



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 04:01 AM UTC

PDB ID : 8P9A / pdb_00008p9a
Title : 80S yeast ribosome in complex with Methyllissoclimide
Authors : Terrosu, S.; Yusupov, M.; Vanderwal, C.
Deposited on : 2023-06-05
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

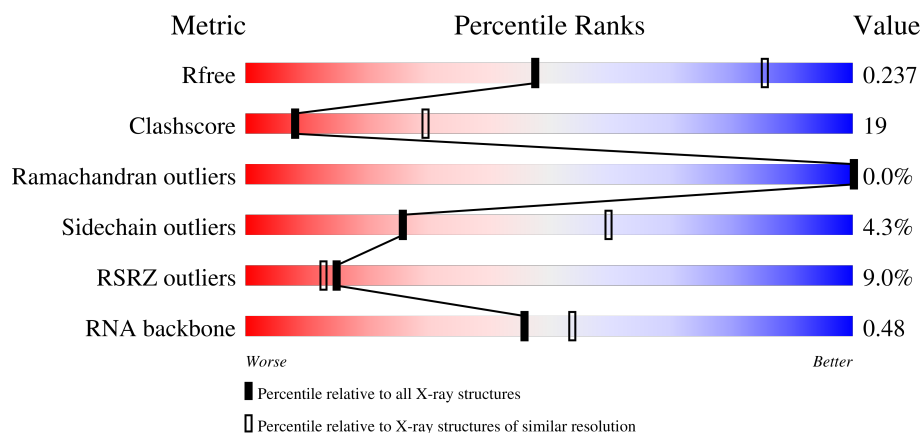
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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

Mol	Chain	Length	Quality of chain
1	1	3149	2% 45% 45% 10%
1	AR	3149	2% 46% 43% 10%
2	3	121	53% 41% 6%
2	AS	121	2% 45% 50% 5%

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Mol	Chain	Length	Quality of chain
3	4	158	
3	AT	158	
4	CD	254	
4	j	254	
5	CE	387	
5	k	387	
6	CF	362	
6	l	362	
7	CG	297	
7	m	297	
8	CH	176	
8	n	176	
9	CI	244	
9	o	244	
10	CJ	256	
10	p	256	
11	CK	191	
11	q	191	
12	CL	221	
12	r	221	
13	CM	174	
13	s	174	
14	CN	199	
14	t	199	
15	CO	138	

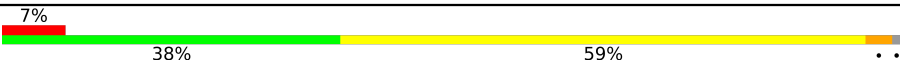
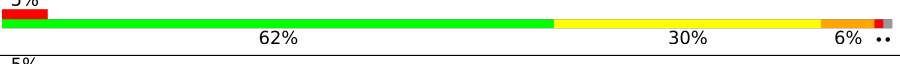
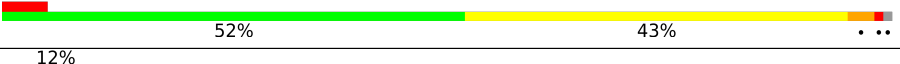
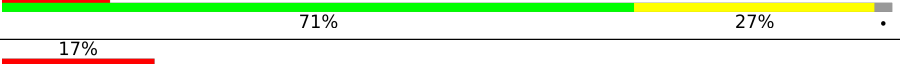
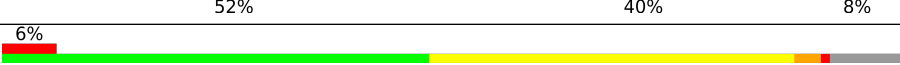
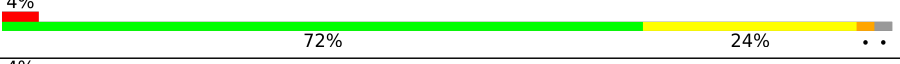
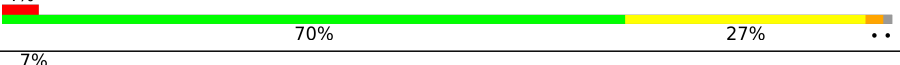
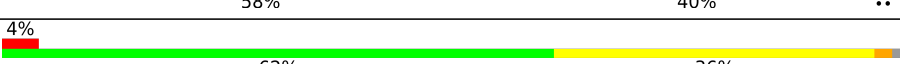
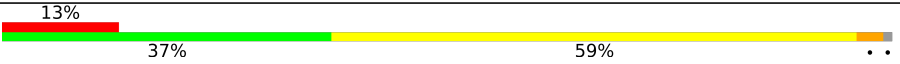
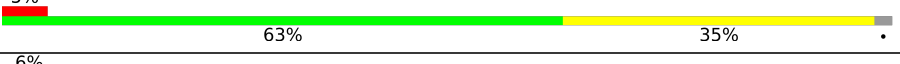
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Mol	Chain	Length	Quality of chain
15	u	138	
16	CP	204	
16	v	204	
17	CQ	199	
17	w	199	
18	CR	184	
18	x	184	
19	CS	186	
19	y	186	
20	CT	189	
20	z	189	
21	0	172	
21	CU	172	
22	2	160	
22	CV	160	
23	5	121	
23	CW	121	
24	6	137	
24	CX	137	
25	7	155	
25	CY	155	
26	8	142	
26	CZ	142	
27	9	127	
27	DA	127	

