wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 12:16 am GMT

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

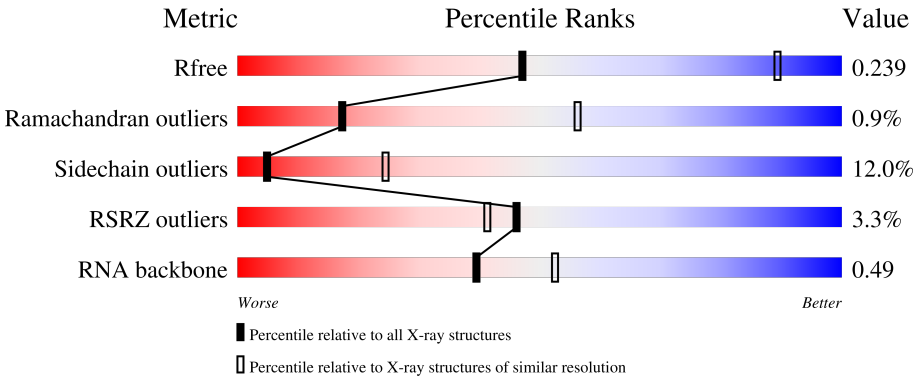
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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)
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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 72% 20% • 7%
1	AR	3396	2% 70% 21% • 7%
2	3	121	84% 16%
2	AS	121	% 83% 17%

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Mol	Chain	Length	Quality of chain
3	4	158	77% 23%
3	AT	158	79% 20%
4	CD	252	89% 11%
4	j	252	92% 8%
5	CE	386	88% 12%
5	k	386	86% 14%
6	CF	361	90% 9%
6	l	361	90% 10%
7	CG	296	88% 12%
7	m	296	91% 9%
8	CH	175	79% 10% 11%
8	n	175	81% 7% 11%
9	CI	222	92% 7%
9	o	222	89% 11%
10	CJ	233	7% 91% 9%
10	p	233	91% 9%
11	CK	191	83% 17%
11	q	191	88% 12%
12	CL	220	84% 12%
12	r	220	85% 11%
13	CM	169	85% 15%
13	s	169	89% 11%
14	CN	193	89% 11%
14	t	193	91% 9%
15	CO	136	85% 15%

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Mol	Chain	Length	Quality of chain
15	u	136	90% 10%
16	CP	203	90% 10%
16	v	203	90% 10%
17	CQ	197	% 88% 12%
17	w	197	87% 12%
18	CR	183	14% 86% 14%
18	x	183	4% 87% 13%
19	CS	185	95% 5%
19	y	185	91% 9%
20	CT	188	2% 87% 13%
20	z	188	2% 93% 6%
21	0	172	% 89% 10%
21	CU	172	87% 13%
22	2	159	84% 16%
22	CV	159	87% 13%
23	5	100	7% 89% 11%
23	CW	100	7% 87% 13%
24	CX	136	93% 7%
24	l2	136	90% 10%
25	6	1800	4% 75% 22%
25	A	1800	5% 74% 24%
26	7	98	34% 93% 7%
26	CY	98	12% 92% 8%
27	8	121	86% 14%
27	CZ	121	2% 88% 11%

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Mol	Chain	Length	Quality of chain
28	9	126	91% 8%
28	DA	126	90% 10%
29	AA	135	3% 92% 8%
29	DB	135	3% 90% 10%
30	AB	148	90% 10%
30	DC	148	91% 9%
31	AC	58	88% 10%
31	DD	58	86% 14%
32	AD	97	4% 89% 11%
32	DE	97	94% 6%
33	AE	109	89% 11%
33	DF	109	83% 17%
34	AF	127	89% 11%
34	DG	127	87% 13%
35	AG	106	92% 8%
35	DH	106	92% 8%
36	AH	112	89% 11%
36	DI	112	88% 12%
37	AI	119	88% 12%
37	DJ	119	86% 14%
38	AJ	99	87% 13%
38	DK	99	85% 15%
39	AK	87	92% 8%
39	DL	87	90% 10%
40	AL	77	87% 13%

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Mol	Chain	Length	Quality of chain
40	DM	77	13% 88% 12%
41	AM	50	90% 10%
41	DN	50	94% 6%
42	AN	52	90% 10%
42	DO	52	90% 10%
43	AO	25	72% 28%
43	DP	25	84% 16%
44	AP	105	2% 86% 13%
44	DQ	105	88% 12%
45	AQ	91	90% 10%
45	DR	91	87% 13%
46	i	168	11% 86% 8% 5%
47	p0	220	11% 57% 8% 35%
48	sM	104	4% 92% 7%
49	B	206	5% 90% 10%
49	s0	206	88% 12%
50	C	216	15% 87% 12%
50	s1	216	% 88% 11%
51	D	217	2% 88% 12%
51	s2	217	85% 14%
52	E	223	3% 89% 11%
52	s3	223	4% 92% 8%
53	F	260	2% 88% 12%
53	s4	260	90% 10%
54	G	206	11% 91% 9%

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Mol	Chain	Length	Quality of chain
54	s5	206	6% 92% 8%
55	H	226	3% 91% 9%
55	s6	226	3% 85% 12%
56	I	186	5% 85% 13%
56	s7	186	4% 92% 7%
57	J	199	5% 85% 9% 6%
57	s8	199	3% 86% 8% 6%
58	K	185	9% 85% 14%
58	s9	185	2% 89% 11%
59	L	105	2% 84% 7% 9%
59	c0	105	26% 79% 10% 9%
60	M	155	10% 92% 7%
60	c1	155	5% 82% 12% 6%
61	N	124	19% 84% 15%
61	c2	124	37% 81% 18%
62	O	150	2% 91% 9%
62	c3	150	91% 9%
63	P	128	12% 88% 12%
63	c4	128	8% 91% 9%
64	Q	141	4% 80% 8% 12%
64	c5	141	8% 87% 8%
65	R	142	12% 86% 13%
65	c6	142	% 87% 13%
66	S	125	2% 85% 10%
67	T	145	7% 88% 11%

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Mol	Chain	Length	Quality of chain
67	c8	145	90% 9%
68	U	143	5% 87% 13%
68	c9	143	93% 7%
69	V	110	7% 87% 10%
69	d0	110	21% 90% 10%
70	W	87	5% 87% 13%
70	d1	87	91% 9%
71	X	129	88% 10%
71	d2	129	91% 9%
72	Y	144	87% 13%
72	d3	144	92% 8%
73	Z	134	4% 94% 6%
73	d4	134	90% 10%
74	a	70	14% 80% 20%
74	d5	70	4% 93% 6%
75	b	97	8% 82% 18%
75	d6	97	90% 10%
76	c	81	11% 94% 6%
76	d7	81	6% 90% 10%
77	d	63	21% 90% 10%
77	d8	63	13% 89% 11%
78	d9	53	87% 11%
78	e	53	91% 9%
79	e0	62	3% 76% 24%
79	f	62	10% 85% 11%

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Mol	Chain	Length	Quality of chain
80	g	71	17% 79% 21%
81	h	318	13% 92% 8%
81	sR	318	13% 94% 6%
82	c7	121	% 84% 12%
83	e1	51	20% 82% 18%

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	3675	-	-	-	X
84	OHX	1	3722	-	-	-	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
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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	S	0	0	0
			1053	675	199	177	2			
15	CO	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	l2	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	0	0	0
			680	403	140	137			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

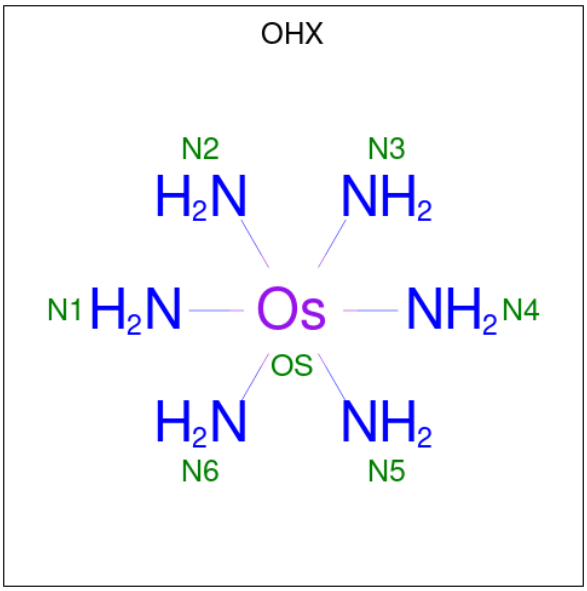
- Molecule 82 is a protein called 40S ribosomal protein S17-A.

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

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

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

- Molecule 84 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



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 7 6 1	0	0
84	1	1	Total N Os 7 6 1	0	0
84	1	1	Total N Os 7 6 1	0	0
84	1	1	Total N Os 7 6 1	0	0
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84	1	1	Total N Os 7 6 1	0	0
84	1	1	Total N Os 7 6 1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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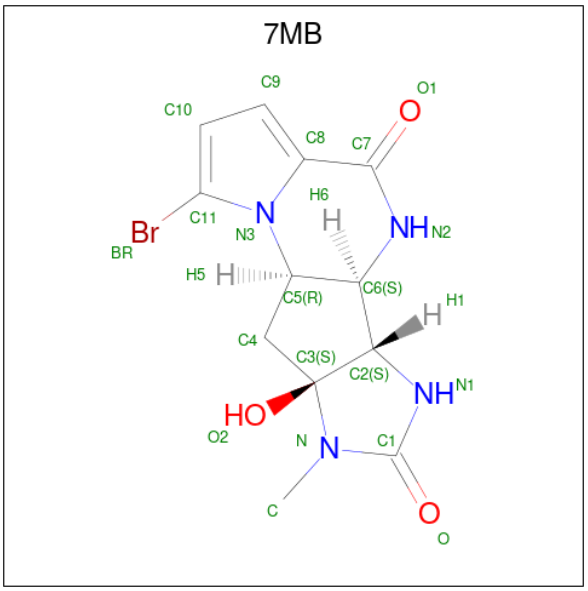
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	DI	1	Total Mg 1 1	0	0
85	DO	1	Total Mg 1 1	0	0
85	DP	1	Total Mg 1 1	0	0
85	DR	2	Total Mg 2 2	0	0
85	sM	1	Total Mg 1 1	0	0
85	A	111	Total Mg 111 111	0	0
85	D	1	Total Mg 1 1	0	0
85	F	1	Total Mg 1 1	0	0
85	Y	1	Total Mg 1 1	0	0
85	b	1	Total Mg 1 1	0	0
85	s1	1	Total Mg 1 1	0	0
85	s2	1	Total Mg 1 1	0	0
85	s6	1	Total Mg 1 1	0	0
85	s8	1	Total Mg 1 1	0	0
85	c6	1	Total Mg 1 1	0	0
85	c9	1	Total Mg 1 1	0	0
85	d3	3	Total Mg 3 3	0	0
85	d5	1	Total Mg 1 1	0	0
85	d6	1	Total Mg 1 1	0	0
85	d9	1	Total Mg 1 1	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	AK	1	Total	Zn	0	0
			1	1		
87	AN	1	Total	Zn	0	0
			1	1		
87	AP	1	Total	Zn	0	0
			1	1		
87	AQ	1	Total	Zn	0	0
			1	1		
87	DL	1	Total	Zn	0	0
			1	1		
87	DO	1	Total	Zn	0	0
			1	1		
87	DQ	1	Total	Zn	0	0
			1	1		
87	DR	1	Total	Zn	0	0
			1	1		
87	b	1	Total	Zn	0	0
			1	1		
87	c	1	Total	Zn	0	0
			1	1		

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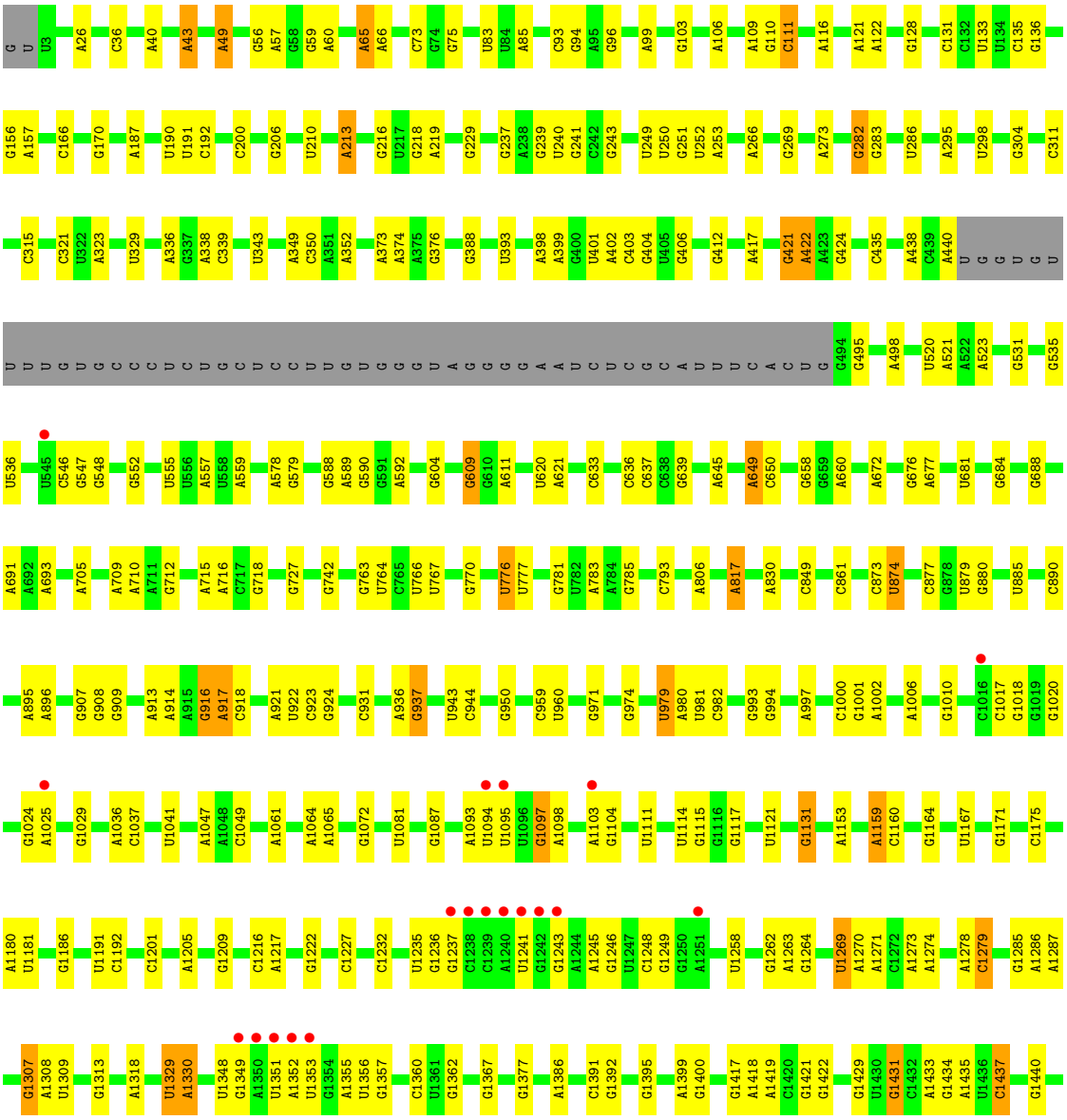
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	e	1	Total Zn 1 1	0	0
87	g	1	Total Zn 1 1	0	0
87	d6	1	Total Zn 1 1	0	0
87	d7	1	Total Zn 1 1	0	0
87	d9	1	Total Zn 1 1	0	0
87	e1	1	Total Zn 1 1	0	0

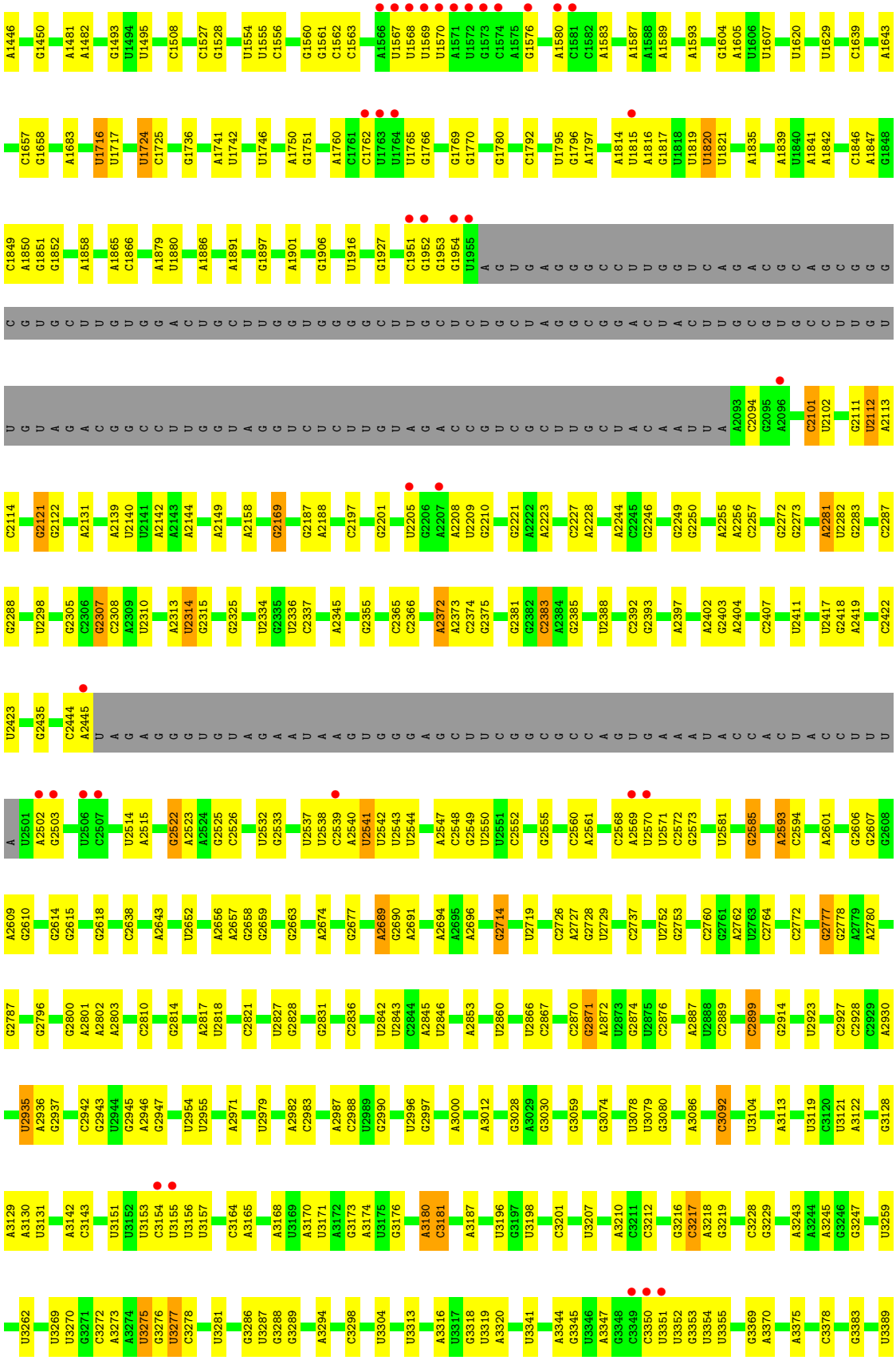
3 Residue-property plots (i)

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

• Molecule 1: 25S ribosomal RNA

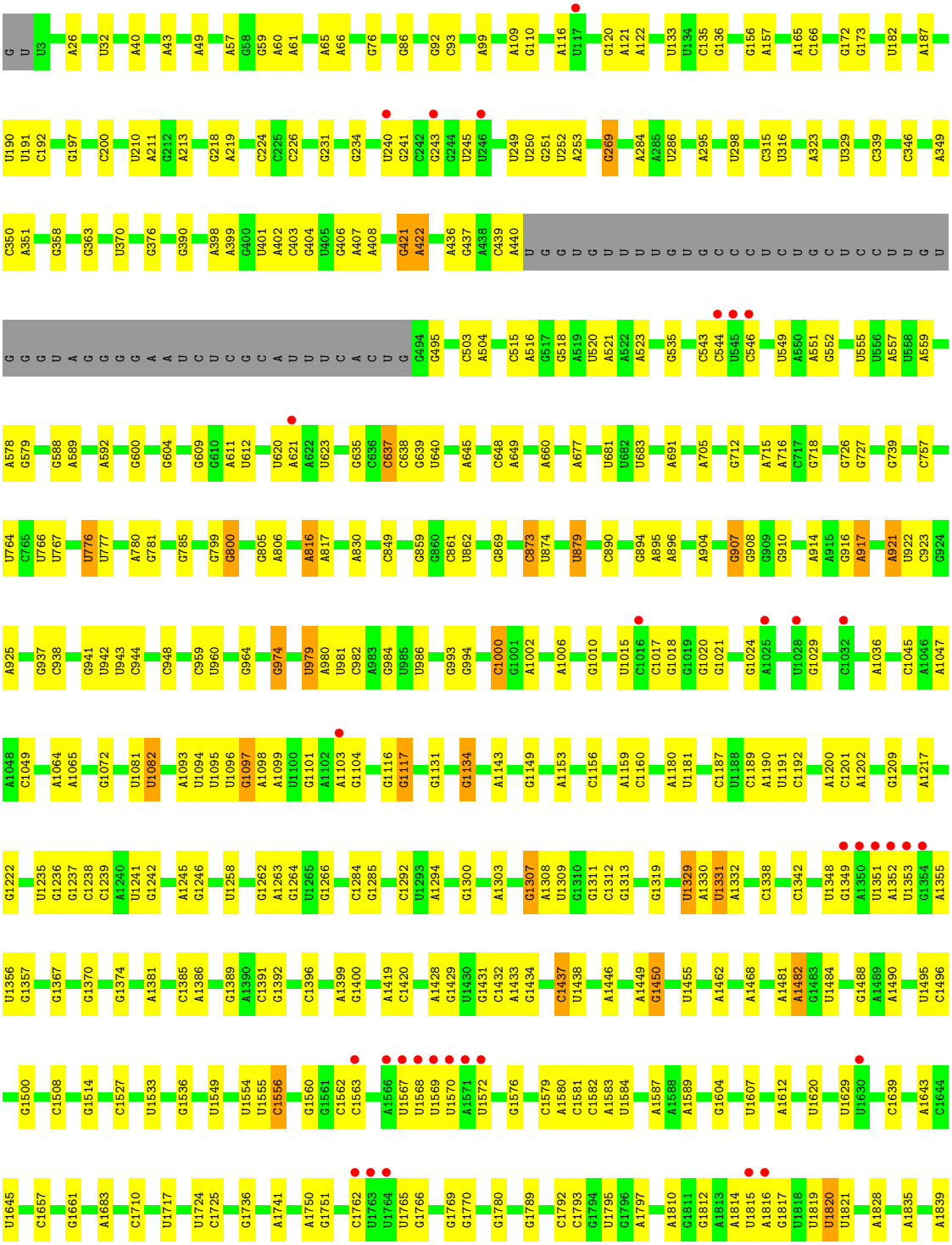
Chain 1: 

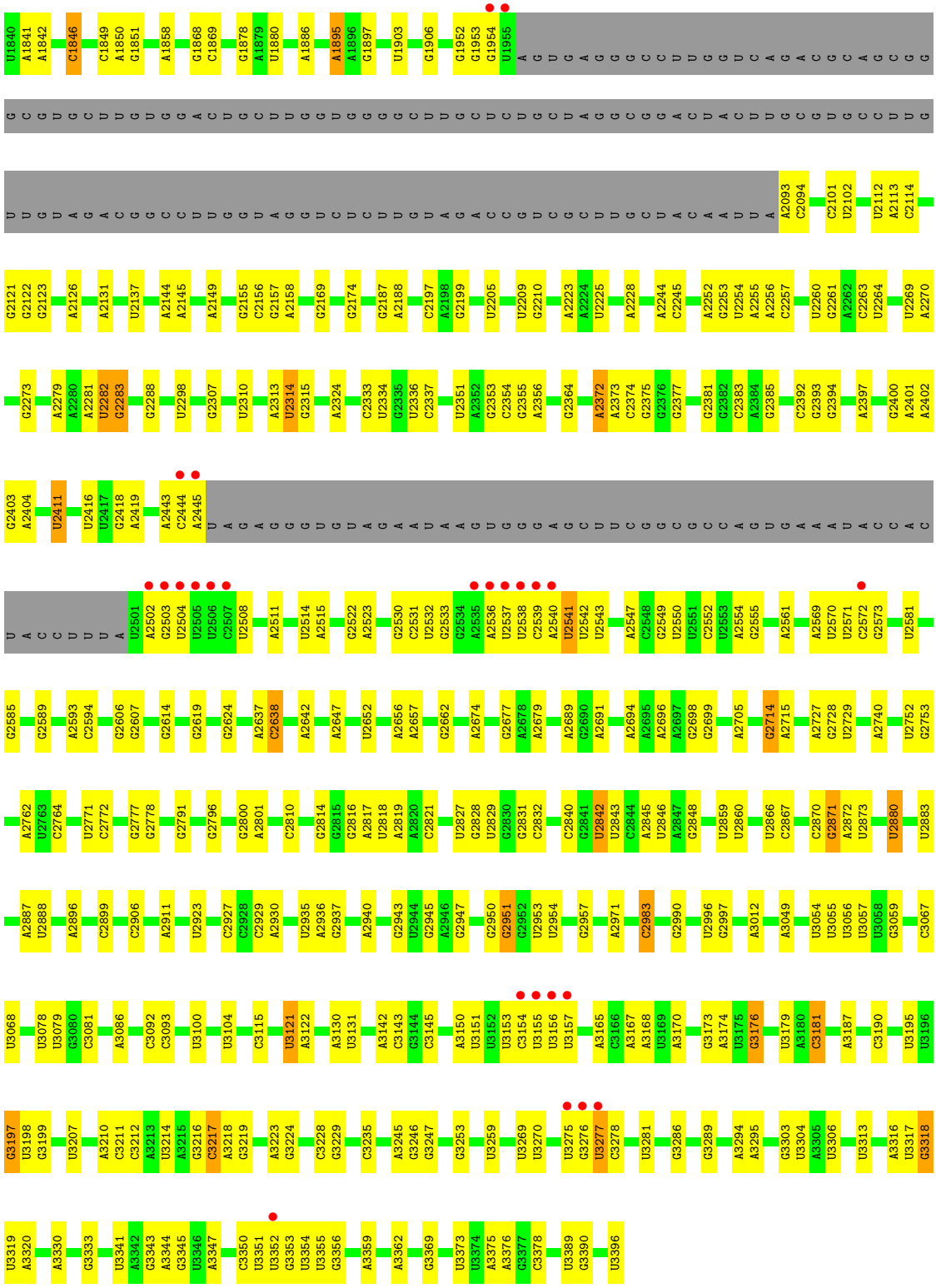




• Molecule 1: 25S ribosomal RNA

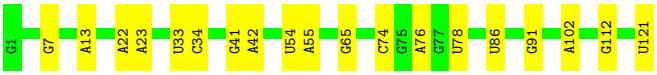
Chain AR:





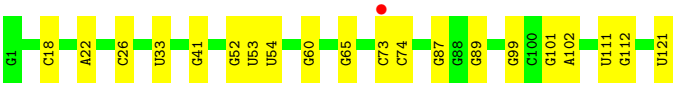
• Molecule 2: 5S ribosomal RNA

Chain 3:



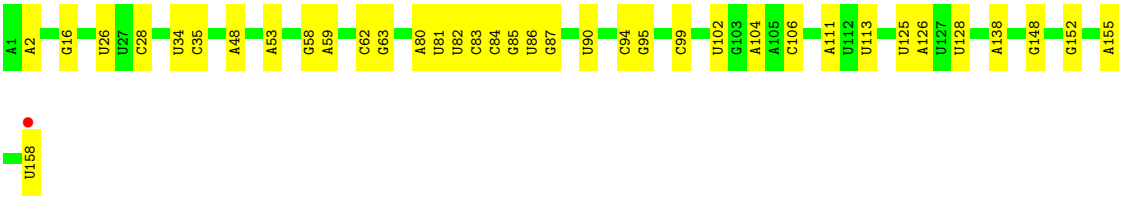
• Molecule 2: 5S ribosomal RNA

Chain AS:



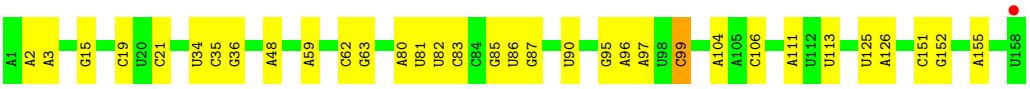
• Molecule 3: 5.8S ribosomal RNA

Chain 4:



• Molecule 3: 5.8S ribosomal RNA

Chain AT:



• Molecule 4: 60S ribosomal protein L2-A

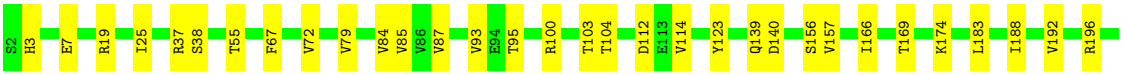
Chain j:

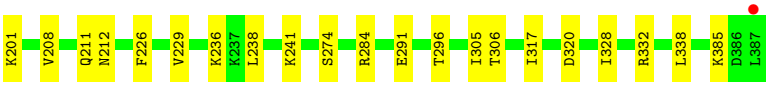
• Molecule 4: 60S ribosomal protein L2-A

Chain CD:

• Molecule 5: 60S ribosomal protein L3

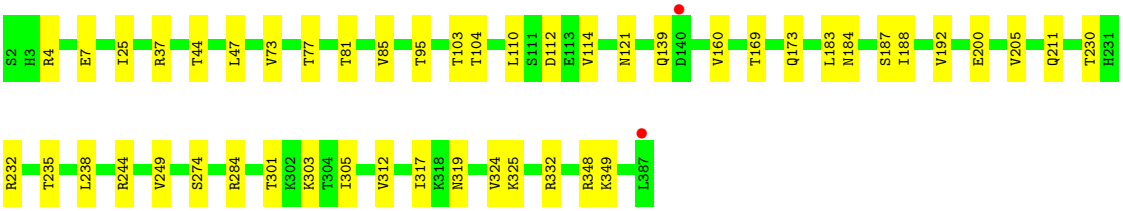
Chain k:





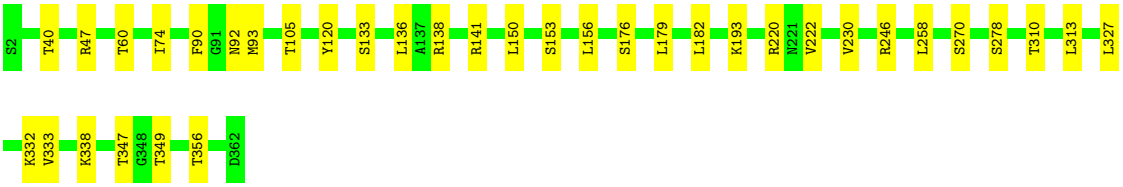
• Molecule 5: 60S ribosomal protein L3

Chain CE:



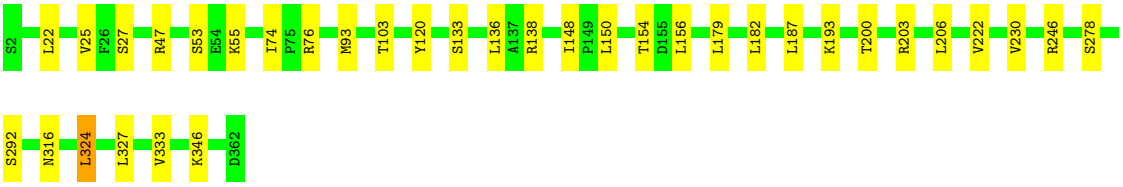
• Molecule 6: 60S ribosomal protein L4-A

Chain l:



• Molecule 6: 60S ribosomal protein L4-A

Chain CF:

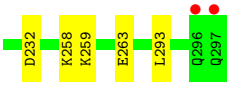


• Molecule 7: 60S ribosomal protein L5

Chain m:

• Molecule 7: 60S ribosomal protein L5

Chain CG:

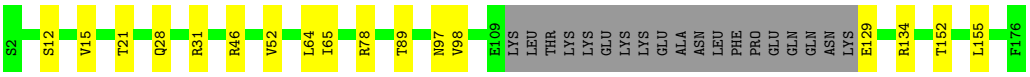


• Molecule 8: 60S ribosomal protein L6-A

Chain n:

• Molecule 8: 60S ribosomal protein L6-A

Chain CH:

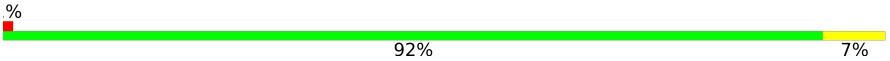


• Molecule 9: 60S ribosomal protein L7-A

Chain o:

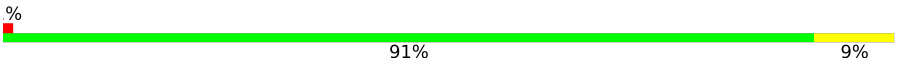
• Molecule 9: 60S ribosomal protein L7-A

Chain CI:



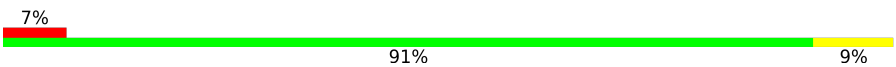
• Molecule 10: 60S ribosomal protein L8-A

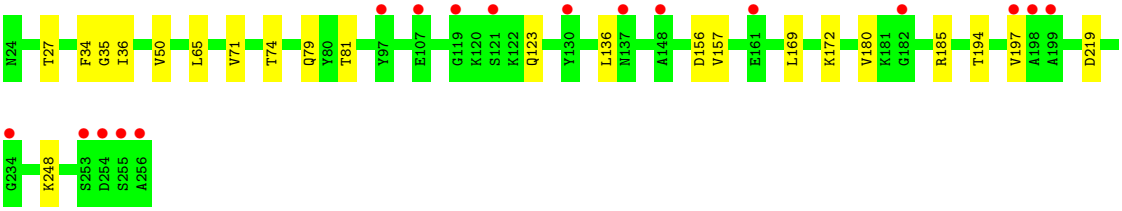
Chain p:



• Molecule 10: 60S ribosomal protein L8-A

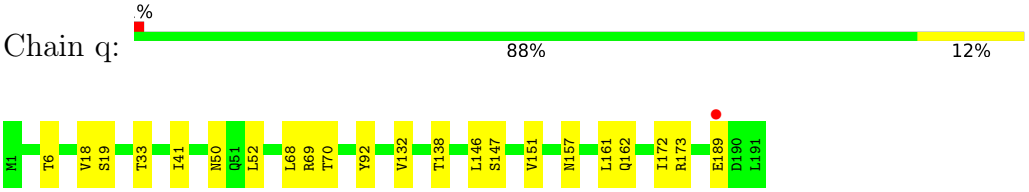
Chain CJ:





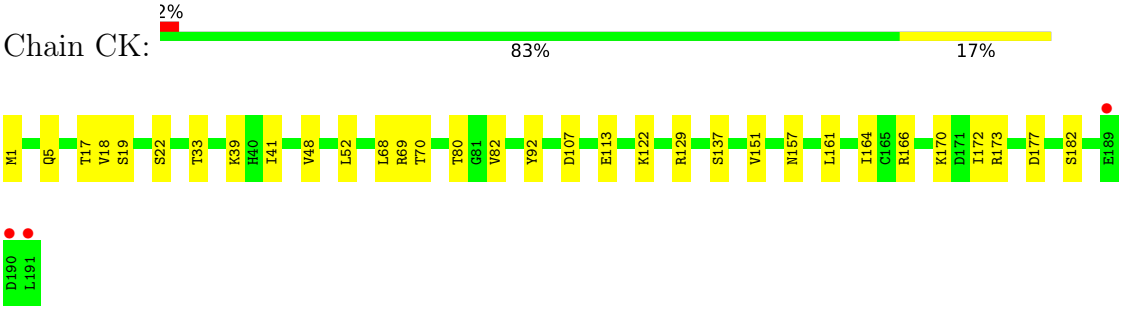
• Molecule 11: 60S ribosomal protein L9-A

Chain q:



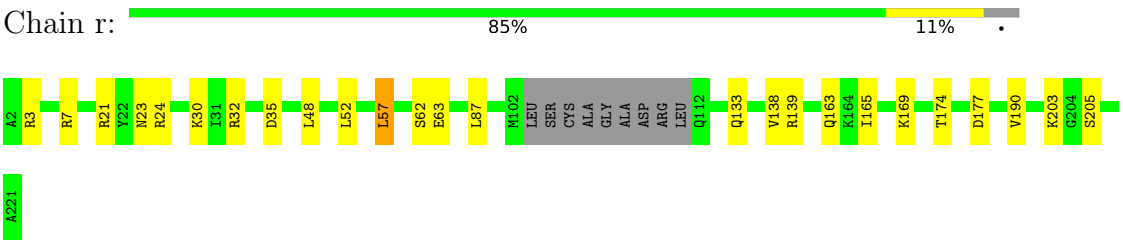
• Molecule 11: 60S ribosomal protein L9-A

Chain CK:



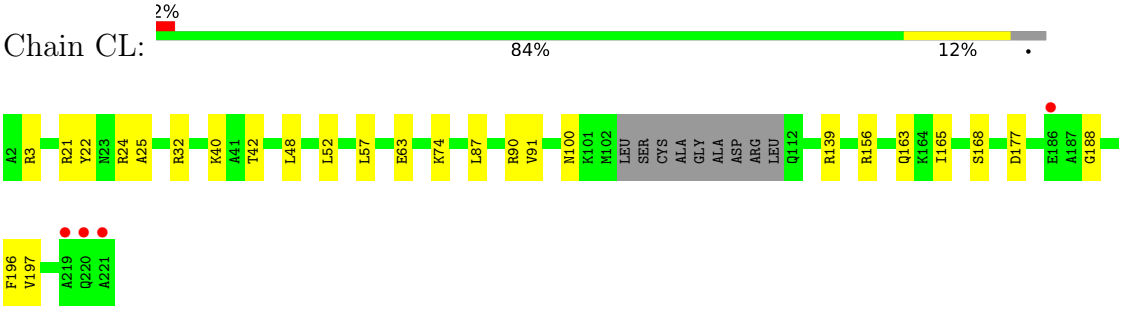
• Molecule 12: 60S ribosomal protein L10

Chain r:



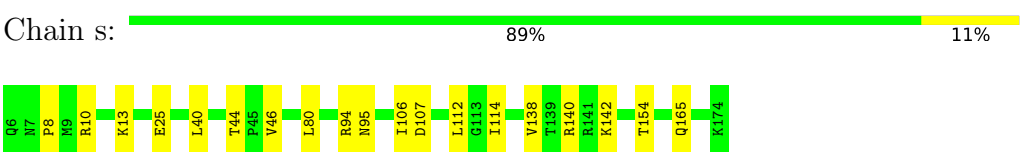
• Molecule 12: 60S ribosomal protein L10

Chain CL:



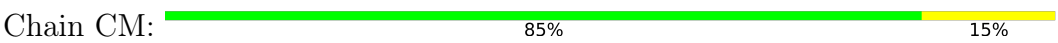
• Molecule 13: 60S ribosomal protein L11-B

Chain s:

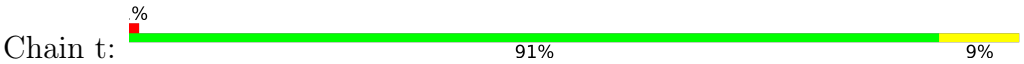


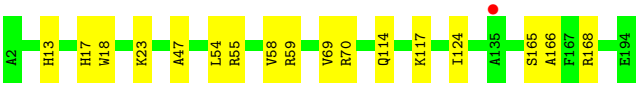
• Molecule 13: 60S ribosomal protein L11-B

Chain CM:

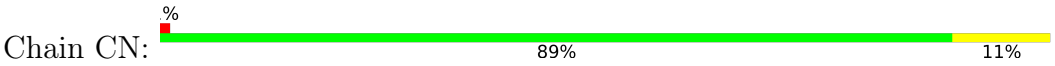


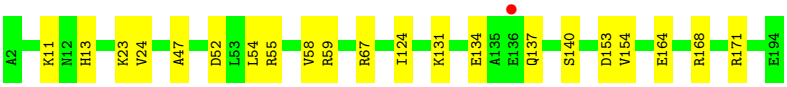
• Molecule 14: 60S ribosomal protein L13-A



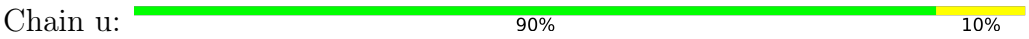


• Molecule 14: 60S ribosomal protein L13-A

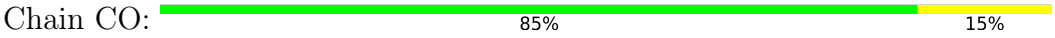


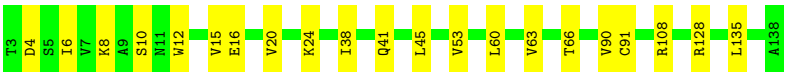


• Molecule 15: 60S ribosomal protein L14-A

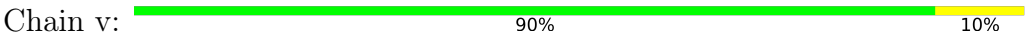


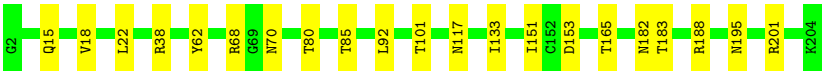
• Molecule 15: 60S ribosomal protein L14-A



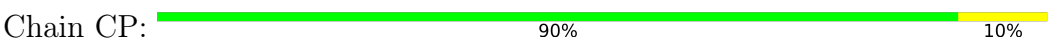


• Molecule 16: 60S ribosomal protein L15-A

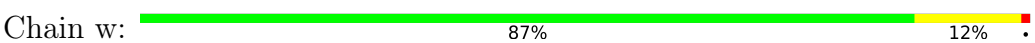




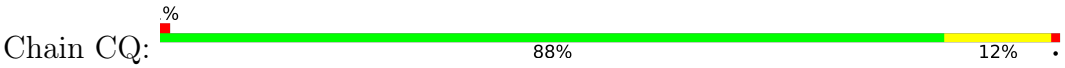
• Molecule 16: 60S ribosomal protein L15-A

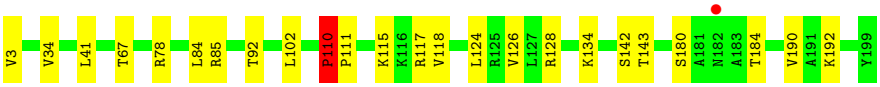


• Molecule 17: 60S ribosomal protein L16-A

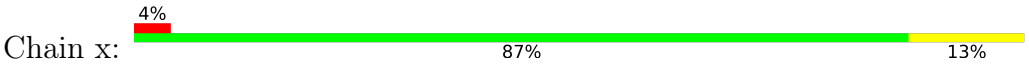


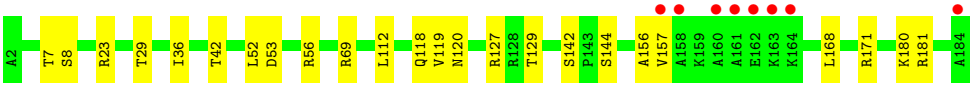
• Molecule 17: 60S ribosomal protein L16-A



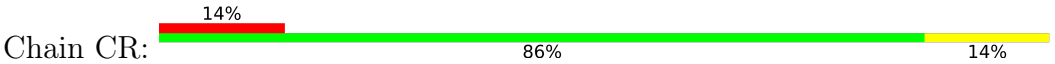


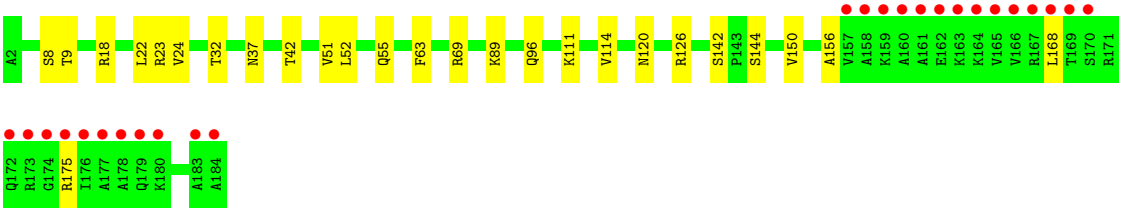
• Molecule 18: 60S ribosomal protein L17-A



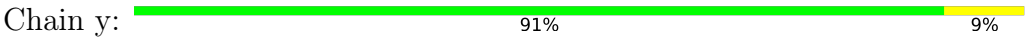


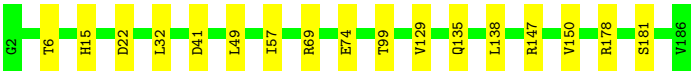
• Molecule 18: 60S ribosomal protein L17-A





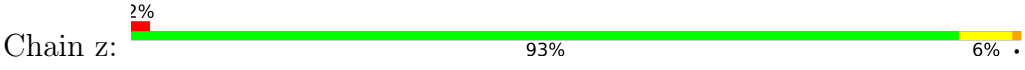
• Molecule 19: 60S ribosomal protein L18-A





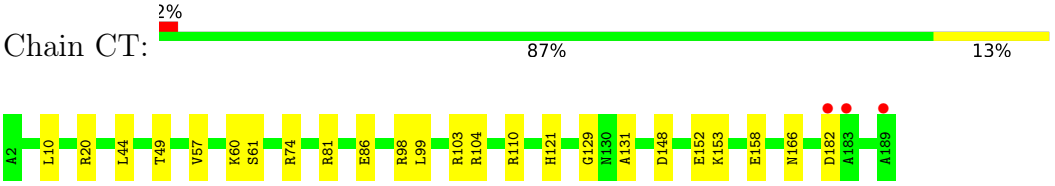
• Molecule 19: 60S ribosomal protein L18-A

• Molecule 20: 60S ribosomal protein L19-A



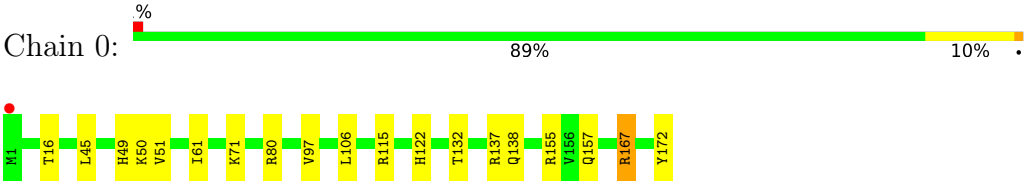
• Molecule 20: 60S ribosomal protein L19-A

Chain CT:



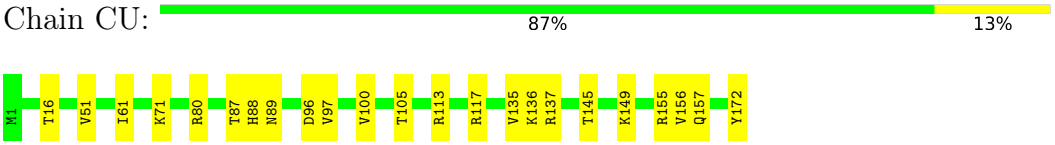
• Molecule 21: 60S ribosomal protein L20-A

Chain 0:



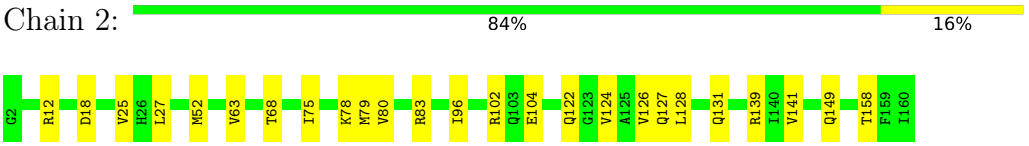
• Molecule 21: 60S ribosomal protein L20-A

Chain CU:



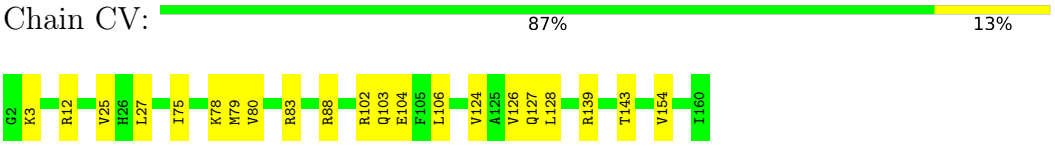
• Molecule 22: 60S ribosomal protein L21-A

Chain 2:



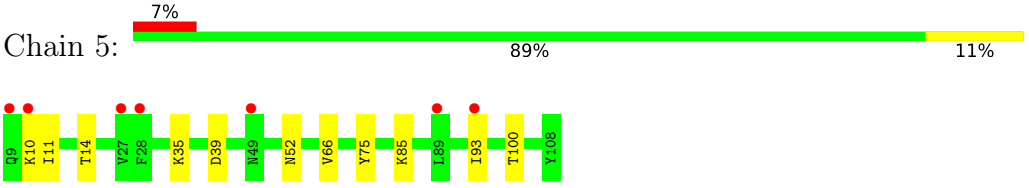
• Molecule 22: 60S ribosomal protein L21-A

Chain CV:



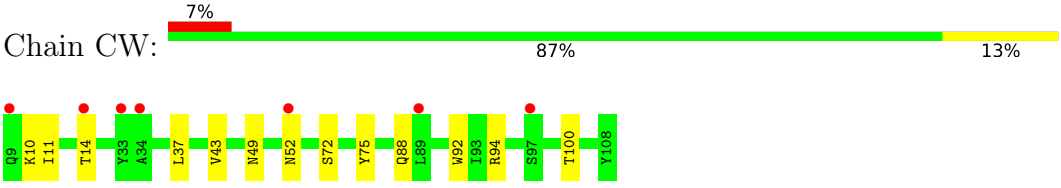
• Molecule 23: 60S ribosomal protein L22-A

Chain 5:



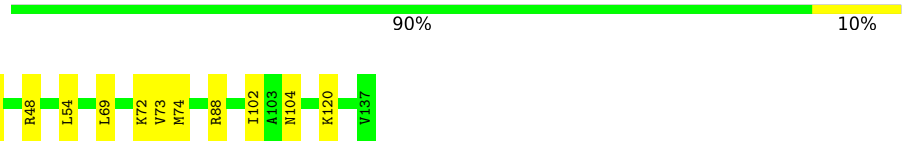
• Molecule 23: 60S ribosomal protein L22-A

Chain CW:



