MG	6	2181	-	-	-	X
85	MG	6	2185	-	-	-	X
85	MG	6	2190	-	-	-	X
85	MG	6	2193	-	-	-	X
85	MG	A	2073	-	-	-	X
85	MG	A	2089	-	-	-	X
85	MG	A	2098	-	-	-	X
85	MG	A	2103	-	-	-	X
85	MG	A	2112	-	-	-	X
85	MG	A	2118	-	-	-	X
85	MG	A	2124	-	-	-	X
85	MG	A	2129	-	-	-	X
85	MG	A	2135	-	-	-	X
85	MG	AR	3804	-	-	-	X
85	MG	AR	3812	-	-	-	X
85	MG	AR	3820	-	-	-	X
85	MG	AR	3826	-	-	-	X
85	MG	AR	3880	-	-	-	X
85	MG	AR	3893	-	-	-	X
85	MG	AR	3958	-	-	-	X
85	MG	AR	4024	-	-	-	X
85	MG	AR	4101	-	-	-	X
85	MG	AR	4122	-	-	-	X
85	MG	AR	4167	-	-	-	X
85	MG	AR	4173	-	-	-	X
85	MG	AR	4193	-	-	-	X
85	MG	AR	4202	-	-	-	X
85	MG	AR	4214	-	-	-	X
85	MG	AR	4233	-	-	-	X
85	MG	AR	4241	-	-	-	X
85	MG	AT	223	-	-	-	X
85	MG	CK	202	-	-	-	X
85	MG	CO	202	-	-	-	X
85	MG	l	402	-	-	-	X

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 409590 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
24	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 46 is a protein called Suppressor protein STM1.

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

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

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

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

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

- Molecule 49 is a protein called 40S ribosomal protein S0-A.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	R	141	Total	C	N	O	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-B.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

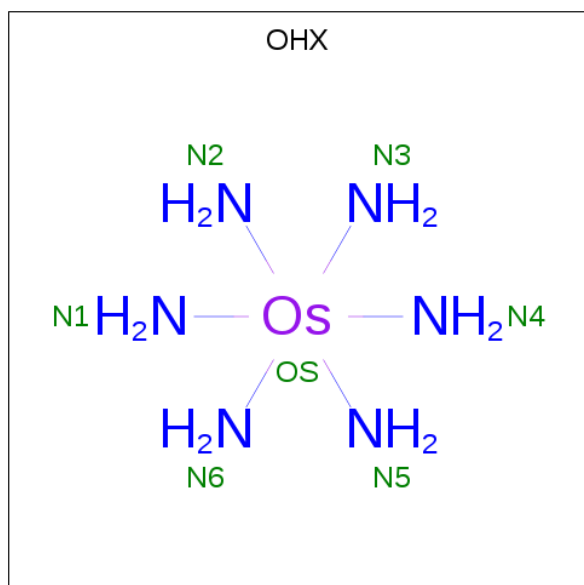
- Molecule 82 is a protein called 40S ribosomal protein S17-A.

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

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

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

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



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

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

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

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

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

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

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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		

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	H	1	Total	N	Os	0	0
			7	6	1		
84	J	1	Total	N	Os	0	0
			7	6	1		
84	M	1	Total	N	Os	0	0
			7	6	1		
84	O	1	Total	N	Os	0	0
			7	6	1		
84	Q	1	Total	N	Os	0	0
			7	6	1		
84	T	1	Total	N	Os	0	0
			7	6	1		
84	e	1	Total	N	Os	0	0
			7	6	1		
84	h	1	Total	N	Os	0	0
			7	6	1		
84	s8	1	Total	N	Os	0	0
			7	6	1		
84	c3	1	Total	N	Os	0	0
			7	6	1		
84	c5	1	Total	N	Os	0	0
			7	6	1		
84	c8	1	Total	N	Os	0	0
			7	6	1		
84	d9	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		

- Molecule 85 is MAGNESIUM ION (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		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AB	4	Total 4	Mg 4	0	0
85	DF	1	Total 1	Mg 1	0	0
85	c6	1	Total 1	Mg 1	0	0
85	6	141	Total 141	Mg 141	0	0
85	DO	1	Total 1	Mg 1	0	0
85	sM	1	Total 1	Mg 1	0	0
85	d5	1	Total 1	Mg 1	0	0
85	t	2	Total 2	Mg 2	0	0
85	CD	2	Total 2	Mg 2	0	0
85	CR	6	Total 6	Mg 6	0	0
85	o	3	Total 3	Mg 3	0	0
85	DC	4	Total 4	Mg 4	0	0
85	AS	20	Total 20	Mg 20	0	0
85	DH	2	Total 2	Mg 2	0	0
85	c9	1	Total 1	Mg 1	0	0
85	k	2	Total 2	Mg 2	0	0
85	CO	2	Total 2	Mg 2	0	0
85	DG	1	Total 1	Mg 1	0	0
85	CU	2	Total 2	Mg 2	0	0
85	b	1	Total 1	Mg 1	0	0
85	DR	2	Total 2	Mg 2	0	0

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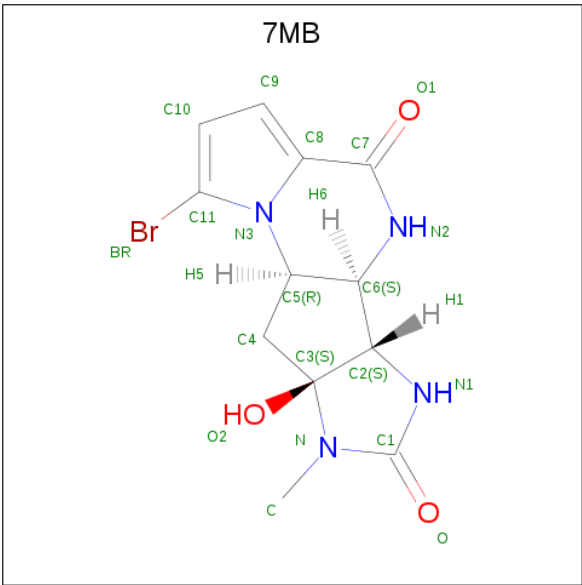
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	w	1	Total 1	Mg 1	0	0
85	CK	1	Total 1	Mg 1	0	0
85	CQ	4	Total 4	Mg 4	0	0
85	x	5	Total 5	Mg 5	0	0
85	AR	504	Total 504	Mg 504	0	0
85	d6	1	Total 1	Mg 1	0	0
85	s6	1	Total 1	Mg 1	0	0
85	s	1	Total 1	Mg 1	0	0
85	DI	1	Total 1	Mg 1	0	0
85	j	2	Total 2	Mg 2	0	0
85	1	490	Total 490	Mg 490	0	0
85	D	1	Total 1	Mg 1	0	0
85	DD	1	Total 1	Mg 1	0	0
85	s2	1	Total 1	Mg 1	0	0
85	d3	3	Total 3	Mg 3	0	0
85	v	1	Total 1	Mg 1	0	0
85	A	111	Total 111	Mg 111	0	0
85	CP	2	Total 2	Mg 2	0	0
85	4	21	Total 21	Mg 21	0	0
85	DA	1	Total 1	Mg 1	0	0
85	r	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	9	1	Total 1	Mg 1	0	0
85	CF	1	Total 1	Mg 1	0	0
85	CX	2	Total 2	Mg 2	0	0
85	DE	1	Total 1	Mg 1	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	i	1	Total 1	Mg 1	0	0
85	CI	1	Total 1	Mg 1	0	0
85	d9	1	Total 1	Mg 1	0	0
85	z	2	Total 2	Mg 2	0	0
85	AT	12	Total 12	Mg 12	0	0
85	F	1	Total 1	Mg 1	0	0
85	l2	2	Total 2	Mg 2	0	0
85	CE	4	Total 4	Mg 4	0	0
85	Y	1	Total 1	Mg 1	0	0
85	l	2	Total 2	Mg 2	0	0
85	3	12	Total 12	Mg 12	0	0
85	AF	2	Total 2	Mg 2	0	0

- Molecule 86 is Agelastatin A (three-letter code: 7MB) (formula: $C_{12}H_{13}BrN_4O_3$).



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

- Molecule 87 is ZINC ION (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		
87	AK	1	Total	Zn	0	0
			1	1		
87	DQ	1	Total	Zn	0	0
			1	1		
87	e	1	Total	Zn	0	0
			1	1		
87	b	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	c	1	Total	Zn	0	0
			1	1		
87	DL	1	Total	Zn	0	0
			1	1		

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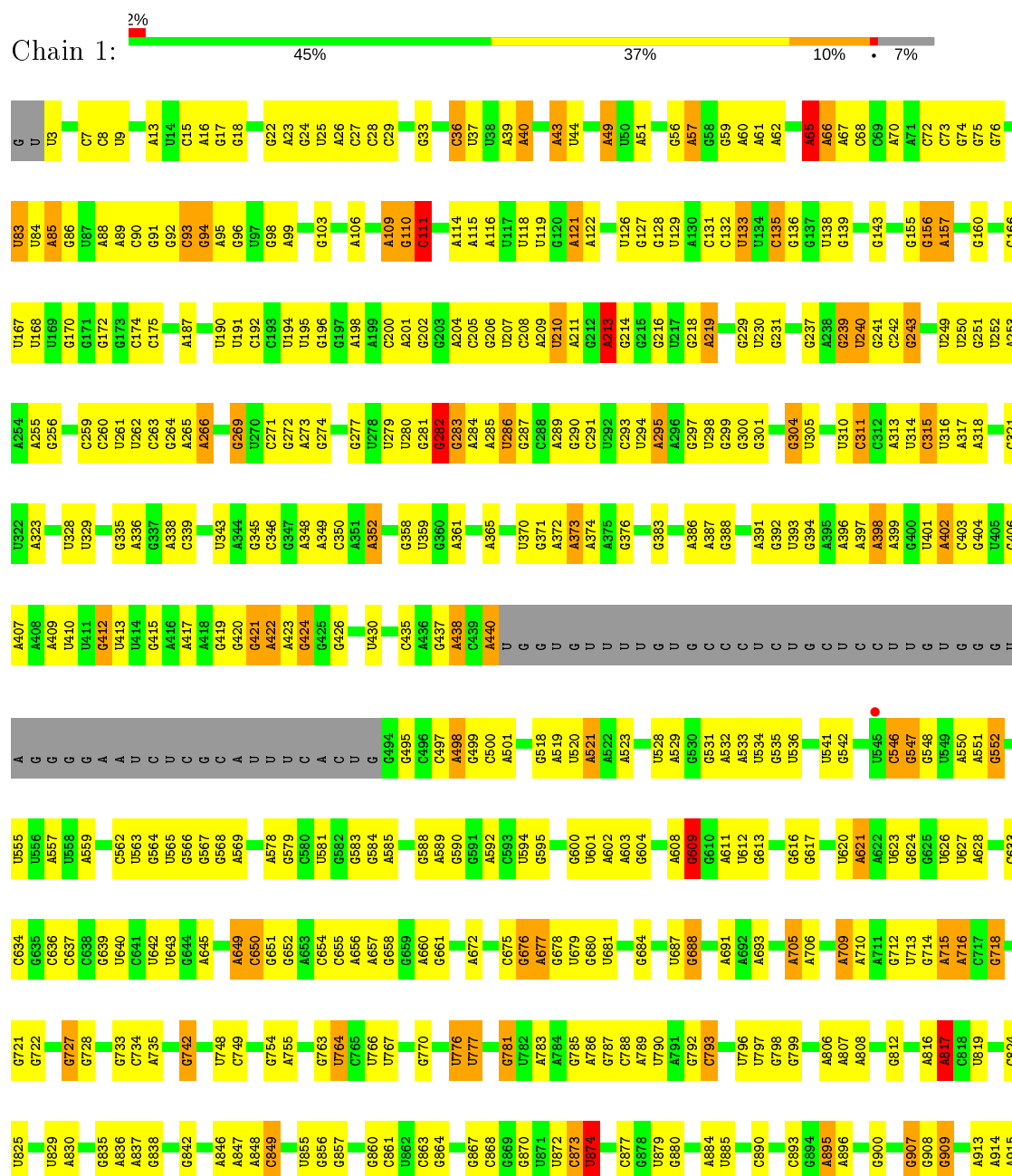
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	d9	1	Total 1	Zn 1	0	0
87	DR	1	Total 1	Zn 1	0	0
87	DO	1	Total 1	Zn 1	0	0
87	AN	1	Total 1	Zn 1	0	0
87	d7	1	Total 1	Zn 1	0	0
87	d6	1	Total 1	Zn 1	0	0

3 Residue-property plots

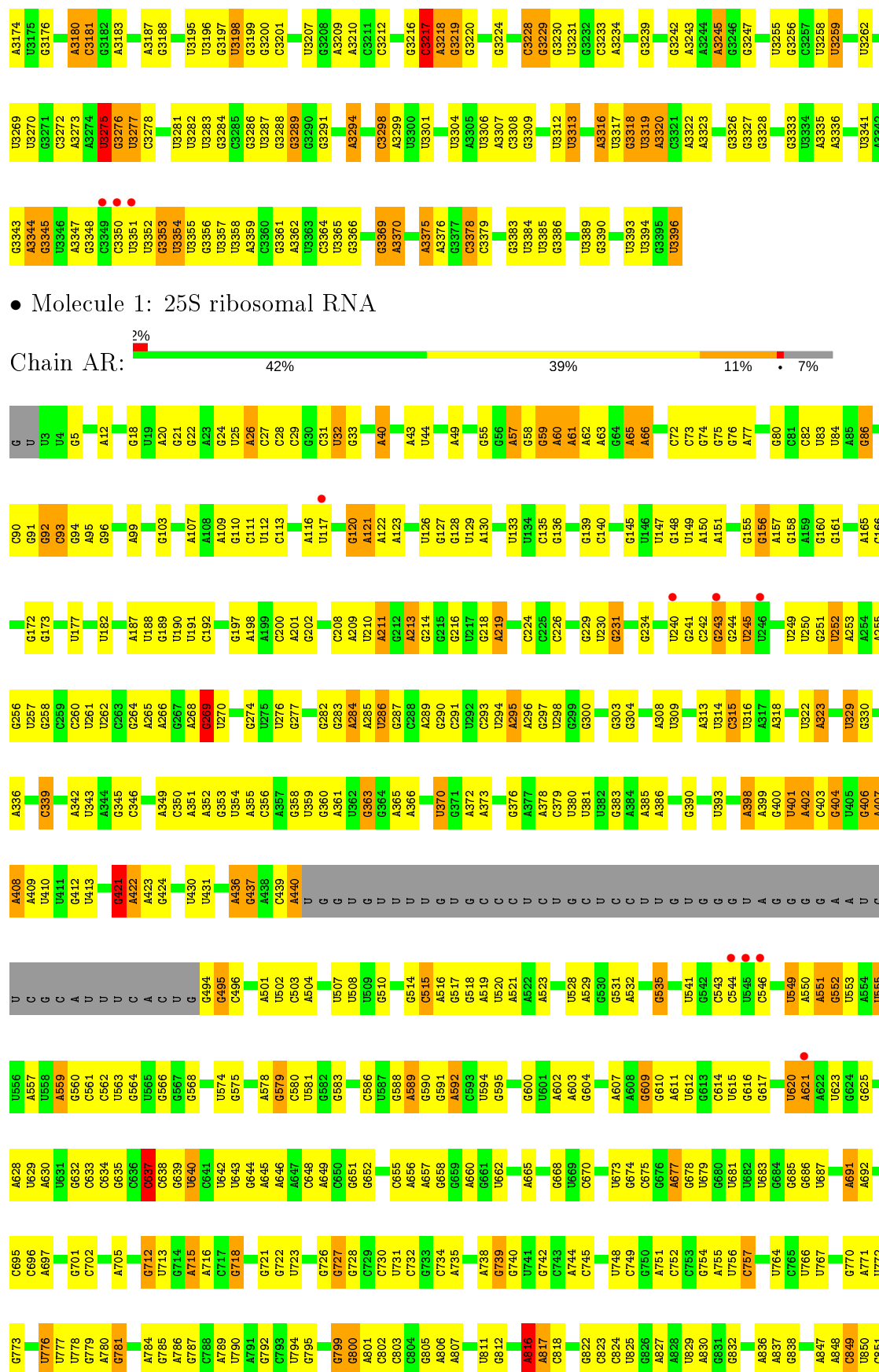
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



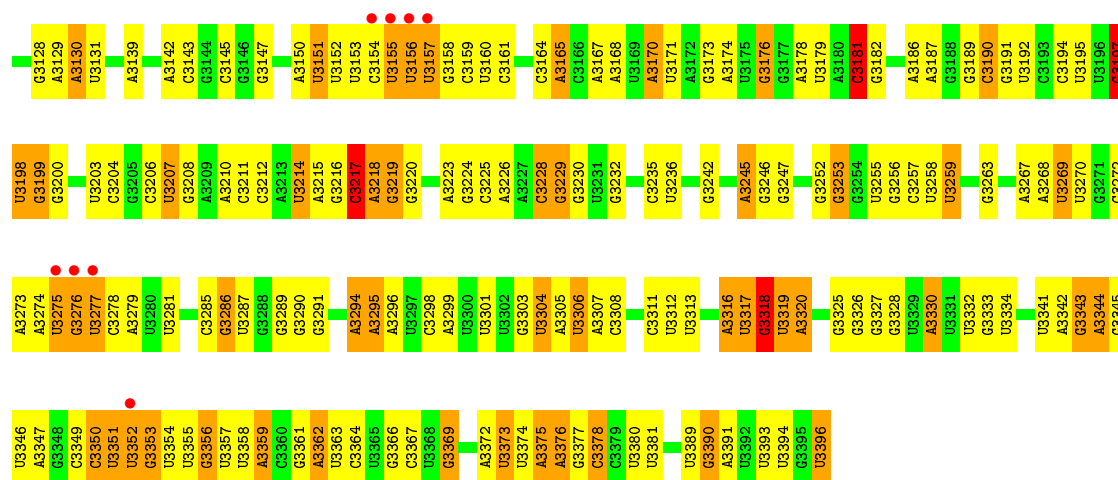
G	A1841	G1767	C1582	U1495	U1415	A1337	A1245	U1073	A998	G916
C	A1842	U1768	A1583	C1496	C1416	C1338	G1246	U1078	G999	A917
U	C1843	G1675	G1586	C1497	A1418	G1339	U1287	U1081	G1000	C918
U	G1844	A1676	G1587	A1498	G1425	G1340	G1248	U1087	G1001	
G	G1845	A1683	A1588	G1500	C1420	U1341	G1249	U1094	A1002	A921
G	A1847	U1686	A1589	C1508	G1422	A1343	A1251	G1087	A1006	U922
U	G1848	U1687	G1590	G1514	U1426	G1344	C1254	U1099	U1007	C923
G	U1784	U1687	G1591	G1514	A1425	U1348	G1254	G1090	U1008	G924
G	U1785	U1687	G1591	G1514	C1426	G1348	G1255	A1091	C928	
G	G1786	U1688	G1592	G1514	U1427	G1349	G1256	A1092	A1009	C929
G	A1787	U1689	A1593	G1517	A1427	A1350	G1257	U1093	A929	U930
C	G1788	U1690	A1594	U1518	A1428	U1351	U1258	A1094	U930	
U	G1789	U1691	U1595	U1518	G1429	A1352	U1259	U1095	C931	
U	G1790	C1596	C1596	U1523	U1430	U1353	G1261	U1096	G934	
G	C1791	G1597	G1597	U1523	A1431	G1354	U1262	G1017	U935	
G	C1792	G1598	G1598	C1527	C1432	A1355	A1263	U1097	U936	
C	G1793	G1599	G1599	G1528	A1433	U1356	A1264	A1098	A936	
U	G1794	U1600	U1600	U1528	G1434	G1357	G1264	G1019	G937	
C	A1858	U1601	U1601	U1528	U1435	U1357	U1265	U1100	C938	
C	A1859	A1603	A1603	U1530	U1436	C1360	U1269	G1024	G939	
U	G1796	G1604	G1604	C1531	A1438	U1361	A1270	A1025	G940	
G	G1797	A1605	A1605	C1531	C1437	U1362	A1271	A1026	U941	
G	A1798	U1606	U1606	A1534	U1438	G1362	C1272	A1027	G942	
A	A1799	U1607	U1607	U1535	G1440	A1273	A1274	U1028	U943	
G	C1802	A1613	A1613	A1536	U1441	G1365	U1274	G1029	C944	
G	C1803	U1721	U1721	A1537	G1442	A1366	U1275	A1030	C945	
C	C1804	U1722	C1615	A1538	A1446	G1367	A1278	U1033	U946	
C	A1805	U1722	C1615	G1538	A1446	U1368	A1279	U1034	G950	
G	A1806	U1722	U1616	G1541	G1450	A1369	C1279	G1035	A951	
C	G1807	U1723	U1616	G1542	A1456	C1372	G1285	A1036	A952	
A	G1808	U1724	U1616	G1543	A1456	A1373	A1286	C1037	G953	
C	A1809	C1725	U1620	G1543	A1456	G1377	U1287	G1038	C959	
A	A1810	U1725	U1620	G1543	A1456	U1378	U1288	U1039	U960	
C	G1811	U1726	C1631	G1554	G1464	G1379	A1294	A1040	G964	
C	A1812	U1727	C1631	U1555	A1465	G1380	G1295	U1041	A965	
C	A1813	U1728	C1631	U1555	A1466	A1381	G1296	C1043		
U	A1814	U1729	C1631	U1555	A1466	A1386	C1297	A1047	G968	
G	A1815	U1730	C1631	U1555	A1466	G1387	C1298	A1048	C969	
C	A1816	U1731	C1631	U1555	A1466	U1388	G1300	A1049	A970	
C	G1817	U1732	C1631	U1555	A1466	G1389	G1301	U1050	G971	
C	U1818	U1733	C1631	U1555	A1466	A1390	A1302	U1051	G974	
C	A1819	U1734	C1631	U1555	A1466	C1391	G1328	A1054	C975	
C	U1820	U1735	C1631	U1555	A1466	G1392	G1329	A1055	U976	
C	A1821	U1736	C1631	U1555	A1466	A1393	U1309	U1056	C977	
C	G1822	U1737	C1631	U1555	A1466	G1394	G1323	U1067	G978	
C	A1823	U1738	C1631	U1555	A1466	G1395	G1324	A1061	U979	
C	U1824	U1739	C1631	U1555	A1466	A1399	C1314	U1064	A980	
C	G1825	U1740	C1631	U1555	A1466	G1400	G1315	A1065	U981	
C	A1826	U1741	C1631	U1555	A1466	G1401	A1317	A1066	C982	
C	G1827	U1742	C1631	U1555	A1466	G1402	A1318	A1067	A983	
C	U1828	U1743	C1631	U1555	A1466	G1403	G1319	U1068	G984	
C	A1829	U1744	C1631	U1555	A1466	G1404	G1320	C1069	U985	
C	G1830	U1745	C1631	U1555	A1466	G1405	G1321	U1070	A996	
C	U1831	U1746	C1631	U1555	A1466	G1406	G1322	U1071	G1072	
C	A1832	U1747	C1631	U1555	A1466	G1407	G1323	U1072		
C	U1833	U1748	C1631	U1555	A1466	G1408	G1324	U1073		
C	G1834	U1749	C1631	U1555	A1466	G1409	G1325	U1074		
C	A1835	U1750	C1631	U1555	A1466	G1410	G1326	U1075		
C	U1836	U1751	C1631	U1555	A1466	G1411	G1327	U1076		
C	G1837	U1752	C1631	U1555	A1466	G1412	G1328	U1077		
C	A1838	U1753	C1631	U1555	A1466	G1413	G1329	U1078		
C	U1839	U1754	C1631	U1555	A1466	G1414	G1330	U1079		
C	A1840	U1755	C1631	U1555	A1466	G1415	G1331	U1080		
C	U1841	U1756	C1631	U1555	A1466	G1416	G1332	U1081		
C	A1842	U1757	C1631	U1555	A1466	G1417	G1333	U1082		
C	U1843	U1758	C1631	U1555	A1466	G1418	G1334	U1083		
C	A1844	U1759	C1631	U1555	A1466	G1419	G1335	U1084		
C	U1845	U1760	C1631	U1555	A1466	G1420	G1336	U1085		
C	A1846	U1761	C1631	U1555	A1466	G1421	G1337	U1086		
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C	A1856	U1771	C1631	U1555	A1466	G1431	G1347	U1096		
C	U1857	U1772	C1631	U1555	A1466	G1432	G1348	U1097		
C	A1858	U1773	C1631	U1555	A1466	G1433	G1349	U1098		
C	U1859	U1774	C1631	U1555	A1466	G1434	G1350	U1099		
C	A1860	U1775	C1631	U1555	A1466	G1435	G1351	U1100		
C	U1861	U1776	C1631	U1555	A1466	G1436	G1352	U1101		
C	A1862	U1777	C1631	U1555	A1466	G1437	G1353	U1102		
C	U1863	U1778	C1631	U1555	A1466	G1438	G1354	U1103		
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C	U1867	U1782	C1631	U1555	A1466	G1442	G1358	U1107		
C	A1868	U1783	C1631	U1555	A1466	G1443	G1359	U1108		
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C	A1870	U1785	C1631	U1555	A1466	G1445	G1361	U1110		
C	U1871	U1786	C1631	U1555	A1466	G1446	G1362	U1111		
C	A1872	U1787	C1631	U1555	A1466	G1447	G1363	U1112		
C	U1873	U1788	C1631	U1555	A1466	G1448	G1364	U1113		
C	A1874	U1789	C1631	U1555	A1466	G1449	G1365	U1114		
C	U1875	U1790	C1631	U1555	A1466	G1450	G1366	U1115		
C	A1876	U1791	C1631	U1555	A1466	G1451	G1367	U1116		
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C	A1878	U1793	C1631	U1555	A1466	G1453	G1369	U1118		
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C	U1891	U1806	C1631	U1555	A1466	G1466	G1382	U1131		
C	A1892	U1807	C1631	U1555	A1466	G1467	G1383	U1132		
C	U1893	U1808	C1631	U1555	A1466	G1468	G1384	U1133		
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C	U1895	U1810	C1631	U1555	A1466	G1470	G1386	U1135		
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C	A1906	U1821	C1631	U1555	A1466	G1481	G1397	U1146		
C	U1907	U1822	C1631	U1555	A1466	G1482	G1398	U1147		

C3092	A3006	U2924	G2834	G3754	G2675	G2586	U2504	C2444	G2370	C2293	G2218	C2128	G
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C3097	C2927	C2927	C2927	A2759	U2683	A2594	C2508	G	A2373	U2298	A2222	U2137	G
G3098	C2928	C2928	C2841	C2760	C2684	A2601	A2511	G	G2374	U2299	A2223	A2138	U
U3104	U3013	A2930	U2842	G2761	A2689	G2602	C2512	G	G2375	A2299	A2224	A2139	C
U3015	U3014	A2933	U2843	A2762	A2690	G2603	U2513	G	G2376	G2300	A2225	A2140	U
A3016	A2845	A2934	C2844	U2763	C2690	G2604	U2514	G	G2377	A2303	U2226	U2141	C
A3017	A2846	A2935	U2846	C2765	A2691	G2605	A2515	U	G2378	C2304	C2227	A2142	U
C3018	A2936	A2936	U2766	C2766	G2695	G2606	G2522	U	U2379	U2380	A2228	A2143	U
U3019	G2937	G2937	G2850	U2767	A2694	G2607	A2523	G	U2380	G2305	A2229	A2144	G
A3113	U3018	G2938	A2851	U2768	A2695	G2608	A2524	A	G2381	C2306	C2230	A	U
A3114	G3028	G2938	A2852	U2769	A2696	A2609	A2525	G	C2382	C2307	C2231	A2149	A
U3119	A3029	C2942	C2852	G2770	A2697	G2610	C2526	A	C2383	A2308	A2232	G2155	G
G3120	G3030	G2943	A2853	U2771	G2698	U2611	G2527	U	A2384	U2310	A2233	G2156	A
U3121	A3035	U2944	U2860	C2772	G2700	U2612	G2527	U	A2385	A2311	G2234	G2157	C
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G3128	U3042	A2946	U2862	U2775	A2702	G2614	G2533	G	U2387	A2313	U2241	G2165	U
A3129	U3043	G2947	U2863	C2776	A2703	G2615	G2534	U	C2392	U2314	A2242	G2169	C
A3130	U3044	C2948	U2864	G2777	A2704	G2616	G2535	G	G2393	U2315	A2243	A	C
U3131	A3046	U2949	U2865	G2778	C2707	G2617	A2536	G	G2396	U2318	A2244	G2172	U
C3132	U3047	G2950	C2867	A2779	C2708	G2620	U2537	G	A2397	A2321	G2245	U2173	U
C3133	A3048	G2952	U2868	U2780	U2712	C2622	U2538	A	G2400	C2322	G2246	G2174	G
U3135	A3049	U2953	C2870	U2783	U2713	G2623	A2540	C	A2401	G2325	G2247	A	U
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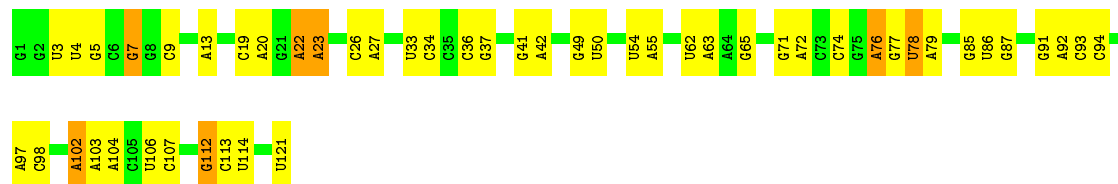


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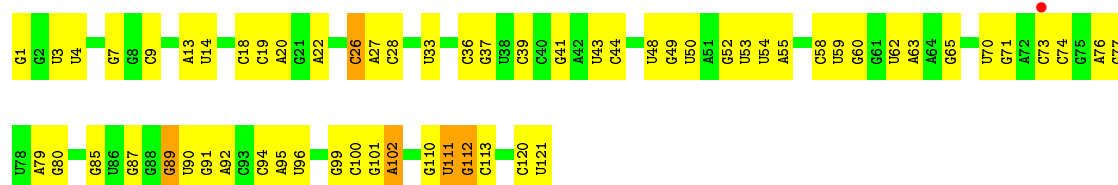
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		U2990	U2846	U2770	U2690	U2602	A	U2426	U2305	U2230	C
		U2991	U2847	U2771	U2691	U2603	U	U2426	U2306	U2231	C
		U2992	U2848	U2772	U2692	U2604	A	U2426	U2307	U2232	C
		U2993	U2849	U2773	U2693	U2605	U	U2426	U2308	U2233	C
		U2994	U2850	U2774	U2694	U2606	A	U2426	U2309	U2234	C
		U2995	U2851	U2775	U2695	U2607	U	U2426	U2310	U2235	C
		U2996	U2852	U2776	U2696	U2608	A	U2426	U2311	U2236	C
		U2997	U2853	U2777	U2697	U2609	U	U2426	U2312	U2237	C
		U2998	U2854	U2778	U2698	U2610	A	U2426	U2313	U2238	C
		U2999	U2855	U2779	U2699	U2611	U	U2426	U2314	U2239	C
		U3000	U2856	U2780	U2700	U2612	A	U2426	U2315	U2240	C
		U3001	U2857	U2781	U2701	U2613	U	U2426	U2316	U2241	C
		U3002	U2858	U2782	U2702	U2614	A	U2426	U2317	U2242	C
		U3003	U2859	U2783	U2703	U2615	U	U2426	U2318	U2243	C
		U3004	U2860	U2784	U2704	U2616	A	U2426	U2319	U2244	C
		U3005	U2861	U2785	U2705	U2617	U	U2426	U2320	U2245	C
		U3006	U2862	U2786	U2706	U2618	A	U2426	U2321	U2246	C
		U3007	U2863	U2787	U2707	U2619	U	U2426	U2322	U2247	C
		U3008	U2864	U2788	U2708	U2620	A	U2426	U2323	U2248	C
		U3009	U2865	U2789	U2709	U2621	U	U2426	U2324	U2249	C
		U3010	U2866	U2790	U2710	U2622	A	U2426	U2325	U2250	C
		U3011	U2867	U2791	U2711	U2623	U	U2426	U2326	U2251	C
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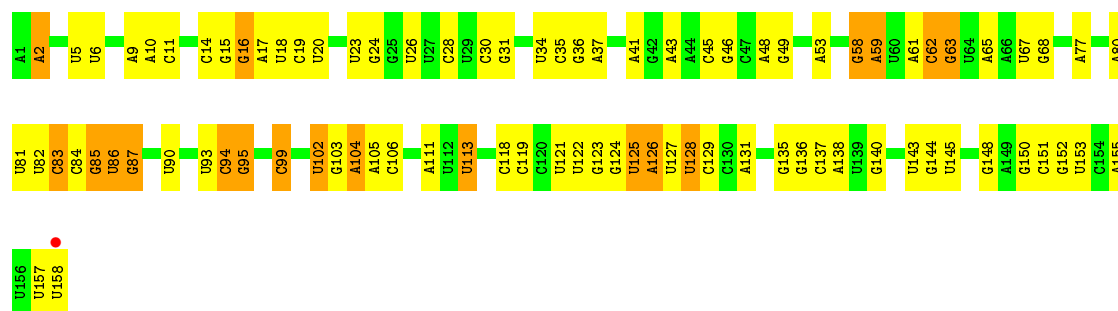
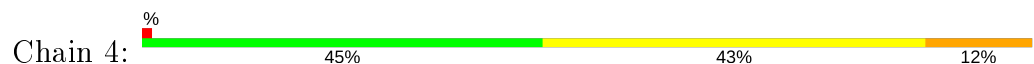
• Molecule 2: 5S ribosomal RNA



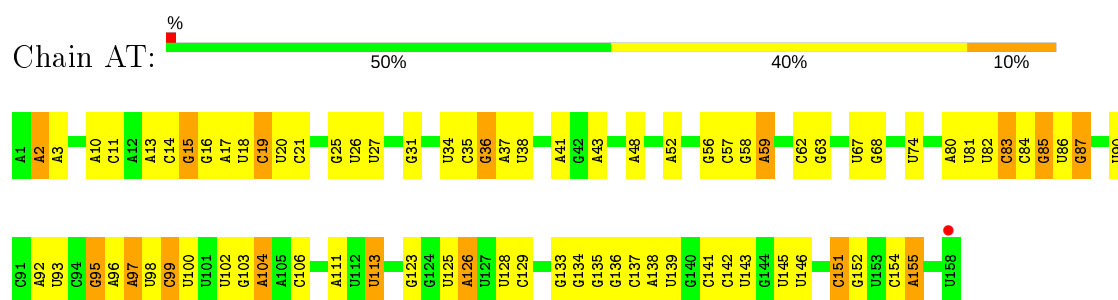
• Molecule 2: 5S ribosomal RNA



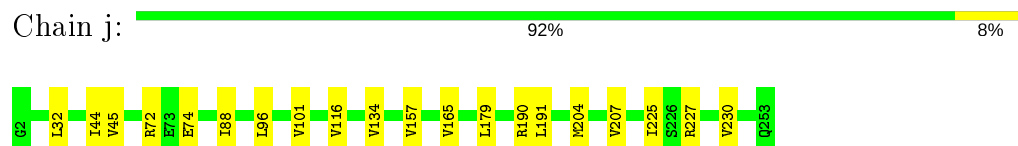
• Molecule 3: 5.8S ribosomal RNA



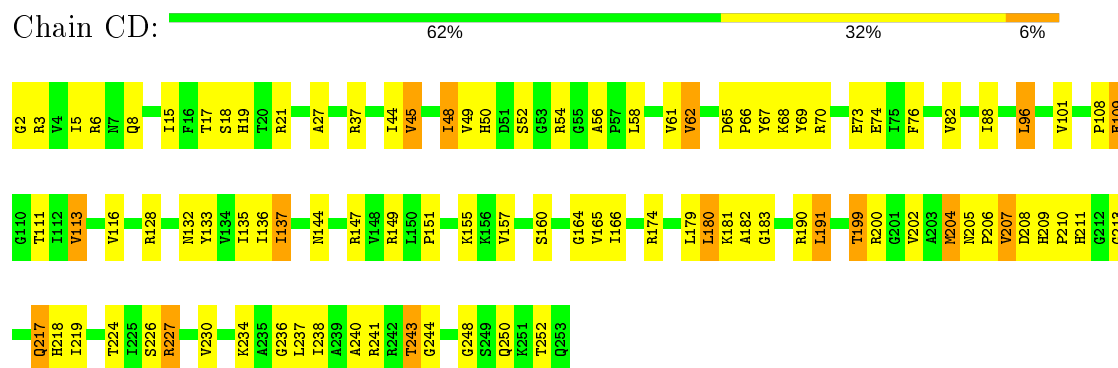
• Molecule 3: 5.8S ribosomal RNA



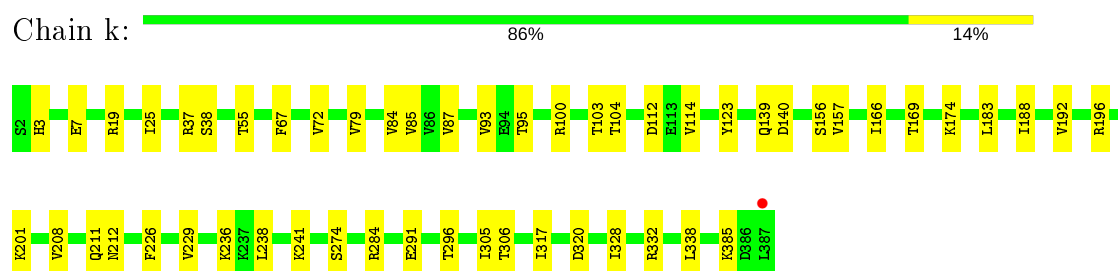
- Molecule 4: 60S ribosomal protein L2-A



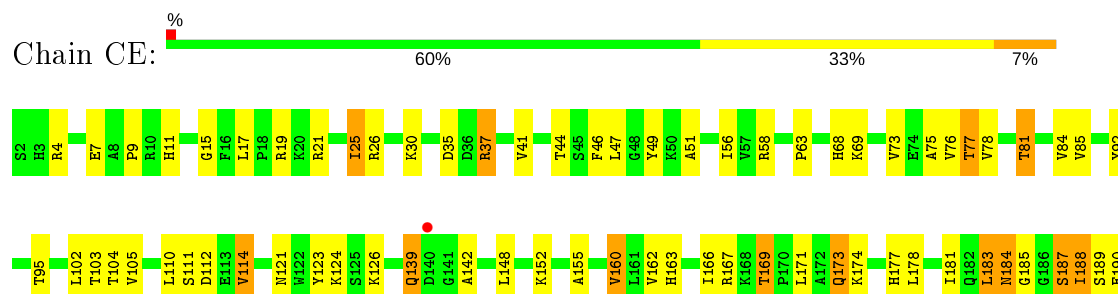
- Molecule 4: 60S ribosomal protein L2-A

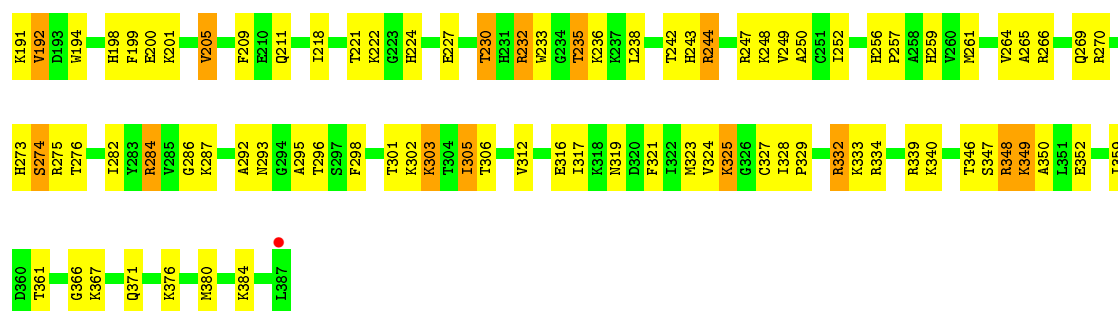


- Molecule 5: 60S ribosomal protein L3



- Molecule 5: 60S ribosomal protein L3





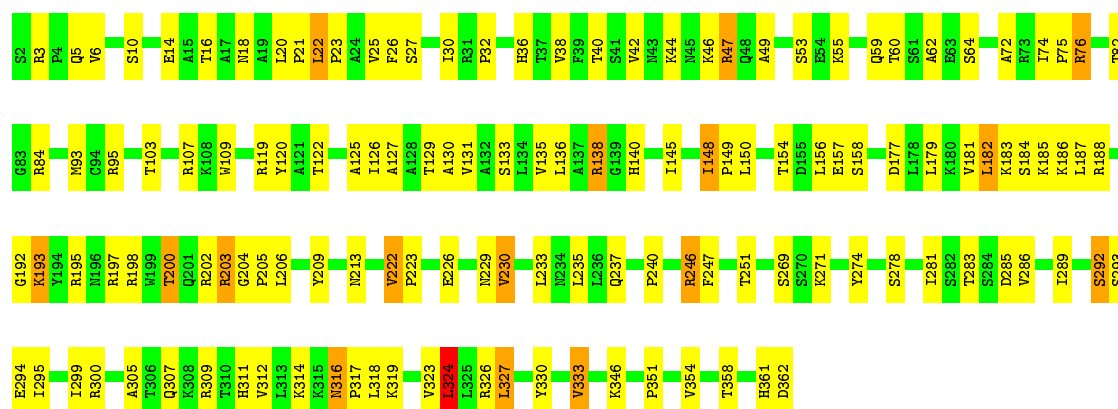
- Molecule 6: 60S ribosomal protein L4-A

Chain l: 90% 10%



- Molecule 6: 60S ribosomal protein L4-A

Chain CF: 63% 33%



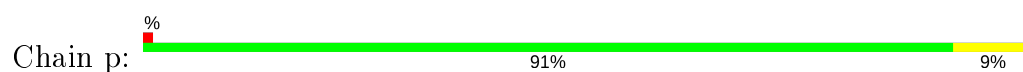
- Molecule 7: 60S ribosomal protein L5

Chain m: 91% 9%

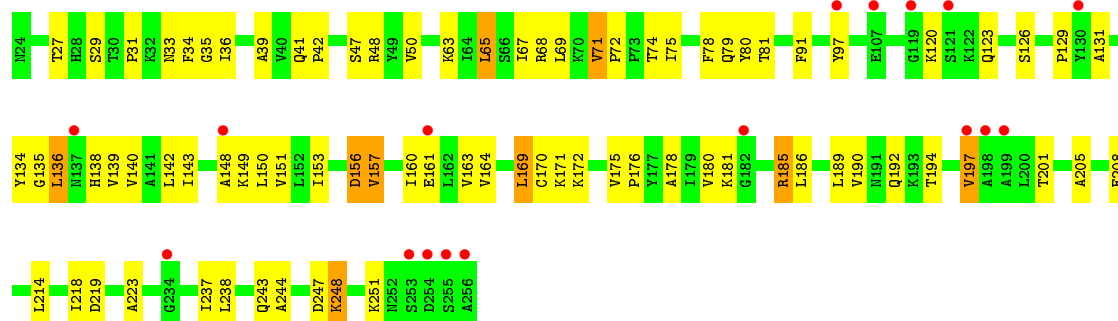


- Molecule 7: 60S ribosomal protein L5

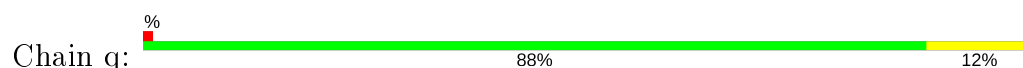
Chain CG: 63% 31% 5%



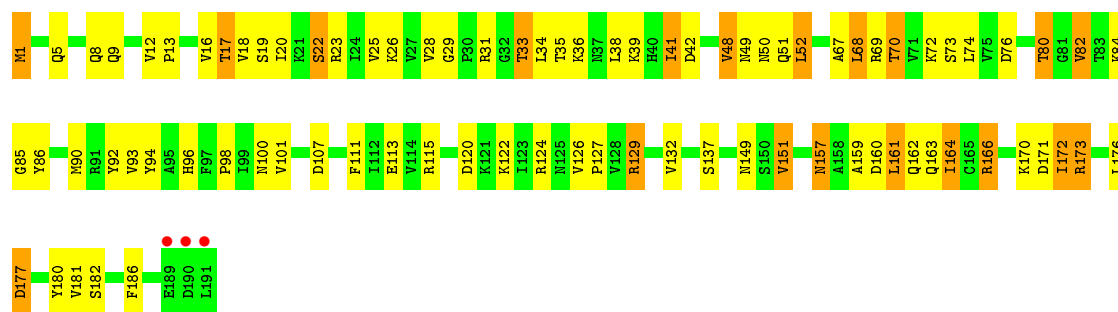
• Molecule 10: 60S ribosomal protein L8-A



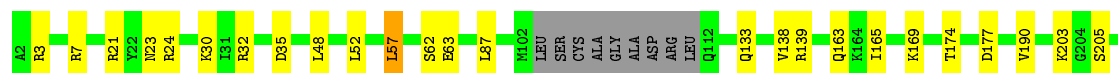
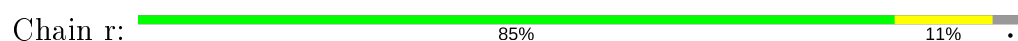
• Molecule 11: 60S ribosomal protein L9-A



• Molecule 11: 60S ribosomal protein L9-A

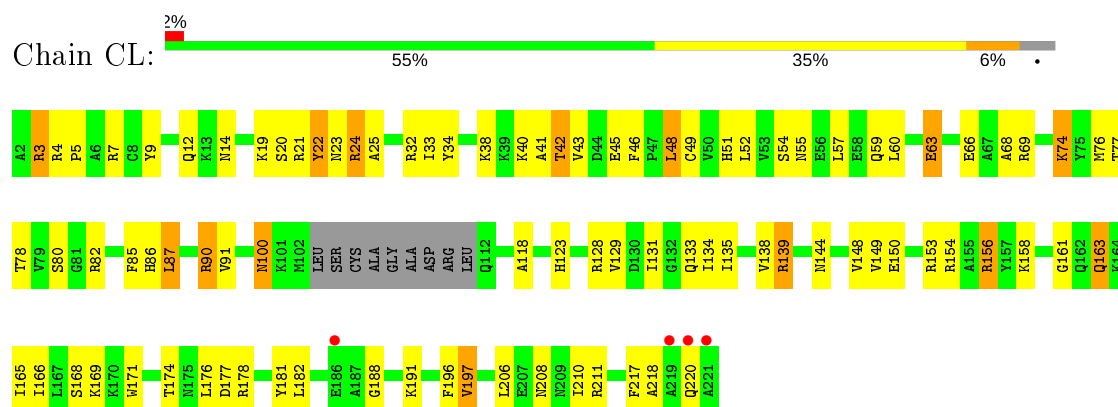


• Molecule 12: 60S ribosomal protein L10

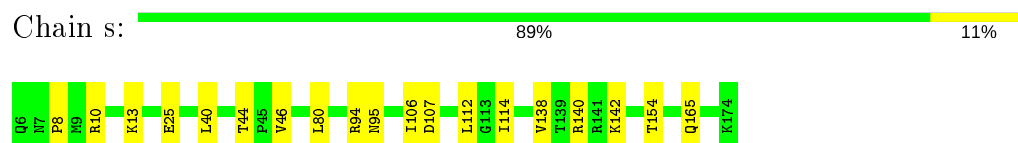


A221

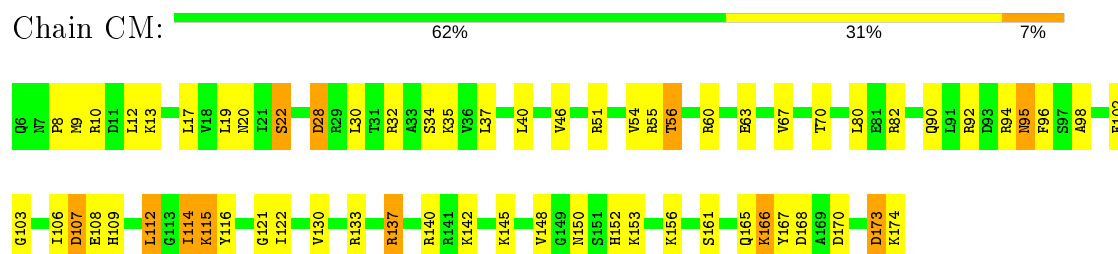
- Molecule 12: 60S ribosomal protein L10



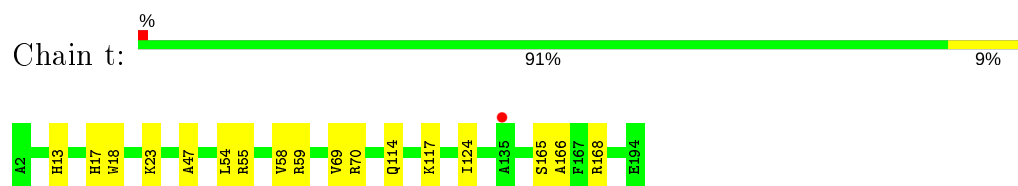
- Molecule 13: 60S ribosomal protein L11-B



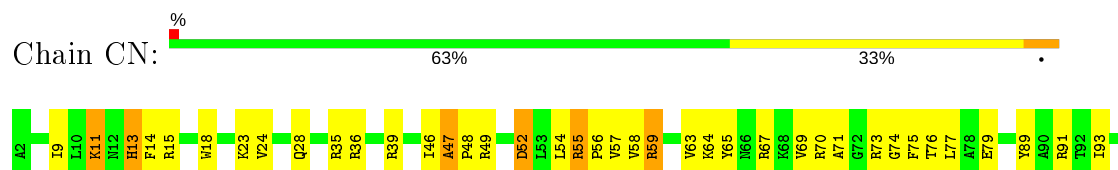
- Molecule 13: 60S ribosomal protein L11-B

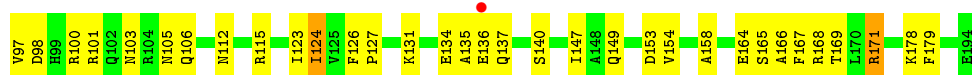


- Molecule 14: 60S ribosomal protein L13-A



- Molecule 14: 60S ribosomal protein L13-A

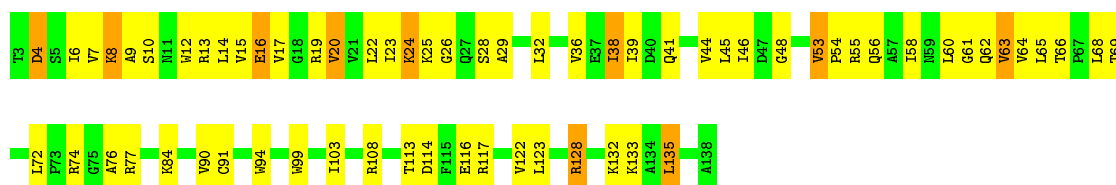




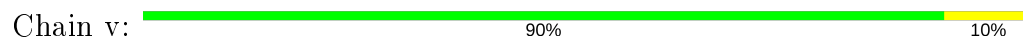
- Molecule 15: 60S ribosomal protein L14-A



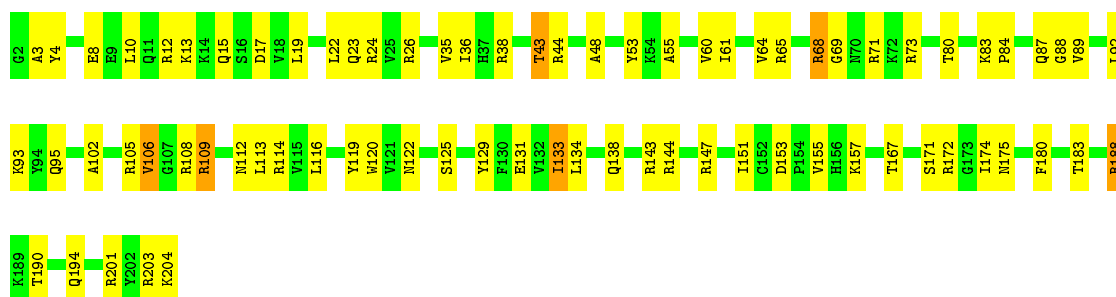
- Molecule 15: 60S ribosomal protein L14-A



- Molecule 16: 60S ribosomal protein L15-A



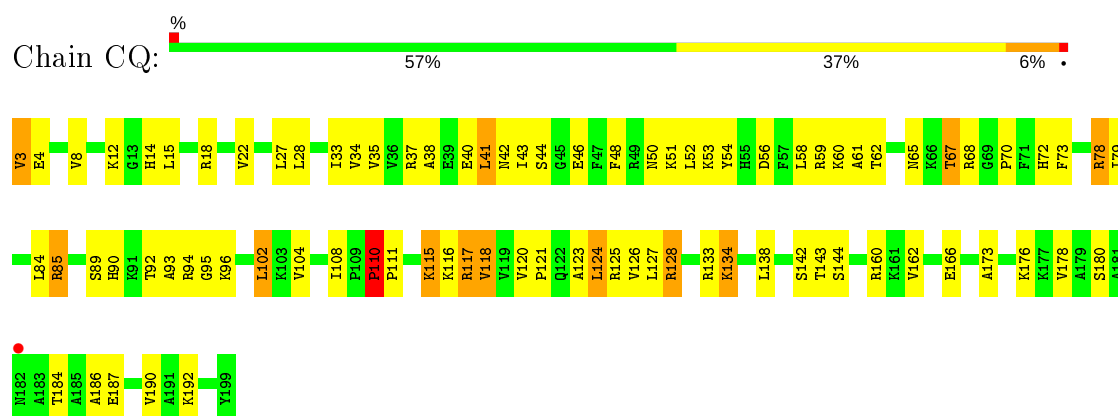
- Molecule 16: 60S ribosomal protein L15-A



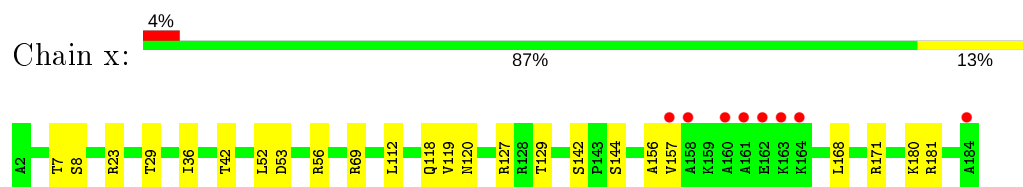
- Molecule 17: 60S ribosomal protein L16-A



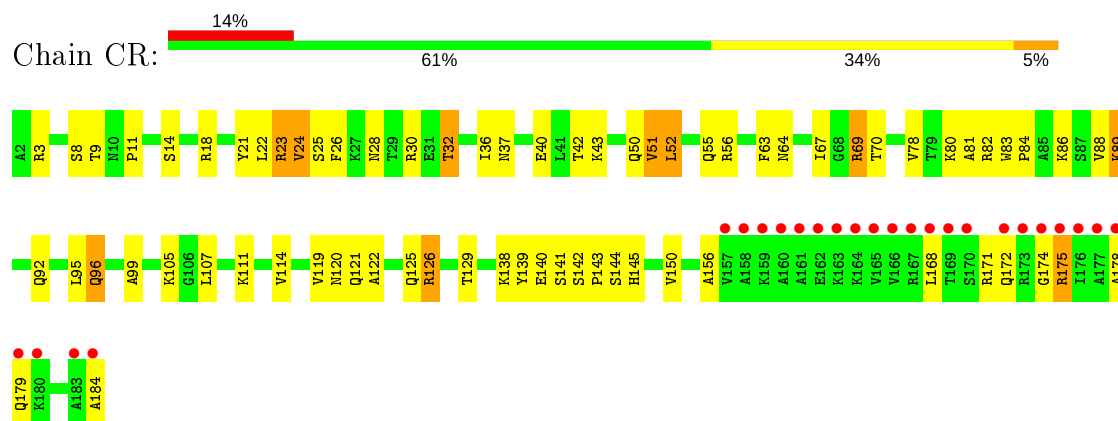
- Molecule 17: 60S ribosomal protein L16-A



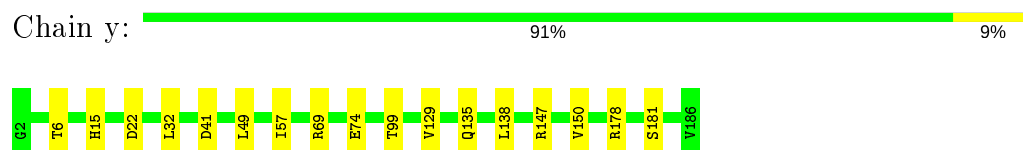
- Molecule 18: 60S ribosomal protein L17-A



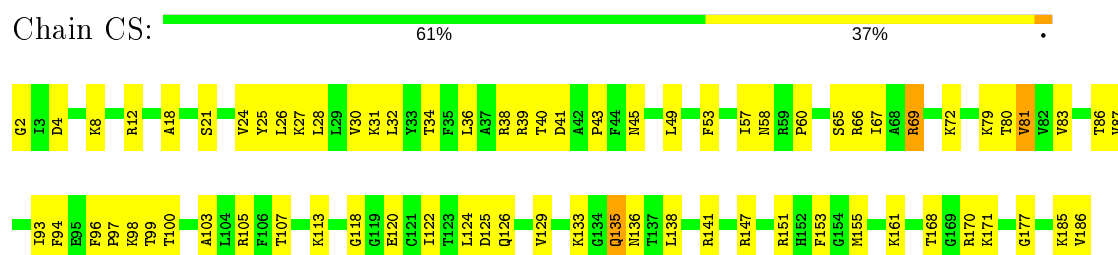
- Molecule 18: 60S ribosomal protein L17-A



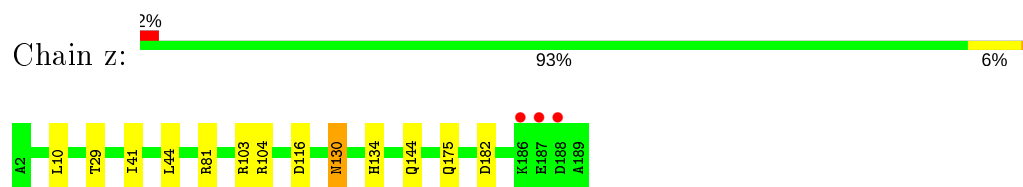
- Molecule 19: 60S ribosomal protein L18-A



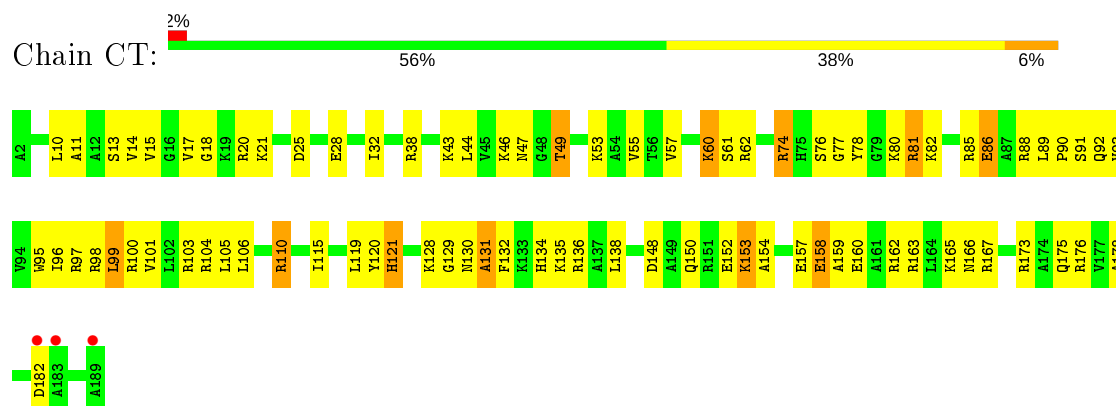
- Molecule 19: 60S ribosomal protein L18-A



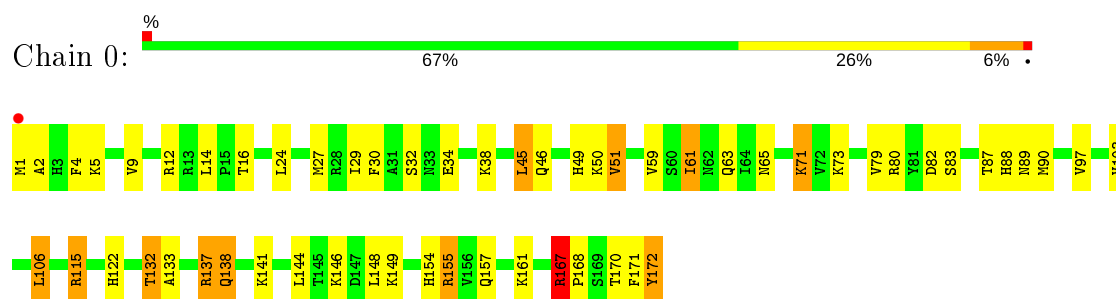
- Molecule 20: 60S ribosomal protein L19-A



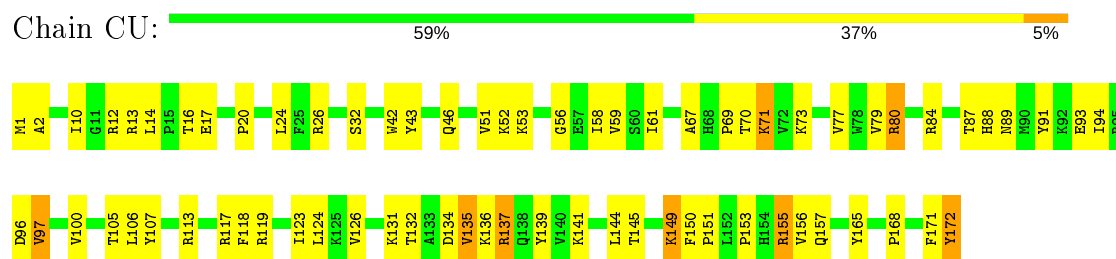
- Molecule 20: 60S ribosomal protein L19-A



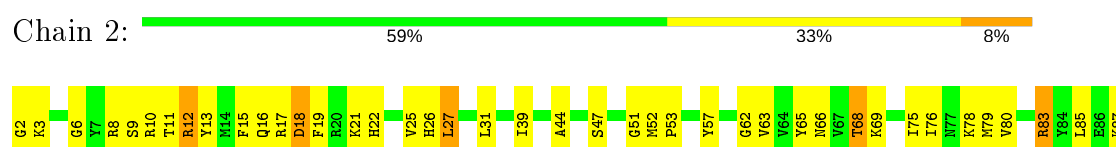
- Molecule 21: 60S ribosomal protein L20-A