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Mol	Chain	Length	Quality of chain
28	AA	136	
28	DB	136	
29	AB	149	
29	DC	149	
30	AC	59	
30	DD	59	
31	AD	105	
31	DE	105	
32	AE	113	
32	DF	113	
33	AF	130	
33	DG	130	
34	AG	107	
34	DH	107	
35	AH	121	
35	DI	121	
36	AI	120	
36	DJ	120	
37	AJ	100	
37	DK	100	
38	AK	88	
38	DL	88	
39	AL	78	
39	DM	78	
40	AM	51	

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Mol	Chain	Length	Quality of chain
40	DN	51	
41	AN	128	
41	DO	128	
42	AO	25	
42	DP	25	
43	AP	106	
43	DQ	106	
44	AQ	92	
44	DR	92	
45	i	273	
45	sM	273	
46	p0	312	
47	A	1800	
47	sR	1800	
48	B	252	
48	s0	252	
49	C	255	
49	s1	255	
50	D	254	
50	s2	254	
51	E	240	
51	s3	240	
52	F	261	
52	s4	261	
53	G	225	

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Mol	Chain	Length	Quality of chain
53	s5	225	
54	H	236	
54	s6	236	
55	I	190	
55	s7	190	
56	J	200	
56	s8	200	
57	K	197	
57	s9	197	
58	L	105	
58	c0	105	
59	M	156	
59	c1	156	
60	N	143	
61	O	151	
61	c3	151	
62	P	138	
62	c4	138	
63	Q	142	
63	c5	142	
64	R	143	
64	c6	143	
65	S	136	
65	c7	136	
66	T	146	

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Mol	Chain	Length	Quality of chain
66	c8	146	
67	U	144	
67	c9	144	
68	V	121	
68	d0	121	
69	W	87	
69	d1	87	
70	X	130	
70	d2	130	
71	Y	145	
71	d3	145	
72	Z	135	
72	d4	135	
73	a	108	
73	d5	108	
74	b	119	
74	d6	119	
75	c	82	
75	d7	82	
76	d	67	
76	d8	67	
77	d9	56	
77	e	56	
78	e0	63	
78	f	63	

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Mol	Chain	Length	Quality of chain
79	e1	152	
79	g	152	
80	Rb	319	
80	h	319	