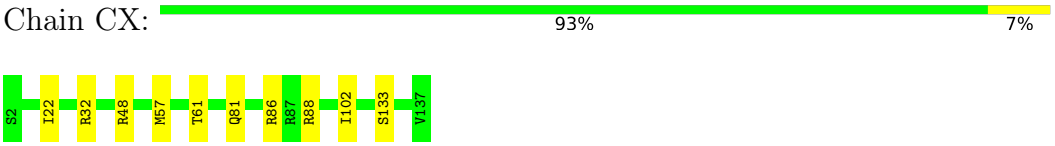
• Molecule 24: 60S ribosomal protein L23-A

Chain l2:



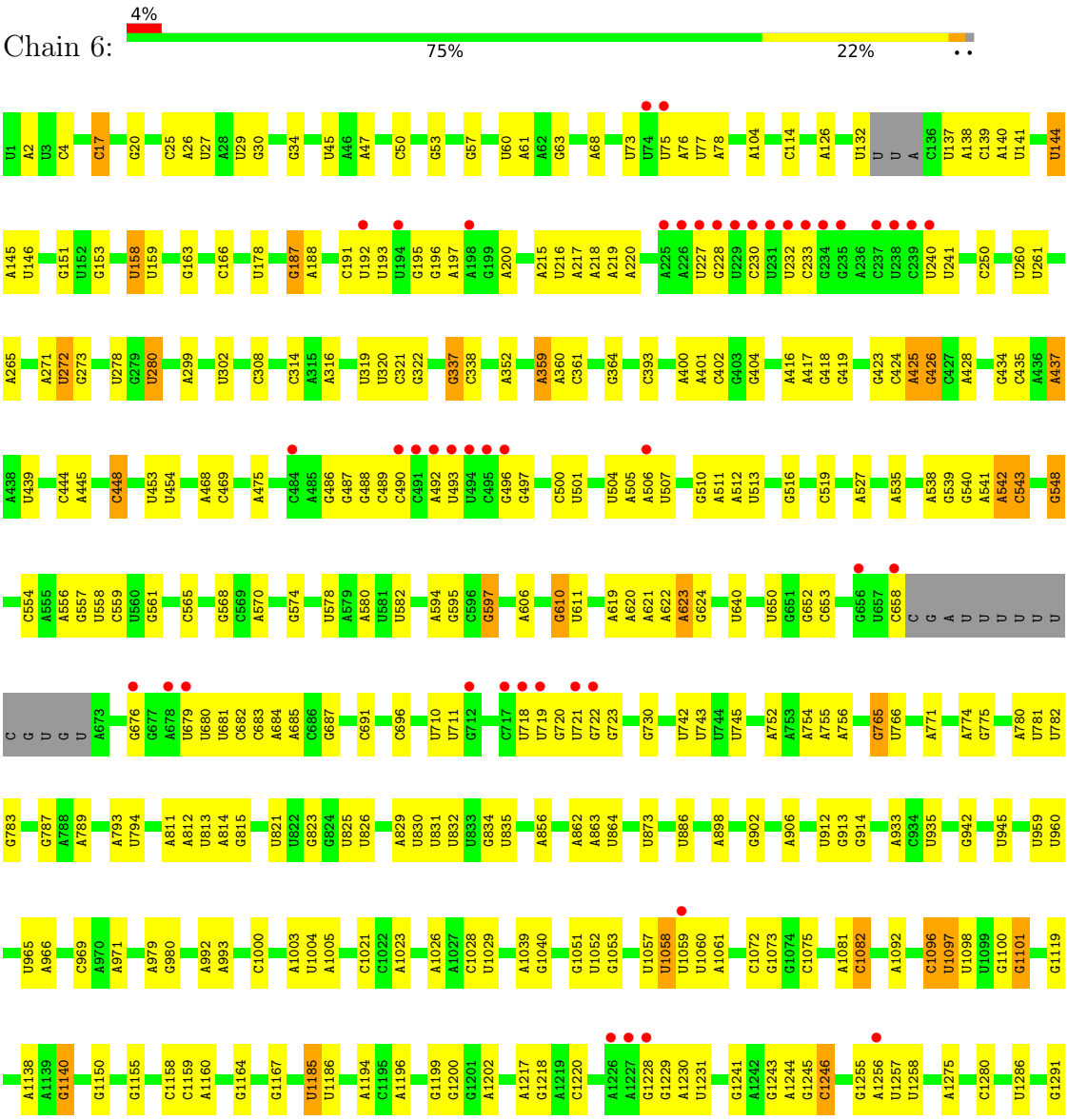
• Molecule 24: 60S ribosomal protein L23-A

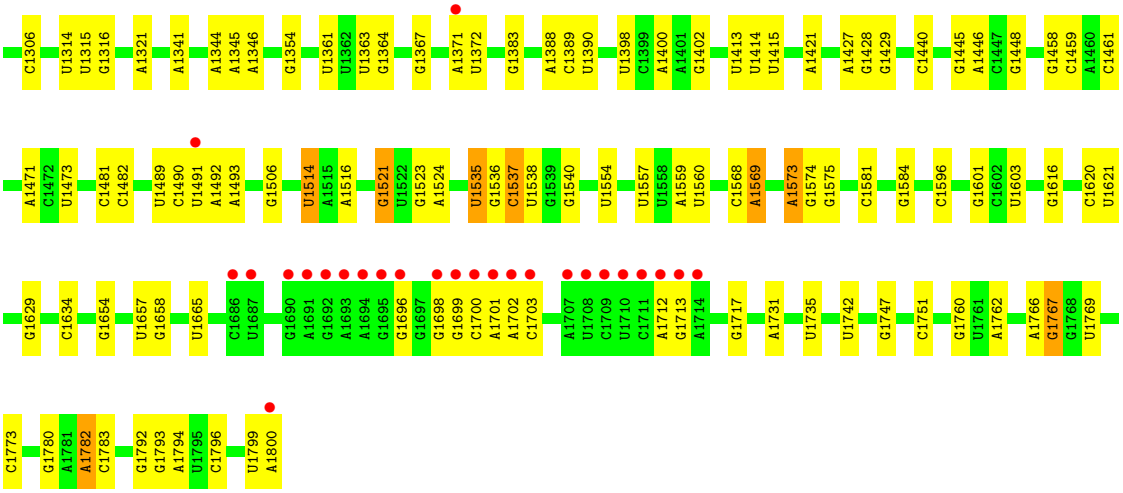
Chain CX:



• Molecule 25: 18S ribosomal RNA

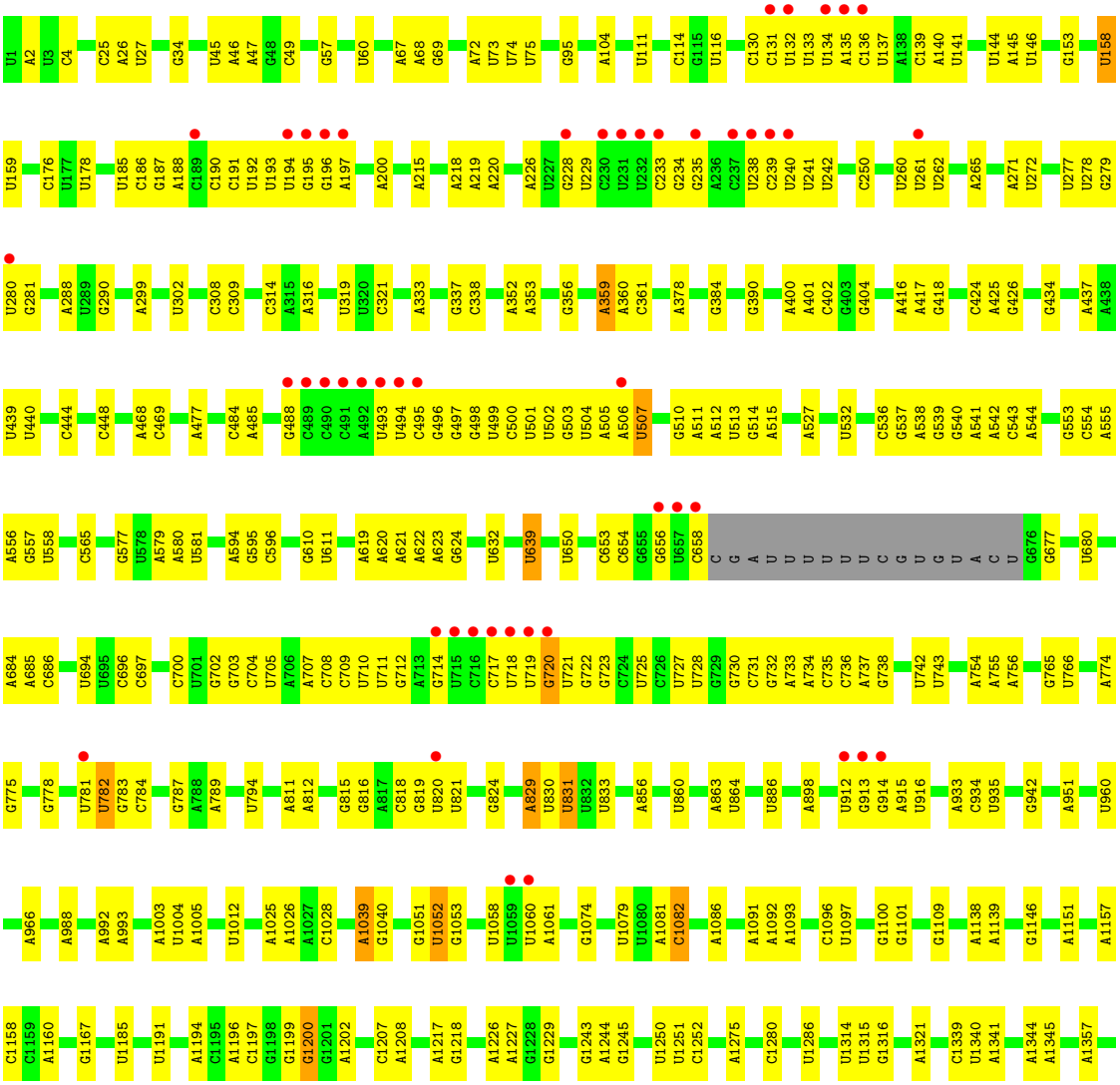
Chain 6:

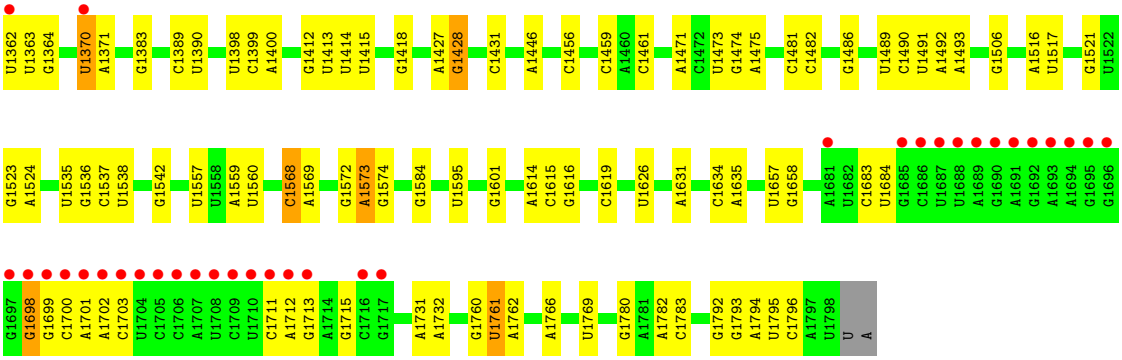




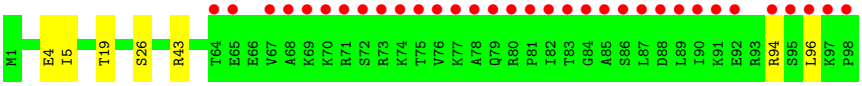
• Molecule 25: 18S ribosomal RNA

Chain A:

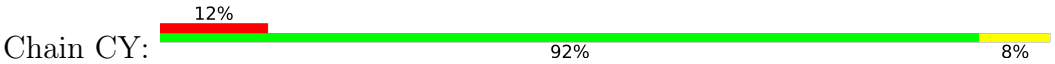


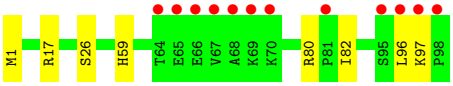


• Molecule 26: 60S ribosomal protein L24-A

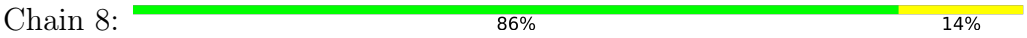


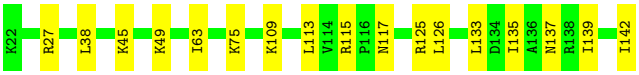
• Molecule 26: 60S ribosomal protein L24-A



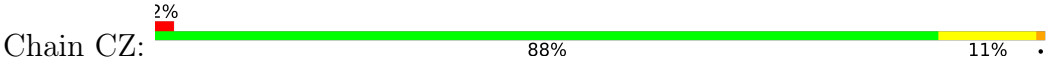


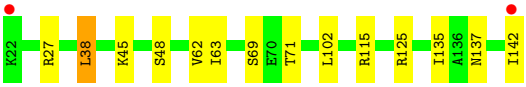
• Molecule 27: 60S ribosomal protein L25



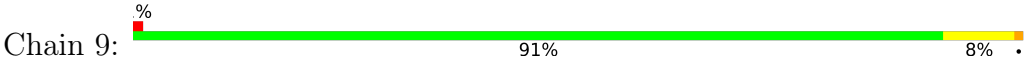


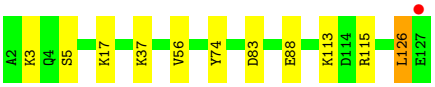
• Molecule 27: 60S ribosomal protein L25





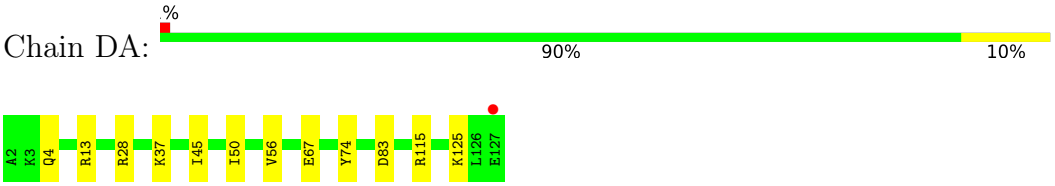
• Molecule 28: 60S ribosomal protein L26-A





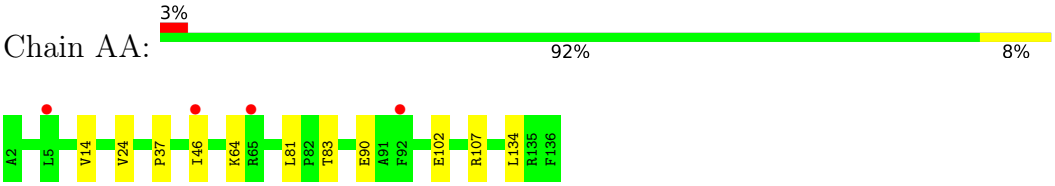
• Molecule 28: 60S ribosomal protein L26-A

Chain DA:



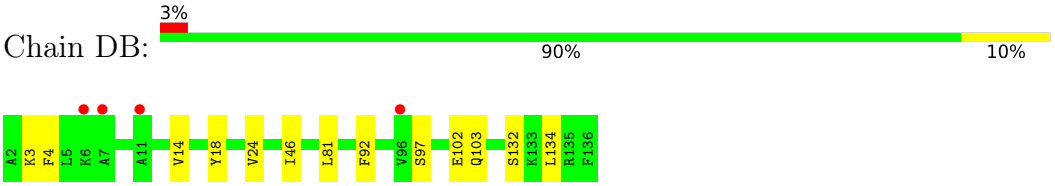
• Molecule 29: 60S ribosomal protein L27-A

Chain AA:



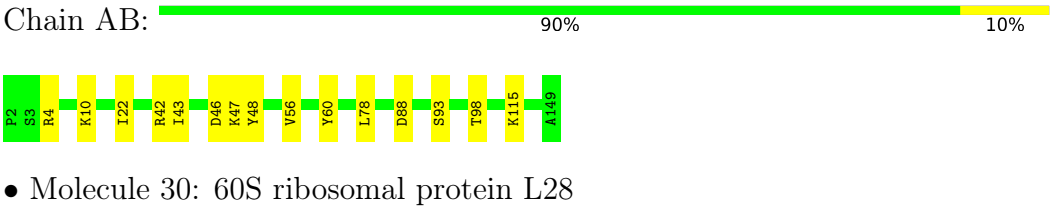
• Molecule 29: 60S ribosomal protein L27-A

Chain DB:



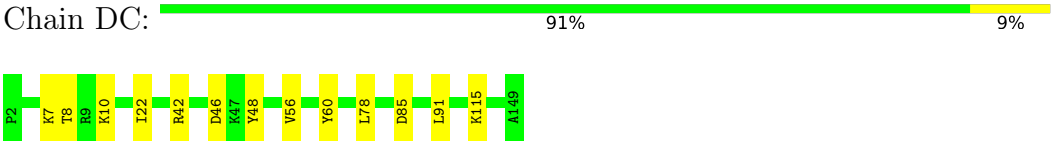
• Molecule 30: 60S ribosomal protein L28

Chain AB:



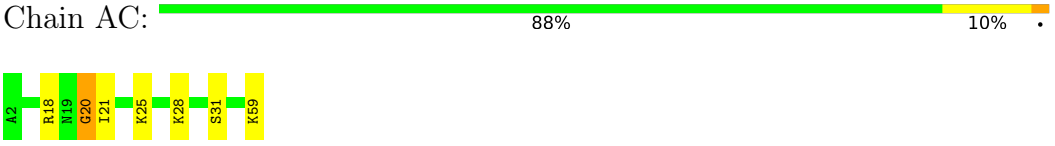
• Molecule 30: 60S ribosomal protein L28

Chain DC:



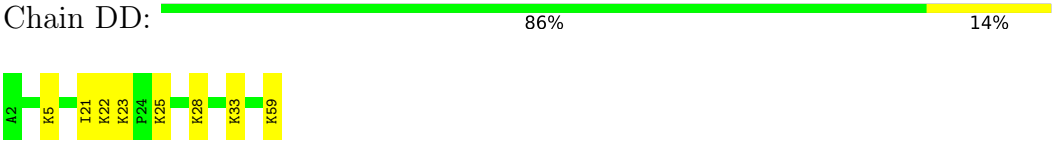
• Molecule 31: 60S ribosomal protein L29

Chain AC:



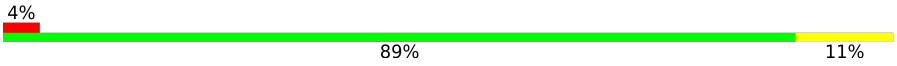
• Molecule 31: 60S ribosomal protein L29

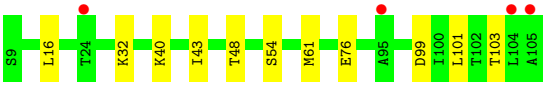
Chain DD:



• Molecule 32: 60S ribosomal protein L30

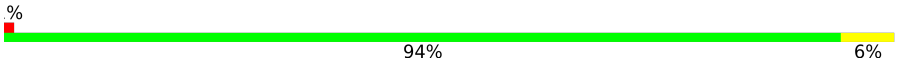
Chain AD:





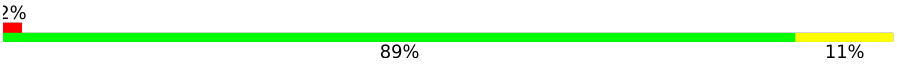
• Molecule 32: 60S ribosomal protein L30

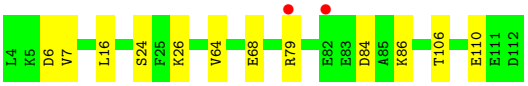
Chain DE:



• Molecule 33: 60S ribosomal protein L31-A

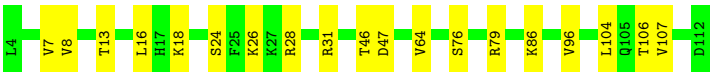
Chain AE:





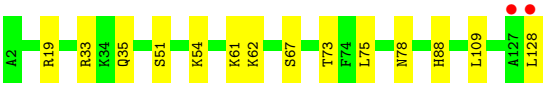
• Molecule 33: 60S ribosomal protein L31-A

Chain DF:



• Molecule 34: 60S ribosomal protein L32

Chain AF:

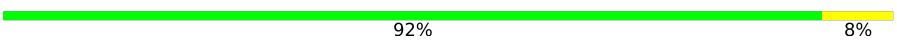


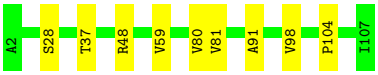
• Molecule 34: 60S ribosomal protein L32

Chain DG:

• Molecule 35: 60S ribosomal protein L33-A

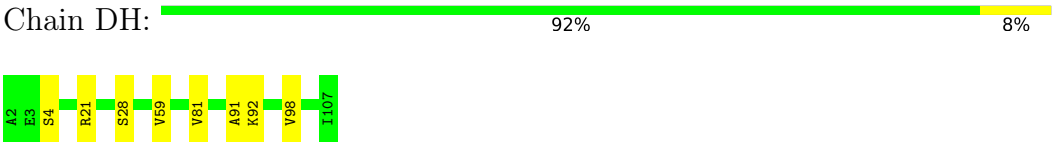
Chain AG:





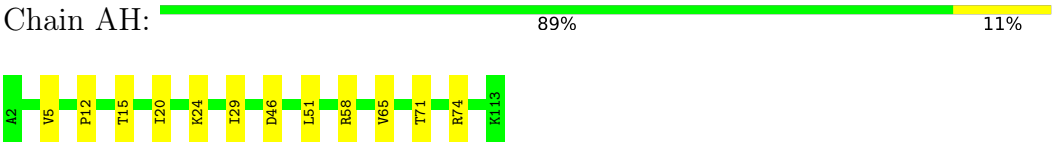
• Molecule 35: 60S ribosomal protein L33-A

Chain DH:



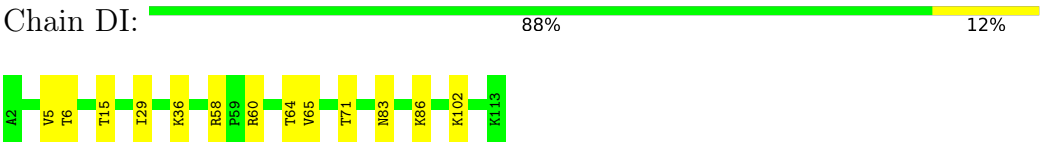
• Molecule 36: 60S ribosomal protein L34-A

Chain AH:



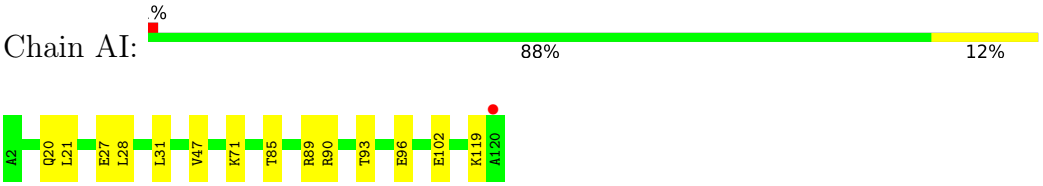
• Molecule 36: 60S ribosomal protein L34-A

Chain DI:



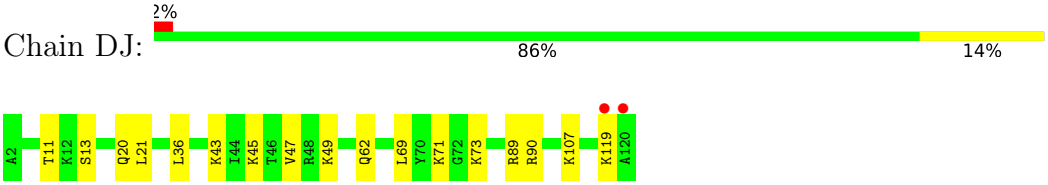
• Molecule 37: 60S ribosomal protein L35-A

Chain AI:



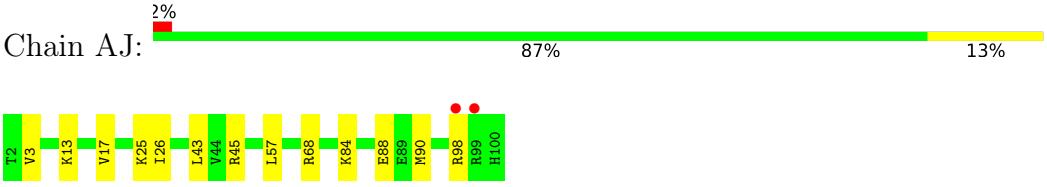
• Molecule 37: 60S ribosomal protein L35-A

Chain DJ:



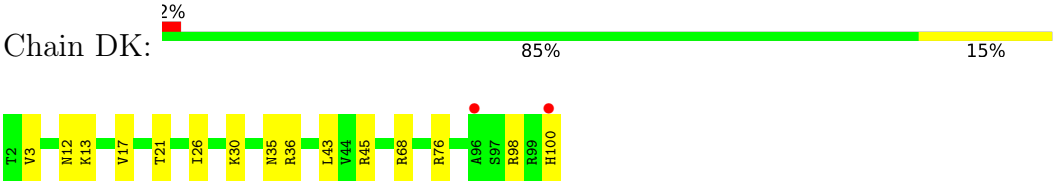
• Molecule 38: 60S ribosomal protein L36-A

Chain AJ:



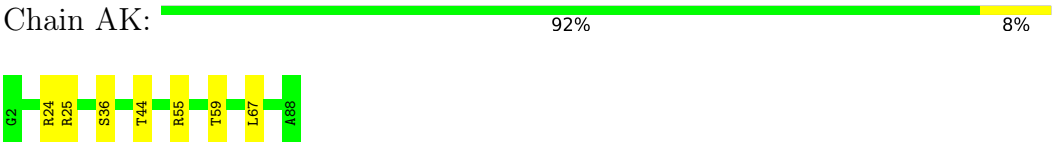
• Molecule 38: 60S ribosomal protein L36-A

Chain DK:



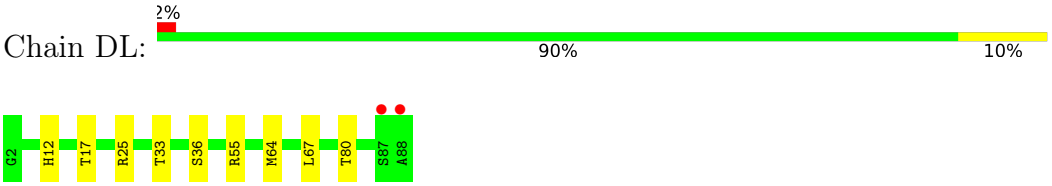
• Molecule 39: 60S ribosomal protein L37-A

Chain AK:



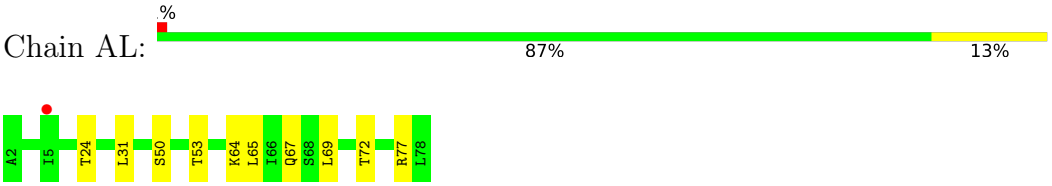
• Molecule 39: 60S ribosomal protein L37-A

Chain DL:



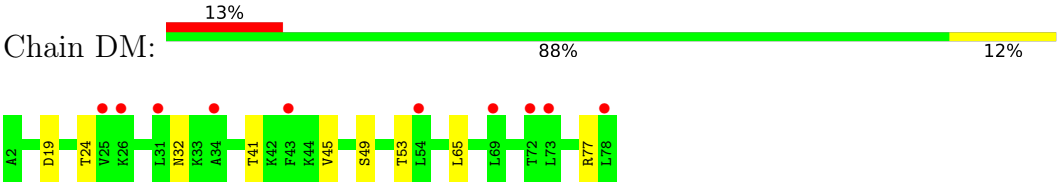
• Molecule 40: 60S ribosomal protein L38

Chain AL:



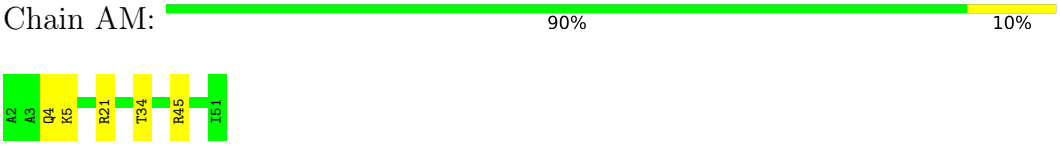
• Molecule 40: 60S ribosomal protein L38

Chain DM:



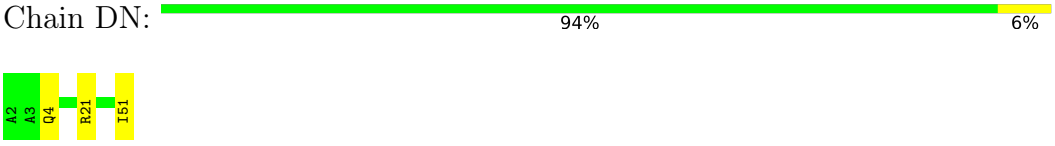
• Molecule 41: 60S ribosomal protein L39

Chain AM:



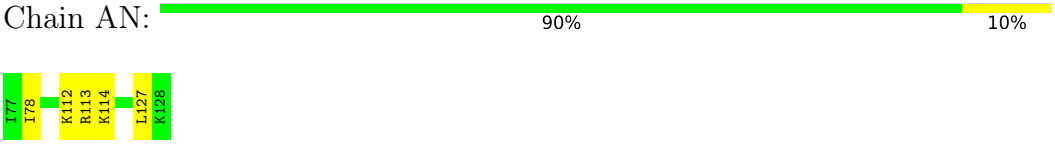
• Molecule 41: 60S ribosomal protein L39

Chain DN:



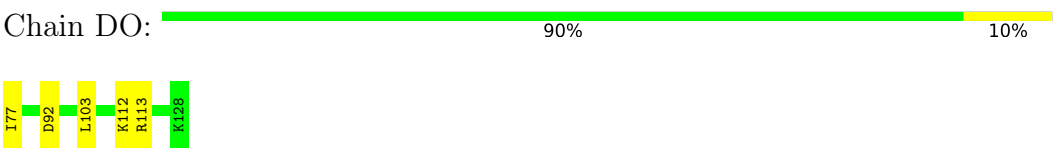
• Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain AN:



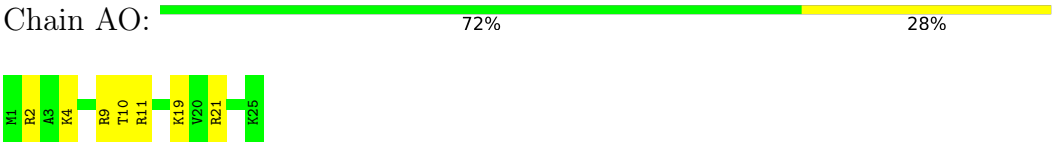
• Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain DO:



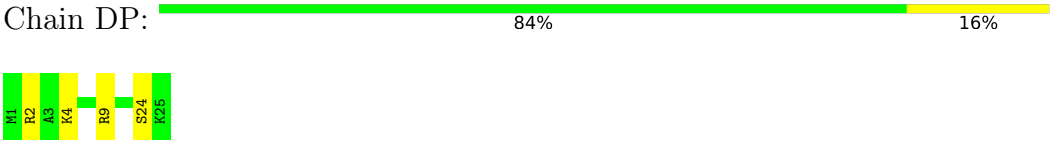
• Molecule 43: 60S ribosomal protein L41-B

Chain AO:



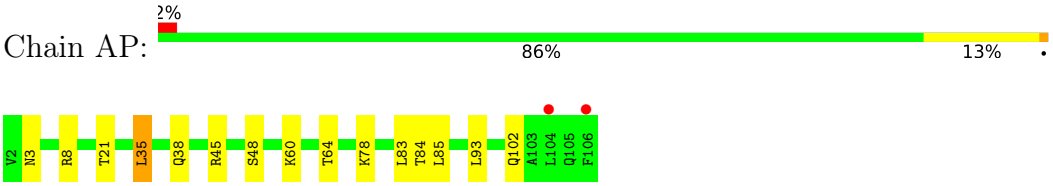
• Molecule 43: 60S ribosomal protein L41-B

Chain DP:



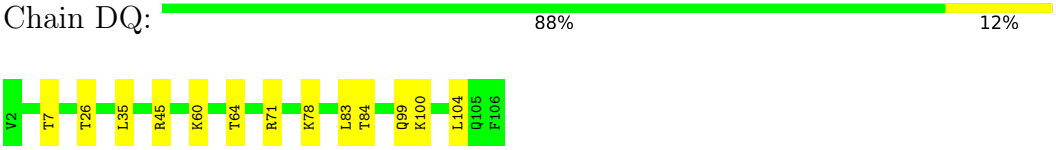
• Molecule 44: 60S ribosomal protein L42-A

Chain AP:



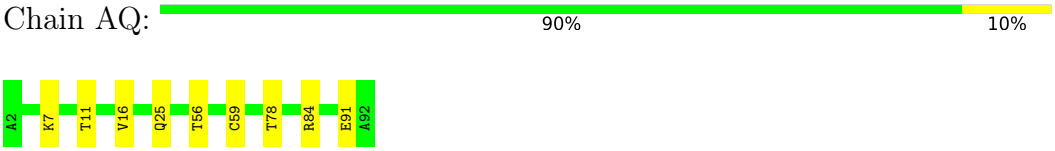
• Molecule 44: 60S ribosomal protein L42-A

Chain DQ:



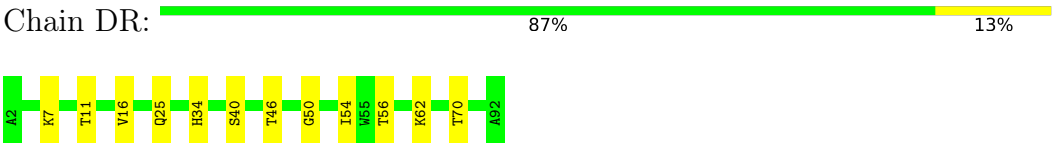
• Molecule 45: 60S ribosomal protein L43-A

Chain AQ:



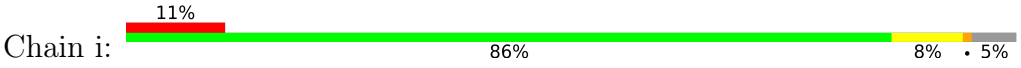
• Molecule 45: 60S ribosomal protein L43-A

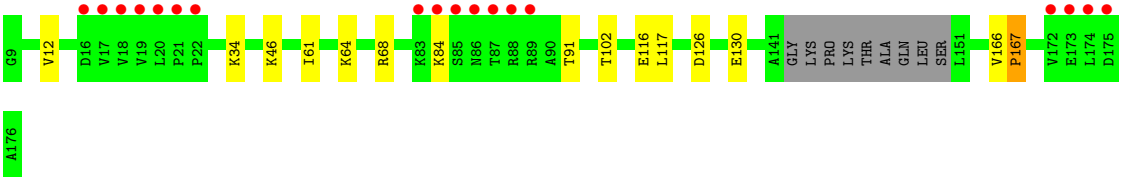
Chain DR:



• Molecule 46: Suppressor protein STM1

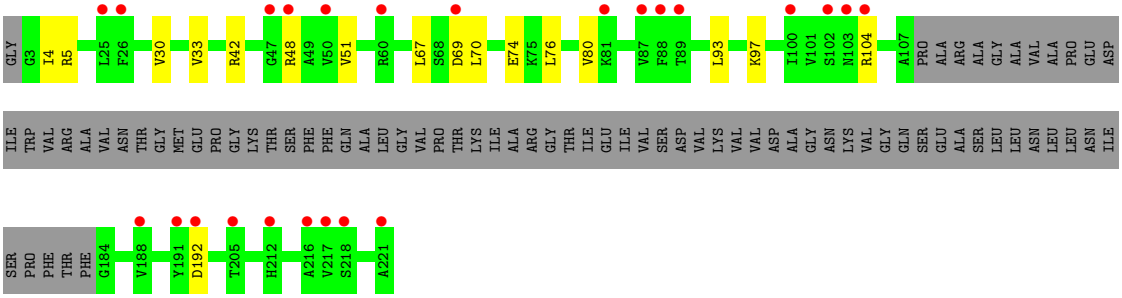
Chain i:





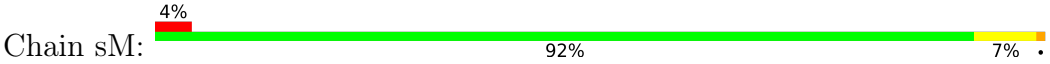
• Molecule 47: 60S acidic ribosomal protein P0

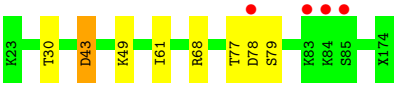
Chain p0:



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

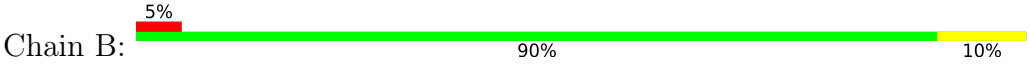
Chain sM:





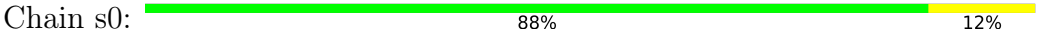
• Molecule 49: 40S ribosomal protein S0-A

Chain B:



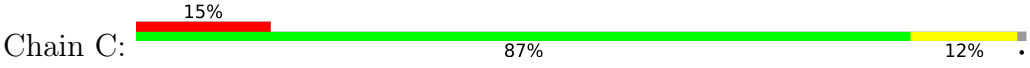
• Molecule 49: 40S ribosomal protein S0-A

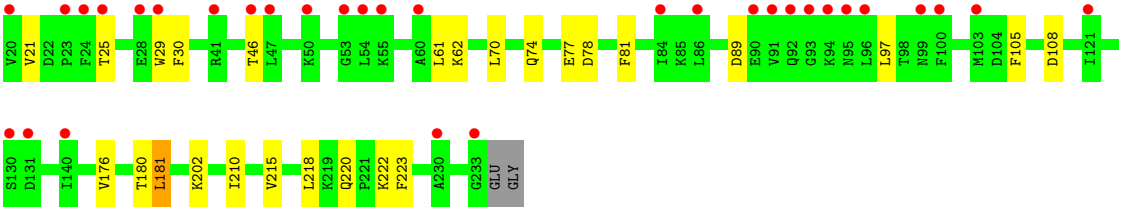
Chain s0:



• Molecule 50: 40S ribosomal protein S1-A

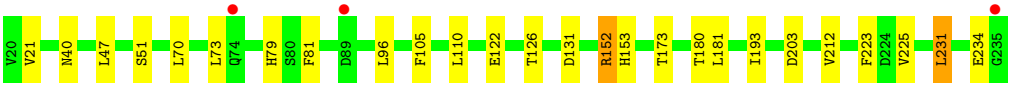
Chain C:





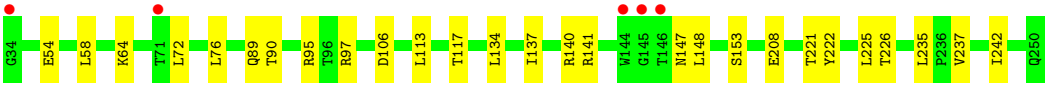
• Molecule 50: 40S ribosomal protein S1-A

Chain s1:



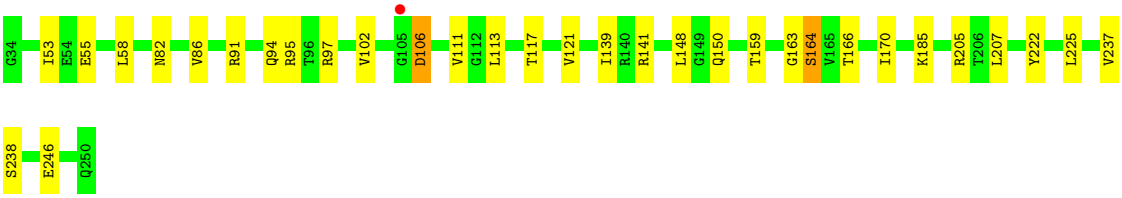
• Molecule 51: 40S ribosomal protein S2

Chain D:



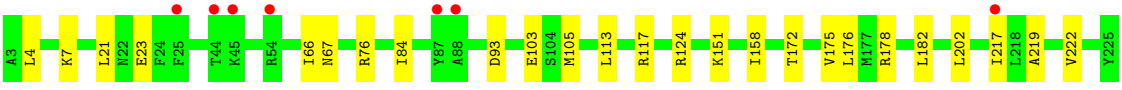
• Molecule 51: 40S ribosomal protein S2

Chain s2:



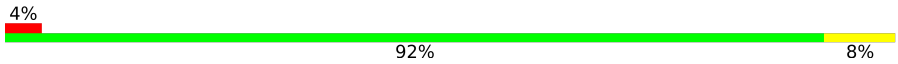
• Molecule 52: 40S ribosomal protein S3

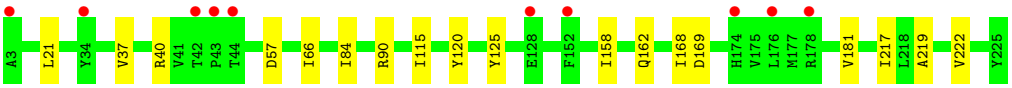
Chain E:



• Molecule 52: 40S ribosomal protein S3

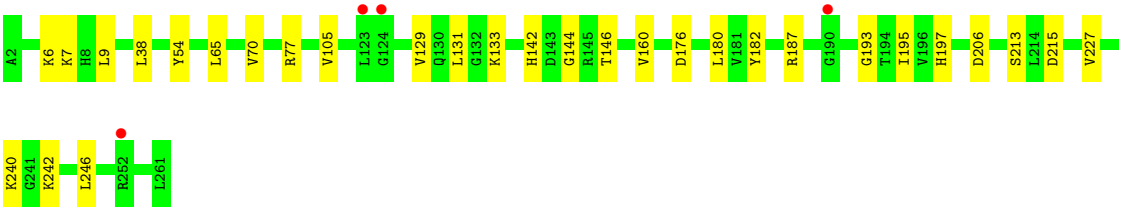
Chain s3:



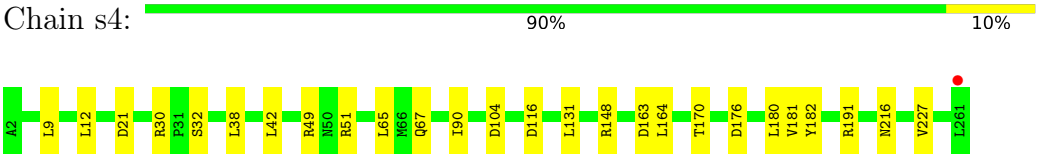


• Molecule 53: 40S ribosomal protein S4-A

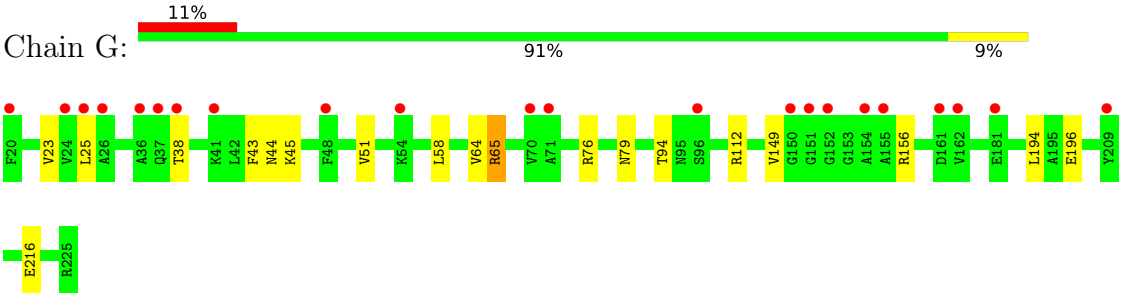
Chain F:



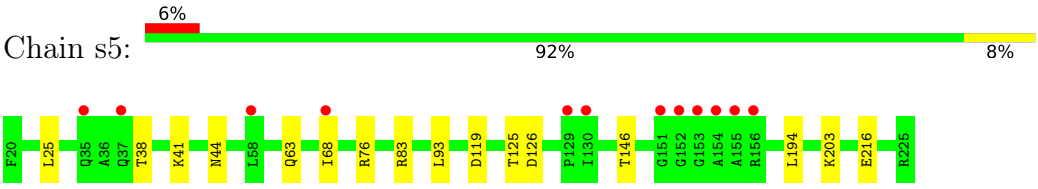
• Molecule 53: 40S ribosomal protein S4-A



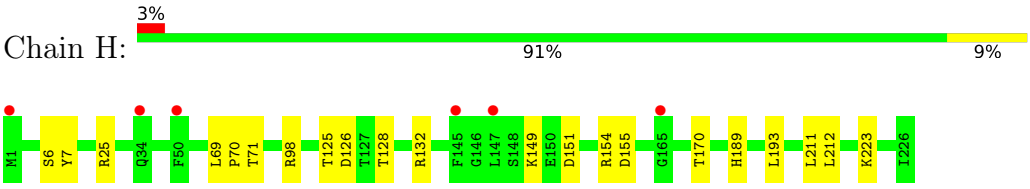
• Molecule 54: 40S ribosomal protein S5



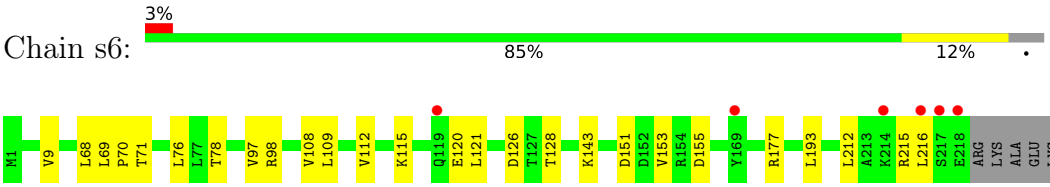
• Molecule 54: 40S ribosomal protein S5



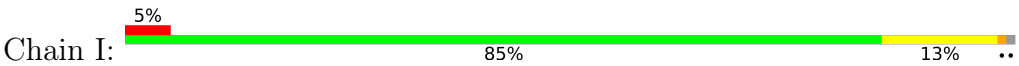
• Molecule 55: 40S ribosomal protein S6-A

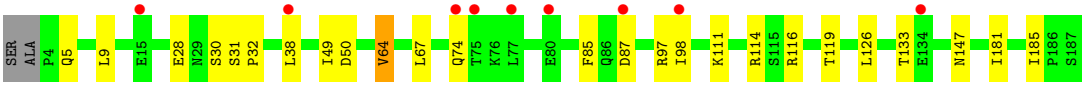


• Molecule 55: 40S ribosomal protein S6-A

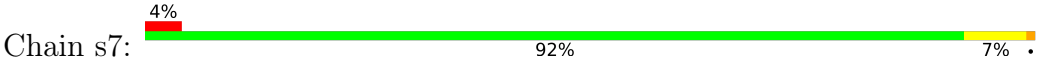


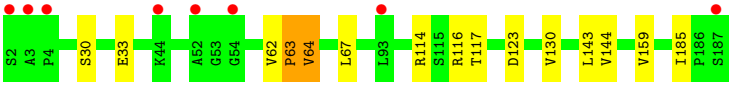
• Molecule 56: 40S ribosomal protein S7-A



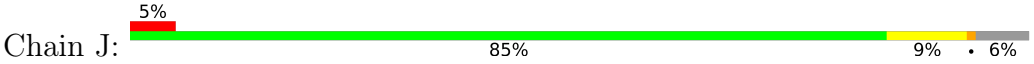


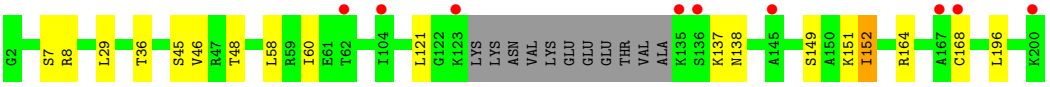
• Molecule 56: 40S ribosomal protein S7-A



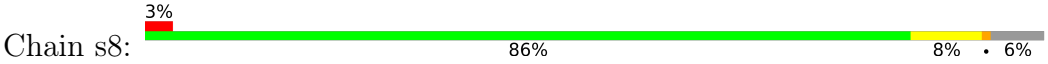


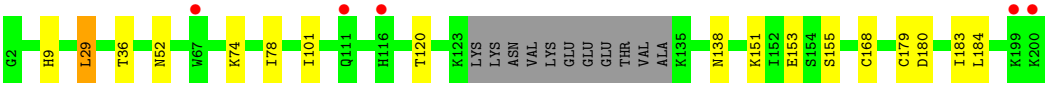
• Molecule 57: 40S ribosomal protein S8-A



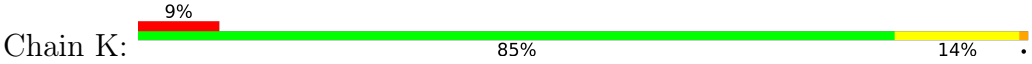


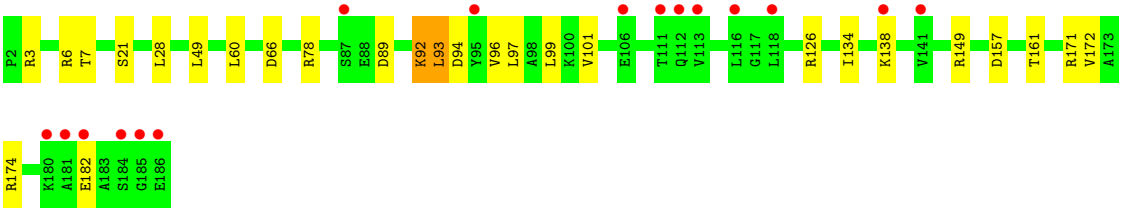
• Molecule 57: 40S ribosomal protein S8-A