- Molecule 21: 60S ribosomal protein L20-A

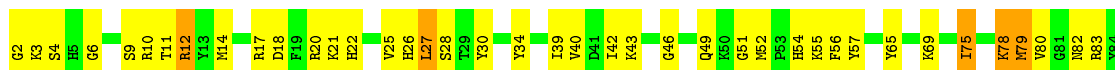


- Molecule 22: 60S ribosomal protein L21-A

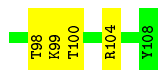
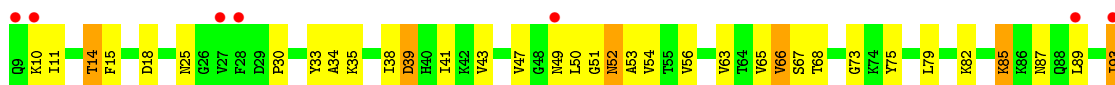




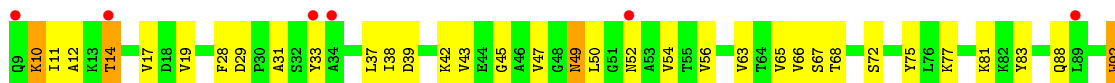
- Molecule 22: 60S ribosomal protein L21-A



- Molecule 23: 60S ribosomal protein L22-A



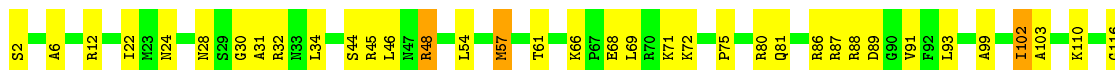
- Molecule 23: 60S ribosomal protein L22-A

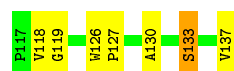


- Molecule 24: 60S ribosomal protein L23-A

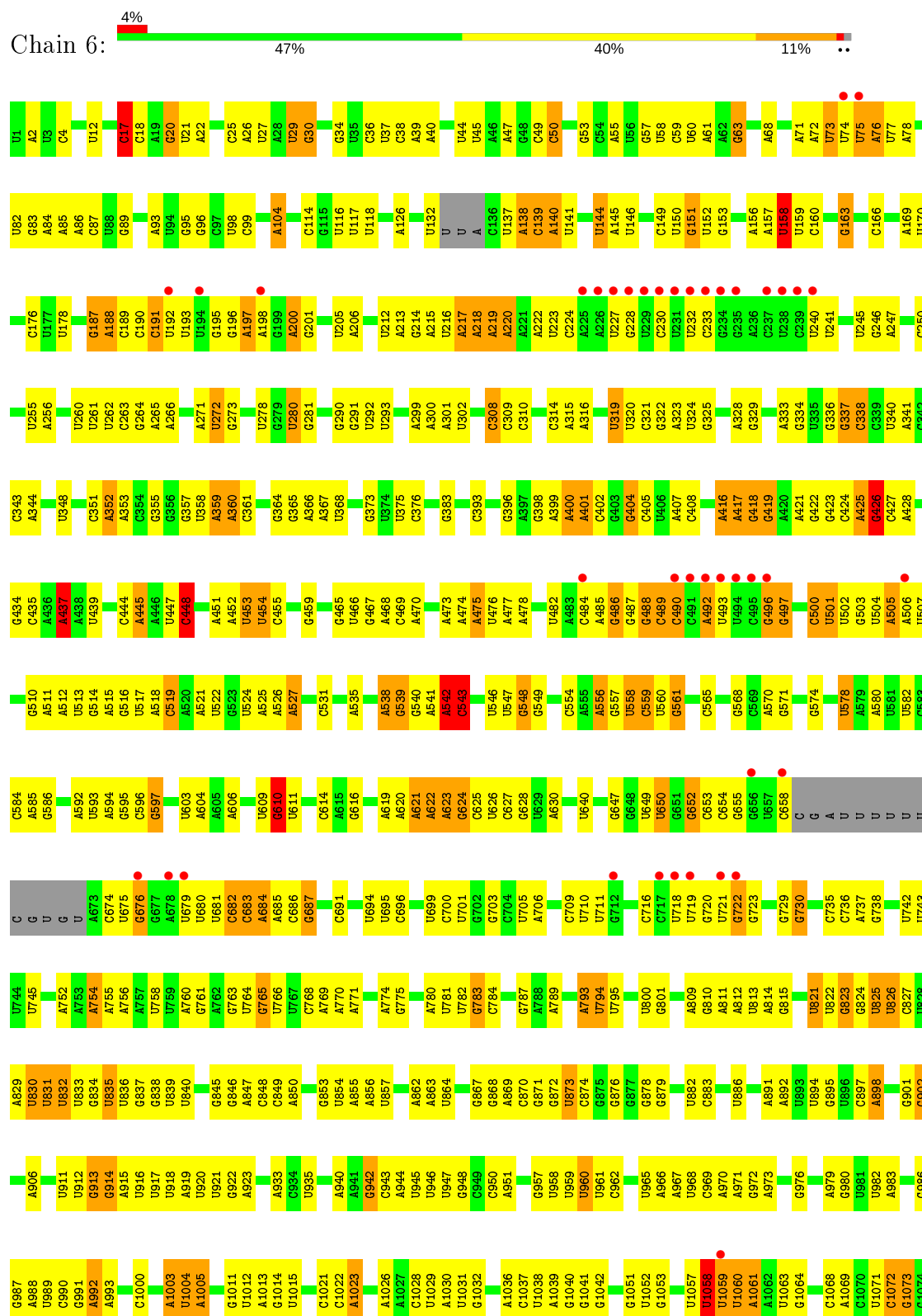


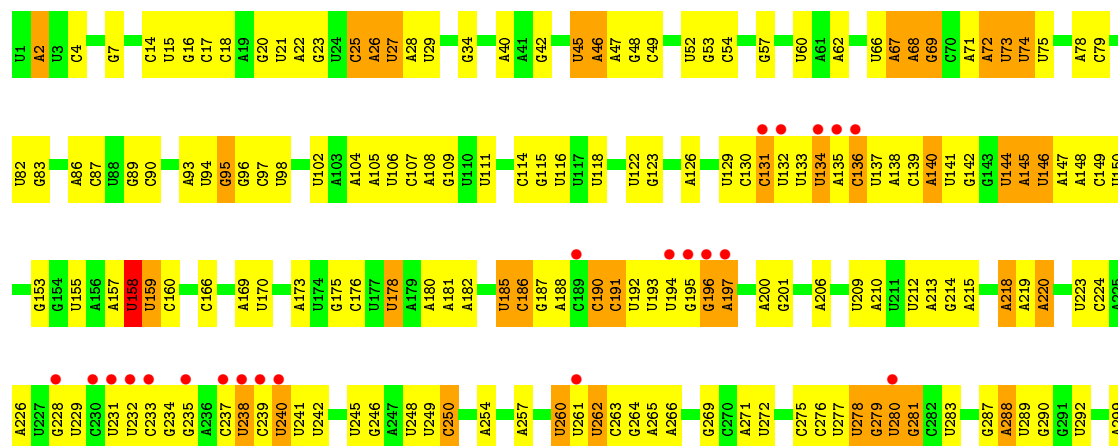
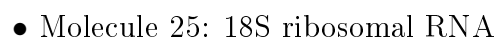
- Molecule 24: 60S ribosomal protein L23-A



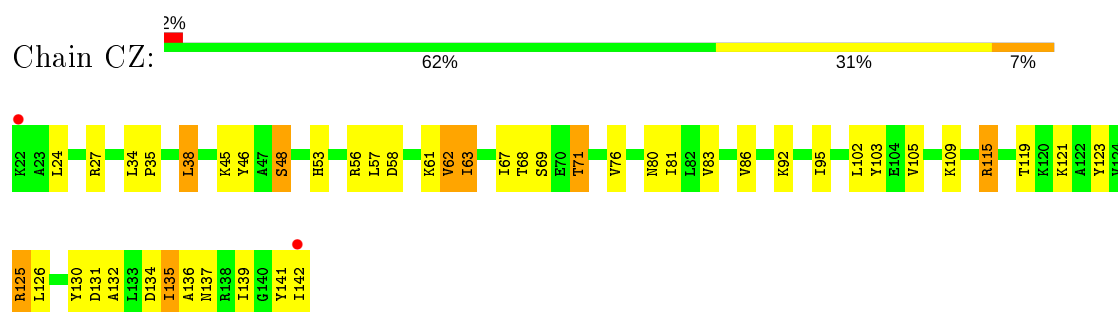


• Molecule 25: 18S ribosomal RNA

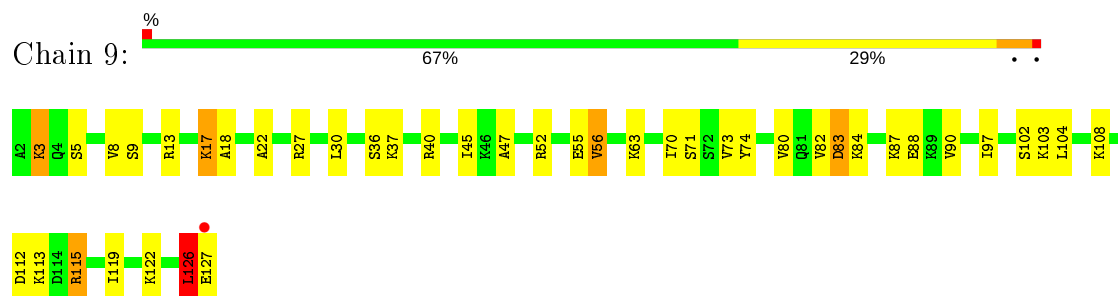




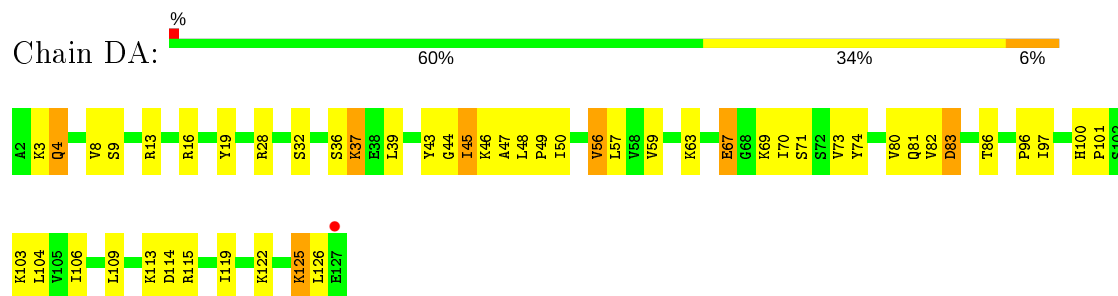
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A1275	C1190	G1102	C1016	A939	U864	U795	G720	U657	U578	U504	C443	G371	U304
U1276	U1191	U1103	U1018	A940	G867	A799	G721	C658	A580	A506	A445	G373	C305
G1277	C1192	U1104	A1019	A941	G868	U800	G722	C	U581	U507	A446	G307	U306
G1278	A1193	G1109	C1022	G942	A869	U801	G723	G	U582	G509	U447	G377	G308
G1279	C1195	G1110	A1025	C943	G870	G802	U724	A	C583	G510	C448	U379	C309
C1280	A1196	G1111	A1026	A944	G871	A806	U725	U	U584	A511	G449	U380	A312
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U1286	G1200	G1119	G954	G876	G876	U808	G730	U	A591	A515	G384	A315	A316
U1286	G1201	A955	A955	G877	G877	A811	C731	C	A592	G516	A456	A385	A316
A1202	C1032	C956	C956	G878	G878	A812	G732	G	U593	G457	G386	A386	A316
A1203	C1033	G879	G879	G879	G879	A812	A733	U	A594	U463	G387	U319	U320
G1291	C1034	U958	U958	C880	C880	G815	A734	G	A595	A521	G388	U320	U320
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A1217	G1041	U965	U965	A884	A884	G819	A739	U	A602	U463	A399	G329	G329
G1218	G1042	A966	A966	C885	C885	U820	A740	G676	A601	A525	A400	G330	G330
A1219	G1046	U968	U968	U886	U886	U821	A741	G677	A602	A526	A401	A331	A331
C1220	G1047	C969	C969	U888	U888	U822	U742	A678	A623	A527	C402	U332	U332
G1226	U1051	G972	G972	U889	U889	G823	U743	U679	A624	U528	G404	G404	G404
A1227	U1052	A973	A973	C890	C890	U825	U744	U680	G625	A529	A473	C405	C405
G1228	G1053	A974	A974	A891	A891	U826	G751	A684	U626	U532	A474	C406	C406
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A1238	U1073	G986	G987	U903	U903	U835	A760	U695	G626	C543	A480	A417	A417
U1239	G1074	A988	A988	U912	U912	G837	G765	C696	U627	A545	A481	G418	G418
A1242	U1079	G991	G991	G914	G914	U838	U766	U698	G628	U547	A482	G418	G418
G1243	U1080	A992	A992	A915	A915	U839	U767	U699	A630	G549	A484	U349	U349
A1244	A1081	A993	A993	U916	U916	A844	G768	U701	G631	G549	A485	C351	C351
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C1246	G1083	A995	A995	U918	U918	C848	C773	G703	U633	G553	G487	C423	C423
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U1254	A1092	A926	A926	U926	U926	A856	U782	G712	G648	C559	U494	A359	A359
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A1262	G1094	C1010	C1010	U928	U928	G858	C784	G714	U650	G565	G497	A436	A436
U1262	U1095	U1011	U1011	A933	A933	A859	G785	U715	G652	G568	G498	A437	A437
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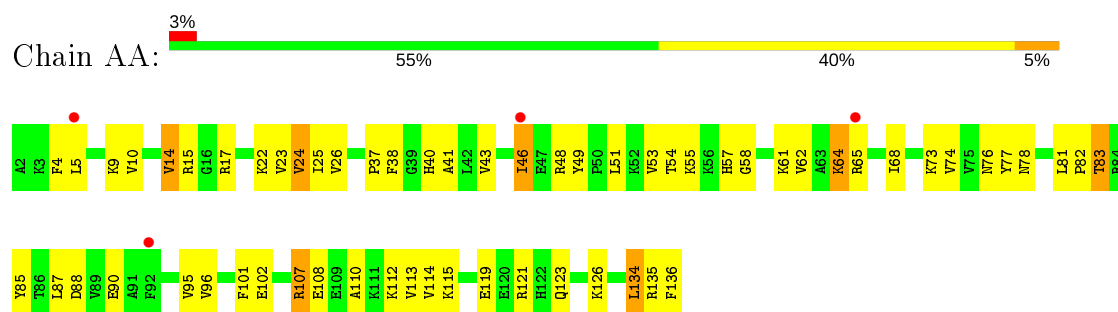
- Molecule 28: 60S ribosomal protein L26-A



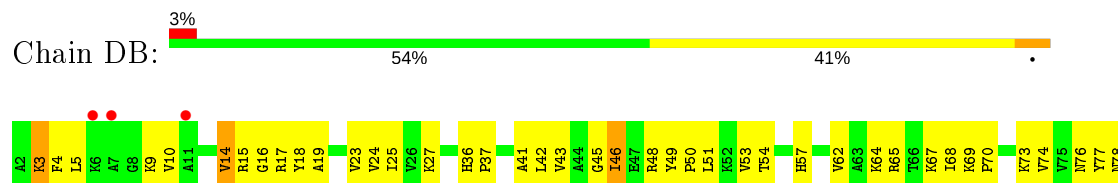
- Molecule 28: 60S ribosomal protein L26-A



- Molecule 29: 60S ribosomal protein L27-A



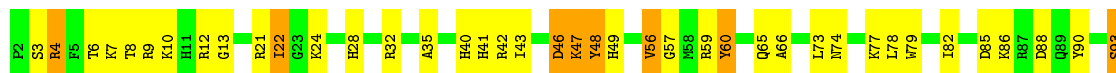
- Molecule 29: 60S ribosomal protein L27-A





- Molecule 30: 60S ribosomal protein L28

Chain AB: 59% 35% 6%



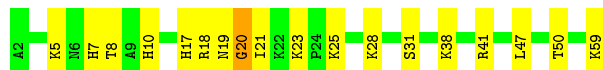
- Molecule 30: 60S ribosomal protein L28

Chain DC: 59% 36% 5%



- Molecule 31: 60S ribosomal protein L29

Chain AC: 69% 29% 2%



- Molecule 31: 60S ribosomal protein L29

Chain DD: 62% 29% 9%



- Molecule 32: 60S ribosomal protein L30

Chain AD: 4% 61% 32% 7%



- Molecule 32: 60S ribosomal protein L30



- Molecule 33: 60S ribosomal protein L31-A



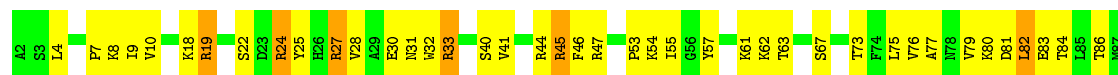
- Molecule 33: 60S ribosomal protein L31-A



- Molecule 34: 60S ribosomal protein L32

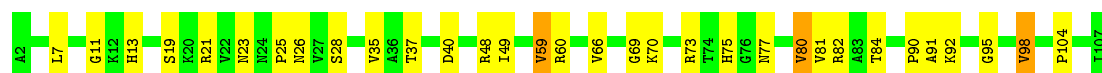


- Molecule 34: 60S ribosomal protein L32



- Molecule 35: 60S ribosomal protein L33-A

Chain AG:  70% 27%



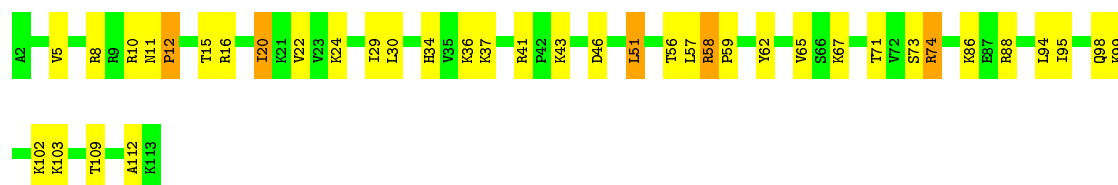
- Molecule 35: 60S ribosomal protein L33-A

Chain DH:  66% 30%



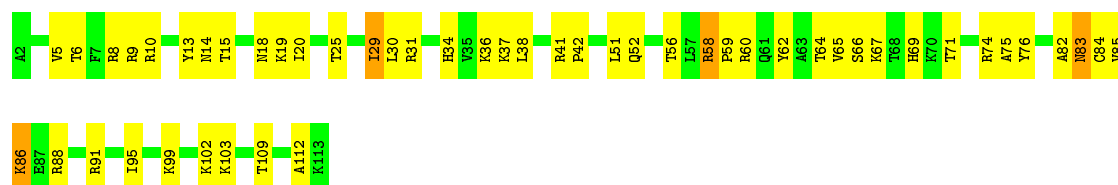
- Molecule 36: 60S ribosomal protein L34-A

Chain AH:  65% 30%



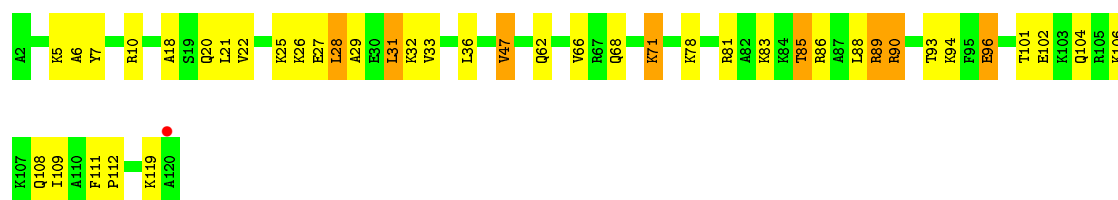
- Molecule 36: 60S ribosomal protein L34-A

Chain DI:  55% 41%



- Molecule 37: 60S ribosomal protein L35-A

Chain AI:  65% 29% 7%



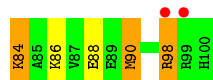
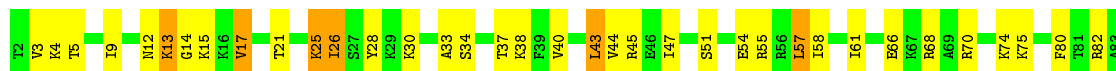
- Molecule 37: 60S ribosomal protein L35-A

Chain DJ:  51% 44% 5%

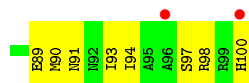
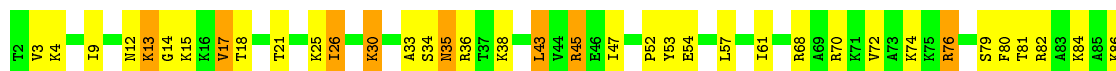




- Molecule 38: 60S ribosomal protein L36-A



- Molecule 38: 60S ribosomal protein L36-A



- Molecule 39: 60S ribosomal protein L37-A



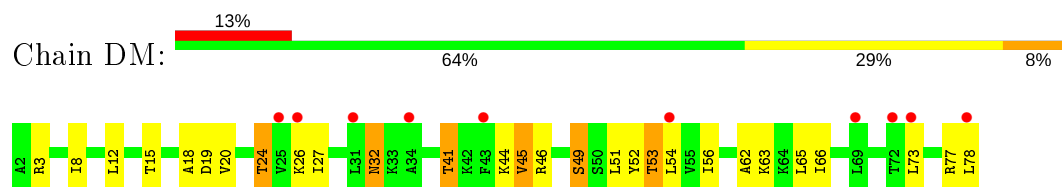
- Molecule 39: 60S ribosomal protein L37-A



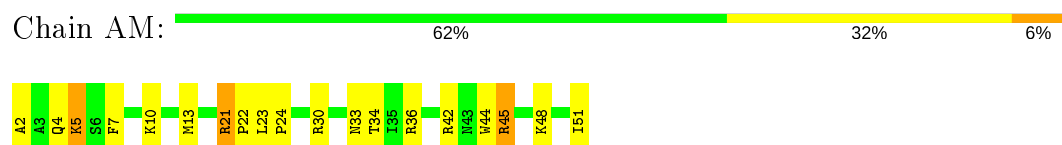
- Molecule 40: 60S ribosomal protein L38



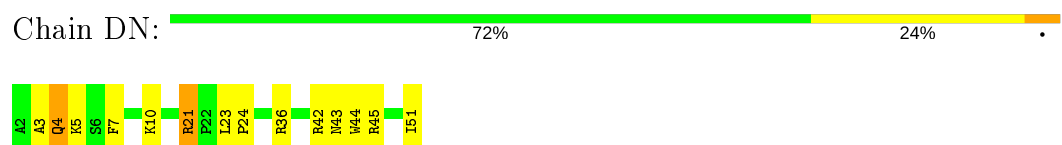
- Molecule 40: 60S ribosomal protein L38



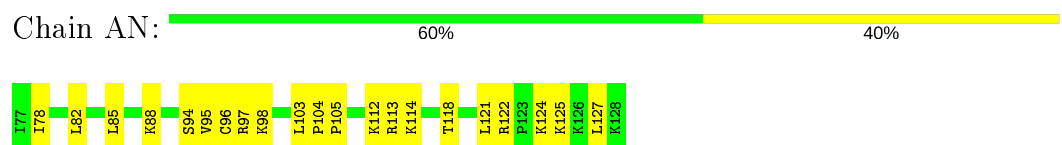
- Molecule 41: 60S ribosomal protein L39



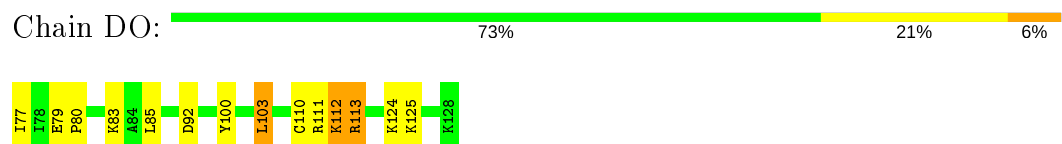
- Molecule 41: 60S ribosomal protein L39



- Molecule 42: Ubiquitin-60S ribosomal protein L40



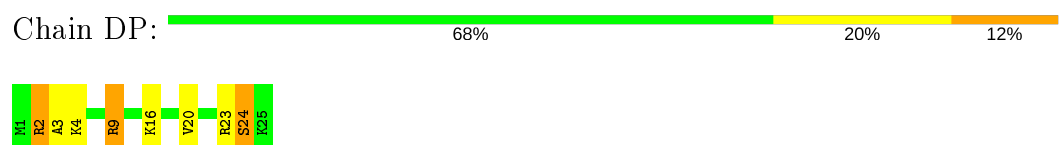
- Molecule 42: Ubiquitin-60S ribosomal protein L40



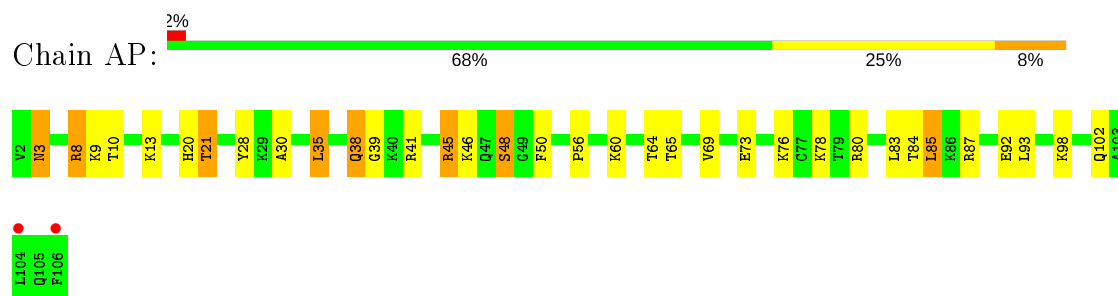
- Molecule 43: 60S ribosomal protein L41-B



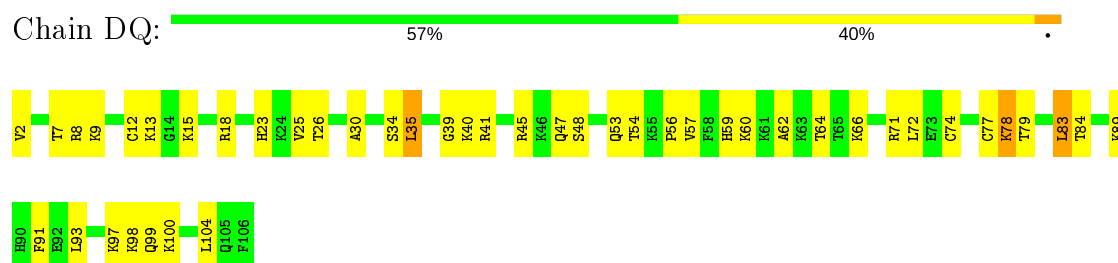
- Molecule 43: 60S ribosomal protein L41-B



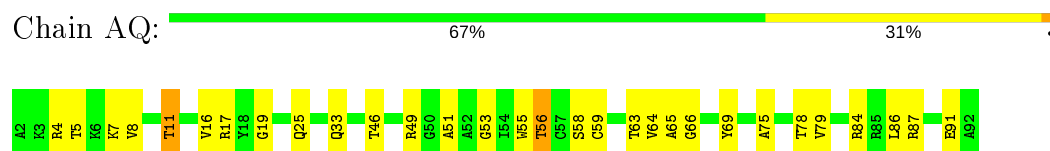
- Molecule 44: 60S ribosomal protein L42-A



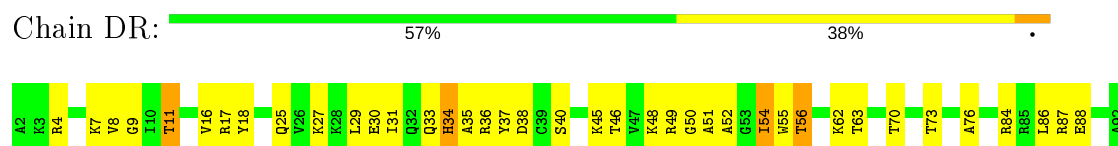
- Molecule 44: 60S ribosomal protein L42-A



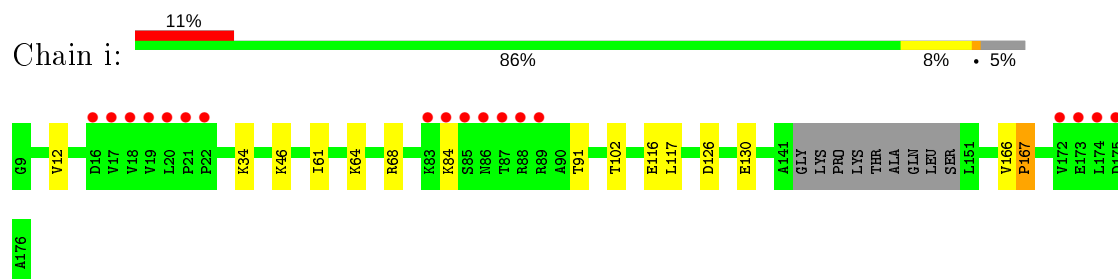
- Molecule 45: 60S ribosomal protein L43-A



- Molecule 45: 60S ribosomal protein L43-A

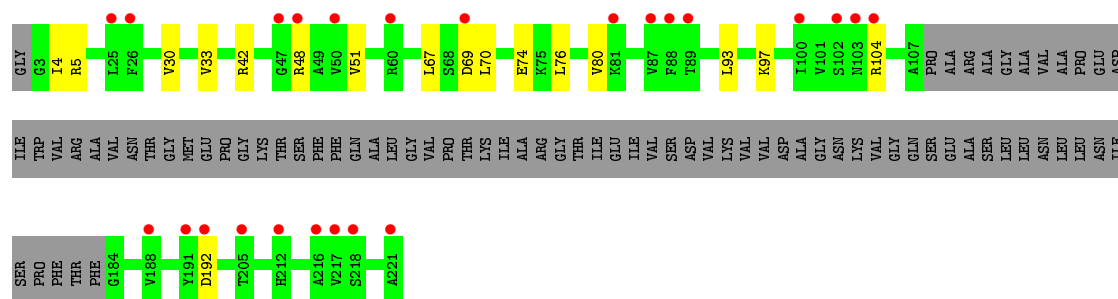


- Molecule 46: Suppressor protein STM1



- Molecule 47: 60S acidic ribosomal protein P0

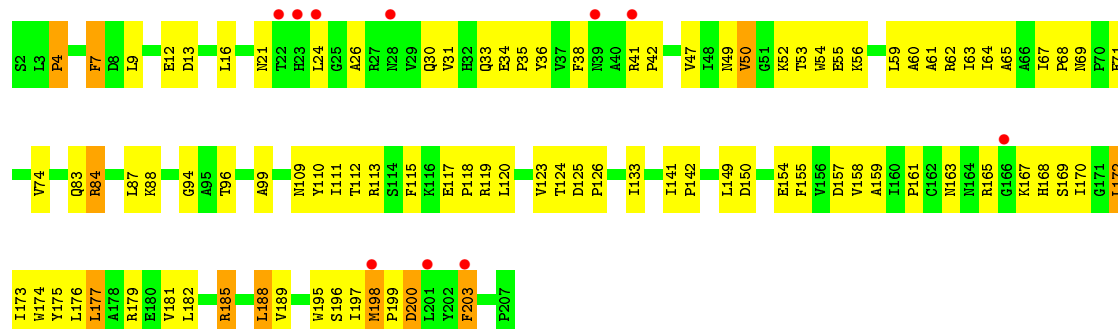




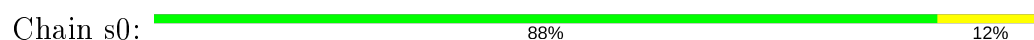
- Molecule 48: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein Stm1 - Mol B



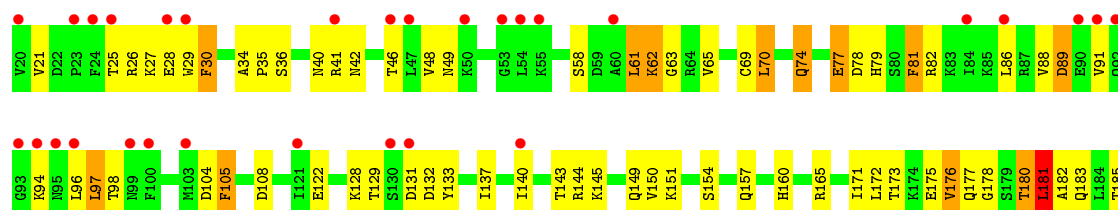
- Molecule 49: 40S ribosomal protein S0-A

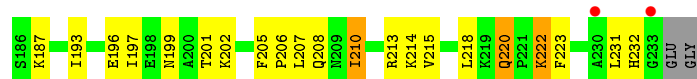


- Molecule 49: 40S ribosomal protein S0-A

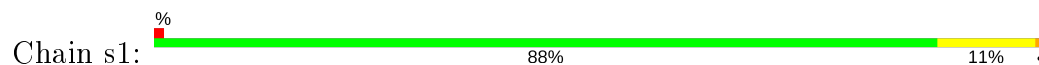


- Molecule 50: 40S ribosomal protein S1-A

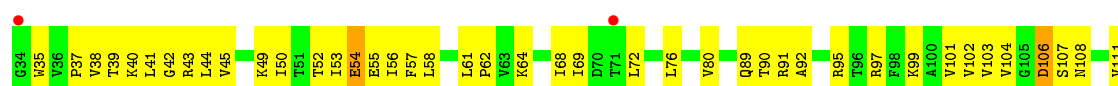




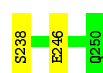
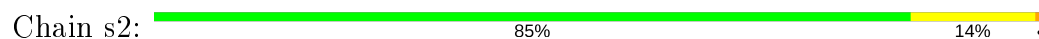
- Molecule 50: 40S ribosomal protein S1-A



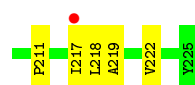
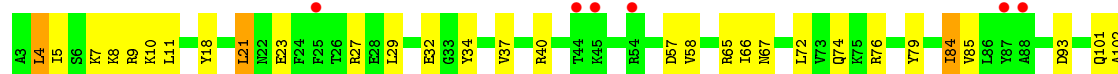
- Molecule 51: 40S ribosomal protein S2



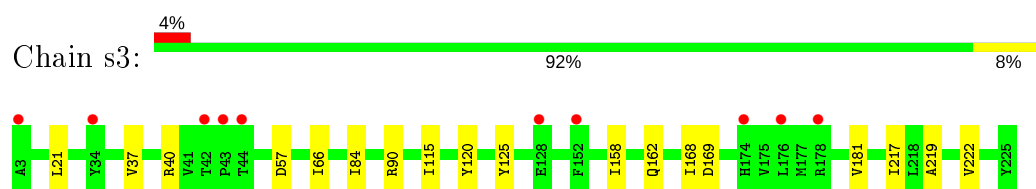
- Molecule 51: 40S ribosomal protein S2



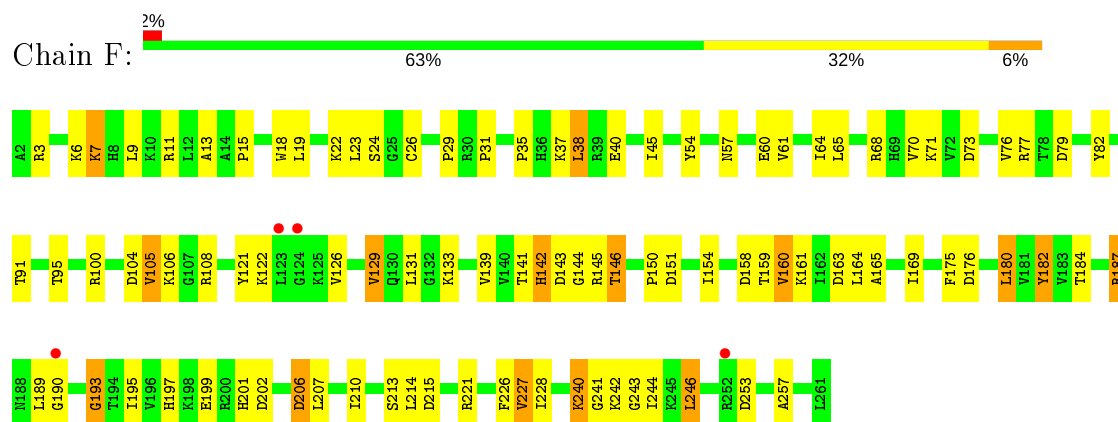
- Molecule 52: 40S ribosomal protein S3



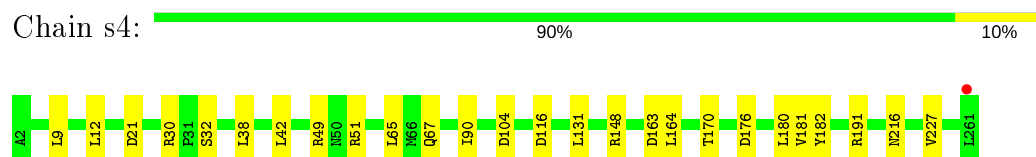
- Molecule 52: 40S ribosomal protein S3



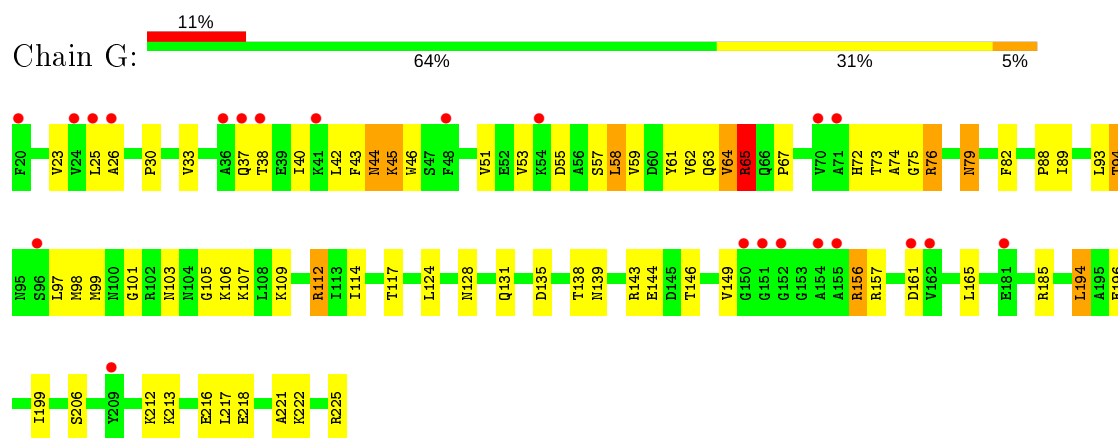
- Molecule 53: 40S ribosomal protein S4-A



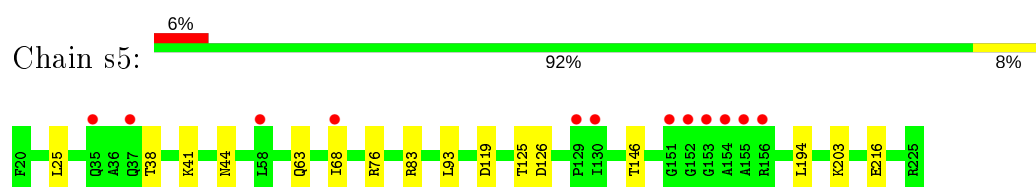
- Molecule 53: 40S ribosomal protein S4-A



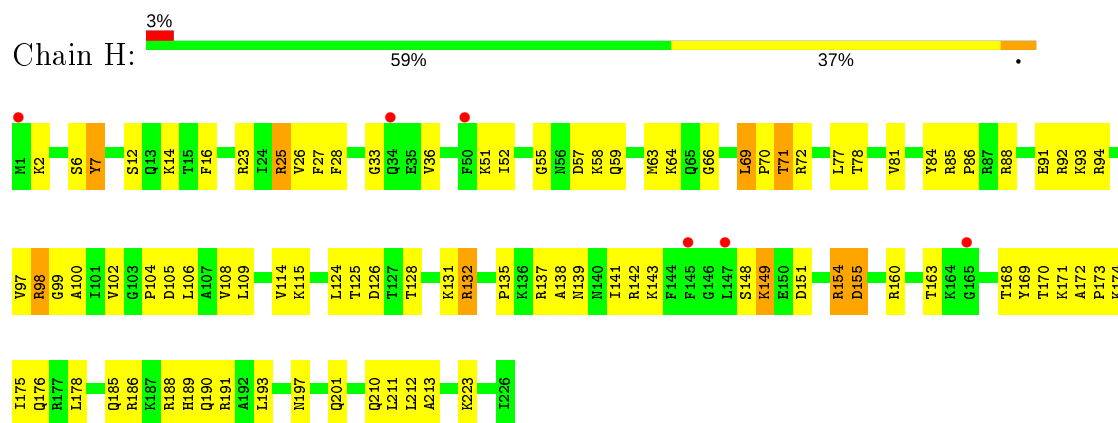
- Molecule 54: 40S ribosomal protein S5



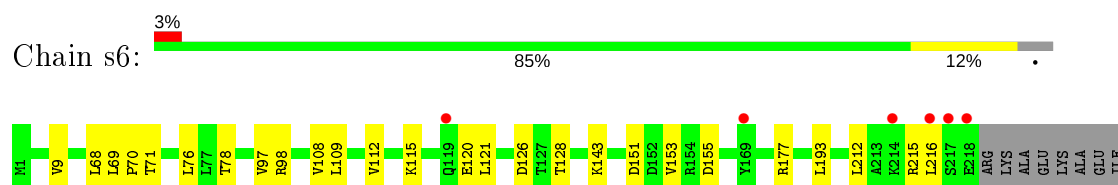
- Molecule 54: 40S ribosomal protein S5



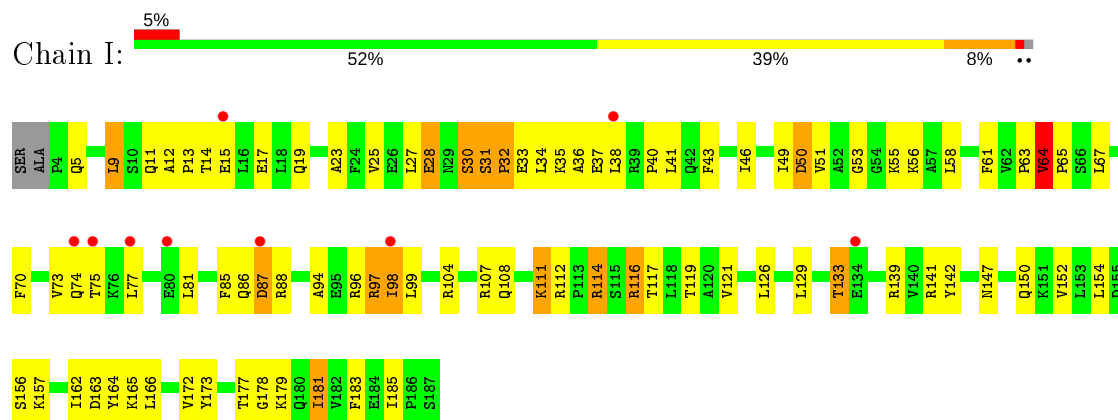
- Molecule 55: 40S ribosomal protein S6-A



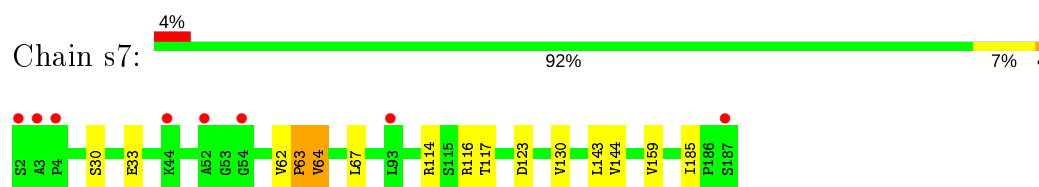
- Molecule 55: 40S ribosomal protein S6-A



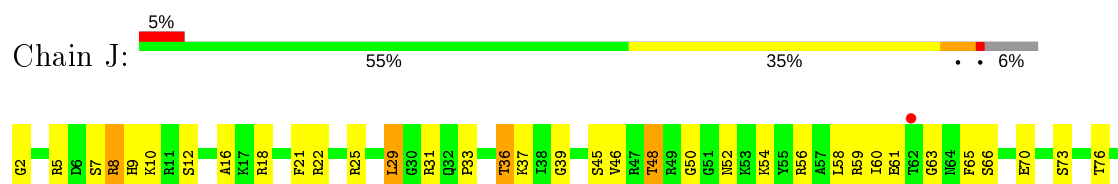
- Molecule 56: 40S ribosomal protein S7-A

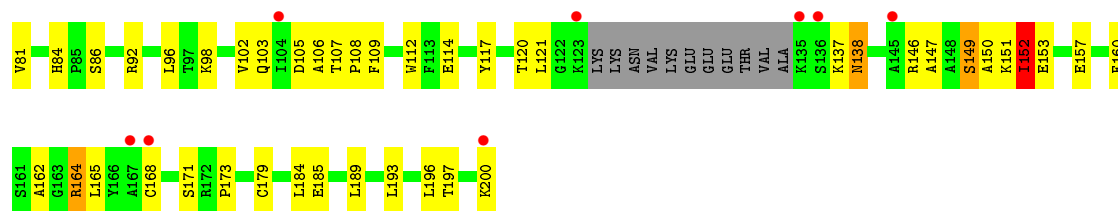


- Molecule 56: 40S ribosomal protein S7-A

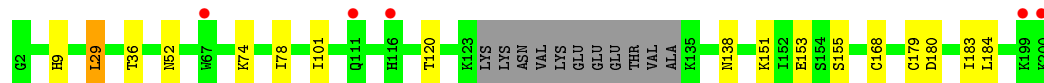
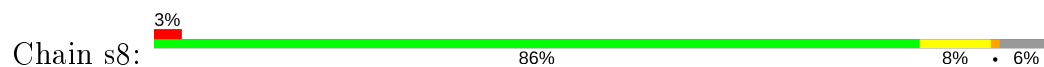


- Molecule 57: 40S ribosomal protein S8-A

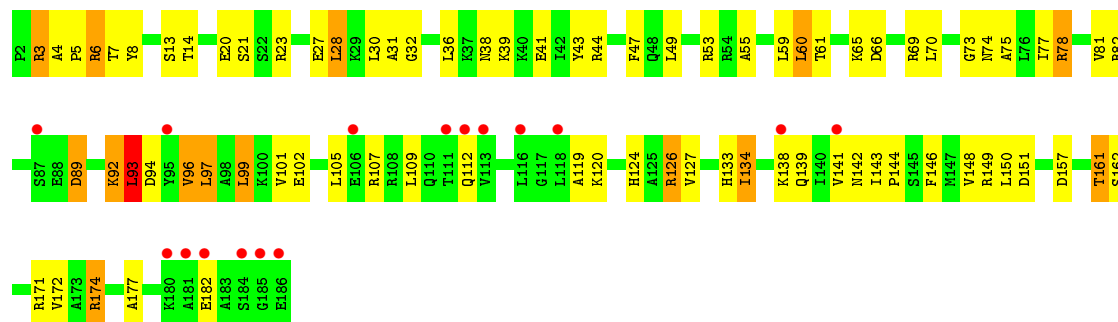




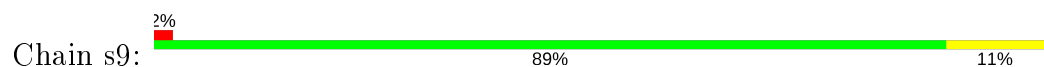
- Molecule 57: 40S ribosomal protein S8-A



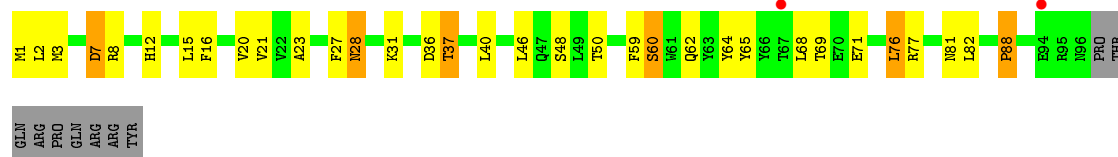
- Molecule 58: 40S ribosomal protein S9-A



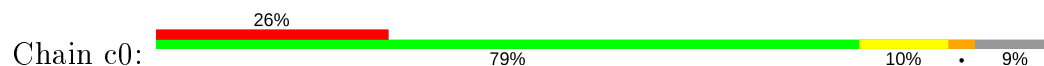
- Molecule 58: 40S ribosomal protein S9-A



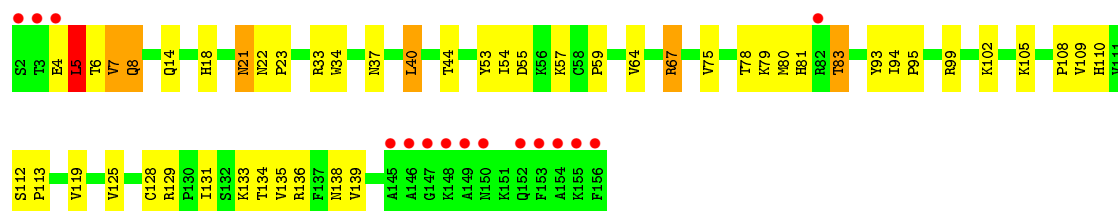
- Molecule 59: 40S ribosomal protein S10-A



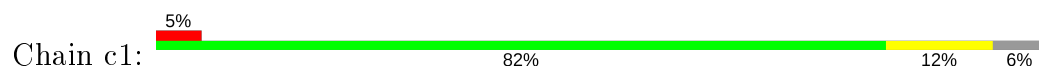
- Molecule 59: 40S ribosomal protein S10-A



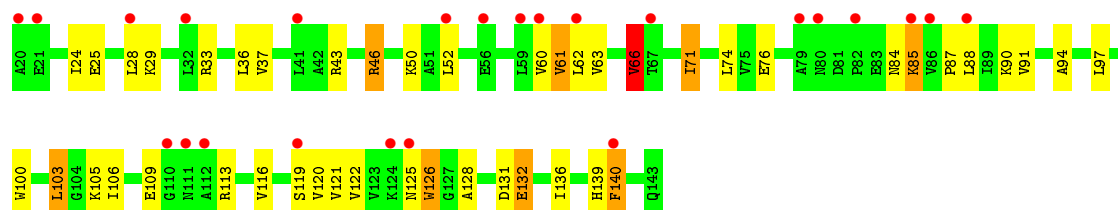
- Molecule 60: 40S ribosomal protein S11-A



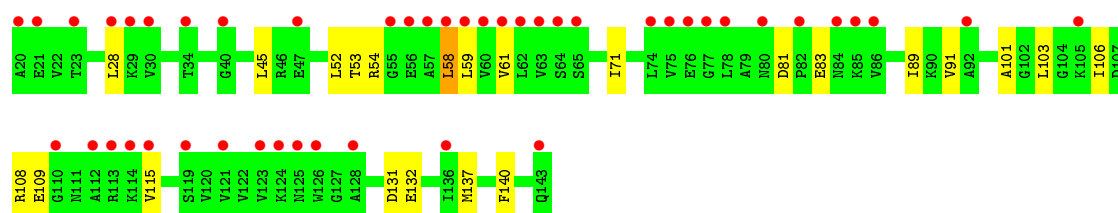
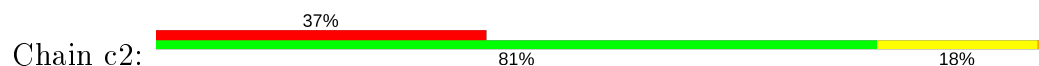
- Molecule 60: 40S ribosomal protein S11-A



- Molecule 61: 40S ribosomal protein S12

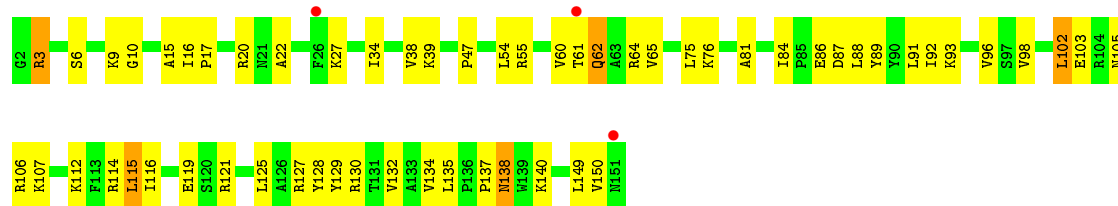


- Molecule 61: 40S ribosomal protein S12



- Molecule 62: 40S ribosomal protein S13





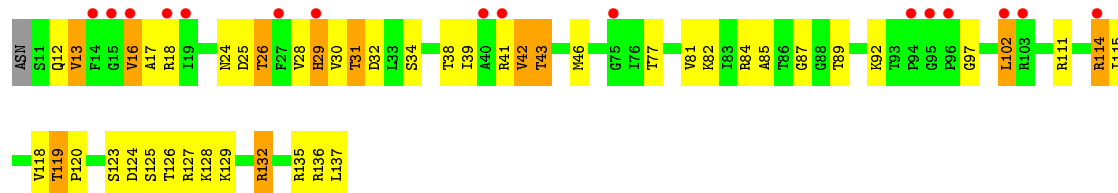
- Molecule 62: 40S ribosomal protein S13

Chain c3: 91% 9% .



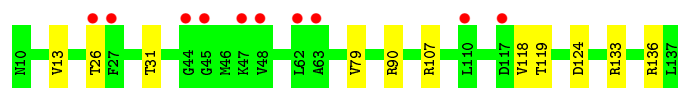
- Molecule 63: 40S ribosomal protein S14-B

Chain P: 13% 63% 28% 9% .



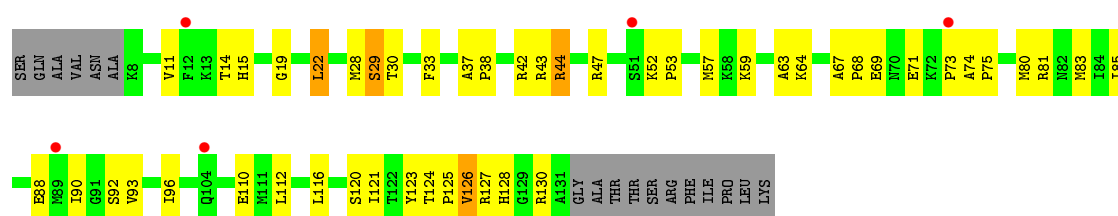
- Molecule 63: 40S ribosomal protein S14-B

Chain c4: 8% 91% 9%



- Molecule 64: 40S ribosomal protein S15

Chain Q: 4% 53% 32% 12%

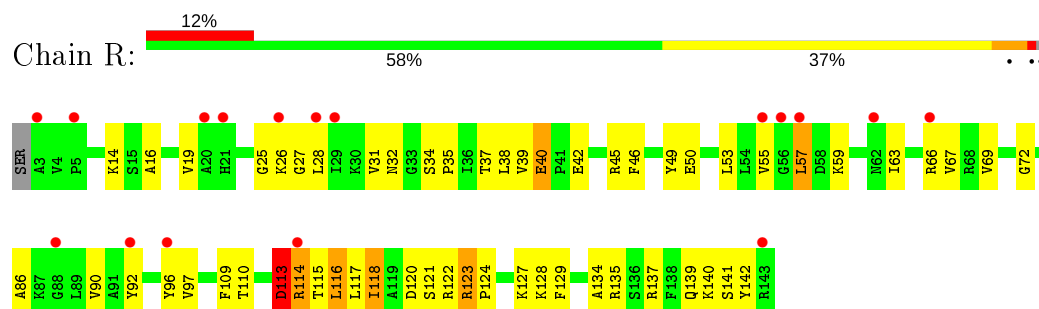


- Molecule 64: 40S ribosomal protein S15

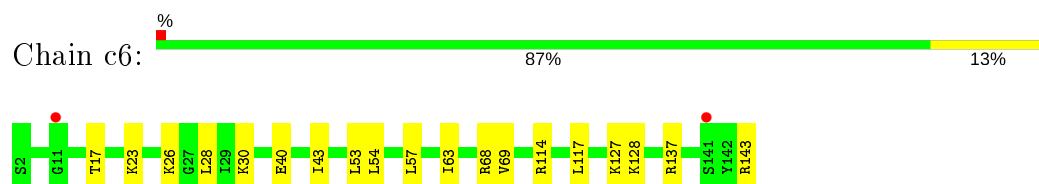
Chain c5: 8% 87% 8% . .