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
81	OHX	1	4090	-	-	X	-
81	OHX	1	4105	-	-	X	-
81	OHX	AR	3425	-	-	X	-
81	OHX	AR	3478[B]	-	-	X	-
81	OHX	AR	3502	-	-	X	-
81	OHX	AR	3539	-	-	X	-
81	OHX	AR	3671	-	-	X	-
81	OHX	AR	4202	-	-	-	X
81	OHX	AS	3501	-	-	X	-
81	OHX	CL	301	-	-	X	-
81	OHX	sR	2022	-	-	X	-
82	MG	1	3867	-	-	-	X
82	MG	1	3992	-	-	-	X
82	MG	1	4039	-	-	-	X
82	MG	A	2001	-	-	-	X
82	MG	A	2096	-	-	-	X
82	MG	AR	3768	-	-	-	X
82	MG	AR	3865	-	-	-	X
82	MG	AR	3952	-	-	-	X
82	MG	AR	4013	-	-	-	X
82	MG	AR	4097	-	-	-	X
82	MG	AR	4162	-	-	-	X
82	MG	AT	205	-	-	-	X
82	MG	s8	301	-	-	-	X
82	MG	s9	201	-	-	-	X
82	MG	x	202	-	-	-	X

2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 405377 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	3130	Total	C	N	O	P	0	0	0
			66954	29906	12075	21843	3130			

- 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 5.8 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	292	Total	C	N	O	S	0	0	0
			2348	1486	408	452	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	226	Total	C	N	O	S	0	0	0
			1757	1125	314	315	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 Large ribosomal subunit protein uL5B.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	x	183	Total	C	N	O	S	0	0	0
			1420	882	281	257				
18	CR	155	Total	C	N	O	S	0	0	0
			1227	764	238	225				

- 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	177	Total	C	N	O	S	0	0	0
			1432	881	310	241				
20	CT	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	6	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
24	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	7	65	Total	C	N	O	S	0	0	0
			533	343	104	85	1			
25	CY	111	Total	C	N	O	S	0	0	0
			769	485	153	130	1			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CZ	117	Total	C	N	O	S	0	0	0
			937	602	164	169	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	9	126	Total	C	N	O		0	0	0
			993	625	192	176				
27	DA	124	Total	C	N	O		0	0	0
			976	614	190	172				

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AG	106	Total	C	N	O	S	0	0	0
			844	537	162	144	1			
34	DH	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AH	111	Total	C	N	O	S	0	0	0
			871	539	177	151	4			
35	DI	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AJ	96	Total	C	N	O	S	0	0	0
			739	463	145	129	2			
37	DK	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AK	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
38	DL	86	Total	C	N	O	S	0	0	0
			676	411	147	113	5			

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

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

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

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

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

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

- Molecule 42 is a protein called Large ribosomal subunit protein eL41B.

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

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

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

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

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

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

- Molecule 45 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	i	142	Total	C	N	O		0	0	0
			1017	599	204	214				
45	sM	63	Total	C	N	O		0	0	0
			475	280	99	96				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	p0	126	Total	C	N	O	S	0	0	0
			992	636	175	178	3			

- Molecule 47 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	A	1741	Total	C	N	O	P	0	0	0
			37101	16586	6569	12205	1741			
47	sR	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			

- Molecule 48 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B	206	Total	C	N	O	S	0	0	0
			1562	1006	273	281	2			
48	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 49 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 50 is a protein called 40S ribosomal protein S2.

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

- Molecule 51 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 52 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 53 is a protein called 40S ribosomal protein S5.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	s5	198	Total	C	N	O	S	0	0	0
			1561	981	286	291	3			

- Molecule 54 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 55 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 56 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 57 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 58 is a protein called 40S ribosomal protein S10-A.

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

- Molecule 59 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	M	142	Total	C	N	O	S	0	0	0
			1149	736	217	193	3			
59	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 60 is a protein called 40S ribosomal protein S12.

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

- Molecule 61 is a protein called 40S ribosomal protein S13.

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

- Molecule 62 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	P	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
62	c4	127	Total	C	N	O	S	0	0	0
			940	577	186	174	3			

- Molecule 63 is a protein called 40S ribosomal protein S15.