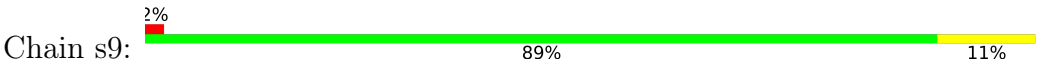


• Molecule 58: 40S ribosomal protein S9-A

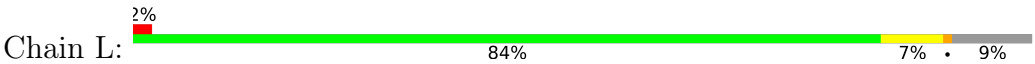




• Molecule 58: 40S ribosomal protein S9-A

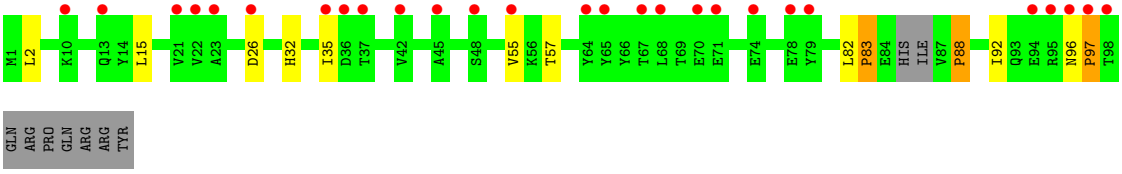


• Molecule 59: 40S ribosomal protein S10-A



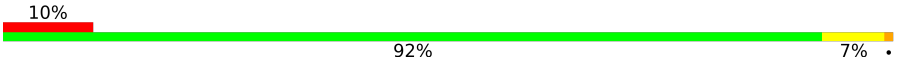
• Molecule 59: 40S ribosomal protein S10-A

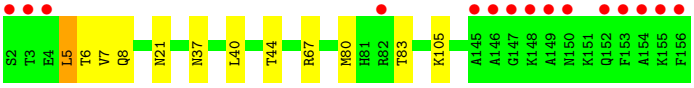
Chain c0:



• Molecule 60: 40S ribosomal protein S11-A

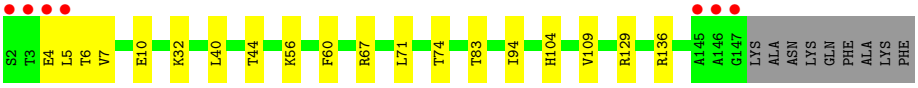
Chain M:





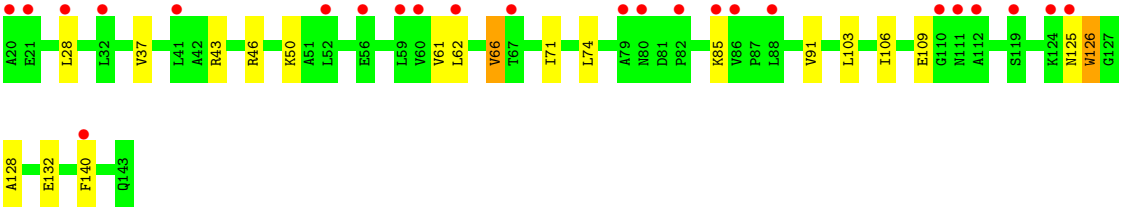
• Molecule 60: 40S ribosomal protein S11-A

Chain c1:



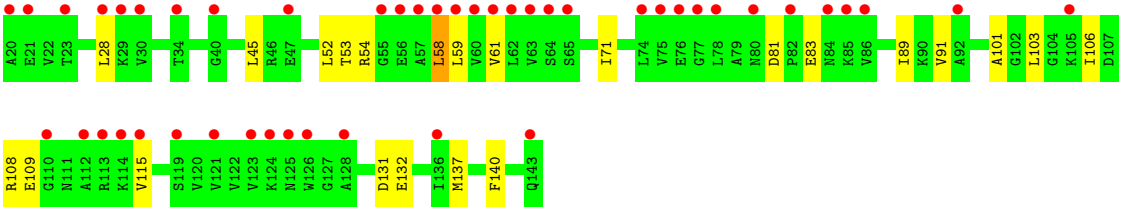
• Molecule 61: 40S ribosomal protein S12

Chain N:



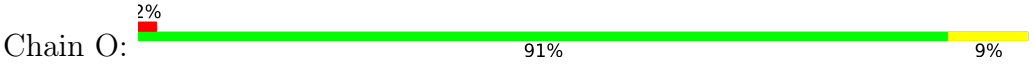
• Molecule 61: 40S ribosomal protein S12

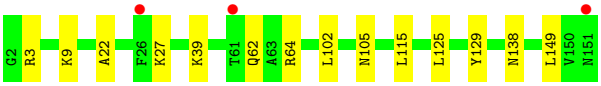
Chain c2:



• Molecule 62: 40S ribosomal protein S13

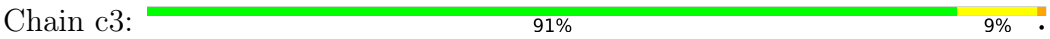
Chain O:

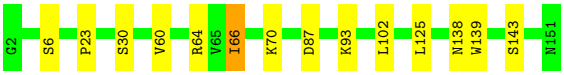




• Molecule 62: 40S ribosomal protein S13

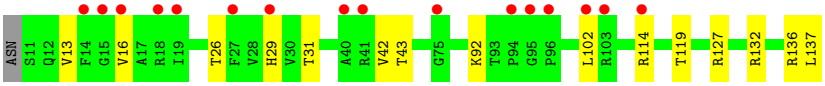
Chain c3:





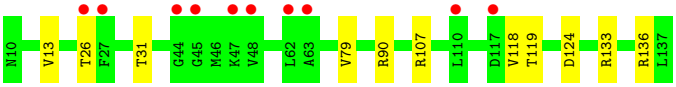
• Molecule 63: 40S ribosomal protein S14-B

Chain P:



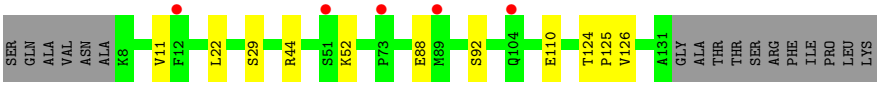
• Molecule 63: 40S ribosomal protein S14-B

Chain c4:



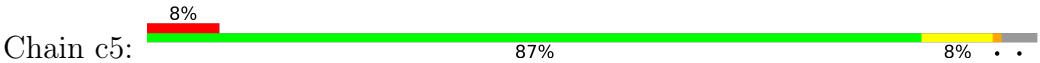
• Molecule 64: 40S ribosomal protein S15

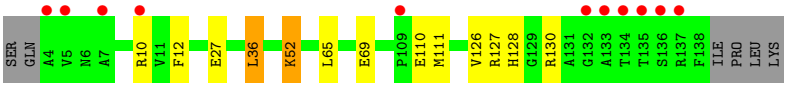
Chain Q:



• Molecule 64: 40S ribosomal protein S15

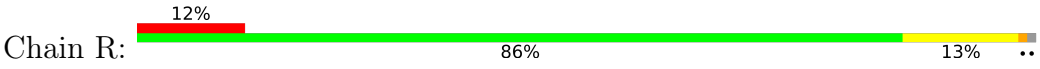
Chain c5:



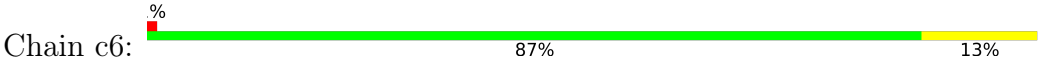


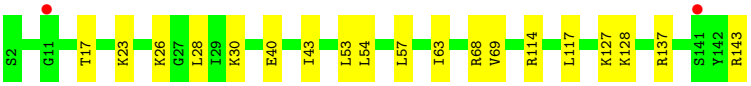
• Molecule 65: 40S ribosomal protein S16-A

Chain R:

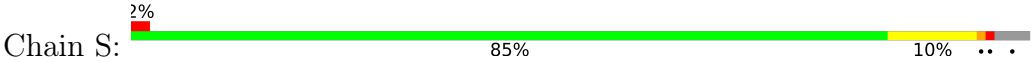


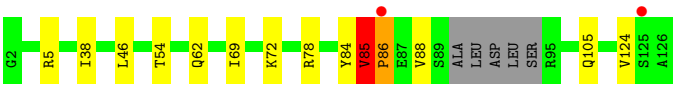
• Molecule 65: 40S ribosomal protein S16-A



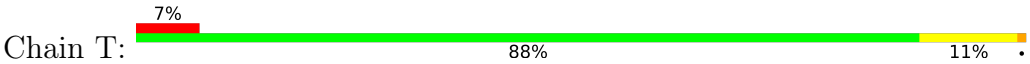


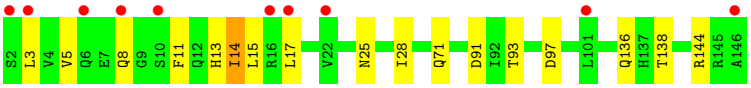
• Molecule 66: 40S ribosomal protein S17-B



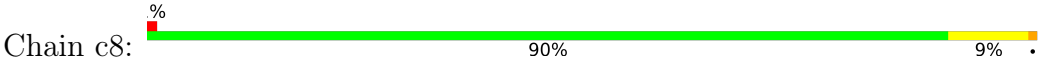


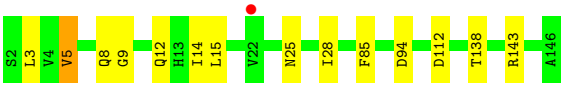
• Molecule 67: 40S ribosomal protein S18-A



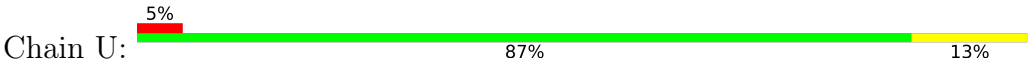


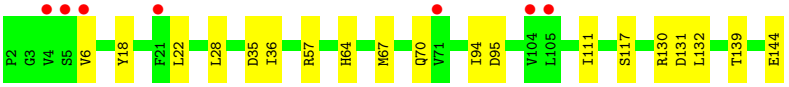
• Molecule 67: 40S ribosomal protein S18-A



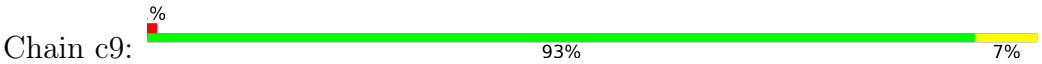


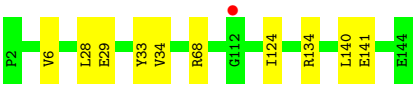
• Molecule 68: 40S ribosomal protein S19-A





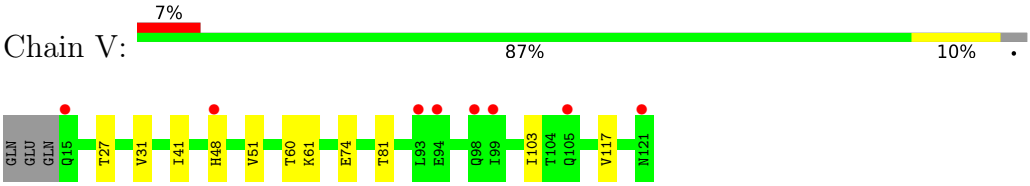
• Molecule 68: 40S ribosomal protein S19-A





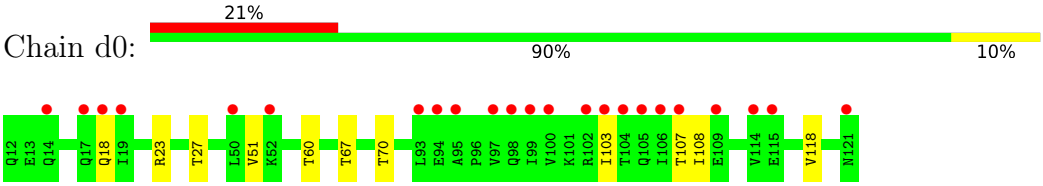
• Molecule 69: 40S ribosomal protein S20

Chain V:



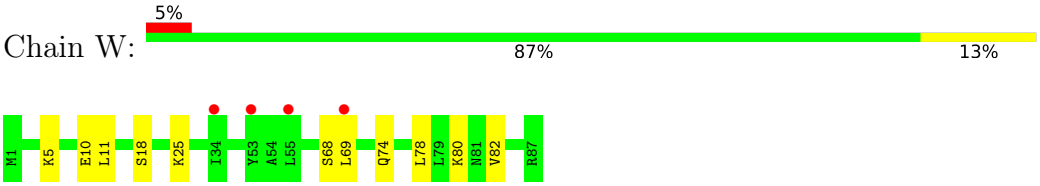
• Molecule 69: 40S ribosomal protein S20

Chain d0:



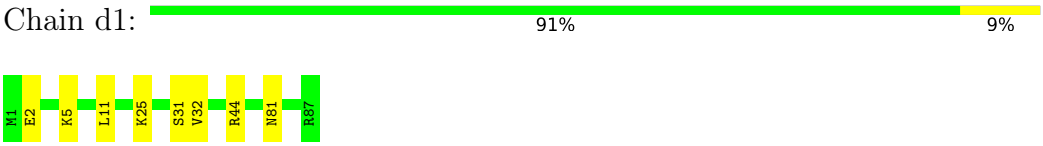
• Molecule 70: 40S ribosomal protein S21-A

Chain W:



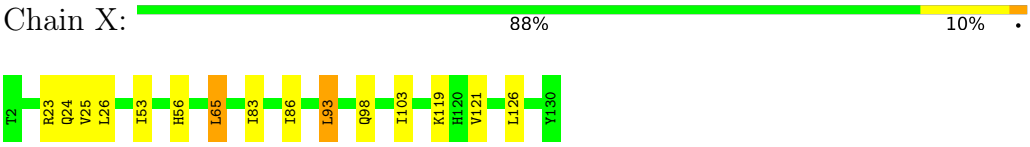
• Molecule 70: 40S ribosomal protein S21-A

Chain d1:



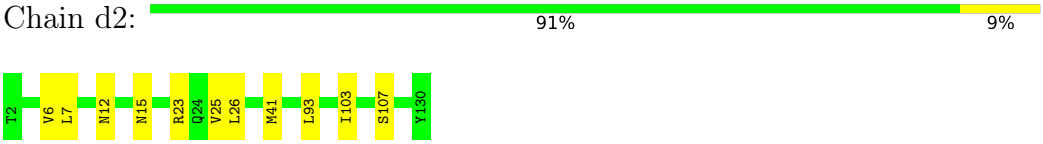
• Molecule 71: 40S ribosomal protein S22-A

Chain X:



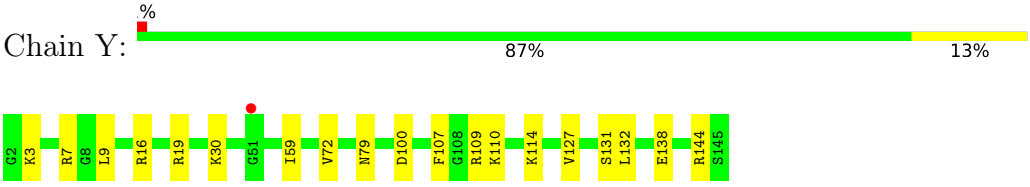
• Molecule 71: 40S ribosomal protein S22-A

Chain d2:



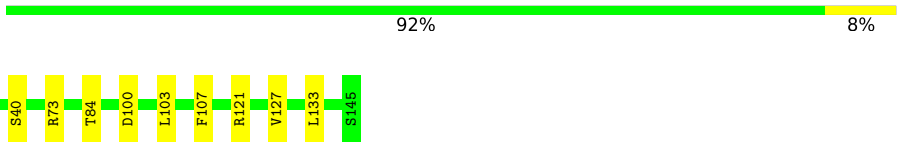
• Molecule 72: 40S ribosomal protein S23-A

Chain Y:



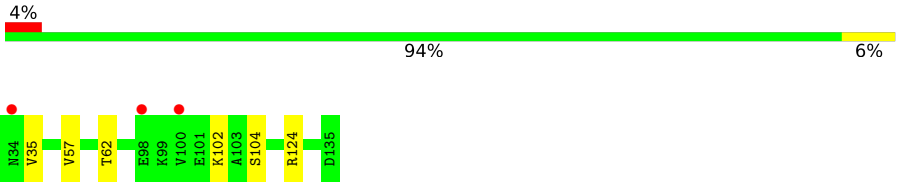
• Molecule 72: 40S ribosomal protein S23-A

Chain d3:



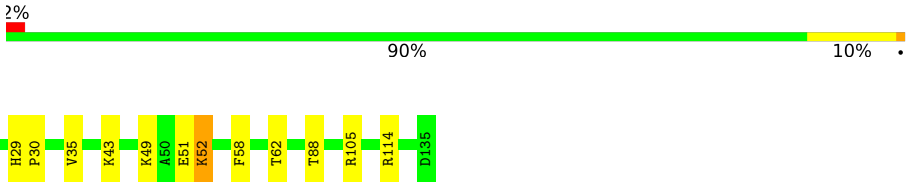
• Molecule 73: 40S ribosomal protein S24-A

Chain Z:



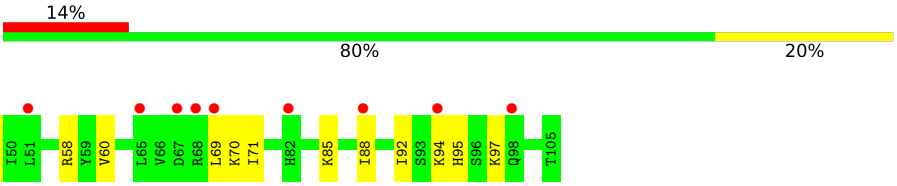
• Molecule 73: 40S ribosomal protein S24-A

Chain d4:



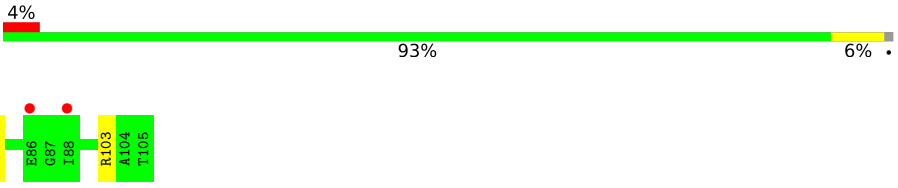
• Molecule 74: 40S ribosomal protein S25-A

Chain a:



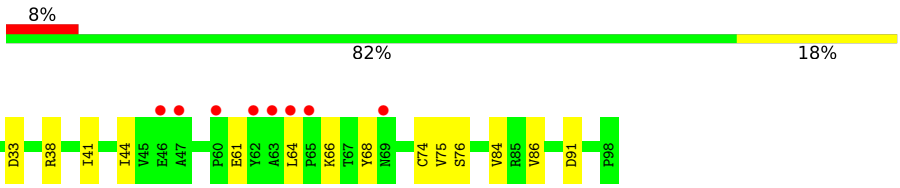
• Molecule 74: 40S ribosomal protein S25-A

Chain d5:



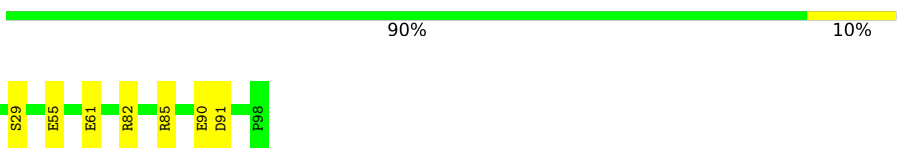
• Molecule 75: 40S ribosomal protein S26-B

Chain b:



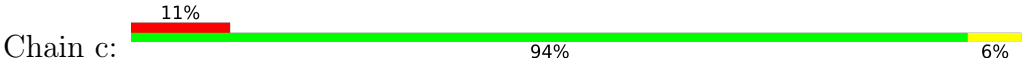
• Molecule 75: 40S ribosomal protein S26-B

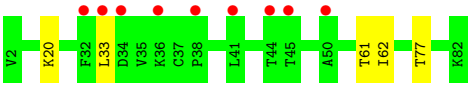
Chain d6:



• Molecule 76: 40S ribosomal protein S27-A

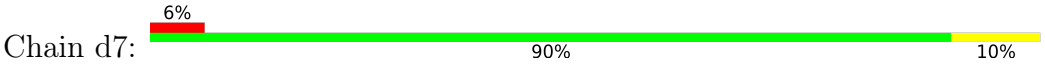
Chain c:





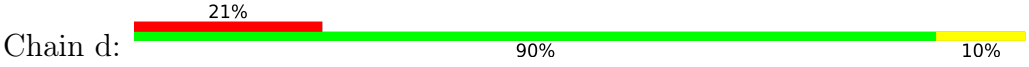
• Molecule 76: 40S ribosomal protein S27-A

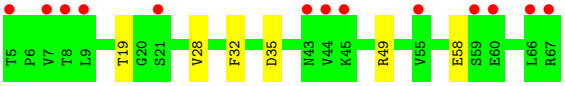
Chain d7:



• Molecule 77: 40S ribosomal protein S28-A

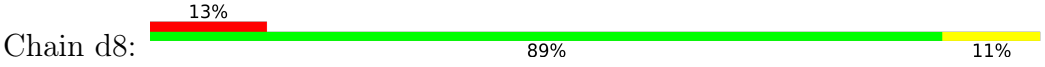
Chain d:

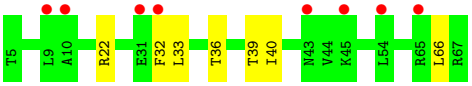




• Molecule 77: 40S ribosomal protein S28-A

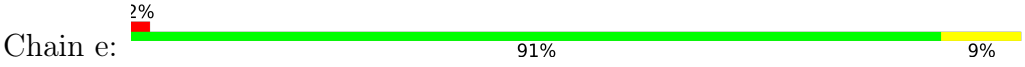
Chain d8:

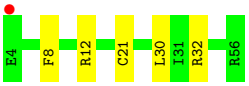




• Molecule 78: 40S ribosomal protein S29-A

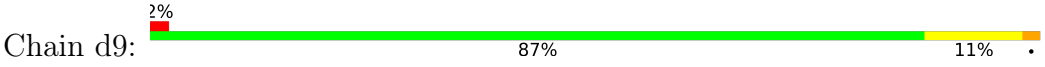
Chain e:





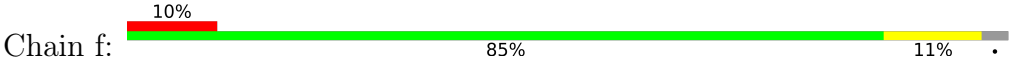
• Molecule 78: 40S ribosomal protein S29-A

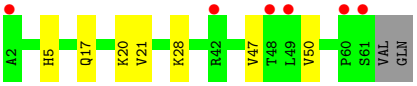
Chain d9:



• Molecule 79: 40S ribosomal protein S30-A

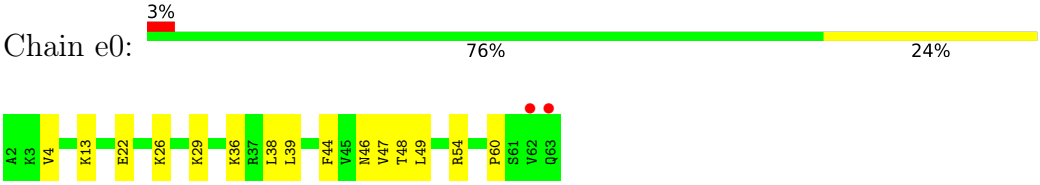
Chain f:





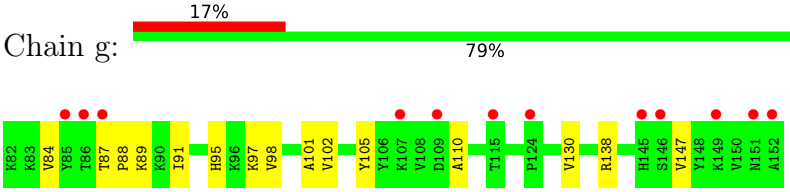
• Molecule 79: 40S ribosomal protein S30-A

Chain e0:



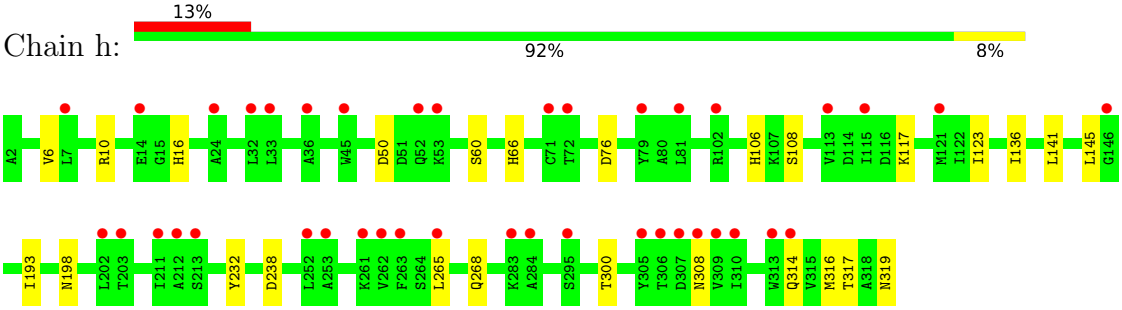
• Molecule 80: Ubiquitin-40S ribosomal protein S31

Chain g:



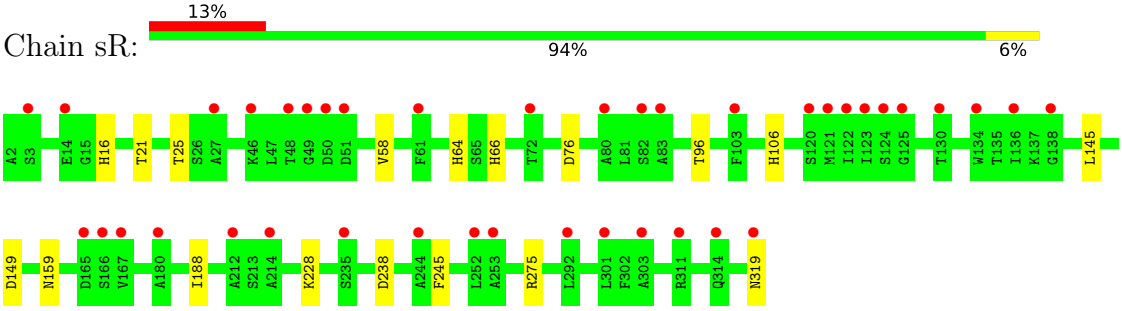
• Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein

Chain h:



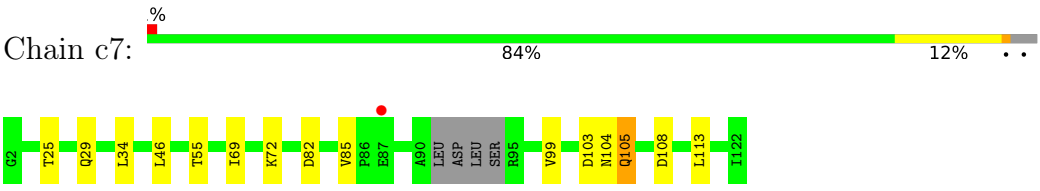
• Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



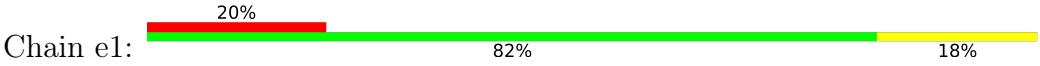
• Molecule 82: 40S ribosomal protein S17-A

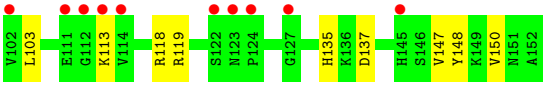
Chain c7:



• Molecule 83: Ubiquitin-40S ribosomal protein S31

Chain e1:




V102
L103
E111
G112
K113
V114
R118
R119
S122
N123
P124
G127
H135
K136
D137
H145
S146
V147
Y148
K149
V150
N151
A152

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.68	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(^{o})	Ideal(^{o})
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 (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	250/252 (99%)	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Res	Type
11	q	50	ASN
30	AB	48	TYR
46	i	167	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	CD	193/194 (100%)	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
51	s2	91	ARG
53	s4	163	ASP
51	s2	82	ASN
65	c6	43	ILE
7	CG	194	LEU

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

Mol	Chain	Res	Type
45	DR	34	HIS
56	s7	150	GLN
62	O	101	HIS
81	h	52	GLN
62	c3	5	HIS