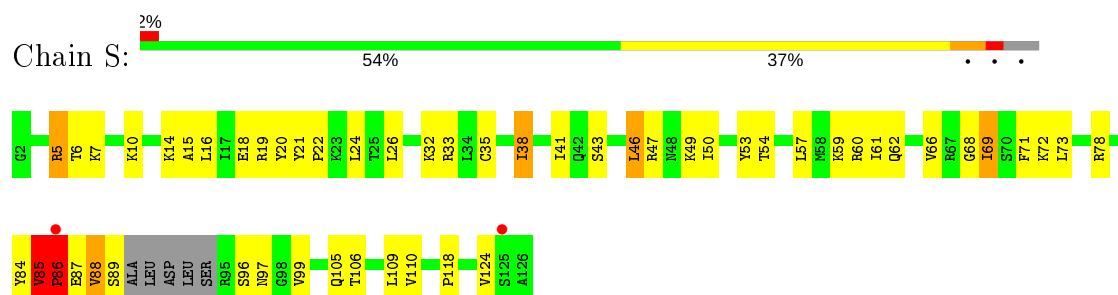
- Molecule 65: 40S ribosomal protein S16-A



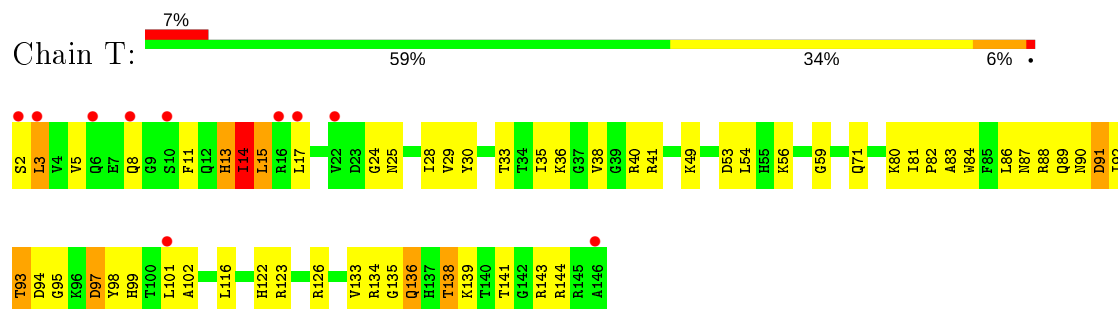
- Molecule 65: 40S ribosomal protein S16-A



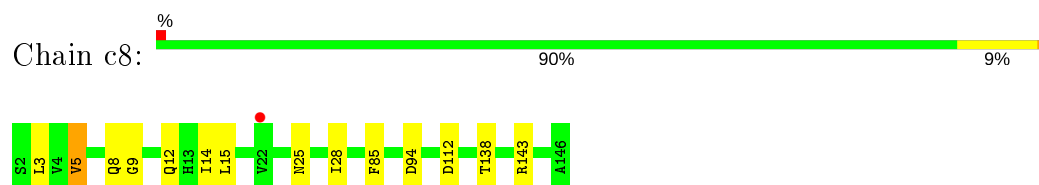
- Molecule 66: 40S ribosomal protein S17-B



- Molecule 67: 40S ribosomal protein S18-A

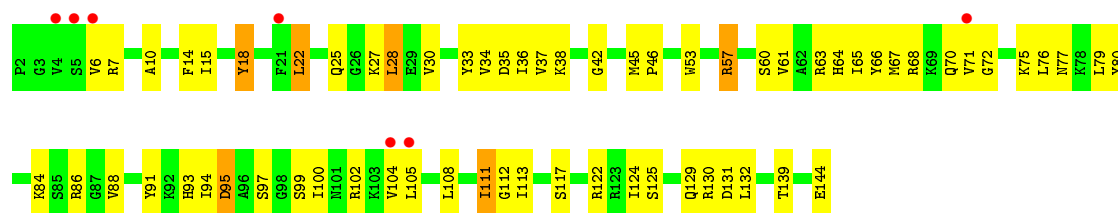


- Molecule 67: 40S ribosomal protein S18-A

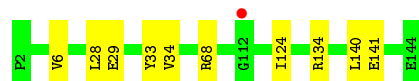


- Molecule 68: 40S ribosomal protein S19-A

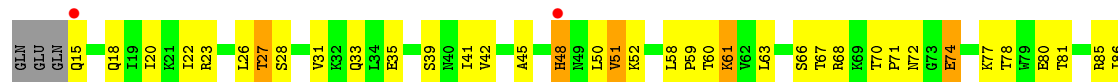




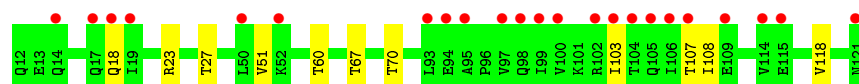
- Molecule 68: 40S ribosomal protein S19-A



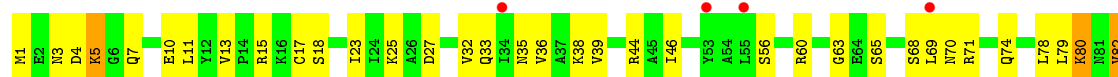
- Molecule 69: 40S ribosomal protein S20



- Molecule 69: 40S ribosomal protein S20



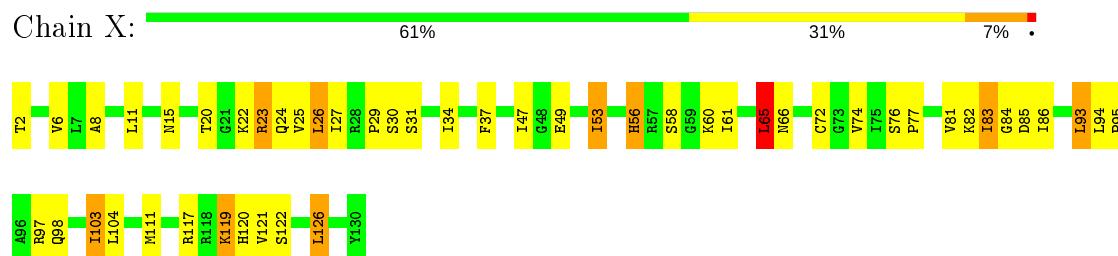
- Molecule 70: 40S ribosomal protein S21-A



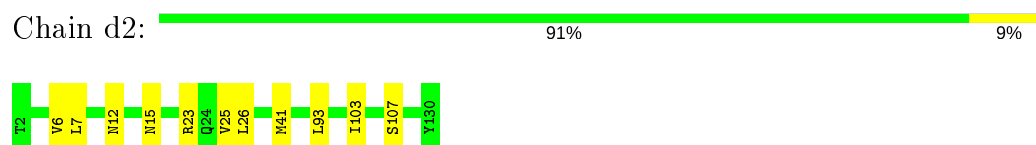
- Molecule 70: 40S ribosomal protein S21-A



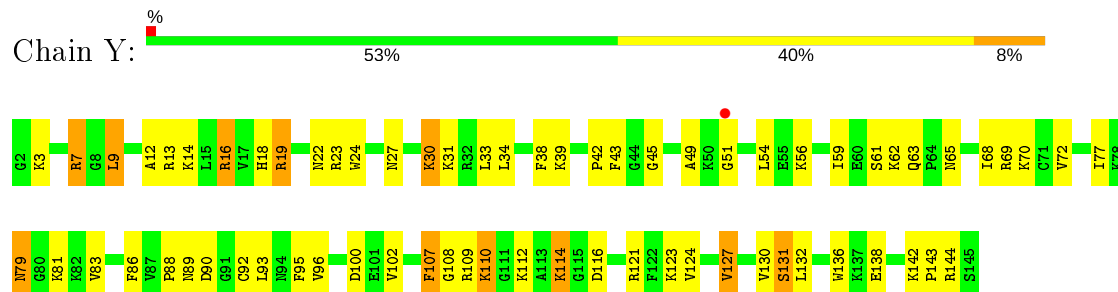
- Molecule 71: 40S ribosomal protein S22-A



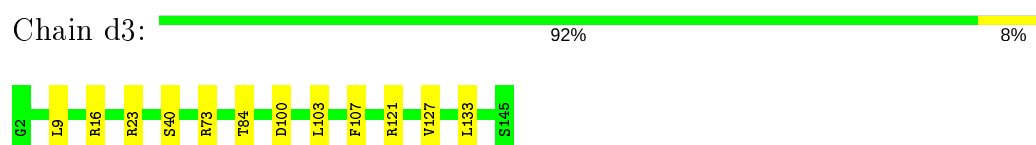
- Molecule 71: 40S ribosomal protein S22-A



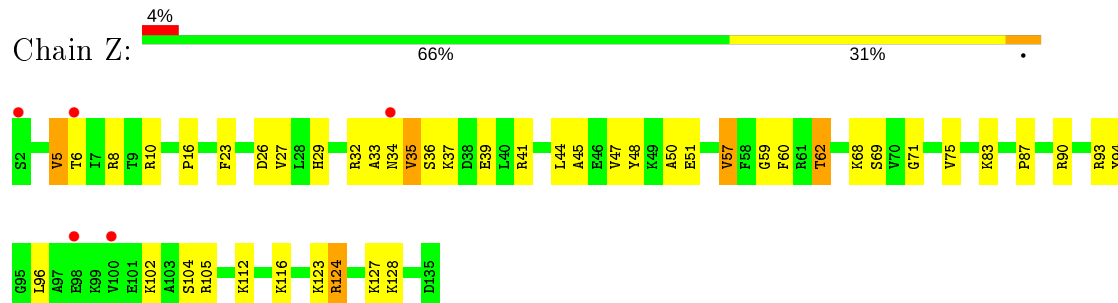
- Molecule 72: 40S ribosomal protein S23-A



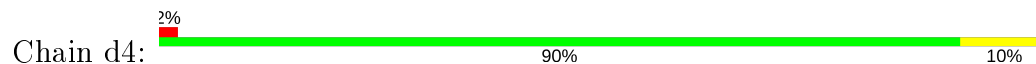
- Molecule 72: 40S ribosomal protein S23-A

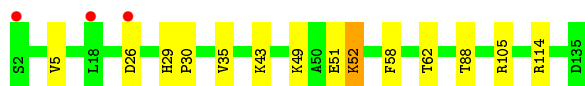


- Molecule 73: 40S ribosomal protein S24-A

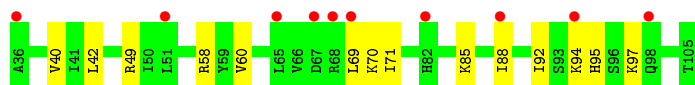
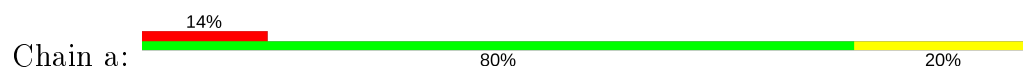


- Molecule 73: 40S ribosomal protein S24-A

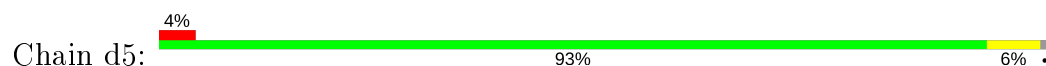




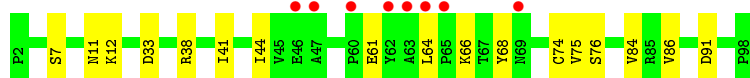
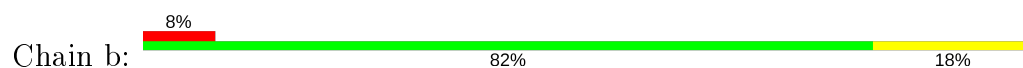
- Molecule 74: 40S ribosomal protein S25-A



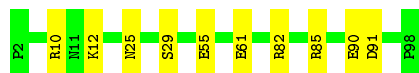
- Molecule 74: 40S ribosomal protein S25-A



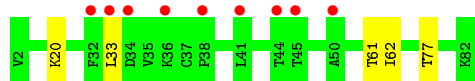
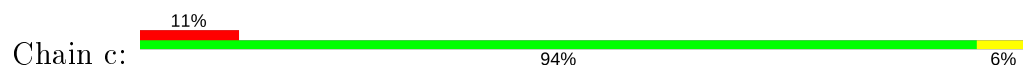
- Molecule 75: 40S ribosomal protein S26-B



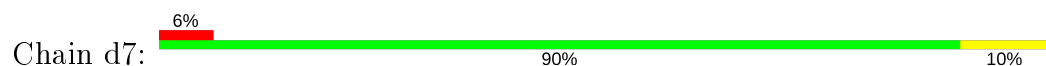
- Molecule 75: 40S ribosomal protein S26-B



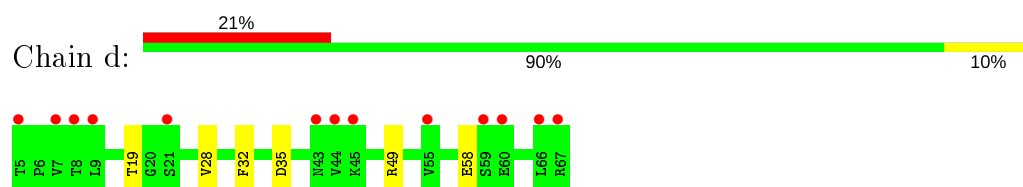
- Molecule 76: 40S ribosomal protein S27-A



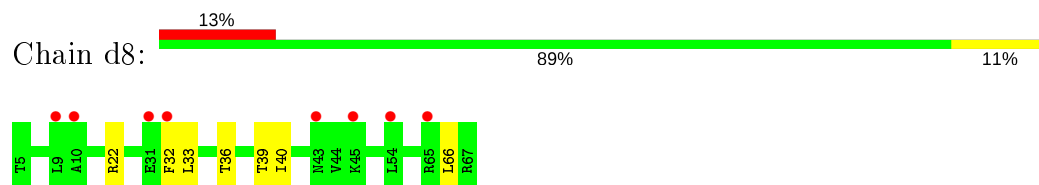
- Molecule 76: 40S ribosomal protein S27-A



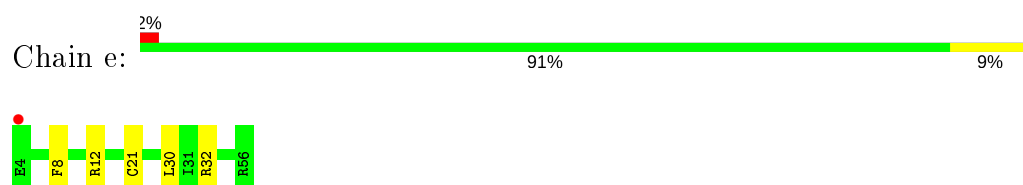
- Molecule 77: 40S ribosomal protein S28-A



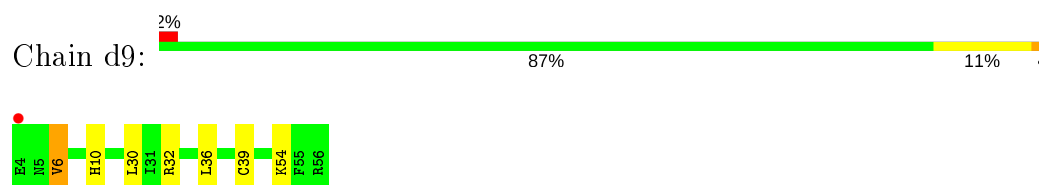
- Molecule 77: 40S ribosomal protein S28-A



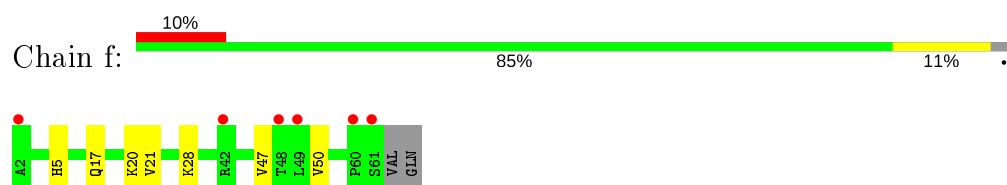
- Molecule 78: 40S ribosomal protein S29-A



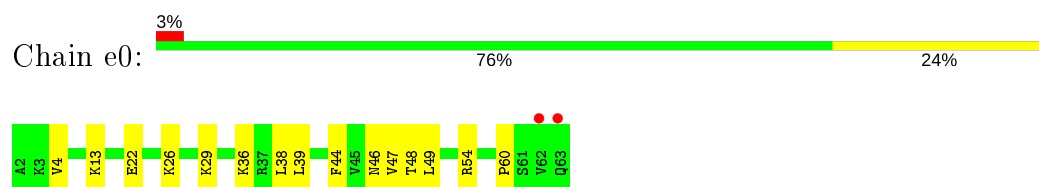
- Molecule 78: 40S ribosomal protein S29-A



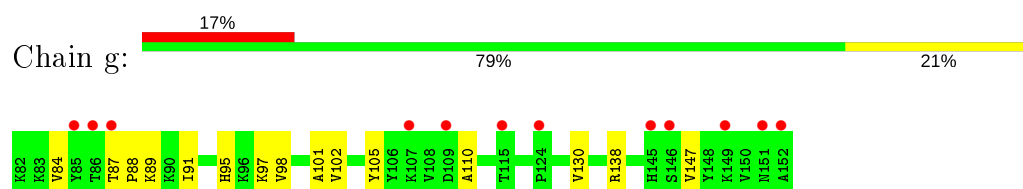
- Molecule 79: 40S ribosomal protein S30-A



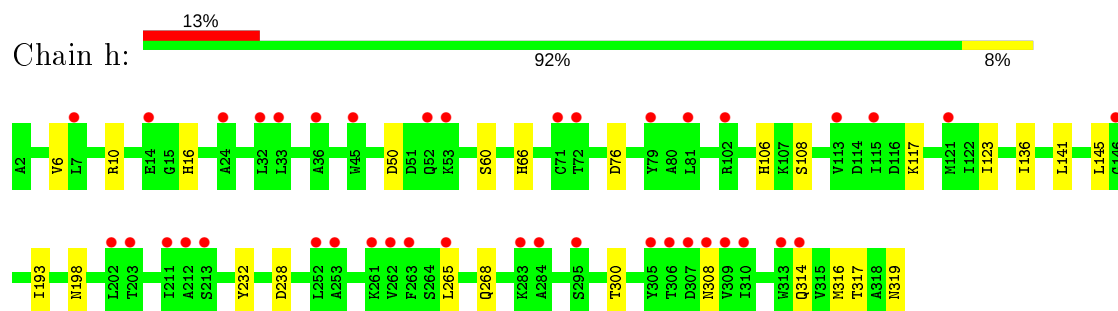
- Molecule 79: 40S ribosomal protein S30-A



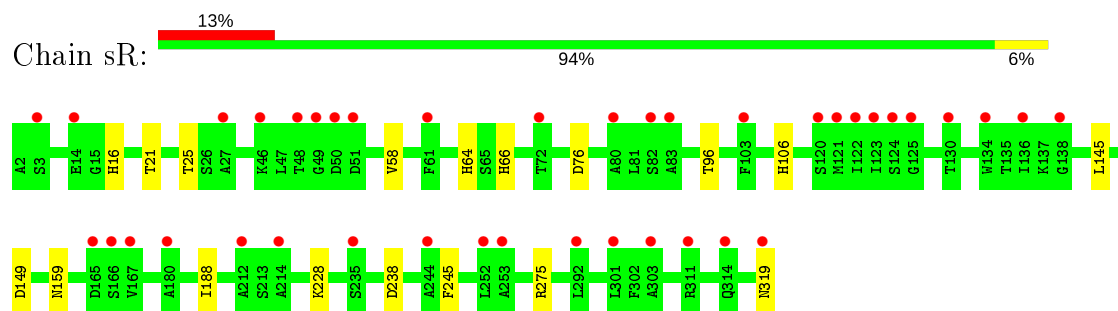
- Molecule 80: Ubiquitin-40S ribosomal protein S31



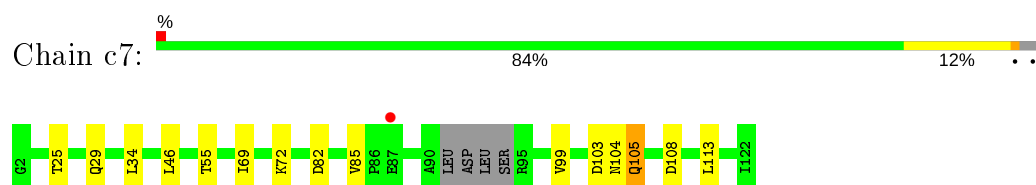
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein



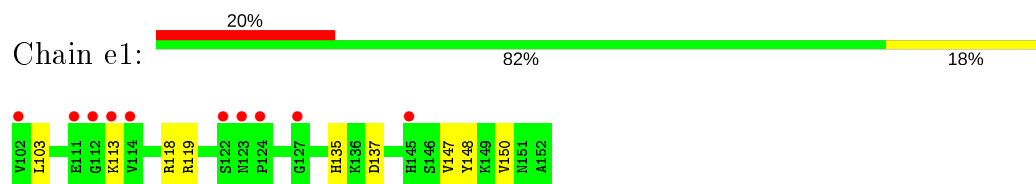
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 82: 40S ribosomal protein S17-A



- Molecule 83: Ubiquitin-40S ribosomal protein S31



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	304.08Å 286.55Å 436.55Å 90.00° 99.05° 90.00°	Depositor
Resolution (Å)	98.38 – 3.50 98.38 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (98.38-3.50) 100.0 (98.38-3.50)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.239 0.197 , 0.239	Depositor DCC
R_{free} test set	18298 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 84.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	409590	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7MB, ZN, 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	0.68	3/75394 (0.0%)	1.16	271/117545 (0.2%)
1	AR	0.72	2/75394 (0.0%)	1.19	322/117545 (0.3%)
2	3	0.63	0/2883	1.06	5/4491 (0.1%)
2	AS	0.68	0/2883	1.09	3/4491 (0.1%)
3	4	0.62	0/3746	1.11	7/5832 (0.1%)
3	AT	0.61	0/3746	1.07	7/5832 (0.1%)
4	CD	0.46	0/1948	0.67	0/2617
4	j	0.47	0/1948	0.66	1/2617 (0.0%)
5	CE	0.56	0/3146	0.69	0/4228
5	k	0.51	0/3146	0.65	0/4228
6	CF	0.49	0/2800	0.71	3/3790 (0.1%)
6	l	0.50	0/2800	0.70	1/3790 (0.0%)
7	CG	0.50	0/2425	0.62	0/3271
7	m	0.41	0/2425	0.58	0/3271
8	CH	0.51	0/1260	0.64	0/1694
8	n	0.50	0/1260	0.64	0/1694
9	CI	0.53	0/1821	0.67	0/2451
9	o	0.52	0/1821	0.66	1/2451 (0.0%)
10	CJ	0.38	0/1836	0.57	1/2481 (0.0%)
10	p	0.38	0/1836	0.56	0/2481
11	CK	0.52	0/1539	0.65	0/2073
11	q	0.46	0/1539	0.59	0/2073
12	CL	0.50	0/1741	0.64	0/2335
12	r	0.49	0/1741	0.62	1/2335 (0.0%)
13	CM	0.48	0/1374	0.64	0/1842
13	s	0.40	0/1374	0.60	0/1842
14	CN	0.47	0/1568	0.64	0/2106
14	t	0.49	0/1568	0.67	0/2106
15	CO	0.53	0/1068	0.64	0/1438
15	u	0.48	0/1068	0.64	0/1438
16	CP	0.47	0/1757	0.61	0/2354
16	v	0.52	0/1757	0.66	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CQ	0.64	0/1585	0.70	1/2128 (0.0%)
17	w	0.56	0/1585	0.67	0/2128
18	CR	0.54	0/1443	0.67	0/1944
18	x	0.52	0/1443	0.66	0/1944
19	CS	0.47	0/1465	0.67	0/1965
19	y	0.51	0/1465	0.68	0/1965
20	CT	0.45	0/1538	0.64	0/2050
20	z	0.37	0/1538	0.55	0/2050
21	0	0.51	0/1481	0.68	0/1990
21	CU	0.55	0/1481	0.69	0/1990
22	2	0.52	0/1300	0.64	0/1743
22	CV	0.52	0/1300	0.64	0/1743
23	5	0.36	0/812	0.55	0/1099
23	CW	0.39	0/812	0.59	0/1099
24	CX	0.58	0/1018	0.69	0/1369
24	l2	0.47	0/1018	0.63	0/1369
25	6	0.57	0/42490	1.06	96/66207 (0.1%)
25	A	0.47	0/42443	0.97	50/66134 (0.1%)
26	7	0.39	0/712	0.55	0/958
26	CY	0.48	0/712	0.66	0/958
27	8	0.43	0/979	0.63	0/1321
27	CZ	0.45	0/979	0.63	1/1321 (0.1%)
28	9	0.45	0/1004	0.69	1/1341 (0.1%)
28	DA	0.44	0/1004	0.67	0/1341
29	AA	0.36	0/1118	0.53	0/1497
29	DB	0.36	0/1118	0.56	0/1497
30	AB	0.48	0/1204	0.70	0/1612
30	DC	0.49	0/1204	0.74	0/1612
31	AC	0.43	0/473	0.65	1/629 (0.2%)
31	DD	0.48	0/473	0.64	0/629
32	AD	0.33	0/751	0.51	0/1008
32	DE	0.38	0/751	0.55	0/1008
33	AE	0.42	0/890	0.58	0/1196
33	DF	0.49	0/890	0.65	0/1196
34	AF	0.55	0/1041	0.66	0/1394
34	DG	0.55	0/1041	0.64	0/1394
35	AG	0.55	0/868	0.70	0/1168
35	DH	0.55	0/868	0.67	0/1168
36	AH	0.40	0/890	0.57	0/1189
36	DI	0.39	0/890	0.60	0/1189
37	AI	0.44	0/978	0.58	0/1301
37	DJ	0.42	0/978	0.53	0/1301
38	AJ	0.44	0/778	0.61	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DK	0.41	0/778	0.58	0/1034
39	AK	0.49	0/696	0.72	0/923
39	DL	0.44	0/696	0.63	0/923
40	AL	0.36	0/618	0.52	0/826
40	DM	0.38	0/618	0.55	0/826
41	AM	0.46	0/443	0.67	0/588
41	DN	0.44	0/443	0.63	0/588
42	AN	0.50	0/423	0.67	0/562
42	DO	0.56	0/423	0.73	1/562 (0.2%)
43	AO	0.42	0/234	0.64	0/300
43	DP	0.49	0/234	0.58	0/300
44	AP	0.48	0/860	0.72	1/1136 (0.1%)
44	DQ	0.48	0/860	0.68	0/1136
45	AQ	0.44	0/701	0.61	0/934
45	DR	0.48	0/701	0.71	1/934 (0.1%)
46	i	0.37	0/1113	0.57	1/1502 (0.1%)
47	p0	0.36	0/1092	0.53	0/1474
48	sM	0.41	0/480	0.64	0/642
49	B	0.37	0/1617	0.59	0/2215
49	s0	0.39	0/1623	0.59	0/2222
50	C	0.32	0/1735	0.57	1/2335 (0.0%)
50	s1	0.36	0/1748	0.60	1/2352 (0.0%)
51	D	0.36	0/1665	0.57	0/2263
51	s2	0.43	0/1665	0.62	0/2263
52	E	0.35	0/1759	0.56	0/2368
52	s3	0.33	0/1759	0.53	0/2368
53	F	0.36	0/2109	0.61	1/2839 (0.0%)
53	s4	0.41	0/2109	0.63	0/2839
54	G	0.32	0/1629	0.52	0/2202
54	s5	0.36	0/1629	0.56	0/2202
55	H	0.34	0/1823	0.53	0/2439
55	s6	0.40	0/1779	0.54	0/2379
56	I	0.33	0/1506	0.59	0/2028
56	s7	0.35	0/1516	0.57	0/2043
57	J	0.40	0/1514	0.60	0/2021
57	s8	0.44	0/1514	0.65	1/2021 (0.0%)
58	K	0.32	0/1519	0.58	0/2035
58	s9	0.40	0/1519	0.58	0/2035
59	L	0.35	0/789	0.66	1/1067 (0.1%)
59	c0	0.33	0/776	0.64	3/1047 (0.3%)
60	M	0.43	0/1239	0.62	1/1673 (0.1%)
60	c1	0.47	0/1194	0.62	0/1610
61	N	0.34	0/898	0.63	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	c2	0.29	0/898	0.59	1/1220 (0.1%)
62	O	0.35	0/1215	0.55	0/1638
62	c3	0.41	0/1215	0.59	0/1638
63	P	0.34	0/901	0.61	0/1217
63	c4	0.40	0/960	0.66	0/1290
64	Q	0.34	0/998	0.59	0/1341
64	c5	0.38	0/1060	0.62	1/1426 (0.1%)
65	R	0.35	0/1125	0.58	0/1510
65	c6	0.39	0/1131	0.57	0/1518
66	S	0.37	0/935	0.65	2/1254 (0.2%)
67	T	0.35	0/1211	0.55	0/1628
67	c8	0.39	0/1211	0.59	0/1628
68	U	0.33	0/1130	0.53	0/1517
68	c9	0.36	0/1130	0.53	0/1517
69	V	0.37	0/865	0.60	0/1169
69	d0	0.37	0/892	0.58	0/1205
70	W	0.35	0/693	0.53	0/935
70	d1	0.38	0/693	0.60	0/935
71	X	0.36	0/1038	0.67	2/1395 (0.1%)
71	d2	0.45	0/1038	0.62	0/1395
72	Y	0.44	0/1139	0.64	0/1518
72	d3	0.51	0/1139	0.67	0/1518
73	Z	0.34	0/1087	0.50	0/1449
73	d4	0.40	0/1087	0.61	0/1449
74	a	0.33	0/571	0.60	0/768
74	d5	0.34	0/566	0.56	0/761
75	b	0.37	0/782	0.59	0/1047
75	d6	0.42	0/782	0.60	0/1047
76	c	0.33	0/620	0.56	0/838
76	d7	0.36	0/620	0.58	0/838
77	d	0.29	0/499	0.52	0/670
77	d8	0.32	0/499	0.54	0/670
78	d9	0.40	0/452	0.57	0/600
78	e	0.42	0/452	0.61	0/600
79	e0	0.41	0/499	0.70	0/665
79	f	0.36	0/483	0.60	0/643
80	g	0.41	0/577	0.73	0/770
81	h	0.31	0/2490	0.51	0/3389
81	sR	0.32	0/2495	0.51	0/3395
82	c7	0.37	0/914	0.58	0/1224
83	e1	0.33	0/404	0.67	0/542
All	All	0.56	5/429965 (0.0%)	0.96	792/631328 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	CG	0	1
10	CJ	0	1
12	CL	0	1
15	u	0	1
17	CQ	0	1
17	w	0	1
20	CT	0	1
22	2	0	1
26	7	0	1
26	CY	0	2
28	9	0	1
28	DA	0	1
29	DB	0	1
30	AB	0	1
31	AC	0	1
48	sM	0	1
49	B	0	1
50	s1	0	1
51	D	0	1
51	s2	0	1
52	E	0	1
52	s3	0	1
53	F	0	1
54	G	0	2
54	s5	0	1
56	I	0	2
56	s7	0	4
58	K	0	1
61	c2	0	4
64	Q	0	1
64	c5	0	1
65	R	0	2
65	c6	0	1
66	S	0	2
73	d4	0	2
74	a	0	1
80	g	0	2
82	c7	0	1
All	All	0	51

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AR	895	A	C5-C6	-5.81	1.35	1.41
1	1	936	A	N9-C4	-5.30	1.34	1.37
1	AR	2911	A	N9-C4	-5.05	1.34	1.37
1	1	1865	A	N9-C4	-5.05	1.34	1.37
1	1	3180	A	N9-C4	-5.03	1.34	1.37

The worst 5 of 792 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	2821	C	C6-N1-C2	-9.74	116.40	120.30
1	1	637	C	C6-N1-C2	9.70	124.18	120.30
3	4	94	C	C6-N1-C2	9.68	124.17	120.30
1	1	2727	A	N1-C6-N6	-9.61	112.84	118.60
25	6	163	G	N3-C4-N9	-9.23	120.46	126.00

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	67355	0	33846	1062	0
1	AR	67355	0	33843	1257	0
2	3	2579	0	1303	32	0
2	AS	2579	0	1304	48	0
3	4	3353	0	1695	64	0
3	AT	3353	0	1695	62	0
4	CD	1914	0	1981	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	j	1914	0	1981	0	0
5	CE	3075	0	3142	128	0
5	k	3075	0	3142	0	0
6	CF	2748	0	2859	91	0
6	l	2748	0	2859	0	0
7	CG	2375	0	2325	78	0
7	m	2375	0	2325	0	0
8	CH	1239	0	1326	39	0
8	n	1239	0	1326	0	0
9	CI	1784	0	1862	59	0
9	o	1784	0	1862	0	0
10	CJ	1804	0	1877	47	0
10	p	1804	0	1877	0	0
11	CK	1518	0	1587	52	0
11	q	1518	0	1587	0	0
12	CL	1705	0	1736	63	0
12	r	1705	0	1736	0	0
13	CM	1353	0	1383	38	0
13	s	1353	0	1383	0	0
14	CN	1543	0	1608	58	0
14	t	1543	0	1608	0	0
15	CO	1053	0	1149	40	0
15	u	1053	0	1149	0	0
16	CP	1720	0	1779	53	0
16	v	1720	0	1778	0	0
17	CQ	1555	0	1659	53	0
17	w	1555	0	1659	0	0
18	CR	1420	0	1437	45	0
18	x	1420	0	1437	0	0
19	CS	1441	0	1543	54	0
19	y	1441	0	1543	0	0
20	CT	1521	0	1617	57	0
20	z	1521	0	1617	0	0
21	0	1445	0	1487	38	0
21	CU	1445	0	1487	48	0
22	2	1276	0	1323	45	0
22	CV	1276	0	1323	63	0
23	5	796	0	812	22	0
23	CW	796	0	812	20	0
24	CX	1003	0	1048	31	0
24	l2	1003	0	1048	0	0
25	6	37990	0	19115	566	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	37948	0	19093	785	0
26	7	699	0	640	9	0
26	CY	699	0	640	14	0
27	8	964	0	1025	33	0
27	CZ	964	0	1025	33	0
28	9	993	0	1081	25	0
28	DA	993	0	1081	35	0
29	AA	1092	0	1155	49	0
29	DB	1092	0	1155	42	0
30	AB	1173	0	1214	52	0
30	DC	1173	0	1215	51	0
31	AC	462	0	491	8	0
31	DD	462	0	491	19	0
32	AD	743	0	797	25	0
32	DE	743	0	797	27	0
33	AE	876	0	912	28	0
33	DF	876	0	912	19	0
34	AF	1020	0	1090	22	0
34	DG	1020	0	1090	38	0
35	AG	850	0	880	22	0
35	DH	850	0	880	27	0
36	AH	880	0	945	27	0
36	DI	880	0	945	37	0
37	AI	969	0	1078	35	0
37	DJ	969	0	1078	40	0
38	AJ	771	0	849	31	0
38	DK	771	0	849	35	0
39	AK	681	0	683	24	0
39	DL	681	0	683	26	0
40	AL	612	0	682	12	0
40	DM	612	0	682	20	0
41	AM	436	0	475	19	0
41	DN	436	0	475	14	0
42	AN	417	0	455	11	0
42	DO	417	0	455	12	0
43	AO	233	0	284	8	0
43	DP	233	0	284	10	0
44	AP	847	0	917	23	0
44	DQ	847	0	918	27	0
45	AQ	694	0	736	17	0
45	DR	694	0	735	24	0
46	i	1104	0	996	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	p0	1077	0	1041	0	0
48	sM	680	0	540	0	0
49	B	1577	0	1567	68	0
49	s0	1583	0	1578	0	0
50	C	1709	0	1784	70	0
50	s1	1722	0	1793	0	0
51	D	1635	0	1723	70	0
51	s2	1635	0	1723	0	0
52	E	1734	0	1817	51	0
52	s3	1734	0	1817	0	0
53	F	2068	0	2154	69	0
53	s4	2068	0	2154	0	0
54	G	1609	0	1675	54	0
54	s5	1609	0	1675	0	0
55	H	1799	0	1879	69	0
55	s6	1755	0	1846	0	0
56	I	1481	0	1572	61	0
56	s7	1491	0	1578	0	0
57	J	1489	0	1525	60	0
57	s8	1489	0	1525	0	0
58	K	1494	0	1573	53	0
58	s9	1494	0	1573	0	0
59	L	772	0	727	25	0
59	c0	761	0	697	0	0
60	M	1213	0	1257	40	0
60	c1	1168	0	1233	0	0
61	N	890	0	887	28	0
61	c2	890	0	887	0	0
62	O	1192	0	1255	39	0
62	c3	1192	0	1255	0	0
63	P	891	0	883	42	0
63	c4	949	0	985	0	0
64	Q	977	0	1002	34	0
64	c5	1039	0	1050	0	0
65	R	1105	0	1166	40	0
65	c6	1111	0	1171	0	0
66	S	926	0	930	44	0
67	T	1192	0	1222	52	0
67	c8	1192	0	1222	0	0
68	U	1112	0	1124	44	0
68	c9	1112	0	1124	0	0
69	V	855	0	917	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	d0	882	0	939	0	0
70	W	684	0	672	27	0
70	d1	684	0	672	0	0
71	X	1021	0	1060	35	0
71	d2	1021	0	1060	0	0
72	Y	1121	0	1196	47	0
72	d3	1121	0	1196	0	0
73	Z	1073	0	1132	37	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	815	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	429	0	0
79	e0	491	0	542	0	0
79	f	475	0	525	0	0
80	g	566	0	602	0	0
81	h	2437	0	2386	0	0
81	sR	2442	0	2392	0	0
82	c7	906	0	909	0	0
83	e1	397	0	396	0	0
84	1	2317	0	0	230	0
84	2	7	0	0	0	0
84	3	56	0	0	5	0
84	4	84	0	0	7	0
84	6	1099	0	0	105	0
84	A	994	0	0	120	0
84	AC	7	0	0	1	0
84	AE	7	0	0	4	0
84	AG	7	0	0	0	0
84	AK	14	0	0	2	0
84	AP	7	0	0	3	0
84	AR	2373	0	0	242	0
84	AS	70	0	0	7	0
84	AT	133	0	0	18	0
84	CE	14	0	0	2	0
84	CF	14	0	0	1	0

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	l	2	0	0	0	0
85	l2	2	0	0	0	0
85	o	3	0	0	0	0
85	r	1	0	0	0	0
85	s	1	0	0	0	0
85	s1	1	0	0	0	0
85	s2	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	1	0	0	0	0
85	sM	1	0	0	0	0
85	t	2	0	0	0	0
85	v	1	0	0	0	0
85	w	1	0	0	0	0
85	x	5	0	0	0	0
85	z	2	0	0	0	0
86	1	20	0	0	4	0
86	AR	20	0	0	3	0
87	AK	1	0	0	0	0
87	AN	1	0	0	0	0
87	AP	1	0	0	0	0
87	AQ	1	0	0	0	0
87	DL	1	0	0	0	0
87	DO	1	0	0	0	0
87	DQ	1	0	0	0	0
87	DR	1	0	0	0	0
87	b	1	0	0	0	0
87	c	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e	1	0	0	0	0
87	e1	1	0	0	0	0
87	g	1	0	0	0	0
All	All	409590	0	296688	6489	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 13.

The worst 5 of 6489 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1171:G:N7	84:1:3496:OHX:N2	2.13	0.96
25:6:1726:G:N7	84:6:2005:OHX:N2	2.12	0.95
1:AR:1481:A:O2'	1:AR:1858:A:N3	2.00	0.95
25:6:1588:G:H1	25:6:1608:U:H3	1.15	0.95
1:AR:1878:G:OP1	84:AR:3457:OHX:N5	2.01	0.94

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	250/252 (99%)	238 (95%)	12 (5%)	0	100	100
4	j	250/252 (99%)	232 (93%)	18 (7%)	0	100	100
5	CE	384/386 (100%)	355 (92%)	27 (7%)	2 (0%)	29	68
5	k	384/386 (100%)	351 (91%)	31 (8%)	2 (0%)	29	68
6	CF	359/361 (99%)	331 (92%)	28 (8%)	0	100	100
6	l	359/361 (99%)	326 (91%)	32 (9%)	1 (0%)	41	75
7	CG	294/296 (99%)	272 (92%)	22 (8%)	0	100	100
7	m	294/296 (99%)	271 (92%)	23 (8%)	0	100	100
8	CH	152/175 (87%)	144 (95%)	6 (4%)	2 (1%)	12	48
8	n	152/175 (87%)	145 (95%)	6 (4%)	1 (1%)	22	61
9	CI	220/222 (99%)	202 (92%)	15 (7%)	3 (1%)	11	46
9	o	220/222 (99%)	204 (93%)	13 (6%)	3 (1%)	11	46
10	CJ	231/233 (99%)	207 (90%)	21 (9%)	3 (1%)	12	48
10	p	231/233 (99%)	209 (90%)	18 (8%)	4 (2%)	9	42
11	CK	189/191 (99%)	178 (94%)	11 (6%)	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%)	195 (94%)	10 (5%)	2 (1%)	15	54
12	r	207/220 (94%)	199 (96%)	8 (4%)	0	100	100
13	CM	167/169 (99%)	146 (87%)	18 (11%)	3 (2%)	8	41
13	s	167/169 (99%)	149 (89%)	15 (9%)	3 (2%)	8	41
14	CN	191/193 (99%)	172 (90%)	18 (9%)	1 (0%)	29	68
14	t	191/193 (99%)	173 (91%)	15 (8%)	3 (2%)	9	43
15	CO	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	10	45
15	u	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	45
16	CP	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
16	v	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
17	CQ	195/197 (99%)	189 (97%)	4 (2%)	2 (1%)	15	54
17	w	195/197 (99%)	188 (96%)	4 (2%)	3 (2%)	10	45
18	CR	181/183 (99%)	166 (92%)	14 (8%)	1 (1%)	25	64
18	x	181/183 (99%)	170 (94%)	10 (6%)	1 (1%)	25	64
19	CS	183/185 (99%)	171 (93%)	11 (6%)	1 (0%)	29	68
19	y	183/185 (99%)	173 (94%)	9 (5%)	1 (0%)	29	68
20	CT	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	68
20	z	186/188 (99%)	178 (96%)	7 (4%)	1 (0%)	29	68
21	0	170/172 (99%)	154 (91%)	15 (9%)	1 (1%)	25	64
21	CU	170/172 (99%)	158 (93%)	12 (7%)	0	100	100
22	2	157/159 (99%)	144 (92%)	12 (8%)	1 (1%)	25	64
22	CV	157/159 (99%)	147 (94%)	9 (6%)	1 (1%)	25	64
23	5	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	15	54
23	CW	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	15	54
24	CX	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
24	l2	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
26	7	96/98 (98%)	85 (88%)	10 (10%)	1 (1%)	15	54
26	CY	96/98 (98%)	83 (86%)	11 (12%)	2 (2%)	7	38
27	8	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
27	CZ	119/121 (98%)	111 (93%)	6 (5%)	2 (2%)	9	42
28	9	124/126 (98%)	120 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	DA	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
29	AA	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
29	DB	133/135 (98%)	121 (91%)	10 (8%)	2 (2%)	10	45
30	AB	146/148 (99%)	127 (87%)	17 (12%)	2 (1%)	11	46
30	DC	146/148 (99%)	130 (89%)	14 (10%)	2 (1%)	11	46
31	AC	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	8	41
31	DD	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	8	41
32	AD	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
32	DE	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
33	AE	107/109 (98%)	101 (94%)	5 (5%)	1 (1%)	17	56
33	DF	107/109 (98%)	103 (96%)	3 (3%)	1 (1%)	17	56
34	AF	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
34	DG	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
35	AG	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	8	40
35	DH	104/106 (98%)	97 (93%)	6 (6%)	1 (1%)	15	54
36	AH	110/112 (98%)	104 (94%)	4 (4%)	2 (2%)	8	41
36	DI	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
37	AI	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
37	DJ	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
38	AJ	97/99 (98%)	83 (86%)	13 (13%)	1 (1%)	15	54
38	DK	97/99 (98%)	86 (89%)	10 (10%)	1 (1%)	15	54
39	AK	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
39	DL	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
40	AL	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
40	DM	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	12	48
41	AM	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
41	DN	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
42	AN	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
42	DO	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
43	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
43	DP	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	AP	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
44	DQ	103/105 (98%)	90 (87%)	12 (12%)	1 (1%)	15	54
45	AQ	89/91 (98%)	77 (86%)	12 (14%)	0	100	100
45	DR	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
46	i	155/168 (92%)	129 (83%)	23 (15%)	3 (2%)	8	40
47	p0	139/220 (63%)	130 (94%)	8 (6%)	1 (1%)	22	61
48	sM	61/104 (59%)	47 (77%)	13 (21%)	1 (2%)	9	43
49	B	204/206 (99%)	175 (86%)	26 (13%)	3 (2%)	10	45
49	s0	204/206 (99%)	184 (90%)	17 (8%)	3 (2%)	10	45
50	C	212/216 (98%)	175 (82%)	35 (16%)	2 (1%)	17	56
50	s1	214/216 (99%)	196 (92%)	18 (8%)	0	100	100
51	D	215/217 (99%)	196 (91%)	18 (8%)	1 (0%)	29	68
51	s2	215/217 (99%)	199 (93%)	13 (6%)	3 (1%)	11	46
52	E	221/223 (99%)	198 (90%)	21 (10%)	2 (1%)	17	56
52	s3	221/223 (99%)	198 (90%)	21 (10%)	2 (1%)	17	56
53	F	258/260 (99%)	236 (92%)	20 (8%)	2 (1%)	19	58
53	s4	258/260 (99%)	233 (90%)	24 (9%)	1 (0%)	34	72
54	G	204/206 (99%)	179 (88%)	22 (11%)	3 (2%)	10	45
54	s5	204/206 (99%)	183 (90%)	21 (10%)	0	100	100
55	H	224/226 (99%)	207 (92%)	13 (6%)	4 (2%)	8	41
55	s6	216/226 (96%)	200 (93%)	14 (6%)	2 (1%)	17	56
56	I	182/186 (98%)	160 (88%)	17 (9%)	5 (3%)	5	33
56	s7	184/186 (99%)	162 (88%)	19 (10%)	3 (2%)	9	43
57	J	184/199 (92%)	160 (87%)	23 (12%)	1 (0%)	29	68
57	s8	184/199 (92%)	167 (91%)	15 (8%)	2 (1%)	14	52
58	K	183/185 (99%)	162 (88%)	19 (10%)	2 (1%)	14	52
58	s9	183/185 (99%)	172 (94%)	11 (6%)	0	100	100
59	L	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	7	38
59	c0	92/105 (88%)	63 (68%)	20 (22%)	9 (10%)	0	7
60	M	153/155 (99%)	138 (90%)	12 (8%)	3 (2%)	7	39
60	c1	144/155 (93%)	133 (92%)	10 (7%)	1 (1%)	22	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	N	122/124 (98%)	86 (70%)	30 (25%)	6 (5%)	2	19
61	c2	122/124 (98%)	91 (75%)	28 (23%)	3 (2%)	5	34
62	O	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	22	61
62	c3	148/150 (99%)	132 (89%)	15 (10%)	1 (1%)	22	61
63	P	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	19	58
63	c4	126/128 (98%)	114 (90%)	12 (10%)	0	100	100
64	Q	122/141 (86%)	107 (88%)	13 (11%)	2 (2%)	9	43
64	c5	133/141 (94%)	107 (80%)	24 (18%)	2 (2%)	10	45
65	R	139/142 (98%)	122 (88%)	14 (10%)	3 (2%)	6	37
65	c6	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
66	S	116/125 (93%)	99 (85%)	13 (11%)	4 (3%)	3	28
67	T	143/145 (99%)	127 (89%)	13 (9%)	3 (2%)	7	38
67	c8	143/145 (99%)	121 (85%)	18 (13%)	4 (3%)	5	32
68	U	141/143 (99%)	129 (92%)	12 (8%)	0	100	100
68	c9	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	22	61
69	V	105/110 (96%)	93 (89%)	12 (11%)	0	100	100
69	d0	108/110 (98%)	92 (85%)	14 (13%)	2 (2%)	8	40
70	W	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	13	50
70	d1	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
71	X	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	58
71	d2	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	58
72	Y	142/144 (99%)	119 (84%)	21 (15%)	2 (1%)	11	46
72	d3	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
73	Z	132/134 (98%)	121 (92%)	9 (7%)	2 (2%)	10	45
73	d4	132/134 (98%)	119 (90%)	10 (8%)	3 (2%)	6	36
74	a	68/70 (97%)	56 (82%)	10 (15%)	2 (3%)	4	31
74	d5	67/70 (96%)	59 (88%)	8 (12%)	0	100	100
75	b	95/97 (98%)	68 (72%)	24 (25%)	3 (3%)	4	29
75	d6	95/97 (98%)	76 (80%)	19 (20%)	0	100	100
76	c	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	12	48
76	d7	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	d	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
77	d8	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
78	d9	51/53 (96%)	46 (90%)	4 (8%)	1 (2%)	7	39
78	e	51/53 (96%)	45 (88%)	6 (12%)	0	100	100
79	e0	60/62 (97%)	50 (83%)	8 (13%)	2 (3%)	4	28
79	f	58/62 (94%)	50 (86%)	7 (12%)	1 (2%)	9	42
80	g	69/71 (97%)	44 (64%)	19 (28%)	6 (9%)	1	9
81	h	316/318 (99%)	292 (92%)	23 (7%)	1 (0%)	41	75
81	sR	316/318 (99%)	292 (92%)	24 (8%)	0	100	100
82	c7	113/121 (93%)	102 (90%)	8 (7%)	3 (3%)	5	33
83	e1	49/51 (96%)	40 (82%)	9 (18%)	0	100	100
All	All	22260/22868 (97%)	20206 (91%)	1851 (8%)	203 (1%)	17	56

5 of 203 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	193/194 (100%)	165 (86%)	28 (14%)	3	18
4	j	193/194 (100%)	174 (90%)	19 (10%)	8	33
5	CE	319/322 (99%)	273 (86%)	46 (14%)	3	18
5	k	319/322 (99%)	268 (84%)	51 (16%)	2	14
6	CF	288/288 (100%)	255 (88%)	33 (12%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	l	288/288 (100%)	254 (88%)	34 (12%)	5	25
7	CG	244/244 (100%)	209 (86%)	35 (14%)	3	19
7	m	244/244 (100%)	216 (88%)	28 (12%)	5	26
8	CH	134/152 (88%)	119 (89%)	15 (11%)	6	27
8	n	134/152 (88%)	120 (90%)	14 (10%)	7	31
9	CI	186/186 (100%)	171 (92%)	15 (8%)	11	41
9	o	186/186 (100%)	164 (88%)	22 (12%)	5	25
10	CJ	187/191 (98%)	170 (91%)	17 (9%)	9	36
10	p	187/191 (98%)	170 (91%)	17 (9%)	9	36
11	CK	171/171 (100%)	139 (81%)	32 (19%)	1	8
11	q	171/171 (100%)	150 (88%)	21 (12%)	4	23
12	CL	177/186 (95%)	154 (87%)	23 (13%)	4	21
12	r	177/186 (95%)	152 (86%)	25 (14%)	3	19
13	CM	147/147 (100%)	124 (84%)	23 (16%)	2	16
13	s	147/147 (100%)	131 (89%)	16 (11%)	6	29
14	CN	154/154 (100%)	134 (87%)	20 (13%)	4	21
14	t	154/154 (100%)	140 (91%)	14 (9%)	9	36
15	CO	107/107 (100%)	88 (82%)	19 (18%)	2	10
15	u	107/107 (100%)	96 (90%)	11 (10%)	7	32
16	CP	175/175 (100%)	155 (89%)	20 (11%)	5	26
16	v	175/175 (100%)	154 (88%)	21 (12%)	5	24
17	CQ	160/160 (100%)	138 (86%)	22 (14%)	3	20
17	w	160/160 (100%)	137 (86%)	23 (14%)	3	18
18	CR	140/145 (97%)	115 (82%)	25 (18%)	2	9
18	x	140/145 (97%)	117 (84%)	23 (16%)	2	13
19	CS	150/150 (100%)	141 (94%)	9 (6%)	19	52
19	y	150/150 (100%)	134 (89%)	16 (11%)	6	30
20	CT	153/153 (100%)	131 (86%)	22 (14%)	3	18
20	z	153/153 (100%)	140 (92%)	13 (8%)	10	39
21	0	156/156 (100%)	137 (88%)	19 (12%)	5	23
21	CU	156/156 (100%)	133 (85%)	23 (15%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	2	136/136 (100%)	113 (83%)	23 (17%)	2	12
22	CV	136/136 (100%)	116 (85%)	20 (15%)	3	18
23	5	87/87 (100%)	77 (88%)	10 (12%)	5	26
23	CW	87/87 (100%)	75 (86%)	12 (14%)	3	20
24	CX	104/104 (100%)	94 (90%)	10 (10%)	8	34
24	l2	104/104 (100%)	91 (88%)	13 (12%)	4	23
26	7	57/86 (66%)	52 (91%)	5 (9%)	10	38
26	CY	57/86 (66%)	53 (93%)	4 (7%)	15	46
27	8	104/105 (99%)	87 (84%)	17 (16%)	2	13
27	CZ	104/105 (99%)	92 (88%)	12 (12%)	5	26
28	9	109/109 (100%)	99 (91%)	10 (9%)	9	36
28	DA	109/109 (100%)	98 (90%)	11 (10%)	7	32
29	AA	115/115 (100%)	104 (90%)	11 (10%)	8	34
29	DB	115/115 (100%)	105 (91%)	10 (9%)	10	38
30	AB	118/118 (100%)	106 (90%)	12 (10%)	7	32
30	DC	118/118 (100%)	107 (91%)	11 (9%)	9	35
31	AC	46/46 (100%)	41 (89%)	5 (11%)	6	29
31	DD	46/46 (100%)	39 (85%)	7 (15%)	3	17
32	AD	81/81 (100%)	70 (86%)	11 (14%)	3	20
32	DE	81/81 (100%)	75 (93%)	6 (7%)	13	44
33	AE	92/96 (96%)	81 (88%)	11 (12%)	5	24
33	DF	92/96 (96%)	74 (80%)	18 (20%)	1	7
34	AF	109/109 (100%)	95 (87%)	14 (13%)	4	22
34	DG	109/109 (100%)	93 (85%)	16 (15%)	3	18
35	AG	90/90 (100%)	83 (92%)	7 (8%)	12	42
35	DH	90/90 (100%)	83 (92%)	7 (8%)	12	42
36	AH	95/95 (100%)	85 (90%)	10 (10%)	7	31
36	DI	95/95 (100%)	82 (86%)	13 (14%)	3	20
37	AI	104/104 (100%)	90 (86%)	14 (14%)	4	21
37	DJ	104/104 (100%)	87 (84%)	17 (16%)	2	13
38	AJ	81/81 (100%)	69 (85%)	12 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DK	81/81 (100%)	67 (83%)	14 (17%)	2	11
39	AK	70/70 (100%)	63 (90%)	7 (10%)	7	32
39	DL	70/70 (100%)	61 (87%)	9 (13%)	4	22
40	AL	68/68 (100%)	58 (85%)	10 (15%)	3	18
40	DM	68/68 (100%)	60 (88%)	8 (12%)	5	25
41	AM	45/45 (100%)	40 (89%)	5 (11%)	6	28
41	DN	45/45 (100%)	42 (93%)	3 (7%)	16	48
42	AN	47/47 (100%)	42 (89%)	5 (11%)	6	30
42	DO	47/47 (100%)	43 (92%)	4 (8%)	10	39
43	AO	23/23 (100%)	16 (70%)	7 (30%)	0	2
43	DP	23/23 (100%)	19 (83%)	4 (17%)	2	11
44	AP	90/90 (100%)	75 (83%)	15 (17%)	2	12
44	DQ	90/90 (100%)	78 (87%)	12 (13%)	4	21
45	AQ	71/71 (100%)	62 (87%)	9 (13%)	4	22
45	DR	71/71 (100%)	60 (84%)	11 (16%)	2	16
46	i	97/137 (71%)	85 (88%)	12 (12%)	4	23
47	p0	105/186 (56%)	89 (85%)	16 (15%)	3	17
48	sM	54/54 (100%)	47 (87%)	7 (13%)	4	21
49	B	164/173 (95%)	148 (90%)	16 (10%)	8	33
49	s0	165/173 (95%)	144 (87%)	21 (13%)	4	22
50	C	191/192 (100%)	167 (87%)	24 (13%)	4	22
50	s1	192/192 (100%)	166 (86%)	26 (14%)	4	21
51	D	176/176 (100%)	151 (86%)	25 (14%)	3	19
51	s2	176/176 (100%)	146 (83%)	30 (17%)	2	12
52	E	182/182 (100%)	160 (88%)	22 (12%)	5	24
52	s3	182/182 (100%)	167 (92%)	15 (8%)	11	40
53	F	221/221 (100%)	195 (88%)	26 (12%)	5	25
53	s4	221/221 (100%)	196 (89%)	25 (11%)	6	27
54	G	173/173 (100%)	158 (91%)	15 (9%)	10	38
54	s5	173/173 (100%)	158 (91%)	15 (9%)	10	38
55	H	188/193 (97%)	171 (91%)	17 (9%)	9	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	s6	187/193 (97%)	163 (87%)	24 (13%)	4	22
56	I	165/166 (99%)	146 (88%)	19 (12%)	5	26
56	s7	165/166 (99%)	155 (94%)	10 (6%)	18	51
57	J	150/160 (94%)	132 (88%)	18 (12%)	5	24
57	s8	150/160 (94%)	135 (90%)	15 (10%)	7	32
58	K	158/158 (100%)	132 (84%)	26 (16%)	2	13
58	s9	158/158 (100%)	138 (87%)	20 (13%)	4	22
59	L	77/98 (79%)	71 (92%)	6 (8%)	12	42
59	c0	73/98 (74%)	69 (94%)	4 (6%)	21	54
60	M	129/136 (95%)	120 (93%)	9 (7%)	15	46
60	c1	129/136 (95%)	111 (86%)	18 (14%)	3	19
61	N	88/100 (88%)	72 (82%)	16 (18%)	1	9
61	c2	88/100 (88%)	72 (82%)	16 (18%)	1	9
62	O	127/127 (100%)	114 (90%)	13 (10%)	7	32
62	c3	127/127 (100%)	113 (89%)	14 (11%)	6	29
63	P	81/97 (84%)	67 (83%)	14 (17%)	2	11
63	c4	97/97 (100%)	86 (89%)	11 (11%)	6	27
64	Q	101/117 (86%)	93 (92%)	8 (8%)	12	41
64	c5	103/117 (88%)	92 (89%)	11 (11%)	6	30
65	R	117/118 (99%)	102 (87%)	15 (13%)	4	22
65	c6	118/118 (100%)	100 (85%)	18 (15%)	2	17
66	S	94/113 (83%)	84 (89%)	10 (11%)	6	30
67	T	128/128 (100%)	113 (88%)	15 (12%)	5	26
67	c8	128/128 (100%)	117 (91%)	11 (9%)	10	38
68	U	115/115 (100%)	96 (84%)	19 (16%)	2	13
68	c9	115/115 (100%)	106 (92%)	9 (8%)	12	42
69	V	100/103 (97%)	89 (89%)	11 (11%)	6	29
69	d0	103/103 (100%)	94 (91%)	9 (9%)	10	38
70	W	74/74 (100%)	64 (86%)	10 (14%)	4	21
70	d1	74/74 (100%)	66 (89%)	8 (11%)	6	30
71	X	110/110 (100%)	96 (87%)	14 (13%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	d2	110/110 (100%)	100 (91%)	10 (9%)	9	36
72	Y	119/119 (100%)	102 (86%)	17 (14%)	3	19
72	d3	119/119 (100%)	107 (90%)	12 (10%)	7	32
73	Z	112/112 (100%)	106 (95%)	6 (5%)	22	55
73	d4	112/112 (100%)	102 (91%)	10 (9%)	9	37
74	a	61/61 (100%)	50 (82%)	11 (18%)	1	9
74	d5	61/61 (100%)	57 (93%)	4 (7%)	16	49
75	b	83/83 (100%)	69 (83%)	14 (17%)	2	12
75	d6	83/83 (100%)	73 (88%)	10 (12%)	5	24
76	c	70/70 (100%)	66 (94%)	4 (6%)	20	53
76	d7	70/70 (100%)	63 (90%)	7 (10%)	7	32
77	d	56/56 (100%)	50 (89%)	6 (11%)	6	30
77	d8	56/56 (100%)	49 (88%)	7 (12%)	4	23
78	d9	47/47 (100%)	40 (85%)	7 (15%)	3	17
78	e	47/47 (100%)	42 (89%)	5 (11%)	6	30
79	e0	53/53 (100%)	40 (76%)	13 (24%)	0	4
79	f	51/53 (96%)	45 (88%)	6 (12%)	5	25
80	g	62/62 (100%)	55 (89%)	7 (11%)	6	27
81	h	259/261 (99%)	234 (90%)	25 (10%)	8	33
81	sR	260/261 (100%)	242 (93%)	18 (7%)	15	47
82	c7	92/110 (84%)	80 (87%)	12 (13%)	4	21
83	e1	43/43 (100%)	34 (79%)	9 (21%)	1	6
All	All	18681/19177 (97%)	16432 (88%)	2249 (12%)	5	24

5 of 2249 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	CS	41	ASP
39	DL	17	THR
65	c6	28	LEU
21	CU	51	VAL
29	DB	92	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
20	CT	92	GLN
37	DJ	59	ASN
67	c8	25	ASN
29	DB	36	HIS
41	DN	33	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3396 (92%)	563 (17%)	51 (1%)
1	AR	3145/3396 (92%)	581 (18%)	51 (1%)
2	3	120/121 (99%)	16 (13%)	0
2	AS	120/121 (99%)	15 (12%)	2 (1%)
25	6	1780/1800 (98%)	383 (21%)	30 (1%)
25	A	1778/1800 (98%)	409 (23%)	47 (2%)
3	4	157/158 (99%)	32 (20%)	2 (1%)
3	AT	157/158 (99%)	28 (17%)	3 (1%)
All	All	10402/10950 (94%)	2027 (19%)	186 (1%)

5 of 2027 RNA backbone outliers are listed below:

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

5 of 186 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AR	588	G
1	AR	1481	A
25	A	1196	A
1	AR	715	A
1	AR	1103	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 2494 ligands modelled in this entry, 1422 are monoatomic - leaving 1072 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
84	OHX	AR	3702	-	0,6,6	0.00	-	-		
84	OHX	AR	3408	-	0,6,6	0.00	-	-		
84	OHX	AR	3685	-	0,6,6	0.00	-	-		
84	OHX	DL	101	-	0,6,6	0.00	-	-		
84	OHX	1	3482	-	0,6,6	0.00	-	-		
84	OHX	AR	3611	-	0,6,6	0.00	-	-		
84	OHX	AR	3537	-	0,6,6	0.00	-	-		
84	OHX	1	3535	-	0,6,6	0.00	-	-		
84	OHX	AR	3466	-	0,6,6	0.00	-	-		
84	OHX	AR	3413	-	0,6,6	0.00	-	-		
84	OHX	6	2051	-	0,6,6	0.00	-	-		
84	OHX	1	401	-	0,6,6	0.00	-	-		
84	OHX	AR	3637	-	0,6,6	0.00	-	-		
84	OHX	AR	3528	-	0,6,6	0.00	-	-		
84	OHX	1	3548	-	0,6,6	0.00	-	-		
84	OHX	AR	3687	-	0,6,6	0.00	-	-		
84	OHX	AR	3429	-	0,6,6	0.00	-	-		
84	OHX	1	3603	-	0,6,6	0.00	-	-		
84	OHX	1	3652	-	0,6,6	0.00	-	-		
84	OHX	DL	102	-	0,6,6	0.00	-	-		
84	OHX	1	3614	-	0,6,6	0.00	-	-		
84	OHX	AR	3710	-	0,6,6	0.00	-	-		
84	OHX	1	3714	-	0,6,6	0.00	-	-		
84	OHX	1	3672	-	0,6,6	0.00	-	-		
84	OHX	AR	3646	-	0,6,6	0.00	-	-		
84	OHX	1	3615	-	0,6,6	0.00	-	-		
84	OHX	6	1930	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3521	-	0,6,6	0.00	-	-		
84	OHX	1	3703	-	0,6,6	0.00	-	-		
84	OHX	6	2038	-	0,6,6	0.00	-	-		
84	OHX	6	1995	-	0,6,6	0.00	-	-		
84	OHX	6	2016	-	0,6,6	0.00	-	-		
84	OHX	1	3558	-	0,6,6	0.00	-	-		
84	OHX	c5	201	-	0,6,6	0.00	-	-		
84	OHX	CF	401	-	0,6,6	0.00	-	-		
84	OHX	6	1961	-	0,6,6	0.00	-	-		
84	OHX	AR	3639	-	0,6,6	0.00	-	-		
84	OHX	1	3712	-	0,6,6	0.00	-	-		
84	OHX	6	1910	-	0,6,6	0.00	-	-		
84	OHX	1	3497	-	0,6,6	0.00	-	-		
84	OHX	AS	208	-	0,6,6	0.00	-	-		
84	OHX	6	1950	-	0,6,6	0.00	-	-		
84	OHX	AR	3437	-	0,6,6	0.00	-	-		
84	OHX	6	1944	-	0,6,6	0.00	-	-		
84	OHX	1	3578	-	0,6,6	0.00	-	-		
84	OHX	6	2027	-	0,6,6	0.00	-	-		
84	OHX	AC	101	-	0,6,6	0.00	-	-		
84	OHX	AR	3730	-	0,6,6	0.00	-	-		
84	OHX	6	1957	-	0,6,6	0.00	-	-		
84	OHX	A	1995	-	0,6,6	0.00	-	-		
84	OHX	1	3528	-	0,6,6	0.00	-	-		
84	OHX	1	3527	-	0,6,6	0.00	-	-		
84	OHX	AR	3477	-	0,6,6	0.00	-	-		
84	OHX	1	3666	-	0,6,6	0.00	-	-		
84	OHX	A	2026	-	0,6,6	0.00	-	-		
84	OHX	6	1904	-	0,6,6	0.00	-	-		
84	OHX	AR	3434	-	0,6,6	0.00	-	-		
84	OHX	6	2007	-	0,6,6	0.00	-	-		
84	OHX	AR	3713	-	0,6,6	0.00	-	-		
84	OHX	1	3487	-	0,6,6	0.00	-	-		
84	OHX	1	3488	-	0,6,6	0.00	-	-		
84	OHX	1	3702	-	0,6,6	0.00	-	-		
84	OHX	6	2011	-	0,6,6	0.00	-	-		
84	OHX	AR	3487	-	0,6,6	0.00	-	-		
84	OHX	A	1946	-	0,6,6	0.00	-	-		
84	OHX	AR	3479	-	0,6,6	0.00	-	-		
84	OHX	AR	3435	-	0,6,6	0.00	-	-		
84	OHX	AR	3728	-	0,6,6	0.00	-	-		
84	OHX	1	3684	-	0,6,6	0.00	-	-		
84	OHX	6	2025	-	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	3600	-	0,6,6	0.00	-	-		
84	OHX	1	3547	-	0,6,6	0.00	-	-		
84	OHX	AR	3682	-	0,6,6	0.00	-	-		
84	OHX	1	3625	-	0,6,6	0.00	-	-		
84	OHX	AR	3485	-	0,6,6	0.00	-	-		
84	OHX	1	3480	-	0,6,6	0.00	-	-		
84	OHX	AR	3416	-	0,6,6	0.00	-	-		
84	OHX	AR	3462	-	0,6,6	0.00	-	-		
84	OHX	1	3402	-	0,6,6	0.00	-	-		
84	OHX	AS	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3624	-	0,6,6	0.00	-	-		
84	OHX	AR	3539	-	0,6,6	0.00	-	-		
84	OHX	AR	3653	-	0,6,6	0.00	-	-		
84	OHX	AR	3670	-	0,6,6	0.00	-	-		
84	OHX	A	2034	-	0,6,6	0.00	-	-		
84	OHX	AR	3704	-	0,6,6	0.00	-	-		
84	OHX	1	3457	-	0,6,6	0.00	-	-		
84	OHX	AR	3560	-	0,6,6	0.00	-	-		
84	OHX	AR	3631	-	0,6,6	0.00	-	-		
84	OHX	AR	3450	-	0,6,6	0.00	-	-		
84	OHX	A	1955	-	0,6,6	0.00	-	-		
84	OHX	M	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3706	-	0,6,6	0.00	-	-		
84	OHX	AR	3549	-	0,6,6	0.00	-	-		
84	OHX	AR	3469	-	0,6,6	0.00	-	-		
84	OHX	1	3446	-	0,6,6	0.00	-	-		
84	OHX	1	3572	-	0,6,6	0.00	-	-		
84	OHX	AT	215	-	0,6,6	0.00	-	-		
84	OHX	1	3554	-	0,6,6	0.00	-	-		
84	OHX	AR	3499	-	0,6,6	0.00	-	-		
84	OHX	A	1920	-	0,6,6	0.00	-	-		
84	OHX	A	2040	-	0,6,6	0.00	-	-		
84	OHX	1	3467	-	0,6,6	0.00	-	-		
84	OHX	6	1937	-	0,6,6	0.00	-	-		
84	OHX	A	1975	-	0,6,6	0.00	-	-		
84	OHX	AR	3558	-	0,6,6	0.00	-	-		
84	OHX	A	1970	-	0,6,6	0.00	-	-		
84	OHX	1	3604	-	0,6,6	0.00	-	-		
84	OHX	AR	3737	-	0,6,6	0.00	-	-		
84	OHX	1	3642	-	0,6,6	0.00	-	-		
84	OHX	AT	205	-	0,6,6	0.00	-	-		
84	OHX	1	3522	-	0,6,6	0.00	-	-		
84	OHX	AR	3649	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3529	-	0,6,6	0.00	-	-		
84	OHX	1	3626	-	0,6,6	0.00	-	-		
84	OHX	A	1988	-	0,6,6	0.00	-	-		
84	OHX	1	3601	-	0,6,6	0.00	-	-		
84	OHX	1	3571	-	0,6,6	0.00	-	-		
84	OHX	6	1964	-	0,6,6	0.00	-	-		
84	OHX	1	3574	-	0,6,6	0.00	-	-		
84	OHX	A	2020	-	0,6,6	0.00	-	-		
84	OHX	AT	203	-	0,6,6	0.00	-	-		
84	OHX	AR	3660	-	0,6,6	0.00	-	-		
84	OHX	1	3664	-	0,6,6	0.00	-	-		
84	OHX	1	3647	-	0,6,6	0.00	-	-		
84	OHX	A	1928	-	0,6,6	0.00	-	-		
84	OHX	1	3585	-	0,6,6	0.00	-	-		
84	OHX	1	3650	-	0,6,6	0.00	-	-		
84	OHX	1	3411	-	0,6,6	0.00	-	-		
84	OHX	1	3673	-	0,6,6	0.00	-	-		
84	OHX	AR	3474	-	0,6,6	0.00	-	-		
84	OHX	AR	3563	-	0,6,6	0.00	-	-		
84	OHX	T	201	-	0,6,6	0.00	-	-		
84	OHX	1	3424	-	0,6,6	0.00	-	-		
84	OHX	6	1973	-	0,6,6	0.00	-	-		
84	OHX	A	1957	-	0,6,6	0.00	-	-		
84	OHX	1	3425	-	0,6,6	0.00	-	-		
84	OHX	AR	3508	-	0,6,6	0.00	-	-		
84	OHX	6	1963	-	0,6,6	0.00	-	-		
84	OHX	1	3671	-	0,6,6	0.00	-	-		
84	OHX	AR	3684	-	0,6,6	0.00	-	-		
84	OHX	AR	3448	-	0,6,6	0.00	-	-		
84	OHX	6	1915	-	0,6,6	0.00	-	-		
84	OHX	1	3567	-	0,6,6	0.00	-	-		
84	OHX	AR	3410	-	0,6,6	0.00	-	-		
84	OHX	A	2004	-	0,6,6	0.00	-	-		
84	OHX	1	3416	-	0,6,6	0.00	-	-		
84	OHX	AR	3714	-	0,6,6	0.00	-	-		
84	OHX	AR	3476	-	0,6,6	0.00	-	-		
84	OHX	6	1905	-	0,6,6	0.00	-	-		
84	OHX	AR	3614	-	0,6,6	0.00	-	-		
84	OHX	6	2041	-	0,6,6	0.00	-	-		
84	OHX	6	1997	-	0,6,6	0.00	-	-		
84	OHX	6	2032	-	0,6,6	0.00	-	-		
84	OHX	AR	3663	-	0,6,6	0.00	-	-		
84	OHX	1	3711	-	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	3657	-	0,6,6	0.00	-	-		
84	OHX	AR	3596	-	0,6,6	0.00	-	-		
84	OHX	A	1942	-	0,6,6	0.00	-	-		
84	OHX	AR	3406	-	0,6,6	0.00	-	-		
84	OHX	A	1978	-	0,6,6	0.00	-	-		
84	OHX	6	1983	-	0,6,6	0.00	-	-		
84	OHX	3	207	-	0,6,6	0.00	-	-		
84	OHX	AR	3590	-	0,6,6	0.00	-	-		
84	OHX	AR	3575	-	0,6,6	0.00	-	-		
84	OHX	1	3654	-	0,6,6	0.00	-	-		
84	OHX	AR	3612	-	0,6,6	0.00	-	-		
84	OHX	AR	3446	-	0,6,6	0.00	-	-		
84	OHX	6	1951	-	0,6,6	0.00	-	-		
84	OHX	1	3686	-	0,6,6	0.00	-	-		
84	OHX	1	3510	-	0,6,6	0.00	-	-		
84	OHX	6	1987	-	0,6,6	0.00	-	-		
84	OHX	1	3499	-	0,6,6	0.00	-	-		
84	OHX	1	3409	-	0,6,6	0.00	-	-		
84	OHX	6	1903	-	0,6,6	0.00	-	-		
84	OHX	A	1997	-	0,6,6	0.00	-	-		
84	OHX	AG	201	-	0,6,6	0.00	-	-		
84	OHX	1	3401	-	0,6,6	0.00	-	-		
84	OHX	1	3483	-	0,6,6	0.00	-	-		
84	OHX	1	3486	-	0,6,6	0.00	-	-		
84	OHX	A	1971	-	0,6,6	0.00	-	-		
84	OHX	1	3660	-	0,6,6	0.00	-	-		
84	OHX	1	3517	-	0,6,6	0.00	-	-		
84	OHX	1	3731	-	0,6,6	0.00	-	-		
84	OHX	1	3530	-	0,6,6	0.00	-	-		
84	OHX	CE	402	-	0,6,6	0.00	-	-		
84	OHX	AK	103	-	0,6,6	0.00	-	-		
84	OHX	s8	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3421	-	0,6,6	0.00	-	-		
86	7MB	1	4216	-	16,23,23	1.32	3 (18%)	8,38,38	1.59	2 (25%)
84	OHX	AR	3676	-	0,6,6	0.00	-	-		
84	OHX	AR	3570	-	0,6,6	0.00	-	-		
84	OHX	AR	3452	-	0,6,6	0.00	-	-		
84	OHX	AR	3678	-	0,6,6	0.00	-	-		
84	OHX	1	3560	-	0,6,6	0.00	-	-		
84	OHX	6	1913	-	0,6,6	0.00	-	-		
84	OHX	AR	3587	-	0,6,6	0.00	-	-		
84	OHX	sR	401	-	0,6,6	0.00	-	-		
84	OHX	AR	3651	-	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	3576	-	0,6,6	0.00	-	-		
84	OHX	1	3687	-	0,6,6	0.00	-	-		
84	OHX	6	1984	-	0,6,6	0.00	-	-		
84	OHX	1	3419	-	0,6,6	0.00	-	-		
84	OHX	AR	3541	-	0,6,6	0.00	-	-		
84	OHX	AR	3504	-	0,6,6	0.00	-	-		
84	OHX	AR	3724	-	0,6,6	0.00	-	-		
84	OHX	6	1958	-	0,6,6	0.00	-	-		
84	OHX	1	3462	-	0,6,6	0.00	-	-		
84	OHX	AT	217	-	0,6,6	0.00	-	-		
84	OHX	AR	3426	-	0,6,6	0.00	-	-		
84	OHX	AR	3668	-	0,6,6	0.00	-	-		
84	OHX	6	1901	-	0,6,6	0.00	-	-		
84	OHX	6	1922	-	0,6,6	0.00	-	-		
84	OHX	AS	210	-	0,6,6	0.00	-	-		
84	OHX	1	3533	-	0,6,6	0.00	-	-		
84	OHX	AR	3534	-	0,6,6	0.00	-	-		
84	OHX	AR	3735	-	0,6,6	0.00	-	-		
84	OHX	1	3591	-	0,6,6	0.00	-	-		
84	OHX	A	1994	-	0,6,6	0.00	-	-		
84	OHX	6	1999	-	0,6,6	0.00	-	-		
84	OHX	AR	3689	-	0,6,6	0.00	-	-		
84	OHX	A	2024	-	0,6,6	0.00	-	-		
84	OHX	6	2055	-	0,6,6	0.00	-	-		
84	OHX	AR	3415	-	0,6,6	0.00	-	-		
84	OHX	1	3519	-	0,6,6	0.00	-	-		
84	OHX	4	205	-	0,6,6	0.00	-	-		
84	OHX	e	101	-	0,6,6	0.00	-	-		
84	OHX	1	3636	-	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	AR	3632	-	0,6,6	0.00	-	-		
84	OHX	A	1979	-	0,6,6	0.00	-	-		
84	OHX	AR	3420	-	0,6,6	0.00	-	-		
84	OHX	1	3644	-	0,6,6	0.00	-	-		
84	OHX	AR	3527	-	0,6,6	0.00	-	-		
84	OHX	AR	3697	-	0,6,6	0.00	-	-		
84	OHX	AR	3522	-	0,6,6	0.00	-	-		
84	OHX	1	3515	-	0,6,6	0.00	-	-		
84	OHX	AR	3692	-	0,6,6	0.00	-	-		
84	OHX	6	1902	-	0,6,6	0.00	-	-		
84	OHX	AR	3559	-	0,6,6	0.00	-	-		
84	OHX	AR	3732	-	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	3713	-	0,6,6	0.00	-	-		
84	OHX	AS	203	-	0,6,6	0.00	-	-		
84	OHX	1	3495	-	0,6,6	0.00	-	-		
84	OHX	AR	3664	-	0,6,6	0.00	-	-		
84	OHX	6	1931	-	0,6,6	0.00	-	-		
84	OHX	AR	3640	-	0,6,6	0.00	-	-		
84	OHX	AR	3584	-	0,6,6	0.00	-	-		
84	OHX	6	1918	-	0,6,6	0.00	-	-		
84	OHX	A	2001	-	0,6,6	0.00	-	-		
84	OHX	AR	3652	-	0,6,6	0.00	-	-		
84	OHX	6	1932	-	0,6,6	0.00	-	-		
84	OHX	AR	3638	-	0,6,6	0.00	-	-		
84	OHX	6	1911	-	0,6,6	0.00	-	-		
84	OHX	AR	3525	-	0,6,6	0.00	-	-		
84	OHX	6	2056	-	0,6,6	0.00	-	-		
84	OHX	6	2010	-	0,6,6	0.00	-	-		
84	OHX	AR	3551	-	0,6,6	0.00	-	-		
84	OHX	1	3454	-	0,6,6	0.00	-	-		
84	OHX	AR	3588	-	0,6,6	0.00	-	-		
84	OHX	A	1906	-	0,6,6	0.00	-	-		
84	OHX	AR	3442	-	0,6,6	0.00	-	-		
84	OHX	1	3447	-	0,6,6	0.00	-	-		
84	OHX	A	1935	-	0,6,6	0.00	-	-		
84	OHX	1	3468	-	0,6,6	0.00	-	-		
84	OHX	6	1912	-	0,6,6	0.00	-	-		
84	OHX	AR	3501	-	0,6,6	0.00	-	-		
84	OHX	AR	3471	-	0,6,6	0.00	-	-		
84	OHX	1	3452	-	0,6,6	0.00	-	-		
84	OHX	AR	3531	-	0,6,6	0.00	-	-		
84	OHX	AR	3454	-	0,6,6	0.00	-	-		
84	OHX	AR	3720	-	0,6,6	0.00	-	-		
84	OHX	AR	3567	-	0,6,6	0.00	-	-		
84	OHX	AR	3443	-	0,6,6	0.00	-	-		
84	OHX	1	3605	-	0,6,6	0.00	-	-		
84	OHX	A	2009	-	0,6,6	0.00	-	-		
84	OHX	AR	3592	-	0,6,6	0.00	-	-		
84	OHX	A	2038	-	0,6,6	0.00	-	-		
84	OHX	1	3418	-	0,6,6	0.00	-	-		
84	OHX	1	3417	-	0,6,6	0.00	-	-		
84	OHX	AR	3561	-	0,6,6	0.00	-	-		
84	OHX	1	3523	-	0,6,6	0.00	-	-		
84	OHX	1	3427	-	0,6,6	0.00	-	-		
84	OHX	A	1934	-	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	3546	-	0,6,6	0.00	-	-		
84	OHX	1	3624	-	0,6,6	0.00	-	-		
84	OHX	AR	3461	-	0,6,6	0.00	-	-		
84	OHX	DI	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3494	-	0,6,6	0.00	-	-		
84	OHX	AR	3679	-	0,6,6	0.00	-	-		
84	OHX	AR	3498	-	0,6,6	0.00	-	-		
84	OHX	1	3720	-	0,6,6	0.00	-	-		
84	OHX	DH	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3708	-	0,6,6	0.00	-	-		
84	OHX	1	3503	-	0,6,6	0.00	-	-		
84	OHX	1	3432	-	0,6,6	0.00	-	-		
84	OHX	AR	3553	-	0,6,6	0.00	-	-		
84	OHX	1	3496	-	0,6,6	0.00	-	-		
84	OHX	6	1946	-	0,6,6	0.00	-	-		
84	OHX	1	3555	-	0,6,6	0.00	-	-		
84	OHX	A	2011	-	0,6,6	0.00	-	-		
84	OHX	AR	3492	-	0,6,6	0.00	-	-		
84	OHX	AS	205	-	0,6,6	0.00	-	-		
84	OHX	AR	3717	-	0,6,6	0.00	-	-		
84	OHX	AR	3569	-	0,6,6	0.00	-	-		
84	OHX	1	3700	-	0,6,6	0.00	-	-		
84	OHX	6	1955	-	0,6,6	0.00	-	-		
84	OHX	1	3436	-	0,6,6	0.00	-	-		
84	OHX	AR	3432	-	0,6,6	0.00	-	-		
84	OHX	AR	3573	-	0,6,6	0.00	-	-		
84	OHX	A	1908	-	0,6,6	0.00	-	-		
84	OHX	z	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3727	-	0,6,6	0.00	-	-		
84	OHX	AR	3602	-	0,6,6	0.00	-	-		
84	OHX	1	3707	-	0,6,6	0.00	-	-		
84	OHX	AS	207	-	0,6,6	0.00	-	-		
84	OHX	AR	3607	-	0,6,6	0.00	-	-		
84	OHX	1	3722	-	0,6,6	0.00	-	-		
84	OHX	A	2027	-	0,6,6	0.00	-	-		
84	OHX	h	401	-	0,6,6	0.00	-	-		
84	OHX	AR	3401	-	0,6,6	0.00	-	-		
84	OHX	AR	3536	-	0,6,6	0.00	-	-		
84	OHX	A	2006	-	0,6,6	0.00	-	-		
84	OHX	A	2003	-	0,6,6	0.00	-	-		
84	OHX	AR	3709	-	0,6,6	0.00	-	-		
84	OHX	AT	219	-	0,6,6	0.00	-	-		
84	OHX	1	3549	-	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	3414	-	0,6,6	0.00	-	-		
84	OHX	1	3456	-	0,6,6	0.00	-	-		
84	OHX	DG	201	-	0,6,6	0.00	-	-		
84	OHX	1	3428	-	0,6,6	0.00	-	-		
84	OHX	A	1931	-	0,6,6	0.00	-	-		
84	OHX	CF	402	-	0,6,6	0.00	-	-		
84	OHX	1	3504	-	0,6,6	0.00	-	-		
84	OHX	1	3656	-	0,6,6	0.00	-	-		
84	OHX	1	3435	-	0,6,6	0.00	-	-		
84	OHX	AR	3507	-	0,6,6	0.00	-	-		
84	OHX	6	1920	-	0,6,6	0.00	-	-		
84	OHX	1	3469	-	0,6,6	0.00	-	-		
84	OHX	AR	3409	-	0,6,6	0.00	-	-		
84	OHX	A	1985	-	0,6,6	0.00	-	-		
84	OHX	AR	3665	-	0,6,6	0.00	-	-		
84	OHX	A	2017	-	0,6,6	0.00	-	-		
84	OHX	A	1961	-	0,6,6	0.00	-	-		
84	OHX	AR	3419	-	0,6,6	0.00	-	-		
84	OHX	6	2046	-	0,6,6	0.00	-	-		
84	OHX	6	1996	-	0,6,6	0.00	-	-		
84	OHX	1	3716	-	0,6,6	0.00	-	-		
84	OHX	A	2035	-	0,6,6	0.00	-	-		
84	OHX	A	2019	-	0,6,6	0.00	-	-		
84	OHX	AR	3630	-	0,6,6	0.00	-	-		
84	OHX	1	3706	-	0,6,6	0.00	-	-		
84	OHX	1	3498	-	0,6,6	0.00	-	-		
84	OHX	AR	3423	-	0,6,6	0.00	-	-		
84	OHX	1	3680	-	0,6,6	0.00	-	-		
84	OHX	AR	3556	-	0,6,6	0.00	-	-		
84	OHX	6	2022	-	0,6,6	0.00	-	-		
84	OHX	AT	220	-	0,6,6	0.00	-	-		
84	OHX	6	2036	-	0,6,6	0.00	-	-		
84	OHX	1	3516	-	0,6,6	0.00	-	-		
84	OHX	6	1916	-	0,6,6	0.00	-	-		
84	OHX	1	3727	-	0,6,6	0.00	-	-		
84	OHX	A	1940	-	0,6,6	0.00	-	-		
84	OHX	6	1993	-	0,6,6	0.00	-	-		
84	OHX	1	3559	-	0,6,6	0.00	-	-		
84	OHX	A	1949	-	0,6,6	0.00	-	-		
84	OHX	AR	3655	-	0,6,6	0.00	-	-		
84	OHX	AP	502	-	0,6,6	0.00	-	-		
84	OHX	CM	201	-	0,6,6	0.00	-	-		
84	OHX	A	1956	-	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	3701	-	0,6,6	0.00	-	-		
84	OHX	1	3598	-	0,6,6	0.00	-	-		
84	OHX	AR	3407	-	0,6,6	0.00	-	-		
84	OHX	6	1938	-	0,6,6	0.00	-	-		
84	OHX	1	3492	-	0,6,6	0.00	-	-		
84	OHX	6	1945	-	0,6,6	0.00	-	-		
84	OHX	6	2052	-	0,6,6	0.00	-	-		
84	OHX	1	3550	-	0,6,6	0.00	-	-		
84	OHX	6	2057	-	0,6,6	0.00	-	-		
84	OHX	A	2037	-	0,6,6	0.00	-	-		
84	OHX	AR	3648	-	0,6,6	0.00	-	-		
84	OHX	6	2021	-	0,6,6	0.00	-	-		
84	OHX	6	1917	-	0,6,6	0.00	-	-		
84	OHX	AR	3585	-	0,6,6	0.00	-	-		
84	OHX	1	3406	-	0,6,6	0.00	-	-		
84	OHX	AK	102	-	0,6,6	0.00	-	-		
84	OHX	CV	201	-	0,6,6	0.00	-	-		
84	OHX	A	2042	-	0,6,6	0.00	-	-		
84	OHX	4	212	-	0,6,6	0.00	-	-		
84	OHX	1	3568	-	0,6,6	0.00	-	-		
84	OHX	6	2000	-	0,6,6	0.00	-	-		
84	OHX	1	3608	-	0,6,6	0.00	-	-		
84	OHX	1	3561	-	0,6,6	0.00	-	-		
84	OHX	1	3429	-	0,6,6	0.00	-	-		
84	OHX	AR	3669	-	0,6,6	0.00	-	-		
84	OHX	AR	3582	-	0,6,6	0.00	-	-		
84	OHX	1	3557	-	0,6,6	0.00	-	-		
84	OHX	4	210	-	0,6,6	0.00	-	-		
84	OHX	1	3670	-	0,6,6	0.00	-	-		
84	OHX	A	1918	-	0,6,6	0.00	-	-		
84	OHX	A	1937	-	0,6,6	0.00	-	-		
84	OHX	1	3443	-	0,6,6	0.00	-	-		
84	OHX	6	2048	-	0,6,6	0.00	-	-		
84	OHX	1	3524	-	0,6,6	0.00	-	-		
84	OHX	AT	212	-	0,6,6	0.00	-	-		
84	OHX	1	3677	-	0,6,6	0.00	-	-		
84	OHX	AR	3597	-	0,6,6	0.00	-	-		
84	OHX	AR	3688	-	0,6,6	0.00	-	-		
84	OHX	6	1977	-	0,6,6	0.00	-	-		
84	OHX	1	3501	-	0,6,6	0.00	-	-		
84	OHX	AR	3482	-	0,6,6	0.00	-	-		
84	OHX	1	3668	-	0,6,6	0.00	-	-		
84	OHX	AR	3491	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AT	214	-	0,6,6	0.00	-	-		
84	OHX	AR	3599	-	0,6,6	0.00	-	-		
84	OHX	6	2029	-	0,6,6	0.00	-	-		
84	OHX	A	2032	-	0,6,6	0.00	-	-		
84	OHX	AR	3643	-	0,6,6	0.00	-	-		
84	OHX	6	1976	-	0,6,6	0.00	-	-		
84	OHX	A	1998	-	0,6,6	0.00	-	-		
84	OHX	1	3577	-	0,6,6	0.00	-	-		
84	OHX	1	3514	-	0,6,6	0.00	-	-		
84	OHX	1	3531	-	0,6,6	0.00	-	-		
84	OHX	AR	3707	-	0,6,6	0.00	-	-		
84	OHX	AR	3591	-	0,6,6	0.00	-	-		
84	OHX	1	3701	-	0,6,6	0.00	-	-		
84	OHX	AS	209	-	0,6,6	0.00	-	-		
84	OHX	1	3470	-	0,6,6	0.00	-	-		
84	OHX	1	3573	-	0,6,6	0.00	-	-		
84	OHX	6	1988	-	0,6,6	0.00	-	-		
84	OHX	1	3415	-	0,6,6	0.00	-	-		
84	OHX	6	1940	-	0,6,6	0.00	-	-		
84	OHX	A	2016	-	0,6,6	0.00	-	-		
84	OHX	A	2008	-	0,6,6	0.00	-	-		
84	OHX	AR	3645	-	0,6,6	0.00	-	-		
84	OHX	AR	3731	-	0,6,6	0.00	-	-		
84	OHX	AR	3455	-	0,6,6	0.00	-	-		
84	OHX	1	3473	-	0,6,6	0.00	-	-		
84	OHX	1	3512	-	0,6,6	0.00	-	-		
84	OHX	AR	3616	-	0,6,6	0.00	-	-		
84	OHX	1	3607	-	0,6,6	0.00	-	-		
84	OHX	6	1968	-	0,6,6	0.00	-	-		
84	OHX	1	3693	-	0,6,6	0.00	-	-		
84	OHX	1	3500	-	0,6,6	0.00	-	-		
84	OHX	6	1906	-	0,6,6	0.00	-	-		
84	OHX	1	3579	-	0,6,6	0.00	-	-		
84	OHX	6	1994	-	0,6,6	0.00	-	-		
84	OHX	A	1943	-	0,6,6	0.00	-	-		
84	OHX	A	2028	-	0,6,6	0.00	-	-		
84	OHX	6	1989	-	0,6,6	0.00	-	-		
84	OHX	1	3479	-	0,6,6	0.00	-	-		
84	OHX	A	1963	-	0,6,6	0.00	-	-		
84	OHX	A	1952	-	0,6,6	0.00	-	-		
84	OHX	1	3708	-	0,6,6	0.00	-	-		
84	OHX	k	401	-	0,6,6	0.00	-	-		
84	OHX	3	204	-	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	3663	-	0,6,6	0.00	-	-		
84	OHX	6	1979	-	0,6,6	0.00	-	-		
84	OHX	A	1913	-	0,6,6	0.00	-	-		
84	OHX	1	3507	-	0,6,6	0.00	-	-		
84	OHX	1	3590	-	0,6,6	0.00	-	-		
84	OHX	1	3612	-	0,6,6	0.00	-	-		
84	OHX	AS	206	-	0,6,6	0.00	-	-		
84	OHX	1	3441	-	0,6,6	0.00	-	-		
84	OHX	1	3460	-	0,6,6	0.00	-	-		
84	OHX	A	2013	-	0,6,6	0.00	-	-		
84	OHX	A	1932	-	0,6,6	0.00	-	-		
84	OHX	AR	3583	-	0,6,6	0.00	-	-		
84	OHX	DD	102	-	0,6,6	0.00	-	-		
84	OHX	AR	3505	-	0,6,6	0.00	-	-		
84	OHX	AR	3524	-	0,6,6	0.00	-	-		
84	OHX	6	2012	-	0,6,6	0.00	-	-		
84	OHX	AR	3562	-	0,6,6	0.00	-	-		
84	OHX	1	3458	-	0,6,6	0.00	-	-		
84	OHX	AT	216	-	0,6,6	0.00	-	-		
84	OHX	1	3451	-	0,6,6	0.00	-	-		
84	OHX	CG	302	-	0,6,6	0.00	-	-		
84	OHX	1	3637	-	0,6,6	0.00	-	-		
84	OHX	6	1936	-	0,6,6	0.00	-	-		
84	OHX	AR	3514	-	0,6,6	0.00	-	-		
84	OHX	6	1933	-	0,6,6	0.00	-	-		
84	OHX	1	3696	-	0,6,6	0.00	-	-		
84	OHX	A	1921	-	0,6,6	0.00	-	-		
84	OHX	AT	213	-	0,6,6	0.00	-	-		
84	OHX	A	1914	-	0,6,6	0.00	-	-		
84	OHX	AR	3718	-	0,6,6	0.00	-	-		
84	OHX	AR	3715	-	0,6,6	0.00	-	-		
84	OHX	AR	3581	-	0,6,6	0.00	-	-		
84	OHX	1	3721	-	0,6,6	0.00	-	-		
84	OHX	AR	3693	-	0,6,6	0.00	-	-		
84	OHX	AR	3480	-	0,6,6	0.00	-	-		
84	OHX	AR	3418	-	0,6,6	0.00	-	-		
84	OHX	1	3541	-	0,6,6	0.00	-	-		
84	OHX	A	1941	-	0,6,6	0.00	-	-		
84	OHX	AR	3598	-	0,6,6	0.00	-	-		
84	OHX	6	1956	-	0,6,6	0.00	-	-		
84	OHX	A	2010	-	0,6,6	0.00	-	-		
84	OHX	AR	3626	-	0,6,6	0.00	-	-		
84	OHX	6	1934	-	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	3695	-	0,6,6	0.00	-	-		
84	OHX	AR	3516	-	0,6,6	0.00	-	-		
84	OHX	1	3538	-	0,6,6	0.00	-	-		
84	OHX	6	2043	-	0,6,6	0.00	-	-		
84	OHX	6	2009	-	0,6,6	0.00	-	-		
84	OHX	1	3688	-	0,6,6	0.00	-	-		
84	OHX	1	3465	-	0,6,6	0.00	-	-		
84	OHX	1	3534	-	0,6,6	0.00	-	-		
84	OHX	AR	3604	-	0,6,6	0.00	-	-		
84	OHX	CG	303	-	0,6,6	0.00	-	-		
84	OHX	A	1980	-	0,6,6	0.00	-	-		
84	OHX	1	3698	-	0,6,6	0.00	-	-		
84	OHX	1	3694	-	0,6,6	0.00	-	-		
84	OHX	6	1974	-	0,6,6	0.00	-	-		
84	OHX	1	3675	-	0,6,6	0.00	-	-		
84	OHX	AR	3568	-	0,6,6	0.00	-	-		
84	OHX	6	1959	-	0,6,6	0.00	-	-		
84	OHX	1	3448	-	0,6,6	0.00	-	-		
84	OHX	1	3599	-	0,6,6	0.00	-	-		
84	OHX	1	3491	-	0,6,6	0.00	-	-		
84	OHX	A	1962	-	0,6,6	0.00	-	-		
84	OHX	AR	3636	-	0,6,6	0.00	-	-		
84	OHX	1	3729	-	0,6,6	0.00	-	-		
84	OHX	AR	3696	-	0,6,6	0.00	-	-		
84	OHX	A	2039	-	0,6,6	0.00	-	-		
84	OHX	6	1909	-	0,6,6	0.00	-	-		
84	OHX	AR	3470	-	0,6,6	0.00	-	-		
84	OHX	A	2041	-	0,6,6	0.00	-	-		
84	OHX	AR	3686	-	0,6,6	0.00	-	-		
84	OHX	1	3669	-	0,6,6	0.00	-	-		
84	OHX	AR	3439	-	0,6,6	0.00	-	-		
84	OHX	6	2039	-	0,6,6	0.00	-	-		
84	OHX	AR	3716	-	0,6,6	0.00	-	-		
84	OHX	AR	3430	-	0,6,6	0.00	-	-		
84	OHX	1	3562	-	0,6,6	0.00	-	-		
84	OHX	AR	3712	-	0,6,6	0.00	-	-		
84	OHX	1	3602	-	0,6,6	0.00	-	-		
84	OHX	1	3705	-	0,6,6	0.00	-	-		
84	OHX	1	3464	-	0,6,6	0.00	-	-		
84	OHX	AR	3736	-	0,6,6	0.00	-	-		
84	OHX	AR	3721	-	0,6,6	0.00	-	-		
84	OHX	6	1981	-	0,6,6	0.00	-	-		
84	OHX	1	3609	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	Q	201	-	0,6,6	0.00	-	-		
84	OHX	CX	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3729	-	0,6,6	0.00	-	-		
84	OHX	AR	3726	-	0,6,6	0.00	-	-		
84	OHX	AR	3647	-	0,6,6	0.00	-	-		
84	OHX	1	3508	-	0,6,6	0.00	-	-		
84	OHX	x	202	-	0,6,6	0.00	-	-		
84	OHX	A	1983	-	0,6,6	0.00	-	-		
84	OHX	AR	3550	-	0,6,6	0.00	-	-		
84	OHX	6	2006	-	0,6,6	0.00	-	-		
84	OHX	6	1978	-	0,6,6	0.00	-	-		
84	OHX	1	3471	-	0,6,6	0.00	-	-		
84	OHX	A	2007	-	0,6,6	0.00	-	-		
86	7MB	AR	4239	-	16,23,23	0.85	0	8,38,38	0.87	0
84	OHX	2	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3545	-	0,6,6	0.00	-	-		
84	OHX	A	1976	-	0,6,6	0.00	-	-		
84	OHX	AR	3449	-	0,6,6	0.00	-	-		
84	OHX	AR	3405	-	0,6,6	0.00	-	-		
84	OHX	y	201	-	0,6,6	0.00	-	-		
84	OHX	6	1939	-	0,6,6	0.00	-	-		
84	OHX	A	2005	-	0,6,6	0.00	-	-		
84	OHX	1	3459	-	0,6,6	0.00	-	-		
84	OHX	1	3438	-	0,6,6	0.00	-	-		
84	OHX	A	1967	-	0,6,6	0.00	-	-		
84	OHX	1	3463	-	0,6,6	0.00	-	-		
84	OHX	AR	3509	-	0,6,6	0.00	-	-		
84	OHX	AR	3441	-	0,6,6	0.00	-	-		
84	OHX	6	2023	-	0,6,6	0.00	-	-		
84	OHX	1	3532	-	0,6,6	0.00	-	-		
84	OHX	AR	3734	-	0,6,6	0.00	-	-		
84	OHX	AR	3580	-	0,6,6	0.00	-	-		
84	OHX	1	3422	-	0,6,6	0.00	-	-		
84	OHX	1	3412	-	0,6,6	0.00	-	-		
84	OHX	1	3674	-	0,6,6	0.00	-	-		
84	OHX	A	1947	-	0,6,6	0.00	-	-		
84	OHX	AR	3496	-	0,6,6	0.00	-	-		
84	OHX	1	3717	-	0,6,6	0.00	-	-		
84	OHX	AR	3515	-	0,6,6	0.00	-	-		
84	OHX	CP	501	-	0,6,6	0.00	-	-		
84	OHX	AR	3427	-	0,6,6	0.00	-	-		
84	OHX	3	205	-	0,6,6	0.00	-	-		
84	OHX	AR	3622	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	6	2019	-	0,6,6	0.00	-	-		
84	OHX	6	2018	-	0,6,6	0.00	-	-		
84	OHX	A	2012	-	0,6,6	0.00	-	-		
84	OHX	A	1959	-	0,6,6	0.00	-	-		
84	OHX	6	1927	-	0,6,6	0.00	-	-		
84	OHX	A	2018	-	0,6,6	0.00	-	-		
84	OHX	1	3430	-	0,6,6	0.00	-	-		
84	OHX	1	3408	-	0,6,6	0.00	-	-		
84	OHX	3	203	-	0,6,6	0.00	-	-		
84	OHX	1	3476	-	0,6,6	0.00	-	-		
84	OHX	1	3520	-	0,6,6	0.00	-	-		
84	OHX	AR	3593	-	0,6,6	0.00	-	-		
84	OHX	4	207	-	0,6,6	0.00	-	-		
84	OHX	1	3645	-	0,6,6	0.00	-	-		
84	OHX	1	3505	-	0,6,6	0.00	-	-		
84	OHX	6	1967	-	0,6,6	0.00	-	-		
84	OHX	1	3640	-	0,6,6	0.00	-	-		
84	OHX	AR	3552	-	0,6,6	0.00	-	-		
84	OHX	6	1962	-	0,6,6	0.00	-	-		
84	OHX	A	1925	-	0,6,6	0.00	-	-		
84	OHX	1	3616	-	0,6,6	0.00	-	-		
84	OHX	AR	3628	-	0,6,6	0.00	-	-		
84	OHX	1	3728	-	0,6,6	0.00	-	-		
84	OHX	6	1954	-	0,6,6	0.00	-	-		
84	OHX	AR	3700	-	0,6,6	0.00	-	-		
84	OHX	1	3513	-	0,6,6	0.00	-	-		
84	OHX	1	3715	-	0,6,6	0.00	-	-		
84	OHX	6	2020	-	0,6,6	0.00	-	-		
84	OHX	1	3584	-	0,6,6	0.00	-	-		
84	OHX	AR	3453	-	0,6,6	0.00	-	-		
84	OHX	A	1977	-	0,6,6	0.00	-	-		
84	OHX	1	3421	-	0,6,6	0.00	-	-		
84	OHX	A	2021	-	0,6,6	0.00	-	-		
84	OHX	AR	3411	-	0,6,6	0.00	-	-		
84	OHX	AR	3650	-	0,6,6	0.00	-	-		
84	OHX	6	1965	-	0,6,6	0.00	-	-		
84	OHX	6	1908	-	0,6,6	0.00	-	-		
84	OHX	6	1982	-	0,6,6	0.00	-	-		
84	OHX	1	3653	-	0,6,6	0.00	-	-		
84	OHX	1	3621	-	0,6,6	0.00	-	-		
84	OHX	A	1923	-	0,6,6	0.00	-	-		
84	OHX	1	3662	-	0,6,6	0.00	-	-		
84	OHX	1	3478	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	4	211	-	0,6,6	0.00	-	-		
84	OHX	A	1954	-	0,6,6	0.00	-	-		
84	OHX	1	3449	-	0,6,6	0.00	-	-		
84	OHX	AR	3535	-	0,6,6	0.00	-	-		
84	OHX	6	2047	-	0,6,6	0.00	-	-		
84	OHX	AR	3681	-	0,6,6	0.00	-	-		
84	OHX	AR	3511	-	0,6,6	0.00	-	-		
84	OHX	AR	3484	-	0,6,6	0.00	-	-		
84	OHX	6	2031	-	0,6,6	0.00	-	-		
84	OHX	AR	3657	-	0,6,6	0.00	-	-		
84	OHX	AR	3603	-	0,6,6	0.00	-	-		
84	OHX	A	1916	-	0,6,6	0.00	-	-		
84	OHX	A	1982	-	0,6,6	0.00	-	-		
84	OHX	1	3404	-	0,6,6	0.00	-	-		
84	OHX	A	1915	-	0,6,6	0.00	-	-		
84	OHX	1	3565	-	0,6,6	0.00	-	-		
84	OHX	1	3489	-	0,6,6	0.00	-	-		
84	OHX	6	2034	-	0,6,6	0.00	-	-		
84	OHX	A	2029	-	0,6,6	0.00	-	-		
84	OHX	k	402	-	0,6,6	0.00	-	-		
84	OHX	1	3592	-	0,6,6	0.00	-	-		
84	OHX	1	3455	-	0,6,6	0.00	-	-		
84	OHX	1	3710	-	0,6,6	0.00	-	-		
84	OHX	A	1973	-	0,6,6	0.00	-	-		
84	OHX	1	3648	-	0,6,6	0.00	-	-		
84	OHX	1	3564	-	0,6,6	0.00	-	-		
84	OHX	AR	3544	-	0,6,6	0.00	-	-		
84	OHX	A	1904	-	0,6,6	0.00	-	-		
84	OHX	1	3676	-	0,6,6	0.00	-	-		
84	OHX	AR	3456	-	0,6,6	0.00	-	-		
84	OHX	1	3618	-	0,6,6	0.00	-	-		
84	OHX	1	3450	-	0,6,6	0.00	-	-		
84	OHX	CL	302	-	0,6,6	0.00	-	-		
84	OHX	1	3594	-	0,6,6	0.00	-	-		
84	OHX	A	1993	-	0,6,6	0.00	-	-		
84	OHX	6	2049	-	0,6,6	0.00	-	-		
84	OHX	AR	3572	-	0,6,6	0.00	-	-		
84	OHX	AR	3578	-	0,6,6	0.00	-	-		
84	OHX	1	3475	-	0,6,6	0.00	-	-		
84	OHX	AR	3579	-	0,6,6	0.00	-	-		
84	OHX	AR	3402	-	0,6,6	0.00	-	-		
84	OHX	1	3678	-	0,6,6	0.00	-	-		
84	OHX	AR	3436	-	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	3638	-	0,6,6	0.00	-	-		
84	OHX	AT	218	-	0,6,6	0.00	-	-		
84	OHX	A	1917	-	0,6,6	0.00	-	-		
84	OHX	1	3641	-	0,6,6	0.00	-	-		
84	OHX	1	3631	-	0,6,6	0.00	-	-		
84	OHX	c3	201	-	0,6,6	0.00	-	-		
84	OHX	6	1970	-	0,6,6	0.00	-	-		
84	OHX	AR	3478	-	0,6,6	0.00	-	-		
84	OHX	A	1929	-	0,6,6	0.00	-	-		
84	OHX	A	1960	-	0,6,6	0.00	-	-		
84	OHX	AR	3595	-	0,6,6	0.00	-	-		
84	OHX	AR	3606	-	0,6,6	0.00	-	-		
84	OHX	AR	3609	-	0,6,6	0.00	-	-		
84	OHX	AR	3547	-	0,6,6	0.00	-	-		
84	OHX	1	3606	-	0,6,6	0.00	-	-		
84	OHX	6	1926	-	0,6,6	0.00	-	-		
84	OHX	1	3502	-	0,6,6	0.00	-	-		
84	OHX	AR	3566	-	0,6,6	0.00	-	-		
84	OHX	AR	3667	-	0,6,6	0.00	-	-		
84	OHX	AR	3500	-	0,6,6	0.00	-	-		
84	OHX	1	3410	-	0,6,6	0.00	-	-		
84	OHX	A	1905	-	0,6,6	0.00	-	-		
84	OHX	1	3474	-	0,6,6	0.00	-	-		
84	OHX	6	1925	-	0,6,6	0.00	-	-		
84	OHX	AR	3472	-	0,6,6	0.00	-	-		
84	OHX	AR	3424	-	0,6,6	0.00	-	-		
84	OHX	AR	3658	-	0,6,6	0.00	-	-		
84	OHX	1	3525	-	0,6,6	0.00	-	-		
84	OHX	AR	3703	-	0,6,6	0.00	-	-		
84	OHX	1	3699	-	0,6,6	0.00	-	-		
84	OHX	A	2022	-	0,6,6	0.00	-	-		
84	OHX	A	1986	-	0,6,6	0.00	-	-		
84	OHX	AR	3629	-	0,6,6	0.00	-	-		
84	OHX	1	3682	-	0,6,6	0.00	-	-		
84	OHX	CO	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3538	-	0,6,6	0.00	-	-		
84	OHX	AR	3540	-	0,6,6	0.00	-	-		
84	OHX	AR	3428	-	0,6,6	0.00	-	-		
84	OHX	1	3613	-	0,6,6	0.00	-	-		
84	OHX	AR	3619	-	0,6,6	0.00	-	-		
84	OHX	6	2045	-	0,6,6	0.00	-	-		
84	OHX	1	3444	-	0,6,6	0.00	-	-		
84	OHX	1	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	3	208	-	0,6,6	0.00	-	-		
84	OHX	CE	403	-	0,6,6	0.00	-	-		
84	OHX	AR	3451	-	0,6,6	0.00	-	-		
84	OHX	A	1964	-	0,6,6	0.00	-	-		
84	OHX	A	1901	-	0,6,6	0.00	-	-		
84	OHX	AR	3605	-	0,6,6	0.00	-	-		
84	OHX	A	1996	-	0,6,6	0.00	-	-		
84	OHX	1	3461	-	0,6,6	0.00	-	-		
84	OHX	6	1935	-	0,6,6	0.00	-	-		
84	OHX	r	301	-	0,6,6	0.00	-	-		
84	OHX	1	3569	-	0,6,6	0.00	-	-		
84	OHX	1	3692	-	0,6,6	0.00	-	-		
84	OHX	6	2035	-	0,6,6	0.00	-	-		
84	OHX	d9	101	-	0,6,6	0.00	-	-		
84	OHX	1	3546	-	0,6,6	0.00	-	-		
84	OHX	6	2013	-	0,6,6	0.00	-	-		
84	OHX	A	2015	-	0,6,6	0.00	-	-		
84	OHX	AR	3513	-	0,6,6	0.00	-	-		
84	OHX	6	2008	-	0,6,6	0.00	-	-		
84	OHX	1	3649	-	0,6,6	0.00	-	-		
84	OHX	A	1974	-	0,6,6	0.00	-	-		
84	OHX	1	3726	-	0,6,6	0.00	-	-		
84	OHX	A	1958	-	0,6,6	0.00	-	-		
84	OHX	1	3405	-	0,6,6	0.00	-	-		
84	OHX	1	3723	-	0,6,6	0.00	-	-		
84	OHX	A	2025	-	0,6,6	0.00	-	-		
84	OHX	6	2030	-	0,6,6	0.00	-	-		
84	OHX	1	3679	-	0,6,6	0.00	-	-		
84	OHX	6	1966	-	0,6,6	0.00	-	-		
84	OHX	6	2028	-	0,6,6	0.00	-	-		
84	OHX	AR	3695	-	0,6,6	0.00	-	-		
84	OHX	1	3589	-	0,6,6	0.00	-	-		
84	OHX	A	1990	-	0,6,6	0.00	-	-		
84	OHX	AR	3481	-	0,6,6	0.00	-	-		
84	OHX	1	3413	-	0,6,6	0.00	-	-		
84	OHX	6	2037	-	0,6,6	0.00	-	-		
84	OHX	AR	3694	-	0,6,6	0.00	-	-		
84	OHX	1	3593	-	0,6,6	0.00	-	-		
84	OHX	AT	206	-	0,6,6	0.00	-	-		
84	OHX	6	2053	-	0,6,6	0.00	-	-		
84	OHX	6	2024	-	0,6,6	0.00	-	-		
84	OHX	1	3627	-	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	1	3724	-	0,6,6	0.00	-	-		
84	OHX	1	3575	-	0,6,6	0.00	-	-		
84	OHX	6	1928	-	0,6,6	0.00	-	-		
84	OHX	AR	3533	-	0,6,6	0.00	-	-		
84	OHX	1	3433	-	0,6,6	0.00	-	-		
84	OHX	CZ	201	-	0,6,6	0.00	-	-		
84	OHX	1	3667	-	0,6,6	0.00	-	-		
84	OHX	A	1945	-	0,6,6	0.00	-	-		
84	OHX	AR	3683	-	0,6,6	0.00	-	-		
84	OHX	1	3685	-	0,6,6	0.00	-	-		
84	OHX	AR	3677	-	0,6,6	0.00	-	-		
84	OHX	1	3620	-	0,6,6	0.00	-	-		
84	OHX	1	3540	-	0,6,6	0.00	-	-		
84	OHX	1	3566	-	0,6,6	0.00	-	-		
84	OHX	1	3511	-	0,6,6	0.00	-	-		
84	OHX	1	3563	-	0,6,6	0.00	-	-		
84	OHX	6	2005	-	0,6,6	0.00	-	-		
84	OHX	1	3709	-	0,6,6	0.00	-	-		
84	OHX	1	3403	-	0,6,6	0.00	-	-		
84	OHX	A	1992	-	0,6,6	0.00	-	-		
84	OHX	AR	3489	-	0,6,6	0.00	-	-		
84	OHX	AR	3739	-	0,6,6	0.00	-	-		
84	OHX	AE	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3711	-	0,6,6	0.00	-	-		
84	OHX	AR	3659	-	0,6,6	0.00	-	-		
84	OHX	AR	3656	-	0,6,6	0.00	-	-		
84	OHX	AR	3722	-	0,6,6	0.00	-	-		
84	OHX	A	1912	-	0,6,6	0.00	-	-		
84	OHX	AR	3608	-	0,6,6	0.00	-	-		
84	OHX	A	1903	-	0,6,6	0.00	-	-		
84	OHX	1	3597	-	0,6,6	0.00	-	-		
84	OHX	1	3490	-	0,6,6	0.00	-	-		
84	OHX	A	2036	-	0,6,6	0.00	-	-		
84	OHX	AR	3642	-	0,6,6	0.00	-	-		
84	OHX	AR	3519	-	0,6,6	0.00	-	-		
84	OHX	1	3596	-	0,6,6	0.00	-	-		
84	OHX	AR	3521	-	0,6,6	0.00	-	-		
84	OHX	AR	3440	-	0,6,6	0.00	-	-		
84	OHX	6	1953	-	0,6,6	0.00	-	-		
84	OHX	AR	3467	-	0,6,6	0.00	-	-		
84	OHX	A	1924	-	0,6,6	0.00	-	-		
84	OHX	1	3632	-	0,6,6	0.00	-	-		
84	OHX	1	3453	-	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	3564	-	0,6,6	0.00	-	-		
84	OHX	6	1941	-	0,6,6	0.00	-	-		
84	OHX	AR	3571	-	0,6,6	0.00	-	-		
84	OHX	1	3659	-	0,6,6	0.00	-	-		
84	OHX	A	1948	-	0,6,6	0.00	-	-		
84	OHX	1	3582	-	0,6,6	0.00	-	-		
84	OHX	1	3407	-	0,6,6	0.00	-	-		
84	OHX	v	301	-	0,6,6	0.00	-	-		
84	OHX	1	3526	-	0,6,6	0.00	-	-		
84	OHX	AR	3523	-	0,6,6	0.00	-	-		
84	OHX	1	3595	-	0,6,6	0.00	-	-		
84	OHX	1	3583	-	0,6,6	0.00	-	-		
84	OHX	AR	3589	-	0,6,6	0.00	-	-		
84	OHX	AR	3674	-	0,6,6	0.00	-	-		
84	OHX	6	1942	-	0,6,6	0.00	-	-		
84	OHX	AR	3555	-	0,6,6	0.00	-	-		
84	OHX	AR	3635	-	0,6,6	0.00	-	-		
84	OHX	6	1998	-	0,6,6	0.00	-	-		
84	OHX	1	3718	-	0,6,6	0.00	-	-		
84	OHX	AR	3486	-	0,6,6	0.00	-	-		
84	OHX	x	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3483	-	0,6,6	0.00	-	-		
84	OHX	6	1952	-	0,6,6	0.00	-	-		
84	OHX	1	3683	-	0,6,6	0.00	-	-		
84	OHX	1	3426	-	0,6,6	0.00	-	-		
84	OHX	AR	3738	-	0,6,6	0.00	-	-		
84	OHX	AR	3733	-	0,6,6	0.00	-	-		
84	OHX	6	1943	-	0,6,6	0.00	-	-		
84	OHX	A	1965	-	0,6,6	0.00	-	-		
84	OHX	AR	3422	-	0,6,6	0.00	-	-		
84	OHX	1	3655	-	0,6,6	0.00	-	-		
84	OHX	1	3442	-	0,6,6	0.00	-	-		
84	OHX	1	3529	-	0,6,6	0.00	-	-		
84	OHX	4	209	-	0,6,6	0.00	-	-		
84	OHX	1	3689	-	0,6,6	0.00	-	-		
84	OHX	CG	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3457	-	0,6,6	0.00	-	-		
84	OHX	6	1929	-	0,6,6	0.00	-	-		
84	OHX	AR	3557	-	0,6,6	0.00	-	-		
84	OHX	AR	3433	-	0,6,6	0.00	-	-		
84	OHX	AR	3460	-	0,6,6	0.00	-	-		
84	OHX	AR	3417	-	0,6,6	0.00	-	-		
84	OHX	AR	3458	-	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	3509	-	0,6,6	0.00	-	-		
84	OHX	6	1914	-	0,6,6	0.00	-	-		
84	OHX	AR	3425	-	0,6,6	0.00	-	-		
84	OHX	6	2015	-	0,6,6	0.00	-	-		
84	OHX	1	3586	-	0,6,6	0.00	-	-		
84	OHX	1	3634	-	0,6,6	0.00	-	-		
84	OHX	A	1910	-	0,6,6	0.00	-	-		
84	OHX	A	1968	-	0,6,6	0.00	-	-		
84	OHX	A	1987	-	0,6,6	0.00	-	-		
84	OHX	AR	3497	-	0,6,6	0.00	-	-		
84	OHX	1	3587	-	0,6,6	0.00	-	-		
84	OHX	AR	3565	-	0,6,6	0.00	-	-		
84	OHX	AR	3548	-	0,6,6	0.00	-	-		
84	OHX	AT	210	-	0,6,6	0.00	-	-		
84	OHX	1	3629	-	0,6,6	0.00	-	-		
84	OHX	1	3484	-	0,6,6	0.00	-	-		
84	OHX	6	1992	-	0,6,6	0.00	-	-		
84	OHX	1	3691	-	0,6,6	0.00	-	-		
84	OHX	1	3544	-	0,6,6	0.00	-	-		
84	OHX	AR	3493	-	0,6,6	0.00	-	-		
84	OHX	A	1953	-	0,6,6	0.00	-	-		
84	OHX	AR	3403	-	0,6,6	0.00	-	-		
84	OHX	A	1938	-	0,6,6	0.00	-	-		
84	OHX	6	1969	-	0,6,6	0.00	-	-		
84	OHX	6	1986	-	0,6,6	0.00	-	-		
84	OHX	3	202	-	0,6,6	0.00	-	-		
84	OHX	6	1960	-	0,6,6	0.00	-	-		
84	OHX	AR	3574	-	0,6,6	0.00	-	-		
84	OHX	AR	3445	-	0,6,6	0.00	-	-		
84	OHX	1	3719	-	0,6,6	0.00	-	-		
84	OHX	A	1919	-	0,6,6	0.00	-	-		
84	OHX	AR	3526	-	0,6,6	0.00	-	-		
84	OHX	1	3439	-	0,6,6	0.00	-	-		
84	OHX	6	2054	-	0,6,6	0.00	-	-		
84	OHX	1	3553	-	0,6,6	0.00	-	-		
84	OHX	AR	3473	-	0,6,6	0.00	-	-		
84	OHX	1	3556	-	0,6,6	0.00	-	-		
84	OHX	AR	3532	-	0,6,6	0.00	-	-		
84	OHX	1	3414	-	0,6,6	0.00	-	-		
84	OHX	AR	3465	-	0,6,6	0.00	-	-		
84	OHX	AR	3719	-	0,6,6	0.00	-	-		
84	OHX	AR	3586	-	0,6,6	0.00	-	-		
84	OHX	AR	3610	-	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	AR	3502	-	0,6,6	0.00	-	-		
84	OHX	4	208	-	0,6,6	0.00	-	-		
84	OHX	1	3704	-	0,6,6	0.00	-	-		
84	OHX	1	3690	-	0,6,6	0.00	-	-		
84	OHX	1	3600	-	0,6,6	0.00	-	-		
84	OHX	1	3730	-	0,6,6	0.00	-	-		
84	OHX	6	1985	-	0,6,6	0.00	-	-		
84	OHX	6	1980	-	0,6,6	0.00	-	-		
84	OHX	AR	3495	-	0,6,6	0.00	-	-		
84	OHX	1	3643	-	0,6,6	0.00	-	-		
84	OHX	1	3661	-	0,6,6	0.00	-	-		
84	OHX	A	1966	-	0,6,6	0.00	-	-		
84	OHX	O	201	-	0,6,6	0.00	-	-		
84	OHX	1	3581	-	0,6,6	0.00	-	-		
84	OHX	1	3543	-	0,6,6	0.00	-	-		
84	OHX	6	1948	-	0,6,6	0.00	-	-		
84	OHX	1	3551	-	0,6,6	0.00	-	-		
84	OHX	CK	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3468	-	0,6,6	0.00	-	-		
84	OHX	AR	3625	-	0,6,6	0.00	-	-		
84	OHX	AR	3543	-	0,6,6	0.00	-	-		
84	OHX	6	2017	-	0,6,6	0.00	-	-		
84	OHX	1	3485	-	0,6,6	0.00	-	-		
84	OHX	1	3506	-	0,6,6	0.00	-	-		
84	OHX	1	3537	-	0,6,6	0.00	-	-		
84	OHX	1	3420	-	0,6,6	0.00	-	-		
84	OHX	6	1949	-	0,6,6	0.00	-	-		
84	OHX	1	3466	-	0,6,6	0.00	-	-		
84	OHX	AR	3475	-	0,6,6	0.00	-	-		
84	OHX	AR	3447	-	0,6,6	0.00	-	-		
84	OHX	AR	3725	-	0,6,6	0.00	-	-		
84	OHX	6	1975	-	0,6,6	0.00	-	-		
84	OHX	A	1972	-	0,6,6	0.00	-	-		
84	OHX	c8	201	-	0,6,6	0.00	-	-		
84	OHX	1	3494	-	0,6,6	0.00	-	-		
84	OHX	1	3570	-	0,6,6	0.00	-	-		
84	OHX	AR	3675	-	0,6,6	0.00	-	-		
84	OHX	6	1990	-	0,6,6	0.00	-	-		
84	OHX	6	1921	-	0,6,6	0.00	-	-		
84	OHX	1	3697	-	0,6,6	0.00	-	-		
84	OHX	1	3445	-	0,6,6	0.00	-	-		
84	OHX	A	1950	-	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	3404	-	0,6,6	0.00	-	-		
84	OHX	AT	207	-	0,6,6	0.00	-	-		
84	OHX	A	2002	-	0,6,6	0.00	-	-		
84	OHX	6	2033	-	0,6,6	0.00	-	-		
84	OHX	AT	211	-	0,6,6	0.00	-	-		
84	OHX	A	2033	-	0,6,6	0.00	-	-		
84	OHX	AR	3615	-	0,6,6	0.00	-	-		
84	OHX	1	3611	-	0,6,6	0.00	-	-		
84	OHX	1	3539	-	0,6,6	0.00	-	-		
84	OHX	AR	3490	-	0,6,6	0.00	-	-		
84	OHX	AR	3723	-	0,6,6	0.00	-	-		
84	OHX	1	3681	-	0,6,6	0.00	-	-		
84	OHX	AR	3691	-	0,6,6	0.00	-	-		
84	OHX	AR	3613	-	0,6,6	0.00	-	-		
84	OHX	1	3477	-	0,6,6	0.00	-	-		
84	OHX	A	1922	-	0,6,6	0.00	-	-		
84	OHX	AT	209	-	0,6,6	0.00	-	-		
84	OHX	A	1902	-	0,6,6	0.00	-	-		
84	OHX	1	3617	-	0,6,6	0.00	-	-		
84	OHX	1	3619	-	0,6,6	0.00	-	-		
84	OHX	AR	3680	-	0,6,6	0.00	-	-		
84	OHX	1	3440	-	0,6,6	0.00	-	-		
84	OHX	AR	3690	-	0,6,6	0.00	-	-		
84	OHX	6	1919	-	0,6,6	0.00	-	-		
84	OHX	1	3493	-	0,6,6	0.00	-	-		
84	OHX	AR	3577	-	0,6,6	0.00	-	-		
84	OHX	AR	3654	-	0,6,6	0.00	-	-		
84	OHX	AR	3673	-	0,6,6	0.00	-	-		
84	OHX	1	3651	-	0,6,6	0.00	-	-		
84	OHX	AR	3633	-	0,6,6	0.00	-	-		
84	OHX	1	3658	-	0,6,6	0.00	-	-		
84	OHX	AR	3488	-	0,6,6	0.00	-	-		
84	OHX	AR	3705	-	0,6,6	0.00	-	-		
84	OHX	A	1907	-	0,6,6	0.00	-	-		
84	OHX	1	3536	-	0,6,6	0.00	-	-		
84	OHX	A	1933	-	0,6,6	0.00	-	-		
84	OHX	AR	3620	-	0,6,6	0.00	-	-		
84	OHX	AR	3627	-	0,6,6	0.00	-	-		
84	OHX	A	1911	-	0,6,6	0.00	-	-		
84	OHX	1	3635	-	0,6,6	0.00	-	-		
84	OHX	6	2002	-	0,6,6	0.00	-	-		
84	OHX	J	301	-	0,6,6	0.00	-	-		
84	OHX	A	1999	-	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	3464	-	0,6,6	0.00	-	-		
84	OHX	6	2044	-	0,6,6	0.00	-	-		
84	OHX	AR	3518	-	0,6,6	0.00	-	-		
84	OHX	A	1981	-	0,6,6	0.00	-	-		
84	OHX	1	3472	-	0,6,6	0.00	-	-		
84	OHX	AR	3698	-	0,6,6	0.00	-	-		
84	OHX	6	2026	-	0,6,6	0.00	-	-		
84	OHX	AT	208	-	0,6,6	0.00	-	-		
84	OHX	A	2030	-	0,6,6	0.00	-	-		
84	OHX	AT	202	-	0,6,6	0.00	-	-		
84	OHX	A	1936	-	0,6,6	0.00	-	-		
84	OHX	1	3481	-	0,6,6	0.00	-	-		
84	OHX	AR	3503	-	0,6,6	0.00	-	-		
84	OHX	6	1972	-	0,6,6	0.00	-	-		
84	OHX	A	2023	-	0,6,6	0.00	-	-		
84	OHX	AR	3662	-	0,6,6	0.00	-	-		
84	OHX	6	2050	-	0,6,6	0.00	-	-		
84	OHX	AR	3576	-	0,6,6	0.00	-	-		
84	OHX	6	1924	-	0,6,6	0.00	-	-		
84	OHX	AR	3412	-	0,6,6	0.00	-	-		
84	OHX	4	201	-	0,6,6	0.00	-	-		
84	OHX	1	3545	-	0,6,6	0.00	-	-		
84	OHX	AT	204	-	0,6,6	0.00	-	-		
84	OHX	AR	3506	-	0,6,6	0.00	-	-		
84	OHX	AR	3671	-	0,6,6	0.00	-	-		
84	OHX	1	3622	-	0,6,6	0.00	-	-		
84	OHX	4	202	-	0,6,6	0.00	-	-		
84	OHX	A	1984	-	0,6,6	0.00	-	-		
84	OHX	AR	3463	-	0,6,6	0.00	-	-		
84	OHX	1	3423	-	0,6,6	0.00	-	-		
84	OHX	AR	3618	-	0,6,6	0.00	-	-		
84	OHX	6	2014	-	0,6,6	0.00	-	-		
84	OHX	6	2040	-	0,6,6	0.00	-	-		
84	OHX	1	3665	-	0,6,6	0.00	-	-		
84	OHX	AR	3512	-	0,6,6	0.00	-	-		
84	OHX	1	3630	-	0,6,6	0.00	-	-		
84	OHX	AR	3634	-	0,6,6	0.00	-	-		
84	OHX	1	3588	-	0,6,6	0.00	-	-		
84	OHX	AS	204	-	0,6,6	0.00	-	-		
84	OHX	1	3725	-	0,6,6	0.00	-	-		
84	OHX	AR	3641	-	0,6,6	0.00	-	-		
84	OHX	6	2004	-	0,6,6	0.00	-	-		
84	OHX	1	3437	-	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	3644	-	0,6,6	0.00	-	-		
84	OHX	6	1947	-	0,6,6	0.00	-	-		
84	OHX	3	206	-	0,6,6	0.00	-	-		
84	OHX	AR	3617	-	0,6,6	0.00	-	-		
84	OHX	1	3639	-	0,6,6	0.00	-	-		
84	OHX	A	1944	-	0,6,6	0.00	-	-		
84	OHX	A	2014	-	0,6,6	0.00	-	-		
84	OHX	4	206	-	0,6,6	0.00	-	-		
84	OHX	AR	3542	-	0,6,6	0.00	-	-		
84	OHX	4	203	-	0,6,6	0.00	-	-		
84	OHX	H	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3672	-	0,6,6	0.00	-	-		
84	OHX	A	1926	-	0,6,6	0.00	-	-		
84	OHX	1	3552	-	0,6,6	0.00	-	-		
84	OHX	6	2001	-	0,6,6	0.00	-	-		
84	OHX	A	2031	-	0,6,6	0.00	-	-		
84	OHX	A	1991	-	0,6,6	0.00	-	-		
84	OHX	AR	3520	-	0,6,6	0.00	-	-		
84	OHX	AR	3661	-	0,6,6	0.00	-	-		
84	OHX	AR	3459	-	0,6,6	0.00	-	-		
84	OHX	AS	202	-	0,6,6	0.00	-	-		
84	OHX	AR	3554	-	0,6,6	0.00	-	-		
84	OHX	AR	3510	-	0,6,6	0.00	-	-		
84	OHX	A	2000	-	0,6,6	0.00	-	-		
84	OHX	A	1969	-	0,6,6	0.00	-	-		
84	OHX	1	3434	-	0,6,6	0.00	-	-		
84	OHX	A	1927	-	0,6,6	0.00	-	-		
84	OHX	CL	301	-	0,6,6	0.00	-	-		
84	OHX	1	3431	-	0,6,6	0.00	-	-		
84	OHX	1	3610	-	0,6,6	0.00	-	-		
84	OHX	3	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3699	-	0,6,6	0.00	-	-		
84	OHX	1	3633	-	0,6,6	0.00	-	-		
84	OHX	AR	3530	-	0,6,6	0.00	-	-		
84	OHX	1	3628	-	0,6,6	0.00	-	-		
84	OHX	4	204	-	0,6,6	0.00	-	-		
84	OHX	1	3518	-	0,6,6	0.00	-	-		
84	OHX	AR	3601	-	0,6,6	0.00	-	-		
84	OHX	6	1923	-	0,6,6	0.00	-	-		
84	OHX	1	3542	-	0,6,6	0.00	-	-		
84	OHX	AR	3621	-	0,6,6	0.00	-	-		
84	OHX	AR	3438	-	0,6,6	0.00	-	-		
84	OHX	A	1939	-	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	3646	-	0,6,6	0.00	-	-		
84	OHX	6	1991	-	0,6,6	0.00	-	-		
84	OHX	6	2003	-	0,6,6	0.00	-	-		
84	OHX	A	1989	-	0,6,6	0.00	-	-		
84	OHX	AR	3666	-	0,6,6	0.00	-	-		
84	OHX	A	1930	-	0,6,6	0.00	-	-		
84	OHX	AR	3444	-	0,6,6	0.00	-	-		
84	OHX	6	1907	-	0,6,6	0.00	-	-		
84	OHX	6	2042	-	0,6,6	0.00	-	-		
84	OHX	A	1951	-	0,6,6	0.00	-	-		
84	OHX	AR	3517	-	0,6,6	0.00	-	-		
84	OHX	6	1971	-	0,6,6	0.00	-	-		
84	OHX	A	1909	-	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	7MB	1	4216	-	-	-	0/3/4/4
86	7MB	AR	4239	-	-	-	0/3/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	4216	7MB	C9-C8	-2.54	1.35	1.40
86	1	4216	7MB	O-C1	-2.22	1.19	1.23
86	1	4216	7MB	C10-C11	-2.11	1.36	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	4216	7MB	C6-C2-N1	-2.82	108.36	113.23
86	1	4216	7MB	C2-N1-C1	-2.34	108.64	113.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