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

- Molecule 64 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
64	R	141	Total	C	N	O	0	0	0
			1105	708	203	194			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
64	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 65 is a protein called 40S ribosomal protein S17-A.

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

- Molecule 66 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 67 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	V	96	Total	C	N	O	S	0	0	0
			765	481	139	144	1			
68	d0	89	Total	C	N	O	S	0	0	0
			715	451	131	132	1			

- Molecule 69 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 71 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 74 is a protein called Small ribosomal subunit protein eS26B.

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

- Molecule 75 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 76 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 77 is a protein called Small ribosomal subunit protein uS14A.

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

- Molecule 78 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 79 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	g	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
79	e1	51	Total	C	N	O		0	0	0
			251	149	51	51				

- Molecule 80 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

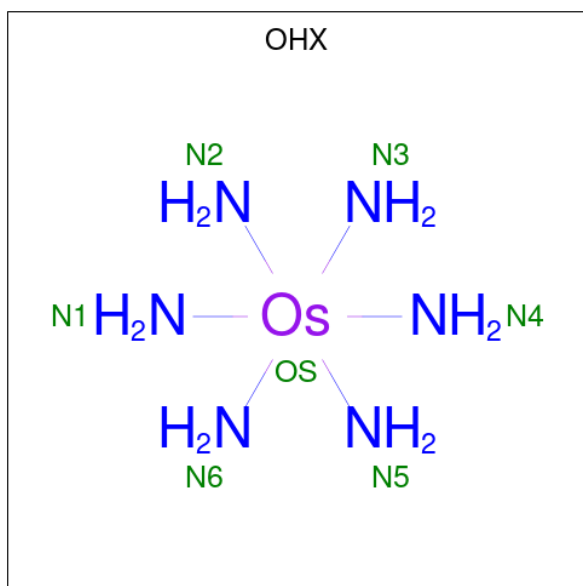
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	h	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			

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

- Molecule 81 is osmium (III) hexammine (CCD ID: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	1
			12	10	2		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	1
			14	12	2		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	1
			14	12	2		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	1
			14	12	2		
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
			7	6	1		
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81	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	1
			14	12	2		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	1
			14	12	2		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			6	5	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			6	5	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			6	5	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	1	1	Total	N	Os	0	0
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
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81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	1	1	Total	N	Os	0	0
			7	6	1		
81	3	1	Total	N	Os	0	0
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			7	6	1		
81	3	1	Total	N	Os	0	0
			7	6	1		
81	3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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81	3	1	Total	N	Os	0	0
			7	6	1		
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81	3	1	Total	N	Os	0	0
			7	6	1		
81	4	1	Total	N	Os	0	0
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			7	6	1		
81	4	1	Total	N	Os	0	0
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81	4	1	Total	N	Os	0	0
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81	4	1	Total	N	Os	0	0
			7	6	1		
81	4	1	Total	N	Os	0	0
			7	6	1		
81	4	1	Total	N	Os	0	0
			7	6	1		
81	4	1	Total	N	Os	0	0
			7	6	1		
81	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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81	k	1	Total	N	Os	0	0
			7	6	1		
81	l	1	Total	N	Os	0	0
			7	6	1		
81	r	1	Total	N	Os	0	0
			7	6	1		
81	v	1	Total	N	Os	0	0
			7	6	1		
81	x	1	Total	N	Os	0	0
			7	6	1		
81	z	1	Total	N	Os	0	0
			7	6	1		
81	z	1	Total	N	Os	0	0
			7	6	1		
81	AC	1	Total	N	Os	0	0
			7	6	1		
81	AG	1	Total	N	Os	0	0
			7	6	1		
81	AK	1	Total	N	Os	0	0
			7	6	1		
81	AP	1	Total	N	Os	0	0
			7	6	1		
81	AR	1	Total	N	Os	0	0
			7	6	1		
81	AR	1	Total	N	Os	0	0
			7	6	1		
81	AR	1	Total	N	Os	0	0
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81	AR	1	Total	N	Os	0	0
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81	AR	1	Total	N	Os	0	0
			7	6	1		
81	AR	1	Total	N	Os	0	0
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81	AR	1	Total	N	Os	0	0
			7	6	1		
81	AR	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	AR	1	Total	N	Os	0	0
			7	6	1		
81	AR	1	Total	N	Os	0	0
			7	6	1		
81	AR	1	Total	N	Os	0	0
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
81	AR	1	Total	N	Os	0	0
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81	AR	1	Total	N	Os	0	0
			7	6	1		
81	AR	1	Total	N	Os	0	0
			7	6	1		
81	AR	1	Total	N	Os	0	1
			14	12	2		
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			7	6	1		
81	AR	1	Total	N	Os	0	0
			7	6	1		
81	AR	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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81	AR	1	Total	N	Os	0	0
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81	AR	1	Total	N	Os	0	0
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81	AR	1	Total	N	Os	0	0
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81	AR	1	Total	N	Os	0	0
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81	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 14	N 12	Os 2	0	1
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
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81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 7	N 6	Os 1	0	0
81	AR	1	Total 6	N 5	Os 1	0	0
81	AS	1	Total 7	N 6	Os 1	0	0
81	AS	1	Total 7	N 6	Os 1	0	0