5.3.3 RNA (i)

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	2209	U
25	A	130	C
1	AR	2269	U
1	AR	3276	G
25	A	278	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	AP	502	-	0,6,6	-	-	-		
84	OHX	1	3699	-	0,6,6	-	-	-		
84	OHX	AR	3582	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3426	-	0,6,6	-	-	-		
84	OHX	6	1905	-	0,6,6	-	-	-		
84	OHX	1	3671	-	0,6,6	-	-	-		
84	OHX	6	1915	-	0,6,6	-	-	-		
84	OHX	A	2001	-	0,6,6	-	-	-		
84	OHX	1	3421	-	0,6,6	-	-	-		
84	OHX	6	2003	-	0,6,6	-	-	-		
84	OHX	1	3669	-	0,6,6	-	-	-		
84	OHX	6	2057	-	0,6,6	-	-	-		
84	OHX	AR	3636	-	0,6,6	-	-	-		
84	OHX	AS	204	-	0,6,6	-	-	-		
84	OHX	6	1936	-	0,6,6	-	-	-		
84	OHX	AR	3545	-	0,6,6	-	-	-		
84	OHX	1	3423	-	0,6,6	-	-	-		
84	OHX	1	3657	-	0,6,6	-	-	-		
84	OHX	6	2017	-	0,6,6	-	-	-		
84	OHX	1	3452	-	0,6,6	-	-	-		
84	OHX	1	3505	-	0,6,6	-	-	-		
84	OHX	1	3475	-	0,6,6	-	-	-		
84	OHX	1	3593	-	0,6,6	-	-	-		
84	OHX	6	1932	-	0,6,6	-	-	-		
84	OHX	AR	3612	-	0,6,6	-	-	-		
84	OHX	A	1997	-	0,6,6	-	-	-		
84	OHX	AS	205	-	0,6,6	-	-	-		
84	OHX	1	3704	-	0,6,6	-	-	-		
84	OHX	A	1933	-	0,6,6	-	-	-		
84	OHX	1	3493	-	0,6,6	-	-	-		
84	OHX	1	3726	-	0,6,6	-	-	-		
84	OHX	6	1950	-	0,6,6	-	-	-		
84	OHX	AR	3579	-	0,6,6	-	-	-		
84	OHX	6	1945	-	0,6,6	-	-	-		
84	OHX	A	2021	-	0,6,6	-	-	-		
84	OHX	6	2034	-	0,6,6	-	-	-		
84	OHX	1	3451	-	0,6,6	-	-	-		
84	OHX	AR	3566	-	0,6,6	-	-	-		
84	OHX	1	3422	-	0,6,6	-	-	-		
84	OHX	1	3638	-	0,6,6	-	-	-		
84	OHX	6	1999	-	0,6,6	-	-	-		
84	OHX	6	2020	-	0,6,6	-	-	-		
84	OHX	AR	3716	-	0,6,6	-	-	-		
84	OHX	1	3450	-	0,6,6	-	-	-		
84	OHX	AR	3565	-	0,6,6	-	-	-		
84	OHX	6	1929	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3682	-	0,6,6	-	-	-		
84	OHX	A	2033	-	0,6,6	-	-	-		
84	OHX	AR	3462	-	0,6,6	-	-	-		
84	OHX	AR	3540	-	0,6,6	-	-	-		
84	OHX	1	3402	-	0,6,6	-	-	-		
84	OHX	1	3690	-	0,6,6	-	-	-		
84	OHX	AR	3603	-	0,6,6	-	-	-		
84	OHX	AR	3647	-	0,6,6	-	-	-		
84	OHX	3	208	-	0,6,6	-	-	-		
84	OHX	AR	3648	-	0,6,6	-	-	-		
84	OHX	AR	3722	-	0,6,6	-	-	-		
84	OHX	A	1986	-	0,6,6	-	-	-		
84	OHX	A	2019	-	0,6,6	-	-	-		
84	OHX	AR	3504	-	0,6,6	-	-	-		
84	OHX	1	3589	-	0,6,6	-	-	-		
84	OHX	1	3660	-	0,6,6	-	-	-		
84	OHX	AR	3630	-	0,6,6	-	-	-		
84	OHX	d9	101	-	0,6,6	-	-	-		
84	OHX	A	1950	-	0,6,6	-	-	-		
84	OHX	AR	3699	-	0,6,6	-	-	-		
84	OHX	1	3471	-	0,6,6	-	-	-		
84	OHX	1	3549	-	0,6,6	-	-	-		
84	OHX	AR	3446	-	0,6,6	-	-	-		
84	OHX	AR	3721	-	0,6,6	-	-	-		
84	OHX	6	1985	-	0,6,6	-	-	-		
84	OHX	AR	3500	-	0,6,6	-	-	-		
84	OHX	AR	3602	-	0,6,6	-	-	-		
84	OHX	A	1934	-	0,6,6	-	-	-		
84	OHX	A	1960	-	0,6,6	-	-	-		
84	OHX	AR	3595	-	0,6,6	-	-	-		
84	OHX	A	1971	-	0,6,6	-	-	-		
84	OHX	AR	3418	-	0,6,6	-	-	-		
84	OHX	AR	3425	-	0,6,6	-	-	-		
84	OHX	DI	201	-	0,6,6	-	-	-		
84	OHX	1	3504	-	0,6,6	-	-	-		
84	OHX	AR	3642	-	0,6,6	-	-	-		
84	OHX	AR	3563	-	0,6,6	-	-	-		
84	OHX	1	3409	-	0,6,6	-	-	-		
84	OHX	AE	201	-	0,6,6	-	-	-		
84	OHX	1	3466	-	0,6,6	-	-	-		
84	OHX	1	3634	-	0,6,6	-	-	-		
84	OHX	4	210	-	0,6,6	-	-	-		
84	OHX	6	2029	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	A	2009	-	0,6,6	-	-	-		
84	OHX	AT	215	-	0,6,6	-	-	-		
84	OHX	1	3558	-	0,6,6	-	-	-		
84	OHX	AR	3730	-	0,6,6	-	-	-		
84	OHX	1	3562	-	0,6,6	-	-	-		
84	OHX	6	1975	-	0,6,6	-	-	-		
84	OHX	6	2028	-	0,6,6	-	-	-		
84	OHX	AK	103	-	0,6,6	-	-	-		
84	OHX	1	3461	-	0,6,6	-	-	-		
84	OHX	AR	3616	-	0,6,6	-	-	-		
84	OHX	1	3480	-	0,6,6	-	-	-		
84	OHX	1	3715	-	0,6,6	-	-	-		
84	OHX	AR	3675	-	0,6,6	-	-	-		
84	OHX	AR	3723	-	0,6,6	-	-	-		
84	OHX	AR	3620	-	0,6,6	-	-	-		
84	OHX	AT	205	-	0,6,6	-	-	-		
84	OHX	AT	208	-	0,6,6	-	-	-		
84	OHX	3	204	-	0,6,6	-	-	-		
84	OHX	1	3601	-	0,6,6	-	-	-		
84	OHX	6	1919	-	0,6,6	-	-	-		
84	OHX	A	1949	-	0,6,6	-	-	-		
84	OHX	AR	3527	-	0,6,6	-	-	-		
84	OHX	AR	3560	-	0,6,6	-	-	-		
84	OHX	A	1957	-	0,6,6	-	-	-		
84	OHX	AR	3530	-	0,6,6	-	-	-		
84	OHX	AR	3738	-	0,6,6	-	-	-		
84	OHX	1	3541	-	0,6,6	-	-	-		
84	OHX	AR	3415	-	0,6,6	-	-	-		
84	OHX	A	1941	-	0,6,6	-	-	-		
84	OHX	A	1947	-	0,6,6	-	-	-		
84	OHX	1	3544	-	0,6,6	-	-	-		
84	OHX	1	3679	-	0,6,6	-	-	-		
84	OHX	AR	3578	-	0,6,6	-	-	-		
84	OHX	AR	3687	-	0,6,6	-	-	-		
84	OHX	AR	3510	-	0,6,6	-	-	-		
84	OHX	AR	3585	-	0,6,6	-	-	-		
84	OHX	1	3706	-	0,6,6	-	-	-		
84	OHX	6	1908	-	0,6,6	-	-	-		
84	OHX	AR	3613	-	0,6,6	-	-	-		
84	OHX	A	2025	-	0,6,6	-	-	-		
84	OHX	6	1933	-	0,6,6	-	-	-		
84	OHX	6	1935	-	0,6,6	-	-	-		
84	OHX	A	1948	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3465	-	0,6,6	-	-	-		
84	OHX	6	1930	-	0,6,6	-	-	-		
84	OHX	A	2010	-	0,6,6	-	-	-		
84	OHX	AR	3431	-	0,6,6	-	-	-		
84	OHX	1	3667	-	0,6,6	-	-	-		
84	OHX	6	2026	-	0,6,6	-	-	-		
84	OHX	AR	3469	-	0,6,6	-	-	-		
84	OHX	1	3559	-	0,6,6	-	-	-		
84	OHX	6	2013	-	0,6,6	-	-	-		
84	OHX	1	3420	-	0,6,6	-	-	-		
84	OHX	6	2033	-	0,6,6	-	-	-		
84	OHX	6	1911	-	0,6,6	-	-	-		
84	OHX	1	3633	-	0,6,6	-	-	-		
84	OHX	AR	3447	-	0,6,6	-	-	-		
84	OHX	1	3572	-	0,6,6	-	-	-		
84	OHX	AT	204	-	0,6,6	-	-	-		
84	OHX	AR	3513	-	0,6,6	-	-	-		
84	OHX	6	2046	-	0,6,6	-	-	-		
84	OHX	AR	3711	-	0,6,6	-	-	-		
84	OHX	1	3604	-	0,6,6	-	-	-		
84	OHX	A	1945	-	0,6,6	-	-	-		
84	OHX	6	1973	-	0,6,6	-	-	-		
84	OHX	1	3566	-	0,6,6	-	-	-		
84	OHX	AR	3408	-	0,6,6	-	-	-		
84	OHX	1	3497	-	0,6,6	-	-	-		
84	OHX	CG	301	-	0,6,6	-	-	-		
84	OHX	1	3456	-	0,6,6	-	-	-		
84	OHX	A	2007	-	0,6,6	-	-	-		
84	OHX	AR	3445	-	0,6,6	-	-	-		
84	OHX	2	201	-	0,6,6	-	-	-		
84	OHX	AR	3518	-	0,6,6	-	-	-		
84	OHX	AR	3529	-	0,6,6	-	-	-		
84	OHX	AR	3543	-	0,6,6	-	-	-		
84	OHX	AR	3646	-	0,6,6	-	-	-		
84	OHX	A	1993	-	0,6,6	-	-	-		
84	OHX	AR	3556	-	0,6,6	-	-	-		
84	OHX	1	3635	-	0,6,6	-	-	-		
84	OHX	1	3650	-	0,6,6	-	-	-		
84	OHX	AR	3658	-	0,6,6	-	-	-		
84	OHX	AR	3639	-	0,6,6	-	-	-		
84	OHX	A	2036	-	0,6,6	-	-	-		
84	OHX	4	209	-	0,6,6	-	-	-		
84	OHX	1	3672	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	6	1978	-	0,6,6	-	-	-		
84	OHX	AR	3405	-	0,6,6	-	-	-		
84	OHX	AR	3411	-	0,6,6	-	-	-		
84	OHX	1	3499	-	0,6,6	-	-	-		
84	OHX	1	3513	-	0,6,6	-	-	-		
84	OHX	AR	3424	-	0,6,6	-	-	-		
84	OHX	6	1916	-	0,6,6	-	-	-		
84	OHX	AT	213	-	0,6,6	-	-	-		
84	OHX	1	3419	-	0,6,6	-	-	-		
84	OHX	AR	3460	-	0,6,6	-	-	-		
84	OHX	A	1917	-	0,6,6	-	-	-		
84	OHX	c3	201	-	0,6,6	-	-	-		
84	OHX	1	3605	-	0,6,6	-	-	-		
84	OHX	6	2001	-	0,6,6	-	-	-		
84	OHX	6	2053	-	0,6,6	-	-	-		
84	OHX	A	1952	-	0,6,6	-	-	-		
84	OHX	O	201	-	0,6,6	-	-	-		
84	OHX	6	1994	-	0,6,6	-	-	-		
84	OHX	6	1938	-	0,6,6	-	-	-		
84	OHX	6	2018	-	0,6,6	-	-	-		
84	OHX	1	3627	-	0,6,6	-	-	-		
84	OHX	6	1998	-	0,6,6	-	-	-		
84	OHX	1	3496	-	0,6,6	-	-	-		
84	OHX	1	3575	-	0,6,6	-	-	-		
84	OHX	AR	3581	-	0,6,6	-	-	-		
84	OHX	6	1957	-	0,6,6	-	-	-		
84	OHX	A	1958	-	0,6,6	-	-	-		
84	OHX	A	2024	-	0,6,6	-	-	-		
84	OHX	6	2040	-	0,6,6	-	-	-		
84	OHX	1	3685	-	0,6,6	-	-	-		
84	OHX	A	1909	-	0,6,6	-	-	-		
84	OHX	1	3581	-	0,6,6	-	-	-		
84	OHX	AR	3521	-	0,6,6	-	-	-		
84	OHX	AR	3672	-	0,6,6	-	-	-		
84	OHX	1	3676	-	0,6,6	-	-	-		
84	OHX	AR	3677	-	0,6,6	-	-	-		
84	OHX	1	3522	-	0,6,6	-	-	-		
84	OHX	A	2017	-	0,6,6	-	-	-		
84	OHX	A	2035	-	0,6,6	-	-	-		
84	OHX	4	201	-	0,6,6	-	-	-		
84	OHX	1	3696	-	0,6,6	-	-	-		
84	OHX	AR	3508	-	0,6,6	-	-	-		
84	OHX	6	1924	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	A	2042	-	0,6,6	-	-	-		
84	OHX	AS	208	-	0,6,6	-	-	-		
84	OHX	AR	3534	-	0,6,6	-	-	-		
84	OHX	1	3610	-	0,6,6	-	-	-		
84	OHX	6	1962	-	0,6,6	-	-	-		
84	OHX	6	2024	-	0,6,6	-	-	-		
84	OHX	AR	3417	-	0,6,6	-	-	-		
84	OHX	AR	3591	-	0,6,6	-	-	-		
84	OHX	AR	3600	-	0,6,6	-	-	-		
84	OHX	A	1998	-	0,6,6	-	-	-		
84	OHX	AT	210	-	0,6,6	-	-	-		
84	OHX	A	2037	-	0,6,6	-	-	-		
84	OHX	1	3490	-	0,6,6	-	-	-		
84	OHX	1	3649	-	0,6,6	-	-	-		
84	OHX	AR	3458	-	0,6,6	-	-	-		
84	OHX	AR	3573	-	0,6,6	-	-	-		
84	OHX	A	1995	-	0,6,6	-	-	-		
84	OHX	1	3680	-	0,6,6	-	-	-		
84	OHX	A	1943	-	0,6,6	-	-	-		
84	OHX	AR	3533	-	0,6,6	-	-	-		
84	OHX	A	2034	-	0,6,6	-	-	-		
84	OHX	1	3722	-	0,6,6	-	-	-		
84	OHX	A	1999	-	0,6,6	-	-	-		
84	OHX	AR	3512	-	0,6,6	-	-	-		
84	OHX	AR	3548	-	0,6,6	-	-	-		
84	OHX	M	201	-	0,6,6	-	-	-		
84	OHX	AR	3624	-	0,6,6	-	-	-		
84	OHX	6	2015	-	0,6,6	-	-	-		
84	OHX	AR	3414	-	0,6,6	-	-	-		
84	OHX	1	3413	-	0,6,6	-	-	-		
84	OHX	AR	3479	-	0,6,6	-	-	-		
84	OHX	1	3644	-	0,6,6	-	-	-		
84	OHX	1	3401	-	0,6,6	-	-	-		
84	OHX	6	1959	-	0,6,6	-	-	-		
84	OHX	AR	3498	-	0,6,6	-	-	-		
84	OHX	1	3598	-	0,6,6	-	-	-		
84	OHX	1	3632	-	0,6,6	-	-	-		
84	OHX	A	2006	-	0,6,6	-	-	-		
84	OHX	6	1931	-	0,6,6	-	-	-		
84	OHX	AR	3410	-	0,6,6	-	-	-		
84	OHX	AR	3464	-	0,6,6	-	-	-		
84	OHX	6	1993	-	0,6,6	-	-	-		
84	OHX	6	1967	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	6	2009	-	0,6,6	-	-	-		
84	OHX	AR	3412	-	0,6,6	-	-	-		
84	OHX	AR	3725	-	0,6,6	-	-	-		
84	OHX	A	1991	-	0,6,6	-	-	-		
84	OHX	CV	201	-	0,6,6	-	-	-		
84	OHX	1	3556	-	0,6,6	-	-	-		
84	OHX	1	3582	-	0,6,6	-	-	-		
84	OHX	AR	3656	-	0,6,6	-	-	-		
84	OHX	A	1915	-	0,6,6	-	-	-		
84	OHX	1	3583	-	0,6,6	-	-	-		
84	OHX	6	1901	-	0,6,6	-	-	-		
84	OHX	AR	3737	-	0,6,6	-	-	-		
84	OHX	1	3531	-	0,6,6	-	-	-		
84	OHX	1	3483	-	0,6,6	-	-	-		
84	OHX	A	1936	-	0,6,6	-	-	-		
84	OHX	A	1974	-	0,6,6	-	-	-		
84	OHX	6	1949	-	0,6,6	-	-	-		
84	OHX	6	1927	-	0,6,6	-	-	-		
84	OHX	AR	3474	-	0,6,6	-	-	-		
84	OHX	1	3662	-	0,6,6	-	-	-		
84	OHX	1	3417	-	0,6,6	-	-	-		
84	OHX	AR	3482	-	0,6,6	-	-	-		
84	OHX	AR	3507	-	0,6,6	-	-	-		
84	OHX	AR	3520	-	0,6,6	-	-	-		
84	OHX	AR	3629	-	0,6,6	-	-	-		
84	OHX	AR	3663	-	0,6,6	-	-	-		
84	OHX	A	1932	-	0,6,6	-	-	-		
84	OHX	1	3532	-	0,6,6	-	-	-		
84	OHX	1	3723	-	0,6,6	-	-	-		
84	OHX	1	3494	-	0,6,6	-	-	-		
84	OHX	A	1975	-	0,6,6	-	-	-		
84	OHX	1	3492	-	0,6,6	-	-	-		
84	OHX	1	3520	-	0,6,6	-	-	-		
84	OHX	A	1916	-	0,6,6	-	-	-		
84	OHX	6	2014	-	0,6,6	-	-	-		
84	OHX	1	3623	-	0,6,6	-	-	-		
84	OHX	1	3670	-	0,6,6	-	-	-		
84	OHX	AR	3470	-	0,6,6	-	-	-		
84	OHX	1	3594	-	0,6,6	-	-	-		
84	OHX	6	1928	-	0,6,6	-	-	-		
84	OHX	1	3443	-	0,6,6	-	-	-		
84	OHX	6	1948	-	0,6,6	-	-	-		
84	OHX	AR	3712	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AR	3707	-	0,6,6	-	-	-		
84	OHX	AR	3586	-	0,6,6	-	-	-		
84	OHX	h	401	-	0,6,6	-	-	-		
84	OHX	1	3570	-	0,6,6	-	-	-		
84	OHX	e	101	-	0,6,6	-	-	-		
84	OHX	1	3568	-	0,6,6	-	-	-		
84	OHX	1	3702	-	0,6,6	-	-	-		
84	OHX	A	1987	-	0,6,6	-	-	-		
84	OHX	1	3525	-	0,6,6	-	-	-		
84	OHX	6	1909	-	0,6,6	-	-	-		
84	OHX	AR	3471	-	0,6,6	-	-	-		
84	OHX	AR	3718	-	0,6,6	-	-	-		
84	OHX	AR	3466	-	0,6,6	-	-	-		
84	OHX	r	301	-	0,6,6	-	-	-		
84	OHX	AR	3596	-	0,6,6	-	-	-		
84	OHX	6	1963	-	0,6,6	-	-	-		
84	OHX	AR	3685	-	0,6,6	-	-	-		
84	OHX	1	3665	-	0,6,6	-	-	-		
84	OHX	AR	3615	-	0,6,6	-	-	-		
84	OHX	J	301	-	0,6,6	-	-	-		
84	OHX	3	201	-	0,6,6	-	-	-		
84	OHX	AR	3700	-	0,6,6	-	-	-		
84	OHX	AR	3623	-	0,6,6	-	-	-		
84	OHX	A	1913	-	0,6,6	-	-	-		
84	OHX	1	3542	-	0,6,6	-	-	-		
84	OHX	AR	3501	-	0,6,6	-	-	-		
84	OHX	1	3553	-	0,6,6	-	-	-		
84	OHX	1	3591	-	0,6,6	-	-	-		
84	OHX	1	3406	-	0,6,6	-	-	-		
84	OHX	1	3697	-	0,6,6	-	-	-		
84	OHX	AR	3489	-	0,6,6	-	-	-		
84	OHX	A	2000	-	0,6,6	-	-	-		
84	OHX	1	3641	-	0,6,6	-	-	-		
84	OHX	AK	102	-	0,6,6	-	-	-		
84	OHX	AS	206	-	0,6,6	-	-	-		
84	OHX	CX	201	-	0,6,6	-	-	-		
84	OHX	6	2049	-	0,6,6	-	-	-		
84	OHX	6	1992	-	0,6,6	-	-	-		
84	OHX	1	3546	-	0,6,6	-	-	-		
84	OHX	6	1997	-	0,6,6	-	-	-		
84	OHX	A	1938	-	0,6,6	-	-	-		
84	OHX	DG	201	-	0,6,6	-	-	-		
84	OHX	1	3403	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3538	-	0,6,6	-	-	-		
84	OHX	1	3429	-	0,6,6	-	-	-		
84	OHX	1	3577	-	0,6,6	-	-	-		
84	OHX	AR	3421	-	0,6,6	-	-	-		
84	OHX	1	3404	-	0,6,6	-	-	-		
84	OHX	1	3713	-	0,6,6	-	-	-		
84	OHX	AR	3457	-	0,6,6	-	-	-		
84	OHX	6	1979	-	0,6,6	-	-	-		
84	OHX	AR	3580	-	0,6,6	-	-	-		
84	OHX	AR	3618	-	0,6,6	-	-	-		
84	OHX	1	3688	-	0,6,6	-	-	-		
84	OHX	6	2039	-	0,6,6	-	-	-		
84	OHX	AR	3715	-	0,6,6	-	-	-		
84	OHX	AT	202	-	0,6,6	-	-	-		
84	OHX	z	201	-	0,6,6	-	-	-		
84	OHX	A	1931	-	0,6,6	-	-	-		
84	OHX	1	3433	-	0,6,6	-	-	-		
84	OHX	AR	3477	-	0,6,6	-	-	-		
84	OHX	AR	3561	-	0,6,6	-	-	-		
84	OHX	AR	3488	-	0,6,6	-	-	-		
84	OHX	AR	3526	-	0,6,6	-	-	-		
84	OHX	1	3606	-	0,6,6	-	-	-		
84	OHX	AR	3640	-	0,6,6	-	-	-		
84	OHX	1	3714	-	0,6,6	-	-	-		
84	OHX	1	3617	-	0,6,6	-	-	-		
84	OHX	1	3447	-	0,6,6	-	-	-		
84	OHX	1	3501	-	0,6,6	-	-	-		
84	OHX	1	3708	-	0,6,6	-	-	-		
84	OHX	1	3485	-	0,6,6	-	-	-		
84	OHX	4	206	-	0,6,6	-	-	-		
84	OHX	AR	3439	-	0,6,6	-	-	-		
84	OHX	1	3555	-	0,6,6	-	-	-		
84	OHX	AR	3628	-	0,6,6	-	-	-		
84	OHX	DL	102	-	0,6,6	-	-	-		
84	OHX	6	2056	-	0,6,6	-	-	-		
84	OHX	AR	3435	-	0,6,6	-	-	-		
84	OHX	A	1926	-	0,6,6	-	-	-		
84	OHX	AR	3592	-	0,6,6	-	-	-		
84	OHX	1	3664	-	0,6,6	-	-	-		
84	OHX	AR	3444	-	0,6,6	-	-	-		
84	OHX	AR	3694	-	0,6,6	-	-	-		
84	OHX	1	3599	-	0,6,6	-	-	-		
84	OHX	A	1976	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	A	1966	-	0,6,6	-	-	-		
84	OHX	AR	3459	-	0,6,6	-	-	-		
84	OHX	A	1964	-	0,6,6	-	-	-		
84	OHX	6	1977	-	0,6,6	-	-	-		
84	OHX	6	1996	-	0,6,6	-	-	-		
84	OHX	1	3430	-	0,6,6	-	-	-		
84	OHX	A	2014	-	0,6,6	-	-	-		
84	OHX	1	3437	-	0,6,6	-	-	-		
84	OHX	1	3580	-	0,6,6	-	-	-		
84	OHX	6	1920	-	0,6,6	-	-	-		
84	OHX	AR	3619	-	0,6,6	-	-	-		
84	OHX	1	3476	-	0,6,6	-	-	-		
84	OHX	1	3689	-	0,6,6	-	-	-		
84	OHX	6	1970	-	0,6,6	-	-	-		
84	OHX	1	3487	-	0,6,6	-	-	-		
84	OHX	A	1962	-	0,6,6	-	-	-		
84	OHX	1	3408	-	0,6,6	-	-	-		
84	OHX	6	1914	-	0,6,6	-	-	-		
84	OHX	AR	3567	-	0,6,6	-	-	-		
84	OHX	1	3472	-	0,6,6	-	-	-		
84	OHX	AR	3682	-	0,6,6	-	-	-		
84	OHX	6	1913	-	0,6,6	-	-	-		
84	OHX	1	3438	-	0,6,6	-	-	-		
84	OHX	AR	3684	-	0,6,6	-	-	-		
84	OHX	6	1984	-	0,6,6	-	-	-		
84	OHX	6	2051	-	0,6,6	-	-	-		
84	OHX	6	1991	-	0,6,6	-	-	-		
84	OHX	1	3597	-	0,6,6	-	-	-		
84	OHX	AR	3571	-	0,6,6	-	-	-		
84	OHX	CK	201	-	0,6,6	-	-	-		
84	OHX	6	1939	-	0,6,6	-	-	-		
84	OHX	1	3498	-	0,6,6	-	-	-		
84	OHX	1	3612	-	0,6,6	-	-	-		
84	OHX	AS	209	-	0,6,6	-	-	-		
84	OHX	4	202	-	0,6,6	-	-	-		
84	OHX	s8	301	-	0,6,6	-	-	-		
84	OHX	A	2018	-	0,6,6	-	-	-		
84	OHX	1	3468	-	0,6,6	-	-	-		
84	OHX	AR	3643	-	0,6,6	-	-	-		
84	OHX	AR	3609	-	0,6,6	-	-	-		
84	OHX	AR	3413	-	0,6,6	-	-	-		
84	OHX	1	3514	-	0,6,6	-	-	-		
84	OHX	AR	3626	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3545	-	0,6,6	-	-	-		
84	OHX	AR	3614	-	0,6,6	-	-	-		
84	OHX	AR	3487	-	0,6,6	-	-	-		
84	OHX	AR	3635	-	0,6,6	-	-	-		
84	OHX	A	1954	-	0,6,6	-	-	-		
84	OHX	AR	3541	-	0,6,6	-	-	-		
84	OHX	AR	3681	-	0,6,6	-	-	-		
84	OHX	A	1937	-	0,6,6	-	-	-		
84	OHX	3	207	-	0,6,6	-	-	-		
84	OHX	AR	3584	-	0,6,6	-	-	-		
84	OHX	1	3540	-	0,6,6	-	-	-		
84	OHX	AR	3705	-	0,6,6	-	-	-		
84	OHX	AR	3733	-	0,6,6	-	-	-		
84	OHX	AS	201	-	0,6,6	-	-	-		
84	OHX	1	3539	-	0,6,6	-	-	-		
84	OHX	AR	3631	-	0,6,6	-	-	-		
84	OHX	1	3663	-	0,6,6	-	-	-		
84	OHX	A	1985	-	0,6,6	-	-	-		
84	OHX	CE	403	-	0,6,6	-	-	-		
84	OHX	AR	3437	-	0,6,6	-	-	-		
84	OHX	AT	217	-	0,6,6	-	-	-		
84	OHX	1	3489	-	0,6,6	-	-	-		
84	OHX	6	1922	-	0,6,6	-	-	-		
84	OHX	AR	3622	-	0,6,6	-	-	-		
84	OHX	1	3565	-	0,6,6	-	-	-		
84	OHX	A	1981	-	0,6,6	-	-	-		
84	OHX	1	3488	-	0,6,6	-	-	-		
84	OHX	1	3462	-	0,6,6	-	-	-		
84	OHX	AR	3679	-	0,6,6	-	-	-		
84	OHX	AR	3686	-	0,6,6	-	-	-		
84	OHX	1	3720	-	0,6,6	-	-	-		
84	OHX	6	1964	-	0,6,6	-	-	-		
84	OHX	AR	3604	-	0,6,6	-	-	-		
84	OHX	AR	3463	-	0,6,6	-	-	-		
84	OHX	AR	3605	-	0,6,6	-	-	-		
84	OHX	1	3648	-	0,6,6	-	-	-		
84	OHX	6	2038	-	0,6,6	-	-	-		
84	OHX	AR	3519	-	0,6,6	-	-	-		
84	OHX	AR	3497	-	0,6,6	-	-	-		
84	OHX	1	3630	-	0,6,6	-	-	-		
84	OHX	AT	206	-	0,6,6	-	-	-		
84	OHX	AR	3537	-	0,6,6	-	-	-		
84	OHX	1	3550	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AT	218	-	0,6,6	-	-	-		
84	OHX	1	3453	-	0,6,6	-	-	-		
84	OHX	1	3608	-	0,6,6	-	-	-		
84	OHX	6	1906	-	0,6,6	-	-	-		
84	OHX	1	3506	-	0,6,6	-	-	-		
84	OHX	6	1952	-	0,6,6	-	-	-		
84	OHX	6	1980	-	0,6,6	-	-	-		
84	OHX	1	3595	-	0,6,6	-	-	-		
84	OHX	AR	3655	-	0,6,6	-	-	-		
84	OHX	AR	3509	-	0,6,6	-	-	-		
84	OHX	AR	3726	-	0,6,6	-	-	-		
84	OHX	AS	203	-	0,6,6	-	-	-		
84	OHX	1	3459	-	0,6,6	-	-	-		
84	OHX	6	2004	-	0,6,6	-	-	-		
84	OHX	1	3434	-	0,6,6	-	-	-		
84	OHX	AR	3401	-	0,6,6	-	-	-		
84	OHX	6	2012	-	0,6,6	-	-	-		
84	OHX	A	1996	-	0,6,6	-	-	-		
84	OHX	6	1974	-	0,6,6	-	-	-		
84	OHX	AR	3554	-	0,6,6	-	-	-		
84	OHX	A	1989	-	0,6,6	-	-	-		
84	OHX	1	3415	-	0,6,6	-	-	-		
84	OHX	1	3656	-	0,6,6	-	-	-		
84	OHX	v	301	-	0,6,6	-	-	-		
84	OHX	6	1965	-	0,6,6	-	-	-		
84	OHX	AR	3576	-	0,6,6	-	-	-		
84	OHX	DH	201	-	0,6,6	-	-	-		
84	OHX	1	3719	-	0,6,6	-	-	-		
84	OHX	A	2027	-	0,6,6	-	-	-		
84	OHX	1	3521	-	0,6,6	-	-	-		
84	OHX	AR	3528	-	0,6,6	-	-	-		
84	OHX	AR	3587	-	0,6,6	-	-	-		
86	7MB	1	4216	-	16,23,23	1.32	3 (18%)	8,38,38	1.59	2 (25%)
84	OHX	1	3503	-	0,6,6	-	-	-		
84	OHX	1	3620	-	0,6,6	-	-	-		
84	OHX	AR	3486	-	0,6,6	-	-	-		
84	OHX	1	3645	-	0,6,6	-	-	-		
84	OHX	CL	301	-	0,6,6	-	-	-		
84	OHX	1	3560	-	0,6,6	-	-	-		
84	OHX	A	1944	-	0,6,6	-	-	-		
84	OHX	1	3416	-	0,6,6	-	-	-		
84	OHX	4	205	-	0,6,6	-	-	-		
84	OHX	AR	3660	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AR	3644	-	0,6,6	-	-	-		
84	OHX	A	2030	-	0,6,6	-	-	-		
84	OHX	1	3463	-	0,6,6	-	-	-		
84	OHX	1	3530	-	0,6,6	-	-	-		
84	OHX	1	3574	-	0,6,6	-	-	-		
84	OHX	6	1986	-	0,6,6	-	-	-		
84	OHX	1	3621	-	0,6,6	-	-	-		
84	OHX	AR	3627	-	0,6,6	-	-	-		
84	OHX	AR	3710	-	0,6,6	-	-	-		
84	OHX	AR	3729	-	0,6,6	-	-	-		
84	OHX	A	1929	-	0,6,6	-	-	-		
84	OHX	1	3585	-	0,6,6	-	-	-		
84	OHX	AR	3676	-	0,6,6	-	-	-		
84	OHX	AR	3683	-	0,6,6	-	-	-		
84	OHX	AT	212	-	0,6,6	-	-	-		
84	OHX	AR	3577	-	0,6,6	-	-	-		
84	OHX	6	2048	-	0,6,6	-	-	-		
84	OHX	1	3446	-	0,6,6	-	-	-		
84	OHX	1	3431	-	0,6,6	-	-	-		
84	OHX	6	2021	-	0,6,6	-	-	-		
84	OHX	AR	3610	-	0,6,6	-	-	-		
84	OHX	1	3640	-	0,6,6	-	-	-		
84	OHX	4	207	-	0,6,6	-	-	-		
84	OHX	AR	3484	-	0,6,6	-	-	-		
84	OHX	1	3628	-	0,6,6	-	-	-		
84	OHX	1	3666	-	0,6,6	-	-	-		
84	OHX	1	3718	-	0,6,6	-	-	-		
84	OHX	k	402	-	0,6,6	-	-	-		
84	OHX	6	1961	-	0,6,6	-	-	-		
84	OHX	AR	3680	-	0,6,6	-	-	-		
84	OHX	AR	3611	-	0,6,6	-	-	-		
84	OHX	6	1942	-	0,6,6	-	-	-		
84	OHX	1	3692	-	0,6,6	-	-	-		
84	OHX	4	204	-	0,6,6	-	-	-		
84	OHX	A	1903	-	0,6,6	-	-	-		
84	OHX	AR	3673	-	0,6,6	-	-	-		
84	OHX	1	3547	-	0,6,6	-	-	-		
84	OHX	1	3639	-	0,6,6	-	-	-		
84	OHX	6	1988	-	0,6,6	-	-	-		
84	OHX	AT	203	-	0,6,6	-	-	-		
84	OHX	A	1922	-	0,6,6	-	-	-		
84	OHX	A	2023	-	0,6,6	-	-	-		
84	OHX	AR	3516	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	6	1976	-	0,6,6	-	-	-		
84	OHX	1	3578	-	0,6,6	-	-	-		
84	OHX	1	3590	-	0,6,6	-	-	-		
84	OHX	AR	3455	-	0,6,6	-	-	-		
84	OHX	AR	3659	-	0,6,6	-	-	-		
84	OHX	A	1969	-	0,6,6	-	-	-		
84	OHX	A	2016	-	0,6,6	-	-	-		
84	OHX	1	3432	-	0,6,6	-	-	-		
84	OHX	A	2031	-	0,6,6	-	-	-		
84	OHX	AR	3423	-	0,6,6	-	-	-		
84	OHX	A	1951	-	0,6,6	-	-	-		
84	OHX	AR	3536	-	0,6,6	-	-	-		
84	OHX	1	3516	-	0,6,6	-	-	-		
84	OHX	AR	3491	-	0,6,6	-	-	-		
84	OHX	1	3543	-	0,6,6	-	-	-		
84	OHX	1	3440	-	0,6,6	-	-	-		
84	OHX	1	3655	-	0,6,6	-	-	-		
84	OHX	6	1982	-	0,6,6	-	-	-		
84	OHX	A	1920	-	0,6,6	-	-	-		
84	OHX	AR	3558	-	0,6,6	-	-	-		
84	OHX	1	3469	-	0,6,6	-	-	-		
84	OHX	CO	201	-	0,6,6	-	-	-		
84	OHX	A	1970	-	0,6,6	-	-	-		
84	OHX	AR	3461	-	0,6,6	-	-	-		
84	OHX	AR	3674	-	0,6,6	-	-	-		
84	OHX	A	1955	-	0,6,6	-	-	-		
84	OHX	1	3460	-	0,6,6	-	-	-		
84	OHX	1	3510	-	0,6,6	-	-	-		
84	OHX	6	2019	-	0,6,6	-	-	-		
84	OHX	AR	3708	-	0,6,6	-	-	-		
84	OHX	A	2039	-	0,6,6	-	-	-		
84	OHX	AR	3436	-	0,6,6	-	-	-		
84	OHX	AR	3483	-	0,6,6	-	-	-		
84	OHX	AR	3552	-	0,6,6	-	-	-		
84	OHX	1	3603	-	0,6,6	-	-	-		
84	OHX	AR	3551	-	0,6,6	-	-	-		
84	OHX	AR	3420	-	0,6,6	-	-	-		
84	OHX	1	3418	-	0,6,6	-	-	-		
84	OHX	1	3727	-	0,6,6	-	-	-		
84	OHX	AR	3688	-	0,6,6	-	-	-		
84	OHX	1	3557	-	0,6,6	-	-	-		
84	OHX	A	1901	-	0,6,6	-	-	-		
84	OHX	AR	3709	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	CL	302	-	0,6,6	-	-	-		
84	OHX	1	3481	-	0,6,6	-	-	-		
84	OHX	AR	3492	-	0,6,6	-	-	-		
84	OHX	DL	101	-	0,6,6	-	-	-		
84	OHX	1	3534	-	0,6,6	-	-	-		
84	OHX	A	1935	-	0,6,6	-	-	-		
84	OHX	1	3584	-	0,6,6	-	-	-		
84	OHX	AR	3555	-	0,6,6	-	-	-		
84	OHX	1	3724	-	0,6,6	-	-	-		
84	OHX	AR	3517	-	0,6,6	-	-	-		
84	OHX	AR	3428	-	0,6,6	-	-	-		
84	OHX	1	3533	-	0,6,6	-	-	-		
84	OHX	1	3502	-	0,6,6	-	-	-		
84	OHX	AR	3441	-	0,6,6	-	-	-		
84	OHX	AR	3402	-	0,6,6	-	-	-		
84	OHX	AR	3442	-	0,6,6	-	-	-		
84	OHX	1	3427	-	0,6,6	-	-	-		
84	OHX	AR	3448	-	0,6,6	-	-	-		
84	OHX	AR	3535	-	0,6,6	-	-	-		
84	OHX	AR	3678	-	0,6,6	-	-	-		
84	OHX	A	1990	-	0,6,6	-	-	-		
84	OHX	AR	3495	-	0,6,6	-	-	-		
84	OHX	A	1924	-	0,6,6	-	-	-		
84	OHX	1	3473	-	0,6,6	-	-	-		
84	OHX	AR	3664	-	0,6,6	-	-	-		
84	OHX	1	3442	-	0,6,6	-	-	-		
84	OHX	6	1960	-	0,6,6	-	-	-		
84	OHX	A	1904	-	0,6,6	-	-	-		
84	OHX	6	1971	-	0,6,6	-	-	-		
84	OHX	A	2011	-	0,6,6	-	-	-		
84	OHX	AR	3452	-	0,6,6	-	-	-		
84	OHX	1	3625	-	0,6,6	-	-	-		
84	OHX	AR	3668	-	0,6,6	-	-	-		
84	OHX	A	2040	-	0,6,6	-	-	-		
84	OHX	6	2025	-	0,6,6	-	-	-		
84	OHX	AR	3632	-	0,6,6	-	-	-		
84	OHX	6	2041	-	0,6,6	-	-	-		
84	OHX	A	1905	-	0,6,6	-	-	-		
84	OHX	A	1963	-	0,6,6	-	-	-		
84	OHX	1	3618	-	0,6,6	-	-	-		
84	OHX	A	1930	-	0,6,6	-	-	-		
84	OHX	AR	3553	-	0,6,6	-	-	-		
84	OHX	CF	401	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	A	2026	-	0,6,6	-	-	-		
84	OHX	A	2038	-	0,6,6	-	-	-		
84	OHX	AR	3499	-	0,6,6	-	-	-		
84	OHX	6	1958	-	0,6,6	-	-	-		
84	OHX	AR	3727	-	0,6,6	-	-	-		
84	OHX	AR	3450	-	0,6,6	-	-	-		
84	OHX	A	2020	-	0,6,6	-	-	-		
84	OHX	1	3412	-	0,6,6	-	-	-		
84	OHX	1	3725	-	0,6,6	-	-	-		
84	OHX	3	203	-	0,6,6	-	-	-		
84	OHX	A	1983	-	0,6,6	-	-	-		
84	OHX	A	2041	-	0,6,6	-	-	-		
84	OHX	AR	3493	-	0,6,6	-	-	-		
84	OHX	AR	3496	-	0,6,6	-	-	-		
84	OHX	A	1906	-	0,6,6	-	-	-		
84	OHX	AR	3662	-	0,6,6	-	-	-		
84	OHX	AR	3713	-	0,6,6	-	-	-		
84	OHX	AR	3524	-	0,6,6	-	-	-		
84	OHX	AC	101	-	0,6,6	-	-	-		
84	OHX	1	3643	-	0,6,6	-	-	-		
84	OHX	AR	3569	-	0,6,6	-	-	-		
84	OHX	CZ	201	-	0,6,6	-	-	-		
84	OHX	1	3507	-	0,6,6	-	-	-		
84	OHX	6	2042	-	0,6,6	-	-	-		
84	OHX	AG	201	-	0,6,6	-	-	-		
84	OHX	A	1953	-	0,6,6	-	-	-		
84	OHX	A	2008	-	0,6,6	-	-	-		
84	OHX	AR	3671	-	0,6,6	-	-	-		
84	OHX	6	1940	-	0,6,6	-	-	-		
84	OHX	AR	3473	-	0,6,6	-	-	-		
84	OHX	1	3730	-	0,6,6	-	-	-		
84	OHX	A	2013	-	0,6,6	-	-	-		
84	OHX	1	3511	-	0,6,6	-	-	-		
84	OHX	6	2036	-	0,6,6	-	-	-		
84	OHX	1	3631	-	0,6,6	-	-	-		
84	OHX	1	3675	-	0,6,6	-	-	-		
84	OHX	1	3569	-	0,6,6	-	-	-		
84	OHX	AR	3522	-	0,6,6	-	-	-		
84	OHX	AR	3735	-	0,6,6	-	-	-		
84	OHX	AT	214	-	0,6,6	-	-	-		
84	OHX	A	1973	-	0,6,6	-	-	-		
84	OHX	1	3470	-	0,6,6	-	-	-		
84	OHX	A	2012	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AR	3485	-	0,6,6	-	-	-		
84	OHX	AR	3426	-	0,6,6	-	-	-		
84	OHX	1	3661	-	0,6,6	-	-	-		
84	OHX	AR	3523	-	0,6,6	-	-	-		
84	OHX	AR	3621	-	0,6,6	-	-	-		
84	OHX	1	3712	-	0,6,6	-	-	-		
84	OHX	1	3674	-	0,6,6	-	-	-		
84	OHX	k	401	-	0,6,6	-	-	-		
84	OHX	AR	3704	-	0,6,6	-	-	-		
84	OHX	6	2055	-	0,6,6	-	-	-		
84	OHX	A	1946	-	0,6,6	-	-	-		
84	OHX	A	2015	-	0,6,6	-	-	-		
84	OHX	A	2029	-	0,6,6	-	-	-		
84	OHX	6	1925	-	0,6,6	-	-	-		
84	OHX	A	1928	-	0,6,6	-	-	-		
84	OHX	1	3678	-	0,6,6	-	-	-		
84	OHX	AR	3724	-	0,6,6	-	-	-		
84	OHX	1	3651	-	0,6,6	-	-	-		
84	OHX	AR	3416	-	0,6,6	-	-	-		
84	OHX	AR	3451	-	0,6,6	-	-	-		
84	OHX	1	3695	-	0,6,6	-	-	-		
84	OHX	AR	3638	-	0,6,6	-	-	-		
84	OHX	6	2005	-	0,6,6	-	-	-		
84	OHX	A	1921	-	0,6,6	-	-	-		
84	OHX	1	3482	-	0,6,6	-	-	-		
84	OHX	1	3654	-	0,6,6	-	-	-		
84	OHX	1	3519	-	0,6,6	-	-	-		
84	OHX	AR	3657	-	0,6,6	-	-	-		
84	OHX	AR	3468	-	0,6,6	-	-	-		
84	OHX	AR	3506	-	0,6,6	-	-	-		
84	OHX	1	3624	-	0,6,6	-	-	-		
84	OHX	1	3615	-	0,6,6	-	-	-		
84	OHX	AR	3531	-	0,6,6	-	-	-		
84	OHX	AR	3544	-	0,6,6	-	-	-		
84	OHX	AR	3689	-	0,6,6	-	-	-		
84	OHX	AR	3728	-	0,6,6	-	-	-		
84	OHX	6	2031	-	0,6,6	-	-	-		
84	OHX	AR	3690	-	0,6,6	-	-	-		
84	OHX	AR	3502	-	0,6,6	-	-	-		
84	OHX	AR	3550	-	0,6,6	-	-	-		
84	OHX	AR	3572	-	0,6,6	-	-	-		
84	OHX	AR	3706	-	0,6,6	-	-	-		
84	OHX	1	3691	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AR	3422	-	0,6,6	-	-	-		
84	OHX	AR	3589	-	0,6,6	-	-	-		
84	OHX	1	3728	-	0,6,6	-	-	-		
84	OHX	AT	216	-	0,6,6	-	-	-		
84	OHX	AR	3549	-	0,6,6	-	-	-		
84	OHX	1	3707	-	0,6,6	-	-	-		
84	OHX	AR	3574	-	0,6,6	-	-	-		
84	OHX	A	2022	-	0,6,6	-	-	-		
84	OHX	1	3717	-	0,6,6	-	-	-		
84	OHX	AR	3434	-	0,6,6	-	-	-		
84	OHX	A	1988	-	0,6,6	-	-	-		
84	OHX	A	1914	-	0,6,6	-	-	-		
84	OHX	6	1955	-	0,6,6	-	-	-		
84	OHX	1	3705	-	0,6,6	-	-	-		
84	OHX	6	1983	-	0,6,6	-	-	-		
84	OHX	AR	3443	-	0,6,6	-	-	-		
84	OHX	AR	3703	-	0,6,6	-	-	-		
84	OHX	4	208	-	0,6,6	-	-	-		
84	OHX	AR	3409	-	0,6,6	-	-	-		
84	OHX	A	1968	-	0,6,6	-	-	-		
84	OHX	1	3646	-	0,6,6	-	-	-		
84	OHX	4	211	-	0,6,6	-	-	-		
84	OHX	1	3587	-	0,6,6	-	-	-		
84	OHX	A	1982	-	0,6,6	-	-	-		
84	OHX	AS	210	-	0,6,6	-	-	-		
84	OHX	AT	220	-	0,6,6	-	-	-		
84	OHX	1	3586	-	0,6,6	-	-	-		
84	OHX	AR	3456	-	0,6,6	-	-	-		
84	OHX	6	2032	-	0,6,6	-	-	-		
84	OHX	6	1953	-	0,6,6	-	-	-		
84	OHX	1	3425	-	0,6,6	-	-	-		
84	OHX	1	3424	-	0,6,6	-	-	-		
84	OHX	1	3703	-	0,6,6	-	-	-		
84	OHX	AR	3480	-	0,6,6	-	-	-		
84	OHX	H	301	-	0,6,6	-	-	-		
84	OHX	AR	3714	-	0,6,6	-	-	-		
84	OHX	6	1923	-	0,6,6	-	-	-		
84	OHX	1	3526	-	0,6,6	-	-	-		
84	OHX	1	3552	-	0,6,6	-	-	-		
84	OHX	3	206	-	0,6,6	-	-	-		
84	OHX	AR	3608	-	0,6,6	-	-	-		
84	OHX	AR	3736	-	0,6,6	-	-	-		
84	OHX	1	3439	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AR	3653	-	0,6,6	-	-	-		
84	OHX	CG	303	-	0,6,6	-	-	-		
84	OHX	1	3435	-	0,6,6	-	-	-		
84	OHX	A	1978	-	0,6,6	-	-	-		
84	OHX	1	3592	-	0,6,6	-	-	-		
84	OHX	6	2023	-	0,6,6	-	-	-		
84	OHX	AR	3601	-	0,6,6	-	-	-		
84	OHX	A	1961	-	0,6,6	-	-	-		
84	OHX	AR	3465	-	0,6,6	-	-	-		
84	OHX	1	3684	-	0,6,6	-	-	-		
84	OHX	CE	402	-	0,6,6	-	-	-		
84	OHX	1	3449	-	0,6,6	-	-	-		
84	OHX	6	1904	-	0,6,6	-	-	-		
84	OHX	6	2011	-	0,6,6	-	-	-		
84	OHX	AR	3720	-	0,6,6	-	-	-		
84	OHX	A	1994	-	0,6,6	-	-	-		
84	OHX	1	3716	-	0,6,6	-	-	-		
84	OHX	4	212	-	0,6,6	-	-	-		
84	OHX	AR	3666	-	0,6,6	-	-	-		
84	OHX	AR	3667	-	0,6,6	-	-	-		
84	OHX	AR	3732	-	0,6,6	-	-	-		
84	OHX	DD	102	-	0,6,6	-	-	-		
84	OHX	AR	3559	-	0,6,6	-	-	-		
84	OHX	6	1918	-	0,6,6	-	-	-		
84	OHX	AR	3633	-	0,6,6	-	-	-		
84	OHX	A	1910	-	0,6,6	-	-	-		
84	OHX	AR	3453	-	0,6,6	-	-	-		
84	OHX	AR	3438	-	0,6,6	-	-	-		
84	OHX	A	1925	-	0,6,6	-	-	-		
84	OHX	1	3607	-	0,6,6	-	-	-		
84	OHX	1	3647	-	0,6,6	-	-	-		
84	OHX	6	1934	-	0,6,6	-	-	-		
84	OHX	CG	302	-	0,6,6	-	-	-		
84	OHX	1	3457	-	0,6,6	-	-	-		
84	OHX	AR	3432	-	0,6,6	-	-	-		
84	OHX	AR	3494	-	0,6,6	-	-	-		
84	OHX	1	3609	-	0,6,6	-	-	-		
84	OHX	AR	3478	-	0,6,6	-	-	-		
84	OHX	AR	3546	-	0,6,6	-	-	-		
84	OHX	AR	3696	-	0,6,6	-	-	-		
84	OHX	1	3477	-	0,6,6	-	-	-		
84	OHX	1	3500	-	0,6,6	-	-	-		
84	OHX	1	3571	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3602	-	0,6,6	-	-	-		
84	OHX	AR	3538	-	0,6,6	-	-	-		
84	OHX	AR	3652	-	0,6,6	-	-	-		
84	OHX	AR	3617	-	0,6,6	-	-	-		
84	OHX	AR	3701	-	0,6,6	-	-	-		
84	OHX	AR	3625	-	0,6,6	-	-	-		
84	OHX	AS	207	-	0,6,6	-	-	-		
84	OHX	1	3642	-	0,6,6	-	-	-		
84	OHX	6	1926	-	0,6,6	-	-	-		
84	OHX	AR	3467	-	0,6,6	-	-	-		
84	OHX	AR	3650	-	0,6,6	-	-	-		
84	OHX	CF	402	-	0,6,6	-	-	-		
84	OHX	AR	3645	-	0,6,6	-	-	-		
84	OHX	AR	3419	-	0,6,6	-	-	-		
84	OHX	1	3464	-	0,6,6	-	-	-		
84	OHX	1	3561	-	0,6,6	-	-	-		
84	OHX	c8	201	-	0,6,6	-	-	-		
84	OHX	1	3614	-	0,6,6	-	-	-		
84	OHX	6	1912	-	0,6,6	-	-	-		
84	OHX	A	1939	-	0,6,6	-	-	-		
84	OHX	1	3636	-	0,6,6	-	-	-		
84	OHX	1	3567	-	0,6,6	-	-	-		
84	OHX	6	2037	-	0,6,6	-	-	-		
84	OHX	1	3681	-	0,6,6	-	-	-		
84	OHX	AR	3557	-	0,6,6	-	-	-		
84	OHX	AR	3649	-	0,6,6	-	-	-		
84	OHX	6	1943	-	0,6,6	-	-	-		
84	OHX	1	3527	-	0,6,6	-	-	-		
84	OHX	6	1987	-	0,6,6	-	-	-		
84	OHX	6	2000	-	0,6,6	-	-	-		
84	OHX	AR	3590	-	0,6,6	-	-	-		
84	OHX	1	3441	-	0,6,6	-	-	-		
84	OHX	6	2008	-	0,6,6	-	-	-		
84	OHX	6	1903	-	0,6,6	-	-	-		
84	OHX	6	1946	-	0,6,6	-	-	-		
84	OHX	AR	3475	-	0,6,6	-	-	-		
84	OHX	AR	3593	-	0,6,6	-	-	-		
84	OHX	Q	201	-	0,6,6	-	-	-		
84	OHX	6	1907	-	0,6,6	-	-	-		
84	OHX	A	2028	-	0,6,6	-	-	-		
84	OHX	1	3564	-	0,6,6	-	-	-		
84	OHX	1	3622	-	0,6,6	-	-	-		
84	OHX	AR	3562	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	A	1967	-	0,6,6	-	-	-		
84	OHX	AR	3731	-	0,6,6	-	-	-		
84	OHX	A	1979	-	0,6,6	-	-	-		
84	OHX	AR	3669	-	0,6,6	-	-	-		
84	OHX	6	2006	-	0,6,6	-	-	-		
84	OHX	AR	3670	-	0,6,6	-	-	-		
84	OHX	A	1919	-	0,6,6	-	-	-		
84	OHX	6	2002	-	0,6,6	-	-	-		
84	OHX	A	1927	-	0,6,6	-	-	-		
84	OHX	AR	3407	-	0,6,6	-	-	-		
84	OHX	AR	3692	-	0,6,6	-	-	-		
84	OHX	1	3563	-	0,6,6	-	-	-		
84	OHX	1	3668	-	0,6,6	-	-	-		
84	OHX	AR	3515	-	0,6,6	-	-	-		
84	OHX	AR	3472	-	0,6,6	-	-	-		
84	OHX	6	1921	-	0,6,6	-	-	-		
84	OHX	1	3537	-	0,6,6	-	-	-		
84	OHX	3	202	-	0,6,6	-	-	-		
84	OHX	1	3711	-	0,6,6	-	-	-		
84	OHX	6	1910	-	0,6,6	-	-	-		
84	OHX	T	201	-	0,6,6	-	-	-		
84	OHX	A	1942	-	0,6,6	-	-	-		
84	OHX	1	3444	-	0,6,6	-	-	-		
84	OHX	AR	3693	-	0,6,6	-	-	-		
84	OHX	A	1902	-	0,6,6	-	-	-		
84	OHX	6	1951	-	0,6,6	-	-	-		
84	OHX	y	201	-	0,6,6	-	-	-		
84	OHX	x	201	-	0,6,6	-	-	-		
84	OHX	1	3509	-	0,6,6	-	-	-		
84	OHX	1	3486	-	0,6,6	-	-	-		
84	OHX	6	2047	-	0,6,6	-	-	-		
84	OHX	sR	401	-	0,6,6	-	-	-		
84	OHX	AR	3570	-	0,6,6	-	-	-		
84	OHX	6	1981	-	0,6,6	-	-	-		
84	OHX	AR	3539	-	0,6,6	-	-	-		
84	OHX	3	205	-	0,6,6	-	-	-		
84	OHX	A	1918	-	0,6,6	-	-	-		
84	OHX	AR	3598	-	0,6,6	-	-	-		
84	OHX	1	3576	-	0,6,6	-	-	-		
84	OHX	1	3700	-	0,6,6	-	-	-		
84	OHX	AR	3525	-	0,6,6	-	-	-		
84	OHX	1	3445	-	0,6,6	-	-	-		
84	OHX	1	3721	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AR	3634	-	0,6,6	-	-	-		
84	OHX	A	1977	-	0,6,6	-	-	-		
84	OHX	AR	3661	-	0,6,6	-	-	-		
84	OHX	A	1992	-	0,6,6	-	-	-		
84	OHX	1	3405	-	0,6,6	-	-	-		
84	OHX	AR	3641	-	0,6,6	-	-	-		
84	OHX	AR	3583	-	0,6,6	-	-	-		
84	OHX	CM	201	-	0,6,6	-	-	-		
84	OHX	1	3407	-	0,6,6	-	-	-		
84	OHX	AR	3568	-	0,6,6	-	-	-		
84	OHX	AR	3403	-	0,6,6	-	-	-		
84	OHX	A	2003	-	0,6,6	-	-	-		
84	OHX	A	1984	-	0,6,6	-	-	-		
84	OHX	1	3710	-	0,6,6	-	-	-		
84	OHX	1	3729	-	0,6,6	-	-	-		
84	OHX	A	2032	-	0,6,6	-	-	-		
84	OHX	1	3478	-	0,6,6	-	-	-		
84	OHX	1	3701	-	0,6,6	-	-	-		
84	OHX	1	3523	-	0,6,6	-	-	-		
84	OHX	1	3467	-	0,6,6	-	-	-		
84	OHX	6	1966	-	0,6,6	-	-	-		
84	OHX	1	3455	-	0,6,6	-	-	-		
84	OHX	1	3454	-	0,6,6	-	-	-		
84	OHX	1	3698	-	0,6,6	-	-	-		
84	OHX	1	3626	-	0,6,6	-	-	-		
84	OHX	6	2045	-	0,6,6	-	-	-		
84	OHX	1	3653	-	0,6,6	-	-	-		
84	OHX	AR	3429	-	0,6,6	-	-	-		
84	OHX	1	401	-	0,6,6	-	-	-		
84	OHX	1	3528	-	0,6,6	-	-	-		
84	OHX	6	1956	-	0,6,6	-	-	-		
84	OHX	AR	3594	-	0,6,6	-	-	-		
84	OHX	AR	3404	-	0,6,6	-	-	-		
84	OHX	AR	3607	-	0,6,6	-	-	-		
84	OHX	A	1923	-	0,6,6	-	-	-		
84	OHX	A	1959	-	0,6,6	-	-	-		
84	OHX	A	2005	-	0,6,6	-	-	-		
84	OHX	6	2043	-	0,6,6	-	-	-		
84	OHX	AR	3406	-	0,6,6	-	-	-		
84	OHX	6	1954	-	0,6,6	-	-	-		
84	OHX	AR	3695	-	0,6,6	-	-	-		
84	OHX	1	3611	-	0,6,6	-	-	-		
84	OHX	AR	3433	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3508	-	0,6,6	-	-	-		
84	OHX	1	3554	-	0,6,6	-	-	-		
84	OHX	AR	3702	-	0,6,6	-	-	-		
84	OHX	A	1956	-	0,6,6	-	-	-		
84	OHX	AR	3734	-	0,6,6	-	-	-		
84	OHX	1	3600	-	0,6,6	-	-	-		
84	OHX	1	3694	-	0,6,6	-	-	-		
84	OHX	AT	211	-	0,6,6	-	-	-		
84	OHX	1	3573	-	0,6,6	-	-	-		
84	OHX	1	3659	-	0,6,6	-	-	-		
84	OHX	6	2054	-	0,6,6	-	-	-		
84	OHX	4	203	-	0,6,6	-	-	-		
84	OHX	AR	3665	-	0,6,6	-	-	-		
84	OHX	AT	207	-	0,6,6	-	-	-		
84	OHX	1	3731	-	0,6,6	-	-	-		
84	OHX	6	1902	-	0,6,6	-	-	-		
84	OHX	1	3512	-	0,6,6	-	-	-		
84	OHX	AR	3564	-	0,6,6	-	-	-		
84	OHX	1	3479	-	0,6,6	-	-	-		
84	OHX	6	2044	-	0,6,6	-	-	-		
84	OHX	6	1990	-	0,6,6	-	-	-		
84	OHX	1	3414	-	0,6,6	-	-	-		
84	OHX	1	3619	-	0,6,6	-	-	-		
84	OHX	AR	3599	-	0,6,6	-	-	-		
84	OHX	1	3529	-	0,6,6	-	-	-		
84	OHX	AR	3717	-	0,6,6	-	-	-		
84	OHX	6	2007	-	0,6,6	-	-	-		
84	OHX	1	3484	-	0,6,6	-	-	-		
84	OHX	6	1937	-	0,6,6	-	-	-		
84	OHX	6	1917	-	0,6,6	-	-	-		
84	OHX	1	3658	-	0,6,6	-	-	-		
84	OHX	AT	209	-	0,6,6	-	-	-		
84	OHX	AR	3697	-	0,6,6	-	-	-		
84	OHX	1	3411	-	0,6,6	-	-	-		
84	OHX	1	3686	-	0,6,6	-	-	-		
84	OHX	AR	3588	-	0,6,6	-	-	-		
84	OHX	6	2050	-	0,6,6	-	-	-		
84	OHX	1	3683	-	0,6,6	-	-	-		
84	OHX	1	3693	-	0,6,6	-	-	-		
84	OHX	1	3458	-	0,6,6	-	-	-		
84	OHX	1	3551	-	0,6,6	-	-	-		
84	OHX	AR	3481	-	0,6,6	-	-	-		
84	OHX	x	202	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3588	-	0,6,6	-	-	-		
84	OHX	AR	3542	-	0,6,6	-	-	-		
84	OHX	CP	501	-	0,6,6	-	-	-		
84	OHX	A	1912	-	0,6,6	-	-	-		
84	OHX	AR	3449	-	0,6,6	-	-	-		
84	OHX	A	2004	-	0,6,6	-	-	-		
84	OHX	c5	201	-	0,6,6	-	-	-		
84	OHX	AR	3532	-	0,6,6	-	-	-		
84	OHX	1	3474	-	0,6,6	-	-	-		
84	OHX	1	3629	-	0,6,6	-	-	-		
84	OHX	1	3536	-	0,6,6	-	-	-		
84	OHX	1	3579	-	0,6,6	-	-	-		
84	OHX	6	1969	-	0,6,6	-	-	-		
84	OHX	6	2030	-	0,6,6	-	-	-		
84	OHX	AR	3511	-	0,6,6	-	-	-		
84	OHX	1	3517	-	0,6,6	-	-	-		
84	OHX	6	1989	-	0,6,6	-	-	-		
84	OHX	6	1947	-	0,6,6	-	-	-		
84	OHX	1	3428	-	0,6,6	-	-	-		
84	OHX	6	2010	-	0,6,6	-	-	-		
84	OHX	6	2027	-	0,6,6	-	-	-		
84	OHX	AR	3427	-	0,6,6	-	-	-		
84	OHX	1	3673	-	0,6,6	-	-	-		
84	OHX	AR	3575	-	0,6,6	-	-	-		
84	OHX	AR	3691	-	0,6,6	-	-	-		
84	OHX	A	1972	-	0,6,6	-	-	-		
84	OHX	1	3410	-	0,6,6	-	-	-		
84	OHX	6	2016	-	0,6,6	-	-	-		
84	OHX	AT	219	-	0,6,6	-	-	-		
84	OHX	1	3535	-	0,6,6	-	-	-		
86	7MB	AR	4239	-	16,23,23	0.85	0	8,38,38	0.87	0
84	OHX	1	3495	-	0,6,6	-	-	-		
84	OHX	AR	3606	-	0,6,6	-	-	-		
84	OHX	1	3677	-	0,6,6	-	-	-		
84	OHX	1	3596	-	0,6,6	-	-	-		
84	OHX	AR	3651	-	0,6,6	-	-	-		
84	OHX	A	1908	-	0,6,6	-	-	-		
84	OHX	AR	3637	-	0,6,6	-	-	-		
84	OHX	6	1944	-	0,6,6	-	-	-		
84	OHX	AR	3514	-	0,6,6	-	-	-		
84	OHX	AR	3547	-	0,6,6	-	-	-		
84	OHX	A	1980	-	0,6,6	-	-	-		
84	OHX	A	1965	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AR	3654	-	0,6,6	-	-	-		
84	OHX	AR	3719	-	0,6,6	-	-	-		
84	OHX	6	2022	-	0,6,6	-	-	-		
84	OHX	A	1907	-	0,6,6	-	-	-		
84	OHX	1	3518	-	0,6,6	-	-	-		
84	OHX	6	2035	-	0,6,6	-	-	-		
84	OHX	1	3436	-	0,6,6	-	-	-		
84	OHX	6	2052	-	0,6,6	-	-	-		
84	OHX	1	3709	-	0,6,6	-	-	-		
84	OHX	AR	3503	-	0,6,6	-	-	-		
84	OHX	A	1911	-	0,6,6	-	-	-		
84	OHX	6	1972	-	0,6,6	-	-	-		
84	OHX	AR	3430	-	0,6,6	-	-	-		
84	OHX	AR	3490	-	0,6,6	-	-	-		
84	OHX	1	3491	-	0,6,6	-	-	-		
84	OHX	AR	3440	-	0,6,6	-	-	-		
84	OHX	AR	3505	-	0,6,6	-	-	-		
84	OHX	6	1995	-	0,6,6	-	-	-		
84	OHX	1	3548	-	0,6,6	-	-	-		
84	OHX	6	1968	-	0,6,6	-	-	-		
84	OHX	1	3613	-	0,6,6	-	-	-		
84	OHX	A	2002	-	0,6,6	-	-	-		
84	OHX	1	3515	-	0,6,6	-	-	-		
84	OHX	1	3524	-	0,6,6	-	-	-		
84	OHX	AR	3454	-	0,6,6	-	-	-		
84	OHX	AR	3476	-	0,6,6	-	-	-		
84	OHX	AR	3739	-	0,6,6	-	-	-		
84	OHX	1	3637	-	0,6,6	-	-	-		
84	OHX	1	3652	-	0,6,6	-	-	-		
84	OHX	AS	202	-	0,6,6	-	-	-		
84	OHX	AR	3698	-	0,6,6	-	-	-		
84	OHX	A	1940	-	0,6,6	-	-	-		
84	OHX	1	3687	-	0,6,6	-	-	-		
84	OHX	1	3616	-	0,6,6	-	-	-		
84	OHX	1	3448	-	0,6,6	-	-	-		
84	OHX	AR	3597	-	0,6,6	-	-	-		
84	OHX	6	1941	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	7MB	AR	4239	-	-	-	0/3/4/4
86	7MB	1	4216	-	-	-	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(^{o})	Ideal(^{o})
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.

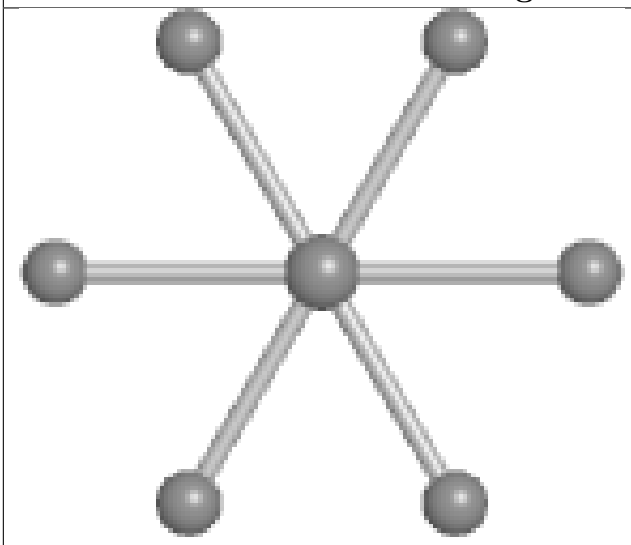
There are no torsion outliers.

There are no ring outliers.

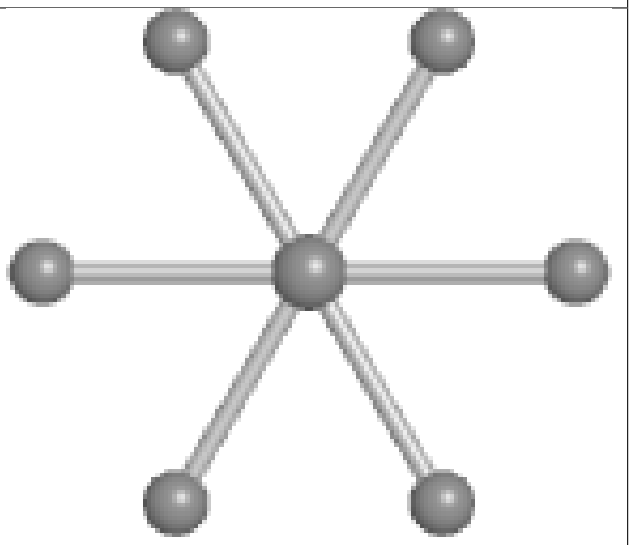
No monomer is involved in short contacts.