538 monomers are involved in 770 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3408	OHX	2	0
84	AR	3685	OHX	1	0
84	DL	101	OHX	1	0
84	1	3482	OHX	2	0
84	AR	3611	OHX	1	0
84	1	3535	OHX	2	0
84	AR	3466	OHX	1	0
84	AR	3413	OHX	1	0
84	1	3548	OHX	1	0
84	AR	3429	OHX	1	0
84	1	3603	OHX	2	0
84	DL	102	OHX	1	0
84	1	3614	OHX	1	0
84	1	3714	OHX	1	0
84	1	3672	OHX	2	0
84	AR	3646	OHX	1	0
84	6	1930	OHX	1	0
84	1	3521	OHX	1	0
84	6	2038	OHX	1	0
84	6	1995	OHX	1	0
84	1	3558	OHX	2	0
84	CF	401	OHX	1	0
84	6	1961	OHX	1	0
84	1	3712	OHX	2	0
84	6	1910	OHX	2	0
84	1	3497	OHX	1	0
84	AR	3437	OHX	2	0
84	1	3578	OHX	1	0
84	AC	101	OHX	1	0
84	6	1957	OHX	1	0
84	1	3527	OHX	1	0
84	1	3666	OHX	2	0
84	A	2026	OHX	2	0
84	6	1904	OHX	1	0
84	6	2007	OHX	1	0
84	AR	3713	OHX	1	0
84	1	3702	OHX	4	0
84	6	2011	OHX	1	0
84	AR	3435	OHX	1	0
84	AR	3728	OHX	1	0
84	1	3684	OHX	1	0
84	1	3547	OHX	1	0
84	AR	3682	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3485	OHX	1	0
84	AR	3416	OHX	2	0
84	AR	3462	OHX	1	0
84	1	3402	OHX	1	0
84	AS	201	OHX	1	0
84	AR	3624	OHX	1	0
84	A	2034	OHX	1	0
84	AR	3560	OHX	1	0
84	AR	3631	OHX	1	0
84	A	1955	OHX	2	0
84	M	201	OHX	2	0
84	AR	3706	OHX	1	0
84	AR	3549	OHX	1	0
84	AR	3469	OHX	3	0
84	1	3446	OHX	1	0
84	1	3572	OHX	3	0
84	1	3554	OHX	1	0
84	AR	3499	OHX	1	0
84	A	1920	OHX	1	0
84	A	1970	OHX	3	0
84	1	3604	OHX	1	0
84	AR	3737	OHX	1	0
84	AT	205	OHX	2	0
84	1	3522	OHX	1	0
84	AR	3649	OHX	1	0
84	A	1988	OHX	3	0
84	AT	203	OHX	3	0
84	A	1928	OHX	2	0
84	1	3585	OHX	1	0
84	1	3650	OHX	1	0
84	AR	3474	OHX	1	0
84	AR	3563	OHX	1	0
84	T	201	OHX	1	0
84	6	1973	OHX	3	0
84	AR	3508	OHX	1	0
84	6	1963	OHX	1	0
84	AR	3684	OHX	1	0
84	AR	3448	OHX	1	0
84	6	1915	OHX	3	0
84	1	3567	OHX	1	0
84	AR	3410	OHX	2	0
84	A	2004	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3416	OHX	2	0
84	AR	3476	OHX	1	0
84	AR	3614	OHX	1	0
84	6	1997	OHX	1	0
84	1	3657	OHX	1	0
84	AR	3596	OHX	1	0
84	AR	3575	OHX	1	0
84	1	3654	OHX	2	0
84	1	3409	OHX	1	0
84	A	1997	OHX	1	0
84	1	3401	OHX	1	0
84	A	1971	OHX	1	0
84	1	3530	OHX	1	0
84	CE	402	OHX	2	0
84	AR	3421	OHX	1	0
86	1	4216	7MB	4	0
84	AR	3570	OHX	1	0
84	AR	3678	OHX	1	0
84	6	1913	OHX	1	0
84	1	3687	OHX	1	0
84	1	3419	OHX	2	0
84	AR	3504	OHX	3	0
84	6	1958	OHX	1	0
84	6	1901	OHX	1	0
84	6	1922	OHX	1	0
84	AR	3534	OHX	1	0
84	AR	3735	OHX	1	0
84	6	1999	OHX	2	0
84	AR	3689	OHX	2	0
84	A	2024	OHX	2	0
84	6	2055	OHX	1	0
84	AR	3594	OHX	1	0
84	AR	3420	OHX	1	0
84	1	3644	OHX	1	0
84	AR	3527	OHX	2	0
84	AR	3697	OHX	3	0
84	AR	3522	OHX	1	0
84	1	3515	OHX	1	0
84	6	1902	OHX	1	0
84	1	3713	OHX	1	0
84	AS	203	OHX	1	0
84	1	3495	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3640	OHX	1	0
84	6	1918	OHX	1	0
84	AR	3652	OHX	1	0
84	6	1932	OHX	1	0
84	6	1911	OHX	1	0
84	1	3454	OHX	1	0
84	AR	3442	OHX	2	0
84	1	3447	OHX	2	0
84	6	1912	OHX	1	0
84	AR	3531	OHX	1	0
84	AR	3454	OHX	2	0
84	AR	3720	OHX	1	0
84	AR	3567	OHX	2	0
84	AR	3443	OHX	7	0
84	1	3605	OHX	1	0
84	A	2009	OHX	2	0
84	AR	3592	OHX	1	0
84	A	2038	OHX	2	0
84	1	3523	OHX	1	0
84	1	3427	OHX	1	0
84	1	3624	OHX	1	0
84	AR	3461	OHX	1	0
84	DI	201	OHX	1	0
84	1	3720	OHX	1	0
84	AR	3708	OHX	1	0
84	1	3503	OHX	1	0
84	1	3496	OHX	4	0
84	AR	3492	OHX	1	0
84	6	1955	OHX	1	0
84	AR	3432	OHX	2	0
84	AR	3573	OHX	1	0
84	AR	3727	OHX	1	0
84	AR	3607	OHX	1	0
84	1	3722	OHX	1	0
84	A	2027	OHX	1	0
84	AR	3401	OHX	1	0
84	AR	3536	OHX	2	0
84	A	2003	OHX	1	0
84	AR	3709	OHX	1	0
84	AT	219	OHX	1	0
84	1	3428	OHX	2	0
84	A	1931	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3504	OHX	2	0
84	1	3656	OHX	1	0
84	AR	3507	OHX	2	0
84	AR	3409	OHX	1	0
84	A	1985	OHX	1	0
84	A	1961	OHX	1	0
84	A	2035	OHX	2	0
84	A	2019	OHX	1	0
84	AR	3630	OHX	2	0
84	AR	3423	OHX	1	0
84	AR	3556	OHX	1	0
84	AT	220	OHX	1	0
84	1	3516	OHX	1	0
84	6	1993	OHX	2	0
84	AP	502	OHX	3	0
84	CM	201	OHX	1	0
84	A	1956	OHX	1	0
84	AR	3701	OHX	2	0
84	1	3598	OHX	1	0
84	AR	3407	OHX	1	0
84	6	1945	OHX	3	0
84	A	2037	OHX	1	0
84	6	2021	OHX	1	0
84	1	3406	OHX	5	0
84	AK	102	OHX	2	0
84	CV	201	OHX	1	0
84	4	212	OHX	1	0
84	1	3568	OHX	1	0
84	6	2000	OHX	2	0
84	AR	3582	OHX	2	0
84	A	1918	OHX	1	0
84	A	1937	OHX	1	0
84	1	3524	OHX	1	0
84	AT	212	OHX	1	0
84	1	3677	OHX	1	0
84	6	1977	OHX	1	0
84	1	3668	OHX	2	0
84	AT	214	OHX	2	0
84	AR	3643	OHX	3	0
84	6	1976	OHX	2	0
84	A	1998	OHX	2	0
84	1	3577	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3514	OHX	2	0
84	AR	3707	OHX	1	0
84	AR	3591	OHX	1	0
84	AS	209	OHX	2	0
84	1	3415	OHX	1	0
84	A	2008	OHX	2	0
84	AR	3645	OHX	1	0
84	AR	3731	OHX	6	0
84	AR	3455	OHX	1	0
84	6	1968	OHX	1	0
84	1	3500	OHX	1	0
84	6	1906	OHX	1	0
84	1	3579	OHX	1	0
84	6	1994	OHX	2	0
84	A	1943	OHX	2	0
84	A	1963	OHX	1	0
84	1	3663	OHX	1	0
84	6	1979	OHX	1	0
84	A	1913	OHX	1	0
84	1	3507	OHX	1	0
84	1	3612	OHX	1	0
84	1	3441	OHX	1	0
84	A	1932	OHX	2	0
84	AR	3505	OHX	1	0
84	AR	3524	OHX	3	0
84	6	2012	OHX	1	0
84	CG	302	OHX	4	0
84	1	3637	OHX	1	0
84	AR	3514	OHX	1	0
84	1	3696	OHX	1	0
84	AT	213	OHX	1	0
84	A	1914	OHX	2	0
84	AR	3715	OHX	2	0
84	AR	3480	OHX	1	0
84	AR	3418	OHX	2	0
84	1	3541	OHX	1	0
84	AR	3598	OHX	1	0
84	6	1956	OHX	3	0
84	A	2010	OHX	1	0
84	6	1934	OHX	1	0
84	AR	3516	OHX	1	0
84	1	3538	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	6	2043	OHX	3	0
84	6	2009	OHX	1	0
84	1	3688	OHX	1	0
84	1	3465	OHX	1	0
84	1	3534	OHX	2	0
84	AR	3604	OHX	4	0
84	1	3698	OHX	2	0
84	AR	3568	OHX	3	0
84	1	3448	OHX	2	0
84	1	3491	OHX	1	0
84	A	1962	OHX	1	0
84	AR	3696	OHX	3	0
84	AR	3470	OHX	1	0
84	A	2041	OHX	1	0
84	1	3669	OHX	1	0
84	AR	3439	OHX	1	0
84	6	2039	OHX	1	0
84	AR	3712	OHX	1	0
84	AR	3736	OHX	1	0
84	AR	3721	OHX	2	0
84	Q	201	OHX	2	0
84	AR	3647	OHX	1	0
84	A	1983	OHX	1	0
84	AR	3550	OHX	2	0
84	6	2006	OHX	1	0
84	6	1978	OHX	1	0
84	1	3471	OHX	4	0
86	AR	4239	7MB	3	0
84	AR	3545	OHX	1	0
84	AR	3449	OHX	1	0
84	6	1939	OHX	1	0
84	A	2005	OHX	1	0
84	1	3459	OHX	1	0
84	1	3438	OHX	2	0
84	1	3463	OHX	1	0
84	AR	3509	OHX	2	0
84	AR	3441	OHX	1	0
84	AR	3580	OHX	2	0
84	1	3422	OHX	2	0
84	1	3674	OHX	1	0
84	A	1947	OHX	1	0
84	1	3717	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3515	OHX	2	0
84	AR	3427	OHX	1	0
84	6	2018	OHX	1	0
84	A	2012	OHX	1	0
84	A	1959	OHX	1	0
84	6	1927	OHX	3	0
84	1	3430	OHX	2	0
84	1	3408	OHX	2	0
84	3	203	OHX	1	0
84	1	3505	OHX	1	0
84	AR	3552	OHX	1	0
84	A	1925	OHX	3	0
84	1	3616	OHX	1	0
84	AR	3628	OHX	1	0
84	AR	3700	OHX	2	0
84	1	3513	OHX	1	0
84	AR	3453	OHX	1	0
84	A	2021	OHX	2	0
84	AR	3650	OHX	2	0
84	6	1965	OHX	1	0
84	6	1908	OHX	1	0
84	6	1982	OHX	3	0
84	A	1923	OHX	1	0
84	1	3662	OHX	1	0
84	1	3478	OHX	2	0
84	4	211	OHX	1	0
84	A	1954	OHX	4	0
84	6	2047	OHX	1	0
84	AR	3511	OHX	2	0
84	AR	3484	OHX	2	0
84	AR	3657	OHX	1	0
84	AR	3603	OHX	2	0
84	A	1916	OHX	1	0
84	1	3404	OHX	1	0
84	A	1915	OHX	2	0
84	1	3565	OHX	1	0
84	A	2029	OHX	1	0
84	A	1973	OHX	2	0
84	A	1904	OHX	1	0
84	1	3676	OHX	2	0
84	AR	3456	OHX	3	0
84	1	3618	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3450	OHX	2	0
84	1	3594	OHX	4	0
84	A	1993	OHX	1	0
84	AR	3578	OHX	1	0
84	AT	218	OHX	1	0
84	A	1917	OHX	1	0
84	1	3641	OHX	1	0
84	1	3631	OHX	1	0
84	6	1970	OHX	1	0
84	AR	3478	OHX	2	0
84	AR	3595	OHX	2	0
84	AR	3606	OHX	3	0
84	6	1926	OHX	1	0
84	1	3502	OHX	3	0
84	AR	3500	OHX	2	0
84	1	3410	OHX	2	0
84	A	1905	OHX	1	0
84	1	3474	OHX	1	0
84	AR	3472	OHX	1	0
84	AR	3658	OHX	1	0
84	A	2022	OHX	1	0
84	A	1986	OHX	1	0
84	1	3682	OHX	2	0
84	AR	3538	OHX	1	0
84	1	3613	OHX	1	0
84	AR	3619	OHX	2	0
84	6	2045	OHX	2	0
84	1	3444	OHX	1	0
84	A	1964	OHX	3	0
84	A	1901	OHX	1	0
84	1	3461	OHX	1	0
84	6	2035	OHX	1	0
84	1	3546	OHX	1	0
84	6	2013	OHX	1	0
84	6	2008	OHX	2	0
84	A	1974	OHX	2	0
84	1	3405	OHX	2	0
84	A	2025	OHX	1	0
84	6	2030	OHX	1	0
84	6	2028	OHX	1	0
84	A	1990	OHX	1	0
84	AR	3481	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3413	OHX	2	0
84	6	2037	OHX	1	0
84	AT	206	OHX	1	0
84	AR	3623	OHX	1	0
84	1	3724	OHX	1	0
84	1	3433	OHX	2	0
84	1	3667	OHX	1	0
84	AR	3683	OHX	3	0
84	1	3540	OHX	2	0
84	1	3511	OHX	1	0
84	1	3563	OHX	1	0
84	6	2005	OHX	2	0
84	1	3709	OHX	1	0
84	1	3403	OHX	1	0
84	A	1992	OHX	3	0
84	AR	3739	OHX	2	0
84	AE	201	OHX	4	0
84	AR	3656	OHX	1	0
84	A	1912	OHX	2	0
84	AR	3608	OHX	1	0
84	1	3597	OHX	1	0
84	AR	3519	OHX	1	0
84	1	3596	OHX	1	0
84	AR	3521	OHX	1	0
84	AR	3440	OHX	2	0
84	6	1953	OHX	2	0
84	1	3632	OHX	1	0
84	1	3453	OHX	1	0
84	AR	3571	OHX	1	0
84	A	1948	OHX	1	0
84	1	3582	OHX	3	0
84	1	3595	OHX	1	0
84	AR	3589	OHX	1	0
84	AR	3674	OHX	1	0
84	6	1942	OHX	2	0
84	AR	3635	OHX	1	0
84	AR	3483	OHX	1	0
84	6	1952	OHX	2	0
84	A	1965	OHX	1	0
84	1	3442	OHX	1	0
84	1	3529	OHX	1	0
84	4	209	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3689	OHX	2	0
84	AR	3457	OHX	2	0
84	AR	3460	OHX	1	0
84	AR	3417	OHX	2	0
84	6	1914	OHX	1	0
84	AR	3425	OHX	2	0
84	1	3586	OHX	2	0
84	1	3634	OHX	1	0
84	A	1910	OHX	2	0
84	A	1968	OHX	1	0
84	A	1987	OHX	1	0
84	1	3587	OHX	1	0
84	AR	3548	OHX	2	0
84	AT	210	OHX	1	0
84	1	3629	OHX	1	0
84	6	1992	OHX	1	0
84	1	3691	OHX	1	0
84	1	3544	OHX	1	0
84	AR	3493	OHX	1	0
84	AR	3403	OHX	1	0
84	A	1938	OHX	2	0
84	6	1969	OHX	1	0
84	6	1986	OHX	3	0
84	3	202	OHX	1	0
84	AR	3574	OHX	1	0
84	A	1919	OHX	1	0
84	AR	3526	OHX	2	0
84	1	3553	OHX	1	0
84	AR	3473	OHX	1	0
84	1	3556	OHX	1	0
84	AR	3532	OHX	1	0
84	1	3414	OHX	1	0
84	AR	3586	OHX	1	0
84	1	3690	OHX	1	0
84	1	3730	OHX	3	0
84	6	1985	OHX	1	0
84	6	1980	OHX	1	0
84	1	3661	OHX	1	0
84	O	201	OHX	1	0
84	CK	201	OHX	1	0
84	AR	3468	OHX	1	0
84	1	3485	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3506	OHX	1	0
84	1	3537	OHX	1	0
84	1	3420	OHX	2	0
84	1	3466	OHX	1	0
84	1	3494	OHX	1	0
84	6	1921	OHX	1	0
84	6	2033	OHX	1	0
84	AT	211	OHX	2	0
84	AR	3615	OHX	1	0
84	1	3539	OHX	1	0
84	AR	3490	OHX	2	0
84	AR	3723	OHX	1	0
84	1	3681	OHX	1	0
84	AR	3691	OHX	1	0
84	AR	3613	OHX	1	0
84	A	1922	OHX	1	0
84	A	1902	OHX	1	0
84	1	3617	OHX	1	0
84	1	3619	OHX	1	0
84	1	3440	OHX	1	0
84	AR	3690	OHX	2	0
84	1	3493	OHX	1	0
84	A	1907	OHX	1	0
84	1	3536	OHX	1	0
84	A	1933	OHX	1	0
84	AR	3620	OHX	1	0
84	A	1911	OHX	1	0
84	A	1999	OHX	1	0
84	6	2044	OHX	1	0
84	AR	3518	OHX	2	0
84	A	1981	OHX	1	0
84	1	3472	OHX	1	0
84	AT	208	OHX	1	0
84	A	2030	OHX	3	0
84	AT	202	OHX	1	0
84	A	2023	OHX	1	0
84	6	2050	OHX	3	0
84	6	1924	OHX	1	0
84	AR	3671	OHX	2	0
84	4	202	OHX	1	0
84	A	1984	OHX	1	0
84	6	2040	OHX	1	0

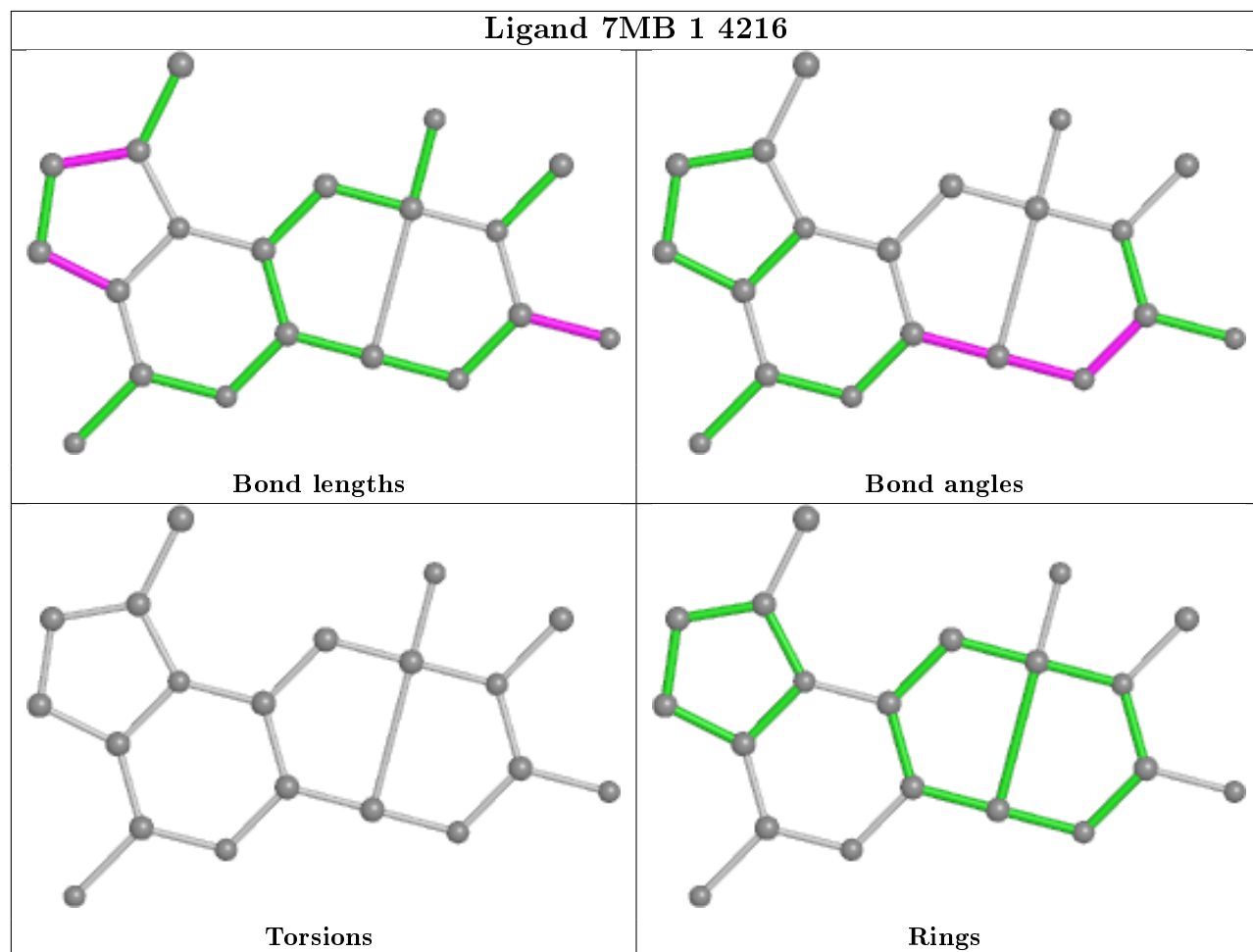
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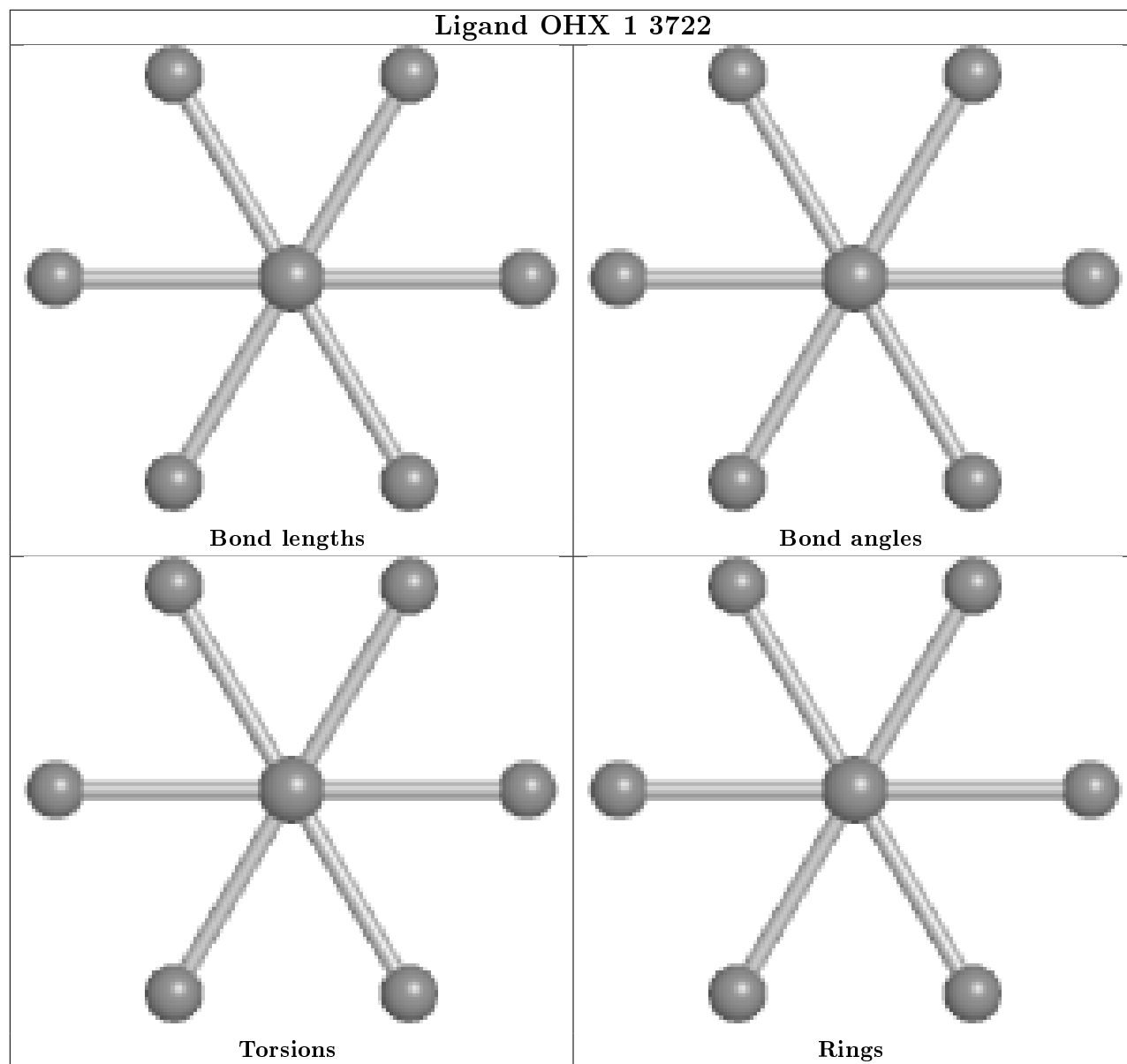
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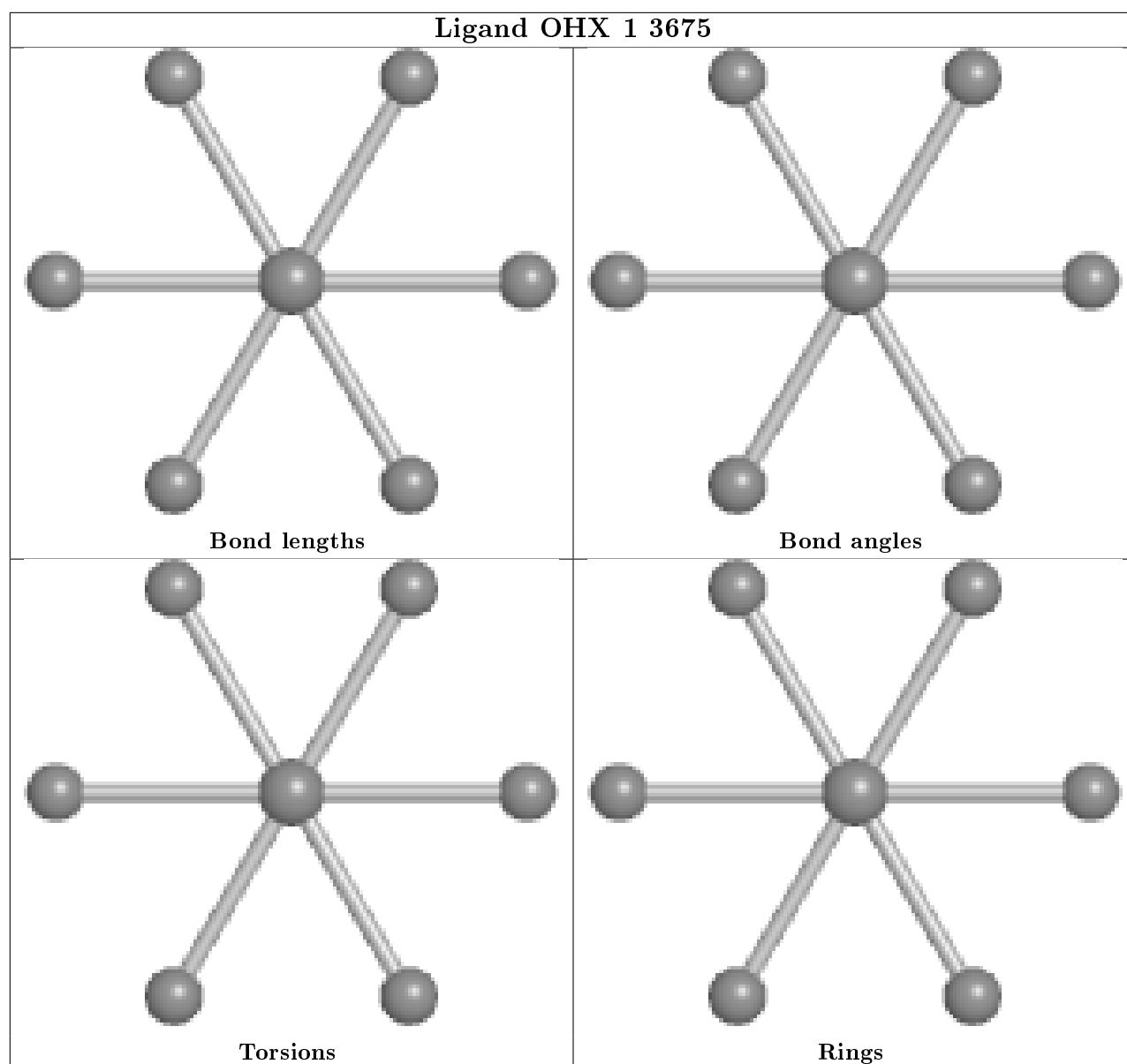
Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3665	OHX	2	0
84	AR	3512	OHX	2	0
84	1	3588	OHX	1	0
84	AS	204	OHX	1	0
84	1	3725	OHX	3	0
84	AR	3641	OHX	1	0
84	1	3437	OHX	2	0
84	3	206	OHX	2	0
84	1	3639	OHX	1	0
84	A	1944	OHX	3	0
84	4	206	OHX	1	0
84	AR	3542	OHX	2	0
84	4	203	OHX	1	0
84	1	3552	OHX	1	0
84	AR	3661	OHX	2	0
84	AR	3459	OHX	1	0
84	AS	202	OHX	2	0
84	A	2000	OHX	1	0
84	CL	301	OHX	2	0
84	1	3610	OHX	1	0
84	3	201	OHX	1	0
84	AR	3530	OHX	1	0
84	1	3628	OHX	1	0
84	4	204	OHX	1	0
84	AR	3601	OHX	2	0
84	1	3542	OHX	2	0
84	A	1939	OHX	3	0
84	1	3646	OHX	1	0
84	6	1991	OHX	1	0
84	AR	3444	OHX	1	0
84	A	1951	OHX	1	0
84	AR	3517	OHX	1	0
84	A	1909	OHX	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	sM	2
25	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	85:SER	C	119:UNK	N	44.36
1	sM	139:UNK	C	155:UNK	N	36.85
1	A	1716:C	O3'	1717:G	P	4.45

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	3149/3396 (92%)	-0.20	55 (1%) 70 64	22, 53, 169, 269	0
1	AR	3149/3396 (92%)	-0.18	58 (1%) 68 62	22, 51, 152, 280	0
2	3	121/121 (100%)	-0.45	0 100 100	33, 69, 92, 108	0
2	AS	121/121 (100%)	-0.51	1 (0%) 86 81	28, 56, 73, 112	0
3	4	158/158 (100%)	-0.18	1 (0%) 89 86	34, 58, 115, 203	0
3	AT	158/158 (100%)	-0.22	1 (0%) 89 86	35, 62, 125, 189	0
4	CD	252/252 (100%)	-0.39	0 100 100	30, 51, 83, 119	0
4	j	252/252 (100%)	-0.39	0 100 100	29, 54, 76, 118	0
5	CE	386/386 (100%)	-0.48	2 (0%) 91 88	21, 40, 65, 139	0
5	k	386/386 (100%)	-0.32	1 (0%) 94 91	28, 54, 77, 122	0
6	CF	361/361 (100%)	-0.37	0 100 100	30, 50, 79, 110	0
6	l	361/361 (100%)	-0.41	0 100 100	28, 49, 82, 101	0
7	CG	296/296 (100%)	-0.22	4 (1%) 75 69	36, 59, 99, 128	0
7	m	296/296 (100%)	0.03	1 (0%) 94 91	46, 78, 115, 168	0
8	CH	156/175 (89%)	-0.30	0 100 100	35, 49, 88, 129	0
8	n	156/175 (89%)	-0.36	0 100 100	35, 46, 79, 132	0
9	CI	222/222 (100%)	-0.49	2 (0%) 84 79	25, 37, 91, 176	0
9	o	222/222 (100%)	-0.42	0 100 100	28, 40, 80, 161	0
10	CJ	233/233 (100%)	0.65	17 (7%) 15 15	64, 87, 146, 191	0
10	p	233/233 (100%)	0.16	3 (1%) 77 71	54, 82, 138, 161	0
11	CK	191/191 (100%)	-0.36	3 (1%) 72 66	33, 46, 77, 143	0
11	q	191/191 (100%)	-0.28	1 (0%) 91 88	46, 62, 84, 149	0
12	CL	211/220 (95%)	-0.06	4 (1%) 66 61	32, 57, 100, 169	0
12	r	211/220 (95%)	-0.36	0 100 100	35, 53, 108, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CM	169/169 (100%)	-0.32	0 100 100	45, 61, 83, 105	0
13	s	169/169 (100%)	-0.00	0 100 100	61, 80, 102, 115	0
14	CN	193/193 (100%)	-0.07	1 (0%) 91 88	33, 67, 131, 148	0
14	t	193/193 (100%)	-0.34	1 (0%) 91 88	30, 60, 113, 144	0
15	CO	136/136 (100%)	-0.57	0 100 100	30, 44, 72, 97	0
15	u	136/136 (100%)	-0.42	0 100 100	42, 52, 77, 105	0
16	CP	203/203 (100%)	-0.32	0 100 100	37, 55, 71, 75	0
16	v	203/203 (100%)	-0.45	0 100 100	30, 51, 64, 74	0
17	CQ	197/197 (100%)	-0.53	1 (0%) 91 88	22, 33, 79, 88	0
17	w	197/197 (100%)	-0.51	0 100 100	27, 41, 75, 85	0
18	CR	183/183 (100%)	0.61	25 (13%) 3 4	25, 41, 181, 234	0
18	x	183/183 (100%)	-0.18	8 (4%) 34 30	33, 42, 124, 165	0
19	CS	185/185 (100%)	-0.40	0 100 100	36, 50, 65, 85	0
19	y	185/185 (100%)	-0.43	0 100 100	36, 49, 84, 123	0
20	CT	188/188 (100%)	-0.13	3 (1%) 72 66	42, 61, 148, 170	0
20	z	188/188 (100%)	0.04	3 (1%) 72 66	53, 73, 158, 171	0
21	0	172/172 (100%)	-0.24	1 (0%) 89 86	37, 46, 72, 91	0
21	CU	172/172 (100%)	-0.54	0 100 100	28, 38, 66, 86	0
22	2	159/159 (100%)	-0.25	0 100 100	31, 48, 111, 126	0
22	CV	159/159 (100%)	-0.37	0 100 100	25, 42, 94, 108	0
23	5	100/100 (100%)	0.55	7 (7%) 16 16	86, 108, 135, 159	0
23	CW	100/100 (100%)	0.69	7 (7%) 16 16	70, 94, 120, 162	0
24	CX	136/136 (100%)	-0.12	0 100 100	21, 37, 66, 96	0
24	l2	136/136 (100%)	-0.06	0 100 100	37, 51, 78, 114	0
25	6	1783/1800 (99%)	-0.05	71 (3%) 38 33	34, 76, 201, 266	0
25	A	1781/1800 (98%)	0.09	82 (4%) 32 28	49, 93, 235, 311	0
26	7	98/98 (100%)	1.65	33 (33%) 0 0	52, 69, 199, 216	0
26	CY	98/98 (100%)	0.57	12 (12%) 4 5	35, 52, 188, 226	0
27	8	121/121 (100%)	-0.04	0 100 100	48, 67, 91, 130	0
27	CZ	121/121 (100%)	-0.07	2 (1%) 70 64	48, 67, 91, 132	0
28	9	126/126 (100%)	-0.06	1 (0%) 86 81	42, 58, 80, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DA	126/126 (100%)	-0.05	1 (0%) 86 81	43, 61, 87, 103	0
29	AA	135/135 (100%)	0.70	4 (2%) 50 44	76, 100, 124, 133	0
29	DB	135/135 (100%)	0.50	4 (2%) 50 44	77, 99, 124, 136	0
30	AB	148/148 (100%)	-0.30	0 100 100	25, 48, 89, 106	0
30	DC	148/148 (100%)	-0.32	0 100 100	26, 52, 87, 95	0
31	AC	58/58 (100%)	-0.41	0 100 100	31, 55, 111, 132	0
31	DD	58/58 (100%)	-0.54	0 100 100	30, 56, 92, 112	0
32	AD	97/97 (100%)	0.42	4 (4%) 37 33	77, 92, 122, 140	0
32	DE	97/97 (100%)	0.16	1 (1%) 82 77	67, 82, 112, 135	0
33	AE	109/109 (100%)	-0.03	2 (1%) 68 62	46, 67, 123, 146	0
33	DF	109/109 (100%)	-0.16	0 100 100	35, 52, 119, 142	0
34	AF	127/127 (100%)	-0.32	2 (1%) 72 66	24, 40, 59, 133	0
34	DG	127/127 (100%)	-0.18	1 (0%) 86 81	24, 46, 66, 132	0
35	AG	106/106 (100%)	-0.58	0 100 100	28, 37, 62, 89	0
35	DH	106/106 (100%)	-0.43	0 100 100	27, 36, 82, 124	0
36	AH	112/112 (100%)	-0.09	0 100 100	53, 73, 130, 149	0
36	DI	112/112 (100%)	-0.20	0 100 100	48, 70, 134, 155	0
37	AI	119/119 (100%)	-0.15	1 (0%) 86 81	45, 68, 85, 92	0
37	DJ	119/119 (100%)	-0.10	2 (1%) 70 64	51, 75, 94, 113	0
38	AJ	99/99 (100%)	0.02	2 (2%) 65 60	50, 69, 116, 148	0
38	DK	99/99 (100%)	0.18	2 (2%) 65 60	59, 74, 118, 154	0
39	AK	87/87 (100%)	-0.46	0 100 100	34, 44, 77, 128	0
39	DL	87/87 (100%)	-0.41	2 (2%) 60 54	33, 47, 88, 167	0
40	AL	77/77 (100%)	0.41	1 (1%) 77 71	78, 94, 120, 130	0
40	DM	77/77 (100%)	1.04	10 (12%) 3 4	75, 94, 120, 129	0
41	AM	50/50 (100%)	-0.44	0 100 100	44, 53, 64, 76	0
41	DN	50/50 (100%)	-0.40	0 100 100	48, 56, 69, 89	0
42	AN	52/52 (100%)	-0.14	0 100 100	43, 53, 81, 108	0
42	DO	52/52 (100%)	-0.49	0 100 100	32, 39, 54, 81	0
43	AO	25/25 (100%)	-0.20	0 100 100	54, 61, 69, 75	0
43	DP	25/25 (100%)	-0.37	0 100 100	42, 50, 62, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AP	105/105 (100%)	0.21	2 (1%) 66 61	36, 59, 96, 156	0
44	DQ	105/105 (100%)	0.08	0 100 100	42, 59, 96, 138	0
45	AQ	91/91 (100%)	-0.37	0 100 100	38, 62, 91, 121	0
45	DR	91/91 (100%)	-0.44	0 100 100	32, 55, 78, 88	0
46	i	159/168 (94%)	0.59	18 (11%) 5 6	56, 101, 165, 178	0
47	p0	143/220 (65%)	1.20	24 (16%) 1 2	100, 113, 177, 185	0
48	sM	63/104 (60%)	0.38	4 (6%) 20 18	54, 106, 129, 136	0
49	B	206/206 (100%)	0.37	10 (4%) 29 26	92, 115, 139, 176	0
49	s0	206/206 (100%)	0.01	1 (0%) 91 88	72, 95, 124, 136	0
50	C	214/216 (99%)	0.87	32 (14%) 2 3	101, 141, 172, 181	0
50	s1	216/216 (100%)	0.34	3 (1%) 75 69	68, 87, 117, 144	0
51	D	217/217 (100%)	0.04	5 (2%) 60 54	69, 91, 118, 142	0
51	s2	217/217 (100%)	0.03	1 (0%) 91 88	55, 75, 97, 121	0
52	E	223/223 (100%)	0.21	7 (3%) 49 43	78, 95, 131, 155	0
52	s3	223/223 (100%)	0.33	10 (4%) 33 29	74, 111, 145, 158	0
53	F	260/260 (100%)	0.37	4 (1%) 73 68	73, 95, 113, 153	0
53	s4	260/260 (100%)	0.02	1 (0%) 92 90	51, 79, 100, 150	0
54	G	206/206 (100%)	0.73	22 (10%) 6 6	98, 121, 152, 179	0
54	s5	206/206 (100%)	0.35	12 (5%) 23 20	71, 92, 124, 157	0
55	H	226/226 (100%)	0.38	6 (2%) 54 48	66, 105, 142, 160	0
55	s6	218/226 (96%)	0.18	6 (2%) 53 47	51, 83, 123, 148	0
56	I	184/186 (98%)	0.58	9 (4%) 29 26	85, 126, 160, 187	0
56	s7	186/186 (100%)	0.32	8 (4%) 35 31	69, 105, 156, 173	0
57	J	188/199 (94%)	0.32	9 (4%) 30 27	58, 77, 128, 150	0
57	s8	188/199 (94%)	0.17	5 (2%) 54 48	43, 68, 121, 138	0
58	K	185/185 (100%)	0.66	16 (8%) 10 11	87, 107, 149, 185	0
58	s9	185/185 (100%)	0.18	3 (1%) 72 66	63, 80, 128, 169	0
59	L	96/105 (91%)	0.41	2 (2%) 63 58	80, 111, 141, 172	0
59	c0	96/105 (91%)	1.29	27 (28%) 0 0	104, 137, 155, 185	0
60	M	155/155 (100%)	0.50	15 (9%) 7 8	60, 76, 162, 194	0
60	c1	146/155 (94%)	0.07	7 (4%) 30 27	42, 64, 118, 151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
61	N	124/124 (100%)	1.26	24 (19%) 1 1	140, 159, 203, 214	0
61	c2	124/124 (100%)	1.71	46 (37%) 0 0	159, 186, 216, 234	0
62	O	150/150 (100%)	0.14	3 (2%) 65 60	60, 90, 112, 129	0
62	c3	150/150 (100%)	-0.23	0 100 100	53, 76, 100, 121	0
63	P	127/128 (99%)	0.67	16 (12%) 3 5	65, 128, 158, 165	0
63	c4	128/128 (100%)	0.61	10 (7%) 13 13	55, 84, 100, 130	0
64	Q	124/141 (87%)	0.36	5 (4%) 38 33	80, 103, 150, 165	0
64	c5	135/141 (95%)	0.41	11 (8%) 12 12	75, 102, 144, 168	0
65	R	141/142 (99%)	0.74	17 (12%) 4 5	83, 110, 129, 132	0
65	c6	142/142 (100%)	0.17	2 (1%) 75 69	62, 88, 109, 141	0
66	S	120/125 (96%)	0.02	2 (1%) 70 64	77, 111, 159, 170	0
67	T	145/145 (100%)	0.42	10 (6%) 16 16	71, 111, 145, 160	0
67	c8	145/145 (100%)	0.01	1 (0%) 87 83	71, 88, 121, 137	0
68	U	143/143 (100%)	0.26	7 (4%) 29 26	89, 112, 136, 148	0
68	c9	143/143 (100%)	0.03	1 (0%) 87 83	66, 85, 109, 139	0
69	V	107/110 (97%)	0.49	8 (7%) 14 14	75, 110, 157, 169	0
69	d0	110/110 (100%)	1.03	23 (20%) 1 1	70, 113, 170, 190	0
70	W	87/87 (100%)	0.42	4 (4%) 32 28	91, 105, 126, 148	0
70	d1	87/87 (100%)	0.18	0 100 100	68, 83, 119, 146	0
71	X	129/129 (100%)	0.01	0 100 100	68, 84, 96, 102	0
71	d2	129/129 (100%)	-0.31	0 100 100	50, 64, 77, 88	0
72	Y	144/144 (100%)	0.03	1 (0%) 87 83	57, 67, 88, 124	0
72	d3	144/144 (100%)	-0.24	0 100 100	40, 49, 73, 108	0
73	Z	134/134 (100%)	0.49	5 (3%) 41 37	82, 111, 137, 155	0
73	d4	134/134 (100%)	0.14	3 (2%) 62 56	59, 89, 117, 159	0
74	a	70/70 (100%)	1.00	10 (14%) 2 3	117, 134, 148, 160	0
74	d5	69/70 (98%)	0.61	3 (4%) 35 31	84, 111, 136, 147	0
75	b	97/97 (100%)	0.38	8 (8%) 11 12	69, 95, 165, 171	0
75	d6	97/97 (100%)	-0.10	0 100 100	54, 68, 110, 126	0
76	c	81/81 (100%)	0.67	9 (11%) 5 6	84, 107, 161, 171	0
76	d7	81/81 (100%)	0.22	5 (6%) 20 18	67, 88, 144, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
77	d	63/63 (100%)	1.19	13 (20%) 1 1	103, 124, 146, 159	0
77	d8	63/63 (100%)	0.94	8 (12%) 3 4	82, 104, 132, 141	0
78	d9	53/53 (100%)	0.21	1 (1%) 66 61	73, 84, 133, 153	0
78	e	53/53 (100%)	-0.24	1 (1%) 66 61	72, 82, 116, 137	0
79	e0	62/62 (100%)	0.27	2 (3%) 47 42	58, 81, 140, 161	0
79	f	60/62 (96%)	0.82	6 (10%) 7 8	65, 98, 158, 164	0
80	g	71/71 (100%)	0.84	12 (16%) 1 2	96, 149, 167, 187	0
81	h	318/318 (100%)	0.85	40 (12%) 3 5	100, 124, 161, 200	0
81	sR	318/318 (100%)	0.79	40 (12%) 3 5	92, 119, 148, 191	0
82	c7	117/121 (96%)	-0.15	1 (0%) 84 79	72, 93, 130, 139	0
83	e1	51/51 (100%)	1.02	10 (19%) 1 1	143, 176, 189, 200	0
All	All	33004/33818 (97%)	0.02	1088 (3%) 46 41	21, 72, 152, 311	0

The worst 5 of 1088 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	A	1709	C	16.0
25	A	1711	C	15.6
25	A	1694	A	14.5
26	7	75	THR	14.4
26	7	76	VAL	13.3