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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81	CE	1	Total	N	Os	0	0
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81	CE	1	Total	N	Os	0	0
			7	6	1		
81	CG	1	Total	N	Os	0	0
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81	CG	1	Total	N	Os	0	0
			7	6	1		
81	CG	1	Total	N	Os	0	0
			7	6	1		
81	CK	1	Total	N	Os	0	0
			7	6	1		
81	CL	1	Total	N	Os	0	0
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81	CL	1	Total	N	Os	0	1
			14	12	2		
81	CP	1	Total	N	Os	0	0
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81	CP	1	Total	N	Os	0	0
			7	6	1		
81	CQ	1	Total	N	Os	0	0
			7	6	1		
81	CS	1	Total	N	Os	0	0
			7	6	1		
81	CX	1	Total	N	Os	0	0
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81	CX	1	Total	N	Os	0	0
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81	DD	1	Total	N	Os	0	0
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81	DK	1	Total	N	Os	0	0
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81	DL	1	Total	N	Os	0	0
			7	6	1		
81	DQ	1	Total	N	Os	0	0
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81	A	1	Total	N	Os	0	0
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81	A	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	A	1	Total	N	Os	0	0
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81	A	1	Total	N	Os	0	0
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81	A	1	Total	N	Os	0	0
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81	A	1	Total	N	Os	0	0
			7	6	1		
81	A	1	Total	N	Os	0	0
			7	6	1		
81	A	1	Total	N	Os	0	0
			7	6	1		
81	A	1	Total	N	Os	0	0
			6	5	1		
81	A	1	Total	N	Os	0	0
			7	6	1		
81	A	1	Total	N	Os	0	0
			7	6	1		
81	J	1	Total	N	Os	0	0
			7	6	1		
81	O	1	Total	N	Os	0	0
			7	6	1		
81	Q	1	Total	N	Os	0	0
			7	6	1		
81	S	1	Total	N	Os	0	0
			7	6	1		
81	T	1	Total	N	Os	0	0
			7	6	1		
81	U	1	Total	N	Os	0	0
			7	6	1		
81	e	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	1
			14	12	2		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	sR	1	Total	N	Os	0	0
			7	6	1		
81	s1	1	Total	N	Os	0	0
			7	6	1		
81	s4	1	Total	N	Os	0	0
			7	6	1		
81	s8	1	Total	N	Os	0	0
			7	6	1		
81	c3	1	Total	N	Os	0	0
			7	6	1		
81	c5	1	Total	N	Os	0	0
			7	6	1		
81	c8	1	Total	N	Os	0	0
			7	6	1		
81	d0	1	Total	N	Os	0	0
			7	6	1		