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

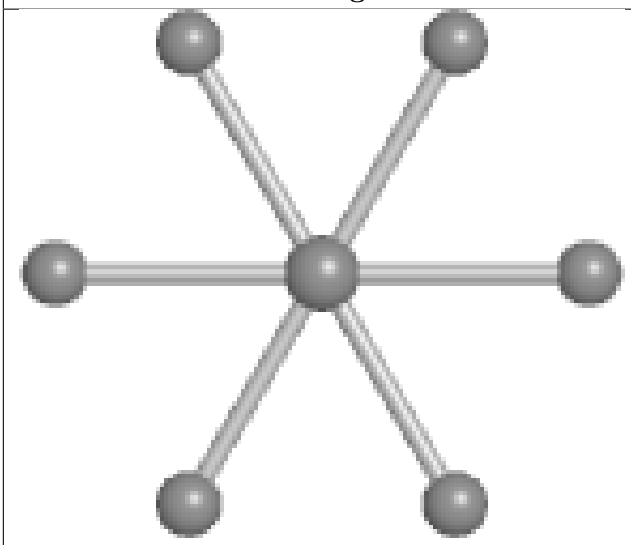
Ligand OHX 1 3722



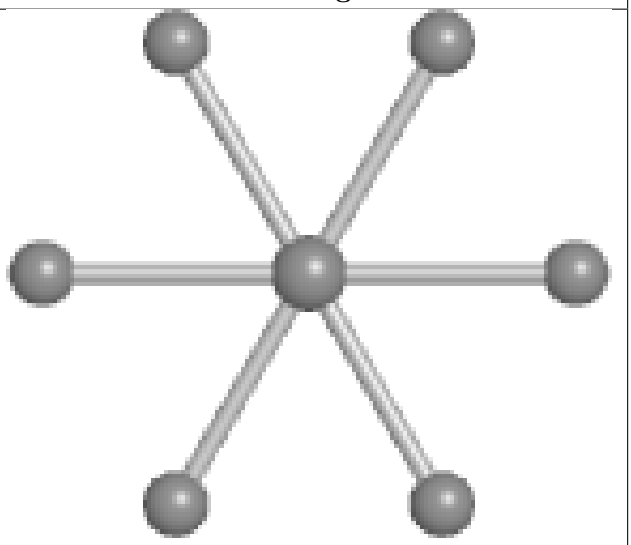
Bond lengths



Bond angles

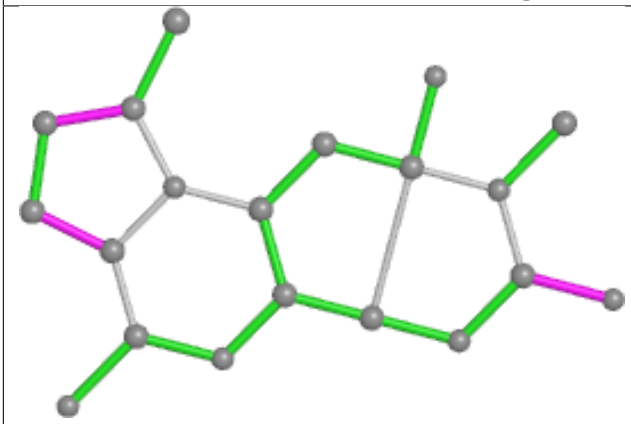


Torsions

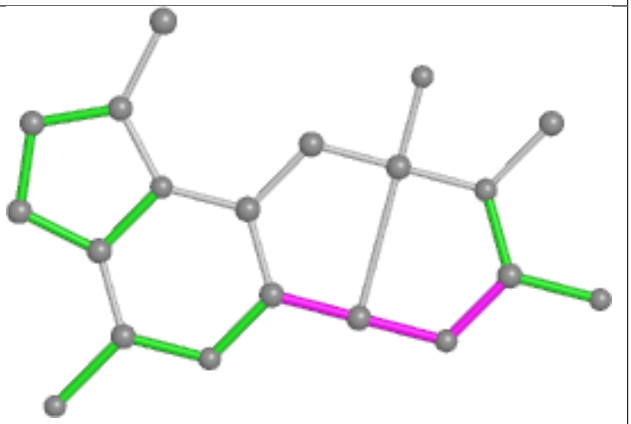


Rings

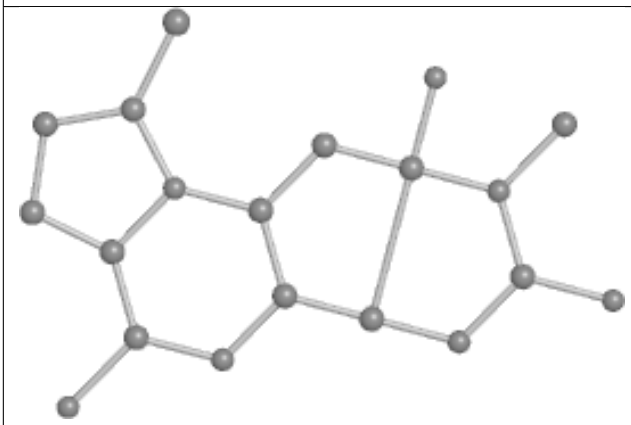
Ligand 7MB 1 4216



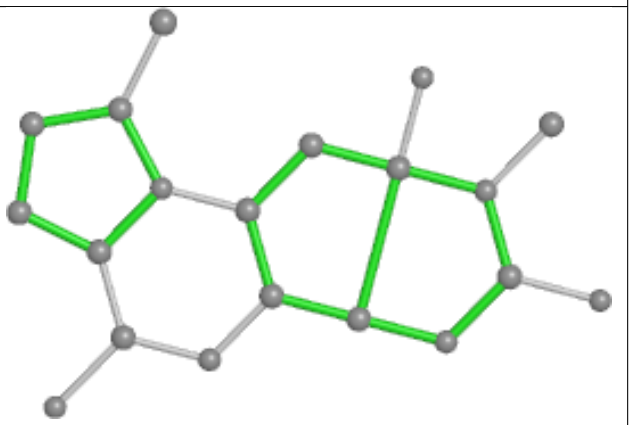
Bond lengths



Bond angles

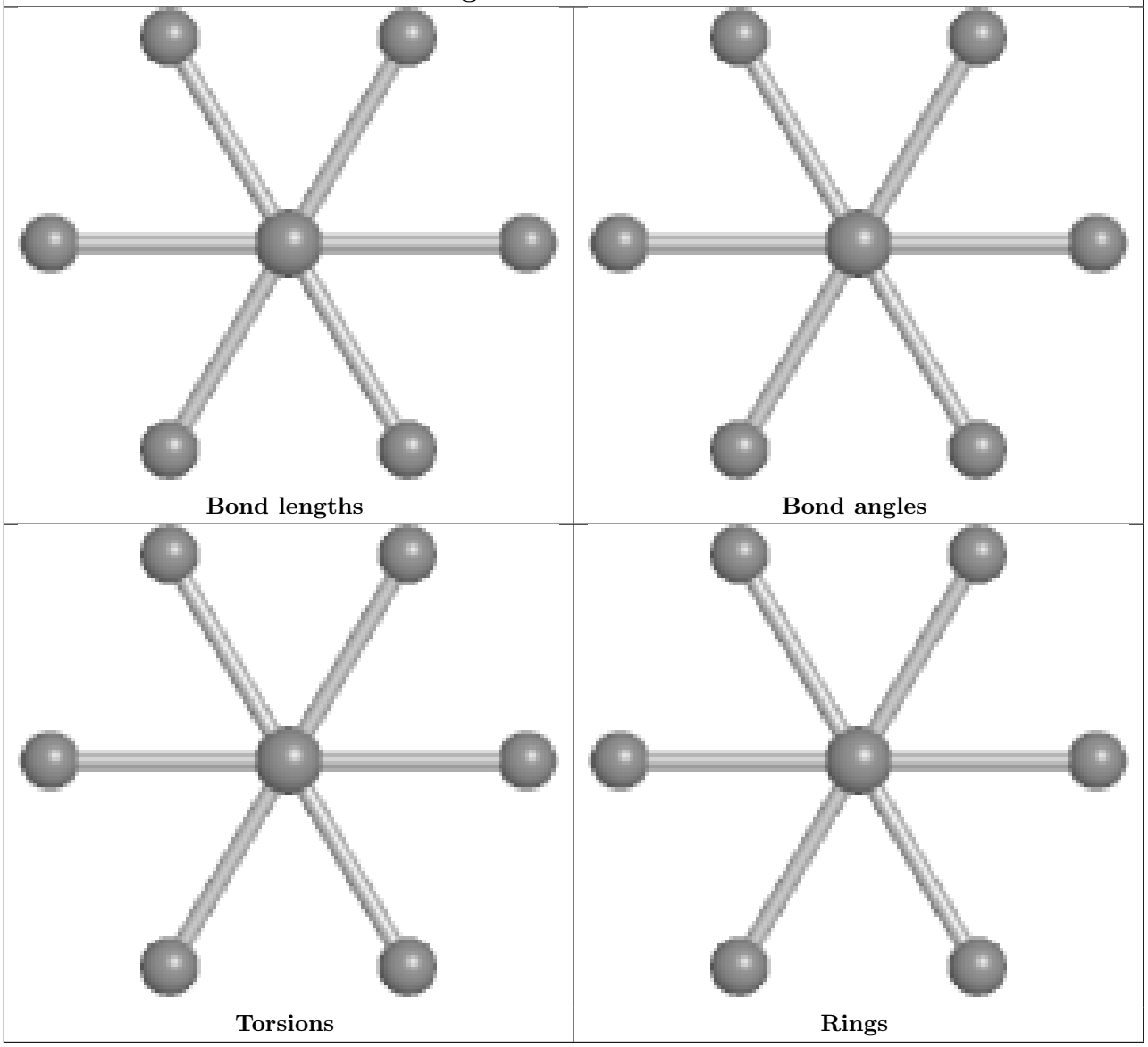


Torsions



Rings

Ligand OHX 1 3675



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, 95^{th} 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, 58, 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, 160	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, 40, 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, 84	0
19	y	185/185 (100%)	-0.43	0 100 100	36, 48, 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	66, 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, 80, 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, 58, 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, 188, 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 (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	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	6	2148	1/1	0.59	0.21	69,69,69,69	0
85	MG	1	3968	1/1	0.59	0.28	50,50,50,50	0
85	MG	CK	202	1/1	0.59	0.64	52,52,52,52	0
85	MG	A	2046	1/1	0.59	0.20	56,56,56,56	0
85	MG	A	2110	1/1	0.59	0.39	108,108,108,108	0
85	MG	AR	3746	1/1	0.59	0.29	39,39,39,39	0
85	MG	1	4107	1/1	0.60	0.28	66,66,66,66	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	A	2112	1/1	0.61	0.41	77,77,77,77	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	6	2190	1/1	0.67	0.41	84,84,84,84	0
85	MG	CO	202	1/1	0.67	0.78	57,57,57,57	0
85	MG	1	4124	1/1	0.67	0.22	52,52,52,52	0
85	MG	AS	228	1/1	0.67	0.25	48,48,48,48	0
85	MG	AR	4167	1/1	0.68	0.51	72,72,72,72	0
85	MG	A	2075	1/1	0.68	0.37	48,48,48,48	0
85	MG	DR	503	1/1	0.69	0.33	54,54,54,54	0
85	MG	6	2139	1/1	0.69	0.31	75,75,75,75	0
85	MG	AR	3813	1/1	0.69	0.33	54,54,54,54	0
85	MG	AR	4217	1/1	0.69	0.24	65,65,65,65	0
85	MG	AR	3826	1/1	0.69	0.61	42,42,42,42	0
85	MG	1	4162	1/1	0.69	0.28	118,118,118,118	0
85	MG	AR	3965	1/1	0.69	0.32	54,54,54,54	0
85	MG	AR	4151	1/1	0.69	0.28	30,30,30,30	0
85	MG	A	2129	1/1	0.69	0.45	58,58,58,58	0
85	MG	AR	4101	1/1	0.70	0.45	48,48,48,48	0
85	MG	1	4092	1/1	0.70	0.16	53,53,53,53	0
84	OHX	AR	3720	7/7	0.70	0.34	267,269,269,270	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	4073	1/1	0.70	0.30	79,79,79,79	0
85	MG	1	4129	1/1	0.70	0.38	51,51,51,51	0
85	MG	1	4140	1/1	0.70	0.48	49,49,49,49	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	3759	1/1	0.71	0.34	69,69,69,69	0
85	MG	1	3801	1/1	0.71	0.52	38,38,38,38	0
85	MG	AT	223	1/1	0.71	0.91	55,55,55,55	0
85	MG	AR	3971	1/1	0.71	0.35	38,38,38,38	0
85	MG	A	2084	1/1	0.72	0.16	53,53,53,53	0
85	MG	1	4135	1/1	0.72	0.33	64,64,64,64	0
85	MG	AR	3804	1/1	0.72	0.45	36,36,36,36	0
85	MG	1	4102	1/1	0.72	0.39	40,40,40,40	0
85	MG	AR	4024	1/1	0.72	0.42	33,33,33,33	0
84	OHX	CZ	201	7/7	0.72	0.34	303,304,305,305	0
85	MG	1	4131	1/1	0.72	0.33	38,38,38,38	0
85	MG	A	2139	1/1	0.72	0.33	86,86,86,86	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	A	2089	1/1	0.73	0.48	65,65,65,65	0
85	MG	6	2174	1/1	0.73	0.25	66,66,66,66	0
85	MG	AR	4147	1/1	0.73	0.21	62,62,62,62	0
85	MG	AR	3893	1/1	0.73	0.58	40,40,40,40	0
85	MG	1	4008	1/1	0.73	1.06	76,76,76,76	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	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
84	OHX	AR	3664	7/7	0.74	0.30	287,287,288,288	0
85	MG	1	3736	1/1	0.74	0.16	82,82,82,82	0
85	MG	6	2195	1/1	0.74	0.37	64,64,64,64	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	1	4027	1/1	0.74	0.35	51,51,51,51	0
85	MG	AR	4202	1/1	0.74	0.50	72,72,72,72	0
85	MG	1	4136	1/1	0.75	0.38	49,49,49,49	0
84	OHX	1	3722	7/7	0.75	0.44	268,268,269,269	0
85	MG	AR	4122	1/1	0.75	0.42	70,70,70,70	0
84	OHX	1	3694	7/7	0.75	0.29	251,252,254,254	0
84	OHX	1	3699	7/7	0.75	0.23	304,306,307,308	0
85	MG	1	3955	1/1	0.75	0.28	52,52,52,52	0
85	MG	AR	3996	1/1	0.76	0.33	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	3820	1/1	0.76	0.64	55,55,55,55	0
85	MG	6	2170	1/1	0.76	0.45	46,46,46,46	0
85	MG	1	3789	1/1	0.76	0.70	51,51,51,51	0
84	OHX	AR	3718	7/7	0.76	0.33	255,256,257,257	0
85	MG	1	4183	1/1	0.76	0.47	41,41,41,41	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	c9	201	1/1	0.76	0.11	73,73,73,73	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	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	AR	3880	1/1	0.77	0.43	20,20,20,20	0
85	MG	A	2127	1/1	0.77	0.30	55,55,55,55	0
85	MG	1	3949	1/1	0.77	0.44	41,41,41,41	0
85	MG	1	4206	1/1	0.77	0.46	28,28,28,28	0
85	MG	1	3758	1/1	0.77	0.46	31,31,31,31	0
85	MG	6	2168	1/1	0.77	0.40	50,50,50,50	0
85	MG	6	2065	1/1	0.77	0.46	32,32,32,32	0
85	MG	1	4095	1/1	0.78	0.37	53,53,53,53	0
85	MG	A	2098	1/1	0.78	0.44	72,72,72,72	0
85	MG	1	3830	1/1	0.78	0.56	60,60,60,60	0
85	MG	AR	4026	1/1	0.78	0.21	62,62,62,62	0
85	MG	3	218	1/1	0.78	0.31	49,49,49,49	0
85	MG	AR	4059	1/1	0.78	0.15	67,67,67,67	0
84	OHX	AR	3687	7/7	0.78	0.37	244,245,246,247	0
85	MG	AR	4193	1/1	0.78	0.55	62,62,62,62	0
85	MG	1	4014	1/1	0.78	0.16	46,46,46,46	0
85	MG	AR	4214	1/1	0.78	0.42	61,61,61,61	0
85	MG	6	2075	1/1	0.78	0.39	49,49,49,49	0
85	MG	AR	4220	1/1	0.78	0.38	54,54,54,54	0
85	MG	F	301	1/1	0.78	0.34	71,71,71,71	0
85	MG	AR	4128	1/1	0.78	0.17	54,54,54,54	0
84	OHX	6	2028	7/7	0.79	0.29	248,250,252,252	0
85	MG	A	2109	1/1	0.79	0.31	50,50,50,50	0
85	MG	1	4063	1/1	0.79	0.59	55,55,55,55	0
84	OHX	AS	210	7/7	0.79	0.33	235,237,238,238	0
85	MG	AH	201	1/1	0.79	0.32	60,60,60,60	0
85	MG	4	217	1/1	0.79	0.48	44,44,44,44	0
84	OHX	1	3675	7/7	0.79	0.57	229,229,230,230	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	x	203	1/1	0.79	0.26	64,64,64,64	0
85	MG	A	2137	1/1	0.79	0.34	40,40,40,40	0
85	MG	AR	4152	1/1	0.79	0.16	152,152,152,152	0
84	OHX	A	1985	7/7	0.79	0.36	221,222,223,224	0
85	MG	6	2071	1/1	0.79	0.20	73,73,73,73	0
85	MG	1	3976	1/1	0.79	0.35	61,61,61,61	0
87	ZN	c	101	1/1	0.79	0.22	197,197,197,197	0
85	MG	AR	4025	1/1	0.80	0.22	40,40,40,40	0
84	OHX	6	2051	7/7	0.80	0.36	228,229,230,231	0
84	OHX	AR	3716	7/7	0.80	0.35	292,293,293,294	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
85	MG	A	2124	1/1	0.80	0.74	57,57,57,57	0
85	MG	AR	3923	1/1	0.80	0.66	32,32,32,32	0
85	MG	AR	4211	1/1	0.80	0.23	86,86,86,86	0
85	MG	6	2081	1/1	0.80	0.31	94,94,94,94	0
84	OHX	AR	3737	7/7	0.80	0.69	260,261,262,262	0
85	MG	6	2179	1/1	0.80	0.30	52,52,52,52	0
85	MG	AR	4233	1/1	0.80	0.40	55,55,55,55	0
85	MG	6	2110	1/1	0.80	0.33	40,40,40,40	0
85	MG	Y	201	1/1	0.80	0.47	51,51,51,51	0
85	MG	AS	216	1/1	0.80	0.68	41,41,41,41	0
85	MG	1	4119	1/1	0.80	0.29	35,35,35,35	0
85	MG	1	3808	1/1	0.81	0.41	54,54,54,54	0
85	MG	AR	4162	1/1	0.81	0.25	54,54,54,54	0
85	MG	AS	229	1/1	0.81	0.29	68,68,68,68	0
84	OHX	1	3693	7/7	0.81	0.45	264,265,266,266	0
85	MG	AT	227	1/1	0.81	0.36	73,73,73,73	0
85	MG	1	4030	1/1	0.81	0.44	45,45,45,45	0
85	MG	AR	4170	1/1	0.81	0.36	128,128,128,128	0
85	MG	AR	3773	1/1	0.81	0.12	113,113,113,113	0
85	MG	AR	4077	1/1	0.81	0.34	49,49,49,49	0
85	MG	AR	4086	1/1	0.81	0.38	28,28,28,28	0
85	MG	6	2182	1/1	0.81	0.28	53,53,53,53	0
84	OHX	CF	401	7/7	0.81	0.27	245,246,247,247	0
85	MG	AR	3990	1/1	0.81	0.41	37,37,37,37	0
85	MG	1	3947	1/1	0.81	0.41	34,34,34,34	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	1	3974	1/1	0.81	0.40	43,43,43,43	0
87	ZN	e1	501	1/1	0.81	0.09	176,176,176,176	0
85	MG	AR	4209	1/1	0.82	0.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	A	2002	7/7	0.82	0.30	242,245,246,247	0
85	MG	AR	4093	1/1	0.82	0.34	46,46,46,46	0
84	OHX	AR	3727	7/7	0.82	0.34	277,279,280,280	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	1	4031	1/1	0.82	0.42	38,38,38,38	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	4040	1/1	0.82	0.53	42,42,42,42	0
85	MG	AS	220	1/1	0.82	0.21	42,42,42,42	0
85	MG	AR	4156	1/1	0.82	0.49	71,71,71,71	0
85	MG	AR	4159	1/1	0.82	0.22	64,64,64,64	0
85	MG	1	4044	1/1	0.82	0.32	40,40,40,40	0
85	MG	AT	226	1/1	0.82	0.34	44,44,44,44	0
85	MG	AR	4050	1/1	0.82	0.28	46,46,46,46	0
85	MG	CI	301	1/1	0.82	0.31	48,48,48,48	0
85	MG	AR	4055	1/1	0.82	0.39	47,47,47,47	0
85	MG	AR	4058	1/1	0.82	0.18	57,57,57,57	0
85	MG	CP	502	1/1	0.82	0.38	25,25,25,25	0
85	MG	D	301	1/1	0.82	0.58	42,42,42,42	0
85	MG	CR	203	1/1	0.82	0.33	74,74,74,74	0
85	MG	1	3864	1/1	0.82	0.50	33,33,33,33	0
85	MG	AR	4071	1/1	0.82	0.37	32,32,32,32	0
84	OHX	AS	208	7/7	0.82	0.30	226,226,228,228	0
85	MG	1	3775	1/1	0.82	0.14	59,59,59,59	0
85	MG	1	3762	1/1	0.83	0.48	40,40,40,40	0
85	MG	AR	4119	1/1	0.83	0.19	77,77,77,77	0
84	OHX	CL	302	7/7	0.83	0.24	200,201,201,202	0
85	MG	s	300	1/1	0.83	0.13	53,53,53,53	0
85	MG	1	4079	1/1	0.83	0.47	47,47,47,47	0
84	OHX	CO	201	7/7	0.83	0.33	281,282,283,284	0
85	MG	1	3978	1/1	0.83	0.30	32,32,32,32	0
85	MG	1	4100	1/1	0.83	0.31	87,87,87,87	0
85	MG	A	2068	1/1	0.83	0.45	68,68,68,68	0
84	OHX	6	1976	7/7	0.83	0.42	182,182,183,184	0
85	MG	6	2085	1/1	0.83	0.42	40,40,40,40	0
85	MG	A	2076	1/1	0.83	0.26	50,50,50,50	0
84	OHX	1	3711	7/7	0.83	0.25	301,302,304,304	0
84	OHX	6	2042	7/7	0.83	0.55	246,246,248,248	0
85	MG	1	4109	1/1	0.83	0.32	37,37,37,37	0
85	MG	1	4113	1/1	0.83	0.65	54,54,54,54	0
85	MG	AR	3976	1/1	0.83	0.40	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	A	2042	7/7	0.83	0.17	240,242,244,245	0
85	MG	1	3840	1/1	0.83	0.18	39,39,39,39	0
85	MG	AR	4021	1/1	0.83	0.33	36,36,36,36	0
84	OHX	1	3707	7/7	0.83	0.25	237,237,239,239	0
85	MG	1	3941	1/1	0.83	0.30	36,36,36,36	0
84	OHX	1	3709	7/7	0.83	0.43	229,231,231,232	0
85	MG	A	2116	1/1	0.83	0.33	49,49,49,49	0
84	OHX	AR	3670	7/7	0.83	0.29	229,230,230,231	0
85	MG	1	4038	1/1	0.83	0.34	33,33,33,33	0
85	MG	A	2125	1/1	0.83	0.54	51,51,51,51	0
85	MG	AR	4223	1/1	0.83	0.35	54,54,54,54	0
84	OHX	1	3726	7/7	0.83	0.42	231,232,233,233	0
85	MG	AR	4056	1/1	0.83	0.29	44,44,44,44	0
85	MG	1	4174	1/1	0.83	0.33	54,54,54,54	0
85	MG	1	4041	1/1	0.83	0.46	38,38,38,38	0
85	MG	1	3963	1/1	0.83	0.16	69,69,69,69	0
85	MG	1	3964	1/1	0.83	0.33	51,51,51,51	0
85	MG	AB	203	1/1	0.83	0.31	37,37,37,37	0
85	MG	1	4070	1/1	0.83	0.29	37,37,37,37	0
84	OHX	4	210	7/7	0.83	0.31	236,236,236,236	0
85	MG	AT	231	1/1	0.83	0.56	46,46,46,46	0
85	MG	CE	406	1/1	0.83	0.59	48,48,48,48	0
85	MG	1	4161	1/1	0.84	0.28	37,37,37,37	0
84	OHX	1	3727	7/7	0.84	0.33	253,254,255,256	0
84	OHX	1	3731	7/7	0.84	0.28	201,202,205,205	0
85	MG	A	2048	1/1	0.84	0.18	42,42,42,42	0
85	MG	AR	4032	1/1	0.84	0.50	47,47,47,47	0
85	MG	AR	4183	1/1	0.84	0.20	93,93,93,93	0
85	MG	AR	3772	1/1	0.84	0.53	81,81,81,81	0
84	OHX	6	2053	7/7	0.84	0.23	250,252,253,254	0
85	MG	AR	3784	1/1	0.84	0.38	29,29,29,29	0
85	MG	AR	3803	1/1	0.84	0.22	54,54,54,54	0
85	MG	A	2088	1/1	0.84	0.27	66,66,66,66	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	1	4184	1/1	0.84	0.23	55,55,55,55	0
85	MG	1	4185	1/1	0.84	0.57	48,48,48,48	0
85	MG	AR	4074	1/1	0.84	0.31	44,44,44,44	0
85	MG	1	4064	1/1	0.84	0.34	59,59,59,59	0
85	MG	AR	4234	1/1	0.84	0.28	17,17,17,17	0
84	OHX	1	3683	7/7	0.84	0.30	197,198,199,199	0
84	OHX	A	2007	7/7	0.84	0.20	275,277,278,279	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4100	1/1	0.84	0.35	67,67,67,67	0
85	MG	AS	221	1/1	0.84	0.20	36,36,36,36	0
85	MG	4	213	1/1	0.84	0.48	34,34,34,34	0
84	OHX	A	2015	7/7	0.84	0.35	248,250,254,254	0
84	OHX	A	2034	7/7	0.84	0.14	277,279,281,282	0
85	MG	AR	4125	1/1	0.84	0.22	62,62,62,62	0
84	OHX	1	3676	7/7	0.84	0.42	223,223,225,225	0
85	MG	1	4085	1/1	0.84	0.28	43,43,43,43	0
85	MG	AR	3986	1/1	0.84	0.86	41,41,41,41	0
85	MG	AR	3988	1/1	0.84	0.31	32,32,32,32	0
84	OHX	6	2025	7/7	0.84	0.20	248,249,250,252	0
84	OHX	1	3703	7/7	0.84	0.58	259,259,260,261	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
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	c5	201	7/7	0.85	0.32	228,229,230,231	0
85	MG	AR	4043	1/1	0.85	0.32	48,48,48,48	0
85	MG	6	2123	1/1	0.85	0.30	60,60,60,60	0
85	MG	6	2134	1/1	0.85	0.21	43,43,43,43	0
85	MG	A	2069	1/1	0.85	0.29	36,36,36,36	0
84	OHX	AR	3669	7/7	0.85	0.16	245,246,247,248	0
84	OHX	6	2054	7/7	0.85	0.24	253,254,256,256	0
85	MG	1	4134	1/1	0.85	0.19	50,50,50,50	0
85	MG	AR	4061	1/1	0.85	0.50	40,40,40,40	0
85	MG	AR	4218	1/1	0.85	0.26	31,31,31,31	0
84	OHX	CG	302	7/7	0.85	0.24	210,211,212,213	0
84	OHX	1	3710	7/7	0.85	0.33	247,248,248,249	0
85	MG	4	222	1/1	0.85	0.44	61,61,61,61	0
85	MG	4	224	1/1	0.85	0.22	51,51,51,51	0
85	MG	AR	3897	1/1	0.85	0.53	18,18,18,18	0
84	OHX	A	2025	7/7	0.85	0.23	249,252,253,253	0
85	MG	AS	214	1/1	0.85	0.26	68,68,68,68	0
85	MG	AR	3950	1/1	0.85	0.25	41,41,41,41	0
84	OHX	AR	3663	7/7	0.85	0.25	208,209,210,210	0
85	MG	t	201	1/1	0.85	0.25	37,37,37,37	0
85	MG	1	4101	1/1	0.85	0.23	37,37,37,37	0
85	MG	x	206	1/1	0.85	0.36	32,32,32,32	0
85	MG	l2	202	1/1	0.85	0.23	48,48,48,48	0
85	MG	AR	4131	1/1	0.85	0.56	59,59,59,59	0
85	MG	6	2194	1/1	0.85	0.44	34,34,34,34	0
84	OHX	6	2045	7/7	0.85	0.39	196,197,198,199	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	4052	1/1	0.85	0.12	48,48,48,48	0
85	MG	AR	4155	1/1	0.85	0.29	27,27,27,27	0
85	MG	1	3950	1/1	0.85	0.11	70,70,70,70	0
85	MG	AR	4015	1/1	0.85	0.35	43,43,43,43	0
85	MG	1	3795	1/1	0.85	0.32	37,37,37,37	0
85	MG	AR	3743	1/1	0.85	0.18	41,41,41,41	0
84	OHX	A	1971	7/7	0.85	0.17	216,218,220,221	0
85	MG	AR	3759	1/1	0.85	0.29	103,103,103,103	0
85	MG	DE	201	1/1	0.85	0.15	55,55,55,55	0
85	MG	1	4017	1/1	0.85	0.21	59,59,59,59	0
85	MG	6	2145	1/1	0.86	0.18	51,51,51,51	0
85	MG	6	2147	1/1	0.86	0.31	75,75,75,75	0
85	MG	1	4150	1/1	0.86	1.01	73,73,73,73	0
85	MG	AR	4012	1/1	0.86	0.24	50,50,50,50	0
84	OHX	6	2027	7/7	0.86	0.32	187,188,189,190	0
84	OHX	AR	3702	7/7	0.86	0.41	218,219,220,220	0
85	MG	6	2167	1/1	0.86	0.42	52,52,52,52	0
85	MG	1	3960	1/1	0.86	0.30	27,27,27,27	0
85	MG	6	2169	1/1	0.86	0.39	39,39,39,39	0
84	OHX	1	3600	7/7	0.86	0.46	258,258,259,259	0
85	MG	1	4177	1/1	0.86	0.20	45,45,45,45	0
85	MG	1	4180	1/1	0.86	0.45	55,55,55,55	0
84	OHX	AR	3717	7/7	0.86	0.32	281,282,283,283	0
84	OHX	6	2055	7/7	0.86	0.18	234,235,236,236	0
85	MG	1	3786	1/1	0.86	0.42	37,37,37,37	0
84	OHX	6	2029	7/7	0.86	0.45	246,248,249,250	0
84	OHX	1	3658	7/7	0.86	0.22	211,212,212,213	0
85	MG	1	4194	1/1	0.86	0.23	82,82,82,82	0
85	MG	AR	4062	1/1	0.86	0.20	54,54,54,54	0
84	OHX	6	2043	7/7	0.86	0.32	196,196,198,198	0
85	MG	DA	201	1/1	0.86	0.20	29,29,29,29	0
85	MG	3	213	1/1	0.86	0.51	23,23,23,23	0
84	OHX	AR	3732	7/7	0.86	0.53	245,246,247,247	0
85	MG	DO	202	1/1	0.86	0.27	46,46,46,46	0
85	MG	1	3983	1/1	0.86	0.38	59,59,59,59	0
85	MG	1	4096	1/1	0.86	0.57	53,53,53,53	0
85	MG	1	3984	1/1	0.86	0.30	33,33,33,33	0
85	MG	1	3821	1/1	0.86	0.56	37,37,37,37	0
85	MG	A	2065	1/1	0.86	0.34	31,31,31,31	0
85	MG	4	233	1/1	0.86	0.61	61,61,61,61	0
85	MG	1	4003	1/1	0.86	0.41	46,46,46,46	0
84	OHX	AR	3735	7/7	0.86	0.31	246,247,248,248	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	3801	1/1	0.86	0.35	30,30,30,30	0
84	OHX	A	2029	7/7	0.86	0.14	261,263,265,265	0
84	OHX	6	2023	7/7	0.86	0.27	201,203,204,205	0
85	MG	AR	4135	1/1	0.86	0.54	66,66,66,66	0
85	MG	AR	3808	1/1	0.86	0.23	33,33,33,33	0
85	MG	1	4111	1/1	0.86	0.65	62,62,62,62	0
85	MG	z	202	1/1	0.86	0.24	62,62,62,62	0
85	MG	AR	3815	1/1	0.86	0.18	75,75,75,75	0
85	MG	1	4112	1/1	0.86	0.28	41,41,41,41	0
85	MG	1	3853	1/1	0.86	0.51	61,61,61,61	0
85	MG	AR	3849	1/1	0.86	0.59	18,18,18,18	0
84	OHX	AR	3738	7/7	0.86	0.24	270,271,272,272	0
85	MG	AR	3888	1/1	0.86	0.46	33,33,33,33	0
85	MG	1	4029	1/1	0.86	0.49	42,42,42,42	0
85	MG	1	3866	1/1	0.86	0.34	46,46,46,46	0
85	MG	AR	4172	1/1	0.86	0.32	25,25,25,25	0
85	MG	AR	3899	1/1	0.86	0.35	46,46,46,46	0
85	MG	1	3887	1/1	0.86	0.12	49,49,49,49	0
85	MG	6	2092	1/1	0.86	0.30	45,45,45,45	0
85	MG	AR	3955	1/1	0.86	0.25	32,32,32,32	0
85	MG	AR	4206	1/1	0.86	0.40	31,31,31,31	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	3939	1/1	0.86	0.32	29,29,29,29	0
85	MG	AR	3968	1/1	0.86	0.33	29,29,29,29	0
84	OHX	4	209	7/7	0.86	0.36	194,194,195,195	0
85	MG	AR	4219	1/1	0.86	0.33	47,47,47,47	0
84	OHX	AR	3671	7/7	0.86	0.27	166,166,167,167	0
84	OHX	AR	3685	7/7	0.86	0.40	187,187,188,188	0
85	MG	6	2142	1/1	0.86	0.10	72,72,72,72	0
84	OHX	AR	3730	7/7	0.87	0.34	271,272,273,273	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
85	MG	A	2054	1/1	0.87	0.21	59,59,59,59	0
85	MG	1	3875	1/1	0.87	0.25	18,18,18,18	0
85	MG	1	3981	1/1	0.87	0.36	59,59,59,59	0
85	MG	AR	3770	1/1	0.87	0.36	36,36,36,36	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	1	4103	1/1	0.87	0.35	60,60,60,60	0
85	MG	AR	3775	1/1	0.87	0.27	16,16,16,16	0
84	OHX	1	3674	7/7	0.87	0.36	212,212,213,213	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3891	1/1	0.87	0.66	16,16,16,16	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
84	OHX	6	2038	7/7	0.87	0.36	213,215,217,217	0
85	MG	z	203	1/1	0.87	0.20	45,45,45,45	0
85	MG	1	4058	1/1	0.87	0.15	37,37,37,37	0
84	OHX	AR	3609	7/7	0.87	0.31	201,201,202,202	0
84	OHX	AR	3641	7/7	0.87	0.40	218,219,219,220	0
84	OHX	AR	3726	7/7	0.87	0.42	220,220,221,221	0
85	MG	AR	4153	1/1	0.87	0.26	52,52,52,52	0
84	OHX	1	3705	7/7	0.87	0.42	222,222,223,223	0
85	MG	1	3749	1/1	0.87	0.35	38,38,38,38	0
85	MG	AR	4029	1/1	0.87	0.35	32,32,32,32	0
85	MG	AR	3834	1/1	0.87	0.18	30,30,30,30	0
85	MG	CF	403	1/1	0.87	0.28	30,30,30,30	0
85	MG	AR	3835	1/1	0.87	0.39	41,41,41,41	0
84	OHX	1	3678	7/7	0.87	0.17	228,228,229,230	0
85	MG	AR	4048	1/1	0.87	0.16	33,33,33,33	0
85	MG	1	3833	1/1	0.87	0.30	41,41,41,41	0
84	OHX	AR	3729	7/7	0.87	0.32	214,215,216,216	0
85	MG	A	2148	1/1	0.87	0.43	103,103,103,103	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	4180	1/1	0.87	0.47	93,93,93,93	0
85	MG	6	2197	1/1	0.87	0.32	57,57,57,57	0
85	MG	1	3761	1/1	0.87	0.42	44,44,44,44	0
85	MG	AF	202	1/1	0.87	0.27	32,32,32,32	0
85	MG	AR	4205	1/1	0.87	0.23	30,30,30,30	0
84	OHX	1	3638	7/7	0.88	0.22	245,246,247,248	0
84	OHX	1	3728	7/7	0.88	0.35	233,233,233,234	0
85	MG	AR	4082	1/1	0.88	0.24	48,48,48,48	0
85	MG	6	2093	1/1	0.88	0.33	47,47,47,47	0
85	MG	AR	3818	1/1	0.88	0.27	45,45,45,45	0
84	OHX	AR	3675	7/7	0.88	0.27	210,211,212,212	0
85	MG	AR	3822	1/1	0.88	0.14	52,52,52,52	0
84	OHX	AR	3734	7/7	0.88	0.29	223,224,224,225	0
85	MG	AR	3832	1/1	0.88	0.18	46,46,46,46	0
84	OHX	A	2031	7/7	0.88	0.23	244,246,248,248	0
85	MG	1	4152	1/1	0.88	0.20	40,40,40,40	0
85	MG	AR	4127	1/1	0.88	0.24	67,67,67,67	0
84	OHX	1	3536	7/7	0.88	0.18	221,221,223,224	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(Å^2)	Q<0.9
84	OHX	A	2036	7/7	0.88	0.12	274,277,278,279	0
84	OHX	A	2039	7/7	0.88	0.28	264,266,268,268	0
85	MG	AR	4146	1/1	0.88	0.41	37,37,37,37	0
84	OHX	A	2040	7/7	0.88	0.24	246,248,249,250	0
84	OHX	1	3666	7/7	0.88	0.39	186,187,188,188	0
84	OHX	AR	3695	7/7	0.88	0.24	225,226,227,227	0
85	MG	1	4179	1/1	0.88	0.15	42,42,42,42	0
85	MG	A	2055	1/1	0.88	0.26	48,48,48,48	0
84	OHX	O	201	7/7	0.88	0.17	249,252,253,253	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	1	3951	1/1	0.88	0.33	43,43,43,43	0
85	MG	AR	3964	1/1	0.88	0.30	28,28,28,28	0
84	OHX	AR	3705	7/7	0.88	0.28	212,213,213,214	0
85	MG	AR	3967	1/1	0.88	0.34	64,64,64,64	0
84	OHX	AR	3711	7/7	0.88	0.20	227,227,228,228	0
85	MG	A	2087	1/1	0.88	0.28	57,57,57,57	0
85	MG	1	3961	1/1	0.88	0.34	26,26,26,26	0
85	MG	1	4199	1/1	0.88	0.62	25,25,25,25	0
85	MG	A	2091	1/1	0.88	0.44	60,60,60,60	0
85	MG	A	2093	1/1	0.88	0.19	93,93,93,93	0
84	OHX	CF	402	7/7	0.88	0.47	254,255,256,256	0
85	MG	1	4217	1/1	0.88	0.29	18,18,18,18	0
85	MG	A	2100	1/1	0.88	0.32	60,60,60,60	0
85	MG	1	4088	1/1	0.88	0.22	28,28,28,28	0
85	MG	1	3751	1/1	0.88	0.16	50,50,50,50	0
84	OHX	AR	3712	7/7	0.88	0.31	183,183,184,184	0
84	OHX	CG	303	7/7	0.88	0.59	212,213,214,214	0
84	OHX	AR	3639	7/7	0.88	0.18	211,212,213,213	0
84	OHX	CM	201	7/7	0.88	0.22	247,248,249,250	0
85	MG	1	3769	1/1	0.88	0.45	61,61,61,61	0
85	MG	1	3774	1/1	0.88	0.21	84,84,84,84	0
85	MG	A	2123	1/1	0.88	0.20	40,40,40,40	0
85	MG	o	303	1/1	0.88	0.21	38,38,38,38	0
85	MG	AR	3740	1/1	0.88	0.45	46,46,46,46	0
84	OHX	AR	3640	7/7	0.88	0.29	197,198,199,199	0
85	MG	1	3779	1/1	0.88	0.31	29,29,29,29	0
84	OHX	6	1960	7/7	0.88	0.21	155,157,157,158	0
85	MG	AR	3762	1/1	0.88	0.19	40,40,40,40	0
85	MG	1	3985	1/1	0.88	0.34	22,22,22,22	0
85	MG	A	2146	1/1	0.88	0.62	29,29,29,29	0
85	MG	AR	3771	1/1	0.88	0.22	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	DL	102	7/7	0.88	0.39	212,212,213,213	0
84	OHX	A	1946	7/7	0.88	0.17	212,214,216,217	0
85	MG	A	2153	1/1	0.88	0.31	66,66,66,66	0
84	OHX	AR	3644	7/7	0.88	0.26	197,197,198,199	0
85	MG	6	2064	1/1	0.88	0.31	62,62,62,62	0
84	OHX	1	3606	7/7	0.88	0.28	193,194,194,195	0
85	MG	b	101	1/1	0.88	0.22	57,57,57,57	0
84	OHX	A	1993	7/7	0.88	0.40	236,237,239,240	0
85	MG	d3	203	1/1	0.88	0.23	29,29,29,29	0
84	OHX	6	1982	7/7	0.88	0.42	171,172,173,174	0
84	OHX	1	3617	7/7	0.88	0.37	201,202,203,204	0
85	MG	4	232	1/1	0.89	0.30	43,43,43,43	0
84	OHX	AR	3646	7/7	0.89	0.30	167,168,169,169	0
84	OHX	x	201	7/7	0.89	0.44	169,169,170,170	0
85	MG	AS	223	1/1	0.89	0.23	59,59,59,59	0
85	MG	AS	224	1/1	0.89	0.26	55,55,55,55	0
85	MG	AR	4042	1/1	0.89	0.26	20,20,20,20	0
84	OHX	x	202	7/7	0.89	0.27	223,224,225,225	0
85	MG	AR	4047	1/1	0.89	0.21	30,30,30,30	0
85	MG	1	3807	1/1	0.89	0.30	37,37,37,37	0
84	OHX	AR	3668	7/7	0.89	0.32	216,216,217,218	0
84	OHX	AR	3733	7/7	0.89	0.52	289,291,292,292	0
85	MG	CD	302	1/1	0.89	0.75	39,39,39,39	0
84	OHX	1	3720	7/7	0.89	0.23	197,197,199,199	0
84	OHX	6	2047	7/7	0.89	0.32	237,239,240,241	0
84	OHX	A	2038	7/7	0.89	0.56	217,217,220,220	0
85	MG	AR	3782	1/1	0.89	0.27	30,30,30,30	0
84	OHX	6	2048	7/7	0.89	0.42	224,224,225,226	0
85	MG	AR	4063	1/1	0.89	0.17	39,39,39,39	0
85	MG	CQ	202	1/1	0.89	0.19	26,26,26,26	0
85	MG	CQ	203	1/1	0.89	0.40	28,28,28,28	0
85	MG	AR	3787	1/1	0.89	0.18	31,31,31,31	0
85	MG	AR	3788	1/1	0.89	0.43	45,45,45,45	0
85	MG	AR	3794	1/1	0.89	0.34	19,19,19,19	0
84	OHX	1	3645	7/7	0.89	0.25	220,221,221,221	0
85	MG	1	4023	1/1	0.89	0.72	44,44,44,44	0
84	OHX	A	2041	7/7	0.89	0.41	201,203,204,204	0
84	OHX	AR	3681	7/7	0.89	0.21	198,199,200,201	0
85	MG	AR	3811	1/1	0.89	0.30	25,25,25,25	0
85	MG	AR	4096	1/1	0.89	0.27	53,53,53,53	0
84	OHX	AR	3682	7/7	0.89	0.42	213,214,214,215	0
85	MG	1	4138	1/1	0.89	0.37	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4107	1/1	0.89	0.26	79,79,79,79	0
85	MG	6	2090	1/1	0.89	0.42	45,45,45,45	0
84	OHX	1	3724	7/7	0.89	0.50	243,244,245,246	0
85	MG	1	3877	1/1	0.89	0.13	44,44,44,44	0
85	MG	AR	4126	1/1	0.89	0.29	73,73,73,73	0
85	MG	1	4142	1/1	0.89	0.58	47,47,47,47	0
85	MG	1	4033	1/1	0.89	0.26	57,57,57,57	0
85	MG	AR	4130	1/1	0.89	0.17	19,19,19,19	0
85	MG	AR	3830	1/1	0.89	0.29	30,30,30,30	0
84	OHX	c3	201	7/7	0.89	0.25	212,213,214,215	0
85	MG	AR	4141	1/1	0.89	0.23	53,53,53,53	0
84	OHX	6	2015	7/7	0.89	0.41	230,231,232,233	0
85	MG	1	3934	1/1	0.89	0.17	61,61,61,61	0
84	OHX	1	3632	7/7	0.89	0.31	202,202,204,204	0
85	MG	1	4169	1/1	0.89	0.22	39,39,39,39	0
85	MG	6	2144	1/1	0.89	0.30	42,42,42,42	0
85	MG	AR	4154	1/1	0.89	0.10	50,50,50,50	0
84	OHX	6	2056	7/7	0.89	0.22	214,215,217,218	0
85	MG	1	4047	1/1	0.89	0.72	39,39,39,39	0
85	MG	1	4050	1/1	0.89	0.30	34,34,34,34	0
85	MG	AR	3913	1/1	0.89	0.35	20,20,20,20	0
84	OHX	1	3698	7/7	0.89	0.46	177,178,178,179	0
85	MG	6	2153	1/1	0.89	0.24	39,39,39,39	0
85	MG	AR	3952	1/1	0.89	0.24	28,28,28,28	0
85	MG	A	2113	1/1	0.89	0.25	35,35,35,35	0
85	MG	AR	3953	1/1	0.89	0.21	35,35,35,35	0
85	MG	A	2117	1/1	0.89	0.20	52,52,52,52	0
85	MG	1	4056	1/1	0.89	0.39	82,82,82,82	0
84	OHX	AE	201	7/7	0.89	0.20	194,195,195,196	0
85	MG	1	4182	1/1	0.89	0.35	49,49,49,49	0
84	OHX	AR	3520	7/7	0.89	0.20	175,175,176,176	0
84	OHX	1	3664	7/7	0.89	0.35	232,233,234,235	0
84	OHX	AR	3638	7/7	0.89	0.41	208,208,209,209	0
84	OHX	1	3715	7/7	0.89	0.43	219,220,222,222	0
84	OHX	AR	3719	7/7	0.89	0.25	220,220,221,221	0
85	MG	1	3766	1/1	0.89	0.29	23,23,23,23	0
84	OHX	1	3597	7/7	0.89	0.13	237,238,240,240	0
85	MG	6	2189	1/1	0.89	0.29	67,67,67,67	0
85	MG	1	4207	1/1	0.89	0.31	44,44,44,44	0
85	MG	AR	3993	1/1	0.89	0.21	62,62,62,62	0
84	OHX	AR	3725	7/7	0.89	0.33	261,263,264,264	0
84	OHX	1	3671	7/7	0.89	0.45	212,213,214,214	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	6	2041	7/7	0.89	0.36	209,209,210,211	0
85	MG	1	3975	1/1	0.89	0.17	43,43,43,43	0
85	MG	9	201	1/1	0.89	0.19	33,33,33,33	0
85	MG	1	3781	1/1	0.89	0.25	24,24,24,24	0
85	MG	1	3977	1/1	0.89	0.35	21,21,21,21	0
84	OHX	A	2012	7/7	0.89	0.20	218,220,220,222	0
85	MG	4	231	1/1	0.89	0.26	30,30,30,30	0
85	MG	AR	3998	1/1	0.90	0.49	18,18,18,18	0
85	MG	1	3897	1/1	0.90	0.38	13,13,13,13	0
85	MG	1	3933	1/1	0.90	0.23	37,37,37,37	0
84	OHX	AR	3688	7/7	0.90	0.28	199,200,201,201	0
84	OHX	AR	3693	7/7	0.90	0.28	238,239,240,240	0
84	OHX	AR	3632	7/7	0.90	0.14	227,227,228,228	0
85	MG	1	3945	1/1	0.90	0.29	17,17,17,17	0
85	MG	AS	218	1/1	0.90	0.22	52,52,52,52	0
85	MG	AS	219	1/1	0.90	0.30	35,35,35,35	0
84	OHX	Q	201	7/7	0.90	0.25	245,246,248,249	0
85	MG	AR	4028	1/1	0.90	0.24	44,44,44,44	0
84	OHX	AR	3696	7/7	0.90	0.34	176,176,177,178	0
84	OHX	CE	403	7/7	0.90	0.50	237,238,239,240	0
85	MG	AS	226	1/1	0.90	0.46	36,36,36,36	0
85	MG	AR	3747	1/1	0.90	0.22	23,23,23,23	0
85	MG	AR	4037	1/1	0.90	0.29	33,33,33,33	0
85	MG	AR	4041	1/1	0.90	0.12	47,47,47,47	0
85	MG	AR	3753	1/1	0.90	0.16	51,51,51,51	0
84	OHX	AR	3701	7/7	0.90	0.41	207,208,208,208	0
84	OHX	AR	3637	7/7	0.90	0.30	204,205,205,205	0
85	MG	AR	3766	1/1	0.90	0.23	21,21,21,21	0
84	OHX	z	201	7/7	0.90	0.23	257,258,259,259	0
84	OHX	AR	3706	7/7	0.90	0.22	209,210,211,212	0
84	OHX	AR	3707	7/7	0.90	0.27	207,207,207,207	0
84	OHX	AR	3710	7/7	0.90	0.32	213,215,216,216	0
84	OHX	1	3692	7/7	0.90	0.31	189,190,191,191	0
85	MG	CO	203	1/1	0.90	0.20	46,46,46,46	0
85	MG	AR	4060	1/1	0.90	0.27	56,56,56,56	0
85	MG	t	202	1/1	0.90	0.21	64,64,64,64	0
84	OHX	1	3635	7/7	0.90	0.26	219,220,221,222	0
85	MG	1	3969	1/1	0.90	0.12	45,45,45,45	0
84	OHX	DI	201	7/7	0.90	0.59	194,195,195,196	0
85	MG	1	4108	1/1	0.90	0.26	33,33,33,33	0
84	OHX	6	1980	7/7	0.90	0.38	206,206,208,208	0
85	MG	1	4110	1/1	0.90	0.27	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3767	1/1	0.90	0.12	34,34,34,34	0
85	MG	DI	202	1/1	0.90	0.26	32,32,32,32	0
85	MG	AR	3805	1/1	0.90	0.17	39,39,39,39	0
84	OHX	1	3648	7/7	0.90	0.27	258,259,260,260	0
85	MG	6	2073	1/1	0.90	0.41	57,57,57,57	0
84	OHX	A	1959	7/7	0.90	0.15	180,182,183,184	0
84	OHX	6	2010	7/7	0.90	0.24	213,214,215,216	0
84	OHX	AR	3652	7/7	0.90	0.36	196,196,197,197	0
85	MG	1	3780	1/1	0.90	0.26	26,26,26,26	0
84	OHX	6	2049	7/7	0.90	0.27	218,219,220,221	0
84	OHX	A	1996	7/7	0.90	0.27	208,209,211,212	0
85	MG	1	3988	1/1	0.90	0.26	46,46,46,46	0
85	MG	1	3998	1/1	0.90	0.24	65,65,65,65	0
85	MG	6	2120	1/1	0.90	0.17	61,61,61,61	0
84	OHX	AR	3722	7/7	0.90	0.30	200,201,201,202	0
84	OHX	A	2005	7/7	0.90	0.45	204,206,207,207	0
85	MG	AR	3839	1/1	0.90	0.38	30,30,30,30	0
85	MG	6	2128	1/1	0.90	0.28	53,53,53,53	0
85	MG	AR	4140	1/1	0.90	0.26	24,24,24,24	0
85	MG	AR	3855	1/1	0.90	0.14	37,37,37,37	0
85	MG	AR	4142	1/1	0.90	0.42	55,55,55,55	0
85	MG	6	2133	1/1	0.90	0.29	51,51,51,51	0
85	MG	AR	3884	1/1	0.90	0.27	27,27,27,27	0
84	OHX	AR	3723	7/7	0.90	0.19	240,241,242,242	0
85	MG	AR	3889	1/1	0.90	0.25	42,42,42,42	0
84	OHX	1	3695	7/7	0.90	0.23	200,201,202,202	0
84	OHX	6	2052	7/7	0.90	0.25	244,244,246,246	0
85	MG	1	3809	1/1	0.90	0.32	23,23,23,23	0
84	OHX	A	2019	7/7	0.90	0.14	252,253,255,256	0
84	OHX	A	2023	7/7	0.90	0.23	202,204,206,206	0
84	OHX	A	2024	7/7	0.90	0.36	219,222,223,223	0
85	MG	AR	3951	1/1	0.90	0.17	26,26,26,26	0
84	OHX	1	3729	7/7	0.90	0.37	206,207,207,208	0
85	MG	1	4171	1/1	0.90	0.14	26,26,26,26	0
84	OHX	1	3649	7/7	0.90	0.21	247,248,249,250	0
84	OHX	1	3670	7/7	0.90	0.30	215,215,217,217	0
84	OHX	1	3680	7/7	0.90	0.39	212,212,213,213	0
85	MG	AR	4176	1/1	0.90	0.20	52,52,52,52	0
85	MG	AR	4179	1/1	0.90	0.21	58,58,58,58	0
85	MG	1	4178	1/1	0.90	0.20	42,42,42,42	0
85	MG	A	2134	1/1	0.90	0.56	34,34,34,34	0
85	MG	AR	4181	1/1	0.90	0.20	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3731	7/7	0.90	0.37	175,176,177,178	0
84	OHX	1	3704	7/7	0.90	0.40	277,278,278,278	0
85	MG	AR	4201	1/1	0.90	0.37	31,31,31,31	0
84	OHX	6	2032	7/7	0.90	0.35	236,237,238,239	0
85	MG	AR	4203	1/1	0.90	0.35	37,37,37,37	0
84	OHX	6	2034	7/7	0.90	0.26	236,238,239,240	0
85	MG	1	4043	1/1	0.90	0.35	40,40,40,40	0
85	MG	AR	3980	1/1	0.90	0.21	32,32,32,32	0
85	MG	1	3880	1/1	0.90	0.50	29,29,29,29	0
85	MG	1	3883	1/1	0.90	0.47	17,17,17,17	0
84	OHX	1	3650	7/7	0.90	0.32	179,181,181,182	0
85	MG	s8	302	1/1	0.90	0.27	44,44,44,44	0
84	OHX	AR	3736	7/7	0.90	0.17	184,185,186,187	0
85	MG	1	3895	1/1	0.90	0.27	29,29,29,29	0
85	MG	AR	3995	1/1	0.90	0.11	38,38,38,38	0
85	MG	1	4202	1/1	0.90	0.33	27,27,27,27	0
85	MG	AR	4084	1/1	0.91	0.19	31,31,31,31	0
85	MG	AR	3864	1/1	0.91	0.26	21,21,21,21	0
84	OHX	AR	3598	7/7	0.91	0.17	205,206,207,208	0
85	MG	1	3986	1/1	0.91	0.13	30,30,30,30	0
84	OHX	AR	3605	7/7	0.91	0.14	194,195,196,196	0
85	MG	1	4105	1/1	0.91	0.51	64,64,64,64	0
84	OHX	J	301	7/7	0.91	0.25	244,245,247,247	0
85	MG	AR	4104	1/1	0.91	0.29	55,55,55,55	0
84	OHX	AR	3678	7/7	0.91	0.53	238,238,239,239	0
85	MG	AR	4117	1/1	0.91	0.23	53,53,53,53	0
85	MG	1	4002	1/1	0.91	0.21	104,104,104,104	0
84	OHX	6	2011	7/7	0.91	0.20	205,205,207,207	0
85	MG	AR	4123	1/1	0.91	0.25	39,39,39,39	0
85	MG	1	3876	1/1	0.91	0.38	39,39,39,39	0
84	OHX	1	3656	7/7	0.91	0.26	229,230,231,231	0
84	OHX	AR	3724	7/7	0.91	0.34	203,204,205,205	0
85	MG	1	4015	1/1	0.91	0.17	38,38,38,38	0
84	OHX	d9	101	7/7	0.91	0.33	234,235,236,237	0
85	MG	6	2196	1/1	0.91	0.38	46,46,46,46	0
85	MG	AR	3956	1/1	0.91	0.20	41,41,41,41	0
85	MG	1	4121	1/1	0.91	0.28	32,32,32,32	0
84	OHX	A	1943	7/7	0.91	0.25	161,163,164,165	0
84	OHX	6	2046	7/7	0.91	0.17	244,245,247,248	0
85	MG	1	4028	1/1	0.91	0.28	24,24,24,24	0
85	MG	1	4133	1/1	0.91	0.45	28,28,28,28	0
85	MG	A	2052	1/1	0.91	0.46	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	4	211	7/7	0.91	0.24	225,225,226,226	0
84	OHX	r	301	7/7	0.91	0.19	167,168,168,169	0
85	MG	1	3930	1/1	0.91	0.21	19,19,19,19	0
85	MG	6	2060	1/1	0.91	0.67	23,23,23,23	0
85	MG	AR	3982	1/1	0.91	0.26	35,35,35,35	0
85	MG	AR	3984	1/1	0.91	0.34	49,49,49,49	0
84	OHX	AR	3689	7/7	0.91	0.23	195,197,198,198	0
84	OHX	A	1989	7/7	0.91	0.29	253,254,256,256	0
84	OHX	1	3557	7/7	0.91	0.20	186,187,188,188	0
84	OHX	AR	3694	7/7	0.91	0.40	212,212,213,213	0
85	MG	6	2074	1/1	0.91	0.31	37,37,37,37	0
84	OHX	A	2000	7/7	0.91	0.22	194,195,196,197	0
85	MG	1	3764	1/1	0.91	0.54	38,38,38,38	0
85	MG	1	4153	1/1	0.91	0.21	39,39,39,39	0
84	OHX	1	3661	7/7	0.91	0.57	251,252,253,253	0
84	OHX	1	3712	7/7	0.91	0.41	215,215,216,217	0
85	MG	A	2095	1/1	0.91	0.18	94,94,94,94	0
84	OHX	6	2031	7/7	0.91	0.27	210,211,213,213	0
85	MG	AR	4016	1/1	0.91	0.44	104,104,104,104	0
84	OHX	1	3713	7/7	0.91	0.33	217,217,218,218	0
85	MG	1	4051	1/1	0.91	0.37	63,63,63,63	0
85	MG	6	2116	1/1	0.91	0.42	41,41,41,41	0
85	MG	AR	3791	1/1	0.91	0.47	32,32,32,32	0
84	OHX	AR	3704	7/7	0.91	0.37	223,224,225,225	0
85	MG	AR	3795	1/1	0.91	0.20	22,22,22,22	0
84	OHX	A	2016	7/7	0.91	0.19	207,209,210,211	0
85	MG	A	2114	1/1	0.91	0.36	41,41,41,41	0
85	MG	AR	4034	1/1	0.91	0.25	42,42,42,42	0
84	OHX	AR	3655	7/7	0.91	0.36	216,218,218,219	0
84	OHX	AR	3659	7/7	0.91	0.26	195,196,196,197	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	4040	1/1	0.91	0.24	27,27,27,27	0
85	MG	6	2130	1/1	0.91	0.26	42,42,42,42	0
85	MG	AR	3807	1/1	0.91	0.24	27,27,27,27	0
85	MG	A	2130	1/1	0.91	0.29	49,49,49,49	0
85	MG	A	2131	1/1	0.91	0.13	88,88,88,88	0
85	MG	A	2132	1/1	0.91	0.27	71,71,71,71	0
84	OHX	1	3633	7/7	0.91	0.17	193,194,195,197	0
84	OHX	AR	3708	7/7	0.91	0.30	228,228,229,229	0
84	OHX	6	2036	7/7	0.91	0.38	172,174,175,176	0
84	OHX	AT	216	7/7	0.91	0.17	193,193,193,193	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AT	218	7/7	0.91	0.39	223,224,224,224	0
84	OHX	A	2032	7/7	0.91	0.19	234,236,237,239	0
84	OHX	AT	220	7/7	0.91	0.26	197,197,198,198	0
84	OHX	AR	3666	7/7	0.91	0.20	217,218,218,219	0
85	MG	6	2151	1/1	0.91	0.71	87,87,87,87	0
84	OHX	1	3651	7/7	0.91	0.30	207,208,209,209	0
85	MG	AR	3831	1/1	0.91	0.32	45,45,45,45	0
84	OHX	AR	3713	7/7	0.91	0.16	247,247,248,249	0
85	MG	6	2156	1/1	0.91	0.14	50,50,50,50	0
85	MG	6	2157	1/1	0.91	0.26	45,45,45,45	0
85	MG	6	2160	1/1	0.91	0.24	121,121,121,121	0
84	OHX	1	3718	7/7	0.91	0.38	220,221,221,222	0
85	MG	d5	201	1/1	0.91	0.09	67,67,67,67	0
85	MG	d6	101	1/1	0.91	0.24	37,37,37,37	0
85	MG	AR	4081	1/1	0.91	0.31	52,52,52,52	0
84	OHX	1	3667	7/7	0.91	0.35	189,189,190,191	0
85	MG	6	2072	1/1	0.92	0.23	36,36,36,36	0
85	MG	AR	3876	1/1	0.92	0.43	30,30,30,30	0
84	OHX	A	2013	7/7	0.92	0.32	203,205,206,206	0
84	OHX	AR	3603	7/7	0.92	0.13	182,183,184,185	0
85	MG	AR	3887	1/1	0.92	0.72	35,35,35,35	0
84	OHX	6	2002	7/7	0.92	0.19	218,220,221,221	0
85	MG	6	2079	1/1	0.92	0.34	37,37,37,37	0
84	OHX	A	2017	7/7	0.92	0.24	220,223,224,224	0
85	MG	AR	4185	1/1	0.92	0.36	40,40,40,40	0
85	MG	1	4084	1/1	0.92	0.21	44,44,44,44	0
85	MG	AR	4194	1/1	0.92	0.27	47,47,47,47	0
85	MG	6	2087	1/1	0.92	0.39	28,28,28,28	0
84	OHX	6	2006	7/7	0.92	0.21	199,199,201,201	0
84	OHX	AR	3621	7/7	0.92	0.22	208,209,210,211	0
85	MG	AR	3943	1/1	0.92	0.26	73,73,73,73	0
85	MG	AR	3948	1/1	0.92	0.23	16,16,16,16	0
85	MG	AR	4208	1/1	0.92	0.24	62,62,62,62	0
84	OHX	AR	3628	7/7	0.92	0.27	209,210,211,211	0
85	MG	1	4093	1/1	0.92	0.47	16,16,16,16	0
84	OHX	AR	3721	7/7	0.92	0.30	212,213,213,214	0
85	MG	1	3898	1/1	0.92	0.33	22,22,22,22	0
85	MG	1	3912	1/1	0.92	0.34	30,30,30,30	0
84	OHX	A	2026	7/7	0.92	0.32	191,192,194,194	0
84	OHX	AR	3629	7/7	0.92	0.32	209,210,211,212	0
85	MG	6	2124	1/1	0.92	0.12	62,62,62,62	0
85	MG	6	2127	1/1	0.92	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3682	7/7	0.92	0.27	204,206,207,207	0
85	MG	1	3938	1/1	0.92	0.11	41,41,41,41	0
84	OHX	AR	3634	7/7	0.92	0.18	213,214,215,216	0
84	OHX	1	3657	7/7	0.92	0.40	170,171,171,171	0
85	MG	AR	3973	1/1	0.92	0.19	27,27,27,27	0
85	MG	AR	4244	1/1	0.92	0.34	44,44,44,44	0
84	OHX	1	3688	7/7	0.92	0.24	220,221,221,222	0
85	MG	AR	3977	1/1	0.92	0.54	26,26,26,26	0
85	MG	AR	3979	1/1	0.92	0.24	45,45,45,45	0
84	OHX	6	2022	7/7	0.92	0.11	235,235,238,239	0
84	OHX	1	3601	7/7	0.92	0.33	200,200,201,202	0
84	OHX	1	3556	7/7	0.92	0.19	180,181,182,183	0
84	OHX	1	3721	7/7	0.92	0.39	191,192,193,193	0
85	MG	1	3952	1/1	0.92	0.16	34,34,34,34	0
84	OHX	1	3608	7/7	0.92	0.28	177,177,179,179	0
85	MG	1	4120	1/1	0.92	0.18	46,46,46,46	0
84	OHX	AR	3647	7/7	0.92	0.31	203,204,205,205	0
85	MG	6	2155	1/1	0.92	0.14	61,61,61,61	0
85	MG	AT	225	1/1	0.92	0.17	60,60,60,60	0
85	MG	1	4123	1/1	0.92	0.23	41,41,41,41	0
84	OHX	1	3665	7/7	0.92	0.16	209,210,211,211	0
85	MG	6	2159	1/1	0.92	0.31	39,39,39,39	0
84	OHX	1	3696	7/7	0.92	0.55	240,240,241,242	0
84	OHX	1	3697	7/7	0.92	0.22	238,240,241,241	0
84	OHX	6	2033	7/7	0.92	0.28	199,200,201,202	0
85	MG	AR	4020	1/1	0.92	0.14	69,69,69,69	0
84	OHX	1	3615	7/7	0.92	0.39	185,186,186,187	0
84	OHX	6	2035	7/7	0.92	0.32	157,158,159,159	0
84	OHX	1	3642	7/7	0.92	0.21	193,193,195,195	0
84	OHX	AS	209	7/7	0.92	0.25	175,176,177,177	0
84	OHX	6	2037	7/7	0.92	0.39	203,204,206,206	0
85	MG	1	3738	1/1	0.92	0.28	57,57,57,57	0
85	MG	1	3742	1/1	0.92	0.36	19,19,19,19	0
85	MG	1	4146	1/1	0.92	0.16	39,39,39,39	0
85	MG	AR	4035	1/1	0.92	0.19	39,39,39,39	0
85	MG	1	3979	1/1	0.92	0.29	47,47,47,47	0
84	OHX	1	3700	7/7	0.92	0.26	161,162,163,163	0
84	OHX	6	2039	7/7	0.92	0.18	204,204,206,206	0
85	MG	1	4157	1/1	0.92	0.21	37,37,37,37	0
84	OHX	AT	219	7/7	0.92	0.38	190,190,190,191	0
85	MG	DP	101	1/1	0.92	0.20	43,43,43,43	0
85	MG	1	3753	1/1	0.92	0.32	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3754	1/1	0.92	0.32	38,38,38,38	0
84	OHX	6	2040	7/7	0.92	0.30	199,200,201,202	0
84	OHX	AR	3677	7/7	0.92	0.36	180,180,181,181	0
84	OHX	3	208	7/7	0.92	0.16	230,231,232,233	0
85	MG	AR	4052	1/1	0.92	0.32	28,28,28,28	0
84	OHX	1	3701	7/7	0.92	0.24	181,182,182,182	0
85	MG	A	2062	1/1	0.92	0.29	48,48,48,48	0
84	OHX	1	3551	7/7	0.92	0.16	191,192,192,193	0
84	OHX	6	2044	7/7	0.92	0.35	238,238,239,240	0
85	MG	1	4005	1/1	0.92	0.63	37,37,37,37	0
85	MG	A	2072	1/1	0.92	0.28	44,44,44,44	0
85	MG	1	4006	1/1	0.92	0.23	33,33,33,33	0
84	OHX	AR	3686	7/7	0.92	0.47	186,187,187,187	0
84	OHX	1	3618	7/7	0.92	0.35	189,190,191,192	0
85	MG	1	4011	1/1	0.92	0.18	38,38,38,38	0
85	MG	A	2085	1/1	0.92	0.20	47,47,47,47	0
84	OHX	4	212	7/7	0.92	0.24	201,202,202,202	0
85	MG	AR	3764	1/1	0.92	0.18	27,27,27,27	0
84	OHX	1	3672	7/7	0.92	0.39	161,162,164,164	0
85	MG	AR	4075	1/1	0.92	0.33	35,35,35,35	0
84	OHX	1	3619	7/7	0.92	0.39	190,191,192,193	0
85	MG	AR	4079	1/1	0.92	0.33	36,36,36,36	0
85	MG	1	4021	1/1	0.92	0.24	29,29,29,29	0
84	OHX	1	3708	7/7	0.92	0.30	210,211,211,211	0
85	MG	A	2097	1/1	0.92	0.32	55,55,55,55	0
84	OHX	1	3621	7/7	0.92	0.24	221,223,224,224	0
85	MG	AR	3774	1/1	0.92	0.21	23,23,23,23	0
85	MG	A	2101	1/1	0.92	0.24	64,64,64,64	0
85	MG	AR	4092	1/1	0.92	0.20	25,25,25,25	0
84	OHX	6	1955	7/7	0.92	0.16	191,193,195,196	0
85	MG	A	2105	1/1	0.92	0.25	71,71,71,71	0
84	OHX	1	3622	7/7	0.92	0.20	211,212,213,213	0
84	OHX	A	1969	7/7	0.92	0.20	220,222,223,223	0
84	OHX	1	3654	7/7	0.92	0.29	192,194,194,194	0
84	OHX	1	3679	7/7	0.92	0.24	230,231,232,232	0
84	OHX	1	3631	7/7	0.92	0.18	198,199,199,199	0
85	MG	AR	3792	1/1	0.92	0.38	28,28,28,28	0
85	MG	AR	4108	1/1	0.92	0.17	25,25,25,25	0
85	MG	AR	4114	1/1	0.92	0.17	30,30,30,30	0
84	OHX	A	1991	7/7	0.92	0.21	218,220,221,221	0
85	MG	4	218	1/1	0.92	0.52	7,7,7,7	0
85	MG	1	4036	1/1	0.92	0.25	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3820	1/1	0.92	0.26	30,30,30,30	0
85	MG	4	227	1/1	0.92	0.21	42,42,42,42	0
85	MG	4	230	1/1	0.92	0.18	54,54,54,54	0
85	MG	AR	3806	1/1	0.92	0.22	68,68,68,68	0
85	MG	1	4039	1/1	0.92	0.23	40,40,40,40	0
84	OHX	6	1990	7/7	0.92	0.33	238,238,239,240	0
85	MG	A	2133	1/1	0.92	0.40	54,54,54,54	0
84	OHX	6	1993	7/7	0.92	0.24	191,192,193,194	0
84	OHX	A	1997	7/7	0.92	0.25	211,214,214,215	0
85	MG	1	3831	1/1	0.92	0.27	42,42,42,42	0
85	MG	1	4045	1/1	0.92	0.11	62,62,62,62	0
85	MG	A	2140	1/1	0.92	0.30	55,55,55,55	0
84	OHX	A	1999	7/7	0.92	0.23	214,215,217,217	0
85	MG	AR	4143	1/1	0.92	0.25	38,38,38,38	0
85	MG	1	3834	1/1	0.92	0.42	18,18,18,18	0
85	MG	A	2149	1/1	0.92	0.36	49,49,49,49	0
84	OHX	6	2000	7/7	0.92	0.16	210,211,212,213	0
85	MG	A	2152	1/1	0.92	0.16	78,78,78,78	0
85	MG	1	3847	1/1	0.92	0.39	23,23,23,23	0
85	MG	AR	3828	1/1	0.92	0.30	47,47,47,47	0
85	MG	1	4055	1/1	0.92	0.24	33,33,33,33	0
84	OHX	AR	3597	7/7	0.92	0.20	176,177,178,178	0
84	OHX	6	2001	7/7	0.92	0.40	211,211,212,213	0
85	MG	1	4062	1/1	0.92	0.19	33,33,33,33	0
85	MG	AR	4158	1/1	0.92	0.30	21,21,21,21	0
84	OHX	A	2006	7/7	0.92	0.25	215,218,219,219	0
84	OHX	AR	3599	7/7	0.92	0.29	201,202,203,203	0
85	MG	AR	3844	1/1	0.92	0.26	25,25,25,25	0
85	MG	6	2069	1/1	0.92	0.59	26,26,26,26	0
84	OHX	AR	3602	7/7	0.92	0.33	192,193,194,194	0
85	MG	6	2125	1/1	0.93	0.26	63,63,63,63	0
85	MG	AR	3933	1/1	0.93	0.53	13,13,13,13	0
85	MG	1	4128	1/1	0.93	0.19	27,27,27,27	0
84	OHX	6	1977	7/7	0.93	0.15	193,194,196,196	0
84	OHX	1	3553	7/7	0.93	0.22	184,185,186,186	0
85	MG	AR	4184	1/1	0.93	0.20	35,35,35,35	0
85	MG	1	3997	1/1	0.93	0.30	37,37,37,37	0
85	MG	AR	4191	1/1	0.93	0.20	38,38,38,38	0
84	OHX	AR	3657	7/7	0.93	0.34	207,207,209,209	0
85	MG	1	4000	1/1	0.93	0.41	36,36,36,36	0
85	MG	AR	4199	1/1	0.93	0.27	64,64,64,64	0
85	MG	6	2140	1/1	0.93	0.23	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3564	7/7	0.93	0.18	173,175,175,175	0
85	MG	6	2143	1/1	0.93	0.18	90,90,90,90	0
84	OHX	AR	3660	7/7	0.93	0.35	167,168,169,170	0
84	OHX	6	1989	7/7	0.93	0.29	169,170,172,172	0
85	MG	1	4004	1/1	0.93	0.21	31,31,31,31	0
84	OHX	1	3566	7/7	0.93	0.24	182,182,183,183	0
85	MG	6	2150	1/1	0.93	0.21	51,51,51,51	0
85	MG	AR	4212	1/1	0.93	0.12	48,48,48,48	0
85	MG	AR	4213	1/1	0.93	0.21	34,34,34,34	0
85	MG	AR	3970	1/1	0.93	0.22	53,53,53,53	0
84	OHX	1	3723	7/7	0.93	0.19	201,202,203,204	0
85	MG	AR	3972	1/1	0.93	0.30	38,38,38,38	0
85	MG	1	3810	1/1	0.93	0.23	86,86,86,86	0
85	MG	AR	3974	1/1	0.93	0.24	28,28,28,28	0
84	OHX	A	2022	7/7	0.93	0.29	229,230,232,233	0
85	MG	6	2154	1/1	0.93	0.20	38,38,38,38	0
84	OHX	6	1998	7/7	0.93	0.19	239,240,243,244	0
85	MG	AR	4226	1/1	0.93	0.51	16,16,16,16	0
85	MG	AR	4230	1/1	0.93	0.40	68,68,68,68	0
84	OHX	1	3623	7/7	0.93	0.10	224,225,226,226	0
85	MG	1	4158	1/1	0.93	0.15	29,29,29,29	0
85	MG	1	4159	1/1	0.93	0.16	42,42,42,42	0
85	MG	1	4160	1/1	0.93	0.26	40,40,40,40	0
85	MG	AR	4242	1/1	0.93	0.73	56,56,56,56	0
85	MG	6	2164	1/1	0.93	0.19	63,63,63,63	0
85	MG	AR	3989	1/1	0.93	0.32	85,85,85,85	0
84	OHX	1	3625	7/7	0.93	0.24	186,186,187,187	0
84	OHX	1	3628	7/7	0.93	0.20	234,235,236,237	0
84	OHX	A	2027	7/7	0.93	0.18	236,239,240,241	0
84	OHX	A	2028	7/7	0.93	0.23	252,254,254,256	0
85	MG	1	4024	1/1	0.93	0.37	15,15,15,15	0
85	MG	1	4025	1/1	0.93	0.24	34,34,34,34	0
85	MG	6	2175	1/1	0.93	0.19	41,41,41,41	0
85	MG	AR	4003	1/1	0.93	0.35	73,73,73,73	0
85	MG	AR	4010	1/1	0.93	0.43	28,28,28,28	0
84	OHX	6	2004	7/7	0.93	0.17	193,194,195,196	0
85	MG	AT	221	1/1	0.93	0.40	26,26,26,26	0
85	MG	1	4176	1/1	0.93	0.19	27,27,27,27	0
85	MG	AT	224	1/1	0.93	0.54	35,35,35,35	0
85	MG	1	3842	1/1	0.93	0.58	27,27,27,27	0
85	MG	AR	4018	1/1	0.93	0.12	40,40,40,40	0
84	OHX	AR	3676	7/7	0.93	0.29	196,197,198,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3653	7/7	0.93	0.41	193,195,196,196	0
85	MG	AR	4023	1/1	0.93	0.10	36,36,36,36	0
85	MG	CE	405	1/1	0.93	0.41	34,34,34,34	0
84	OHX	6	2008	7/7	0.93	0.29	211,213,214,216	0
84	OHX	AR	3680	7/7	0.93	0.41	220,222,222,223	0
84	OHX	1	3630	7/7	0.93	0.19	199,200,200,201	0
84	OHX	A	2037	7/7	0.93	0.28	238,240,241,241	0
84	OHX	AT	211	7/7	0.93	0.26	179,179,180,180	0
85	MG	AR	4030	1/1	0.93	0.26	37,37,37,37	0
84	OHX	1	3655	7/7	0.93	0.20	203,204,205,205	0
85	MG	1	3879	1/1	0.93	0.30	47,47,47,47	0
84	OHX	3	205	7/7	0.93	0.13	169,171,171,173	0
85	MG	AF	201	1/1	0.93	0.24	27,27,27,27	0
85	MG	1	4198	1/1	0.93	0.56	36,36,36,36	0
84	OHX	6	2016	7/7	0.93	0.21	194,194,196,196	0
85	MG	DC	202	1/1	0.93	0.21	28,28,28,28	0
84	OHX	AR	3577	7/7	0.93	0.30	201,201,202,202	0
85	MG	1	4203	1/1	0.93	0.52	34,34,34,34	0
85	MG	AR	3742	1/1	0.93	0.34	29,29,29,29	0
84	OHX	AR	3581	7/7	0.93	0.32	205,205,205,205	0
85	MG	AR	4044	1/1	0.93	0.25	51,51,51,51	0
84	OHX	AR	3586	7/7	0.93	0.14	182,184,185,185	0
84	OHX	M	201	7/7	0.93	0.33	202,204,205,206	0
85	MG	AR	3748	1/1	0.93	0.25	41,41,41,41	0
85	MG	A	2045	1/1	0.93	0.42	35,35,35,35	0
84	OHX	AR	3591	7/7	0.93	0.40	168,169,169,169	0
85	MG	3	215	1/1	0.93	0.23	39,39,39,39	0
85	MG	A	2051	1/1	0.93	0.26	62,62,62,62	0
85	MG	1	3903	1/1	0.93	0.32	32,32,32,32	0
84	OHX	CG	301	7/7	0.93	0.13	191,193,193,195	0
85	MG	4	215	1/1	0.93	0.49	23,23,23,23	0
85	MG	AR	3769	1/1	0.93	0.13	35,35,35,35	0
85	MG	1	3914	1/1	0.93	0.54	31,31,31,31	0
85	MG	A	2067	1/1	0.93	0.57	32,32,32,32	0
84	OHX	6	2021	7/7	0.93	0.33	210,210,212,213	0
84	OHX	1	3568	7/7	0.93	0.20	195,196,196,197	0
85	MG	AR	4064	1/1	0.93	0.21	30,30,30,30	0
85	MG	AR	4069	1/1	0.93	0.20	53,53,53,53	0
85	MG	1	4060	1/1	0.93	0.55	16,16,16,16	0
84	OHX	4	206	7/7	0.93	0.27	179,179,180,180	0
85	MG	4	229	1/1	0.93	0.26	57,57,57,57	0
84	OHX	sR	401	7/7	0.93	0.15	215,216,219,219	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	6	2024	7/7	0.93	0.18	207,208,210,211	0
85	MG	1	3940	1/1	0.93	0.21	21,21,21,21	0
85	MG	1	4072	1/1	0.93	0.23	55,55,55,55	0
85	MG	1	3735	1/1	0.93	0.23	39,39,39,39	0
85	MG	1	4075	1/1	0.93	0.23	20,20,20,20	0
84	OHX	1	3681	7/7	0.93	0.28	210,211,212,212	0
85	MG	AR	4090	1/1	0.93	0.27	62,62,62,62	0
85	MG	1	3737	1/1	0.93	0.26	36,36,36,36	0
85	MG	AR	3796	1/1	0.93	0.59	32,32,32,32	0
84	OHX	6	2026	7/7	0.93	0.21	218,219,220,222	0
85	MG	v	302	1/1	0.93	0.39	43,43,43,43	0
85	MG	AR	4097	1/1	0.93	0.33	26,26,26,26	0
84	OHX	1	3609	7/7	0.93	0.21	191,193,194,195	0
84	OHX	AR	3616	7/7	0.93	0.35	210,210,211,212	0
85	MG	AR	4103	1/1	0.93	0.16	35,35,35,35	0
85	MG	1	3747	1/1	0.93	0.31	28,28,28,28	0
85	MG	1	4089	1/1	0.93	0.21	30,30,30,30	0
85	MG	1	4090	1/1	0.93	0.10	54,54,54,54	0
85	MG	A	2111	1/1	0.93	0.22	68,68,68,68	0
85	MG	AR	3809	1/1	0.93	0.12	86,86,86,86	0
85	MG	6	2058	1/1	0.93	0.39	33,33,33,33	0
84	OHX	1	3587	7/7	0.93	0.25	188,189,189,190	0
85	MG	AR	4120	1/1	0.93	0.22	32,32,32,32	0
85	MG	AR	4121	1/1	0.93	0.37	42,42,42,42	0
85	MG	1	3957	1/1	0.93	0.42	29,29,29,29	0
85	MG	A	2121	1/1	0.93	0.08	66,66,66,66	0
85	MG	A	2122	1/1	0.93	0.41	42,42,42,42	0
85	MG	1	3958	1/1	0.93	0.20	54,54,54,54	0
85	MG	AR	4124	1/1	0.93	0.17	54,54,54,54	0
84	OHX	1	3686	7/7	0.93	0.33	207,208,209,209	0
85	MG	A	2126	1/1	0.93	0.16	48,48,48,48	0
84	OHX	l	401	7/7	0.93	0.38	208,209,210,210	0
84	OHX	1	3687	7/7	0.93	0.32	196,196,197,197	0
85	MG	AR	3823	1/1	0.93	0.56	15,15,15,15	0
85	MG	1	3757	1/1	0.93	0.13	46,46,46,46	0
84	OHX	1	3659	7/7	0.93	0.14	208,210,211,211	0
84	OHX	1	3714	7/7	0.93	0.17	155,156,157,158	0
84	OHX	AR	3714	7/7	0.93	0.43	192,193,193,194	0
84	OHX	y	201	7/7	0.93	0.26	204,205,207,208	0
85	MG	6	2083	1/1	0.93	0.47	35,35,35,35	0
85	MG	6	2084	1/1	0.93	0.27	35,35,35,35	0
85	MG	AR	4145	1/1	0.93	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	A	2143	1/1	0.93	0.21	151,151,151,151	0
84	OHX	1	3634	7/7	0.93	0.21	206,207,207,209	0
85	MG	1	3765	1/1	0.93	0.13	41,41,41,41	0
85	MG	AR	4148	1/1	0.93	0.14	36,36,36,36	0
85	MG	6	2089	1/1	0.93	0.25	34,34,34,34	0
84	OHX	A	1995	7/7	0.93	0.15	206,207,208,209	0
84	OHX	1	3595	7/7	0.93	0.44	190,191,192,192	0
85	MG	AR	3875	1/1	0.93	0.20	48,48,48,48	0
84	OHX	1	3491	7/7	0.93	0.18	138,138,139,139	0
85	MG	6	2095	1/1	0.93	0.58	32,32,32,32	0
85	MG	1	3980	1/1	0.93	0.26	19,19,19,19	0
85	MG	1	3772	1/1	0.93	0.34	32,32,32,32	0
85	MG	6	2111	1/1	0.93	0.16	42,42,42,42	0
84	OHX	6	1964	7/7	0.93	0.20	175,175,177,177	0
85	MG	d3	202	1/1	0.93	0.54	56,56,56,56	0
84	OHX	6	1974	7/7	0.93	0.20	176,176,178,178	0
84	OHX	1	3640	7/7	0.93	0.19	194,195,196,196	0
84	OHX	AR	3648	7/7	0.93	0.39	196,197,198,198	0
85	MG	d9	102	1/1	0.93	0.44	106,106,106,106	0
85	MG	AR	3907	1/1	0.93	0.36	20,20,20,20	0
85	MG	1	4127	1/1	0.93	0.16	58,58,58,58	0
84	OHX	1	3660	7/7	0.94	0.29	208,209,210,210	0
85	MG	1	3743	1/1	0.94	0.39	23,23,23,23	0
84	OHX	6	1978	7/7	0.94	0.13	176,178,180,181	0
84	OHX	1	3605	7/7	0.94	0.31	171,171,172,172	0
84	OHX	AT	214	7/7	0.94	0.26	173,173,174,174	0
85	MG	1	3989	1/1	0.94	0.48	20,20,20,20	0
84	OHX	AR	3656	7/7	0.94	0.20	187,187,189,189	0
85	MG	1	4188	1/1	0.94	0.21	34,34,34,34	0
85	MG	1	4190	1/1	0.94	0.25	26,26,26,26	0
85	MG	AR	3778	1/1	0.94	0.37	42,42,42,42	0
84	OHX	1	3662	7/7	0.94	0.22	178,179,180,180	0
85	MG	AR	4136	1/1	0.94	0.22	41,41,41,41	0
85	MG	1	3999	1/1	0.94	0.29	38,38,38,38	0
84	OHX	AR	3658	7/7	0.94	0.27	177,177,179,179	0
84	OHX	6	1985	7/7	0.94	0.16	191,193,194,195	0
84	OHX	1	3725	7/7	0.94	0.08	203,204,205,206	0
84	OHX	AR	3661	7/7	0.94	0.53	176,177,178,178	0
85	MG	1	3760	1/1	0.94	0.61	26,26,26,26	0
84	OHX	1	3461	7/7	0.94	0.17	136,137,137,138	0
85	MG	1	4213	1/1	0.94	0.21	36,36,36,36	0
84	OHX	6	1992	7/7	0.94	0.22	185,186,187,188	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	3	210	1/1	0.94	0.25	41,41,41,41	0
85	MG	1	3763	1/1	0.94	0.31	34,34,34,34	0
84	OHX	1	3542	7/7	0.94	0.28	156,157,158,158	0
85	MG	3	216	1/1	0.94	0.21	35,35,35,35	0
85	MG	3	217	1/1	0.94	0.15	48,48,48,48	0
84	OHX	AR	3667	7/7	0.94	0.23	207,209,210,210	0
85	MG	3	219	1/1	0.94	0.14	77,77,77,77	0
85	MG	1	4012	1/1	0.94	0.20	26,26,26,26	0
84	OHX	CK	201	7/7	0.94	0.24	185,185,186,187	0
84	OHX	6	1995	7/7	0.94	0.18	171,173,174,175	0
85	MG	1	4016	1/1	0.94	0.17	11,11,11,11	0
85	MG	AR	4169	1/1	0.94	0.14	34,34,34,34	0
84	OHX	6	1996	7/7	0.94	0.17	190,191,192,193	0
85	MG	AR	4171	1/1	0.94	0.43	59,59,59,59	0
84	OHX	6	1997	7/7	0.94	0.20	198,199,201,201	0
85	MG	4	226	1/1	0.94	0.10	54,54,54,54	0
84	OHX	1	3544	7/7	0.94	0.17	187,188,190,190	0
85	MG	AR	4178	1/1	0.94	0.23	48,48,48,48	0
85	MG	AR	3824	1/1	0.94	0.14	62,62,62,62	0
84	OHX	AR	3673	7/7	0.94	0.20	179,180,180,180	0
85	MG	AR	3827	1/1	0.94	0.45	40,40,40,40	0
85	MG	1	3778	1/1	0.94	0.19	20,20,20,20	0
84	OHX	AR	3674	7/7	0.94	0.41	215,215,216,216	0
84	OHX	A	1932	7/7	0.94	0.17	178,180,182,182	0
84	OHX	A	1934	7/7	0.94	0.14	176,177,179,179	0
85	MG	AR	4192	1/1	0.94	0.18	44,44,44,44	0
85	MG	1	3782	1/1	0.94	0.41	44,44,44,44	0
85	MG	o	301	1/1	0.94	0.25	39,39,39,39	0
85	MG	AR	4196	1/1	0.94	0.22	39,39,39,39	0
85	MG	AR	3838	1/1	0.94	0.61	21,21,21,21	0
85	MG	1	3783	1/1	0.94	0.30	27,27,27,27	0
84	OHX	1	3611	7/7	0.94	0.23	184,185,185,186	0
85	MG	1	3788	1/1	0.94	0.33	34,34,34,34	0
85	MG	AR	4204	1/1	0.94	0.21	31,31,31,31	0
85	MG	AR	3850	1/1	0.94	0.52	11,11,11,11	0
84	OHX	1	3641	7/7	0.94	0.23	195,196,197,197	0
85	MG	AR	3859	1/1	0.94	0.27	28,28,28,28	0
84	OHX	A	1958	7/7	0.94	0.18	206,207,210,210	0
85	MG	1	3796	1/1	0.94	0.19	33,33,33,33	0
85	MG	1	3798	1/1	0.94	0.19	29,29,29,29	0
85	MG	AR	3879	1/1	0.94	0.54	21,21,21,21	0
84	OHX	1	3702	7/7	0.94	0.33	179,180,181,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3802	1/1	0.94	0.21	32,32,32,32	0
85	MG	AR	4216	1/1	0.94	0.30	67,67,67,67	0
85	MG	AR	3885	1/1	0.94	0.37	38,38,38,38	0
85	MG	1	4042	1/1	0.94	0.16	65,65,65,65	0
85	MG	1	3804	1/1	0.94	0.61	18,18,18,18	0
84	OHX	A	1960	7/7	0.94	0.15	225,226,227,228	0
85	MG	AR	3891	1/1	0.94	0.36	36,36,36,36	0
85	MG	6	2062	1/1	0.94	0.36	32,32,32,32	0
85	MG	AR	3896	1/1	0.94	0.43	37,37,37,37	0
84	OHX	3	207	7/7	0.94	0.17	188,189,190,191	0
84	OHX	AR	3679	7/7	0.94	0.24	218,220,221,221	0
84	OHX	A	1977	7/7	0.94	0.17	202,205,207,207	0
85	MG	1	3811	1/1	0.94	0.21	42,42,42,42	0
85	MG	AR	4240	1/1	0.94	0.14	33,33,33,33	0
85	MG	AR	3916	1/1	0.94	0.41	3,3,3,3	0
85	MG	AR	3918	1/1	0.94	0.40	21,21,21,21	0
85	MG	1	3812	1/1	0.94	0.37	29,29,29,29	0
85	MG	AR	3928	1/1	0.94	0.26	10,10,10,10	0
85	MG	AS	215	1/1	0.94	0.67	12,12,12,12	0
84	OHX	A	1978	7/7	0.94	0.14	210,212,214,214	0
85	MG	AR	3936	1/1	0.94	0.32	20,20,20,20	0
85	MG	AR	3938	1/1	0.94	0.52	20,20,20,20	0
85	MG	AR	3941	1/1	0.94	0.08	46,46,46,46	0
85	MG	AR	3942	1/1	0.94	0.10	45,45,45,45	0
84	OHX	A	1980	7/7	0.94	0.26	194,196,197,197	0
85	MG	AR	3946	1/1	0.94	0.19	28,28,28,28	0
84	OHX	A	1981	7/7	0.94	0.10	231,234,235,236	0
85	MG	AS	227	1/1	0.94	0.51	43,43,43,43	0
84	OHX	6	2005	7/7	0.94	0.27	152,153,155,155	0
85	MG	6	2080	1/1	0.94	0.15	53,53,53,53	0
85	MG	AT	201	1/1	0.94	0.29	31,31,31,31	0
85	MG	1	4061	1/1	0.94	0.40	23,23,23,23	0
84	OHX	1	3613	7/7	0.94	0.23	166,166,167,168	0
84	OHX	AR	3530	7/7	0.94	0.20	147,148,148,148	0
84	OHX	AR	3684	7/7	0.94	0.47	181,182,183,183	0
85	MG	1	3839	1/1	0.94	0.60	7,7,7,7	0
85	MG	AR	3959	1/1	0.94	0.22	32,32,32,32	0
85	MG	AR	3960	1/1	0.94	0.15	17,17,17,17	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
85	MG	AR	3963	1/1	0.94	0.38	23,23,23,23	0
84	OHX	AR	3539	7/7	0.94	0.12	169,170,172,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3556	7/7	0.94	0.19	138,139,140,140	0
85	MG	6	2091	1/1	0.94	0.33	54,54,54,54	0
84	OHX	AR	3564	7/7	0.94	0.17	189,190,190,190	0
85	MG	AR	3969	1/1	0.94	0.25	38,38,38,38	0
85	MG	1	3851	1/1	0.94	0.24	34,34,34,34	0
85	MG	CP	503	1/1	0.94	0.25	95,95,95,95	0
84	OHX	AR	3565	7/7	0.94	0.16	161,162,163,164	0
85	MG	1	3855	1/1	0.94	0.44	26,26,26,26	0
85	MG	CR	201	1/1	0.94	0.44	14,14,14,14	0
85	MG	6	2099	1/1	0.94	0.22	19,19,19,19	0
85	MG	CR	204	1/1	0.94	0.21	46,46,46,46	0
85	MG	6	2102	1/1	0.94	0.31	14,14,14,14	0
85	MG	CR	206	1/1	0.94	0.15	30,30,30,30	0
85	MG	CU	201	1/1	0.94	0.19	44,44,44,44	0
85	MG	CX	203	1/1	0.94	0.15	45,45,45,45	0
85	MG	6	2104	1/1	0.94	0.24	22,22,22,22	0
85	MG	6	2106	1/1	0.94	0.58	32,32,32,32	0
85	MG	1	4080	1/1	0.94	0.33	55,55,55,55	0
85	MG	1	3862	1/1	0.94	0.34	18,18,18,18	0
84	OHX	AR	3573	7/7	0.94	0.19	178,178,179,180	0
85	MG	DF	201	1/1	0.94	0.31	30,30,30,30	0
85	MG	DG	202	1/1	0.94	0.36	21,21,21,21	0
85	MG	DH	202	1/1	0.94	0.16	30,30,30,30	0
84	OHX	A	2001	7/7	0.94	0.18	185,188,189,189	0
85	MG	AR	3985	1/1	0.94	0.23	19,19,19,19	0
84	OHX	AR	3690	7/7	0.94	0.23	179,179,180,181	0
84	OHX	A	2003	7/7	0.94	0.41	196,198,199,199	0
84	OHX	1	3644	7/7	0.94	0.27	170,171,173,173	0
85	MG	sM	201	1/1	0.94	0.10	41,41,41,41	0
84	OHX	1	3547	7/7	0.94	0.20	168,169,170,170	0
85	MG	AR	3992	1/1	0.94	0.50	19,19,19,19	0
85	MG	6	2126	1/1	0.94	0.33	39,39,39,39	0
84	OHX	AR	3582	7/7	0.94	0.21	166,167,167,168	0
84	OHX	A	2011	7/7	0.94	0.17	208,209,211,211	0
85	MG	6	2129	1/1	0.94	0.22	53,53,53,53	0
85	MG	AR	3997	1/1	0.94	0.26	45,45,45,45	0
85	MG	A	2061	1/1	0.94	0.22	27,27,27,27	0
84	OHX	1	3646	7/7	0.94	0.22	182,183,184,185	0
85	MG	6	2132	1/1	0.94	0.23	38,38,38,38	0
84	OHX	AR	3700	7/7	0.94	0.37	174,175,175,176	0
84	OHX	A	2014	7/7	0.94	0.34	198,199,200,200	0
85	MG	6	2138	1/1	0.94	0.58	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	A	2071	1/1	0.94	0.32	45,45,45,45	0
84	OHX	AR	3589	7/7	0.94	0.19	186,187,188,189	0
84	OHX	6	2012	7/7	0.94	0.11	188,189,190,191	0
84	OHX	AR	3703	7/7	0.94	0.42	214,214,214,214	0
85	MG	1	3900	1/1	0.94	0.74	34,34,34,34	0
84	OHX	AR	3592	7/7	0.94	0.28	151,152,152,153	0
84	OHX	AR	3593	7/7	0.94	0.20	173,174,174,174	0
84	OHX	6	2014	7/7	0.94	0.23	219,220,221,221	0
85	MG	1	3920	1/1	0.94	0.31	29,29,29,29	0
84	OHX	1	3647	7/7	0.94	0.30	203,204,205,206	0
84	OHX	1	3570	7/7	0.94	0.15	202,203,204,205	0
85	MG	1	4116	1/1	0.94	0.12	81,81,81,81	0
84	OHX	AR	3601	7/7	0.94	0.29	171,172,173,173	0
84	OHX	1	3575	7/7	0.94	0.21	187,188,189,189	0
84	OHX	1	3578	7/7	0.94	0.24	168,170,170,171	0
84	OHX	1	3580	7/7	0.94	0.17	162,164,164,165	0
84	OHX	AR	3606	7/7	0.94	0.30	155,156,157,157	0
85	MG	A	2099	1/1	0.94	0.76	64,64,64,64	0
85	MG	1	4125	1/1	0.94	0.20	58,58,58,58	0
84	OHX	1	3548	7/7	0.94	0.20	179,180,181,181	0
84	OHX	AR	3612	7/7	0.94	0.19	182,183,184,184	0
84	OHX	1	3592	7/7	0.94	0.26	166,166,167,167	0
85	MG	1	4130	1/1	0.94	0.28	68,68,68,68	0
84	OHX	AR	3618	7/7	0.94	0.19	195,196,196,196	0
84	OHX	AR	3620	7/7	0.94	0.27	180,182,183,184	0
84	OHX	1	3550	7/7	0.94	0.15	196,197,198,199	0
85	MG	6	2172	1/1	0.94	0.20	32,32,32,32	0
85	MG	1	3953	1/1	0.94	0.29	32,32,32,32	0
84	OHX	AR	3622	7/7	0.94	0.29	203,203,204,205	0
85	MG	AR	4054	1/1	0.94	0.24	33,33,33,33	0
85	MG	6	2177	1/1	0.94	0.23	25,25,25,25	0
84	OHX	AR	3623	7/7	0.94	0.17	186,187,188,188	0
84	OHX	AR	3624	7/7	0.94	0.30	210,211,212,212	0
85	MG	1	3959	1/1	0.94	0.23	54,54,54,54	0
85	MG	6	2184	1/1	0.94	0.27	43,43,43,43	0
84	OHX	AR	3625	7/7	0.94	0.19	216,216,218,219	0
85	MG	6	2186	1/1	0.94	0.15	82,82,82,82	0
85	MG	6	2188	1/1	0.94	0.32	55,55,55,55	0
85	MG	1	4144	1/1	0.94	0.19	59,59,59,59	0
84	OHX	6	1932	7/7	0.94	0.21	129,129,131,131	0
85	MG	A	2128	1/1	0.94	0.26	53,53,53,53	0
85	MG	AR	4070	1/1	0.94	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	2192	1/1	0.94	0.63	54,54,54,54	0
85	MG	1	4149	1/1	0.94	0.22	45,45,45,45	0
85	MG	1	3962	1/1	0.94	0.25	33,33,33,33	0
84	OHX	6	1941	7/7	0.94	0.17	158,159,160,161	0
84	OHX	1	3504	7/7	0.94	0.12	154,156,157,158	0
85	MG	1	3965	1/1	0.94	0.12	32,32,32,32	0
84	OHX	AR	3633	7/7	0.94	0.32	173,173,174,174	0
85	MG	1	3967	1/1	0.94	0.16	47,47,47,47	0
84	OHX	1	3511	7/7	0.94	0.17	166,167,168,168	0
85	MG	AR	4085	1/1	0.94	0.30	37,37,37,37	0
84	OHX	6	1962	7/7	0.94	0.21	187,188,189,190	0
85	MG	AR	4088	1/1	0.94	0.15	50,50,50,50	0
84	OHX	1	3691	7/7	0.94	0.30	206,207,208,208	0
84	OHX	c8	201	7/7	0.94	0.15	198,199,200,201	0
85	MG	A	2150	1/1	0.94	0.17	52,52,52,52	0
85	MG	1	4168	1/1	0.94	0.20	51,51,51,51	0
84	OHX	6	1969	7/7	0.94	0.14	163,163,165,165	0
85	MG	1	4170	1/1	0.94	0.22	33,33,33,33	0
85	MG	AR	3744	1/1	0.94	0.47	20,20,20,20	0
85	MG	AR	4099	1/1	0.94	0.15	44,44,44,44	0
84	OHX	6	1971	7/7	0.94	0.18	177,178,179,180	0
84	OHX	6	1972	7/7	0.94	0.34	196,197,198,199	0
85	MG	s2	301	1/1	0.94	0.60	46,46,46,46	0
85	MG	AR	4102	1/1	0.94	0.32	24,24,24,24	0
84	OHX	6	1973	7/7	0.94	0.26	161,162,163,163	0
85	MG	AR	3750	1/1	0.94	0.39	19,19,19,19	0
85	MG	AR	3752	1/1	0.94	0.53	16,16,16,16	0
84	OHX	AR	3645	7/7	0.94	0.25	174,175,176,176	0
85	MG	AR	3755	1/1	0.94	0.18	34,34,34,34	0
85	MG	AR	3757	1/1	0.94	0.28	32,32,32,32	0