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	6	2193	1/1	0.19	0.90	76,76,76,76	0
85	MG	1	3982	1/1	0.38	0.26	98,98,98,98	0
85	MG	AR	4241	1/1	0.42	0.56	59,59,59,59	0
85	MG	6	2185	1/1	0.50	0.59	60,60,60,60	0
85	MG	6	2181	1/1	0.52	0.49	78,78,78,78	0
85	MG	A	2118	1/1	0.52	0.95	75,75,75,75	0
85	MG	AR	3958	1/1	0.55	0.59	90,90,90,90	0
85	MG	1	4010	1/1	0.56	0.61	44,44,44,44	0
85	MG	A	2110	1/1	0.59	0.39	108,108,108,108	0
85	MG	CK	202	1/1	0.59	0.64	52,52,52,52	0
85	MG	AR	3746	1/1	0.59	0.29	39,39,39,39	0
85	MG	6	2148	1/1	0.59	0.21	69,69,69,69	0
85	MG	A	2046	1/1	0.59	0.20	56,56,56,56	0
85	MG	1	3968	1/1	0.59	0.28	50,50,50,50	0
85	MG	1	4107	1/1	0.60	0.28	66,66,66,66	0
85	MG	A	2112	1/1	0.61	0.41	77,77,77,77	0
85	MG	A	2073	1/1	0.61	0.41	65,65,65,65	0
85	MG	AP	503	1/1	0.61	0.20	61,61,61,61	0
85	MG	1	3966	1/1	0.61	0.21	62,62,62,62	0
85	MG	AR	3812	1/1	0.62	0.41	46,46,46,46	0
85	MG	A	2094	1/1	0.63	0.28	110,110,110,110	0
85	MG	AR	4173	1/1	0.64	0.47	38,38,38,38	0
85	MG	l	402	1/1	0.65	0.45	32,32,32,32	0
85	MG	1	3824	1/1	0.65	0.26	77,77,77,77	0
85	MG	AS	228	1/1	0.67	0.25	48,48,48,48	0
85	MG	1	4124	1/1	0.67	0.22	52,52,52,52	0
85	MG	CO	202	1/1	0.67	0.78	57,57,57,57	0
85	MG	6	2190	1/1	0.67	0.41	84,84,84,84	0
85	MG	A	2075	1/1	0.68	0.37	48,48,48,48	0
85	MG	AR	4167	1/1	0.68	0.51	72,72,72,72	0
85	MG	A	2129	1/1	0.69	0.45	58,58,58,58	0
85	MG	AR	4217	1/1	0.69	0.24	65,65,65,65	0
85	MG	DR	503	1/1	0.69	0.33	54,54,54,54	0
85	MG	1	4162	1/1	0.69	0.28	118,118,118,118	0
85	MG	6	2139	1/1	0.69	0.31	75,75,75,75	0
85	MG	AR	4151	1/1	0.69	0.28	30,30,30,30	0
85	MG	AR	3826	1/1	0.69	0.61	42,42,42,42	0
85	MG	AR	3965	1/1	0.69	0.32	54,54,54,54	0
85	MG	AR	3813	1/1	0.69	0.33	54,54,54,54	0
85	MG	1	4129	1/1	0.70	0.38	51,51,51,51	0
84	OHX	AR	3720	7/7	0.70	0.34	267,269,269,270	0
85	MG	AR	4101	1/1	0.70	0.45	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4092	1/1	0.70	0.16	53,53,53,53	0
85	MG	1	4073	1/1	0.70	0.30	79,79,79,79	0
85	MG	1	4140	1/1	0.70	0.48	49,49,49,49	0
85	MG	AR	3971	1/1	0.71	0.35	38,38,38,38	0
85	MG	AT	223	1/1	0.71	0.91	55,55,55,55	0
85	MG	1	4175	1/1	0.71	0.80	91,91,91,91	0
85	MG	A	2103	1/1	0.71	0.43	64,64,64,64	0
85	MG	1	3801	1/1	0.71	0.52	38,38,38,38	0
85	MG	1	3759	1/1	0.71	0.34	69,69,69,69	0
85	MG	A	2139	1/1	0.72	0.33	86,86,86,86	0
85	MG	A	2084	1/1	0.72	0.16	53,53,53,53	0
85	MG	AR	3804	1/1	0.72	0.45	36,36,36,36	0
85	MG	AR	4024	1/1	0.72	0.42	33,33,33,33	0
85	MG	1	4135	1/1	0.72	0.33	64,64,64,64	0
85	MG	1	4131	1/1	0.72	0.33	38,38,38,38	0
85	MG	1	4102	1/1	0.72	0.39	40,40,40,40	0
84	OHX	CZ	201	7/7	0.72	0.34	303,304,305,305	0
85	MG	AR	4147	1/1	0.73	0.21	62,62,62,62	0
85	MG	AR	4072	1/1	0.73	0.36	71,71,71,71	0
85	MG	A	2086	1/1	0.73	0.30	50,50,50,50	0
85	MG	1	4008	1/1	0.73	1.06	76,76,76,76	0
85	MG	AR	3893	1/1	0.73	0.58	40,40,40,40	0
85	MG	1	4076	1/1	0.73	0.27	71,71,71,71	0
85	MG	1	4078	1/1	0.73	0.21	44,44,44,44	0
85	MG	6	2174	1/1	0.73	0.25	66,66,66,66	0
85	MG	A	2135	1/1	0.73	0.61	50,50,50,50	0
84	OHX	H	301	7/7	0.73	0.32	231,233,235,235	0
85	MG	A	2089	1/1	0.73	0.48	65,65,65,65	0
85	MG	AR	4202	1/1	0.74	0.50	72,72,72,72	0
85	MG	1	3736	1/1	0.74	0.16	82,82,82,82	0
85	MG	AR	4161	1/1	0.74	0.38	56,56,56,56	0
85	MG	6	2097	1/1	0.74	0.30	79,79,79,79	0
85	MG	6	2195	1/1	0.74	0.37	64,64,64,64	0
84	OHX	AR	3664	7/7	0.74	0.30	287,287,288,288	0
85	MG	1	4027	1/1	0.74	0.35	51,51,51,51	0
84	OHX	1	3699	7/7	0.75	0.23	304,306,307,308	0
85	MG	AR	4122	1/1	0.75	0.42	70,70,70,70	0
85	MG	1	3955	1/1	0.75	0.28	52,52,52,52	0
84	OHX	1	3694	7/7	0.75	0.29	251,252,254,254	0
84	OHX	1	3722	7/7	0.75	0.44	268,268,269,269	0
85	MG	1	4136	1/1	0.75	0.38	49,49,49,49	0
84	OHX	AR	3718	7/7	0.76	0.33	255,256,257,257	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3789	1/1	0.76	0.70	51,51,51,51	0
85	MG	c9	201	1/1	0.76	0.11	73,73,73,73	0
85	MG	6	2152	1/1	0.76	0.31	57,57,57,57	0
85	MG	A	2107	1/1	0.76	0.24	69,69,69,69	0
85	MG	AR	3996	1/1	0.76	0.33	38,38,38,38	0
85	MG	1	4183	1/1	0.76	0.47	41,41,41,41	0
85	MG	6	2170	1/1	0.76	0.45	46,46,46,46	0
85	MG	1	4192	1/1	0.76	0.44	38,38,38,38	0
85	MG	A	2147	1/1	0.76	0.20	106,106,106,106	0
85	MG	AR	3820	1/1	0.76	0.64	55,55,55,55	0
85	MG	6	2065	1/1	0.77	0.46	32,32,32,32	0
85	MG	1	4034	1/1	0.77	0.16	33,33,33,33	0
85	MG	AR	4036	1/1	0.77	0.25	68,68,68,68	0
85	MG	1	3758	1/1	0.77	0.46	31,31,31,31	0
85	MG	1	4206	1/1	0.77	0.46	28,28,28,28	0
85	MG	6	2168	1/1	0.77	0.40	50,50,50,50	0
85	MG	A	2127	1/1	0.77	0.30	55,55,55,55	0
85	MG	AR	3880	1/1	0.77	0.43	20,20,20,20	0
85	MG	AR	4164	1/1	0.77	0.31	30,30,30,30	0
85	MG	DR	502	1/1	0.77	0.36	76,76,76,76	0
85	MG	1	3949	1/1	0.77	0.44	41,41,41,41	0
85	MG	A	2098	1/1	0.78	0.44	72,72,72,72	0
85	MG	1	4095	1/1	0.78	0.37	53,53,53,53	0
85	MG	AR	4128	1/1	0.78	0.17	54,54,54,54	0
84	OHX	AR	3687	7/7	0.78	0.37	244,245,246,247	0
85	MG	AR	4220	1/1	0.78	0.38	54,54,54,54	0
85	MG	6	2075	1/1	0.78	0.39	49,49,49,49	0
85	MG	1	4014	1/1	0.78	0.16	46,46,46,46	0
85	MG	F	301	1/1	0.78	0.34	71,71,71,71	0
85	MG	3	218	1/1	0.78	0.31	49,49,49,49	0
85	MG	AR	4214	1/1	0.78	0.42	61,61,61,61	0
85	MG	AR	4026	1/1	0.78	0.21	62,62,62,62	0
85	MG	1	3830	1/1	0.78	0.56	60,60,60,60	0
85	MG	AR	4193	1/1	0.78	0.55	62,62,62,62	0
85	MG	AR	4059	1/1	0.78	0.15	67,67,67,67	0
84	OHX	6	2028	7/7	0.79	0.29	248,250,252,252	0
85	MG	AR	4152	1/1	0.79	0.16	152,152,152,152	0
85	MG	4	217	1/1	0.79	0.48	44,44,44,44	0
84	OHX	A	1985	7/7	0.79	0.36	221,222,223,224	0
84	OHX	1	3675	7/7	0.79	0.57	229,229,230,230	0
84	OHX	AS	210	7/7	0.79	0.33	235,237,238,238	0
85	MG	1	4063	1/1	0.79	0.59	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	ZN	c	101	1/1	0.79	0.22	197,197,197,197	0
85	MG	x	203	1/1	0.79	0.26	64,64,64,64	0
85	MG	A	2109	1/1	0.79	0.31	50,50,50,50	0
85	MG	AH	201	1/1	0.79	0.32	60,60,60,60	0
85	MG	1	3976	1/1	0.79	0.35	61,61,61,61	0
85	MG	A	2137	1/1	0.79	0.34	40,40,40,40	0
85	MG	6	2071	1/1	0.79	0.20	73,73,73,73	0
84	OHX	AR	3716	7/7	0.80	0.35	292,293,293,294	0
85	MG	1	4119	1/1	0.80	0.29	35,35,35,35	0
85	MG	Y	201	1/1	0.80	0.47	51,51,51,51	0
85	MG	6	2179	1/1	0.80	0.30	52,52,52,52	0
85	MG	AS	216	1/1	0.80	0.68	41,41,41,41	0
85	MG	6	2166	1/1	0.80	0.16	36,36,36,36	0
85	MG	1	4001	1/1	0.80	0.31	65,65,65,65	0
84	OHX	AR	3737	7/7	0.80	0.69	260,261,262,262	0
85	MG	AR	4025	1/1	0.80	0.22	40,40,40,40	0
85	MG	AR	3923	1/1	0.80	0.66	32,32,32,32	0
84	OHX	6	2051	7/7	0.80	0.36	228,229,230,231	0
85	MG	AR	4211	1/1	0.80	0.23	86,86,86,86	0
85	MG	AR	4233	1/1	0.80	0.40	55,55,55,55	0
85	MG	6	2081	1/1	0.80	0.31	94,94,94,94	0
85	MG	A	2124	1/1	0.80	0.74	57,57,57,57	0
85	MG	6	2110	1/1	0.80	0.33	40,40,40,40	0
85	MG	AR	3990	1/1	0.81	0.41	37,37,37,37	0
84	OHX	CF	401	7/7	0.81	0.27	245,246,247,247	0
85	MG	AR	4162	1/1	0.81	0.25	54,54,54,54	0
85	MG	AR	4077	1/1	0.81	0.34	49,49,49,49	0
85	MG	AR	4170	1/1	0.81	0.36	128,128,128,128	0
85	MG	1	3974	1/1	0.81	0.40	43,43,43,43	0
85	MG	AR	4221	1/1	0.81	0.27	49,49,49,49	0
85	MG	1	4106	1/1	0.81	0.38	30,30,30,30	0
85	MG	AR	3773	1/1	0.81	0.12	113,113,113,113	0
85	MG	AS	229	1/1	0.81	0.29	68,68,68,68	0
85	MG	AR	4086	1/1	0.81	0.38	28,28,28,28	0
85	MG	1	3947	1/1	0.81	0.41	34,34,34,34	0
84	OHX	1	3693	7/7	0.81	0.45	264,265,266,266	0
85	MG	6	2182	1/1	0.81	0.28	53,53,53,53	0
85	MG	1	3808	1/1	0.81	0.41	54,54,54,54	0
85	MG	1	4030	1/1	0.81	0.44	45,45,45,45	0
87	ZN	e1	501	1/1	0.81	0.09	176,176,176,176	0
85	MG	AT	227	1/1	0.81	0.36	73,73,73,73	0
85	MG	AR	4156	1/1	0.82	0.49	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3727	7/7	0.82	0.34	277,279,280,280	0
85	MG	1	3864	1/1	0.82	0.50	33,33,33,33	0
85	MG	1	3775	1/1	0.82	0.14	59,59,59,59	0
84	OHX	A	2002	7/7	0.82	0.30	242,245,246,247	0
85	MG	AR	4055	1/1	0.82	0.39	47,47,47,47	0
85	MG	AR	4071	1/1	0.82	0.37	32,32,32,32	0
85	MG	AR	4159	1/1	0.82	0.22	64,64,64,64	0
84	OHX	AR	3728	7/7	0.82	0.35	238,238,239,239	0
85	MG	1	3746	1/1	0.82	0.27	59,59,59,59	0
85	MG	CR	203	1/1	0.82	0.33	74,74,74,74	0
85	MG	1	4040	1/1	0.82	0.53	42,42,42,42	0
85	MG	AR	4209	1/1	0.82	0.27	48,48,48,48	0
85	MG	CI	301	1/1	0.82	0.31	48,48,48,48	0
85	MG	CP	502	1/1	0.82	0.38	25,25,25,25	0
85	MG	AR	4058	1/1	0.82	0.18	57,57,57,57	0
85	MG	AT	226	1/1	0.82	0.34	44,44,44,44	0
85	MG	D	301	1/1	0.82	0.58	42,42,42,42	0
85	MG	1	4044	1/1	0.82	0.32	40,40,40,40	0
84	OHX	AS	208	7/7	0.82	0.30	226,226,228,228	0
85	MG	AS	220	1/1	0.82	0.21	42,42,42,42	0
85	MG	AR	4050	1/1	0.82	0.28	46,46,46,46	0
85	MG	A	2104	1/1	0.82	0.27	131,131,131,131	0
84	OHX	1	3717	7/7	0.82	0.48	217,218,219,219	0
85	MG	1	4031	1/1	0.82	0.42	38,38,38,38	0
85	MG	AR	4093	1/1	0.82	0.34	46,46,46,46	0
84	OHX	1	3707	7/7	0.83	0.25	237,237,239,239	0
84	OHX	1	3711	7/7	0.83	0.25	301,302,304,304	0
84	OHX	1	3709	7/7	0.83	0.43	229,231,231,232	0
85	MG	AR	4223	1/1	0.83	0.35	54,54,54,54	0
85	MG	1	3941	1/1	0.83	0.30	36,36,36,36	0
84	OHX	CO	201	7/7	0.83	0.33	281,282,283,284	0
85	MG	AR	3976	1/1	0.83	0.40	42,42,42,42	0
85	MG	1	3963	1/1	0.83	0.16	69,69,69,69	0
85	MG	1	4113	1/1	0.83	0.65	54,54,54,54	0
84	OHX	4	210	7/7	0.83	0.31	236,236,236,236	0
85	MG	1	3964	1/1	0.83	0.33	51,51,51,51	0
85	MG	s	300	1/1	0.83	0.13	53,53,53,53	0
84	OHX	AR	3670	7/7	0.83	0.29	229,230,230,231	0
85	MG	A	2116	1/1	0.83	0.33	49,49,49,49	0
84	OHX	6	1976	7/7	0.83	0.42	182,182,183,184	0
85	MG	CE	406	1/1	0.83	0.59	48,48,48,48	0
85	MG	1	4174	1/1	0.83	0.33	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4070	1/1	0.83	0.29	37,37,37,37	0
85	MG	1	4041	1/1	0.83	0.46	38,38,38,38	0
85	MG	1	4109	1/1	0.83	0.32	37,37,37,37	0
85	MG	AB	203	1/1	0.83	0.31	37,37,37,37	0
85	MG	1	3762	1/1	0.83	0.48	40,40,40,40	0
85	MG	1	4079	1/1	0.83	0.47	47,47,47,47	0
84	OHX	CL	302	7/7	0.83	0.24	200,201,201,202	0
85	MG	1	3840	1/1	0.83	0.18	39,39,39,39	0
84	OHX	1	3726	7/7	0.83	0.42	231,232,233,233	0
85	MG	1	4100	1/1	0.83	0.31	87,87,87,87	0
85	MG	A	2125	1/1	0.83	0.54	51,51,51,51	0
85	MG	1	4038	1/1	0.83	0.34	33,33,33,33	0
85	MG	A	2076	1/1	0.83	0.26	50,50,50,50	0
85	MG	AR	4056	1/1	0.83	0.29	44,44,44,44	0
84	OHX	A	2042	7/7	0.83	0.17	240,242,244,245	0
85	MG	AR	4119	1/1	0.83	0.19	77,77,77,77	0
85	MG	A	2068	1/1	0.83	0.45	68,68,68,68	0
85	MG	AR	4021	1/1	0.83	0.33	36,36,36,36	0
85	MG	AT	231	1/1	0.83	0.56	46,46,46,46	0
85	MG	1	3978	1/1	0.83	0.30	32,32,32,32	0
85	MG	6	2085	1/1	0.83	0.42	40,40,40,40	0
84	OHX	6	2042	7/7	0.83	0.55	246,246,248,248	0
85	MG	AR	4100	1/1	0.84	0.35	67,67,67,67	0
85	MG	1	4184	1/1	0.84	0.23	55,55,55,55	0
85	MG	AR	4234	1/1	0.84	0.28	17,17,17,17	0
85	MG	4	213	1/1	0.84	0.48	34,34,34,34	0
85	MG	AR	3803	1/1	0.84	0.22	54,54,54,54	0
85	MG	1	4161	1/1	0.84	0.28	37,37,37,37	0
84	OHX	6	2025	7/7	0.84	0.20	248,249,250,252	0
85	MG	CR	205	1/1	0.84	0.44	29,29,29,29	0
85	MG	DC	203	1/1	0.84	0.25	35,35,35,35	0
84	OHX	1	3683	7/7	0.84	0.30	197,198,199,199	0
84	OHX	A	2034	7/7	0.84	0.14	277,279,281,282	0
85	MG	1	4185	1/1	0.84	0.57	48,48,48,48	0
85	MG	AR	4001	1/1	0.84	0.43	41,41,41,41	0
85	MG	1	4141	1/1	0.84	0.33	36,36,36,36	0
84	OHX	A	2007	7/7	0.84	0.20	275,277,278,279	0
85	MG	AS	221	1/1	0.84	0.20	36,36,36,36	0
84	OHX	1	3727	7/7	0.84	0.33	253,254,255,256	0
85	MG	AR	3986	1/1	0.84	0.86	41,41,41,41	0
85	MG	A	2088	1/1	0.84	0.27	66,66,66,66	0
85	MG	AR	4125	1/1	0.84	0.22	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3772	1/1	0.84	0.53	81,81,81,81	0
85	MG	AR	3988	1/1	0.84	0.31	32,32,32,32	0
85	MG	AR	4032	1/1	0.84	0.50	47,47,47,47	0
84	OHX	1	3676	7/7	0.84	0.42	223,223,225,225	0
84	OHX	6	2053	7/7	0.84	0.23	250,252,253,254	0
85	MG	1	4064	1/1	0.84	0.34	59,59,59,59	0
85	MG	1	4085	1/1	0.84	0.28	43,43,43,43	0
84	OHX	A	2015	7/7	0.84	0.35	248,250,254,254	0
85	MG	AR	4183	1/1	0.84	0.20	93,93,93,93	0
85	MG	A	2048	1/1	0.84	0.18	42,42,42,42	0
85	MG	AR	4074	1/1	0.84	0.31	44,44,44,44	0
84	OHX	1	3703	7/7	0.84	0.58	259,259,260,261	0
84	OHX	1	3731	7/7	0.84	0.28	201,202,205,205	0
85	MG	AR	3784	1/1	0.84	0.38	29,29,29,29	0
85	MG	1	4181	1/1	0.84	0.23	50,50,50,50	0
84	OHX	6	2057	7/7	0.84	0.17	247,247,250,250	0
85	MG	A	2069	1/1	0.85	0.29	36,36,36,36	0
85	MG	AR	4043	1/1	0.85	0.32	48,48,48,48	0
85	MG	AR	4061	1/1	0.85	0.50	40,40,40,40	0
85	MG	6	2134	1/1	0.85	0.21	43,43,43,43	0
85	MG	AR	3950	1/1	0.85	0.25	41,41,41,41	0
85	MG	AR	4218	1/1	0.85	0.26	31,31,31,31	0
84	OHX	AR	3663	7/7	0.85	0.25	208,209,210,210	0
84	OHX	c5	201	7/7	0.85	0.32	228,229,230,231	0
85	MG	1	4052	1/1	0.85	0.12	48,48,48,48	0
84	OHX	A	2025	7/7	0.85	0.23	249,252,253,253	0
85	MG	6	2123	1/1	0.85	0.30	60,60,60,60	0
85	MG	1	4017	1/1	0.85	0.21	59,59,59,59	0
85	MG	4	222	1/1	0.85	0.44	61,61,61,61	0
85	MG	x	206	1/1	0.85	0.36	32,32,32,32	0
84	OHX	A	1971	7/7	0.85	0.17	216,218,220,221	0
84	OHX	1	3710	7/7	0.85	0.33	247,248,248,249	0
85	MG	DE	201	1/1	0.85	0.15	55,55,55,55	0
84	OHX	6	2054	7/7	0.85	0.24	253,254,256,256	0
84	OHX	6	2045	7/7	0.85	0.39	196,197,198,199	0
85	MG	AR	4155	1/1	0.85	0.29	27,27,27,27	0
85	MG	AR	4015	1/1	0.85	0.35	43,43,43,43	0
85	MG	6	2194	1/1	0.85	0.44	34,34,34,34	0
85	MG	AR	3759	1/1	0.85	0.29	103,103,103,103	0
85	MG	1	4101	1/1	0.85	0.23	37,37,37,37	0
85	MG	AR	3897	1/1	0.85	0.53	18,18,18,18	0
85	MG	t	201	1/1	0.85	0.25	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4131	1/1	0.85	0.56	59,59,59,59	0
85	MG	1	3950	1/1	0.85	0.11	70,70,70,70	0
85	MG	1	4134	1/1	0.85	0.19	50,50,50,50	0
85	MG	4	224	1/1	0.85	0.22	51,51,51,51	0
84	OHX	AR	3669	7/7	0.85	0.16	245,246,247,248	0
85	MG	l2	202	1/1	0.85	0.23	48,48,48,48	0
85	MG	AR	3743	1/1	0.85	0.18	41,41,41,41	0
85	MG	AS	214	1/1	0.85	0.26	68,68,68,68	0
85	MG	1	3795	1/1	0.85	0.32	37,37,37,37	0
84	OHX	CG	302	7/7	0.85	0.24	210,211,212,213	0
85	MG	AR	3955	1/1	0.86	0.25	32,32,32,32	0
85	MG	DA	201	1/1	0.86	0.20	29,29,29,29	0
85	MG	AR	4062	1/1	0.86	0.20	54,54,54,54	0
85	MG	3	213	1/1	0.86	0.51	23,23,23,23	0
84	OHX	6	2027	7/7	0.86	0.32	187,188,189,190	0
85	MG	1	3983	1/1	0.86	0.38	59,59,59,59	0
84	OHX	4	209	7/7	0.86	0.36	194,194,195,195	0
85	MG	1	4032	1/1	0.86	0.29	49,49,49,49	0
85	MG	AR	3962	1/1	0.86	0.20	43,43,43,43	0
85	MG	1	4150	1/1	0.86	1.01	73,73,73,73	0
85	MG	1	3853	1/1	0.86	0.51	61,61,61,61	0
85	MG	1	4194	1/1	0.86	0.23	82,82,82,82	0
84	OHX	6	2029	7/7	0.86	0.45	246,248,249,250	0
85	MG	AR	3899	1/1	0.86	0.35	46,46,46,46	0
85	MG	AR	3849	1/1	0.86	0.59	18,18,18,18	0
85	MG	6	2169	1/1	0.86	0.39	39,39,39,39	0
85	MG	6	2147	1/1	0.86	0.31	75,75,75,75	0
85	MG	1	3960	1/1	0.86	0.30	27,27,27,27	0
85	MG	AR	3808	1/1	0.86	0.23	33,33,33,33	0
85	MG	6	2142	1/1	0.86	0.10	72,72,72,72	0
84	OHX	AR	3702	7/7	0.86	0.41	218,219,220,220	0
85	MG	z	202	1/1	0.86	0.24	62,62,62,62	0
84	OHX	AR	3735	7/7	0.86	0.31	246,247,248,248	0
84	OHX	1	3600	7/7	0.86	0.46	258,258,259,259	0
85	MG	6	2092	1/1	0.86	0.30	45,45,45,45	0
85	MG	1	4180	1/1	0.86	0.45	55,55,55,55	0
85	MG	1	4096	1/1	0.86	0.57	53,53,53,53	0
85	MG	1	4112	1/1	0.86	0.28	41,41,41,41	0
85	MG	AR	3968	1/1	0.86	0.33	29,29,29,29	0
85	MG	DO	202	1/1	0.86	0.27	46,46,46,46	0
84	OHX	AR	3738	7/7	0.86	0.24	270,271,272,272	0
85	MG	1	3984	1/1	0.86	0.30	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3801	1/1	0.86	0.35	30,30,30,30	0
85	MG	1	3887	1/1	0.86	0.12	49,49,49,49	0
85	MG	1	4111	1/1	0.86	0.65	62,62,62,62	0
85	MG	1	4177	1/1	0.86	0.20	45,45,45,45	0
84	OHX	AR	3685	7/7	0.86	0.40	187,187,188,188	0
84	OHX	AR	3717	7/7	0.86	0.32	281,282,283,283	0
85	MG	1	3866	1/1	0.86	0.34	46,46,46,46	0
85	MG	1	3939	1/1	0.86	0.32	29,29,29,29	0
85	MG	AR	4206	1/1	0.86	0.40	31,31,31,31	0
85	MG	AR	3815	1/1	0.86	0.18	75,75,75,75	0
85	MG	AR	3888	1/1	0.86	0.46	33,33,33,33	0
85	MG	AR	4135	1/1	0.86	0.54	66,66,66,66	0
85	MG	1	3821	1/1	0.86	0.56	37,37,37,37	0
85	MG	1	4003	1/1	0.86	0.41	46,46,46,46	0
85	MG	AR	4219	1/1	0.86	0.33	47,47,47,47	0
85	MG	1	4029	1/1	0.86	0.49	42,42,42,42	0
84	OHX	6	2055	7/7	0.86	0.18	234,235,236,236	0
85	MG	AR	4012	1/1	0.86	0.24	50,50,50,50	0
84	OHX	6	2023	7/7	0.86	0.27	201,203,204,205	0
85	MG	6	2167	1/1	0.86	0.42	52,52,52,52	0
84	OHX	AR	3732	7/7	0.86	0.53	245,246,247,247	0
85	MG	AR	4172	1/1	0.86	0.32	25,25,25,25	0
85	MG	4	233	1/1	0.86	0.61	61,61,61,61	0
84	OHX	1	3658	7/7	0.86	0.22	211,212,212,213	0
84	OHX	AR	3671	7/7	0.86	0.27	166,166,167,167	0
85	MG	1	3786	1/1	0.86	0.42	37,37,37,37	0
84	OHX	6	2043	7/7	0.86	0.32	196,196,198,198	0
85	MG	6	2145	1/1	0.86	0.18	51,51,51,51	0
85	MG	A	2065	1/1	0.86	0.34	31,31,31,31	0
84	OHX	A	2029	7/7	0.86	0.14	261,263,265,265	0
84	OHX	AR	3726	7/7	0.87	0.42	220,220,221,221	0
84	OHX	A	2030	7/7	0.87	0.24	208,209,211,212	0
85	MG	1	3871	1/1	0.87	0.28	27,27,27,27	0
84	OHX	1	3705	7/7	0.87	0.42	222,222,223,223	0
85	MG	1	4103	1/1	0.87	0.35	60,60,60,60	0
85	MG	1	3875	1/1	0.87	0.25	18,18,18,18	0
85	MG	1	3833	1/1	0.87	0.30	41,41,41,41	0
85	MG	6	2197	1/1	0.87	0.32	57,57,57,57	0
85	MG	AR	4237	1/1	0.87	0.31	26,26,26,26	0
85	MG	AR	3994	1/1	0.87	0.40	44,44,44,44	0
85	MG	CF	403	1/1	0.87	0.28	30,30,30,30	0
85	MG	AR	4205	1/1	0.87	0.23	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3678	7/7	0.87	0.17	228,228,229,230	0
85	MG	AR	4180	1/1	0.87	0.47	93,93,93,93	0
84	OHX	1	3674	7/7	0.87	0.36	212,212,213,213	0
85	MG	A	2151	1/1	0.87	0.10	72,72,72,72	0
85	MG	6	2121	1/1	0.87	0.22	71,71,71,71	0
85	MG	AR	3835	1/1	0.87	0.39	41,41,41,41	0
85	MG	1	3761	1/1	0.87	0.42	44,44,44,44	0
84	OHX	AR	3609	7/7	0.87	0.31	201,201,202,202	0
85	MG	1	3749	1/1	0.87	0.35	38,38,38,38	0
84	OHX	AR	3729	7/7	0.87	0.32	214,215,216,216	0
85	MG	AR	4029	1/1	0.87	0.35	32,32,32,32	0
85	MG	AR	4153	1/1	0.87	0.26	52,52,52,52	0
85	MG	AR	3834	1/1	0.87	0.18	30,30,30,30	0
85	MG	1	3891	1/1	0.87	0.66	16,16,16,16	0
85	MG	A	2054	1/1	0.87	0.21	59,59,59,59	0
85	MG	AR	3775	1/1	0.87	0.27	16,16,16,16	0
85	MG	z	203	1/1	0.87	0.20	45,45,45,45	0
85	MG	AF	202	1/1	0.87	0.27	32,32,32,32	0
85	MG	AR	4048	1/1	0.87	0.16	33,33,33,33	0
84	OHX	AR	3730	7/7	0.87	0.34	271,272,273,273	0
85	MG	1	4163	1/1	0.87	0.40	68,68,68,68	0
85	MG	AR	4095	1/1	0.87	0.34	36,36,36,36	0
85	MG	AR	3770	1/1	0.87	0.36	36,36,36,36	0
85	MG	1	3981	1/1	0.87	0.36	59,59,59,59	0
85	MG	1	4058	1/1	0.87	0.15	37,37,37,37	0
85	MG	A	2148	1/1	0.87	0.43	103,103,103,103	0
84	OHX	6	2038	7/7	0.87	0.36	213,215,217,217	0
84	OHX	AR	3641	7/7	0.87	0.40	218,219,219,220	0
85	MG	b	101	1/1	0.88	0.22	57,57,57,57	0
85	MG	1	4152	1/1	0.88	0.20	40,40,40,40	0
84	OHX	CM	201	7/7	0.88	0.22	247,248,249,250	0
85	MG	1	4199	1/1	0.88	0.62	25,25,25,25	0
85	MG	1	3961	1/1	0.88	0.34	26,26,26,26	0
84	OHX	1	3719	7/7	0.88	0.38	264,264,265,265	0
85	MG	1	3733	1/1	0.88	0.44	33,33,33,33	0
85	MG	AR	3822	1/1	0.88	0.14	52,52,52,52	0
84	OHX	AR	3695	7/7	0.88	0.24	225,226,227,227	0
84	OHX	1	3638	7/7	0.88	0.22	245,246,247,248	0
84	OHX	O	201	7/7	0.88	0.17	249,252,253,253	0
85	MG	A	2123	1/1	0.88	0.20	40,40,40,40	0
84	OHX	AR	3639	7/7	0.88	0.18	211,212,213,213	0
85	MG	DD	101	1/1	0.88	0.23	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4088	1/1	0.88	0.22	28,28,28,28	0
85	MG	AR	4082	1/1	0.88	0.24	48,48,48,48	0
84	OHX	AR	3705	7/7	0.88	0.28	212,213,213,214	0
85	MG	1	3779	1/1	0.88	0.31	29,29,29,29	0
85	MG	A	2153	1/1	0.88	0.31	66,66,66,66	0
84	OHX	CG	303	7/7	0.88	0.59	212,213,214,214	0
85	MG	AR	4146	1/1	0.88	0.41	37,37,37,37	0
85	MG	o	303	1/1	0.88	0.21	38,38,38,38	0
85	MG	AR	3818	1/1	0.88	0.27	45,45,45,45	0
84	OHX	1	3666	7/7	0.88	0.39	186,187,188,188	0
84	OHX	AR	3644	7/7	0.88	0.26	197,197,198,199	0
84	OHX	AR	3712	7/7	0.88	0.31	183,183,184,184	0
85	MG	AR	3967	1/1	0.88	0.34	64,64,64,64	0
85	MG	AR	3740	1/1	0.88	0.45	46,46,46,46	0
85	MG	1	4217	1/1	0.88	0.29	18,18,18,18	0
84	OHX	1	3728	7/7	0.88	0.35	233,233,233,234	0
84	OHX	CF	402	7/7	0.88	0.47	254,255,256,256	0
85	MG	6	2064	1/1	0.88	0.31	62,62,62,62	0
84	OHX	6	1982	7/7	0.88	0.42	171,172,173,174	0
85	MG	A	2087	1/1	0.88	0.28	57,57,57,57	0
85	MG	AR	3762	1/1	0.88	0.19	40,40,40,40	0
85	MG	1	3951	1/1	0.88	0.33	43,43,43,43	0
84	OHX	A	2040	7/7	0.88	0.24	246,248,249,250	0
85	MG	AR	3964	1/1	0.88	0.30	28,28,28,28	0
85	MG	6	2093	1/1	0.88	0.33	47,47,47,47	0
84	OHX	AR	3711	7/7	0.88	0.20	227,227,228,228	0
85	MG	1	3751	1/1	0.88	0.16	50,50,50,50	0
85	MG	A	2100	1/1	0.88	0.32	60,60,60,60	0
85	MG	1	3774	1/1	0.88	0.21	84,84,84,84	0
84	OHX	A	2031	7/7	0.88	0.23	244,246,248,248	0
85	MG	AR	3771	1/1	0.88	0.22	24,24,24,24	0
85	MG	1	3769	1/1	0.88	0.45	61,61,61,61	0
84	OHX	A	2036	7/7	0.88	0.12	274,277,278,279	0
84	OHX	AR	3734	7/7	0.88	0.29	223,224,224,225	0
84	OHX	AR	3640	7/7	0.88	0.29	197,198,199,199	0
85	MG	d3	203	1/1	0.88	0.23	29,29,29,29	0
84	OHX	A	1993	7/7	0.88	0.40	236,237,239,240	0
84	OHX	6	1960	7/7	0.88	0.21	155,157,157,158	0
85	MG	A	2146	1/1	0.88	0.62	29,29,29,29	0
84	OHX	1	3606	7/7	0.88	0.28	193,194,194,195	0
85	MG	A	2093	1/1	0.88	0.19	93,93,93,93	0
84	OHX	AR	3675	7/7	0.88	0.27	210,211,212,212	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	A	2091	1/1	0.88	0.44	60,60,60,60	0
84	OHX	1	3617	7/7	0.88	0.37	201,202,203,204	0
84	OHX	1	3536	7/7	0.88	0.18	221,221,223,224	0
85	MG	A	2055	1/1	0.88	0.26	48,48,48,48	0
84	OHX	A	1946	7/7	0.88	0.17	212,214,216,217	0
85	MG	AR	3832	1/1	0.88	0.18	46,46,46,46	0
84	OHX	A	2039	7/7	0.88	0.28	264,266,268,268	0
85	MG	1	4179	1/1	0.88	0.15	42,42,42,42	0
85	MG	1	3985	1/1	0.88	0.34	22,22,22,22	0
84	OHX	DL	102	7/7	0.88	0.39	212,212,213,213	0
85	MG	AR	4127	1/1	0.88	0.24	67,67,67,67	0
84	OHX	1	3645	7/7	0.89	0.25	220,221,221,221	0
84	OHX	6	2015	7/7	0.89	0.41	230,231,232,233	0
85	MG	1	3807	1/1	0.89	0.30	37,37,37,37	0
84	OHX	x	201	7/7	0.89	0.44	169,169,170,170	0
85	MG	1	4169	1/1	0.89	0.22	39,39,39,39	0
84	OHX	AR	3668	7/7	0.89	0.32	216,216,217,218	0
85	MG	AS	223	1/1	0.89	0.23	59,59,59,59	0
85	MG	1	3975	1/1	0.89	0.17	43,43,43,43	0
85	MG	1	3781	1/1	0.89	0.25	24,24,24,24	0
84	OHX	AR	3520	7/7	0.89	0.20	175,175,176,176	0
85	MG	AR	4096	1/1	0.89	0.27	53,53,53,53	0
84	OHX	6	2056	7/7	0.89	0.22	214,215,217,218	0
84	OHX	1	3664	7/7	0.89	0.35	232,233,234,235	0
85	MG	1	4142	1/1	0.89	0.58	47,47,47,47	0
85	MG	AR	3913	1/1	0.89	0.35	20,20,20,20	0
85	MG	1	4182	1/1	0.89	0.35	49,49,49,49	0
84	OHX	x	202	7/7	0.89	0.27	223,224,225,225	0
85	MG	6	2189	1/1	0.89	0.29	67,67,67,67	0
85	MG	AR	3830	1/1	0.89	0.29	30,30,30,30	0
85	MG	6	2090	1/1	0.89	0.42	45,45,45,45	0
84	OHX	A	2012	7/7	0.89	0.20	218,220,220,222	0
84	OHX	6	2048	7/7	0.89	0.42	224,224,225,226	0
85	MG	CD	302	1/1	0.89	0.75	39,39,39,39	0
85	MG	AR	3782	1/1	0.89	0.27	30,30,30,30	0
84	OHX	A	2038	7/7	0.89	0.56	217,217,220,220	0
84	OHX	AE	201	7/7	0.89	0.20	194,195,195,196	0
85	MG	A	2117	1/1	0.89	0.20	52,52,52,52	0
85	MG	AR	4042	1/1	0.89	0.26	20,20,20,20	0
85	MG	AR	4130	1/1	0.89	0.17	19,19,19,19	0
85	MG	1	3766	1/1	0.89	0.29	23,23,23,23	0
85	MG	AR	4126	1/1	0.89	0.29	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4063	1/1	0.89	0.17	39,39,39,39	0
85	MG	9	201	1/1	0.89	0.19	33,33,33,33	0
85	MG	AR	4107	1/1	0.89	0.26	79,79,79,79	0
84	OHX	AR	3681	7/7	0.89	0.21	198,199,200,201	0
85	MG	AS	224	1/1	0.89	0.26	55,55,55,55	0
84	OHX	1	3715	7/7	0.89	0.43	219,220,222,222	0
85	MG	AR	3787	1/1	0.89	0.18	31,31,31,31	0
85	MG	4	232	1/1	0.89	0.30	43,43,43,43	0
85	MG	AR	4154	1/1	0.89	0.10	50,50,50,50	0
85	MG	6	2153	1/1	0.89	0.24	39,39,39,39	0
85	MG	1	4047	1/1	0.89	0.72	39,39,39,39	0
85	MG	CQ	203	1/1	0.89	0.40	28,28,28,28	0
85	MG	6	2144	1/1	0.89	0.30	42,42,42,42	0
85	MG	1	4056	1/1	0.89	0.39	82,82,82,82	0
84	OHX	1	3671	7/7	0.89	0.45	212,213,214,214	0
84	OHX	c3	201	7/7	0.89	0.25	212,213,214,215	0
85	MG	1	3877	1/1	0.89	0.13	44,44,44,44	0
84	OHX	AR	3682	7/7	0.89	0.42	213,214,214,215	0
85	MG	AR	3953	1/1	0.89	0.21	35,35,35,35	0
85	MG	AR	4141	1/1	0.89	0.23	53,53,53,53	0
84	OHX	6	2041	7/7	0.89	0.36	209,209,210,211	0
85	MG	1	3977	1/1	0.89	0.35	21,21,21,21	0
84	OHX	6	2047	7/7	0.89	0.32	237,239,240,241	0
85	MG	1	4023	1/1	0.89	0.72	44,44,44,44	0
85	MG	AR	3993	1/1	0.89	0.21	62,62,62,62	0
85	MG	1	3934	1/1	0.89	0.17	61,61,61,61	0
84	OHX	1	3724	7/7	0.89	0.50	243,244,245,246	0
84	OHX	AR	3638	7/7	0.89	0.41	208,208,209,209	0
85	MG	AR	3952	1/1	0.89	0.24	28,28,28,28	0
84	OHX	1	3720	7/7	0.89	0.23	197,197,199,199	0
84	OHX	A	2041	7/7	0.89	0.41	201,203,204,204	0
84	OHX	AR	3719	7/7	0.89	0.25	220,220,221,221	0
84	OHX	AR	3646	7/7	0.89	0.30	167,168,169,169	0
85	MG	1	4207	1/1	0.89	0.31	44,44,44,44	0
84	OHX	AR	3725	7/7	0.89	0.33	261,263,264,264	0
85	MG	4	231	1/1	0.89	0.26	30,30,30,30	0
85	MG	CQ	202	1/1	0.89	0.19	26,26,26,26	0
85	MG	1	4138	1/1	0.89	0.37	37,37,37,37	0
84	OHX	1	3698	7/7	0.89	0.46	177,178,178,179	0
85	MG	1	4050	1/1	0.89	0.30	34,34,34,34	0
84	OHX	1	3597	7/7	0.89	0.13	237,238,240,240	0
85	MG	A	2113	1/1	0.89	0.25	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3632	7/7	0.89	0.31	202,202,204,204	0
84	OHX	AR	3733	7/7	0.89	0.52	289,291,292,292	0
85	MG	AR	4047	1/1	0.89	0.21	30,30,30,30	0
85	MG	1	4033	1/1	0.89	0.26	57,57,57,57	0
85	MG	AR	3794	1/1	0.89	0.34	19,19,19,19	0
85	MG	AR	3811	1/1	0.89	0.30	25,25,25,25	0
85	MG	AR	3788	1/1	0.89	0.43	45,45,45,45	0
84	OHX	1	3695	7/7	0.90	0.23	200,201,202,202	0
84	OHX	1	3692	7/7	0.90	0.31	189,190,191,191	0
84	OHX	1	3635	7/7	0.90	0.26	219,220,221,222	0
84	OHX	AR	3696	7/7	0.90	0.34	176,176,177,178	0
84	OHX	AR	3652	7/7	0.90	0.36	196,196,197,197	0
85	MG	AR	4176	1/1	0.90	0.20	52,52,52,52	0
85	MG	AR	4142	1/1	0.90	0.42	55,55,55,55	0
84	OHX	A	2005	7/7	0.90	0.45	204,206,207,207	0
85	MG	6	2133	1/1	0.90	0.29	51,51,51,51	0
85	MG	AR	4179	1/1	0.90	0.21	58,58,58,58	0
84	OHX	DI	201	7/7	0.90	0.59	194,195,195,196	0
85	MG	AR	4140	1/1	0.90	0.26	24,24,24,24	0
84	OHX	AR	3693	7/7	0.90	0.28	238,239,240,240	0
84	OHX	1	3670	7/7	0.90	0.30	215,215,217,217	0
85	MG	AR	3753	1/1	0.90	0.16	51,51,51,51	0
84	OHX	1	3729	7/7	0.90	0.37	206,207,207,208	0
85	MG	1	4178	1/1	0.90	0.20	42,42,42,42	0
85	MG	1	3809	1/1	0.90	0.32	23,23,23,23	0
85	MG	6	2073	1/1	0.90	0.41	57,57,57,57	0
85	MG	1	4110	1/1	0.90	0.27	37,37,37,37	0
85	MG	AR	3980	1/1	0.90	0.21	32,32,32,32	0
84	OHX	AR	3637	7/7	0.90	0.30	204,205,205,205	0
85	MG	6	2128	1/1	0.90	0.28	53,53,53,53	0
84	OHX	1	3650	7/7	0.90	0.32	179,181,181,182	0
85	MG	AR	4041	1/1	0.90	0.12	47,47,47,47	0
84	OHX	AR	3736	7/7	0.90	0.17	184,185,186,187	0
84	OHX	AR	3710	7/7	0.90	0.32	213,215,216,216	0
84	OHX	AR	3731	7/7	0.90	0.37	175,176,177,178	0
84	OHX	6	2049	7/7	0.90	0.27	218,219,220,221	0
84	OHX	z	201	7/7	0.90	0.23	257,258,259,259	0
84	OHX	AR	3722	7/7	0.90	0.30	200,201,201,202	0
84	OHX	A	1959	7/7	0.90	0.15	180,182,183,184	0
85	MG	DI	202	1/1	0.90	0.26	32,32,32,32	0
85	MG	1	3969	1/1	0.90	0.12	45,45,45,45	0
85	MG	AR	4201	1/1	0.90	0.37	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	A	2134	1/1	0.90	0.56	34,34,34,34	0
84	OHX	A	1996	7/7	0.90	0.27	208,209,211,212	0
85	MG	AS	219	1/1	0.90	0.30	35,35,35,35	0
85	MG	1	3895	1/1	0.90	0.27	29,29,29,29	0
85	MG	AR	3998	1/1	0.90	0.49	18,18,18,18	0
85	MG	AR	4203	1/1	0.90	0.35	37,37,37,37	0
84	OHX	1	3649	7/7	0.90	0.21	247,248,249,250	0
85	MG	AR	3766	1/1	0.90	0.23	21,21,21,21	0
85	MG	1	3897	1/1	0.90	0.38	13,13,13,13	0
85	MG	1	3945	1/1	0.90	0.29	17,17,17,17	0
85	MG	s8	302	1/1	0.90	0.27	44,44,44,44	0
85	MG	1	3988	1/1	0.90	0.26	46,46,46,46	0
85	MG	t	202	1/1	0.90	0.21	64,64,64,64	0
85	MG	AR	4037	1/1	0.90	0.29	33,33,33,33	0
85	MG	1	3767	1/1	0.90	0.12	34,34,34,34	0
85	MG	AR	3855	1/1	0.90	0.14	37,37,37,37	0
84	OHX	CE	403	7/7	0.90	0.50	237,238,239,240	0
85	MG	AR	4060	1/1	0.90	0.27	56,56,56,56	0
85	MG	1	4171	1/1	0.90	0.14	26,26,26,26	0
84	OHX	AR	3688	7/7	0.90	0.28	199,200,201,201	0
84	OHX	AR	3632	7/7	0.90	0.14	227,227,228,228	0
85	MG	1	4108	1/1	0.90	0.26	33,33,33,33	0
85	MG	CO	203	1/1	0.90	0.20	46,46,46,46	0
85	MG	AS	218	1/1	0.90	0.22	52,52,52,52	0
84	OHX	A	2019	7/7	0.90	0.14	252,253,255,256	0
85	MG	AR	3805	1/1	0.90	0.17	39,39,39,39	0
84	OHX	6	2032	7/7	0.90	0.35	236,237,238,239	0
84	OHX	6	2010	7/7	0.90	0.24	213,214,215,216	0
84	OHX	1	3648	7/7	0.90	0.27	258,259,260,260	0
85	MG	AR	3747	1/1	0.90	0.22	23,23,23,23	0
85	MG	1	3780	1/1	0.90	0.26	26,26,26,26	0
85	MG	AR	3951	1/1	0.90	0.17	26,26,26,26	0
85	MG	AR	3839	1/1	0.90	0.38	30,30,30,30	0
84	OHX	AR	3707	7/7	0.90	0.27	207,207,207,207	0
85	MG	6	2120	1/1	0.90	0.17	61,61,61,61	0
84	OHX	6	2052	7/7	0.90	0.25	244,244,246,246	0
84	OHX	1	3680	7/7	0.90	0.39	212,212,213,213	0
84	OHX	1	3704	7/7	0.90	0.40	277,278,278,278	0
84	OHX	6	1980	7/7	0.90	0.38	206,206,208,208	0
85	MG	1	3933	1/1	0.90	0.23	37,37,37,37	0
85	MG	AS	226	1/1	0.90	0.46	36,36,36,36	0
85	MG	1	3880	1/1	0.90	0.50	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3889	1/1	0.90	0.25	42,42,42,42	0
84	OHX	A	2024	7/7	0.90	0.36	219,222,223,223	0
85	MG	1	4043	1/1	0.90	0.35	40,40,40,40	0
85	MG	AR	4181	1/1	0.90	0.20	37,37,37,37	0
84	OHX	AR	3706	7/7	0.90	0.22	209,210,211,212	0
84	OHX	Q	201	7/7	0.90	0.25	245,246,248,249	0
84	OHX	AR	3723	7/7	0.90	0.19	240,241,242,242	0
85	MG	AR	4028	1/1	0.90	0.24	44,44,44,44	0
84	OHX	AR	3701	7/7	0.90	0.41	207,208,208,208	0
85	MG	1	3883	1/1	0.90	0.47	17,17,17,17	0
85	MG	1	4202	1/1	0.90	0.33	27,27,27,27	0
85	MG	1	3998	1/1	0.90	0.24	65,65,65,65	0
85	MG	AR	3884	1/1	0.90	0.27	27,27,27,27	0
84	OHX	A	2023	7/7	0.90	0.23	202,204,206,206	0
85	MG	AR	3995	1/1	0.90	0.11	38,38,38,38	0
84	OHX	6	2034	7/7	0.90	0.26	236,238,239,240	0
85	MG	6	2060	1/1	0.91	0.67	23,23,23,23	0
85	MG	AR	4123	1/1	0.91	0.25	39,39,39,39	0
84	OHX	A	1989	7/7	0.91	0.29	253,254,256,256	0
85	MG	AR	3791	1/1	0.91	0.47	32,32,32,32	0
84	OHX	AT	218	7/7	0.91	0.39	223,224,224,224	0
84	OHX	AT	216	7/7	0.91	0.17	193,193,193,193	0
84	OHX	1	3667	7/7	0.91	0.35	189,189,190,191	0
84	OHX	1	3712	7/7	0.91	0.41	215,215,216,217	0
85	MG	AR	3956	1/1	0.91	0.20	41,41,41,41	0
84	OHX	AT	220	7/7	0.91	0.26	197,197,198,198	0
85	MG	1	4133	1/1	0.91	0.45	28,28,28,28	0
85	MG	1	4153	1/1	0.91	0.21	39,39,39,39	0
85	MG	AR	3984	1/1	0.91	0.34	49,49,49,49	0
85	MG	6	2156	1/1	0.91	0.14	50,50,50,50	0
84	OHX	AR	3713	7/7	0.91	0.16	247,247,248,249	0
85	MG	AR	4081	1/1	0.91	0.31	52,52,52,52	0
85	MG	6	2116	1/1	0.91	0.42	41,41,41,41	0
84	OHX	AR	3678	7/7	0.91	0.53	238,238,239,239	0
84	OHX	AR	3724	7/7	0.91	0.34	203,204,205,205	0
85	MG	A	2052	1/1	0.91	0.46	27,27,27,27	0
84	OHX	AR	3689	7/7	0.91	0.23	195,197,198,198	0
84	OHX	6	2046	7/7	0.91	0.17	244,245,247,248	0
85	MG	AR	4084	1/1	0.91	0.19	31,31,31,31	0
84	OHX	1	3661	7/7	0.91	0.57	251,252,253,253	0
85	MG	1	4051	1/1	0.91	0.37	63,63,63,63	0
84	OHX	AR	3598	7/7	0.91	0.17	205,206,207,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	A	2114	1/1	0.91	0.36	41,41,41,41	0
84	OHX	6	2031	7/7	0.91	0.27	210,211,213,213	0
84	OHX	A	2016	7/7	0.91	0.19	207,209,210,211	0
85	MG	AR	3864	1/1	0.91	0.26	21,21,21,21	0
85	MG	1	3876	1/1	0.91	0.38	39,39,39,39	0
85	MG	1	3986	1/1	0.91	0.13	30,30,30,30	0
85	MG	AR	3831	1/1	0.91	0.32	45,45,45,45	0
84	OHX	1	3718	7/7	0.91	0.38	220,221,221,222	0
84	OHX	AR	3708	7/7	0.91	0.30	228,228,229,229	0
84	OHX	AR	3704	7/7	0.91	0.37	223,224,225,225	0
85	MG	6	2151	1/1	0.91	0.71	87,87,87,87	0
85	MG	6	2160	1/1	0.91	0.24	121,121,121,121	0
85	MG	A	2130	1/1	0.91	0.29	49,49,49,49	0
85	MG	1	4015	1/1	0.91	0.17	38,38,38,38	0
84	OHX	AR	3655	7/7	0.91	0.36	216,218,218,219	0
85	MG	AR	4040	1/1	0.91	0.24	27,27,27,27	0
84	OHX	1	3713	7/7	0.91	0.33	217,217,218,218	0
85	MG	1	3930	1/1	0.91	0.21	19,19,19,19	0
85	MG	1	4002	1/1	0.91	0.21	104,104,104,104	0
85	MG	A	2131	1/1	0.91	0.13	88,88,88,88	0
85	MG	A	2095	1/1	0.91	0.18	94,94,94,94	0
85	MG	d6	101	1/1	0.91	0.24	37,37,37,37	0
84	OHX	1	3651	7/7	0.91	0.30	207,208,209,209	0
85	MG	6	2074	1/1	0.91	0.31	37,37,37,37	0
85	MG	1	4121	1/1	0.91	0.28	32,32,32,32	0
84	OHX	6	2036	7/7	0.91	0.38	172,174,175,176	0
85	MG	AR	4034	1/1	0.91	0.25	42,42,42,42	0
85	MG	6	2157	1/1	0.91	0.26	45,45,45,45	0
85	MG	1	3764	1/1	0.91	0.54	38,38,38,38	0
84	OHX	1	3557	7/7	0.91	0.20	186,187,188,188	0
84	OHX	J	301	7/7	0.91	0.25	244,245,247,247	0
85	MG	AR	4016	1/1	0.91	0.44	104,104,104,104	0
85	MG	AR	4215	1/1	0.91	0.23	72,72,72,72	0
85	MG	AR	4039	1/1	0.91	0.28	37,37,37,37	0
85	MG	AR	4104	1/1	0.91	0.29	55,55,55,55	0
85	MG	AR	3795	1/1	0.91	0.20	22,22,22,22	0
85	MG	d5	201	1/1	0.91	0.09	67,67,67,67	0
84	OHX	AR	3605	7/7	0.91	0.14	194,195,196,196	0
85	MG	AR	3982	1/1	0.91	0.26	35,35,35,35	0
84	OHX	d9	101	7/7	0.91	0.33	234,235,236,237	0
85	MG	AR	4117	1/1	0.91	0.23	53,53,53,53	0
84	OHX	A	2000	7/7	0.91	0.22	194,195,196,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3633	7/7	0.91	0.17	193,194,195,197	0
85	MG	1	4028	1/1	0.91	0.28	24,24,24,24	0
84	OHX	4	211	7/7	0.91	0.24	225,225,226,226	0
84	OHX	A	2032	7/7	0.91	0.19	234,236,237,239	0
84	OHX	6	2011	7/7	0.91	0.20	205,205,207,207	0
84	OHX	AR	3694	7/7	0.91	0.40	212,212,213,213	0
85	MG	6	2196	1/1	0.91	0.38	46,46,46,46	0
85	MG	1	4105	1/1	0.91	0.51	64,64,64,64	0
84	OHX	A	1943	7/7	0.91	0.25	161,163,164,165	0
85	MG	AR	3807	1/1	0.91	0.24	27,27,27,27	0
85	MG	A	2132	1/1	0.91	0.27	71,71,71,71	0
84	OHX	r	301	7/7	0.91	0.19	167,168,168,169	0
84	OHX	1	3656	7/7	0.91	0.26	229,230,231,231	0
85	MG	6	2130	1/1	0.91	0.26	42,42,42,42	0
84	OHX	AR	3666	7/7	0.91	0.20	217,218,218,219	0
84	OHX	AR	3659	7/7	0.91	0.26	195,196,196,197	0
85	MG	1	4120	1/1	0.92	0.18	46,46,46,46	0
84	OHX	AR	3677	7/7	0.92	0.36	180,180,181,181	0
85	MG	AR	4158	1/1	0.92	0.30	21,21,21,21	0
84	OHX	6	2035	7/7	0.92	0.32	157,158,159,159	0
84	OHX	6	2033	7/7	0.92	0.28	199,200,201,202	0
85	MG	DP	101	1/1	0.92	0.20	43,43,43,43	0
85	MG	4	230	1/1	0.92	0.18	54,54,54,54	0
85	MG	1	4045	1/1	0.92	0.11	62,62,62,62	0
85	MG	AR	3764	1/1	0.92	0.18	27,27,27,27	0
84	OHX	6	2044	7/7	0.92	0.35	238,238,239,240	0
84	OHX	6	1993	7/7	0.92	0.24	191,192,193,194	0
84	OHX	6	2022	7/7	0.92	0.11	235,235,238,239	0
84	OHX	AR	3628	7/7	0.92	0.27	209,210,211,211	0
85	MG	AR	4052	1/1	0.92	0.32	28,28,28,28	0
84	OHX	AS	209	7/7	0.92	0.25	175,176,177,177	0
85	MG	AR	4208	1/1	0.92	0.24	62,62,62,62	0
85	MG	A	2152	1/1	0.92	0.16	78,78,78,78	0
85	MG	AR	3979	1/1	0.92	0.24	45,45,45,45	0
84	OHX	6	2000	7/7	0.92	0.16	210,211,212,213	0
84	OHX	AR	3634	7/7	0.92	0.18	213,214,215,216	0
85	MG	AR	4143	1/1	0.92	0.25	38,38,38,38	0
85	MG	AR	4185	1/1	0.92	0.36	40,40,40,40	0
85	MG	6	2087	1/1	0.92	0.39	28,28,28,28	0
85	MG	1	3738	1/1	0.92	0.28	57,57,57,57	0
85	MG	AR	3943	1/1	0.92	0.26	73,73,73,73	0
84	OHX	6	2001	7/7	0.92	0.40	211,211,212,213	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4062	1/1	0.92	0.19	33,33,33,33	0
85	MG	AR	4020	1/1	0.92	0.14	69,69,69,69	0
84	OHX	1	3631	7/7	0.92	0.18	198,199,199,199	0
85	MG	1	4093	1/1	0.92	0.47	16,16,16,16	0
85	MG	AR	3774	1/1	0.92	0.21	23,23,23,23	0
85	MG	AR	4035	1/1	0.92	0.19	39,39,39,39	0
85	MG	6	2155	1/1	0.92	0.14	61,61,61,61	0
85	MG	1	3742	1/1	0.92	0.36	19,19,19,19	0
85	MG	6	2079	1/1	0.92	0.34	37,37,37,37	0
85	MG	A	2101	1/1	0.92	0.24	64,64,64,64	0
85	MG	6	2069	1/1	0.92	0.59	26,26,26,26	0
84	OHX	1	3657	7/7	0.92	0.40	170,171,171,171	0
85	MG	1	4157	1/1	0.92	0.21	37,37,37,37	0
85	MG	1	3754	1/1	0.92	0.32	38,38,38,38	0
84	OHX	1	3708	7/7	0.92	0.30	210,211,211,211	0
84	OHX	A	2006	7/7	0.92	0.25	215,218,219,219	0
84	OHX	AT	219	7/7	0.92	0.38	190,190,190,191	0
85	MG	AR	3828	1/1	0.92	0.30	47,47,47,47	0
84	OHX	AR	3599	7/7	0.92	0.29	201,202,203,203	0
84	OHX	6	2002	7/7	0.92	0.19	218,220,221,221	0
84	OHX	A	1999	7/7	0.92	0.23	214,215,217,217	0
84	OHX	A	1997	7/7	0.92	0.25	211,214,214,215	0
84	OHX	A	2013	7/7	0.92	0.32	203,205,206,206	0
84	OHX	A	2026	7/7	0.92	0.32	191,192,194,194	0
85	MG	1	4006	1/1	0.92	0.23	33,33,33,33	0
85	MG	1	3912	1/1	0.92	0.34	30,30,30,30	0
84	OHX	1	3696	7/7	0.92	0.55	240,240,241,242	0
85	MG	AR	4114	1/1	0.92	0.17	30,30,30,30	0
84	OHX	AR	3647	7/7	0.92	0.31	203,204,205,205	0
85	MG	AR	3977	1/1	0.92	0.54	26,26,26,26	0
85	MG	AR	3973	1/1	0.92	0.19	27,27,27,27	0
84	OHX	1	3701	7/7	0.92	0.24	181,182,182,182	0
85	MG	A	2072	1/1	0.92	0.28	44,44,44,44	0
85	MG	AR	4244	1/1	0.92	0.34	44,44,44,44	0
84	OHX	1	3615	7/7	0.92	0.39	185,186,186,187	0
85	MG	6	2072	1/1	0.92	0.23	36,36,36,36	0
85	MG	AT	225	1/1	0.92	0.17	60,60,60,60	0
85	MG	1	4055	1/1	0.92	0.24	33,33,33,33	0
84	OHX	1	3621	7/7	0.92	0.24	221,223,224,224	0
85	MG	1	3831	1/1	0.92	0.27	42,42,42,42	0
85	MG	1	4005	1/1	0.92	0.63	37,37,37,37	0
84	OHX	1	3672	7/7	0.92	0.39	161,162,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3721	7/7	0.92	0.30	212,213,213,214	0
84	OHX	6	2006	7/7	0.92	0.21	199,199,201,201	0
84	OHX	1	3654	7/7	0.92	0.29	192,194,194,194	0
84	OHX	1	3556	7/7	0.92	0.19	180,181,182,183	0
84	OHX	AR	3597	7/7	0.92	0.20	176,177,178,178	0
85	MG	AR	3806	1/1	0.92	0.22	68,68,68,68	0
85	MG	1	4084	1/1	0.92	0.21	44,44,44,44	0
85	MG	1	3979	1/1	0.92	0.29	47,47,47,47	0
84	OHX	3	208	7/7	0.92	0.16	230,231,232,233	0
85	MG	A	2097	1/1	0.92	0.32	55,55,55,55	0
85	MG	1	3820	1/1	0.92	0.26	30,30,30,30	0
84	OHX	1	3697	7/7	0.92	0.22	238,240,241,241	0
84	OHX	1	3682	7/7	0.92	0.27	204,206,207,207	0
84	OHX	1	3618	7/7	0.92	0.35	189,190,191,192	0
85	MG	1	3898	1/1	0.92	0.33	22,22,22,22	0
84	OHX	1	3601	7/7	0.92	0.33	200,200,201,202	0
85	MG	6	2124	1/1	0.92	0.12	62,62,62,62	0
84	OHX	1	3679	7/7	0.92	0.24	230,231,232,232	0
85	MG	A	2062	1/1	0.92	0.29	48,48,48,48	0
85	MG	AR	4194	1/1	0.92	0.27	47,47,47,47	0
84	OHX	1	3551	7/7	0.92	0.16	191,192,192,193	0
84	OHX	4	212	7/7	0.92	0.24	201,202,202,202	0
85	MG	6	2159	1/1	0.92	0.31	39,39,39,39	0
85	MG	AR	3948	1/1	0.92	0.23	16,16,16,16	0
85	MG	AR	4108	1/1	0.92	0.17	25,25,25,25	0
85	MG	A	2105	1/1	0.92	0.25	71,71,71,71	0
85	MG	AR	3844	1/1	0.92	0.26	25,25,25,25	0
85	MG	1	4146	1/1	0.92	0.16	39,39,39,39	0
85	MG	A	2133	1/1	0.92	0.40	54,54,54,54	0
84	OHX	1	3688	7/7	0.92	0.24	220,221,221,222	0
85	MG	1	4123	1/1	0.92	0.23	41,41,41,41	0
84	OHX	1	3642	7/7	0.92	0.21	193,193,195,195	0
85	MG	1	3834	1/1	0.92	0.42	18,18,18,18	0
85	MG	1	3847	1/1	0.92	0.39	23,23,23,23	0
85	MG	1	3938	1/1	0.92	0.11	41,41,41,41	0
84	OHX	AR	3603	7/7	0.92	0.13	182,183,184,185	0
85	MG	1	4021	1/1	0.92	0.24	29,29,29,29	0
85	MG	AR	4079	1/1	0.92	0.33	36,36,36,36	0
85	MG	AR	4092	1/1	0.92	0.20	25,25,25,25	0
85	MG	1	4011	1/1	0.92	0.18	38,38,38,38	0
85	MG	1	4036	1/1	0.92	0.25	35,35,35,35	0
84	OHX	1	3721	7/7	0.92	0.39	191,192,193,193	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3621	7/7	0.92	0.22	208,209,210,211	0
85	MG	1	3753	1/1	0.92	0.32	28,28,28,28	0
85	MG	AR	3887	1/1	0.92	0.72	35,35,35,35	0
85	MG	A	2140	1/1	0.92	0.30	55,55,55,55	0
85	MG	6	2127	1/1	0.92	0.17	52,52,52,52	0
84	OHX	1	3700	7/7	0.92	0.26	161,162,163,163	0
85	MG	1	4039	1/1	0.92	0.23	40,40,40,40	0
85	MG	4	218	1/1	0.92	0.52	7,7,7,7	0
84	OHX	1	3619	7/7	0.92	0.39	190,191,192,193	0
85	MG	1	3952	1/1	0.92	0.16	34,34,34,34	0
85	MG	A	2149	1/1	0.92	0.36	49,49,49,49	0
85	MG	AR	3792	1/1	0.92	0.38	28,28,28,28	0
85	MG	AR	3876	1/1	0.92	0.43	30,30,30,30	0
85	MG	AR	4075	1/1	0.92	0.33	35,35,35,35	0
84	OHX	AR	3602	7/7	0.92	0.33	192,193,194,194	0
84	OHX	1	3622	7/7	0.92	0.20	211,212,213,213	0
84	OHX	AR	3629	7/7	0.92	0.32	209,210,211,212	0
84	OHX	6	2040	7/7	0.92	0.30	199,200,201,202	0
84	OHX	1	3665	7/7	0.92	0.16	209,210,211,211	0
85	MG	4	227	1/1	0.92	0.21	42,42,42,42	0
84	OHX	AR	3686	7/7	0.92	0.47	186,187,187,187	0
84	OHX	1	3608	7/7	0.92	0.28	177,177,179,179	0
84	OHX	6	2037	7/7	0.92	0.39	203,204,206,206	0
84	OHX	6	1955	7/7	0.92	0.16	191,193,195,196	0
84	OHX	A	1991	7/7	0.92	0.21	218,220,221,221	0
84	OHX	6	1990	7/7	0.92	0.33	238,238,239,240	0
84	OHX	A	1969	7/7	0.92	0.20	220,222,223,223	0
85	MG	A	2085	1/1	0.92	0.20	47,47,47,47	0
84	OHX	6	2039	7/7	0.92	0.18	204,204,206,206	0
84	OHX	A	2017	7/7	0.92	0.24	220,223,224,224	0
85	MG	1	4004	1/1	0.93	0.21	31,31,31,31	0
84	OHX	AR	3586	7/7	0.93	0.14	182,184,185,185	0
85	MG	AT	221	1/1	0.93	0.40	26,26,26,26	0
84	OHX	1	3568	7/7	0.93	0.20	195,196,196,197	0
84	OHX	1	3686	7/7	0.93	0.33	207,208,209,209	0
84	OHX	1	3587	7/7	0.93	0.25	188,189,189,190	0
84	OHX	6	2021	7/7	0.93	0.33	210,210,212,213	0
84	OHX	AR	3714	7/7	0.93	0.43	192,193,193,194	0
85	MG	A	2126	1/1	0.93	0.16	48,48,48,48	0
85	MG	6	2058	1/1	0.93	0.39	33,33,33,33	0
84	OHX	1	3564	7/7	0.93	0.18	173,175,175,175	0
85	MG	1	4128	1/1	0.93	0.19	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3591	7/7	0.93	0.40	168,169,169,169	0
84	OHX	1	3653	7/7	0.93	0.41	193,195,196,196	0
84	OHX	6	2004	7/7	0.93	0.17	193,194,195,196	0
85	MG	1	4203	1/1	0.93	0.52	34,34,34,34	0
85	MG	6	2154	1/1	0.93	0.20	38,38,38,38	0
85	MG	AF	201	1/1	0.93	0.24	27,27,27,27	0
85	MG	AR	4003	1/1	0.93	0.35	73,73,73,73	0
85	MG	AR	3933	1/1	0.93	0.53	13,13,13,13	0
84	OHX	1	3491	7/7	0.93	0.18	138,138,139,139	0
84	OHX	1	3625	7/7	0.93	0.24	186,186,187,187	0
85	MG	A	2067	1/1	0.93	0.57	32,32,32,32	0
84	OHX	6	1998	7/7	0.93	0.19	239,240,243,244	0
85	MG	1	3980	1/1	0.93	0.26	19,19,19,19	0
85	MG	v	302	1/1	0.93	0.39	43,43,43,43	0
85	MG	1	4158	1/1	0.93	0.15	29,29,29,29	0
84	OHX	AR	3581	7/7	0.93	0.32	205,205,205,205	0
85	MG	1	4072	1/1	0.93	0.23	55,55,55,55	0
85	MG	1	3842	1/1	0.93	0.58	27,27,27,27	0
85	MG	AR	3742	1/1	0.93	0.34	29,29,29,29	0
85	MG	d3	202	1/1	0.93	0.54	56,56,56,56	0
84	OHX	1	3681	7/7	0.93	0.28	210,211,212,212	0
85	MG	AR	3907	1/1	0.93	0.36	20,20,20,20	0
85	MG	A	2122	1/1	0.93	0.41	42,42,42,42	0
85	MG	AR	4069	1/1	0.93	0.20	53,53,53,53	0
85	MG	AR	4121	1/1	0.93	0.37	42,42,42,42	0
84	OHX	AR	3616	7/7	0.93	0.35	210,210,211,212	0
85	MG	1	4000	1/1	0.93	0.41	36,36,36,36	0
85	MG	1	3735	1/1	0.93	0.23	39,39,39,39	0
85	MG	1	3914	1/1	0.93	0.54	31,31,31,31	0
85	MG	AR	4145	1/1	0.93	0.14	38,38,38,38	0
85	MG	4	229	1/1	0.93	0.26	57,57,57,57	0
84	OHX	A	2028	7/7	0.93	0.23	252,254,254,256	0
85	MG	1	3940	1/1	0.93	0.21	21,21,21,21	0
84	OHX	1	3630	7/7	0.93	0.19	199,200,200,201	0
85	MG	1	3879	1/1	0.93	0.30	47,47,47,47	0
85	MG	6	2083	1/1	0.93	0.47	35,35,35,35	0
84	OHX	6	2008	7/7	0.93	0.29	211,213,214,216	0
84	OHX	y	201	7/7	0.93	0.26	204,205,207,208	0
85	MG	AR	4044	1/1	0.93	0.25	51,51,51,51	0
84	OHX	4	206	7/7	0.93	0.27	179,179,180,180	0
85	MG	1	3772	1/1	0.93	0.34	32,32,32,32	0
84	OHX	1	3640	7/7	0.93	0.19	194,195,196,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4090	1/1	0.93	0.10	54,54,54,54	0
85	MG	6	2150	1/1	0.93	0.21	51,51,51,51	0
84	OHX	1	401	7/7	0.93	0.38	208,209,210,210	0
85	MG	6	2175	1/1	0.93	0.19	41,41,41,41	0
84	OHX	1	3609	7/7	0.93	0.21	191,193,194,195	0
84	OHX	3	205	7/7	0.93	0.13	169,171,171,173	0
84	OHX	1	3628	7/7	0.93	0.20	234,235,236,237	0
85	MG	AR	4148	1/1	0.93	0.14	36,36,36,36	0
85	MG	4	215	1/1	0.93	0.49	23,23,23,23	0
84	OHX	6	1989	7/7	0.93	0.29	169,170,172,172	0
84	OHX	AR	3660	7/7	0.93	0.35	167,168,169,170	0
84	OHX	1	3714	7/7	0.93	0.17	155,156,157,158	0
85	MG	6	2089	1/1	0.93	0.25	34,34,34,34	0
84	OHX	AR	3676	7/7	0.93	0.29	196,197,198,198	0
85	MG	6	2125	1/1	0.93	0.26	63,63,63,63	0
85	MG	AR	4023	1/1	0.93	0.10	36,36,36,36	0
84	OHX	1	3687	7/7	0.93	0.32	196,196,197,197	0
85	MG	3	215	1/1	0.93	0.23	39,39,39,39	0
85	MG	AR	3972	1/1	0.93	0.30	38,38,38,38	0
85	MG	1	4127	1/1	0.93	0.16	58,58,58,58	0
85	MG	AR	4226	1/1	0.93	0.51	16,16,16,16	0
84	OHX	6	2016	7/7	0.93	0.21	194,194,196,196	0
85	MG	AR	4030	1/1	0.93	0.26	37,37,37,37	0
84	OHX	M	201	7/7	0.93	0.33	202,204,205,206	0
85	MG	1	4024	1/1	0.93	0.37	15,15,15,15	0
85	MG	AR	3875	1/1	0.93	0.20	48,48,48,48	0
85	MG	AR	4018	1/1	0.93	0.12	40,40,40,40	0
84	OHX	CG	301	7/7	0.93	0.13	191,193,193,195	0
84	OHX	A	1995	7/7	0.93	0.15	206,207,208,209	0
85	MG	1	3757	1/1	0.93	0.13	46,46,46,46	0
85	MG	1	4160	1/1	0.93	0.26	40,40,40,40	0
85	MG	1	4060	1/1	0.93	0.55	16,16,16,16	0
85	MG	1	3958	1/1	0.93	0.20	54,54,54,54	0
85	MG	A	2143	1/1	0.93	0.21	151,151,151,151	0
84	OHX	AT	211	7/7	0.93	0.26	179,179,180,180	0
85	MG	6	2095	1/1	0.93	0.58	32,32,32,32	0
85	MG	AR	3989	1/1	0.93	0.32	85,85,85,85	0
85	MG	AR	4090	1/1	0.93	0.27	62,62,62,62	0
84	OHX	AR	3648	7/7	0.93	0.39	196,197,198,198	0
85	MG	AR	4184	1/1	0.93	0.20	35,35,35,35	0
85	MG	AR	4124	1/1	0.93	0.17	54,54,54,54	0
85	MG	AR	4120	1/1	0.93	0.22	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	DC	202	1/1	0.93	0.21	28,28,28,28	0
85	MG	AR	3970	1/1	0.93	0.22	53,53,53,53	0
85	MG	AR	3823	1/1	0.93	0.56	15,15,15,15	0
85	MG	1	3957	1/1	0.93	0.42	29,29,29,29	0
85	MG	AR	4191	1/1	0.93	0.20	38,38,38,38	0
84	OHX	A	2022	7/7	0.93	0.29	229,230,232,233	0
85	MG	A	2121	1/1	0.93	0.08	66,66,66,66	0
85	MG	1	3903	1/1	0.93	0.32	32,32,32,32	0
85	MG	1	3747	1/1	0.93	0.31	28,28,28,28	0
85	MG	AT	224	1/1	0.93	0.54	35,35,35,35	0
85	MG	AR	3769	1/1	0.93	0.13	35,35,35,35	0
84	OHX	1	3723	7/7	0.93	0.19	201,202,203,204	0
85	MG	AR	4213	1/1	0.93	0.21	34,34,34,34	0
84	OHX	1	3634	7/7	0.93	0.21	206,207,207,209	0
84	OHX	AR	3577	7/7	0.93	0.30	201,201,202,202	0
84	OHX	sR	401	7/7	0.93	0.15	215,216,219,219	0
85	MG	1	4159	1/1	0.93	0.16	42,42,42,42	0
84	OHX	6	2024	7/7	0.93	0.18	207,208,210,211	0
85	MG	1	4176	1/1	0.93	0.19	27,27,27,27	0
84	OHX	1	3553	7/7	0.93	0.22	184,185,186,186	0
85	MG	d9	102	1/1	0.93	0.44	106,106,106,106	0
85	MG	AR	3748	1/1	0.93	0.25	41,41,41,41	0
85	MG	1	3737	1/1	0.93	0.26	36,36,36,36	0
85	MG	A	2051	1/1	0.93	0.26	62,62,62,62	0
85	MG	AR	4242	1/1	0.93	0.73	56,56,56,56	0
85	MG	AR	3974	1/1	0.93	0.24	28,28,28,28	0
84	OHX	6	1977	7/7	0.93	0.15	193,194,196,196	0
85	MG	AR	3796	1/1	0.93	0.59	32,32,32,32	0
85	MG	AR	4064	1/1	0.93	0.21	30,30,30,30	0
85	MG	CE	405	1/1	0.93	0.41	34,34,34,34	0
85	MG	1	4075	1/1	0.93	0.23	20,20,20,20	0
84	OHX	A	2027	7/7	0.93	0.18	236,239,240,241	0
85	MG	A	2045	1/1	0.93	0.42	35,35,35,35	0
85	MG	6	2140	1/1	0.93	0.23	46,46,46,46	0
85	MG	AR	4103	1/1	0.93	0.16	35,35,35,35	0
85	MG	AR	4097	1/1	0.93	0.33	26,26,26,26	0
85	MG	AR	4010	1/1	0.93	0.43	28,28,28,28	0
84	OHX	1	3566	7/7	0.93	0.24	182,182,183,183	0
84	OHX	AR	3680	7/7	0.93	0.41	220,222,222,223	0
85	MG	6	2143	1/1	0.93	0.18	90,90,90,90	0
85	MG	AR	3809	1/1	0.93	0.12	86,86,86,86	0
84	OHX	6	2026	7/7	0.93	0.21	218,219,220,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3765	1/1	0.93	0.13	41,41,41,41	0
84	OHX	1	3623	7/7	0.93	0.10	224,225,226,226	0
85	MG	6	2084	1/1	0.93	0.27	35,35,35,35	0
84	OHX	AR	3657	7/7	0.93	0.34	207,207,209,209	0
85	MG	AR	4230	1/1	0.93	0.40	68,68,68,68	0
84	OHX	A	2037	7/7	0.93	0.28	238,240,241,241	0
85	MG	1	4198	1/1	0.93	0.56	36,36,36,36	0
85	MG	AR	4199	1/1	0.93	0.27	64,64,64,64	0
85	MG	1	4025	1/1	0.93	0.24	34,34,34,34	0
85	MG	6	2164	1/1	0.93	0.19	63,63,63,63	0
85	MG	A	2111	1/1	0.93	0.22	68,68,68,68	0
85	MG	AR	4212	1/1	0.93	0.12	48,48,48,48	0
85	MG	1	3810	1/1	0.93	0.23	86,86,86,86	0
84	OHX	6	1964	7/7	0.93	0.20	175,175,177,177	0
85	MG	1	3997	1/1	0.93	0.30	37,37,37,37	0
84	OHX	1	3655	7/7	0.93	0.20	203,204,205,205	0
85	MG	6	2111	1/1	0.93	0.16	42,42,42,42	0
84	OHX	1	3595	7/7	0.93	0.44	190,191,192,192	0
84	OHX	1	3659	7/7	0.93	0.14	208,210,211,211	0
84	OHX	6	1974	7/7	0.93	0.20	176,176,178,178	0
85	MG	1	4089	1/1	0.93	0.21	30,30,30,30	0
85	MG	sM	201	1/1	0.94	0.10	41,41,41,41	0
84	OHX	AR	3679	7/7	0.94	0.24	218,220,221,221	0
85	MG	1	3862	1/1	0.94	0.34	18,18,18,18	0
85	MG	1	3965	1/1	0.94	0.12	32,32,32,32	0
84	OHX	1	3550	7/7	0.94	0.15	196,197,198,199	0
85	MG	1	4130	1/1	0.94	0.28	68,68,68,68	0
84	OHX	1	3580	7/7	0.94	0.17	162,164,164,165	0
84	OHX	A	2001	7/7	0.94	0.18	185,188,189,189	0
85	MG	1	4016	1/1	0.94	0.17	11,11,11,11	0
84	OHX	1	3461	7/7	0.94	0.17	136,137,137,138	0
84	OHX	AR	3573	7/7	0.94	0.19	178,178,179,180	0
85	MG	6	2126	1/1	0.94	0.33	39,39,39,39	0
84	OHX	6	1962	7/7	0.94	0.21	187,188,189,190	0
85	MG	AS	227	1/1	0.94	0.51	43,43,43,43	0
85	MG	1	3900	1/1	0.94	0.74	34,34,34,34	0
85	MG	CP	503	1/1	0.94	0.25	95,95,95,95	0
85	MG	1	3920	1/1	0.94	0.31	29,29,29,29	0
84	OHX	1	3702	7/7	0.94	0.33	179,180,181,182	0
84	OHX	1	3644	7/7	0.94	0.27	170,171,173,173	0
85	MG	CX	203	1/1	0.94	0.15	45,45,45,45	0
85	MG	6	2192	1/1	0.94	0.63	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	6	1941	7/7	0.94	0.17	158,159,160,161	0
85	MG	AR	4169	1/1	0.94	0.14	34,34,34,34	0
84	OHX	1	3605	7/7	0.94	0.31	171,171,172,172	0
84	OHX	AR	3592	7/7	0.94	0.28	151,152,152,153	0
84	OHX	AR	3623	7/7	0.94	0.17	186,187,188,188	0
85	MG	AR	3750	1/1	0.94	0.39	19,19,19,19	0
85	MG	1	3788	1/1	0.94	0.33	34,34,34,34	0
85	MG	A	2071	1/1	0.94	0.32	45,45,45,45	0
85	MG	1	3855	1/1	0.94	0.44	26,26,26,26	0
85	MG	DG	202	1/1	0.94	0.36	21,21,21,21	0
84	OHX	AR	3625	7/7	0.94	0.19	216,216,218,219	0
85	MG	1	4061	1/1	0.94	0.40	23,23,23,23	0
84	OHX	AR	3673	7/7	0.94	0.20	179,180,180,180	0
84	OHX	6	2005	7/7	0.94	0.27	152,153,155,155	0
84	OHX	6	1971	7/7	0.94	0.18	177,178,179,180	0
85	MG	1	4125	1/1	0.94	0.20	58,58,58,58	0
84	OHX	AR	3645	7/7	0.94	0.25	174,175,176,176	0
85	MG	1	3778	1/1	0.94	0.19	20,20,20,20	0
85	MG	AR	4136	1/1	0.94	0.22	41,41,41,41	0
85	MG	6	2184	1/1	0.94	0.27	43,43,43,43	0
84	OHX	AR	3656	7/7	0.94	0.20	187,187,189,189	0
84	OHX	1	3646	7/7	0.94	0.22	182,183,184,185	0
84	OHX	6	1969	7/7	0.94	0.14	163,163,165,165	0
84	OHX	AR	3624	7/7	0.94	0.30	210,211,212,212	0
84	OHX	A	2011	7/7	0.94	0.17	208,209,211,211	0
84	OHX	1	3660	7/7	0.94	0.29	208,209,210,210	0
85	MG	6	2091	1/1	0.94	0.33	54,54,54,54	0
85	MG	1	4188	1/1	0.94	0.21	34,34,34,34	0
85	MG	6	2172	1/1	0.94	0.20	32,32,32,32	0
85	MG	AR	3916	1/1	0.94	0.41	3,3,3,3	0
84	OHX	1	3575	7/7	0.94	0.21	187,188,189,189	0
84	OHX	AR	3674	7/7	0.94	0.41	215,215,216,216	0
85	MG	6	2129	1/1	0.94	0.22	53,53,53,53	0
85	MG	AR	3942	1/1	0.94	0.10	45,45,45,45	0
84	OHX	6	2012	7/7	0.94	0.11	188,189,190,191	0
85	MG	1	3796	1/1	0.94	0.19	33,33,33,33	0
84	OHX	A	1932	7/7	0.94	0.17	178,180,182,182	0
85	MG	A	2128	1/1	0.94	0.26	53,53,53,53	0
85	MG	1	3760	1/1	0.94	0.61	26,26,26,26	0
85	MG	1	4144	1/1	0.94	0.19	59,59,59,59	0
85	MG	6	2080	1/1	0.94	0.15	53,53,53,53	0
85	MG	AR	3896	1/1	0.94	0.43	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3985	1/1	0.94	0.23	19,19,19,19	0
85	MG	s2	301	1/1	0.94	0.60	46,46,46,46	0
85	MG	1	3812	1/1	0.94	0.37	29,29,29,29	0
84	OHX	AR	3556	7/7	0.94	0.19	138,139,140,140	0
85	MG	AR	3918	1/1	0.94	0.40	21,21,21,21	0
84	OHX	AR	3565	7/7	0.94	0.16	161,162,163,164	0
85	MG	1	4213	1/1	0.94	0.21	36,36,36,36	0
85	MG	AR	3961	1/1	0.94	0.19	23,23,23,23	0
85	MG	6	2088	1/1	0.94	0.38	30,30,30,30	0
84	OHX	1	3544	7/7	0.94	0.17	187,188,190,190	0
85	MG	6	2132	1/1	0.94	0.23	38,38,38,38	0
85	MG	1	3743	1/1	0.94	0.39	23,23,23,23	0
85	MG	3	210	1/1	0.94	0.25	41,41,41,41	0
85	MG	1	4149	1/1	0.94	0.22	45,45,45,45	0
85	MG	1	3999	1/1	0.94	0.29	38,38,38,38	0
84	OHX	AR	3620	7/7	0.94	0.27	180,182,183,184	0
85	MG	6	2186	1/1	0.94	0.15	82,82,82,82	0
84	OHX	6	1996	7/7	0.94	0.17	190,191,192,193	0
85	MG	AR	3859	1/1	0.94	0.27	28,28,28,28	0
85	MG	AR	3959	1/1	0.94	0.22	32,32,32,32	0
85	MG	AR	4178	1/1	0.94	0.23	48,48,48,48	0
85	MG	AR	4192	1/1	0.94	0.18	44,44,44,44	0
84	OHX	6	2014	7/7	0.94	0.23	219,220,221,221	0
85	MG	1	3811	1/1	0.94	0.21	42,42,42,42	0
84	OHX	1	3504	7/7	0.94	0.12	154,156,157,158	0
85	MG	1	3989	1/1	0.94	0.48	20,20,20,20	0
85	MG	AR	3879	1/1	0.94	0.54	21,21,21,21	0
85	MG	6	2188	1/1	0.94	0.32	55,55,55,55	0
85	MG	AR	4196	1/1	0.94	0.22	39,39,39,39	0
85	MG	AR	3757	1/1	0.94	0.28	32,32,32,32	0
84	OHX	AR	3633	7/7	0.94	0.32	173,173,174,174	0
84	OHX	6	1995	7/7	0.94	0.18	171,173,174,175	0
84	OHX	1	3725	7/7	0.94	0.08	203,204,205,206	0
85	MG	AR	3838	1/1	0.94	0.61	21,21,21,21	0
85	MG	AR	3992	1/1	0.94	0.50	19,19,19,19	0
85	MG	1	4012	1/1	0.94	0.20	26,26,26,26	0
84	OHX	A	2014	7/7	0.94	0.34	198,199,200,200	0
85	MG	AR	3946	1/1	0.94	0.19	28,28,28,28	0
84	OHX	1	3602	7/7	0.94	0.29	228,229,229,230	0
84	OHX	A	1977	7/7	0.94	0.17	202,205,207,207	0
85	MG	1	3851	1/1	0.94	0.24	34,34,34,34	0
85	MG	1	4170	1/1	0.94	0.22	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3850	1/1	0.94	0.52	11,11,11,11	0
84	OHX	1	3662	7/7	0.94	0.22	178,179,180,180	0
84	OHX	A	1981	7/7	0.94	0.10	231,234,235,236	0
85	MG	1	4116	1/1	0.94	0.12	81,81,81,81	0
84	OHX	1	3570	7/7	0.94	0.15	202,203,204,205	0
85	MG	AR	3963	1/1	0.94	0.38	23,23,23,23	0
85	MG	A	2061	1/1	0.94	0.22	27,27,27,27	0
84	OHX	A	1980	7/7	0.94	0.26	194,196,197,197	0
84	OHX	6	1973	7/7	0.94	0.26	161,162,163,163	0
85	MG	AR	4070	1/1	0.94	0.12	42,42,42,42	0
84	OHX	1	3641	7/7	0.94	0.23	195,196,197,197	0
85	MG	1	4080	1/1	0.94	0.33	55,55,55,55	0
85	MG	1	3967	1/1	0.94	0.16	47,47,47,47	0
84	OHX	AR	3601	7/7	0.94	0.29	171,172,173,173	0
84	OHX	AR	3658	7/7	0.94	0.27	177,177,179,179	0
84	OHX	6	1992	7/7	0.94	0.22	185,186,187,188	0
84	OHX	AR	3703	7/7	0.94	0.42	214,214,214,214	0
85	MG	CR	204	1/1	0.94	0.21	46,46,46,46	0
84	OHX	AR	3667	7/7	0.94	0.23	207,209,210,210	0
84	OHX	1	3511	7/7	0.94	0.17	166,167,168,168	0
85	MG	6	2138	1/1	0.94	0.58	49,49,49,49	0
84	OHX	AR	3690	7/7	0.94	0.23	179,179,180,181	0
84	OHX	1	3691	7/7	0.94	0.30	206,207,208,208	0
85	MG	6	2177	1/1	0.94	0.23	25,25,25,25	0
84	OHX	AR	3684	7/7	0.94	0.47	181,182,183,183	0
85	MG	6	2104	1/1	0.94	0.24	22,22,22,22	0
84	OHX	AR	3539	7/7	0.94	0.12	169,170,172,172	0
84	OHX	AR	3606	7/7	0.94	0.30	155,156,157,157	0
84	OHX	A	1958	7/7	0.94	0.18	206,207,210,210	0
85	MG	1	4042	1/1	0.94	0.16	65,65,65,65	0
85	MG	4	226	1/1	0.94	0.10	54,54,54,54	0
85	MG	1	3959	1/1	0.94	0.23	54,54,54,54	0
85	MG	3	219	1/1	0.94	0.14	77,77,77,77	0
84	OHX	6	1997	7/7	0.94	0.20	198,199,201,201	0
85	MG	CR	206	1/1	0.94	0.15	30,30,30,30	0
85	MG	1	3798	1/1	0.94	0.19	29,29,29,29	0
85	MG	6	2102	1/1	0.94	0.31	14,14,14,14	0
85	MG	AR	4085	1/1	0.94	0.30	37,37,37,37	0
84	OHX	6	1932	7/7	0.94	0.21	129,129,131,131	0
85	MG	DF	201	1/1	0.94	0.31	30,30,30,30	0
85	MG	AR	3827	1/1	0.94	0.45	40,40,40,40	0
85	MG	AR	4216	1/1	0.94	0.30	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3744	1/1	0.94	0.47	20,20,20,20	0
85	MG	1	3953	1/1	0.94	0.29	32,32,32,32	0
85	MG	A	2150	1/1	0.94	0.17	52,52,52,52	0
84	OHX	AR	3564	7/7	0.94	0.17	189,190,190,190	0
85	MG	AR	4102	1/1	0.94	0.32	24,24,24,24	0
84	OHX	AR	3589	7/7	0.94	0.19	186,187,188,189	0
85	MG	AR	4054	1/1	0.94	0.24	33,33,33,33	0
84	OHX	AR	3582	7/7	0.94	0.21	166,167,167,168	0
85	MG	AR	4240	1/1	0.94	0.14	33,33,33,33	0
85	MG	AR	3778	1/1	0.94	0.37	42,42,42,42	0
84	OHX	1	3547	7/7	0.94	0.20	168,169,170,170	0
85	MG	A	2099	1/1	0.94	0.76	64,64,64,64	0
85	MG	AS	215	1/1	0.94	0.67	12,12,12,12	0
85	MG	AT	201	1/1	0.94	0.29	31,31,31,31	0
84	OHX	1	3542	7/7	0.94	0.28	156,157,158,158	0
85	MG	6	2099	1/1	0.94	0.22	19,19,19,19	0
85	MG	6	2062	1/1	0.94	0.36	32,32,32,32	0
84	OHX	AR	3593	7/7	0.94	0.20	173,174,174,174	0
85	MG	AR	4099	1/1	0.94	0.15	44,44,44,44	0
85	MG	AR	3885	1/1	0.94	0.37	38,38,38,38	0
85	MG	AR	4204	1/1	0.94	0.21	31,31,31,31	0
84	OHX	6	1985	7/7	0.94	0.16	191,193,194,195	0
85	MG	AR	3755	1/1	0.94	0.18	34,34,34,34	0
84	OHX	AR	3612	7/7	0.94	0.19	182,183,184,184	0
84	OHX	AR	3618	7/7	0.94	0.19	195,196,196,196	0
85	MG	AR	3997	1/1	0.94	0.26	45,45,45,45	0
84	OHX	A	1960	7/7	0.94	0.15	225,226,227,228	0
85	MG	6	2106	1/1	0.94	0.58	32,32,32,32	0
85	MG	AR	3941	1/1	0.94	0.08	46,46,46,46	0
85	MG	AR	3960	1/1	0.94	0.15	17,17,17,17	0
85	MG	AR	3936	1/1	0.94	0.32	20,20,20,20	0
84	OHX	A	2003	7/7	0.94	0.41	196,198,199,199	0
85	MG	AR	4171	1/1	0.94	0.43	59,59,59,59	0
85	MG	1	4190	1/1	0.94	0.25	26,26,26,26	0
84	OHX	c8	201	7/7	0.94	0.15	198,199,200,201	0
85	MG	AR	3969	1/1	0.94	0.25	38,38,38,38	0
84	OHX	1	3611	7/7	0.94	0.23	184,185,185,186	0
85	MG	o	301	1/1	0.94	0.25	39,39,39,39	0
85	MG	1	3962	1/1	0.94	0.25	33,33,33,33	0
84	OHX	A	1978	7/7	0.94	0.14	210,212,214,214	0
84	OHX	1	3531	7/7	0.94	0.17	179,180,181,181	0
84	OHX	AR	3700	7/7	0.94	0.37	174,175,175,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3938	1/1	0.94	0.52	20,20,20,20	0
85	MG	1	3783	1/1	0.94	0.30	27,27,27,27	0
84	OHX	1	3613	7/7	0.94	0.23	166,166,167,168	0
85	MG	AR	3928	1/1	0.94	0.26	10,10,10,10	0
84	OHX	6	1972	7/7	0.94	0.34	196,197,198,199	0
85	MG	CU	201	1/1	0.94	0.19	44,44,44,44	0
86	7MB	1	4216	20/20	0.94	0.20	48,48,48,48	0
84	OHX	1	3548	7/7	0.94	0.20	179,180,181,181	0
85	MG	1	3763	1/1	0.94	0.31	34,34,34,34	0
85	MG	3	216	1/1	0.94	0.21	35,35,35,35	0
85	MG	1	3802	1/1	0.94	0.21	32,32,32,32	0
85	MG	AR	3824	1/1	0.94	0.14	62,62,62,62	0
84	OHX	CK	201	7/7	0.94	0.24	185,185,186,187	0
84	OHX	1	3592	7/7	0.94	0.26	166,166,167,167	0
84	OHX	AT	214	7/7	0.94	0.26	173,173,174,174	0
84	OHX	1	3647	7/7	0.94	0.30	203,204,205,206	0
84	OHX	3	207	7/7	0.94	0.17	188,189,190,191	0
85	MG	1	4168	1/1	0.94	0.20	51,51,51,51	0
85	MG	CR	201	1/1	0.94	0.44	14,14,14,14	0
85	MG	1	3839	1/1	0.94	0.60	7,7,7,7	0
85	MG	1	3782	1/1	0.94	0.41	44,44,44,44	0
85	MG	DH	202	1/1	0.94	0.16	30,30,30,30	0
84	OHX	AR	3622	7/7	0.94	0.29	203,203,204,205	0
85	MG	AR	3752	1/1	0.94	0.53	16,16,16,16	0
85	MG	AR	3891	1/1	0.94	0.36	36,36,36,36	0
84	OHX	AR	3661	7/7	0.94	0.53	176,177,178,178	0
85	MG	3	217	1/1	0.94	0.15	48,48,48,48	0
84	OHX	1	3578	7/7	0.94	0.24	168,170,170,171	0
87	ZN	d7	101	1/1	0.94	0.29	176,176,176,176	0
84	OHX	AR	3530	7/7	0.94	0.20	147,148,148,148	0
84	OHX	6	1978	7/7	0.94	0.13	176,178,180,181	0
85	MG	AR	4088	1/1	0.94	0.15	50,50,50,50	0
84	OHX	A	1934	7/7	0.94	0.14	176,177,179,179	0
85	MG	1	3804	1/1	0.94	0.61	18,18,18,18	0
84	OHX	AR	3653	7/7	0.95	0.31	178,178,179,179	0
85	MG	1	4081	1/1	0.95	0.11	35,35,35,35	0
84	OHX	1	3596	7/7	0.95	0.29	183,184,185,185	0
84	OHX	AR	3651	7/7	0.95	0.23	229,230,231,231	0
84	OHX	1	3612	7/7	0.95	0.24	173,174,175,175	0
84	OHX	AR	3547	7/7	0.95	0.20	147,147,147,148	0
84	OHX	6	1979	7/7	0.95	0.29	165,165,166,167	0
84	OHX	A	1998	7/7	0.95	0.19	213,217,219,219	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4098	1/1	0.95	0.19	33,33,33,33	0
85	MG	AR	4053	1/1	0.95	0.27	50,50,50,50	0
85	MG	AT	228	1/1	0.95	0.22	34,34,34,34	0
85	MG	AR	4065	1/1	0.95	0.17	54,54,54,54	0
84	OHX	AR	3555	7/7	0.95	0.17	148,149,149,150	0
85	MG	1	4077	1/1	0.95	0.15	42,42,42,42	0
85	MG	1	4009	1/1	0.95	0.40	41,41,41,41	0
84	OHX	6	1994	7/7	0.95	0.26	168,169,171,171	0
84	OHX	4	203	7/7	0.95	0.25	181,182,183,184	0
84	OHX	A	1970	7/7	0.95	0.31	178,180,182,182	0
85	MG	AR	4022	1/1	0.95	0.21	41,41,41,41	0
84	OHX	1	3636	7/7	0.95	0.36	170,171,172,172	0
84	OHX	AR	3626	7/7	0.95	0.32	204,205,205,205	0
85	MG	A	2092	1/1	0.95	0.37	87,87,87,87	0
84	OHX	A	2033	7/7	0.95	0.19	210,212,214,214	0
84	OHX	AR	3615	7/7	0.95	0.23	169,170,171,171	0
84	OHX	AR	3529	7/7	0.95	0.18	161,162,163,163	0
85	MG	6	2198	1/1	0.95	0.19	53,53,53,53	0
84	OHX	1	3534	7/7	0.95	0.18	148,149,149,150	0
85	MG	AR	4002	1/1	0.95	0.41	42,42,42,42	0
85	MG	6	2158	1/1	0.95	0.19	64,64,64,64	0
84	OHX	A	2004	7/7	0.95	0.22	192,194,196,196	0
84	OHX	AR	3496	7/7	0.95	0.15	147,147,148,149	0
85	MG	AR	3921	1/1	0.95	0.27	10,10,10,10	0
84	OHX	CP	501	7/7	0.95	0.23	177,178,178,178	0
85	MG	1	4122	1/1	0.95	0.50	45,45,45,45	0
84	OHX	6	2019	7/7	0.95	0.31	191,192,193,194	0
85	MG	1	4145	1/1	0.95	0.19	48,48,48,48	0
85	MG	1	4049	1/1	0.95	0.18	36,36,36,36	0
85	MG	4	228	1/1	0.95	0.59	42,42,42,42	0
85	MG	AR	4129	1/1	0.95	0.32	21,21,21,21	0
84	OHX	AR	3590	7/7	0.95	0.19	172,173,173,173	0
85	MG	A	2044	1/1	0.95	0.52	25,25,25,25	0
85	MG	AR	3776	1/1	0.95	0.17	32,32,32,32	0
84	OHX	1	3599	7/7	0.95	0.11	190,191,192,193	0
85	MG	AS	212	1/1	0.95	0.38	13,13,13,13	0
84	OHX	AG	201	7/7	0.95	0.27	186,187,188,188	0
85	MG	1	3776	1/1	0.95	0.28	29,29,29,29	0
84	OHX	A	2010	7/7	0.95	0.14	192,195,197,197	0
85	MG	1	3906	1/1	0.95	0.23	29,29,29,29	0
85	MG	AR	3930	1/1	0.95	0.39	14,14,14,14	0
85	MG	A	2079	1/1	0.95	0.58	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3567	7/7	0.95	0.16	159,159,160,160	0
85	MG	1	3745	1/1	0.95	0.48	20,20,20,20	0
85	MG	s6	301	1/1	0.95	0.26	64,64,64,64	0
84	OHX	6	1981	7/7	0.95	0.34	195,197,199,199	0
85	MG	AR	4004	1/1	0.95	0.33	27,27,27,27	0
84	OHX	6	1958	7/7	0.95	0.21	153,153,155,156	0
84	OHX	AR	3554	7/7	0.95	0.29	159,160,161,161	0
85	MG	AR	4137	1/1	0.95	0.16	57,57,57,57	0
85	MG	A	2074	1/1	0.95	0.55	38,38,38,38	0
85	MG	AR	3857	1/1	0.95	0.14	46,46,46,46	0
85	MG	4	214	1/1	0.95	0.46	18,18,18,18	0
85	MG	1	4066	1/1	0.95	0.28	66,66,66,66	0
85	MG	AR	3902	1/1	0.95	0.69	24,24,24,24	0
85	MG	AR	3939	1/1	0.95	0.43	16,16,16,16	0
85	MG	1	4091	1/1	0.95	0.15	49,49,49,49	0
84	OHX	6	2009	7/7	0.95	0.22	181,181,183,183	0
84	OHX	AR	3517	7/7	0.95	0.15	134,135,135,136	0
84	OHX	A	2009	7/7	0.95	0.32	191,192,194,195	0
84	OHX	A	2018	7/7	0.95	0.16	214,215,216,217	0
84	OHX	4	205	7/7	0.95	0.23	172,173,174,174	0
84	OHX	k	402	7/7	0.95	0.20	156,157,158,158	0
84	OHX	1	3512	7/7	0.95	0.12	170,172,172,173	0
85	MG	AR	3749	1/1	0.95	0.26	19,19,19,19	0
84	OHX	6	1983	7/7	0.95	0.35	169,169,170,170	0
84	OHX	6	1954	7/7	0.95	0.11	181,182,184,185	0
84	OHX	AR	3594	7/7	0.95	0.17	169,170,171,171	0
84	OHX	1	3584	7/7	0.95	0.29	154,155,156,156	0
85	MG	AR	3862	1/1	0.95	0.27	20,20,20,20	0
84	OHX	AR	3650	7/7	0.95	0.39	177,177,178,178	0
85	MG	AR	3758	1/1	0.95	0.34	81,81,81,81	0
84	OHX	6	2020	7/7	0.95	0.23	177,178,179,179	0
85	MG	AR	3780	1/1	0.95	0.27	20,20,20,20	0
84	OHX	AR	3546	7/7	0.95	0.17	140,140,141,141	0
85	MG	AR	4177	1/1	0.95	0.23	18,18,18,18	0
85	MG	6	2114	1/1	0.95	0.36	28,28,28,28	0
84	OHX	A	2020	7/7	0.95	0.17	188,191,192,192	0
84	OHX	1	3545	7/7	0.95	0.18	156,157,158,159	0
84	OHX	AR	3559	7/7	0.95	0.14	177,178,179,179	0
85	MG	1	3740	1/1	0.95	0.41	7,7,7,7	0
85	MG	1	3852	1/1	0.95	0.59	22,22,22,22	0
84	OHX	AR	3588	7/7	0.95	0.16	176,177,178,178	0
85	MG	1	3918	1/1	0.95	0.37	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4026	1/1	0.95	0.54	44,44,44,44	0
84	OHX	6	2050	7/7	0.95	0.27	190,191,192,193	0
84	OHX	AR	3584	7/7	0.95	0.36	169,169,170,171	0
85	MG	A	2053	1/1	0.95	0.33	39,39,39,39	0
84	OHX	1	3523	7/7	0.95	0.20	157,158,159,160	0
85	MG	1	4210	1/1	0.95	0.31	32,32,32,32	0
84	OHX	A	1929	7/7	0.95	0.22	157,159,160,160	0
85	MG	1	3818	1/1	0.95	0.39	19,19,19,19	0
84	OHX	AR	3631	7/7	0.95	0.15	153,155,155,155	0
85	MG	6	2173	1/1	0.95	0.19	69,69,69,69	0
84	OHX	A	1982	7/7	0.95	0.29	164,166,167,167	0
85	MG	1	4154	1/1	0.95	0.20	92,92,92,92	0
84	OHX	1	3565	7/7	0.95	0.16	168,169,170,170	0
85	MG	AR	3919	1/1	0.95	0.56	11,11,11,11	0
85	MG	1	3829	1/1	0.95	0.38	25,25,25,25	0
84	OHX	AT	215	7/7	0.95	0.23	212,213,213,213	0
85	MG	1	4068	1/1	0.95	0.20	39,39,39,39	0
84	OHX	1	3663	7/7	0.95	0.32	214,216,217,217	0
84	OHX	1	3594	7/7	0.95	0.26	150,150,151,151	0
84	OHX	1	3543	7/7	0.95	0.14	166,166,167,167	0
85	MG	AR	3966	1/1	0.95	0.24	24,24,24,24	0
85	MG	3	212	1/1	0.95	0.30	27,27,27,27	0
85	MG	AR	4186	1/1	0.95	0.34	33,33,33,33	0
85	MG	AR	4187	1/1	0.95	0.67	27,27,27,27	0
85	MG	6	2131	1/1	0.95	0.38	32,32,32,32	0
85	MG	1	3919	1/1	0.95	0.65	30,30,30,30	0
85	MG	AR	3797	1/1	0.95	0.38	18,18,18,18	0
84	OHX	A	1947	7/7	0.95	0.30	162,164,165,165	0
85	MG	1	3755	1/1	0.95	0.21	41,41,41,41	0
84	OHX	1	3673	7/7	0.95	0.16	192,193,194,194	0
84	OHX	6	2030	7/7	0.95	0.38	160,161,162,162	0
84	OHX	1	3539	7/7	0.95	0.20	169,169,170,170	0
84	OHX	1	3668	7/7	0.95	0.28	179,179,180,181	0
85	MG	1	3915	1/1	0.95	0.55	19,19,19,19	0
85	MG	6	2108	1/1	0.95	0.29	44,44,44,44	0
84	OHX	AR	3566	7/7	0.95	0.17	205,206,207,207	0
84	OHX	AR	3500	7/7	0.95	0.12	136,138,139,140	0
84	OHX	1	3526	7/7	0.95	0.13	167,168,169,170	0
85	MG	1	3888	1/1	0.95	0.26	21,21,21,21	0
84	OHX	AR	3613	7/7	0.95	0.29	165,166,167,167	0
85	MG	AR	4175	1/1	0.95	0.14	27,27,27,27	0
85	MG	AR	3848	1/1	0.95	0.25	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3846	1/1	0.95	0.57	17,17,17,17	0
85	MG	1	403	1/1	0.95	0.26	20,20,20,20	0
85	MG	1	3799	1/1	0.95	0.30	28,28,28,28	0
85	MG	1	3734	1/1	0.95	0.32	27,27,27,27	0
84	OHX	AR	3524	7/7	0.95	0.23	152,153,154,155	0
84	OHX	AR	3709	7/7	0.95	0.18	163,163,164,164	0
85	MG	1	3907	1/1	0.95	0.37	13,13,13,13	0
85	MG	AR	3945	1/1	0.95	0.43	22,22,22,22	0
85	MG	1	3937	1/1	0.95	0.29	58,58,58,58	0
85	MG	6	2171	1/1	0.95	0.23	34,34,34,34	0
85	MG	1	4114	1/1	0.95	0.13	33,33,33,33	0
84	OHX	s8	301	7/7	0.95	0.33	214,216,216,218	0
85	MG	1	4053	1/1	0.95	0.18	32,32,32,32	0
85	MG	AR	3810	1/1	0.95	0.29	28,28,28,28	0
85	MG	A	2115	1/1	0.95	0.27	85,85,85,85	0
84	OHX	A	1966	7/7	0.95	0.14	194,195,196,197	0
84	OHX	1	3540	7/7	0.95	0.24	145,146,146,148	0
85	MG	AR	3789	1/1	0.95	0.24	36,36,36,36	0
84	OHX	A	2035	7/7	0.95	0.30	177,178,180,181	0
85	MG	3	220	1/1	0.95	0.34	31,31,31,31	0
84	OHX	AR	3526	7/7	0.95	0.21	164,166,167,167	0
84	OHX	6	1966	7/7	0.95	0.14	164,165,166,167	0
85	MG	6	2161	1/1	0.95	0.17	51,51,51,51	0
84	OHX	1	3593	7/7	0.95	0.15	206,207,208,209	0
85	MG	A	2059	1/1	0.95	0.40	25,25,25,25	0
84	OHX	1	3537	7/7	0.95	0.25	160,161,162,162	0
84	OHX	AR	3558	7/7	0.95	0.22	159,160,160,160	0
85	MG	1	3910	1/1	0.95	0.20	30,30,30,30	0
84	OHX	1	3706	7/7	0.95	0.17	144,145,146,146	0
85	MG	AR	3944	1/1	0.95	0.38	39,39,39,39	0
85	MG	1	4196	1/1	0.95	0.36	35,35,35,35	0
85	MG	CQ	201	1/1	0.95	0.30	23,23,23,23	0
85	MG	AR	4033	1/1	0.95	0.30	63,63,63,63	0
84	OHX	A	1951	7/7	0.95	0.20	203,205,207,207	0
84	OHX	A	1936	7/7	0.95	0.15	160,162,163,163	0
85	MG	AR	4049	1/1	0.95	0.09	74,74,74,74	0
84	OHX	1	3620	7/7	0.95	0.28	208,208,209,209	0
85	MG	w	201	1/1	0.95	0.17	33,33,33,33	0
85	MG	1	3860	1/1	0.95	0.47	19,19,19,19	0
84	OHX	AR	3571	7/7	0.95	0.18	194,194,195,195	0
85	MG	AR	3947	1/1	0.95	0.18	26,26,26,26	0
84	OHX	AR	3699	7/7	0.95	0.38	194,195,196,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4067	1/1	0.95	0.28	98,98,98,98	0
85	MG	6	2178	1/1	0.95	0.25	26,26,26,26	0
85	MG	A	2050	1/1	0.95	0.32	68,68,68,68	0
85	MG	AR	3756	1/1	0.95	0.71	11,11,11,11	0
85	MG	x	204	1/1	0.95	0.15	18,18,18,18	0
84	OHX	1	3555	7/7	0.95	0.11	190,191,192,192	0
85	MG	1	3946	1/1	0.95	0.17	68,68,68,68	0
85	MG	1	3995	1/1	0.95	0.28	54,54,54,54	0
84	OHX	1	3521	7/7	0.95	0.16	144,145,147,147	0
84	OHX	AR	3505	7/7	0.95	0.17	138,140,141,141	0
84	OHX	A	1974	7/7	0.95	0.10	196,198,200,201	0
85	MG	1	3867	1/1	0.95	0.37	26,26,26,26	0
85	MG	1	4214	1/1	0.95	0.17	50,50,50,50	0
84	OHX	AR	3665	7/7	0.95	0.26	189,189,189,189	0
85	MG	AR	3847	1/1	0.95	0.29	35,35,35,35	0
84	OHX	1	3614	7/7	0.95	0.18	199,200,201,203	0
85	MG	AR	4038	1/1	0.95	0.26	30,30,30,30	0
84	OHX	1	3581	7/7	0.95	0.24	153,153,154,154	0
84	OHX	6	1986	7/7	0.95	0.12	157,157,159,159	0
85	MG	AR	4013	1/1	0.95	0.34	38,38,38,38	0
84	OHX	1	3627	7/7	0.95	0.15	176,176,178,179	0
84	OHX	A	2021	7/7	0.95	0.34	176,177,179,179	0
85	MG	1	3990	1/1	0.95	0.41	36,36,36,36	0
84	OHX	1	3716	7/7	0.95	0.17	205,206,208,209	0
84	OHX	AR	3600	7/7	0.95	0.13	172,173,173,174	0
85	MG	1	3826	1/1	0.95	0.26	44,44,44,44	0
85	MG	6	2076	1/1	0.95	0.32	18,18,18,18	0
85	MG	6	2078	1/1	0.95	0.42	25,25,25,25	0
84	OHX	A	1945	7/7	0.95	0.16	201,203,204,205	0
85	MG	AR	4009	1/1	0.95	0.28	25,25,25,25	0
85	MG	1	4132	1/1	0.95	0.38	42,42,42,42	0
84	OHX	AR	3570	7/7	0.95	0.17	161,162,163,163	0
84	OHX	1	3559	7/7	0.95	0.16	182,183,184,184	0
84	OHX	1	3607	7/7	0.95	0.24	190,192,193,193	0
85	MG	AR	3957	1/1	0.95	0.55	37,37,37,37	0
84	OHX	AR	3533	7/7	0.95	0.15	166,166,167,167	0
84	OHX	6	1991	7/7	0.95	0.20	184,185,187,187	0
84	OHX	AR	3473	7/7	0.95	0.16	121,122,122,122	0
85	MG	AR	3837	1/1	0.95	0.17	16,16,16,16	0
85	MG	AR	4019	1/1	0.95	0.14	29,29,29,29	0
84	OHX	1	3484	7/7	0.95	0.14	131,131,133,133	0
84	OHX	1	3522	7/7	0.96	0.15	133,134,134,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3608	7/7	0.96	0.32	186,187,188,188	0
84	OHX	1	3432	7/7	0.96	0.15	131,131,132,132	0
85	MG	1	4208	1/1	0.96	0.30	30,30,30,30	0
84	OHX	1	3561	7/7	0.96	0.14	184,184,185,186	0
85	MG	1	3739	1/1	0.96	0.46	15,15,15,15	0
85	MG	AR	3981	1/1	0.96	0.18	17,17,17,17	0
85	MG	AT	222	1/1	0.96	0.43	35,35,35,35	0
84	OHX	AR	3499	7/7	0.96	0.14	130,131,133,133	0
84	OHX	1	3492	7/7	0.96	0.15	127,128,128,128	0
85	MG	1	3927	1/1	0.96	0.50	6,6,6,6	0
84	OHX	A	1949	7/7	0.96	0.11	165,167,169,169	0
84	OHX	A	1948	7/7	0.96	0.09	166,169,170,170	0
84	OHX	AR	3642	7/7	0.96	0.28	189,189,191,191	0
84	OHX	AR	3611	7/7	0.96	0.33	194,196,197,197	0
85	MG	4	216	1/1	0.96	0.20	42,42,42,42	0
84	OHX	1	3517	7/7	0.96	0.17	141,142,143,143	0
85	MG	1	3911	1/1	0.96	0.33	20,20,20,20	0
84	OHX	AR	3585	7/7	0.96	0.16	165,166,167,167	0
85	MG	1	4022	1/1	0.96	0.18	24,24,24,24	0
85	MG	1	3756	1/1	0.96	0.15	22,22,22,22	0
84	OHX	AT	212	7/7	0.96	0.16	160,160,161,161	0
84	OHX	1	3677	7/7	0.96	0.14	170,171,171,171	0
85	MG	AR	4116	1/1	0.96	0.29	105,105,105,105	0
85	MG	1	3777	1/1	0.96	0.26	40,40,40,40	0
85	MG	k	404	1/1	0.96	0.44	71,71,71,71	0
85	MG	c6	201	1/1	0.96	0.16	67,67,67,67	0
84	OHX	1	3501	7/7	0.96	0.16	123,124,125,125	0
84	OHX	6	1914	7/7	0.96	0.14	119,120,121,123	0
85	MG	A	2082	1/1	0.96	0.19	65,65,65,65	0
85	MG	6	2149	1/1	0.96	0.32	75,75,75,75	0
85	MG	AR	4229	1/1	0.96	0.46	23,23,23,23	0
84	OHX	AR	3643	7/7	0.96	0.28	157,158,159,160	0
84	OHX	6	1961	7/7	0.96	0.15	152,153,154,155	0
85	MG	1	3956	1/1	0.96	0.22	15,15,15,15	0
84	OHX	6	2003	7/7	0.96	0.18	180,182,183,184	0
85	MG	AR	4083	1/1	0.96	0.35	23,23,23,23	0
85	MG	AR	3860	1/1	0.96	0.47	6,6,6,6	0
85	MG	AR	3741	1/1	0.96	0.24	14,14,14,14	0
85	MG	1	4186	1/1	0.96	0.27	51,51,51,51	0
84	OHX	A	1953	7/7	0.96	0.18	180,182,184,184	0
85	MG	A	2070	1/1	0.96	0.49	59,59,59,59	0
84	OHX	6	1940	7/7	0.96	0.15	149,151,152,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4074	1/1	0.96	0.15	45,45,45,45	0
85	MG	6	2162	1/1	0.96	0.31	69,69,69,69	0
84	OHX	AR	3569	7/7	0.96	0.10	182,182,183,183	0
85	MG	AR	3871	1/1	0.96	0.50	20,20,20,20	0
85	MG	A	2080	1/1	0.96	0.52	45,45,45,45	0
84	OHX	A	1928	7/7	0.96	0.12	156,158,159,159	0
84	OHX	AR	3466	7/7	0.96	0.17	114,115,116,116	0
84	OHX	AR	3495	7/7	0.96	0.14	163,165,166,166	0
85	MG	AR	3892	1/1	0.96	0.44	19,19,19,19	0
84	OHX	A	1983	7/7	0.96	0.20	188,190,192,192	0
85	MG	A	2077	1/1	0.96	0.19	25,25,25,25	0
85	MG	1	3916	1/1	0.96	0.50	14,14,14,14	0
84	OHX	A	1986	7/7	0.96	0.25	215,218,220,222	0
85	MG	AR	4182	1/1	0.96	0.47	48,48,48,48	0
85	MG	1	3841	1/1	0.96	0.31	19,19,19,19	0
85	MG	6	2137	1/1	0.96	0.40	82,82,82,82	0
84	OHX	1	3576	7/7	0.96	0.14	189,189,191,191	0
85	MG	1	3905	1/1	0.96	0.59	14,14,14,14	0
85	MG	1	3928	1/1	0.96	0.13	32,32,32,32	0
84	OHX	AR	3472	7/7	0.96	0.12	129,130,130,130	0
85	MG	DC	201	1/1	0.96	0.36	16,16,16,16	0
85	MG	AR	4017	1/1	0.96	0.17	27,27,27,27	0
84	OHX	3	206	7/7	0.96	0.09	176,177,179,179	0
84	OHX	1	3441	7/7	0.96	0.17	168,169,169,170	0
85	MG	A	2108	1/1	0.96	0.39	39,39,39,39	0
85	MG	AR	3873	1/1	0.96	0.31	23,23,23,23	0
84	OHX	1	3458	7/7	0.96	0.14	131,132,133,133	0
84	OHX	AR	3538	7/7	0.96	0.20	184,185,186,186	0
85	MG	AS	211	1/1	0.96	0.29	22,22,22,22	0
84	OHX	AR	3541	7/7	0.96	0.12	170,171,172,174	0
85	MG	AR	4198	1/1	0.96	0.24	34,34,34,34	0
85	MG	6	2105	1/1	0.96	0.34	24,24,24,24	0
84	OHX	1	3533	7/7	0.96	0.19	196,197,198,199	0
85	MG	AR	3868	1/1	0.96	0.13	33,33,33,33	0
85	MG	AR	4011	1/1	0.96	0.47	31,31,31,31	0
84	OHX	1	3529	7/7	0.96	0.22	143,144,145,146	0
84	OHX	AR	3508	7/7	0.96	0.21	139,139,140,140	0
84	OHX	AR	3715	7/7	0.96	0.21	144,146,147,147	0
84	OHX	A	1994	7/7	0.96	0.23	200,203,204,205	0
85	MG	o	302	1/1	0.96	0.23	27,27,27,27	0
85	MG	AR	3768	1/1	0.96	0.24	23,23,23,23	0
84	OHX	AR	3550	7/7	0.96	0.17	164,164,165,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	4	219	1/1	0.96	0.39	24,24,24,24	0
84	OHX	AR	3516	7/7	0.96	0.09	174,176,178,178	0
85	MG	1	3890	1/1	0.96	0.39	23,23,23,23	0
85	MG	AR	4057	1/1	0.96	0.17	46,46,46,46	0
85	MG	AR	4045	1/1	0.96	0.12	33,33,33,33	0
85	MG	6	2107	1/1	0.96	0.41	24,24,24,24	0
84	OHX	1	3528	7/7	0.96	0.14	169,170,171,171	0
84	OHX	AR	3683	7/7	0.96	0.36	178,179,179,180	0
84	OHX	AR	3604	7/7	0.96	0.15	150,151,151,151	0
85	MG	AR	3949	1/1	0.96	0.38	19,19,19,19	0
85	MG	AR	3978	1/1	0.96	0.26	20,20,20,20	0
84	OHX	AR	3568	7/7	0.96	0.17	162,163,164,165	0
85	MG	6	2098	1/1	0.96	0.23	38,38,38,38	0
85	MG	6	2165	1/1	0.96	0.28	45,45,45,45	0
85	MG	AK	104	1/1	0.96	0.39	44,44,44,44	0
85	MG	6	2163	1/1	0.96	0.12	60,60,60,60	0
84	OHX	3	203	7/7	0.96	0.14	143,144,145,145	0
84	OHX	A	1962	7/7	0.96	0.14	175,176,177,178	0
85	MG	1	3970	1/1	0.96	0.25	59,59,59,59	0
84	OHX	6	1967	7/7	0.96	0.13	157,159,160,160	0
84	OHX	AR	3739	7/7	0.96	0.37	151,152,152,152	0
85	MG	1	3923	1/1	0.96	0.50	7,7,7,7	0
84	OHX	AR	3540	7/7	0.96	0.16	151,152,153,154	0
85	MG	AR	3833	1/1	0.96	0.15	37,37,37,37	0
85	MG	AR	4087	1/1	0.96	0.35	31,31,31,31	0
84	OHX	1	3546	7/7	0.96	0.19	147,148,149,150	0
84	OHX	A	1992	7/7	0.96	0.13	167,169,170,171	0
84	OHX	AR	3514	7/7	0.96	0.26	146,147,147,148	0
85	MG	AR	4068	1/1	0.96	0.18	25,25,25,25	0
84	OHX	6	1950	7/7	0.96	0.12	171,171,173,174	0
84	OHX	6	1936	7/7	0.96	0.18	145,146,146,146	0
84	OHX	AT	213	7/7	0.96	0.11	175,176,176,177	0
85	MG	1	3926	1/1	0.96	0.54	21,21,21,21	0
85	MG	6	2112	1/1	0.96	0.54	25,25,25,25	0
84	OHX	A	1988	7/7	0.96	0.12	158,160,162,162	0
85	MG	AR	3867	1/1	0.96	0.50	13,13,13,13	0
84	OHX	AR	3596	7/7	0.96	0.30	208,209,210,211	0
85	MG	1	4172	1/1	0.96	0.16	76,76,76,76	0
84	OHX	3	202	7/7	0.96	0.13	176,177,177,178	0
85	MG	AR	4046	1/1	0.96	0.19	45,45,45,45	0
85	MG	AR	4073	1/1	0.96	0.15	33,33,33,33	0
85	MG	AR	4109	1/1	0.96	0.23	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3575	7/7	0.96	0.21	156,158,159,159	0
84	OHX	A	1967	7/7	0.96	0.14	167,168,169,170	0
85	MG	1	3813	1/1	0.96	0.18	24,24,24,24	0
84	OHX	1	3558	7/7	0.96	0.19	166,167,168,168	0
85	MG	1	3881	1/1	0.96	0.31	35,35,35,35	0
84	OHX	6	1987	7/7	0.96	0.15	179,179,180,181	0
85	MG	1	4221	1/1	0.96	0.36	22,22,22,22	0
84	OHX	A	1941	7/7	0.96	0.17	195,197,198,198	0
84	OHX	AR	3587	7/7	0.96	0.19	175,176,177,177	0
85	MG	AR	4113	1/1	0.96	0.30	17,17,17,17	0
85	MG	6	2115	1/1	0.96	0.36	36,36,36,36	0
84	OHX	6	2018	7/7	0.96	0.27	186,187,188,189	0
84	OHX	AR	3635	7/7	0.96	0.33	173,175,175,175	0
85	MG	AR	4115	1/1	0.96	0.34	64,64,64,64	0
85	MG	AR	4144	1/1	0.96	0.15	35,35,35,35	0
85	MG	AR	4094	1/1	0.96	0.14	38,38,38,38	0
85	MG	AR	4008	1/1	0.96	0.16	33,33,33,33	0
85	MG	AR	3825	1/1	0.96	0.18	30,30,30,30	0
84	OHX	AR	3619	7/7	0.96	0.28	169,169,170,170	0
84	OHX	AR	3477	7/7	0.96	0.18	119,119,119,120	0
84	OHX	1	3669	7/7	0.96	0.23	125,126,127,127	0
84	OHX	1	3604	7/7	0.96	0.08	204,205,206,206	0
85	MG	1	3794	1/1	0.96	0.22	31,31,31,31	0
85	MG	1	3744	1/1	0.96	0.73	43,43,43,43	0
84	OHX	A	1964	7/7	0.96	0.29	168,169,170,170	0
85	MG	1	3803	1/1	0.96	0.23	22,22,22,22	0
84	OHX	1	3466	7/7	0.96	0.18	120,121,122,123	0
85	MG	d3	201	1/1	0.96	0.13	48,48,48,48	0
84	OHX	AR	3494	7/7	0.96	0.23	144,145,146,146	0
85	MG	A	2081	1/1	0.96	0.41	48,48,48,48	0
85	MG	1	3935	1/1	0.96	0.24	24,24,24,24	0
84	OHX	AR	3636	7/7	0.96	0.17	187,188,188,189	0
85	MG	1	4069	1/1	0.96	0.18	39,39,39,39	0
85	MG	AR	4112	1/1	0.96	0.13	70,70,70,70	0
84	OHX	A	1990	7/7	0.96	0.42	212,215,216,216	0
84	OHX	1	3598	7/7	0.96	0.13	173,173,174,175	0
85	MG	1	3954	1/1	0.96	0.16	45,45,45,45	0
84	OHX	AT	206	7/7	0.96	0.17	155,155,156,156	0
85	MG	1	3790	1/1	0.96	0.52	15,15,15,15	0
84	OHX	AR	3560	7/7	0.96	0.12	173,174,175,175	0
84	OHX	AT	217	7/7	0.96	0.24	184,185,185,186	0
85	MG	6	2070	1/1	0.96	0.56	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3732	1/1	0.96	0.31	27,27,27,27	0
84	OHX	AR	3492	7/7	0.96	0.16	134,135,135,135	0
85	MG	1	3921	1/1	0.96	0.23	45,45,45,45	0
85	MG	1	3902	1/1	0.96	0.52	4,4,4,4	0
85	MG	A	2058	1/1	0.96	0.48	27,27,27,27	0
84	OHX	A	1979	7/7	0.96	0.15	200,203,204,205	0
84	OHX	1	3589	7/7	0.96	0.15	179,180,181,181	0
84	OHX	1	3567	7/7	0.96	0.23	177,178,178,179	0
84	OHX	1	3554	7/7	0.96	0.22	167,168,169,169	0
85	MG	6	2086	1/1	0.96	0.24	49,49,49,49	0
84	OHX	AR	3535	7/7	0.96	0.14	157,157,158,158	0
84	OHX	AR	3545	7/7	0.96	0.23	181,182,182,183	0
85	MG	AR	3975	1/1	0.96	0.27	31,31,31,31	0
84	OHX	AR	3561	7/7	0.96	0.19	171,171,172,172	0
85	MG	A	2090	1/1	0.96	0.28	46,46,46,46	0
85	MG	AR	3900	1/1	0.96	0.33	29,29,29,29	0
84	OHX	1	3470	7/7	0.96	0.13	141,142,143,143	0
84	OHX	1	3643	7/7	0.96	0.14	192,193,194,194	0
85	MG	1	4151	1/1	0.96	0.15	53,53,53,53	0
84	OHX	6	1988	7/7	0.96	0.12	191,193,195,195	0
84	OHX	AR	3662	7/7	0.96	0.19	168,169,169,170	0
84	OHX	A	1968	7/7	0.96	0.20	168,170,171,172	0
84	OHX	1	3685	7/7	0.96	0.16	173,173,175,175	0
85	MG	1	4193	1/1	0.96	0.37	9,9,9,9	0
85	MG	6	2096	1/1	0.96	0.38	48,48,48,48	0
84	OHX	AR	3572	7/7	0.96	0.20	174,175,176,176	0
84	OHX	DH	201	7/7	0.96	0.13	155,156,157,157	0
85	MG	1	3835	1/1	0.96	0.29	19,19,19,19	0
84	OHX	AR	3549	7/7	0.96	0.19	156,157,158,158	0
84	OHX	4	208	7/7	0.96	0.27	187,187,188,188	0
84	OHX	1	3507	7/7	0.96	0.17	149,149,150,150	0
85	MG	1	3823	1/1	0.96	0.20	51,51,51,51	0
84	OHX	1	3610	7/7	0.96	0.28	212,212,212,212	0
85	MG	AR	3863	1/1	0.96	0.60	15,15,15,15	0
85	MG	AR	3798	1/1	0.96	0.39	21,21,21,21	0
85	MG	AR	3777	1/1	0.96	0.14	50,50,50,50	0
84	OHX	AR	3649	7/7	0.96	0.30	207,208,208,208	0
84	OHX	1	3535	7/7	0.96	0.10	196,198,199,200	0
85	MG	AR	4098	1/1	0.96	0.18	27,27,27,27	0
85	MG	AR	3802	1/1	0.96	0.58	16,16,16,16	0
85	MG	AR	3861	1/1	0.96	0.42	16,16,16,16	0
84	OHX	1	3462	7/7	0.96	0.16	115,116,117,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3586	7/7	0.96	0.17	182,183,185,186	0
85	MG	CE	401	1/1	0.96	0.14	30,30,30,30	0
85	MG	AR	3761	1/1	0.96	0.10	41,41,41,41	0
85	MG	AR	3853	1/1	0.96	0.58	17,17,17,17	0
84	OHX	A	1952	7/7	0.96	0.25	181,183,185,185	0
85	MG	CD	301	1/1	0.96	0.20	28,28,28,28	0
85	MG	AR	3760	1/1	0.96	0.39	21,21,21,21	0
85	MG	AR	3854	1/1	0.96	0.21	28,28,28,28	0
85	MG	6	2061	1/1	0.96	0.21	64,64,64,64	0
85	MG	1	3854	1/1	0.96	0.40	13,13,13,13	0
84	OHX	1	3624	7/7	0.96	0.20	171,172,173,174	0
84	OHX	AT	209	7/7	0.96	0.18	163,163,163,163	0
85	MG	6	2122	1/1	0.96	0.18	48,48,48,48	0
84	OHX	1	3629	7/7	0.96	0.14	161,162,162,163	0
85	MG	AR	4163	1/1	0.96	0.12	30,30,30,30	0
85	MG	1	4018	1/1	0.96	0.24	26,26,26,26	0
84	OHX	1	3616	7/7	0.96	0.22	177,177,178,178	0
84	OHX	1	3690	7/7	0.96	0.28	174,175,176,176	0
84	OHX	1	3585	7/7	0.96	0.24	173,174,174,175	0
85	MG	A	2043	1/1	0.96	0.26	47,47,47,47	0
85	MG	AT	229	1/1	0.96	0.33	30,30,30,30	0
85	MG	AR	4224	1/1	0.96	0.25	26,26,26,26	0
85	MG	1	3844	1/1	0.96	0.44	9,9,9,9	0
85	MG	AR	4168	1/1	0.96	0.32	45,45,45,45	0
85	MG	1	4067	1/1	0.96	0.19	24,24,24,24	0
85	MG	1	4164	1/1	0.96	0.16	48,48,48,48	0
85	MG	1	3894	1/1	0.96	0.42	26,26,26,26	0
85	MG	AR	4111	1/1	0.96	0.60	48,48,48,48	0
84	OHX	A	1973	7/7	0.96	0.15	201,204,206,208	0
84	OHX	AR	3576	7/7	0.96	0.14	168,169,169,170	0
84	OHX	A	1954	7/7	0.96	0.20	172,174,175,175	0
87	ZN	g	501	1/1	0.96	0.04	143,143,143,143	0
84	OHX	AR	3563	7/7	0.96	0.17	173,173,174,174	0
85	MG	AR	3869	1/1	0.96	0.40	12,12,12,12	0
84	OHX	1	3549	7/7	0.96	0.13	190,190,191,192	0
84	OHX	4	201	7/7	0.96	0.16	143,143,144,144	0
84	OHX	6	1952	7/7	0.96	0.13	183,184,185,186	0
85	MG	1	3800	1/1	0.96	0.40	37,37,37,37	0
84	OHX	AR	3630	7/7	0.96	0.10	172,173,174,175	0
84	OHX	6	1947	7/7	0.96	0.12	142,144,145,145	0
84	OHX	A	1976	7/7	0.96	0.16	165,166,167,168	0
85	MG	AR	3898	1/1	0.96	0.42	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	A	1931	7/7	0.96	0.11	166,168,169,169	0
85	MG	A	2083	1/1	0.96	0.37	62,62,62,62	0
84	OHX	AR	3579	7/7	0.96	0.13	183,184,185,185	0
85	MG	AR	4076	1/1	0.96	0.16	38,38,38,38	0
85	MG	1	3748	1/1	0.96	0.25	23,23,23,23	0
85	MG	AR	3781	1/1	0.96	0.34	11,11,11,11	0
85	MG	AR	4106	1/1	0.96	0.19	55,55,55,55	0
84	OHX	1	3552	7/7	0.96	0.20	173,174,175,175	0
84	OHX	AR	3691	7/7	0.96	0.45	170,171,172,172	0
85	MG	AR	3920	1/1	0.96	0.34	19,19,19,19	0
84	OHX	A	1927	7/7	0.96	0.12	158,160,162,162	0
85	MG	AR	4005	1/1	0.96	0.35	24,24,24,24	0
85	MG	6	2141	1/1	0.96	0.21	56,56,56,56	0
84	OHX	4	204	7/7	0.96	0.28	160,160,161,161	0
85	MG	1	4020	1/1	0.96	0.12	38,38,38,38	0
84	OHX	AR	3692	7/7	0.96	0.34	184,186,186,187	0
85	MG	AS	225	1/1	0.96	0.15	67,67,67,67	0
85	MG	1	4139	1/1	0.96	0.18	29,29,29,29	0
85	MG	AR	4031	1/1	0.96	0.25	31,31,31,31	0
84	OHX	1	3574	7/7	0.97	0.20	138,139,140,140	0
84	OHX	AR	3578	7/7	0.97	0.39	188,188,189,189	0
84	OHX	AT	208	7/7	0.97	0.12	154,154,155,155	0
85	MG	1	4155	1/1	0.97	0.48	66,66,66,66	0
84	OHX	AR	3583	7/7	0.97	0.18	148,149,150,150	0
85	MG	1	3994	1/1	0.97	0.21	32,32,32,32	0
85	MG	1	3770	1/1	0.97	0.47	11,11,11,11	0
85	MG	6	2119	1/1	0.97	0.36	31,31,31,31	0
84	OHX	AS	206	7/7	0.97	0.14	146,146,148,148	0
85	MG	1	4195	1/1	0.97	0.37	52,52,52,52	0
85	MG	6	2067	1/1	0.97	0.34	41,41,41,41	0
85	MG	6	2113	1/1	0.97	0.42	23,23,23,23	0
85	MG	AR	3924	1/1	0.97	0.47	13,13,13,13	0
84	OHX	1	3516	7/7	0.97	0.23	131,132,133,133	0
84	OHX	6	1933	7/7	0.97	0.14	121,122,123,123	0
87	ZN	DQ	501	1/1	0.97	0.15	105,105,105,105	0
84	OHX	1	3503	7/7	0.97	0.19	145,146,147,148	0
84	OHX	1	3513	7/7	0.97	0.13	140,141,142,142	0
84	OHX	1	3482	7/7	0.97	0.14	116,116,117,117	0
84	OHX	AR	3617	7/7	0.97	0.28	158,158,159,159	0
84	OHX	1	3541	7/7	0.97	0.12	154,155,156,156	0
84	OHX	A	1944	7/7	0.97	0.11	161,163,165,165	0
84	OHX	AT	207	7/7	0.97	0.10	162,163,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3496	7/7	0.97	0.18	115,116,117,117	0
85	MG	1	3922	1/1	0.97	0.50	15,15,15,15	0
84	OHX	AR	3510	7/7	0.97	0.09	154,155,156,157	0
84	OHX	AR	3543	7/7	0.97	0.17	181,181,182,182	0
84	OHX	AR	3627	7/7	0.97	0.20	173,173,174,174	0
84	OHX	6	1949	7/7	0.97	0.13	165,167,168,168	0
85	MG	1	4048	1/1	0.97	0.32	27,27,27,27	0
85	MG	AR	3999	1/1	0.97	0.37	28,28,28,28	0
85	MG	1	3791	1/1	0.97	0.44	21,21,21,21	0
85	MG	AR	3793	1/1	0.97	0.55	23,23,23,23	0
84	OHX	AR	3463	7/7	0.97	0.18	114,114,115,115	0
85	MG	1	3908	1/1	0.97	0.36	14,14,14,14	0
85	MG	3	211	1/1	0.97	0.30	33,33,33,33	0
85	MG	1	3741	1/1	0.97	0.21	40,40,40,40	0
85	MG	1	3943	1/1	0.97	0.32	22,22,22,22	0
85	MG	6	2180	1/1	0.97	0.16	94,94,94,94	0
84	OHX	CL	301	7/7	0.97	0.10	165,166,167,168	0
84	OHX	AP	502	7/7	0.97	0.14	124,124,126,127	0
85	MG	AR	3894	1/1	0.97	0.50	24,24,24,24	0
85	MG	AR	3954	1/1	0.97	0.34	36,36,36,36	0
84	OHX	1	3603	7/7	0.97	0.34	162,162,164,164	0
85	MG	AR	4006	1/1	0.97	0.10	33,33,33,33	0
85	MG	1	4215	1/1	0.97	0.34	28,28,28,28	0
84	OHX	AR	3528	7/7	0.97	0.11	147,147,148,149	0
84	OHX	1	3652	7/7	0.97	0.17	173,174,174,174	0
84	OHX	1	3562	7/7	0.97	0.08	200,200,201,202	0
84	OHX	1	3588	7/7	0.97	0.16	168,169,170,170	0
85	MG	A	2057	1/1	0.97	0.42	50,50,50,50	0
85	MG	1	4222	1/1	0.97	0.14	30,30,30,30	0
85	MG	CU	202	1/1	0.97	0.20	31,31,31,31	0
85	MG	1	4211	1/1	0.97	0.37	21,21,21,21	0
84	OHX	AR	3467	7/7	0.97	0.13	137,138,138,139	0
84	OHX	k	401	7/7	0.97	0.24	169,170,170,170	0
84	OHX	A	1940	7/7	0.97	0.16	174,175,177,178	0
84	OHX	AR	3614	7/7	0.97	0.15	164,165,165,166	0
84	OHX	CE	402	7/7	0.97	0.12	142,143,144,144	0
85	MG	x	205	1/1	0.97	0.48	20,20,20,20	0
86	7MB	AR	4239	20/20	0.97	0.19	44,44,44,44	0
84	OHX	DL	101	7/7	0.97	0.14	144,144,144,144	0
85	MG	AR	3866	1/1	0.97	0.26	20,20,20,20	0
85	MG	AR	3983	1/1	0.97	0.28	24,24,24,24	0
85	MG	A	2102	1/1	0.97	0.31	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	A	2136	1/1	0.97	0.08	110,110,110,110	0
84	OHX	1	3527	7/7	0.97	0.18	138,139,140,140	0
85	MG	1	3858	1/1	0.97	0.64	12,12,12,12	0
85	MG	1	4220	1/1	0.97	0.22	25,25,25,25	0
84	OHX	AR	3480	7/7	0.97	0.12	132,132,132,133	0
85	MG	AR	4228	1/1	0.97	0.31	12,12,12,12	0
85	MG	6	2176	1/1	0.97	0.16	73,73,73,73	0
84	OHX	A	1918	7/7	0.97	0.17	120,122,123,123	0
84	OHX	1	3475	7/7	0.97	0.17	128,129,130,130	0
85	MG	AR	4238	1/1	0.97	0.47	27,27,27,27	0
85	MG	AR	3905	1/1	0.97	0.52	24,24,24,24	0
85	MG	AR	3922	1/1	0.97	0.36	20,20,20,20	0
84	OHX	A	1955	7/7	0.97	0.11	145,148,150,150	0
85	MG	1	4104	1/1	0.97	0.22	32,32,32,32	0
85	MG	AR	3940	1/1	0.97	0.10	34,34,34,34	0
85	MG	1	3944	1/1	0.97	0.33	33,33,33,33	0
85	MG	1	3827	1/1	0.97	0.27	21,21,21,21	0
84	OHX	1	3477	7/7	0.97	0.13	118,119,120,120	0
85	MG	6	2101	1/1	0.97	0.28	37,37,37,37	0
84	OHX	4	207	7/7	0.97	0.10	174,175,175,176	0
84	OHX	AR	3595	7/7	0.97	0.20	160,161,161,162	0
84	OHX	AR	3481	7/7	0.97	0.11	132,132,133,133	0
84	OHX	1	3497	7/7	0.97	0.12	140,141,142,142	0
84	OHX	1	3467	7/7	0.97	0.13	124,125,126,126	0
85	MG	1	3784	1/1	0.97	0.30	30,30,30,30	0
85	MG	AR	3799	1/1	0.97	0.17	83,83,83,83	0
84	OHX	6	1919	7/7	0.97	0.14	112,113,114,114	0
85	MG	1	3936	1/1	0.97	0.13	48,48,48,48	0
84	OHX	6	1968	7/7	0.97	0.17	145,146,147,148	0
85	MG	AR	3934	1/1	0.97	0.37	14,14,14,14	0
85	MG	AR	4160	1/1	0.97	0.26	31,31,31,31	0
85	MG	AR	3890	1/1	0.97	0.50	33,33,33,33	0
85	MG	1	4147	1/1	0.97	0.25	28,28,28,28	0
84	OHX	6	2007	7/7	0.97	0.15	148,150,151,151	0
85	MG	A	2063	1/1	0.97	0.42	36,36,36,36	0
85	MG	AR	3991	1/1	0.97	0.26	15,15,15,15	0
85	MG	AR	4174	1/1	0.97	0.21	23,23,23,23	0
85	MG	1	4173	1/1	0.97	0.14	33,33,33,33	0
85	MG	6	2118	1/1	0.97	0.25	54,54,54,54	0
84	OHX	AR	3474	7/7	0.97	0.15	119,120,121,121	0
84	OHX	1	3569	7/7	0.97	0.27	166,166,167,168	0
85	MG	AR	4138	1/1	0.97	0.41	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3842	1/1	0.97	0.38	10,10,10,10	0
84	OHX	AT	210	7/7	0.97	0.11	164,164,165,165	0
84	OHX	1	3563	7/7	0.97	0.14	151,152,152,152	0
84	OHX	T	201	7/7	0.97	0.13	133,135,137,138	0
85	MG	AR	3814	1/1	0.97	0.33	27,27,27,27	0
85	MG	1	4007	1/1	0.97	0.30	16,16,16,16	0
84	OHX	A	1961	7/7	0.97	0.13	175,176,179,180	0
85	MG	AR	3786	1/1	0.97	0.19	16,16,16,16	0
85	MG	AR	4139	1/1	0.97	0.64	37,37,37,37	0
85	MG	A	2142	1/1	0.97	0.28	90,90,90,90	0
85	MG	AR	4133	1/1	0.97	0.13	35,35,35,35	0
85	MG	CQ	204	1/1	0.97	0.33	48,48,48,48	0
85	MG	1	3929	1/1	0.97	0.43	20,20,20,20	0
85	MG	AR	3836	1/1	0.97	0.31	15,15,15,15	0
85	MG	1	3885	1/1	0.97	0.49	10,10,10,10	0
85	MG	1	3973	1/1	0.97	0.26	33,33,33,33	0
85	MG	AR	3816	1/1	0.97	0.21	27,27,27,27	0
84	OHX	A	1935	7/7	0.97	0.13	191,193,195,195	0
85	MG	1	4087	1/1	0.97	0.13	37,37,37,37	0
84	OHX	1	3577	7/7	0.97	0.25	177,178,179,179	0
84	OHX	6	1965	7/7	0.97	0.27	161,162,163,163	0
84	OHX	1	3488	7/7	0.97	0.14	140,140,141,141	0
84	OHX	v	301	7/7	0.97	0.14	155,155,156,156	0
85	MG	AR	3877	1/1	0.97	0.39	14,14,14,14	0
85	MG	6	2100	1/1	0.97	0.44	16,16,16,16	0
85	MG	1	4035	1/1	0.97	0.18	131,131,131,131	0
85	MG	AR	3745	1/1	0.97	0.19	32,32,32,32	0
84	OHX	1	3518	7/7	0.97	0.17	134,135,135,136	0
85	MG	6	2109	1/1	0.97	0.24	39,39,39,39	0
84	OHX	6	1984	7/7	0.97	0.18	198,200,201,201	0
84	OHX	A	1975	7/7	0.97	0.08	190,193,195,195	0
84	OHX	1	3530	7/7	0.97	0.13	151,151,151,152	0
84	OHX	1	3579	7/7	0.97	0.12	175,175,177,177	0
85	MG	AR	4091	1/1	0.97	0.16	53,53,53,53	0
85	MG	1	3991	1/1	0.97	0.25	30,30,30,30	0
84	OHX	AR	3453	7/7	0.97	0.12	127,128,128,128	0
84	OHX	AR	3536	7/7	0.97	0.17	141,141,142,142	0
84	OHX	6	2013	7/7	0.97	0.20	149,151,152,153	0
85	MG	1	3942	1/1	0.97	0.37	20,20,20,20	0
85	MG	A	2119	1/1	0.97	0.38	55,55,55,55	0
85	MG	4	223	1/1	0.97	0.26	44,44,44,44	0
84	OHX	A	2008	7/7	0.97	0.13	156,158,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	A	2056	1/1	0.97	0.39	39,39,39,39	0
87	ZN	AP	501	1/1	0.97	0.26	115,115,115,115	0
85	MG	CR	202	1/1	0.97	0.20	20,20,20,20	0
85	MG	AR	4235	1/1	0.97	0.40	15,15,15,15	0
85	MG	3	209	1/1	0.97	0.26	46,46,46,46	0
84	OHX	1	3591	7/7	0.97	0.12	185,186,187,188	0
84	OHX	AR	3484	7/7	0.97	0.20	133,134,135,135	0
84	OHX	1	3500	7/7	0.97	0.07	156,157,159,159	0
84	OHX	AR	3503	7/7	0.97	0.33	152,153,154,154	0
84	OHX	1	3730	7/7	0.97	0.13	141,142,143,143	0
84	OHX	6	1963	7/7	0.97	0.15	159,159,161,161	0
84	OHX	AR	3489	7/7	0.97	0.12	149,150,151,152	0
84	OHX	A	1950	7/7	0.97	0.17	168,169,170,171	0
85	MG	AB	204	1/1	0.97	0.27	42,42,42,42	0
85	MG	1	3863	1/1	0.97	0.43	25,25,25,25	0
84	OHX	AR	3515	7/7	0.97	0.16	159,160,161,162	0
84	OHX	1	3498	7/7	0.97	0.11	150,150,151,152	0
85	MG	AR	4195	1/1	0.97	0.17	21,21,21,21	0
84	OHX	1	3590	7/7	0.97	0.18	208,209,210,211	0
85	MG	x	207	1/1	0.97	0.15	17,17,17,17	0
84	OHX	6	1953	7/7	0.97	0.13	154,155,157,158	0
84	OHX	A	1987	7/7	0.97	0.14	172,173,174,175	0
85	MG	AR	3870	1/1	0.97	0.23	14,14,14,14	0
85	MG	1	4204	1/1	0.97	0.41	12,12,12,12	0
85	MG	1	4057	1/1	0.97	0.17	30,30,30,30	0
85	MG	AR	3901	1/1	0.97	0.26	17,17,17,17	0
84	OHX	AR	3523	7/7	0.97	0.23	175,176,176,177	0
84	OHX	A	1957	7/7	0.97	0.18	169,171,172,173	0
84	OHX	6	1927	7/7	0.97	0.16	128,128,130,130	0
84	OHX	1	3583	7/7	0.97	0.29	144,144,145,145	0
84	OHX	1	3582	7/7	0.97	0.20	152,153,154,155	0
84	OHX	AR	3525	7/7	0.97	0.13	150,151,151,152	0
85	MG	AS	213	1/1	0.97	0.23	40,40,40,40	0
85	MG	AR	3925	1/1	0.97	0.38	14,14,14,14	0
85	MG	AR	4225	1/1	0.97	0.25	23,23,23,23	0
85	MG	1	4200	1/1	0.97	0.34	18,18,18,18	0
85	MG	AR	3858	1/1	0.97	0.47	22,22,22,22	0
84	OHX	6	1943	7/7	0.97	0.11	147,149,150,150	0
85	MG	AR	4150	1/1	0.97	0.12	49,49,49,49	0
84	OHX	1	3476	7/7	0.97	0.16	121,121,122,123	0
85	MG	6	2136	1/1	0.97	0.25	29,29,29,29	0
84	OHX	1	3689	7/7	0.97	0.14	140,141,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3637	7/7	0.97	0.21	180,181,181,181	0
84	OHX	A	1925	7/7	0.97	0.09	171,172,174,175	0
85	MG	AR	4232	1/1	0.97	0.26	33,33,33,33	0
85	MG	i	201	1/1	0.97	0.06	57,57,57,57	0
84	OHX	A	1921	7/7	0.97	0.17	139,141,143,143	0
85	MG	1	3822	1/1	0.97	0.31	22,22,22,22	0
85	MG	A	2064	1/1	0.97	0.15	49,49,49,49	0
85	MG	1	4205	1/1	0.97	0.53	26,26,26,26	0
84	OHX	A	1933	7/7	0.97	0.12	154,155,156,157	0
84	OHX	6	1951	7/7	0.97	0.14	165,167,169,170	0
85	MG	AR	4066	1/1	0.97	0.17	35,35,35,35	0
84	OHX	6	1946	7/7	0.97	0.12	160,161,163,164	0
85	MG	AR	3935	1/1	0.97	0.28	22,22,22,22	0
85	MG	AR	4134	1/1	0.97	0.28	10,10,10,10	0
84	OHX	AR	3497	7/7	0.97	0.22	140,140,141,141	0
85	MG	1	3815	1/1	0.97	0.18	40,40,40,40	0
85	MG	AS	230	1/1	0.97	0.27	67,67,67,67	0
84	OHX	AR	3610	7/7	0.97	0.13	139,140,140,140	0
84	OHX	A	1972	7/7	0.97	0.12	195,196,198,199	0
84	OHX	1	3486	7/7	0.97	0.12	146,146,147,147	0
84	OHX	AR	3574	7/7	0.97	0.27	171,172,173,173	0
85	MG	6	2082	1/1	0.97	0.54	25,25,25,25	0
85	MG	1	3805	1/1	0.97	0.19	60,60,60,60	0
85	MG	AR	3874	1/1	0.97	0.31	18,18,18,18	0
84	OHX	h	401	7/7	0.97	0.09	203,206,208,210	0
84	OHX	e	101	7/7	0.97	0.22	205,208,210,210	0
85	MG	1	3948	1/1	0.97	0.40	46,46,46,46	0
85	MG	1	3817	1/1	0.97	0.30	32,32,32,32	0
84	OHX	A	1920	7/7	0.97	0.13	141,142,143,144	0
85	MG	1	3750	1/1	0.97	0.09	70,70,70,70	0
84	OHX	1	3485	7/7	0.97	0.19	151,152,153,153	0
85	MG	1	3909	1/1	0.97	0.19	24,24,24,24	0
84	OHX	1	3524	7/7	0.97	0.22	164,164,166,167	0
85	MG	1	3785	1/1	0.97	0.33	21,21,21,21	0
85	MG	AR	4000	1/1	0.97	0.38	30,30,30,30	0
84	OHX	AR	3460	7/7	0.97	0.12	109,109,110,110	0
84	OHX	6	1975	7/7	0.97	0.16	160,161,162,162	0
84	OHX	AR	3464	7/7	0.97	0.13	117,118,118,118	0
85	MG	AR	4027	1/1	0.97	0.27	33,33,33,33	0
84	OHX	1	3684	7/7	0.97	0.22	170,171,172,173	0
84	OHX	1	3639	7/7	0.97	0.30	201,203,203,204	0
85	MG	AR	4165	1/1	0.97	0.07	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3430	7/7	0.97	0.15	137,137,138,138	0
84	OHX	1	3573	7/7	0.97	0.10	196,196,197,197	0
84	OHX	1	3515	7/7	0.97	0.13	128,128,129,129	0
84	OHX	AR	3698	7/7	0.97	0.19	166,167,167,168	0
84	OHX	6	2017	7/7	0.97	0.20	158,159,160,161	0
85	MG	A	2144	1/1	0.97	0.24	49,49,49,49	0
85	MG	AR	3785	1/1	0.97	0.29	29,29,29,29	0
84	OHX	AR	3518	7/7	0.97	0.16	161,162,163,163	0
84	OHX	1	3495	7/7	0.97	0.12	133,134,135,135	0
85	MG	AR	4231	1/1	0.97	0.33	9,9,9,9	0
84	OHX	6	1938	7/7	0.97	0.13	145,146,148,148	0
84	OHX	AR	3534	7/7	0.97	0.12	162,163,164,165	0
84	OHX	6	1931	7/7	0.97	0.12	151,152,153,153	0
84	OHX	AR	3506	7/7	0.97	0.17	158,159,159,160	0
85	MG	AR	3763	1/1	0.97	0.26	18,18,18,18	0
85	MG	A	2138	1/1	0.97	0.29	35,35,35,35	0
84	OHX	AR	3475	7/7	0.97	0.17	114,115,115,116	0
87	ZN	AQ	501	1/1	0.97	0.08	77,77,77,77	0
85	MG	1	4082	1/1	0.97	0.13	22,22,22,22	0
85	MG	AR	4200	1/1	0.97	0.57	30,30,30,30	0
84	OHX	4	202	7/7	0.97	0.10	157,158,158,158	0
85	MG	1	3861	1/1	0.97	0.15	65,65,65,65	0
85	MG	1	4197	1/1	0.97	0.13	48,48,48,48	0
84	OHX	1	3572	7/7	0.97	0.28	168,168,169,170	0
84	OHX	6	1945	7/7	0.97	0.16	149,150,151,152	0
85	MG	1	3792	1/1	0.97	0.26	16,16,16,16	0
84	OHX	A	1937	7/7	0.97	0.14	152,154,157,157	0
85	MG	AR	4227	1/1	0.97	0.53	18,18,18,18	0
84	OHX	AR	3544	7/7	0.97	0.11	177,178,179,179	0
85	MG	1	4019	1/1	0.97	0.20	31,31,31,31	0
84	OHX	AR	3672	7/7	0.97	0.32	137,138,138,138	0
84	OHX	AR	3488	7/7	0.97	0.13	129,130,130,131	0
84	OHX	AR	3522	7/7	0.97	0.14	134,135,136,136	0
84	OHX	AR	3607	7/7	0.97	0.22	166,166,167,167	0
85	MG	1	4059	1/1	0.97	0.26	32,32,32,32	0
85	MG	CX	202	1/1	0.97	0.32	6,6,6,6	0
85	MG	AR	4007	1/1	0.97	0.11	23,23,23,23	0
84	OHX	1	3514	7/7	0.97	0.13	148,148,149,149	0
85	MG	A	2106	1/1	0.97	0.47	30,30,30,30	0
85	MG	AR	3904	1/1	0.97	0.73	11,11,11,11	0
85	MG	1	3843	1/1	0.97	0.66	11,11,11,11	0
85	MG	1	3859	1/1	0.97	0.21	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	A	2078	1/1	0.97	0.51	28,28,28,28	0
84	OHX	A	1930	7/7	0.97	0.16	164,165,166,167	0
85	MG	AR	4149	1/1	0.97	0.13	28,28,28,28	0
84	OHX	AR	3551	7/7	0.97	0.19	161,162,163,164	0
84	OHX	A	1956	7/7	0.97	0.13	171,173,174,175	0
85	MG	1	3874	1/1	0.98	0.42	19,19,19,19	0
84	OHX	6	1999	7/7	0.98	0.18	177,179,179,181	0
84	OHX	1	3456	7/7	0.98	0.13	114,115,116,117	0
85	MG	4	225	1/1	0.98	0.18	43,43,43,43	0
85	MG	1	3870	1/1	0.98	0.51	11,11,11,11	0
85	MG	AR	3779	1/1	0.98	0.28	20,20,20,20	0
85	MG	1	4209	1/1	0.98	0.40	22,22,22,22	0
85	MG	1	4218	1/1	0.98	0.07	84,84,84,84	0
84	OHX	1	3532	7/7	0.98	0.13	133,133,134,134	0
87	ZN	DR	501	1/1	0.98	0.07	73,73,73,73	0
84	OHX	AR	3454	7/7	0.98	0.12	120,120,121,121	0
85	MG	1	3814	1/1	0.98	0.32	39,39,39,39	0
85	MG	1	3846	1/1	0.98	0.38	16,16,16,16	0
85	MG	1	4083	1/1	0.98	0.11	34,34,34,34	0
84	OHX	AT	204	7/7	0.98	0.10	143,143,143,143	0
84	OHX	1	3435	7/7	0.98	0.15	103,104,105,105	0
85	MG	1	4046	1/1	0.98	0.09	54,54,54,54	0
84	OHX	AR	3468	7/7	0.98	0.11	111,112,113,114	0
84	OHX	AR	3532	7/7	0.98	0.17	129,130,130,131	0
85	MG	A	2066	1/1	0.98	0.44	62,62,62,62	0
84	OHX	1	3469	7/7	0.98	0.13	118,118,119,120	0
85	MG	AR	3987	1/1	0.98	0.33	50,50,50,50	0
84	OHX	6	1942	7/7	0.98	0.09	142,143,144,145	0
85	MG	1	3996	1/1	0.98	0.26	51,51,51,51	0
84	OHX	1	3493	7/7	0.98	0.16	147,148,148,149	0
85	MG	AR	3829	1/1	0.98	0.41	16,16,16,16	0
85	MG	AR	3915	1/1	0.98	0.29	20,20,20,20	0
84	OHX	6	1920	7/7	0.98	0.12	124,126,127,128	0
84	OHX	6	1928	7/7	0.98	0.09	150,151,152,152	0
85	MG	1	3971	1/1	0.98	0.18	63,63,63,63	0
84	OHX	1	3487	7/7	0.98	0.10	139,140,142,142	0
84	OHX	A	1924	7/7	0.98	0.10	153,154,155,156	0
84	OHX	A	1911	7/7	0.98	0.13	115,117,118,120	0
84	OHX	AR	3427	7/7	0.98	0.22	87,87,87,87	0
84	OHX	AK	103	7/7	0.98	0.12	145,146,146,146	0
84	OHX	AR	3457	7/7	0.98	0.13	107,107,108,108	0
85	MG	CE	404	1/1	0.98	0.27	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3445	7/7	0.98	0.13	94,94,94,95	0
84	OHX	AR	3451	7/7	0.98	0.15	104,105,106,106	0
84	OHX	AR	3511	7/7	0.98	0.15	96,96,96,97	0
84	OHX	1	3505	7/7	0.98	0.13	139,139,140,140	0
84	OHX	AR	3485	7/7	0.98	0.25	135,136,137,137	0
84	OHX	AR	3479	7/7	0.98	0.15	119,119,120,120	0
84	OHX	AR	3452	7/7	0.98	0.11	108,109,110,111	0
85	MG	AR	3895	1/1	0.98	0.39	21,21,21,21	0
85	MG	1	3893	1/1	0.98	0.28	38,38,38,38	0
85	MG	j	301	1/1	0.98	0.13	26,26,26,26	0
85	MG	AR	4243	1/1	0.98	0.43	22,22,22,22	0
85	MG	AR	3790	1/1	0.98	0.28	17,17,17,17	0
84	OHX	1	3560	7/7	0.98	0.13	155,156,158,158	0
85	MG	1	3872	1/1	0.98	0.39	23,23,23,23	0
85	MG	1	3878	1/1	0.98	0.18	36,36,36,36	0
84	OHX	AS	201	7/7	0.98	0.16	98,99,100,101	0
84	OHX	AR	3429	7/7	0.98	0.09	105,105,106,106	0
84	OHX	AR	3504	7/7	0.98	0.21	116,117,117,118	0
85	MG	1	4117	1/1	0.98	0.34	26,26,26,26	0
84	OHX	AR	3548	7/7	0.98	0.18	165,166,166,166	0
85	MG	1	3993	1/1	0.98	0.10	27,27,27,27	0
84	OHX	AR	3552	7/7	0.98	0.12	148,148,149,149	0
84	OHX	1	3626	7/7	0.98	0.16	137,137,138,138	0
84	OHX	AR	3527	7/7	0.98	0.10	138,139,140,141	0
84	OHX	A	1938	7/7	0.98	0.14	138,139,140,141	0
85	MG	AR	3865	1/1	0.98	0.27	23,23,23,23	0
85	MG	AR	4080	1/1	0.98	0.16	16,16,16,16	0
85	MG	AR	4189	1/1	0.98	0.14	32,32,32,32	0
84	OHX	AS	203	7/7	0.98	0.11	118,119,120,120	0
85	MG	1	3816	1/1	0.98	0.36	28,28,28,28	0
84	OHX	6	1937	7/7	0.98	0.11	140,141,141,141	0
84	OHX	1	3480	7/7	0.98	0.13	141,141,142,142	0
85	MG	AR	4118	1/1	0.98	0.27	29,29,29,29	0
85	MG	4	221	1/1	0.98	0.15	52,52,52,52	0
85	MG	A	2120	1/1	0.98	0.08	74,74,74,74	0
85	MG	1	4189	1/1	0.98	0.22	48,48,48,48	0
84	OHX	A	1942	7/7	0.98	0.14	163,165,166,167	0
84	OHX	A	1913	7/7	0.98	0.14	121,122,123,124	0
84	OHX	1	3454	7/7	0.98	0.14	111,112,113,113	0
84	OHX	AR	3478	7/7	0.98	0.12	102,103,103,104	0
85	MG	AR	3926	1/1	0.98	0.51	10,10,10,10	0
85	MG	AR	3908	1/1	0.98	0.46	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3889	1/1	0.98	0.28	19,19,19,19	0
84	OHX	1	3490	7/7	0.98	0.10	134,135,136,136	0
84	OHX	AR	3580	7/7	0.98	0.18	139,139,140,140	0
84	OHX	6	1944	7/7	0.98	0.12	154,155,157,158	0
84	OHX	AR	3697	7/7	0.98	0.21	115,116,116,116	0
85	MG	AR	4236	1/1	0.98	0.32	22,22,22,22	0
84	OHX	1	3471	7/7	0.98	0.13	118,118,121,121	0
84	OHX	6	1956	7/7	0.98	0.09	192,194,195,196	0
85	MG	6	2068	1/1	0.98	0.35	76,76,76,76	0
85	MG	AR	4222	1/1	0.98	0.15	27,27,27,27	0
84	OHX	1	3483	7/7	0.98	0.10	118,119,120,121	0
85	MG	1	4219	1/1	0.98	0.34	47,47,47,47	0
84	OHX	1	3446	7/7	0.98	0.16	107,108,109,110	0
85	MG	AR	3800	1/1	0.98	0.28	22,22,22,22	0
85	MG	6	2187	1/1	0.98	0.12	82,82,82,82	0
85	MG	AR	3903	1/1	0.98	0.41	5,5,5,5	0
85	MG	AR	4188	1/1	0.98	0.19	35,35,35,35	0
85	MG	AR	3754	1/1	0.98	0.14	35,35,35,35	0
84	OHX	6	1921	7/7	0.98	0.14	121,124,124,126	0
84	OHX	1	3571	7/7	0.98	0.27	144,145,145,146	0
85	MG	4	220	1/1	0.98	0.37	37,37,37,37	0
85	MG	AR	3881	1/1	0.98	0.41	12,12,12,12	0
84	OHX	AR	3553	7/7	0.98	0.12	160,160,161,162	0
85	MG	AR	4132	1/1	0.98	0.08	36,36,36,36	0
84	OHX	AS	202	7/7	0.98	0.11	122,123,124,124	0
84	OHX	AR	3521	7/7	0.98	0.12	160,161,161,162	0
84	OHX	AS	205	7/7	0.98	0.11	144,146,147,147	0
85	MG	1	3771	1/1	0.98	0.48	23,23,23,23	0
84	OHX	6	1970	7/7	0.98	0.19	178,179,180,180	0
84	OHX	A	1922	7/7	0.98	0.10	138,140,141,141	0
84	OHX	AR	3557	7/7	0.98	0.11	144,145,146,146	0
85	MG	6	2066	1/1	0.98	0.27	87,87,87,87	0
84	OHX	1	3442	7/7	0.98	0.12	98,99,99,100	0
85	MG	1	3865	1/1	0.98	0.47	13,13,13,13	0
85	MG	6	2103	1/1	0.98	0.41	40,40,40,40	0
84	OHX	AR	3502	7/7	0.98	0.11	131,132,132,133	0
84	OHX	AS	207	7/7	0.98	0.11	163,165,166,166	0
85	MG	1	4118	1/1	0.98	0.23	87,87,87,87	0
84	OHX	AR	3442	7/7	0.98	0.15	110,111,111,111	0
85	MG	AR	4166	1/1	0.98	0.11	58,58,58,58	0
84	OHX	1	3520	7/7	0.98	0.07	149,150,152,152	0
84	OHX	AR	3513	7/7	0.98	0.11	152,153,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3917	1/1	0.98	0.33	29,29,29,29	0
85	MG	1	3768	1/1	0.98	0.30	24,24,24,24	0
85	MG	1	4115	1/1	0.98	0.17	97,97,97,97	0
85	MG	1	3868	1/1	0.98	0.58	9,9,9,9	0
84	OHX	DG	201	7/7	0.98	0.16	132,133,133,134	0
85	MG	1	3819	1/1	0.98	0.25	25,25,25,25	0
84	OHX	AR	3519	7/7	0.98	0.12	135,135,136,136	0
85	MG	1	3932	1/1	0.98	0.26	24,24,24,24	0
84	OHX	AR	3509	7/7	0.98	0.14	135,136,136,137	0
84	OHX	AR	3507	7/7	0.98	0.16	136,136,137,137	0
85	MG	AR	3821	1/1	0.98	0.35	26,26,26,26	0
84	OHX	1	3506	7/7	0.98	0.08	159,160,161,162	0
84	OHX	AT	205	7/7	0.98	0.09	151,151,151,151	0
84	OHX	CX	201	7/7	0.98	0.17	121,122,123,124	0
84	OHX	1	3449	7/7	0.98	0.10	119,120,121,121	0
85	MG	1	3849	1/1	0.98	0.44	21,21,21,21	0
85	MG	AR	4210	1/1	0.98	0.37	33,33,33,33	0
85	MG	1	3828	1/1	0.98	0.41	29,29,29,29	0
85	MG	1	4126	1/1	0.98	0.33	30,30,30,30	0
85	MG	1	3773	1/1	0.98	0.46	15,15,15,15	0
84	OHX	A	1916	7/7	0.98	0.11	128,130,131,131	0
85	MG	r	302	1/1	0.98	0.10	40,40,40,40	0
84	OHX	1	3508	7/7	0.98	0.12	140,142,143,144	0
84	OHX	1	3525	7/7	0.98	0.10	151,152,153,154	0
85	MG	1	4013	1/1	0.98	0.22	56,56,56,56	0
84	OHX	6	1929	7/7	0.98	0.14	147,148,151,152	0
84	OHX	AR	3470	7/7	0.98	0.09	125,127,127,128	0
85	MG	A	2096	1/1	0.98	0.27	51,51,51,51	0
84	OHX	1	3509	7/7	0.98	0.18	155,155,157,157	0
84	OHX	1	3452	7/7	0.98	0.14	111,111,112,113	0
84	OHX	6	1924	7/7	0.98	0.12	123,124,126,127	0
84	OHX	A	1915	7/7	0.98	0.09	149,151,152,154	0
87	ZN	d9	103	1/1	0.98	0.10	86,86,86,86	0
84	OHX	AR	3512	7/7	0.98	0.10	132,132,132,133	0
84	OHX	AR	3476	7/7	0.98	0.12	127,128,129,130	0
85	MG	AR	4078	1/1	0.98	0.31	23,23,23,23	0
85	MG	1	3787	1/1	0.98	0.28	15,15,15,15	0
84	OHX	AR	3443	7/7	0.98	0.14	98,99,100,101	0
85	MG	A	2049	1/1	0.98	0.34	35,35,35,35	0
84	OHX	6	1935	7/7	0.98	0.12	136,137,138,139	0
84	OHX	1	3478	7/7	0.98	0.11	133,134,135,135	0
85	MG	1	4165	1/1	0.98	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4014	1/1	0.98	0.35	32,32,32,32	0
85	MG	AR	3751	1/1	0.98	0.21	29,29,29,29	0
84	OHX	AK	102	7/7	0.98	0.10	121,122,122,122	0
85	MG	AR	3843	1/1	0.98	0.24	13,13,13,13	0
85	MG	AS	217	1/1	0.98	0.16	18,18,18,18	0
84	OHX	AR	3471	7/7	0.98	0.12	127,127,128,128	0
84	OHX	AR	3459	7/7	0.98	0.14	97,97,98,99	0
84	OHX	1	3455	7/7	0.98	0.13	104,104,105,105	0
85	MG	AR	3817	1/1	0.98	0.31	20,20,20,20	0
84	OHX	AR	3537	7/7	0.98	0.11	133,134,135,135	0
85	MG	6	2094	1/1	0.98	0.28	24,24,24,24	0
84	OHX	6	1939	7/7	0.98	0.11	131,133,134,135	0
84	OHX	A	1912	7/7	0.98	0.09	132,133,135,136	0
85	MG	AR	3914	1/1	0.98	0.35	13,13,13,13	0
84	OHX	6	1948	7/7	0.98	0.10	145,147,148,148	0
85	MG	1	3793	1/1	0.98	0.46	12,12,12,12	0
84	OHX	AR	3441	7/7	0.98	0.14	109,110,110,111	0
85	MG	1	3992	1/1	0.98	0.14	53,53,53,53	0
85	MG	AR	3911	1/1	0.98	0.43	16,16,16,16	0
84	OHX	1	3479	7/7	0.98	0.15	136,137,138,138	0
84	OHX	AR	3491	7/7	0.98	0.10	130,131,132,132	0
85	MG	AR	3886	1/1	0.98	0.25	15,15,15,15	0
85	MG	6	2191	1/1	0.98	0.30	47,47,47,47	0
84	OHX	A	1965	7/7	0.98	0.19	167,169,170,171	0
85	MG	AR	3912	1/1	0.98	0.54	1,1,1,1	0
85	MG	A	2141	1/1	0.98	0.32	73,73,73,73	0
84	OHX	A	1963	7/7	0.98	0.10	185,187,189,190	0
84	OHX	1	3494	7/7	0.98	0.11	141,142,144,144	0
84	OHX	1	3468	7/7	0.98	0.14	104,104,104,105	0
84	OHX	AR	3456	7/7	0.98	0.12	109,110,110,111	0
84	OHX	1	3445	7/7	0.98	0.14	95,95,95,96	0
85	MG	1	3917	1/1	0.98	0.36	18,18,18,18	0
84	OHX	1	3538	7/7	0.98	0.14	135,135,137,137	0
84	OHX	A	1910	7/7	0.98	0.11	123,125,127,128	0
84	OHX	AR	3433	7/7	0.98	0.17	94,94,94,95	0
85	MG	AT	230	1/1	0.98	0.23	48,48,48,48	0
85	MG	1	3972	1/1	0.98	0.31	31,31,31,31	0
85	MG	1	3825	1/1	0.98	0.17	42,42,42,42	0
84	OHX	1	3473	7/7	0.98	0.12	119,120,121,121	0
84	OHX	1	3450	7/7	0.98	0.12	116,117,118,118	0
85	MG	1	3797	1/1	0.98	0.13	41,41,41,41	0
85	MG	1	4201	1/1	0.98	0.53	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	6	1915	7/7	0.98	0.12	100,101,102,102	0
85	MG	AR	4089	1/1	0.98	0.39	15,15,15,15	0
84	OHX	1	3444	7/7	0.98	0.16	103,104,104,105	0
85	MG	1	3838	1/1	0.98	0.36	20,20,20,20	0
85	MG	1	3913	1/1	0.98	0.27	38,38,38,38	0
85	MG	AR	3932	1/1	0.98	0.38	25,25,25,25	0
85	MG	1	3869	1/1	0.98	0.33	33,33,33,33	0
84	OHX	AR	3531	7/7	0.98	0.10	123,124,124,124	0
85	MG	1	3925	1/1	0.98	0.38	15,15,15,15	0
84	OHX	6	1930	7/7	0.98	0.12	114,115,116,117	0
85	MG	AR	3929	1/1	0.98	0.13	75,75,75,75	0
85	MG	1	3896	1/1	0.98	0.41	10,10,10,10	0
85	MG	AR	3931	1/1	0.98	0.18	13,13,13,13	0
85	MG	A	2060	1/1	0.98	0.41	20,20,20,20	0
84	OHX	6	1957	7/7	0.98	0.14	144,145,146,147	0
84	OHX	A	1909	7/7	0.98	0.13	124,125,128,129	0
85	MG	1	3892	1/1	0.98	0.52	14,14,14,14	0
85	MG	AR	3765	1/1	0.98	0.44	23,23,23,23	0
84	OHX	AR	3450	7/7	0.98	0.11	109,110,112,113	0
84	OHX	AR	3493	7/7	0.98	0.12	137,139,139,140	0
84	OHX	AR	3448	7/7	0.98	0.12	109,110,110,110	0
85	MG	AR	3878	1/1	0.98	0.27	12,12,12,12	0
84	OHX	AR	3498	7/7	0.98	0.09	143,144,145,146	0
84	OHX	AR	3654	7/7	0.98	0.20	161,162,163,164	0
85	MG	1	3857	1/1	0.98	0.39	12,12,12,12	0
84	OHX	AR	3487	7/7	0.98	0.12	116,117,117,117	0
84	OHX	A	1908	7/7	0.98	0.16	111,111,113,114	0
84	OHX	3	204	7/7	0.98	0.08	163,164,165,166	0
85	MG	AR	4197	1/1	0.98	0.24	29,29,29,29	0
84	OHX	AS	204	7/7	0.98	0.12	140,141,141,141	0
84	OHX	1	3437	7/7	0.98	0.14	100,101,102,102	0
84	OHX	AR	3455	7/7	0.98	0.17	106,107,108,108	0
85	MG	1	3836	1/1	0.98	0.24	17,17,17,17	0
85	MG	1	4037	1/1	0.98	0.19	61,61,61,61	0
84	OHX	AR	3562	7/7	0.98	0.07	173,174,175,176	0
84	OHX	A	1923	7/7	0.98	0.09	137,138,140,140	0
85	MG	1	3886	1/1	0.98	0.43	24,24,24,24	0
85	MG	1	3904	1/1	0.98	0.44	4,4,4,4	0
84	OHX	A	1926	7/7	0.98	0.11	149,150,151,152	0
85	MG	AS	222	1/1	0.98	0.22	13,13,13,13	0
85	MG	6	2063	1/1	0.98	0.28	31,31,31,31	0
85	MG	6	2183	1/1	0.98	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3433	7/7	0.98	0.21	90,90,90,90	0
85	MG	AR	3845	1/1	0.98	0.23	32,32,32,32	0
85	MG	6	2059	1/1	0.98	0.42	40,40,40,40	0
84	OHX	1	3510	7/7	0.98	0.22	148,148,149,149	0
85	MG	AR	3856	1/1	0.98	0.53	10,10,10,10	0
85	MG	6	2077	1/1	0.98	0.56	51,51,51,51	0
84	OHX	1	3448	7/7	0.98	0.24	104,105,106,106	0
84	OHX	6	1959	7/7	0.98	0.11	154,155,156,157	0
85	MG	1	4148	1/1	0.98	0.57	35,35,35,35	0
84	OHX	1	3481	7/7	0.98	0.11	130,131,132,133	0
84	OHX	1	3464	7/7	0.98	0.11	136,137,138,139	0
84	OHX	AR	3469	7/7	0.98	0.10	122,124,125,125	0
84	OHX	1	3474	7/7	0.98	0.14	131,132,133,133	0
84	OHX	6	1907	7/7	0.98	0.19	100,101,101,101	0
85	MG	1	3884	1/1	0.98	0.38	27,27,27,27	0
85	MG	AR	3783	1/1	0.98	0.39	15,15,15,15	0
84	OHX	1	3404	7/7	0.99	0.20	93,93,93,93	0
84	OHX	6	1925	7/7	0.99	0.12	116,116,118,118	0
84	OHX	AR	3421	7/7	0.99	0.12	89,89,89,89	0
84	OHX	1	3409	7/7	0.99	0.21	85,85,85,85	0
85	MG	1	3752	1/1	0.99	0.29	27,27,27,27	0
84	OHX	1	3430	7/7	0.99	0.14	97,97,97,98	0
85	MG	1	4054	1/1	0.99	0.14	40,40,40,40	0
85	MG	1	3837	1/1	0.99	0.64	25,25,25,25	0
85	MG	1	3882	1/1	0.99	0.38	11,11,11,11	0
84	OHX	1	3416	7/7	0.99	0.15	86,86,86,86	0
84	OHX	1	3443	7/7	0.99	0.12	95,95,95,95	0
84	OHX	6	1905	7/7	0.99	0.20	100,100,101,101	0
84	OHX	1	3436	7/7	0.99	0.11	101,102,104,104	0
84	OHX	AR	3432	7/7	0.99	0.13	91,91,91,91	0
84	OHX	AR	3482	7/7	0.99	0.10	116,117,117,117	0
84	OHX	AT	203	7/7	0.99	0.21	83,83,83,83	0
85	MG	AR	3852	1/1	0.99	0.44	18,18,18,18	0
84	OHX	6	1922	7/7	0.99	0.10	111,112,113,114	0
84	OHX	A	1905	7/7	0.99	0.18	102,102,103,103	0
84	OHX	6	1934	7/7	0.99	0.09	141,141,143,144	0
87	ZN	e	102	1/1	0.99	0.06	74,74,74,74	0
84	OHX	AR	3415	7/7	0.99	0.23	86,86,86,87	0
85	MG	6	2117	1/1	0.99	0.41	21,21,21,21	0
84	OHX	2	201	7/7	0.99	0.17	94,94,94,94	0
84	OHX	6	1918	7/7	0.99	0.11	103,104,105,105	0
84	OHX	1	3410	7/7	0.99	0.20	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	A	1903	7/7	0.99	0.26	117,118,118,119	0
84	OHX	1	3413	7/7	0.99	0.18	88,88,89,89	0
85	MG	AR	3906	1/1	0.99	0.23	15,15,15,15	0
84	OHX	1	3465	7/7	0.99	0.10	113,114,114,114	0
84	OHX	AR	3437	7/7	0.99	0.11	89,89,89,89	0
85	MG	6	2146	1/1	0.99	0.14	44,44,44,44	0
84	OHX	AR	3401	7/7	0.99	0.26	93,93,93,93	0
85	MG	A	2145	1/1	0.99	0.21	83,83,83,83	0
85	MG	1	3856	1/1	0.99	0.31	15,15,15,15	0
84	OHX	1	3429	7/7	0.99	0.13	89,89,90,90	0
85	MG	l2	201	1/1	0.99	0.28	21,21,21,21	0
84	OHX	AR	3414	7/7	0.99	0.18	90,90,90,90	0
85	MG	AR	3909	1/1	0.99	0.37	14,14,14,14	0
84	OHX	6	1913	7/7	0.99	0.13	105,105,106,107	0
84	OHX	AR	3444	7/7	0.99	0.10	101,102,102,103	0
87	ZN	AK	101	1/1	0.99	0.13	38,38,38,38	0
85	MG	AR	3883	1/1	0.99	0.34	12,12,12,12	0
85	MG	AR	3819	1/1	0.99	0.49	53,53,53,53	0
85	MG	1	4094	1/1	0.99	0.13	43,43,43,43	0
84	OHX	A	1984	7/7	0.99	0.12	151,152,153,154	0
84	OHX	6	1909	7/7	0.99	0.16	103,104,104,104	0
84	OHX	AR	3404	7/7	0.99	0.19	88,89,89,89	0
84	OHX	AR	3440	7/7	0.99	0.12	98,98,98,99	0
84	OHX	AR	3465	7/7	0.99	0.12	100,101,102,102	0
84	OHX	1	3425	7/7	0.99	0.16	93,93,93,93	0
84	OHX	1	3431	7/7	0.99	0.12	95,95,95,95	0
85	MG	AR	3841	1/1	0.99	0.32	25,25,25,25	0
84	OHX	1	3424	7/7	0.99	0.19	92,93,93,93	0
85	MG	1	3806	1/1	0.99	0.28	31,31,31,31	0
84	OHX	AR	3462	7/7	0.99	0.11	106,107,108,108	0
84	OHX	6	1917	7/7	0.99	0.10	113,114,116,117	0
84	OHX	6	1923	7/7	0.99	0.14	136,138,139,139	0
84	OHX	AR	3418	7/7	0.99	0.14	92,92,93,93	0
84	OHX	AR	3422	7/7	0.99	0.15	86,86,86,86	0
85	MG	AR	4051	1/1	0.99	0.12	62,62,62,62	0
85	MG	6	2135	1/1	0.99	0.22	38,38,38,38	0
85	MG	AB	201	1/1	0.99	0.50	15,15,15,15	0
85	MG	1	4086	1/1	0.99	0.32	16,16,16,16	0
84	OHX	AR	3431	7/7	0.99	0.14	86,86,86,86	0
85	MG	DC	204	1/1	0.99	0.17	45,45,45,45	0
84	OHX	1	3408	7/7	0.99	0.12	89,89,89,89	0
84	OHX	6	1903	7/7	0.99	0.20	89,89,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3439	7/7	0.99	0.16	91,91,92,92	0
84	OHX	AR	3417	7/7	0.99	0.14	86,86,86,86	0
84	OHX	1	3453	7/7	0.99	0.09	130,132,133,133	0
87	ZN	b	102	1/1	0.99	0.10	68,68,68,68	0
84	OHX	1	3415	7/7	0.99	0.15	89,90,90,90	0
84	OHX	AR	3408	7/7	0.99	0.22	83,83,83,83	0
84	OHX	AR	3425	7/7	0.99	0.10	85,85,85,85	0
85	MG	AB	202	1/1	0.99	0.22	34,34,34,34	0
84	OHX	1	3423	7/7	0.99	0.15	91,92,92,92	0
85	MG	1	3832	1/1	0.99	0.34	13,13,13,13	0
84	OHX	1	3447	7/7	0.99	0.14	95,95,95,95	0
84	OHX	AR	3413	7/7	0.99	0.16	84,84,84,84	0
84	OHX	AR	3449	7/7	0.99	0.12	98,99,99,100	0
84	OHX	1	3502	7/7	0.99	0.10	100,101,102,102	0
84	OHX	AR	3419	7/7	0.99	0.13	94,94,95,95	0
84	OHX	AR	3542	7/7	0.99	0.19	133,134,134,134	0
85	MG	1	3845	1/1	0.99	0.36	14,14,14,14	0
84	OHX	6	1916	7/7	0.99	0.11	102,103,104,104	0
84	OHX	AR	3501	7/7	0.99	0.11	118,118,120,120	0
85	MG	AR	3910	1/1	0.99	0.32	17,17,17,17	0
85	MG	1	3848	1/1	0.99	0.20	26,26,26,26	0
85	MG	1	4191	1/1	0.99	0.45	22,22,22,22	0
85	MG	1	4099	1/1	0.99	0.31	16,16,16,16	0
84	OHX	1	3438	7/7	0.99	0.13	91,91,92,92	0
85	MG	1	4065	1/1	0.99	0.26	35,35,35,35	0
84	OHX	A	1919	7/7	0.99	0.10	113,115,116,116	0
84	OHX	1	3463	7/7	0.99	0.08	108,109,109,109	0
84	OHX	6	1906	7/7	0.99	0.19	94,94,95,95	0
84	OHX	1	3499	7/7	0.99	0.10	124,125,126,126	0
84	OHX	1	3428	7/7	0.99	0.14	96,96,96,96	0
84	OHX	A	1939	7/7	0.99	0.08	153,155,156,157	0
84	OHX	AR	3403	7/7	0.99	0.19	86,86,86,86	0
84	OHX	1	3451	7/7	0.99	0.10	101,101,102,103	0
84	OHX	6	1901	7/7	0.99	0.23	92,92,92,92	0
84	OHX	AR	3458	7/7	0.99	0.11	100,101,101,102	0
85	MG	1	3987	1/1	0.99	0.24	32,32,32,32	0
84	OHX	AR	3405	7/7	0.99	0.23	94,94,94,94	0
84	OHX	1	3422	7/7	0.99	0.17	94,94,94,94	0
84	OHX	AR	3402	7/7	0.99	0.27	89,89,89,89	0
84	OHX	1	3402	7/7	0.99	0.24	90,90,91,91	0
84	OHX	AR	3428	7/7	0.99	0.10	97,97,98,98	0
84	OHX	1	3421	7/7	0.99	0.11	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3447	7/7	0.99	0.13	88,88,89,89	0
84	OHX	AR	3423	7/7	0.99	0.14	85,85,85,85	0
84	OHX	1	3418	7/7	0.99	0.13	85,85,85,85	0
84	OHX	A	1906	7/7	0.99	0.17	112,113,113,113	0
87	ZN	d6	102	1/1	0.99	0.10	59,59,59,59	0
85	MG	AR	4190	1/1	0.99	0.24	107,107,107,107	0
84	OHX	A	1901	7/7	0.99	0.21	101,101,102,102	0
85	MG	1	3931	1/1	0.99	0.12	31,31,31,31	0
84	OHX	6	1911	7/7	0.99	0.15	99,100,100,100	0
85	MG	1	4137	1/1	0.99	0.20	38,38,38,38	0
84	OHX	1	3459	7/7	0.99	0.09	134,134,135,136	0
84	OHX	AR	3486	7/7	0.99	0.09	118,119,120,121	0
84	OHX	AR	3483	7/7	0.99	0.16	124,125,125,126	0
85	MG	AR	3840	1/1	0.99	0.33	22,22,22,22	0
84	OHX	AR	3490	7/7	0.99	0.09	108,108,109,110	0
84	OHX	1	3460	7/7	0.99	0.12	112,114,115,116	0
85	MG	AR	3882	1/1	0.99	0.58	11,11,11,11	0
84	OHX	AR	3420	7/7	0.99	0.16	87,87,87,87	0
85	MG	AR	4157	1/1	0.99	0.22	29,29,29,29	0
84	OHX	1	3412	7/7	0.99	0.22	88,88,88,88	0
85	MG	k	403	1/1	0.99	0.21	24,24,24,24	0
84	OHX	1	3439	7/7	0.99	0.11	102,103,103,104	0
84	OHX	6	1902	7/7	0.99	0.24	102,102,102,102	0
84	OHX	AR	3411	7/7	0.99	0.20	83,83,83,83	0
84	OHX	AR	3461	7/7	0.99	0.11	108,109,109,110	0
84	OHX	A	1917	7/7	0.99	0.12	126,128,129,130	0
85	MG	1	3873	1/1	0.99	0.40	18,18,18,18	0
85	MG	1	3899	1/1	0.99	0.41	12,12,12,12	0
84	OHX	6	1910	7/7	0.99	0.14	93,93,93,93	0
85	MG	AR	3872	1/1	0.99	0.45	0,0,0,0	0
84	OHX	1	3403	7/7	0.99	0.23	90,90,90,90	0
84	OHX	AR	3434	7/7	0.99	0.16	87,87,88,88	0
85	MG	AR	3851	1/1	0.99	0.34	29,29,29,29	0
85	MG	3	214	1/1	0.99	0.42	12,12,12,12	0
84	OHX	AR	3446	7/7	0.99	0.09	99,100,100,101	0
85	MG	1	4143	1/1	0.99	0.07	53,53,53,53	0
84	OHX	6	1926	7/7	0.99	0.10	122,123,124,124	0
84	OHX	AR	3412	7/7	0.99	0.16	85,85,85,85	0
84	OHX	AR	3410	7/7	0.99	0.13	86,86,86,86	0
84	OHX	AR	3435	7/7	0.99	0.11	96,96,96,96	0
84	OHX	AR	3407	7/7	0.99	0.24	88,88,88,88	0
85	MG	AR	4105	1/1	0.99	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	6	1908	7/7	0.99	0.16	91,91,91,91	0
84	OHX	1	3457	7/7	0.99	0.14	108,108,109,109	0
85	MG	1	3924	1/1	0.99	0.54	8,8,8,8	0
84	OHX	AR	3409	7/7	0.99	0.20	92,92,92,92	0
85	MG	1	4212	1/1	0.99	0.32	27,27,27,27	0
84	OHX	A	1902	7/7	0.99	0.16	96,97,97,97	0
84	OHX	1	3440	7/7	0.99	0.14	94,95,95,95	0
84	OHX	1	3426	7/7	0.99	0.15	93,93,93,94	0
85	MG	AR	3937	1/1	0.99	0.43	9,9,9,9	0
85	MG	DH	203	1/1	0.99	0.23	41,41,41,41	0
85	MG	A	2047	1/1	0.99	0.39	55,55,55,55	0
84	OHX	1	3489	7/7	0.99	0.11	114,115,116,117	0
84	OHX	AR	3426	7/7	0.99	0.13	88,88,88,89	0
84	OHX	6	1912	7/7	0.99	0.09	107,108,110,110	0
85	MG	1	3901	1/1	0.99	0.49	12,12,12,12	0
84	OHX	3	201	7/7	0.99	0.10	106,107,108,108	0
84	OHX	1	3419	7/7	0.99	0.19	93,93,93,93	0
85	MG	1	4167	1/1	0.99	0.15	52,52,52,52	0
84	OHX	1	3420	7/7	0.99	0.20	91,91,92,92	0
85	MG	1	4071	1/1	0.99	0.37	16,16,16,16	0
85	MG	AR	3927	1/1	0.99	0.64	11,11,11,11	0
84	OHX	A	1914	7/7	0.99	0.11	109,110,111,112	0
85	MG	j	302	1/1	0.99	0.14	29,29,29,29	0
84	OHX	AR	3436	7/7	0.99	0.16	87,87,87,87	0
84	OHX	DD	102	7/7	0.99	0.17	88,89,89,89	0
84	OHX	A	1904	7/7	0.99	0.12	107,107,108,108	0
84	OHX	1	3411	7/7	0.99	0.19	93,93,93,93	0
84	OHX	1	3405	7/7	0.99	0.26	97,98,98,98	0
84	OHX	1	3434	7/7	0.99	0.14	94,95,95,95	0
84	OHX	1	3519	7/7	0.99	0.10	112,112,113,113	0
84	OHX	1	3417	7/7	0.99	0.19	97,97,97,97	0
84	OHX	1	3414	7/7	0.99	0.17	90,90,90,90	0
84	OHX	1	3472	7/7	0.99	0.12	114,115,115,116	0
84	OHX	AR	3416	7/7	0.99	0.17	88,88,88,89	0
84	OHX	AR	3438	7/7	0.99	0.12	89,89,89,90	0
84	OHX	A	1907	7/7	0.99	0.09	117,118,120,121	0
84	OHX	1	3407	7/7	0.99	0.20	83,83,83,83	0
84	OHX	1	3427	7/7	0.99	0.15	87,87,87,87	0
84	OHX	AR	3424	7/7	0.99	0.19	86,87,87,87	0
84	OHX	1	3406	7/7	0.99	0.22	85,85,85,85	0
84	OHX	CV	201	7/7	0.99	0.21	91,91,91,91	0
84	OHX	AR	3406	7/7	0.99	0.23	86,86,86,86	0