- Molecule 82 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	1	476	Total	Mg	0	0
			476	476		
82	3	11	Total	Mg	0	0
			11	11		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	4	20	Total 20	Mg 20	0	0
82	j	3	Total 3	Mg 3	0	0
82	k	1	Total 1	Mg 1	0	0
82	l	3	Total 3	Mg 3	0	0
82	n	1	Total 1	Mg 1	0	0
82	o	1	Total 1	Mg 1	0	0
82	r	3	Total 3	Mg 3	0	0
82	s	1	Total 1	Mg 1	0	0
82	t	3	Total 3	Mg 3	0	0
82	v	3	Total 3	Mg 3	0	0
82	w	1	Total 1	Mg 1	0	0
82	x	8	Total 8	Mg 8	0	0
82	z	1	Total 1	Mg 1	0	0
82	6	3	Total 3	Mg 3	0	0
82	AB	5	Total 5	Mg 5	0	0
82	AF	4	Total 4	Mg 4	0	0
82	AG	2	Total 2	Mg 2	0	0
82	AK	1	Total 1	Mg 1	0	0
82	AR	519	Total 519	Mg 519	0	0
82	AS	20	Total 20	Mg 20	0	0
82	AT	17	Total 17	Mg 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	CD	3	Total 3	Mg 3	0	0
82	CE	6	Total 6	Mg 6	0	0
82	CF	2	Total 2	Mg 2	0	0
82	CG	1	Total 1	Mg 1	0	0
82	CI	3	Total 3	Mg 3	0	0
82	CK	1	Total 1	Mg 1	0	0
82	CL	1	Total 1	Mg 1	0	0
82	CM	2	Total 2	Mg 2	0	0
82	CO	1	Total 1	Mg 1	0	0
82	CP	3	Total 3	Mg 3	0	0
82	CQ	4	Total 4	Mg 4	0	0
82	CR	5	Total 5	Mg 5	0	0
82	CU	1	Total 1	Mg 1	0	0
82	CX	1	Total 1	Mg 1	0	0
82	CY	1	Total 1	Mg 1	0	0
82	DA	2	Total 2	Mg 2	0	0
82	DC	3	Total 3	Mg 3	0	0
82	DF	1	Total 1	Mg 1	0	0
82	DH	2	Total 2	Mg 2	0	0
82	DI	1	Total 1	Mg 1	0	0
82	DL	1	Total 1	Mg 1	0	0

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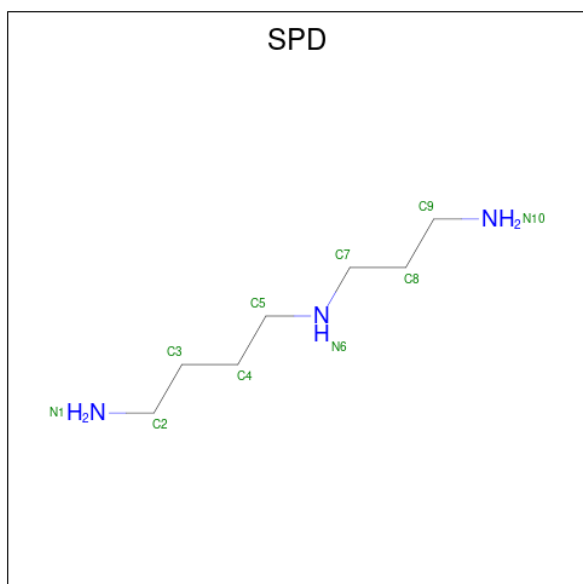
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	DO	1	Total 1	Mg 1	0	0
82	DP	1	Total 1	Mg 1	0	0
82	DQ	2	Total 2	Mg 2	0	0
82	sM	2	Total 2	Mg 2	0	0
82	A	132	Total 132	Mg 132	0	0
82	F	1	Total 1	Mg 1	0	0
82	H	1	Total 1	Mg 1	0	0
82	O	1	Total 1	Mg 1	0	0
82	P	1	Total 1	Mg 1	0	0
82	X	1	Total 1	Mg 1	0	0
82	Y	1	Total 1	Mg 1	0	0
82	b	1	Total 1	Mg 1	0	0
82	sR	144	Total 144	Mg 144	0	0
82	s1	1	Total 1	Mg 1	0	0
82	s2	1	Total 1	Mg 1	0	0
82	s4	1	Total 1	Mg 1	0	0
82	s8	2	Total 2	Mg 2	0	0
82	s9	1	Total 1	Mg 1	0	0
82	c1	1	Total 1	Mg 1	0	0
82	c4	2	Total 2	Mg 2	0	0
82	c6	2	Total 2	Mg 2	0	0