86	7MB	1	4216	20/20	0.94	0.20	48,48,48,48	0
84	OHX	1	3531	7/7	0.94	0.17	179,180,181,181	0
87	ZN	d7	101	1/1	0.94	0.29	176,176,176,176	0
84	OHX	1	3602	7/7	0.94	0.29	228,229,229,230	0
85	MG	AR	3837	1/1	0.95	0.17	16,16,16,16	0
84	OHX	1	3594	7/7	0.95	0.26	150,150,151,151	0
84	OHX	A	2009	7/7	0.95	0.32	191,192,194,195	0
84	OHX	A	2010	7/7	0.95	0.14	192,195,197,197	0
85	MG	AR	3846	1/1	0.95	0.57	17,17,17,17	0
85	MG	AR	3847	1/1	0.95	0.29	35,35,35,35	0
85	MG	AR	3848	1/1	0.95	0.25	15,15,15,15	0
85	MG	1	3852	1/1	0.95	0.59	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3600	7/7	0.95	0.13	172,173,173,174	0
84	OHX	1	3555	7/7	0.95	0.11	190,191,192,192	0
85	MG	AR	3857	1/1	0.95	0.14	46,46,46,46	0
85	MG	1	4066	1/1	0.95	0.28	66,66,66,66	0
85	MG	AR	3862	1/1	0.95	0.27	20,20,20,20	0
85	MG	1	4068	1/1	0.95	0.20	39,39,39,39	0
85	MG	1	3860	1/1	0.95	0.47	19,19,19,19	0
85	MG	AR	4175	1/1	0.95	0.14	27,27,27,27	0
85	MG	6	2076	1/1	0.95	0.32	18,18,18,18	0
85	MG	AR	4177	1/1	0.95	0.23	18,18,18,18	0
85	MG	6	2078	1/1	0.95	0.42	25,25,25,25	0
84	OHX	6	2030	7/7	0.95	0.38	160,161,162,162	0
84	OHX	1	3627	7/7	0.95	0.15	176,176,178,179	0
84	OHX	AR	3709	7/7	0.95	0.18	163,163,164,164	0
85	MG	1	3867	1/1	0.95	0.37	26,26,26,26	0
85	MG	1	4077	1/1	0.95	0.15	42,42,42,42	0
84	OHX	1	3596	7/7	0.95	0.29	183,184,185,185	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
84	OHX	1	3539	7/7	0.95	0.20	169,169,170,170	0
84	OHX	A	2018	7/7	0.95	0.16	214,215,216,217	0
85	MG	1	4081	1/1	0.95	0.11	35,35,35,35	0
84	OHX	1	3599	7/7	0.95	0.11	190,191,192,193	0
84	OHX	A	2020	7/7	0.95	0.17	188,191,192,192	0
85	MG	AR	3902	1/1	0.95	0.69	24,24,24,24	0
84	OHX	A	2021	7/7	0.95	0.34	176,177,179,179	0
84	OHX	6	1979	7/7	0.95	0.29	165,165,166,167	0
84	OHX	AR	3613	7/7	0.95	0.29	165,166,167,167	0
85	MG	1	4091	1/1	0.95	0.15	49,49,49,49	0
85	MG	AR	3919	1/1	0.95	0.56	11,11,11,11	0
85	MG	AR	3921	1/1	0.95	0.27	10,10,10,10	0
85	MG	1	3888	1/1	0.95	0.26	21,21,21,21	0
84	OHX	AR	3615	7/7	0.95	0.23	169,170,171,171	0
85	MG	AR	3930	1/1	0.95	0.39	14,14,14,14	0
84	OHX	1	3540	7/7	0.95	0.24	145,146,146,148	0
84	OHX	6	1981	7/7	0.95	0.34	195,197,199,199	0
85	MG	6	2108	1/1	0.95	0.29	44,44,44,44	0
85	MG	AR	3939	1/1	0.95	0.43	16,16,16,16	0
85	MG	1	4098	1/1	0.95	0.19	33,33,33,33	0
84	OHX	1	3663	7/7	0.95	0.32	214,216,217,217	0
85	MG	6	2114	1/1	0.95	0.36	28,28,28,28	0
85	MG	AR	3944	1/1	0.95	0.38	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	3945	1/1	0.95	0.43	22,22,22,22	0
84	OHX	6	1983	7/7	0.95	0.35	169,169,170,170	0
85	MG	AR	3947	1/1	0.95	0.18	26,26,26,26	0
84	OHX	1	3559	7/7	0.95	0.16	182,183,184,184	0
85	MG	1	3906	1/1	0.95	0.23	29,29,29,29	0
85	MG	1	3907	1/1	0.95	0.37	13,13,13,13	0
85	MG	1	3910	1/1	0.95	0.20	30,30,30,30	0
84	OHX	6	1986	7/7	0.95	0.12	157,157,159,159	0
84	OHX	1	3521	7/7	0.95	0.16	144,145,147,147	0
85	MG	1	3915	1/1	0.95	0.55	19,19,19,19	0
85	MG	AR	3957	1/1	0.95	0.55	37,37,37,37	0
85	MG	1	3918	1/1	0.95	0.37	26,26,26,26	0
85	MG	AS	212	1/1	0.95	0.38	13,13,13,13	0
85	MG	1	3919	1/1	0.95	0.65	30,30,30,30	0
84	OHX	1	3565	7/7	0.95	0.16	168,169,170,170	0
85	MG	6	2131	1/1	0.95	0.38	32,32,32,32	0
84	OHX	A	2033	7/7	0.95	0.19	210,212,214,214	0
85	MG	1	4114	1/1	0.95	0.13	33,33,33,33	0
84	OHX	AR	3626	7/7	0.95	0.32	204,205,205,205	0
84	OHX	A	2035	7/7	0.95	0.30	177,178,180,181	0
85	MG	AR	3966	1/1	0.95	0.24	24,24,24,24	0
85	MG	1	3937	1/1	0.95	0.29	58,58,58,58	0
84	OHX	6	1991	7/7	0.95	0.20	184,185,187,187	0
85	MG	1	4122	1/1	0.95	0.50	45,45,45,45	0
84	OHX	1	3636	7/7	0.95	0.36	170,171,172,172	0
84	OHX	AR	3631	7/7	0.95	0.15	153,155,155,155	0
84	OHX	4	203	7/7	0.95	0.25	181,182,183,184	0
84	OHX	6	1994	7/7	0.95	0.26	168,169,171,171	0
85	MG	1	3946	1/1	0.95	0.17	68,68,68,68	0
84	OHX	4	205	7/7	0.95	0.23	172,173,174,174	0
84	OHX	1	3668	7/7	0.95	0.28	179,179,180,181	0
84	OHX	6	2050	7/7	0.95	0.27	190,191,192,193	0
85	MG	1	4132	1/1	0.95	0.38	42,42,42,42	0
85	MG	AT	228	1/1	0.95	0.22	34,34,34,34	0
84	OHX	1	3543	7/7	0.95	0.14	166,166,167,167	0
84	OHX	1	3607	7/7	0.95	0.24	190,192,193,193	0
84	OHX	1	3706	7/7	0.95	0.17	144,145,146,146	0
84	OHX	1	3523	7/7	0.95	0.20	157,158,159,160	0
85	MG	6	2158	1/1	0.95	0.19	64,64,64,64	0
84	OHX	s8	301	7/7	0.95	0.33	214,216,216,218	0
84	OHX	k	402	7/7	0.95	0.20	156,157,158,158	0
85	MG	6	2161	1/1	0.95	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3673	7/7	0.95	0.16	192,193,194,194	0
84	OHX	1	3545	7/7	0.95	0.18	156,157,158,159	0
84	OHX	1	3526	7/7	0.95	0.13	167,168,169,170	0
85	MG	CQ	201	1/1	0.95	0.30	23,23,23,23	0
85	MG	1	4145	1/1	0.95	0.19	48,48,48,48	0
84	OHX	AR	3650	7/7	0.95	0.39	177,177,178,178	0
84	OHX	AR	3651	7/7	0.95	0.23	229,230,231,231	0
85	MG	6	2171	1/1	0.95	0.23	34,34,34,34	0
85	MG	AR	4002	1/1	0.95	0.41	42,42,42,42	0
85	MG	1	3734	1/1	0.95	0.32	27,27,27,27	0
85	MG	AR	4004	1/1	0.95	0.33	27,27,27,27	0
85	MG	AR	4009	1/1	0.95	0.28	25,25,25,25	0
85	MG	6	2173	1/1	0.95	0.19	69,69,69,69	0
84	OHX	AT	215	7/7	0.95	0.23	212,213,213,213	0
85	MG	AR	4013	1/1	0.95	0.34	38,38,38,38	0
84	OHX	AG	201	7/7	0.95	0.27	186,187,188,188	0
85	MG	1	4154	1/1	0.95	0.20	92,92,92,92	0
85	MG	6	2178	1/1	0.95	0.25	26,26,26,26	0
85	MG	AR	4019	1/1	0.95	0.14	29,29,29,29	0
84	OHX	AR	3653	7/7	0.95	0.31	178,178,179,179	0
84	OHX	AR	3473	7/7	0.95	0.16	121,122,122,122	0
85	MG	AR	4022	1/1	0.95	0.21	41,41,41,41	0
85	MG	1	3740	1/1	0.95	0.41	7,7,7,7	0
84	OHX	AR	3496	7/7	0.95	0.15	147,147,148,149	0
84	OHX	AR	3500	7/7	0.95	0.12	136,138,139,140	0
85	MG	1	3745	1/1	0.95	0.48	20,20,20,20	0
84	OHX	AR	3505	7/7	0.95	0.17	138,140,141,141	0
85	MG	A	2044	1/1	0.95	0.52	25,25,25,25	0
84	OHX	AR	3517	7/7	0.95	0.15	134,135,135,136	0
84	OHX	1	3612	7/7	0.95	0.24	173,174,175,175	0
84	OHX	AR	3524	7/7	0.95	0.23	152,153,154,155	0
85	MG	A	2050	1/1	0.95	0.32	68,68,68,68	0
85	MG	AR	4033	1/1	0.95	0.30	63,63,63,63	0
84	OHX	AR	3526	7/7	0.95	0.21	164,166,167,167	0
85	MG	A	2053	1/1	0.95	0.33	39,39,39,39	0
84	OHX	AR	3529	7/7	0.95	0.18	161,162,163,163	0
85	MG	1	3755	1/1	0.95	0.21	41,41,41,41	0
85	MG	A	2059	1/1	0.95	0.40	25,25,25,25	0
84	OHX	AR	3665	7/7	0.95	0.26	189,189,189,189	0
85	MG	AR	4038	1/1	0.95	0.26	30,30,30,30	0
84	OHX	6	2009	7/7	0.95	0.22	181,181,183,183	0
85	MG	6	2198	1/1	0.95	0.19	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3533	7/7	0.95	0.15	166,166,167,167	0
84	OHX	CP	501	7/7	0.95	0.23	177,178,178,178	0
84	OHX	1	3484	7/7	0.95	0.14	131,131,133,133	0
85	MG	1	3990	1/1	0.95	0.41	36,36,36,36	0
85	MG	1	3995	1/1	0.95	0.28	54,54,54,54	0
85	MG	A	2074	1/1	0.95	0.55	38,38,38,38	0
84	OHX	AR	3546	7/7	0.95	0.17	140,140,141,141	0
85	MG	AR	4049	1/1	0.95	0.09	74,74,74,74	0
85	MG	A	2079	1/1	0.95	0.58	46,46,46,46	0
84	OHX	AR	3547	7/7	0.95	0.20	147,147,147,148	0
84	OHX	A	1929	7/7	0.95	0.22	157,159,160,160	0
85	MG	AR	4053	1/1	0.95	0.27	50,50,50,50	0
84	OHX	AR	3554	7/7	0.95	0.29	159,160,161,161	0
84	OHX	AR	3555	7/7	0.95	0.17	148,149,149,150	0
84	OHX	A	1936	7/7	0.95	0.15	160,162,163,163	0
84	OHX	1	3614	7/7	0.95	0.18	199,200,201,203	0
85	MG	A	2092	1/1	0.95	0.37	87,87,87,87	0
85	MG	1	4196	1/1	0.95	0.36	35,35,35,35	0
85	MG	AR	3749	1/1	0.95	0.26	19,19,19,19	0
84	OHX	A	1945	7/7	0.95	0.16	201,203,204,205	0
84	OHX	AR	3558	7/7	0.95	0.22	159,160,160,160	0
84	OHX	A	1947	7/7	0.95	0.30	162,164,165,165	0
85	MG	1	3776	1/1	0.95	0.28	29,29,29,29	0
85	MG	AR	4065	1/1	0.95	0.17	54,54,54,54	0
85	MG	AR	4067	1/1	0.95	0.28	98,98,98,98	0
85	MG	AR	3756	1/1	0.95	0.71	11,11,11,11	0
85	MG	1	4009	1/1	0.95	0.40	41,41,41,41	0
85	MG	AR	3758	1/1	0.95	0.34	81,81,81,81	0
84	OHX	A	1951	7/7	0.95	0.20	203,205,207,207	0
85	MG	1	4210	1/1	0.95	0.31	32,32,32,32	0
84	OHX	AR	3559	7/7	0.95	0.14	177,178,179,179	0
85	MG	1	4214	1/1	0.95	0.17	50,50,50,50	0
84	OHX	1	3534	7/7	0.95	0.18	148,149,149,150	0
84	OHX	1	3581	7/7	0.95	0.24	153,153,154,154	0
85	MG	3	212	1/1	0.95	0.30	27,27,27,27	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	AR	3566	7/7	0.95	0.17	205,206,207,207	0
84	OHX	A	1970	7/7	0.95	0.31	178,180,182,182	0
84	OHX	AR	3567	7/7	0.95	0.16	159,159,160,160	0
85	MG	AR	3776	1/1	0.95	0.17	32,32,32,32	0
84	OHX	A	1974	7/7	0.95	0.10	196,198,200,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	3780	1/1	0.95	0.27	20,20,20,20	0
84	OHX	AR	3570	7/7	0.95	0.17	161,162,163,163	0
85	MG	3	220	1/1	0.95	0.34	31,31,31,31	0
84	OHX	AR	3571	7/7	0.95	0.18	194,194,195,195	0
85	MG	4	214	1/1	0.95	0.46	18,18,18,18	0
85	MG	AR	3789	1/1	0.95	0.24	36,36,36,36	0
85	MG	1	4026	1/1	0.95	0.54	44,44,44,44	0
84	OHX	6	1954	7/7	0.95	0.11	181,182,184,185	0
85	MG	1	3799	1/1	0.95	0.30	28,28,28,28	0
84	OHX	1	3716	7/7	0.95	0.17	205,206,208,209	0
84	OHX	A	1982	7/7	0.95	0.29	164,166,167,167	0
85	MG	AR	3797	1/1	0.95	0.38	18,18,18,18	0
84	OHX	6	2019	7/7	0.95	0.31	191,192,193,194	0
84	OHX	6	2020	7/7	0.95	0.23	177,178,179,179	0
85	MG	4	228	1/1	0.95	0.59	42,42,42,42	0
84	OHX	AR	3584	7/7	0.95	0.36	169,169,170,171	0
84	OHX	6	1958	7/7	0.95	0.21	153,153,155,156	0
84	OHX	AR	3588	7/7	0.95	0.16	176,177,178,178	0
84	OHX	1	3584	7/7	0.95	0.29	154,155,156,156	0
84	OHX	AR	3590	7/7	0.95	0.19	172,173,173,173	0
85	MG	AR	3810	1/1	0.95	0.29	28,28,28,28	0
85	MG	1	3818	1/1	0.95	0.39	19,19,19,19	0
85	MG	l	403	1/1	0.95	0.26	20,20,20,20	0
84	OHX	A	1998	7/7	0.95	0.19	213,217,219,219	0
85	MG	AR	4129	1/1	0.95	0.32	21,21,21,21	0
84	OHX	1	3512	7/7	0.95	0.12	170,172,172,173	0
84	OHX	1	3620	7/7	0.95	0.28	208,208,209,209	0
85	MG	1	3826	1/1	0.95	0.26	44,44,44,44	0
85	MG	1	3829	1/1	0.95	0.38	25,25,25,25	0
85	MG	s6	301	1/1	0.95	0.26	64,64,64,64	0
85	MG	AR	4137	1/1	0.95	0.16	57,57,57,57	0
84	OHX	AR	3699	7/7	0.95	0.38	194,195,196,196	0
85	MG	w	201	1/1	0.95	0.17	33,33,33,33	0
85	MG	1	4049	1/1	0.95	0.18	36,36,36,36	0
85	MG	x	204	1/1	0.95	0.15	18,18,18,18	0
84	OHX	6	1966	7/7	0.95	0.14	164,165,166,167	0
84	OHX	AR	3594	7/7	0.95	0.17	169,170,171,171	0
84	OHX	A	2004	7/7	0.95	0.22	192,194,196,196	0
85	MG	1	4053	1/1	0.95	0.18	32,32,32,32	0
84	OHX	1	3537	7/7	0.95	0.25	160,161,162,162	0
84	OHX	1	3593	7/7	0.95	0.15	206,207,208,209	0
85	MG	AR	4116	1/1	0.96	0.29	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	6	1950	7/7	0.96	0.12	171,171,173,174	0
85	MG	AR	3798	1/1	0.96	0.39	21,21,21,21	0
85	MG	4	216	1/1	0.96	0.20	42,42,42,42	0
85	MG	AR	3802	1/1	0.96	0.58	16,16,16,16	0
84	OHX	6	1952	7/7	0.96	0.13	183,184,185,186	0
84	OHX	A	1941	7/7	0.96	0.17	195,197,198,198	0
85	MG	4	219	1/1	0.96	0.39	24,24,24,24	0
84	OHX	1	3604	7/7	0.96	0.08	204,205,206,206	0
84	OHX	1	3462	7/7	0.96	0.16	115,116,117,118	0
84	OHX	AR	3560	7/7	0.96	0.12	173,174,175,175	0
85	MG	1	3777	1/1	0.96	0.26	40,40,40,40	0
84	OHX	AR	3561	7/7	0.96	0.19	171,171,172,172	0
85	MG	1	4018	1/1	0.96	0.24	26,26,26,26	0
85	MG	1	4020	1/1	0.96	0.12	38,38,38,38	0
84	OHX	A	1948	7/7	0.96	0.09	166,169,170,170	0
85	MG	1	4022	1/1	0.96	0.18	24,24,24,24	0
84	OHX	A	1949	7/7	0.96	0.11	165,167,169,169	0
85	MG	k	404	1/1	0.96	0.44	71,71,71,71	0
84	OHX	AR	3563	7/7	0.96	0.17	173,173,174,174	0
84	OHX	A	1952	7/7	0.96	0.25	181,183,185,185	0
84	OHX	A	1953	7/7	0.96	0.18	180,182,184,184	0
85	MG	AR	4144	1/1	0.96	0.15	35,35,35,35	0
85	MG	AR	3825	1/1	0.96	0.18	30,30,30,30	0
85	MG	o	302	1/1	0.96	0.23	27,27,27,27	0
84	OHX	A	1954	7/7	0.96	0.20	172,174,175,175	0
84	OHX	1	3466	7/7	0.96	0.18	120,121,122,123	0
84	OHX	1	3677	7/7	0.96	0.14	170,171,171,171	0
85	MG	1	3790	1/1	0.96	0.52	15,15,15,15	0
85	MG	1	3794	1/1	0.96	0.22	31,31,31,31	0
85	MG	AR	3833	1/1	0.96	0.15	37,37,37,37	0
84	OHX	6	1961	7/7	0.96	0.15	152,153,154,155	0
84	OHX	A	1962	7/7	0.96	0.14	175,176,177,178	0
84	OHX	A	1964	7/7	0.96	0.29	168,169,170,170	0
84	OHX	1	3517	7/7	0.96	0.17	141,142,143,143	0
85	MG	1	3800	1/1	0.96	0.40	37,37,37,37	0
84	OHX	A	1967	7/7	0.96	0.14	167,168,169,170	0
85	MG	AR	4163	1/1	0.96	0.12	30,30,30,30	0
84	OHX	A	1968	7/7	0.96	0.20	168,170,171,172	0
85	MG	1	3803	1/1	0.96	0.23	22,22,22,22	0
85	MG	AR	4168	1/1	0.96	0.32	45,45,45,45	0
84	OHX	AR	3568	7/7	0.96	0.17	162,163,164,165	0
85	MG	6	2061	1/1	0.96	0.21	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3569	7/7	0.96	0.10	182,182,183,183	0
85	MG	AR	3853	1/1	0.96	0.58	17,17,17,17	0
85	MG	AR	3854	1/1	0.96	0.21	28,28,28,28	0
84	OHX	1	3643	7/7	0.96	0.14	192,193,194,194	0
84	OHX	A	1973	7/7	0.96	0.15	201,204,206,208	0
84	OHX	1	3567	7/7	0.96	0.23	177,178,178,179	0
85	MG	AR	3860	1/1	0.96	0.47	6,6,6,6	0
85	MG	AR	3861	1/1	0.96	0.42	16,16,16,16	0
85	MG	6	2070	1/1	0.96	0.56	17,17,17,17	0
85	MG	AR	3863	1/1	0.96	0.60	15,15,15,15	0
85	MG	AR	4182	1/1	0.96	0.47	48,48,48,48	0
84	OHX	A	1976	7/7	0.96	0.16	165,166,167,168	0
85	MG	AR	3867	1/1	0.96	0.50	13,13,13,13	0
85	MG	AR	3868	1/1	0.96	0.13	33,33,33,33	0
85	MG	AR	3869	1/1	0.96	0.40	12,12,12,12	0
85	MG	AR	3871	1/1	0.96	0.50	20,20,20,20	0
85	MG	AR	3873	1/1	0.96	0.31	23,23,23,23	0
84	OHX	AR	3572	7/7	0.96	0.20	174,175,176,176	0
85	MG	1	3813	1/1	0.96	0.18	24,24,24,24	0
84	OHX	6	1967	7/7	0.96	0.13	157,159,160,160	0
84	OHX	A	1979	7/7	0.96	0.15	200,203,204,205	0
85	MG	AR	4198	1/1	0.96	0.24	34,34,34,34	0
84	OHX	AR	3575	7/7	0.96	0.21	156,158,159,159	0
85	MG	1	3823	1/1	0.96	0.20	51,51,51,51	0
84	OHX	AR	3576	7/7	0.96	0.14	168,169,169,170	0
84	OHX	AR	3683	7/7	0.96	0.36	178,179,179,180	0
84	OHX	A	1983	7/7	0.96	0.20	188,190,192,192	0
84	OHX	1	3470	7/7	0.96	0.13	141,142,143,143	0
85	MG	AR	3892	1/1	0.96	0.44	19,19,19,19	0
84	OHX	A	1986	7/7	0.96	0.25	215,218,220,222	0
84	OHX	A	1988	7/7	0.96	0.12	158,160,162,162	0
85	MG	6	2086	1/1	0.96	0.24	49,49,49,49	0
85	MG	AR	3898	1/1	0.96	0.42	16,16,16,16	0
84	OHX	AR	3579	7/7	0.96	0.13	183,184,185,185	0
85	MG	AR	3900	1/1	0.96	0.33	29,29,29,29	0
85	MG	1	4067	1/1	0.96	0.19	24,24,24,24	0
85	MG	1	3835	1/1	0.96	0.29	19,19,19,19	0
85	MG	1	4069	1/1	0.96	0.18	39,39,39,39	0
84	OHX	A	1990	7/7	0.96	0.42	212,215,216,216	0
84	OHX	1	3610	7/7	0.96	0.28	212,212,212,212	0
85	MG	1	3841	1/1	0.96	0.31	19,19,19,19	0
85	MG	AR	3920	1/1	0.96	0.34	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	4074	1/1	0.96	0.15	45,45,45,45	0
85	MG	AR	4224	1/1	0.96	0.25	26,26,26,26	0
85	MG	6	2096	1/1	0.96	0.38	48,48,48,48	0
85	MG	AR	4229	1/1	0.96	0.46	23,23,23,23	0
84	OHX	A	1992	7/7	0.96	0.13	167,169,170,171	0
85	MG	6	2098	1/1	0.96	0.23	38,38,38,38	0
85	MG	1	3844	1/1	0.96	0.44	9,9,9,9	0
84	OHX	1	3522	7/7	0.96	0.15	133,134,134,135	0
84	OHX	A	1994	7/7	0.96	0.23	200,203,204,205	0
85	MG	6	2105	1/1	0.96	0.34	24,24,24,24	0
84	OHX	1	3685	7/7	0.96	0.16	173,173,175,175	0
85	MG	6	2107	1/1	0.96	0.41	24,24,24,24	0
85	MG	AS	211	1/1	0.96	0.29	22,22,22,22	0
84	OHX	AR	3585	7/7	0.96	0.16	165,166,167,167	0
85	MG	1	3854	1/1	0.96	0.40	13,13,13,13	0
84	OHX	1	3441	7/7	0.96	0.17	168,169,169,170	0
85	MG	6	2112	1/1	0.96	0.54	25,25,25,25	0
84	OHX	AR	3691	7/7	0.96	0.45	170,171,172,172	0
85	MG	6	2115	1/1	0.96	0.36	36,36,36,36	0
85	MG	AR	3949	1/1	0.96	0.38	19,19,19,19	0
84	OHX	AR	3692	7/7	0.96	0.34	184,186,186,187	0
84	OHX	AR	3587	7/7	0.96	0.19	175,176,177,177	0
84	OHX	1	3576	7/7	0.96	0.14	189,189,191,191	0
85	MG	AS	225	1/1	0.96	0.15	67,67,67,67	0
85	MG	6	2122	1/1	0.96	0.18	48,48,48,48	0
84	OHX	1	3546	7/7	0.96	0.19	147,148,149,150	0
84	OHX	1	3690	7/7	0.96	0.28	174,175,176,176	0
84	OHX	1	3458	7/7	0.96	0.14	131,132,133,133	0
84	OHX	1	3616	7/7	0.96	0.22	177,177,178,178	0
84	OHX	1	3528	7/7	0.96	0.14	169,170,171,171	0
85	MG	AT	222	1/1	0.96	0.43	35,35,35,35	0
84	OHX	3	202	7/7	0.96	0.13	176,177,177,178	0
84	OHX	AR	3596	7/7	0.96	0.30	208,209,210,211	0
85	MG	1	3881	1/1	0.96	0.31	35,35,35,35	0
84	OHX	3	203	7/7	0.96	0.14	143,144,145,145	0
84	OHX	1	3549	7/7	0.96	0.13	190,190,191,192	0
84	OHX	3	206	7/7	0.96	0.09	176,177,179,179	0
85	MG	AT	229	1/1	0.96	0.33	30,30,30,30	0
85	MG	1	3890	1/1	0.96	0.39	23,23,23,23	0
85	MG	CD	301	1/1	0.96	0.20	28,28,28,28	0
85	MG	6	2137	1/1	0.96	0.40	82,82,82,82	0
85	MG	CE	401	1/1	0.96	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	6	1987	7/7	0.96	0.15	179,179,180,181	0
85	MG	1	3894	1/1	0.96	0.42	26,26,26,26	0
84	OHX	6	1988	7/7	0.96	0.12	191,193,195,195	0
85	MG	6	2141	1/1	0.96	0.21	56,56,56,56	0
84	OHX	1	3585	7/7	0.96	0.24	173,174,174,175	0
84	OHX	1	3586	7/7	0.96	0.17	182,183,185,186	0
84	OHX	AR	3604	7/7	0.96	0.15	150,151,151,151	0
85	MG	AR	3975	1/1	0.96	0.27	31,31,31,31	0
85	MG	1	3902	1/1	0.96	0.52	4,4,4,4	0
84	OHX	4	201	7/7	0.96	0.16	143,143,144,144	0
85	MG	AR	3978	1/1	0.96	0.26	20,20,20,20	0
85	MG	1	3905	1/1	0.96	0.59	14,14,14,14	0
85	MG	6	2149	1/1	0.96	0.32	75,75,75,75	0
85	MG	AR	3981	1/1	0.96	0.18	17,17,17,17	0
84	OHX	1	3529	7/7	0.96	0.22	143,144,145,146	0
84	OHX	AR	3608	7/7	0.96	0.32	186,187,188,188	0
84	OHX	AR	3715	7/7	0.96	0.21	144,146,147,147	0
85	MG	1	3911	1/1	0.96	0.33	20,20,20,20	0
84	OHX	4	204	7/7	0.96	0.28	160,160,161,161	0
84	OHX	AR	3611	7/7	0.96	0.33	194,196,197,197	0
85	MG	DC	201	1/1	0.96	0.36	16,16,16,16	0
84	OHX	1	3589	7/7	0.96	0.15	179,180,181,181	0
85	MG	1	3916	1/1	0.96	0.50	14,14,14,14	0
84	OHX	1	3492	7/7	0.96	0.15	127,128,128,128	0
84	OHX	4	208	7/7	0.96	0.27	187,187,188,188	0
84	OHX	1	3624	7/7	0.96	0.20	171,172,173,174	0
85	MG	1	3921	1/1	0.96	0.23	45,45,45,45	0
85	MG	6	2162	1/1	0.96	0.31	69,69,69,69	0
85	MG	6	2163	1/1	0.96	0.12	60,60,60,60	0
85	MG	1	3923	1/1	0.96	0.50	7,7,7,7	0
85	MG	6	2165	1/1	0.96	0.28	45,45,45,45	0
85	MG	1	3926	1/1	0.96	0.54	21,21,21,21	0
85	MG	1	3927	1/1	0.96	0.50	6,6,6,6	0
85	MG	AR	4005	1/1	0.96	0.35	24,24,24,24	0
85	MG	A	2043	1/1	0.96	0.26	47,47,47,47	0
85	MG	AR	4008	1/1	0.96	0.16	33,33,33,33	0
85	MG	1	3928	1/1	0.96	0.13	32,32,32,32	0
84	OHX	1	3552	7/7	0.96	0.20	173,174,175,175	0
85	MG	AR	4011	1/1	0.96	0.47	31,31,31,31	0
84	OHX	AR	3619	7/7	0.96	0.28	169,169,170,170	0
85	MG	1	4139	1/1	0.96	0.18	29,29,29,29	0
84	OHX	1	3533	7/7	0.96	0.19	196,197,198,199	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3935	1/1	0.96	0.24	24,24,24,24	0
85	MG	AR	4017	1/1	0.96	0.17	27,27,27,27	0
84	OHX	1	3554	7/7	0.96	0.22	167,168,169,169	0
85	MG	A	2058	1/1	0.96	0.48	27,27,27,27	0
84	OHX	AR	3466	7/7	0.96	0.17	114,115,116,116	0
84	OHX	AR	3472	7/7	0.96	0.12	129,130,130,130	0
84	OHX	1	3629	7/7	0.96	0.14	161,162,162,163	0
84	OHX	AR	3477	7/7	0.96	0.18	119,119,119,120	0
84	OHX	AR	3492	7/7	0.96	0.16	134,135,135,135	0
85	MG	1	4151	1/1	0.96	0.15	53,53,53,53	0
84	OHX	AR	3494	7/7	0.96	0.23	144,145,146,146	0
85	MG	A	2070	1/1	0.96	0.49	59,59,59,59	0
84	OHX	AR	3495	7/7	0.96	0.14	163,165,166,166	0
84	OHX	AR	3630	7/7	0.96	0.10	172,173,174,175	0
84	OHX	6	2003	7/7	0.96	0.18	180,182,183,184	0
84	OHX	AR	3499	7/7	0.96	0.14	130,131,133,133	0
85	MG	AR	4031	1/1	0.96	0.25	31,31,31,31	0
84	OHX	1	3501	7/7	0.96	0.16	123,124,125,125	0
85	MG	A	2077	1/1	0.96	0.19	25,25,25,25	0
84	OHX	1	3535	7/7	0.96	0.10	196,198,199,200	0
85	MG	A	2080	1/1	0.96	0.52	45,45,45,45	0
85	MG	A	2081	1/1	0.96	0.41	48,48,48,48	0
85	MG	A	2082	1/1	0.96	0.19	65,65,65,65	0
85	MG	A	2083	1/1	0.96	0.37	62,62,62,62	0
85	MG	1	3954	1/1	0.96	0.16	45,45,45,45	0
84	OHX	AR	3635	7/7	0.96	0.33	173,175,175,175	0
85	MG	1	3956	1/1	0.96	0.22	15,15,15,15	0
85	MG	1	4164	1/1	0.96	0.16	48,48,48,48	0
84	OHX	AR	3739	7/7	0.96	0.37	151,152,152,152	0
84	OHX	AR	3636	7/7	0.96	0.17	187,188,188,189	0
85	MG	A	2090	1/1	0.96	0.28	46,46,46,46	0
84	OHX	AR	3508	7/7	0.96	0.21	139,139,140,140	0
84	OHX	AR	3514	7/7	0.96	0.26	146,147,147,148	0
85	MG	1	4172	1/1	0.96	0.16	76,76,76,76	0
84	OHX	AT	206	7/7	0.96	0.17	155,155,156,156	0
84	OHX	AT	209	7/7	0.96	0.18	163,163,163,163	0
85	MG	AR	4045	1/1	0.96	0.12	33,33,33,33	0
85	MG	AR	4046	1/1	0.96	0.19	45,45,45,45	0
85	MG	AK	104	1/1	0.96	0.39	44,44,44,44	0
84	OHX	AR	3516	7/7	0.96	0.09	174,176,178,178	0
84	OHX	AT	212	7/7	0.96	0.16	160,160,161,161	0
85	MG	AR	3741	1/1	0.96	0.24	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AT	213	7/7	0.96	0.11	175,176,176,177	0
85	MG	1	3732	1/1	0.96	0.31	27,27,27,27	0
84	OHX	1	3598	7/7	0.96	0.13	173,173,174,175	0
85	MG	A	2108	1/1	0.96	0.39	39,39,39,39	0
84	OHX	1	3669	7/7	0.96	0.23	125,126,127,127	0
84	OHX	AR	3642	7/7	0.96	0.28	189,189,191,191	0
85	MG	AR	4057	1/1	0.96	0.17	46,46,46,46	0
85	MG	1	3970	1/1	0.96	0.25	59,59,59,59	0
84	OHX	AT	217	7/7	0.96	0.24	184,185,185,186	0
84	OHX	AR	3643	7/7	0.96	0.28	157,158,159,160	0
85	MG	1	4186	1/1	0.96	0.27	51,51,51,51	0
84	OHX	1	3432	7/7	0.96	0.15	131,131,132,132	0
85	MG	1	3739	1/1	0.96	0.46	15,15,15,15	0
84	OHX	1	3558	7/7	0.96	0.19	166,167,168,168	0
85	MG	1	4193	1/1	0.96	0.37	9,9,9,9	0
84	OHX	6	1914	7/7	0.96	0.14	119,120,121,123	0
85	MG	AR	4068	1/1	0.96	0.18	25,25,25,25	0
84	OHX	1	3507	7/7	0.96	0.17	149,149,150,150	0
85	MG	AR	3760	1/1	0.96	0.39	21,21,21,21	0
85	MG	AR	3761	1/1	0.96	0.10	41,41,41,41	0
85	MG	1	3744	1/1	0.96	0.73	43,43,43,43	0
85	MG	AR	4073	1/1	0.96	0.15	33,33,33,33	0
84	OHX	6	1936	7/7	0.96	0.18	145,146,146,146	0
84	OHX	AR	3649	7/7	0.96	0.30	207,208,208,208	0
85	MG	AR	4076	1/1	0.96	0.16	38,38,38,38	0
85	MG	AR	3768	1/1	0.96	0.24	23,23,23,23	0
84	OHX	AR	3535	7/7	0.96	0.14	157,157,158,158	0
85	MG	1	3748	1/1	0.96	0.25	23,23,23,23	0
84	OHX	AR	3538	7/7	0.96	0.20	184,185,186,186	0
85	MG	AR	4083	1/1	0.96	0.35	23,23,23,23	0
85	MG	1	4208	1/1	0.96	0.30	30,30,30,30	0
84	OHX	6	1940	7/7	0.96	0.15	149,151,152,153	0
84	OHX	AR	3540	7/7	0.96	0.16	151,152,153,154	0
85	MG	AR	4087	1/1	0.96	0.35	31,31,31,31	0
84	OHX	AR	3541	7/7	0.96	0.12	170,171,172,174	0
84	OHX	AR	3545	7/7	0.96	0.23	181,182,182,183	0
85	MG	AR	3777	1/1	0.96	0.14	50,50,50,50	0
85	MG	1	4221	1/1	0.96	0.36	22,22,22,22	0
85	MG	AR	4094	1/1	0.96	0.14	38,38,38,38	0
85	MG	1	3756	1/1	0.96	0.15	22,22,22,22	0
85	MG	AR	3781	1/1	0.96	0.34	11,11,11,11	0
84	OHX	1	3561	7/7	0.96	0.14	184,184,185,186	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4098	1/1	0.96	0.18	27,27,27,27	0
84	OHX	6	2018	7/7	0.96	0.27	186,187,188,189	0
84	OHX	DH	201	7/7	0.96	0.13	155,156,157,157	0
84	OHX	AR	3549	7/7	0.96	0.19	156,157,158,158	0
84	OHX	AR	3550	7/7	0.96	0.17	164,164,165,165	0
84	OHX	A	1927	7/7	0.96	0.12	158,160,162,162	0
85	MG	c6	201	1/1	0.96	0.16	67,67,67,67	0
84	OHX	A	1928	7/7	0.96	0.12	156,158,159,159	0
85	MG	d3	201	1/1	0.96	0.13	48,48,48,48	0
85	MG	AR	4106	1/1	0.96	0.19	55,55,55,55	0
84	OHX	6	1947	7/7	0.96	0.12	142,144,145,145	0
84	OHX	A	1931	7/7	0.96	0.11	166,168,169,169	0
85	MG	AR	4109	1/1	0.96	0.23	42,42,42,42	0
85	MG	AR	4111	1/1	0.96	0.60	48,48,48,48	0
85	MG	AR	4112	1/1	0.96	0.13	70,70,70,70	0
85	MG	AR	4113	1/1	0.96	0.30	17,17,17,17	0
87	ZN	g	501	1/1	0.96	0.04	143,143,143,143	0
84	OHX	AR	3662	7/7	0.96	0.19	168,169,169,170	0
85	MG	AR	4115	1/1	0.96	0.34	64,64,64,64	0
85	MG	AR	4150	1/1	0.97	0.12	49,49,49,49	0
85	MG	1	4087	1/1	0.97	0.13	37,37,37,37	0
85	MG	AR	3874	1/1	0.97	0.31	18,18,18,18	0
84	OHX	AR	3515	7/7	0.97	0.16	159,160,161,162	0
84	OHX	6	2007	7/7	0.97	0.15	148,150,151,151	0
85	MG	AR	3877	1/1	0.97	0.39	14,14,14,14	0
84	OHX	1	3530	7/7	0.97	0.13	151,151,151,152	0
85	MG	6	2100	1/1	0.97	0.44	16,16,16,16	0
85	MG	6	2101	1/1	0.97	0.28	37,37,37,37	0
85	MG	AR	4160	1/1	0.97	0.26	31,31,31,31	0
84	OHX	AR	3518	7/7	0.97	0.16	161,162,163,163	0
84	OHX	AT	207	7/7	0.97	0.10	162,163,164,164	0
84	OHX	AT	208	7/7	0.97	0.12	154,154,155,155	0
84	OHX	6	1933	7/7	0.97	0.14	121,122,123,123	0
85	MG	AR	4165	1/1	0.97	0.07	88,88,88,88	0
85	MG	AR	3890	1/1	0.97	0.50	33,33,33,33	0
84	OHX	AT	210	7/7	0.97	0.11	164,164,165,165	0
84	OHX	AR	3522	7/7	0.97	0.14	134,135,136,136	0
85	MG	6	2109	1/1	0.97	0.24	39,39,39,39	0
85	MG	AR	3894	1/1	0.97	0.50	24,24,24,24	0
84	OHX	AR	3523	7/7	0.97	0.23	175,176,176,177	0
84	OHX	1	3500	7/7	0.97	0.07	156,157,159,159	0
85	MG	AR	4174	1/1	0.97	0.21	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3525	7/7	0.97	0.13	150,151,151,152	0
85	MG	6	2113	1/1	0.97	0.42	23,23,23,23	0
84	OHX	6	1938	7/7	0.97	0.13	145,146,148,148	0
85	MG	AR	3901	1/1	0.97	0.26	17,17,17,17	0
85	MG	1	4104	1/1	0.97	0.22	32,32,32,32	0
85	MG	AR	3904	1/1	0.97	0.73	11,11,11,11	0
85	MG	AR	3905	1/1	0.97	0.52	24,24,24,24	0
85	MG	1	3908	1/1	0.97	0.36	14,14,14,14	0
85	MG	6	2118	1/1	0.97	0.25	54,54,54,54	0
85	MG	6	2119	1/1	0.97	0.36	31,31,31,31	0
85	MG	1	3909	1/1	0.97	0.19	24,24,24,24	0
84	OHX	AR	3528	7/7	0.97	0.11	147,147,148,149	0
84	OHX	1	3477	7/7	0.97	0.13	118,119,120,120	0
84	OHX	6	2013	7/7	0.97	0.20	149,151,152,153	0
85	MG	AR	3922	1/1	0.97	0.36	20,20,20,20	0
84	OHX	1	3503	7/7	0.97	0.19	145,146,147,148	0
85	MG	AR	3924	1/1	0.97	0.47	13,13,13,13	0
85	MG	AR	4195	1/1	0.97	0.17	21,21,21,21	0
85	MG	AR	3925	1/1	0.97	0.38	14,14,14,14	0
84	OHX	AR	3534	7/7	0.97	0.12	162,163,164,165	0
84	OHX	CE	402	7/7	0.97	0.12	142,143,144,144	0
85	MG	AR	4200	1/1	0.97	0.57	30,30,30,30	0
84	OHX	6	1943	7/7	0.97	0.11	147,149,150,150	0
85	MG	AR	3934	1/1	0.97	0.37	14,14,14,14	0
85	MG	AR	3935	1/1	0.97	0.28	22,22,22,22	0
84	OHX	AR	3536	7/7	0.97	0.17	141,141,142,142	0
84	OHX	6	1945	7/7	0.97	0.16	149,150,151,152	0
84	OHX	6	2017	7/7	0.97	0.20	158,159,160,161	0
85	MG	AR	3940	1/1	0.97	0.10	34,34,34,34	0
85	MG	1	3922	1/1	0.97	0.50	15,15,15,15	0
84	OHX	T	201	7/7	0.97	0.13	133,135,137,138	0
84	OHX	e	101	7/7	0.97	0.22	205,208,210,210	0
84	OHX	h	401	7/7	0.97	0.09	203,206,208,210	0
85	MG	6	2136	1/1	0.97	0.25	29,29,29,29	0
84	OHX	6	1946	7/7	0.97	0.12	160,161,163,164	0
85	MG	1	3929	1/1	0.97	0.43	20,20,20,20	0
84	OHX	1	3482	7/7	0.97	0.14	116,116,117,117	0
84	OHX	AR	3543	7/7	0.97	0.17	181,181,182,182	0
84	OHX	CL	301	7/7	0.97	0.10	165,166,167,168	0
84	OHX	AR	3544	7/7	0.97	0.11	177,178,179,179	0
85	MG	1	3936	1/1	0.97	0.13	48,48,48,48	0
84	OHX	6	1949	7/7	0.97	0.13	165,167,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	3954	1/1	0.97	0.34	36,36,36,36	0
85	MG	AR	4225	1/1	0.97	0.25	23,23,23,23	0
84	OHX	1	3467	7/7	0.97	0.13	124,125,126,126	0
85	MG	AR	4227	1/1	0.97	0.53	18,18,18,18	0
85	MG	AR	4228	1/1	0.97	0.31	12,12,12,12	0
84	OHX	6	1951	7/7	0.97	0.14	165,167,169,170	0
84	OHX	1	3637	7/7	0.97	0.21	180,181,181,181	0
85	MG	AR	4231	1/1	0.97	0.33	9,9,9,9	0
85	MG	AR	4232	1/1	0.97	0.26	33,33,33,33	0
84	OHX	6	1953	7/7	0.97	0.13	154,155,157,158	0
85	MG	1	3942	1/1	0.97	0.37	20,20,20,20	0
85	MG	AR	4235	1/1	0.97	0.40	15,15,15,15	0
85	MG	1	3943	1/1	0.97	0.32	22,22,22,22	0
85	MG	AR	4238	1/1	0.97	0.47	27,27,27,27	0
85	MG	1	3944	1/1	0.97	0.33	33,33,33,33	0
84	OHX	AR	3551	7/7	0.97	0.19	161,162,163,164	0
84	OHX	DL	101	7/7	0.97	0.14	144,144,144,144	0
84	OHX	1	3562	7/7	0.97	0.08	200,200,201,202	0
85	MG	1	3948	1/1	0.97	0.40	46,46,46,46	0
84	OHX	A	1918	7/7	0.97	0.17	120,122,123,123	0
85	MG	AS	213	1/1	0.97	0.23	40,40,40,40	0
85	MG	1	4147	1/1	0.97	0.25	28,28,28,28	0
84	OHX	A	1920	7/7	0.97	0.13	141,142,143,144	0
85	MG	1	3741	1/1	0.97	0.21	40,40,40,40	0
84	OHX	A	1921	7/7	0.97	0.17	139,141,143,143	0
84	OHX	A	1925	7/7	0.97	0.09	171,172,174,175	0
84	OHX	1	3639	7/7	0.97	0.30	201,203,203,204	0
84	OHX	1	3563	7/7	0.97	0.14	151,152,152,152	0
85	MG	1	4155	1/1	0.97	0.48	66,66,66,66	0
84	OHX	1	3485	7/7	0.97	0.19	151,152,153,153	0
84	OHX	A	1930	7/7	0.97	0.16	164,165,166,167	0
84	OHX	1	3486	7/7	0.97	0.12	146,146,147,147	0
84	OHX	1	3603	7/7	0.97	0.34	162,162,164,164	0
85	MG	1	3750	1/1	0.97	0.09	70,70,70,70	0
84	OHX	A	1933	7/7	0.97	0.12	154,155,156,157	0
85	MG	AS	230	1/1	0.97	0.27	67,67,67,67	0
84	OHX	6	1963	7/7	0.97	0.15	159,159,161,161	0
84	OHX	A	1935	7/7	0.97	0.13	191,193,195,195	0
85	MG	AR	3983	1/1	0.97	0.28	24,24,24,24	0
84	OHX	1	3684	7/7	0.97	0.22	170,171,172,173	0
84	OHX	A	1937	7/7	0.97	0.14	152,154,157,157	0
85	MG	6	2176	1/1	0.97	0.16	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	A	1940	7/7	0.97	0.16	174,175,177,178	0
84	OHX	6	1965	7/7	0.97	0.27	161,162,163,163	0
84	OHX	1	3513	7/7	0.97	0.13	140,141,142,142	0
85	MG	AR	3991	1/1	0.97	0.26	15,15,15,15	0
85	MG	6	2180	1/1	0.97	0.16	94,94,94,94	0
85	MG	1	4173	1/1	0.97	0.14	33,33,33,33	0
84	OHX	A	1944	7/7	0.97	0.11	161,163,165,165	0
84	OHX	AR	3672	7/7	0.97	0.32	137,138,138,138	0
85	MG	1	3973	1/1	0.97	0.26	33,33,33,33	0
84	OHX	1	3541	7/7	0.97	0.12	154,155,156,156	0
84	OHX	6	1968	7/7	0.97	0.17	145,146,147,148	0
85	MG	AR	3999	1/1	0.97	0.37	28,28,28,28	0
85	MG	AR	4000	1/1	0.97	0.38	30,30,30,30	0
84	OHX	1	3514	7/7	0.97	0.13	148,148,149,149	0
84	OHX	1	3730	7/7	0.97	0.13	141,142,143,143	0
84	OHX	A	1950	7/7	0.97	0.17	168,169,170,171	0
84	OHX	1	3569	7/7	0.97	0.27	166,166,167,168	0
84	OHX	1	3689	7/7	0.97	0.14	140,141,142,142	0
85	MG	AR	4006	1/1	0.97	0.10	33,33,33,33	0
85	MG	AR	4007	1/1	0.97	0.11	23,23,23,23	0
85	MG	CQ	204	1/1	0.97	0.33	48,48,48,48	0
85	MG	1	3770	1/1	0.97	0.47	11,11,11,11	0
85	MG	CR	202	1/1	0.97	0.20	20,20,20,20	0
84	OHX	1	3515	7/7	0.97	0.13	128,128,129,129	0
84	OHX	6	1975	7/7	0.97	0.16	160,161,162,162	0
84	OHX	A	1955	7/7	0.97	0.11	145,148,150,150	0
84	OHX	A	1956	7/7	0.97	0.13	171,173,174,175	0
84	OHX	A	1957	7/7	0.97	0.18	169,171,172,173	0
85	MG	CU	202	1/1	0.97	0.20	31,31,31,31	0
85	MG	CX	202	1/1	0.97	0.32	6,6,6,6	0
85	MG	AB	204	1/1	0.97	0.27	42,42,42,42	0
84	OHX	AR	3574	7/7	0.97	0.27	171,172,173,173	0
84	OHX	1	3572	7/7	0.97	0.28	168,168,169,170	0
85	MG	1	4195	1/1	0.97	0.37	52,52,52,52	0
84	OHX	1	3573	7/7	0.97	0.10	196,196,197,197	0
85	MG	1	4197	1/1	0.97	0.13	48,48,48,48	0
85	MG	i	201	1/1	0.97	0.06	57,57,57,57	0
85	MG	1	3991	1/1	0.97	0.25	30,30,30,30	0
85	MG	1	3994	1/1	0.97	0.21	32,32,32,32	0
85	MG	1	4200	1/1	0.97	0.34	18,18,18,18	0
84	OHX	A	1961	7/7	0.97	0.13	175,176,179,180	0
84	OHX	1	3574	7/7	0.97	0.20	138,139,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4027	1/1	0.97	0.27	33,33,33,33	0
85	MG	AR	3745	1/1	0.97	0.19	32,32,32,32	0
85	MG	1	4204	1/1	0.97	0.41	12,12,12,12	0
85	MG	1	4205	1/1	0.97	0.53	26,26,26,26	0
84	OHX	AR	3578	7/7	0.97	0.39	188,188,189,189	0
85	MG	1	3784	1/1	0.97	0.30	30,30,30,30	0
85	MG	1	3785	1/1	0.97	0.33	21,21,21,21	0
84	OHX	1	3652	7/7	0.97	0.17	173,174,174,174	0
85	MG	1	4211	1/1	0.97	0.37	21,21,21,21	0
84	OHX	1	3516	7/7	0.97	0.23	131,132,133,133	0
84	OHX	4	202	7/7	0.97	0.10	157,158,158,158	0
85	MG	1	4215	1/1	0.97	0.34	28,28,28,28	0
84	OHX	AR	3583	7/7	0.97	0.18	148,149,150,150	0
85	MG	1	4220	1/1	0.97	0.22	25,25,25,25	0
85	MG	1	3791	1/1	0.97	0.44	21,21,21,21	0
85	MG	A	2056	1/1	0.97	0.39	39,39,39,39	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	3	209	1/1	0.97	0.26	46,46,46,46	0
85	MG	AR	3763	1/1	0.97	0.26	18,18,18,18	0
85	MG	1	3792	1/1	0.97	0.26	16,16,16,16	0
85	MG	A	2063	1/1	0.97	0.42	36,36,36,36	0
85	MG	A	2064	1/1	0.97	0.15	49,49,49,49	0
85	MG	3	211	1/1	0.97	0.30	33,33,33,33	0
85	MG	1	4007	1/1	0.97	0.30	16,16,16,16	0
84	OHX	1	3488	7/7	0.97	0.14	140,140,141,141	0
84	OHX	1	3577	7/7	0.97	0.25	177,178,179,179	0
84	OHX	A	1972	7/7	0.97	0.12	195,196,198,199	0
84	OHX	6	1984	7/7	0.97	0.18	198,200,201,201	0
84	OHX	1	3518	7/7	0.97	0.17	134,135,135,136	0
84	OHX	A	1975	7/7	0.97	0.08	190,193,195,195	0
84	OHX	1	3579	7/7	0.97	0.12	175,175,177,177	0
84	OHX	4	207	7/7	0.97	0.10	174,175,175,176	0
84	OHX	1	3475	7/7	0.97	0.17	128,129,130,130	0
84	OHX	AR	3698	7/7	0.97	0.19	166,167,167,168	0
85	MG	A	2078	1/1	0.97	0.51	28,28,28,28	0
85	MG	1	4019	1/1	0.97	0.20	31,31,31,31	0
85	MG	1	3805	1/1	0.97	0.19	60,60,60,60	0
84	OHX	1	3476	7/7	0.97	0.16	121,121,122,123	0
84	OHX	1	3582	7/7	0.97	0.20	152,153,154,155	0
85	MG	AR	3785	1/1	0.97	0.29	29,29,29,29	0
85	MG	AR	3786	1/1	0.97	0.19	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3583	7/7	0.97	0.29	144,144,145,145	0
85	MG	AR	4066	1/1	0.97	0.17	35,35,35,35	0
85	MG	4	223	1/1	0.97	0.26	44,44,44,44	0
84	OHX	1	3495	7/7	0.97	0.12	133,134,135,135	0
84	OHX	AR	3595	7/7	0.97	0.20	160,161,161,162	0
84	OHX	AP	502	7/7	0.97	0.14	124,124,126,127	0
85	MG	AR	3793	1/1	0.97	0.55	23,23,23,23	0
84	OHX	A	1987	7/7	0.97	0.14	172,173,174,175	0
85	MG	1	3815	1/1	0.97	0.18	40,40,40,40	0
85	MG	1	3817	1/1	0.97	0.30	32,32,32,32	0
84	OHX	AR	3430	7/7	0.97	0.15	137,137,138,138	0
84	OHX	AR	3453	7/7	0.97	0.12	127,128,128,128	0
85	MG	AR	3799	1/1	0.97	0.17	83,83,83,83	0
84	OHX	AR	3460	7/7	0.97	0.12	109,109,110,110	0
85	MG	1	3822	1/1	0.97	0.31	22,22,22,22	0
84	OHX	AR	3463	7/7	0.97	0.18	114,114,115,115	0
85	MG	A	2102	1/1	0.97	0.31	52,52,52,52	0
85	MG	1	4035	1/1	0.97	0.18	131,131,131,131	0
84	OHX	AR	3464	7/7	0.97	0.13	117,118,118,118	0
84	OHX	k	401	7/7	0.97	0.24	169,170,170,170	0
85	MG	A	2106	1/1	0.97	0.47	30,30,30,30	0
85	MG	1	3827	1/1	0.97	0.27	21,21,21,21	0
84	OHX	AR	3467	7/7	0.97	0.13	137,138,138,139	0
84	OHX	1	3524	7/7	0.97	0.22	164,164,166,167	0
84	OHX	1	3496	7/7	0.97	0.18	115,116,117,117	0
85	MG	AR	4091	1/1	0.97	0.16	53,53,53,53	0
84	OHX	AR	3474	7/7	0.97	0.15	119,120,121,121	0
84	OHX	AR	3607	7/7	0.97	0.22	166,166,167,167	0
84	OHX	AR	3475	7/7	0.97	0.17	114,115,115,116	0
85	MG	AR	3814	1/1	0.97	0.33	27,27,27,27	0
84	OHX	1	3527	7/7	0.97	0.18	138,139,140,140	0
85	MG	AR	3816	1/1	0.97	0.21	27,27,27,27	0
85	MG	x	205	1/1	0.97	0.48	20,20,20,20	0
85	MG	A	2119	1/1	0.97	0.38	55,55,55,55	0
85	MG	1	4048	1/1	0.97	0.32	27,27,27,27	0
85	MG	x	207	1/1	0.97	0.15	17,17,17,17	0
84	OHX	AR	3610	7/7	0.97	0.13	139,140,140,140	0
84	OHX	AR	3480	7/7	0.97	0.12	132,132,132,133	0
84	OHX	AR	3481	7/7	0.97	0.11	132,132,133,133	0
85	MG	1	3843	1/1	0.97	0.66	11,11,11,11	0
84	OHX	AR	3484	7/7	0.97	0.20	133,134,135,135	0
84	OHX	AR	3614	7/7	0.97	0.15	164,165,165,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3488	7/7	0.97	0.13	129,130,130,131	0
85	MG	1	4057	1/1	0.97	0.17	30,30,30,30	0
84	OHX	AR	3489	7/7	0.97	0.12	149,150,151,152	0
85	MG	6	2067	1/1	0.97	0.34	41,41,41,41	0
85	MG	1	4059	1/1	0.97	0.26	32,32,32,32	0
84	OHX	A	2008	7/7	0.97	0.13	156,158,159,159	0
85	MG	AR	3836	1/1	0.97	0.31	15,15,15,15	0
85	MG	A	2136	1/1	0.97	0.08	110,110,110,110	0
84	OHX	AR	3617	7/7	0.97	0.28	158,158,159,159	0
85	MG	A	2138	1/1	0.97	0.29	35,35,35,35	0
84	OHX	v	301	7/7	0.97	0.14	155,155,156,156	0
85	MG	1	3858	1/1	0.97	0.64	12,12,12,12	0
85	MG	A	2142	1/1	0.97	0.28	90,90,90,90	0
85	MG	AR	3842	1/1	0.97	0.38	10,10,10,10	0
85	MG	A	2144	1/1	0.97	0.24	49,49,49,49	0
85	MG	1	3859	1/1	0.97	0.21	33,33,33,33	0
84	OHX	1	3588	7/7	0.97	0.16	168,169,170,170	0
85	MG	1	3861	1/1	0.97	0.15	65,65,65,65	0
84	OHX	1	3497	7/7	0.97	0.12	140,141,142,142	0
85	MG	1	3863	1/1	0.97	0.43	25,25,25,25	0
84	OHX	1	3590	7/7	0.97	0.18	208,209,210,211	0
84	OHX	AR	3497	7/7	0.97	0.22	140,140,141,141	0
85	MG	6	2082	1/1	0.97	0.54	25,25,25,25	0
84	OHX	1	3591	7/7	0.97	0.12	185,186,187,188	0
84	OHX	1	3498	7/7	0.97	0.11	150,150,151,152	0
85	MG	AR	3858	1/1	0.97	0.47	22,22,22,22	0
85	MG	AR	4133	1/1	0.97	0.13	35,35,35,35	0
85	MG	AR	4134	1/1	0.97	0.28	10,10,10,10	0
84	OHX	AR	3503	7/7	0.97	0.33	152,153,154,154	0
84	OHX	6	1919	7/7	0.97	0.14	112,113,114,114	0
84	OHX	AR	3627	7/7	0.97	0.20	173,173,174,174	0
85	MG	AR	4138	1/1	0.97	0.41	44,44,44,44	0
85	MG	AR	4139	1/1	0.97	0.64	37,37,37,37	0
84	OHX	AR	3506	7/7	0.97	0.17	158,159,159,160	0
84	OHX	6	1927	7/7	0.97	0.16	128,128,130,130	0
84	OHX	AR	3510	7/7	0.97	0.09	154,155,156,157	0
85	MG	AR	3866	1/1	0.97	0.26	20,20,20,20	0
84	OHX	6	1931	7/7	0.97	0.12	151,152,153,153	0
85	MG	1	4082	1/1	0.97	0.13	22,22,22,22	0
86	7MB	AR	4239	20/20	0.97	0.19	44,44,44,44	0
87	ZN	AP	501	1/1	0.97	0.26	115,115,115,115	0
87	ZN	AQ	501	1/1	0.97	0.08	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	ZN	DQ	501	1/1	0.97	0.15	105,105,105,105	0
85	MG	1	3885	1/1	0.97	0.49	10,10,10,10	0
85	MG	AR	3870	1/1	0.97	0.23	14,14,14,14	0
84	OHX	AS	206	7/7	0.97	0.14	146,146,148,148	0
85	MG	AR	4149	1/1	0.97	0.13	28,28,28,28	0
85	MG	AR	4188	1/1	0.98	0.19	35,35,35,35	0
85	MG	AR	4189	1/1	0.98	0.14	32,32,32,32	0
84	OHX	A	1963	7/7	0.98	0.10	185,187,189,190	0
84	OHX	6	1948	7/7	0.98	0.10	145,147,148,148	0
85	MG	1	4165	1/1	0.98	0.19	38,38,38,38	0
84	OHX	A	1965	7/7	0.98	0.19	167,169,170,171	0
84	OHX	1	3435	7/7	0.98	0.15	103,104,105,105	0
84	OHX	AR	3476	7/7	0.98	0.12	127,128,129,130	0
85	MG	AR	4197	1/1	0.98	0.24	29,29,29,29	0
85	MG	1	3971	1/1	0.98	0.18	63,63,63,63	0
85	MG	1	3972	1/1	0.98	0.31	31,31,31,31	0
84	OHX	1	3437	7/7	0.98	0.14	100,101,102,102	0
85	MG	1	3787	1/1	0.98	0.28	15,15,15,15	0
84	OHX	AR	3478	7/7	0.98	0.12	102,103,103,104	0
84	OHX	AR	3479	7/7	0.98	0.15	119,119,120,120	0
84	OHX	3	204	7/7	0.98	0.08	163,164,165,166	0
84	OHX	1	3571	7/7	0.98	0.27	144,145,145,146	0
84	OHX	1	3532	7/7	0.98	0.13	133,133,134,134	0
85	MG	1	3793	1/1	0.98	0.46	12,12,12,12	0
84	OHX	AR	3485	7/7	0.98	0.25	135,136,137,137	0
85	MG	AR	4210	1/1	0.98	0.37	33,33,33,33	0
84	OHX	AR	3487	7/7	0.98	0.12	116,117,117,117	0
84	OHX	1	3493	7/7	0.98	0.16	147,148,148,149	0
85	MG	1	3797	1/1	0.98	0.13	41,41,41,41	0
84	OHX	1	3494	7/7	0.98	0.11	141,142,144,144	0
84	OHX	AR	3491	7/7	0.98	0.10	130,131,132,132	0
84	OHX	6	1956	7/7	0.98	0.09	192,194,195,196	0
85	MG	1	4189	1/1	0.98	0.22	48,48,48,48	0
84	OHX	AR	3493	7/7	0.98	0.12	137,139,139,140	0
85	MG	6	2183	1/1	0.98	0.23	44,44,44,44	0
84	OHX	6	1957	7/7	0.98	0.14	144,145,146,147	0
84	OHX	1	3433	7/7	0.98	0.21	90,90,90,90	0
85	MG	AR	4222	1/1	0.98	0.15	27,27,27,27	0
85	MG	1	3992	1/1	0.98	0.14	53,53,53,53	0
85	MG	6	2187	1/1	0.98	0.12	82,82,82,82	0
85	MG	1	3993	1/1	0.98	0.10	27,27,27,27	0
84	OHX	6	1959	7/7	0.98	0.11	154,155,156,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3464	7/7	0.98	0.11	136,137,138,139	0
85	MG	6	2191	1/1	0.98	0.30	47,47,47,47	0
85	MG	1	3996	1/1	0.98	0.26	51,51,51,51	0
84	OHX	AR	3498	7/7	0.98	0.09	143,144,145,146	0
84	OHX	1	3442	7/7	0.98	0.12	98,99,99,100	0
85	MG	1	4201	1/1	0.98	0.53	31,31,31,31	0
84	OHX	1	3538	7/7	0.98	0.14	135,135,137,137	0
84	OHX	AR	3502	7/7	0.98	0.11	131,132,132,133	0
84	OHX	1	3444	7/7	0.98	0.16	103,104,104,105	0
85	MG	AR	4236	1/1	0.98	0.32	22,22,22,22	0
84	OHX	AR	3504	7/7	0.98	0.21	116,117,117,118	0
84	OHX	1	3468	7/7	0.98	0.14	104,104,104,105	0
85	MG	1	3814	1/1	0.98	0.32	39,39,39,39	0
84	OHX	1	3469	7/7	0.98	0.13	118,118,119,120	0
85	MG	1	4209	1/1	0.98	0.40	22,22,22,22	0
85	MG	AR	4243	1/1	0.98	0.43	22,22,22,22	0
85	MG	1	3816	1/1	0.98	0.36	28,28,28,28	0
85	MG	AR	3987	1/1	0.98	0.33	50,50,50,50	0
84	OHX	AR	3507	7/7	0.98	0.16	136,136,137,137	0
84	OHX	1	3445	7/7	0.98	0.14	95,95,95,96	0
85	MG	1	3819	1/1	0.98	0.25	25,25,25,25	0
84	OHX	AR	3509	7/7	0.98	0.14	135,136,136,137	0
84	OHX	1	3471	7/7	0.98	0.13	118,118,121,121	0
85	MG	AS	217	1/1	0.98	0.16	18,18,18,18	0
85	MG	1	4218	1/1	0.98	0.07	84,84,84,84	0
85	MG	1	4219	1/1	0.98	0.34	47,47,47,47	0
84	OHX	AR	3511	7/7	0.98	0.15	96,96,96,97	0
85	MG	1	4013	1/1	0.98	0.22	56,56,56,56	0
85	MG	AS	222	1/1	0.98	0.22	13,13,13,13	0
84	OHX	AR	3512	7/7	0.98	0.10	132,132,132,133	0
84	OHX	AR	3513	7/7	0.98	0.11	152,153,154,154	0
85	MG	1	3825	1/1	0.98	0.17	42,42,42,42	0
84	OHX	1	3505	7/7	0.98	0.13	139,139,140,140	0
84	OHX	1	3506	7/7	0.98	0.08	159,160,161,162	0
85	MG	AR	3751	1/1	0.98	0.21	29,29,29,29	0
85	MG	1	3828	1/1	0.98	0.41	29,29,29,29	0
84	OHX	6	1970	7/7	0.98	0.19	178,179,180,180	0
85	MG	AR	3754	1/1	0.98	0.14	35,35,35,35	0
84	OHX	AS	201	7/7	0.98	0.16	98,99,100,101	0
84	OHX	AS	202	7/7	0.98	0.11	122,123,124,124	0
84	OHX	AS	203	7/7	0.98	0.11	118,119,120,120	0
84	OHX	AS	204	7/7	0.98	0.12	140,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AS	205	7/7	0.98	0.11	144,146,147,147	0
85	MG	1	3836	1/1	0.98	0.24	17,17,17,17	0
85	MG	1	3838	1/1	0.98	0.36	20,20,20,20	0
84	OHX	1	3626	7/7	0.98	0.16	137,137,138,138	0
85	MG	AR	4014	1/1	0.98	0.35	32,32,32,32	0
85	MG	AT	230	1/1	0.98	0.23	48,48,48,48	0
84	OHX	AS	207	7/7	0.98	0.11	163,165,166,166	0
84	OHX	1	3473	7/7	0.98	0.12	119,120,121,121	0
85	MG	AR	3765	1/1	0.98	0.44	23,23,23,23	0
84	OHX	AR	3519	7/7	0.98	0.12	135,135,136,136	0
85	MG	CE	404	1/1	0.98	0.27	24,24,24,24	0
84	OHX	1	3508	7/7	0.98	0.12	140,142,143,144	0
85	MG	4	220	1/1	0.98	0.37	37,37,37,37	0
85	MG	4	221	1/1	0.98	0.15	52,52,52,52	0
84	OHX	AT	204	7/7	0.98	0.10	143,143,143,143	0
85	MG	1	3846	1/1	0.98	0.38	16,16,16,16	0
84	OHX	AT	205	7/7	0.98	0.09	151,151,151,151	0
85	MG	4	225	1/1	0.98	0.18	43,43,43,43	0
85	MG	1	3849	1/1	0.98	0.44	21,21,21,21	0
85	MG	1	4037	1/1	0.98	0.19	61,61,61,61	0
84	OHX	AR	3521	7/7	0.98	0.12	160,161,161,162	0
84	OHX	1	3509	7/7	0.98	0.18	155,155,157,157	0
85	MG	AR	3779	1/1	0.98	0.28	20,20,20,20	0
84	OHX	1	3510	7/7	0.98	0.22	148,148,149,149	0
84	OHX	1	3474	7/7	0.98	0.14	131,132,133,133	0
84	OHX	1	3446	7/7	0.98	0.16	107,108,109,110	0
85	MG	AR	3783	1/1	0.98	0.39	15,15,15,15	0
85	MG	1	3857	1/1	0.98	0.39	12,12,12,12	0
85	MG	j	301	1/1	0.98	0.13	26,26,26,26	0
84	OHX	1	3448	7/7	0.98	0.24	104,105,106,106	0
84	OHX	AR	3527	7/7	0.98	0.10	138,139,140,141	0
85	MG	1	4046	1/1	0.98	0.09	54,54,54,54	0
84	OHX	1	3449	7/7	0.98	0.10	119,120,121,121	0
85	MG	AR	3790	1/1	0.98	0.28	17,17,17,17	0
84	OHX	1	3478	7/7	0.98	0.11	133,134,135,135	0
84	OHX	6	1907	7/7	0.98	0.19	100,101,101,101	0
85	MG	r	302	1/1	0.98	0.10	40,40,40,40	0
84	OHX	AR	3531	7/7	0.98	0.10	123,124,124,124	0
84	OHX	AR	3532	7/7	0.98	0.17	129,130,130,131	0
85	MG	1	3865	1/1	0.98	0.47	13,13,13,13	0
84	OHX	1	3479	7/7	0.98	0.15	136,137,138,138	0
84	OHX	6	1915	7/7	0.98	0.12	100,101,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3868	1/1	0.98	0.58	9,9,9,9	0
85	MG	AR	3800	1/1	0.98	0.28	22,22,22,22	0
85	MG	1	3869	1/1	0.98	0.33	33,33,33,33	0
85	MG	1	3870	1/1	0.98	0.51	11,11,11,11	0
84	OHX	1	3480	7/7	0.98	0.13	141,141,142,142	0
85	MG	1	3872	1/1	0.98	0.39	23,23,23,23	0
85	MG	1	3874	1/1	0.98	0.42	19,19,19,19	0
84	OHX	6	1920	7/7	0.98	0.12	124,126,127,128	0
84	OHX	AR	3537	7/7	0.98	0.11	133,134,135,135	0
84	OHX	6	1921	7/7	0.98	0.14	121,124,124,126	0
85	MG	6	2059	1/1	0.98	0.42	40,40,40,40	0
85	MG	1	3878	1/1	0.98	0.18	36,36,36,36	0
85	MG	A	2049	1/1	0.98	0.34	35,35,35,35	0
84	OHX	6	1924	7/7	0.98	0.12	123,124,126,127	0
84	OHX	1	3481	7/7	0.98	0.11	130,131,132,133	0
85	MG	6	2063	1/1	0.98	0.28	31,31,31,31	0
84	OHX	6	1928	7/7	0.98	0.09	150,151,152,152	0
84	OHX	6	1929	7/7	0.98	0.14	147,148,151,152	0
85	MG	6	2066	1/1	0.98	0.27	87,87,87,87	0
85	MG	AR	3817	1/1	0.98	0.31	20,20,20,20	0
85	MG	1	3884	1/1	0.98	0.38	27,27,27,27	0
85	MG	6	2068	1/1	0.98	0.35	76,76,76,76	0
85	MG	AR	3821	1/1	0.98	0.35	26,26,26,26	0
85	MG	A	2060	1/1	0.98	0.41	20,20,20,20	0
84	OHX	AR	3654	7/7	0.98	0.20	161,162,163,164	0
85	MG	1	3886	1/1	0.98	0.43	24,24,24,24	0
84	OHX	6	1930	7/7	0.98	0.12	114,115,116,117	0
84	OHX	1	3520	7/7	0.98	0.07	149,150,152,152	0
85	MG	1	3889	1/1	0.98	0.28	19,19,19,19	0
85	MG	A	2066	1/1	0.98	0.44	62,62,62,62	0
85	MG	AR	4078	1/1	0.98	0.31	23,23,23,23	0
84	OHX	1	3450	7/7	0.98	0.12	116,117,118,118	0
85	MG	AR	4080	1/1	0.98	0.16	16,16,16,16	0
84	OHX	1	3560	7/7	0.98	0.13	155,156,158,158	0
85	MG	AR	3829	1/1	0.98	0.41	16,16,16,16	0
85	MG	1	3892	1/1	0.98	0.52	14,14,14,14	0
85	MG	6	2077	1/1	0.98	0.56	51,51,51,51	0
85	MG	1	3893	1/1	0.98	0.28	38,38,38,38	0
84	OHX	AR	3548	7/7	0.98	0.18	165,166,166,166	0
85	MG	1	4083	1/1	0.98	0.11	34,34,34,34	0
84	OHX	CX	201	7/7	0.98	0.17	121,122,123,124	0
85	MG	AR	4089	1/1	0.98	0.39	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3896	1/1	0.98	0.41	10,10,10,10	0
84	OHX	6	1935	7/7	0.98	0.12	136,137,138,139	0
84	OHX	DG	201	7/7	0.98	0.16	132,133,133,134	0
84	OHX	1	3483	7/7	0.98	0.10	118,119,120,121	0
84	OHX	6	1937	7/7	0.98	0.11	140,141,141,141	0
85	MG	AR	3843	1/1	0.98	0.24	13,13,13,13	0
84	OHX	AR	3552	7/7	0.98	0.12	148,148,149,149	0
85	MG	AR	3845	1/1	0.98	0.23	32,32,32,32	0
85	MG	1	3904	1/1	0.98	0.44	4,4,4,4	0
84	OHX	AR	3553	7/7	0.98	0.12	160,160,161,162	0
84	OHX	A	1908	7/7	0.98	0.16	111,111,113,114	0
84	OHX	A	1909	7/7	0.98	0.13	124,125,128,129	0
84	OHX	A	1910	7/7	0.98	0.11	123,125,127,128	0
84	OHX	A	1911	7/7	0.98	0.13	115,117,118,120	0
85	MG	6	2094	1/1	0.98	0.28	24,24,24,24	0
84	OHX	A	1912	7/7	0.98	0.09	132,133,135,136	0
85	MG	AR	3856	1/1	0.98	0.53	10,10,10,10	0
85	MG	A	2096	1/1	0.98	0.27	51,51,51,51	0
84	OHX	A	1913	7/7	0.98	0.14	121,122,123,124	0
84	OHX	A	1915	7/7	0.98	0.09	149,151,152,154	0
85	MG	1	3913	1/1	0.98	0.27	38,38,38,38	0
84	OHX	A	1916	7/7	0.98	0.11	128,130,131,131	0
84	OHX	1	3452	7/7	0.98	0.14	111,111,112,113	0
84	OHX	AK	102	7/7	0.98	0.10	121,122,122,122	0
85	MG	1	3917	1/1	0.98	0.36	18,18,18,18	0
85	MG	6	2103	1/1	0.98	0.41	40,40,40,40	0
85	MG	AR	3865	1/1	0.98	0.27	23,23,23,23	0
85	MG	AR	4118	1/1	0.98	0.27	29,29,29,29	0
84	OHX	AK	103	7/7	0.98	0.12	145,146,146,146	0
84	OHX	A	1922	7/7	0.98	0.10	138,140,141,141	0
84	OHX	A	1923	7/7	0.98	0.09	137,138,140,140	0
84	OHX	A	1924	7/7	0.98	0.10	153,154,155,156	0
84	OHX	AR	3557	7/7	0.98	0.11	144,145,146,146	0
84	OHX	A	1926	7/7	0.98	0.11	149,150,151,152	0
85	MG	1	4115	1/1	0.98	0.17	97,97,97,97	0
85	MG	1	3925	1/1	0.98	0.38	15,15,15,15	0
85	MG	1	4117	1/1	0.98	0.34	26,26,26,26	0
85	MG	1	4118	1/1	0.98	0.23	87,87,87,87	0
84	OHX	6	1999	7/7	0.98	0.18	177,179,179,181	0
85	MG	AR	3878	1/1	0.98	0.27	12,12,12,12	0
84	OHX	AR	3427	7/7	0.98	0.22	87,87,87,87	0
85	MG	A	2120	1/1	0.98	0.08	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4132	1/1	0.98	0.08	36,36,36,36	0
84	OHX	AR	3429	7/7	0.98	0.09	105,105,106,106	0
85	MG	AR	3881	1/1	0.98	0.41	12,12,12,12	0
84	OHX	6	1939	7/7	0.98	0.11	131,133,134,135	0
84	OHX	AR	3562	7/7	0.98	0.07	173,174,175,176	0
85	MG	AR	3886	1/1	0.98	0.25	15,15,15,15	0
85	MG	1	3932	1/1	0.98	0.26	24,24,24,24	0
84	OHX	AR	3433	7/7	0.98	0.17	94,94,94,95	0
85	MG	1	4126	1/1	0.98	0.33	30,30,30,30	0
84	OHX	AR	3441	7/7	0.98	0.14	109,110,110,111	0
84	OHX	AR	3442	7/7	0.98	0.15	110,111,111,111	0
84	OHX	AR	3443	7/7	0.98	0.14	98,99,100,101	0
84	OHX	AR	3445	7/7	0.98	0.13	94,94,94,95	0
84	OHX	AR	3448	7/7	0.98	0.12	109,110,110,110	0
85	MG	AR	3895	1/1	0.98	0.39	21,21,21,21	0
84	OHX	A	1938	7/7	0.98	0.14	138,139,140,141	0
84	OHX	AR	3450	7/7	0.98	0.11	109,110,112,113	0
84	OHX	AR	3451	7/7	0.98	0.15	104,105,106,106	0
84	OHX	A	1942	7/7	0.98	0.14	163,165,166,167	0
84	OHX	AR	3452	7/7	0.98	0.11	108,109,110,111	0
85	MG	A	2141	1/1	0.98	0.32	73,73,73,73	0
84	OHX	1	3454	7/7	0.98	0.14	111,112,113,113	0
84	OHX	AR	3454	7/7	0.98	0.12	120,120,121,121	0
85	MG	AR	3903	1/1	0.98	0.41	5,5,5,5	0
84	OHX	AR	3455	7/7	0.98	0.17	106,107,108,108	0
84	OHX	AR	3456	7/7	0.98	0.12	109,110,110,111	0
84	OHX	AR	3457	7/7	0.98	0.13	107,107,108,108	0
85	MG	AR	3908	1/1	0.98	0.46	18,18,18,18	0
85	MG	AR	3911	1/1	0.98	0.43	16,16,16,16	0
85	MG	AR	3912	1/1	0.98	0.54	1,1,1,1	0
84	OHX	AR	3459	7/7	0.98	0.14	97,97,98,99	0
85	MG	AR	3914	1/1	0.98	0.35	13,13,13,13	0
85	MG	AR	3915	1/1	0.98	0.29	20,20,20,20	0
84	OHX	1	3525	7/7	0.98	0.10	151,152,153,154	0
85	MG	AR	4166	1/1	0.98	0.11	58,58,58,58	0
85	MG	AR	3917	1/1	0.98	0.33	29,29,29,29	0
84	OHX	6	1942	7/7	0.98	0.09	142,143,144,145	0
84	OHX	AR	3580	7/7	0.98	0.18	139,139,140,140	0
85	MG	1	4148	1/1	0.98	0.57	35,35,35,35	0
85	MG	1	3768	1/1	0.98	0.30	24,24,24,24	0
84	OHX	1	3455	7/7	0.98	0.13	104,104,105,105	0
84	OHX	6	1944	7/7	0.98	0.12	154,155,157,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3771	1/1	0.98	0.48	23,23,23,23	0
84	OHX	1	3487	7/7	0.98	0.10	139,140,142,142	0
85	MG	AR	3926	1/1	0.98	0.51	10,10,10,10	0
85	MG	1	3773	1/1	0.98	0.46	15,15,15,15	0
85	MG	AR	3929	1/1	0.98	0.13	75,75,75,75	0
84	OHX	AR	3468	7/7	0.98	0.11	111,112,113,114	0
85	MG	AR	3931	1/1	0.98	0.18	13,13,13,13	0
85	MG	AR	3932	1/1	0.98	0.38	25,25,25,25	0
84	OHX	AR	3469	7/7	0.98	0.10	122,124,125,125	0
84	OHX	AR	3697	7/7	0.98	0.21	115,116,116,116	0
87	ZN	DR	501	1/1	0.98	0.07	73,73,73,73	0
84	OHX	AR	3470	7/7	0.98	0.09	125,127,127,128	0
84	OHX	AR	3471	7/7	0.98	0.12	127,127,128,128	0
84	OHX	1	3456	7/7	0.98	0.13	114,115,116,117	0
87	ZN	d9	103	1/1	0.98	0.10	86,86,86,86	0
84	OHX	1	3490	7/7	0.98	0.10	134,135,136,136	0
84	OHX	1	3416	7/7	0.99	0.15	86,86,86,86	0
84	OHX	AR	3482	7/7	0.99	0.10	116,117,117,117	0
84	OHX	AR	3483	7/7	0.99	0.16	124,125,125,126	0
84	OHX	1	3417	7/7	0.99	0.19	97,97,97,97	0
84	OHX	1	3457	7/7	0.99	0.14	108,108,109,109	0
84	OHX	AR	3486	7/7	0.99	0.09	118,119,120,121	0
85	MG	1	3931	1/1	0.99	0.12	31,31,31,31	0
84	OHX	1	3418	7/7	0.99	0.13	85,85,85,85	0
84	OHX	1	3459	7/7	0.99	0.09	134,134,135,136	0
85	MG	1	4086	1/1	0.99	0.32	16,16,16,16	0
85	MG	AR	3906	1/1	0.99	0.23	15,15,15,15	0
84	OHX	1	3460	7/7	0.99	0.12	112,114,115,116	0
84	OHX	AR	3490	7/7	0.99	0.09	108,108,109,110	0
85	MG	AR	3909	1/1	0.99	0.37	14,14,14,14	0
85	MG	AR	3910	1/1	0.99	0.32	17,17,17,17	0
85	MG	AB	201	1/1	0.99	0.50	15,15,15,15	0
85	MG	AB	202	1/1	0.99	0.22	34,34,34,34	0
84	OHX	1	3419	7/7	0.99	0.19	93,93,93,93	0
84	OHX	1	3420	7/7	0.99	0.20	91,91,92,92	0
85	MG	j	302	1/1	0.99	0.14	29,29,29,29	0
85	MG	k	403	1/1	0.99	0.21	24,24,24,24	0
84	OHX	1	3463	7/7	0.99	0.08	108,109,109,109	0
84	OHX	1	3421	7/7	0.99	0.11	84,84,84,84	0
84	OHX	1	3465	7/7	0.99	0.10	113,114,114,114	0
85	MG	1	4094	1/1	0.99	0.13	43,43,43,43	0
84	OHX	1	3422	7/7	0.99	0.17	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4105	1/1	0.99	0.08	41,41,41,41	0
84	OHX	2	201	7/7	0.99	0.17	94,94,94,94	0
84	OHX	6	1901	7/7	0.99	0.23	92,92,92,92	0
85	MG	1	4099	1/1	0.99	0.31	16,16,16,16	0
84	OHX	A	1984	7/7	0.99	0.12	151,152,153,154	0
84	OHX	6	1902	7/7	0.99	0.24	102,102,102,102	0
85	MG	AR	3927	1/1	0.99	0.64	11,11,11,11	0
84	OHX	6	1903	7/7	0.99	0.20	89,89,90,90	0
84	OHX	AR	3501	7/7	0.99	0.11	118,118,120,120	0
84	OHX	6	1905	7/7	0.99	0.20	100,100,101,101	0
84	OHX	6	1906	7/7	0.99	0.19	94,94,95,95	0
84	OHX	1	3423	7/7	0.99	0.15	91,92,92,92	0
84	OHX	6	1908	7/7	0.99	0.16	91,91,91,91	0
84	OHX	6	1909	7/7	0.99	0.16	103,104,104,104	0
85	MG	DC	204	1/1	0.99	0.17	45,45,45,45	0
84	OHX	6	1910	7/7	0.99	0.14	93,93,93,93	0
84	OHX	6	1911	7/7	0.99	0.15	99,100,100,100	0
85	MG	AR	3937	1/1	0.99	0.43	9,9,9,9	0
85	MG	l2	201	1/1	0.99	0.28	21,21,21,21	0
85	MG	1	3806	1/1	0.99	0.28	31,31,31,31	0
85	MG	DH	203	1/1	0.99	0.23	41,41,41,41	0
84	OHX	6	1912	7/7	0.99	0.09	107,108,110,110	0
84	OHX	AT	203	7/7	0.99	0.21	83,83,83,83	0
84	OHX	6	1913	7/7	0.99	0.13	105,105,106,107	0
84	OHX	1	3424	7/7	0.99	0.19	92,93,93,93	0
84	OHX	1	3425	7/7	0.99	0.16	93,93,93,93	0
84	OHX	6	1916	7/7	0.99	0.11	102,103,104,104	0
84	OHX	6	1917	7/7	0.99	0.10	113,114,116,117	0
84	OHX	6	1918	7/7	0.99	0.11	103,104,105,105	0
84	OHX	1	3426	7/7	0.99	0.15	93,93,93,94	0
84	OHX	1	3519	7/7	0.99	0.10	112,112,113,113	0
85	MG	A	2047	1/1	0.99	0.39	55,55,55,55	0
84	OHX	1	3427	7/7	0.99	0.15	87,87,87,87	0
84	OHX	6	1922	7/7	0.99	0.10	111,112,113,114	0
84	OHX	AR	3401	7/7	0.99	0.26	93,93,93,93	0
84	OHX	AR	3402	7/7	0.99	0.27	89,89,89,89	0
84	OHX	AR	3403	7/7	0.99	0.19	86,86,86,86	0
84	OHX	AR	3404	7/7	0.99	0.19	88,89,89,89	0
84	OHX	AR	3405	7/7	0.99	0.23	94,94,94,94	0
84	OHX	AR	3406	7/7	0.99	0.23	86,86,86,86	0
84	OHX	AR	3407	7/7	0.99	0.24	88,88,88,88	0
84	OHX	AR	3408	7/7	0.99	0.22	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3409	7/7	0.99	0.20	92,92,92,92	0
84	OHX	AR	3410	7/7	0.99	0.13	86,86,86,86	0
84	OHX	AR	3411	7/7	0.99	0.20	83,83,83,83	0
84	OHX	AR	3412	7/7	0.99	0.16	85,85,85,85	0
84	OHX	AR	3413	7/7	0.99	0.16	84,84,84,84	0
85	MG	1	4137	1/1	0.99	0.20	38,38,38,38	0
85	MG	1	3832	1/1	0.99	0.34	13,13,13,13	0
84	OHX	AR	3414	7/7	0.99	0.18	90,90,90,90	0
84	OHX	AR	3415	7/7	0.99	0.23	86,86,86,87	0
84	OHX	AR	3416	7/7	0.99	0.17	88,88,88,89	0
84	OHX	AR	3417	7/7	0.99	0.14	86,86,86,86	0
85	MG	1	4143	1/1	0.99	0.07	53,53,53,53	0
85	MG	AR	4157	1/1	0.99	0.22	29,29,29,29	0
85	MG	1	3837	1/1	0.99	0.64	25,25,25,25	0
85	MG	1	3987	1/1	0.99	0.24	32,32,32,32	0
84	OHX	AR	3418	7/7	0.99	0.14	92,92,93,93	0
84	OHX	AR	3419	7/7	0.99	0.13	94,94,95,95	0
84	OHX	AR	3420	7/7	0.99	0.16	87,87,87,87	0
84	OHX	CV	201	7/7	0.99	0.21	91,91,91,91	0
84	OHX	AR	3421	7/7	0.99	0.12	89,89,89,89	0
84	OHX	AR	3422	7/7	0.99	0.15	86,86,86,86	0
84	OHX	DD	102	7/7	0.99	0.17	88,89,89,89	0
85	MG	1	3845	1/1	0.99	0.36	14,14,14,14	0
84	OHX	AR	3542	7/7	0.99	0.19	133,134,134,134	0
84	OHX	AR	3423	7/7	0.99	0.14	85,85,85,85	0
85	MG	1	3848	1/1	0.99	0.20	26,26,26,26	0
84	OHX	AR	3424	7/7	0.99	0.19	86,87,87,87	0
84	OHX	AR	3425	7/7	0.99	0.10	85,85,85,85	0
84	OHX	AR	3426	7/7	0.99	0.13	88,88,88,89	0
84	OHX	A	1901	7/7	0.99	0.21	101,101,102,102	0
84	OHX	A	1902	7/7	0.99	0.16	96,97,97,97	0
84	OHX	A	1903	7/7	0.99	0.26	117,118,118,119	0
85	MG	1	3856	1/1	0.99	0.31	15,15,15,15	0
84	OHX	A	1904	7/7	0.99	0.12	107,107,108,108	0
85	MG	1	4167	1/1	0.99	0.15	52,52,52,52	0
84	OHX	A	1905	7/7	0.99	0.18	102,102,103,103	0
84	OHX	A	1906	7/7	0.99	0.17	112,113,113,113	0
84	OHX	A	1907	7/7	0.99	0.09	117,118,120,121	0
84	OHX	6	1923	7/7	0.99	0.14	136,138,139,139	0
84	OHX	AR	3428	7/7	0.99	0.10	97,97,98,98	0
85	MG	6	2117	1/1	0.99	0.41	21,21,21,21	0
84	OHX	1	3472	7/7	0.99	0.12	114,115,115,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	3819	1/1	0.99	0.49	53,53,53,53	0
84	OHX	6	1925	7/7	0.99	0.12	116,116,118,118	0
84	OHX	AR	3431	7/7	0.99	0.14	86,86,86,86	0
85	MG	AR	4190	1/1	0.99	0.24	107,107,107,107	0
84	OHX	AR	3432	7/7	0.99	0.13	91,91,91,91	0
84	OHX	A	1914	7/7	0.99	0.11	109,110,111,112	0
84	OHX	6	1926	7/7	0.99	0.10	122,123,124,124	0
84	OHX	AR	3434	7/7	0.99	0.16	87,87,88,88	0
84	OHX	A	1917	7/7	0.99	0.12	126,128,129,130	0
84	OHX	AR	3435	7/7	0.99	0.11	96,96,96,96	0
84	OHX	A	1919	7/7	0.99	0.10	113,115,116,116	0
85	MG	1	3873	1/1	0.99	0.40	18,18,18,18	0
84	OHX	AR	3436	7/7	0.99	0.16	87,87,87,87	0
84	OHX	AR	3437	7/7	0.99	0.11	89,89,89,89	0
84	OHX	AR	3438	7/7	0.99	0.12	89,89,89,90	0
84	OHX	AR	3439	7/7	0.99	0.16	91,91,92,92	0
84	OHX	AR	3440	7/7	0.99	0.12	98,98,98,99	0
84	OHX	1	3428	7/7	0.99	0.14	96,96,96,96	0
85	MG	6	2135	1/1	0.99	0.22	38,38,38,38	0
85	MG	1	4191	1/1	0.99	0.45	22,22,22,22	0
84	OHX	1	3429	7/7	0.99	0.13	89,89,90,90	0
84	OHX	1	3430	7/7	0.99	0.14	97,97,97,98	0
85	MG	AR	3840	1/1	0.99	0.33	22,22,22,22	0
85	MG	AR	3841	1/1	0.99	0.32	25,25,25,25	0
85	MG	1	3882	1/1	0.99	0.38	11,11,11,11	0
84	OHX	AR	3444	7/7	0.99	0.10	101,102,102,103	0
84	OHX	1	3431	7/7	0.99	0.12	95,95,95,95	0
84	OHX	AR	3446	7/7	0.99	0.09	99,100,100,101	0
84	OHX	AR	3447	7/7	0.99	0.13	88,88,89,89	0
84	OHX	1	3402	7/7	0.99	0.24	90,90,91,91	0
84	OHX	AR	3449	7/7	0.99	0.12	98,99,99,100	0
85	MG	6	2146	1/1	0.99	0.14	44,44,44,44	0
84	OHX	1	3403	7/7	0.99	0.23	90,90,90,90	0
85	MG	AR	3851	1/1	0.99	0.34	29,29,29,29	0
85	MG	AR	3852	1/1	0.99	0.44	18,18,18,18	0
84	OHX	1	3434	7/7	0.99	0.14	94,95,95,95	0
84	OHX	6	1934	7/7	0.99	0.09	141,141,143,144	0
84	OHX	1	3404	7/7	0.99	0.20	93,93,93,93	0
84	OHX	1	3436	7/7	0.99	0.11	101,102,104,104	0
84	OHX	A	1939	7/7	0.99	0.08	153,155,156,157	0
84	OHX	1	3405	7/7	0.99	0.26	97,98,98,98	0
84	OHX	1	3438	7/7	0.99	0.13	91,91,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3752	1/1	0.99	0.29	27,27,27,27	0
84	OHX	1	3439	7/7	0.99	0.11	102,103,103,104	0
85	MG	1	3899	1/1	0.99	0.41	12,12,12,12	0
85	MG	A	2145	1/1	0.99	0.21	83,83,83,83	0
85	MG	1	4212	1/1	0.99	0.32	27,27,27,27	0
84	OHX	AR	3458	7/7	0.99	0.11	100,101,101,102	0
85	MG	1	3901	1/1	0.99	0.49	12,12,12,12	0
84	OHX	1	3440	7/7	0.99	0.14	94,95,95,95	0
84	OHX	1	3406	7/7	0.99	0.22	85,85,85,85	0
84	OHX	AR	3461	7/7	0.99	0.11	108,109,109,110	0
85	MG	AR	4051	1/1	0.99	0.12	62,62,62,62	0
85	MG	1	4054	1/1	0.99	0.14	40,40,40,40	0
84	OHX	AR	3462	7/7	0.99	0.11	106,107,108,108	0
84	OHX	3	201	7/7	0.99	0.10	106,107,108,108	0
85	MG	AR	3872	1/1	0.99	0.45	0,0,0,0	0
84	OHX	1	3407	7/7	0.99	0.20	83,83,83,83	0
84	OHX	AR	3465	7/7	0.99	0.12	100,101,102,102	0
84	OHX	1	3443	7/7	0.99	0.12	95,95,95,95	0
84	OHX	1	3489	7/7	0.99	0.11	114,115,116,117	0
84	OHX	1	3408	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	3	214	1/1	0.99	0.42	12,12,12,12	0
84	OHX	1	3410	7/7	0.99	0.20	88,88,88,88	0
84	OHX	1	3447	7/7	0.99	0.14	95,95,95,95	0
85	MG	AR	3882	1/1	0.99	0.58	11,11,11,11	0
85	MG	AR	3883	1/1	0.99	0.34	12,12,12,12	0
85	MG	1	4065	1/1	0.99	0.26	35,35,35,35	0
84	OHX	1	3411	7/7	0.99	0.19	93,93,93,93	0
84	OHX	1	3412	7/7	0.99	0.22	88,88,88,88	0
87	ZN	AK	101	1/1	0.99	0.13	38,38,38,38	0
84	OHX	1	3413	7/7	0.99	0.18	88,88,89,89	0
84	OHX	1	3451	7/7	0.99	0.10	101,101,102,103	0
84	OHX	1	3414	7/7	0.99	0.17	90,90,90,90	0
85	MG	1	4071	1/1	0.99	0.37	16,16,16,16	0
87	ZN	b	102	1/1	0.99	0.10	68,68,68,68	0
84	OHX	1	3499	7/7	0.99	0.10	124,125,126,126	0
87	ZN	e	102	1/1	0.99	0.06	74,74,74,74	0
84	OHX	1	3453	7/7	0.99	0.09	130,132,133,133	0
87	ZN	d6	102	1/1	0.99	0.10	59,59,59,59	0
84	OHX	1	3415	7/7	0.99	0.15	89,90,90,90	0
84	OHX	1	3502	7/7	0.99	0.10	100,101,102,102	0
85	MG	1	3924	1/1	0.99	0.54	8,8,8,8	0