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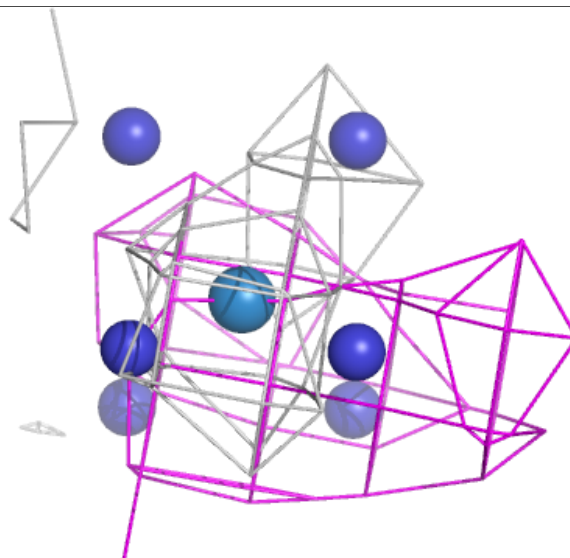
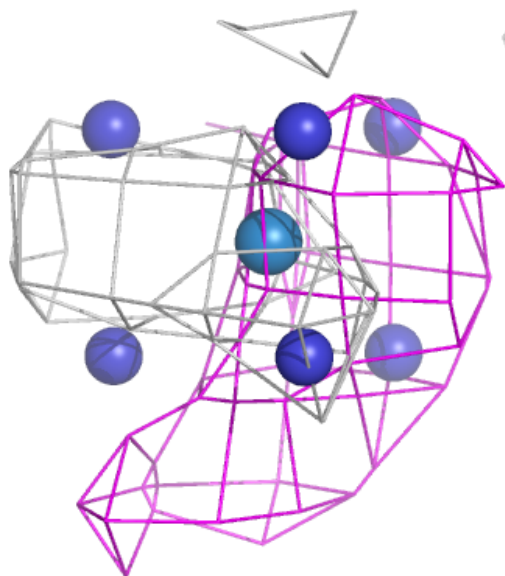
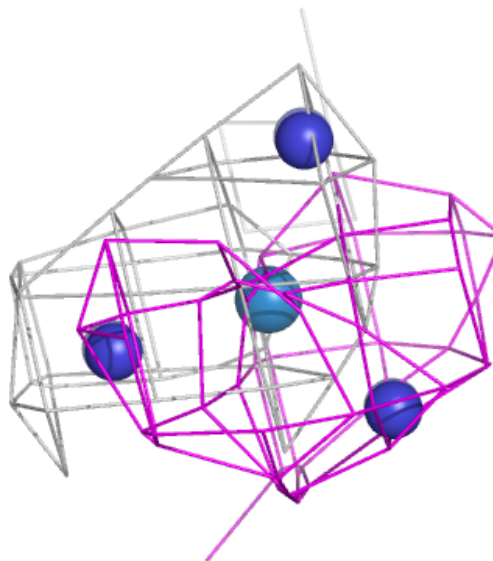
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AT	202	7/7	1.00	0.20	86,86,87,87	0
84	OHX	AC	101	7/7	1.00	0.18	89,90,90,90	0
85	MG	AR	3767	1/1	1.00	0.11	34,34,34,34	0
85	MG	1	4156	1/1	1.00	0.13	65,65,65,65	0
85	MG	1	3850	1/1	1.00	0.12	29,29,29,29	0
85	MG	1	4166	1/1	1.00	0.12	30,30,30,30	0
87	ZN	DO	201	1/1	1.00	0.13	31,31,31,31	0
85	MG	AR	4110	1/1	1.00	0.11	45,45,45,45	0
85	MG	AR	4207	1/1	1.00	0.14	50,50,50,50	0
84	OHX	6	1904	7/7	1.00	0.15	96,96,96,96	0
85	MG	1	4097	1/1	1.00	0.17	61,61,61,61	0
84	OHX	1	3401	7/7	1.00	0.26	89,89,90,90	0
85	MG	1	4187	1/1	1.00	0.10	55,55,55,55	0
87	ZN	DL	103	1/1	1.00	0.12	37,37,37,37	0
87	ZN	AN	500	1/1	1.00	0.11	43,43,43,43	0
85	MG	s1	301	1/1	1.00	0.16	67,67,67,67	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.

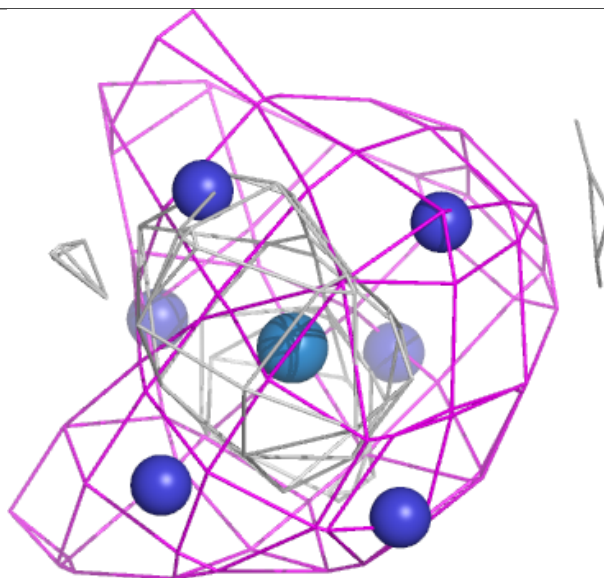
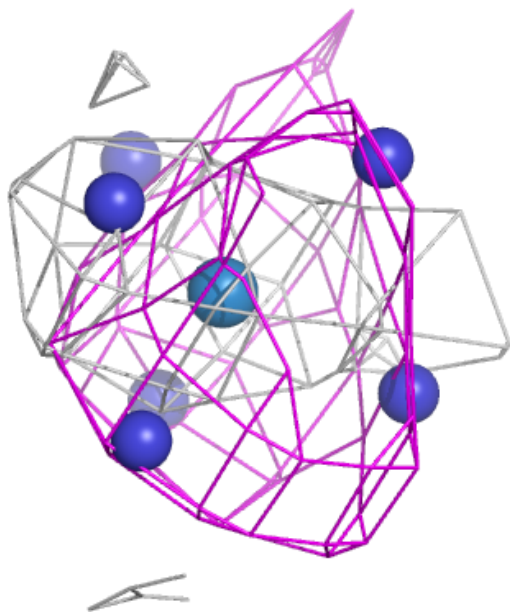
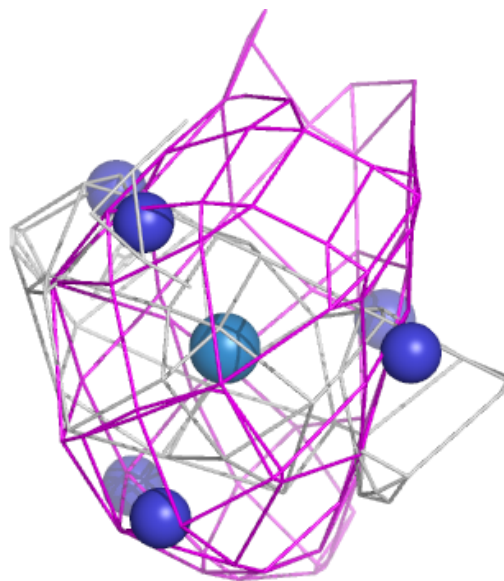
Electron density around OHX 1 3722:

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



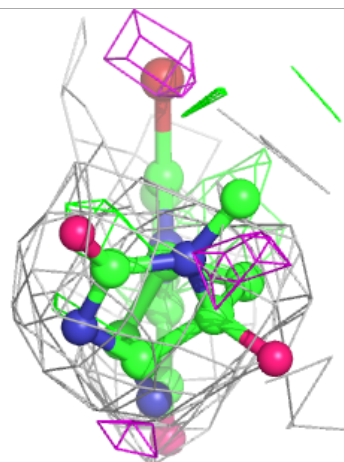
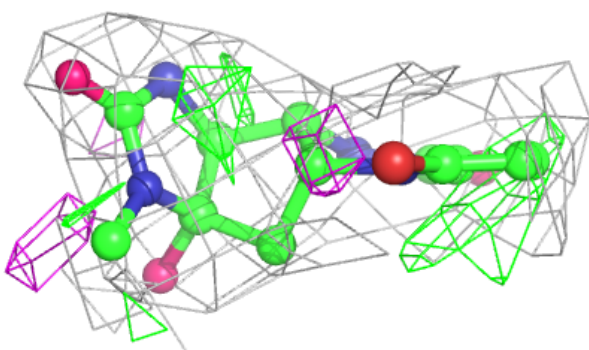
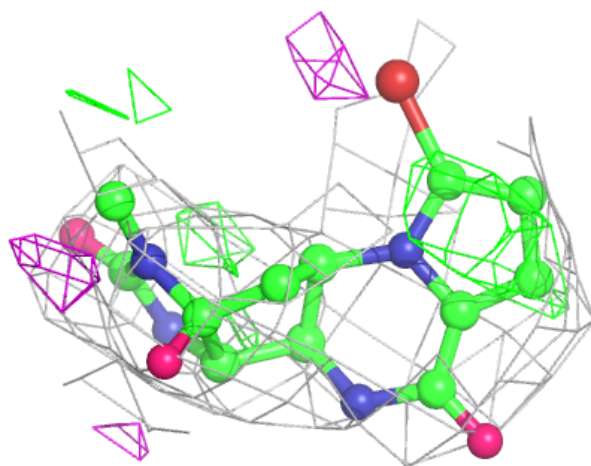
Electron density around OHX 1 3675:

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



Electron density around 7MB 1 4216:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.