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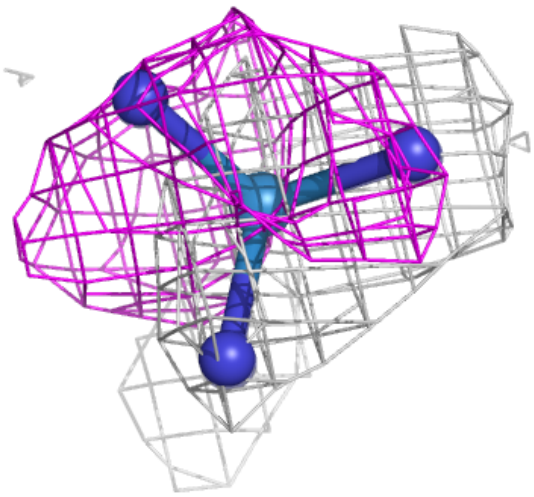
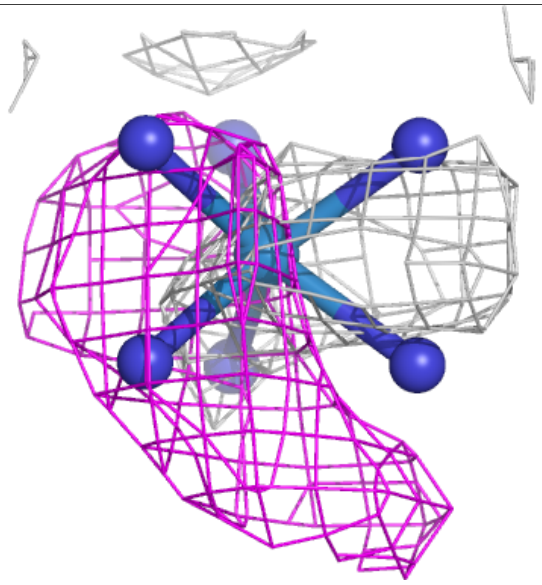
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4207	1/1	1.00	0.14	50,50,50,50	0
87	ZN	AN	500	1/1	1.00	0.11	43,43,43,43	0
85	MG	1	4156	1/1	1.00	0.13	65,65,65,65	0
84	OHX	AC	101	7/7	1.00	0.18	89,90,90,90	0
87	ZN	DL	103	1/1	1.00	0.12	37,37,37,37	0
87	ZN	DO	201	1/1	1.00	0.13	31,31,31,31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

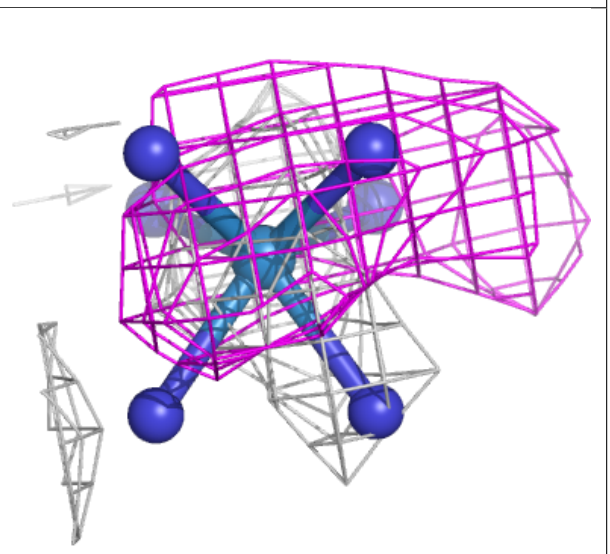
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

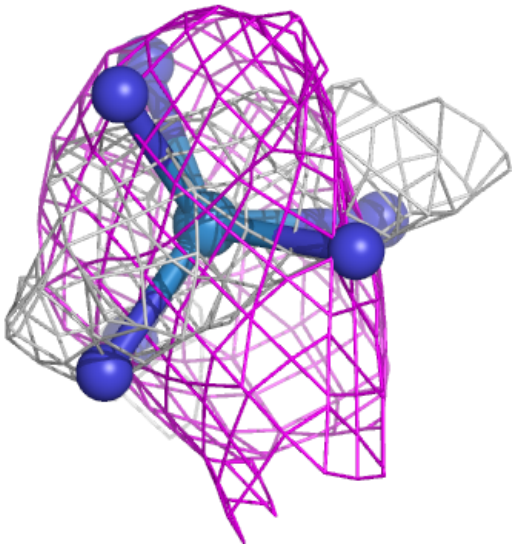


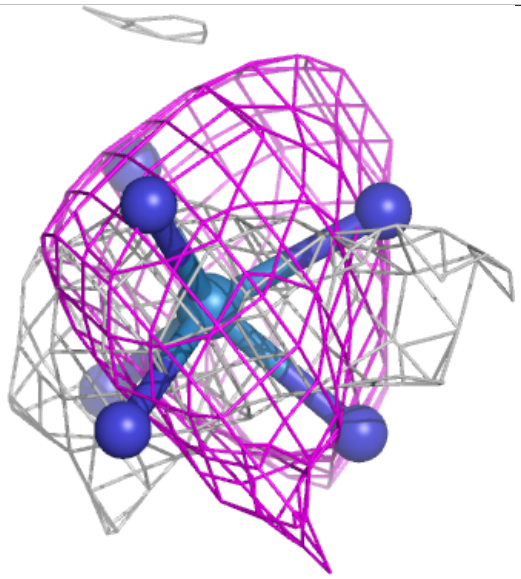


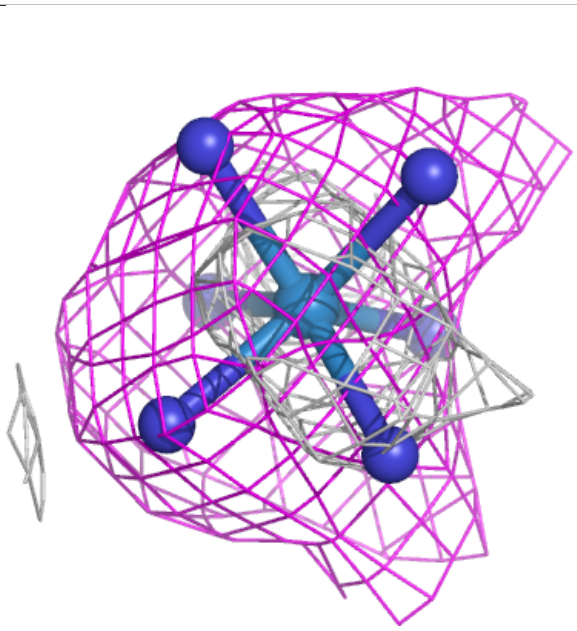


Electron density around OHX 1 3675:

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

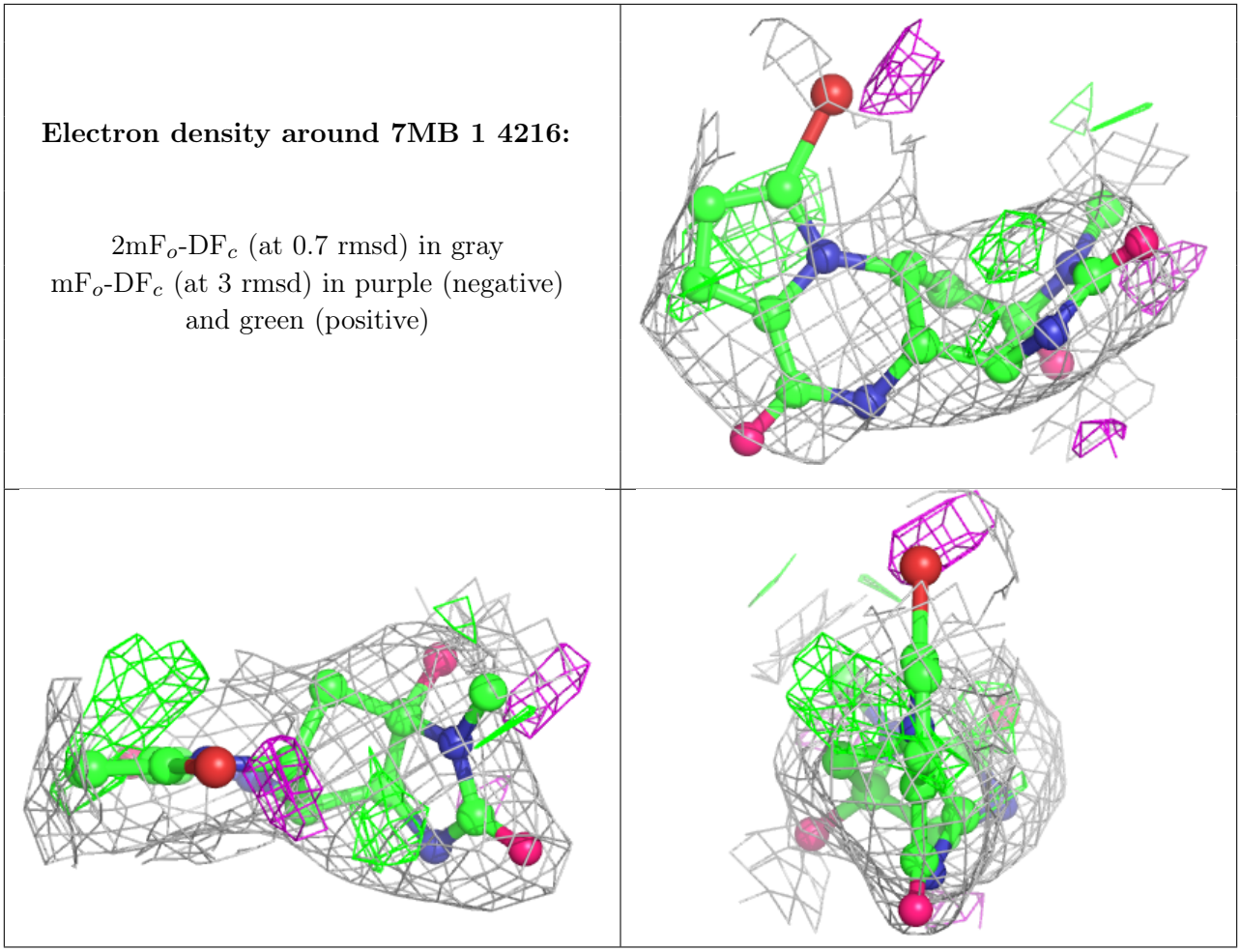






Electron density around 7MB 1 4216:

$2mF_o$-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.