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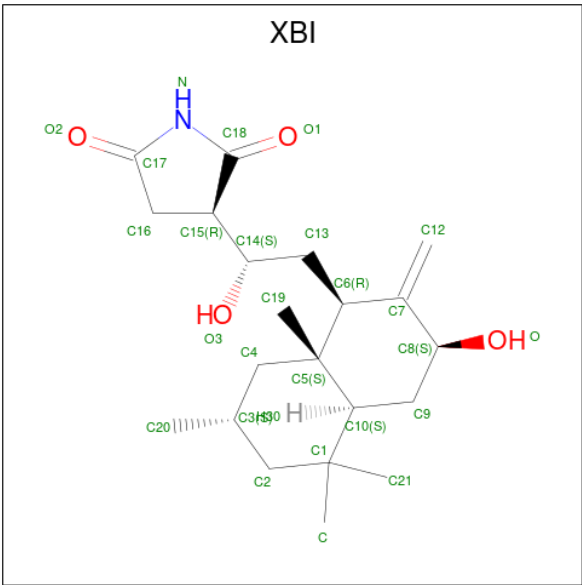
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	c8	1	Total	Mg	0	0
			1	1		
82	c9	1	Total	Mg	0	0
			1	1		
82	d3	4	Total	Mg	0	0
			4	4		
82	d4	3	Total	Mg	0	0
			3	3		
82	d6	2	Total	Mg	0	0
			2	2		
82	d9	1	Total	Mg	0	0
			1	1		

- Molecule 83 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
83	1	1	Total	C	N	0	0
			10	7	3		
83	AR	1	Total	C	N	0	0
			10	7	3		

- Molecule 84 is (3 {R})-3-[(1 {S})-2-[(1 {R},3 {S},4 {a} {S},7 {S},8 {a} {S})-5,5,7,8 {a}-tetramethyl-2-methylidene-3-oxidanyl-3,4,4 {a},6,7,8-hexahydro-1 {H}-naphthalen-1-yl]-1-oxidanyl-ethyl]pyrrolidine-2,5-dione (CCD ID: XBI) (formula: $C_{21}H_{33}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
84	1	1	Total	C	N	O	0	0
			26	21	1	4		
84	AR	1	Total	C	N	O	0	0
			26	21	1	4		

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AH	1	Total	Zn	0	0
			1	1		
85	AK	1	Total	Zn	0	0
			1	1		
85	AN	1	Total	Zn	0	0
			1	1		
85	AP	1	Total	Zn	0	0
			1	1		
85	AQ	1	Total	Zn	0	0
			1	1		
85	DI	1	Total	Zn	0	0
			1	1		
85	DL	1	Total	Zn	0	0
			1	1		
85	DO	1	Total	Zn	0	0
			1	1		
85	DQ	1	Total	Zn	0	0
			1	1		
85	DR	1	Total	Zn	0	0
			1	1		

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

- Molecule 86 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	1	53	Total 53	O 53	0	0
86	j	1	Total 1	O 1	0	0
86	AE	1	Total 1	O 1	0	0
86	AF	3	Total 3	O 3	0	0
86	AR	82	Total 82	O 82	0	0
86	AT	3	Total 3	O 3	0	0
86	CP	2	Total 2	O 2	0	0
86	CR	1	Total 1	O 1	0	0
86	DG	3	Total 3	O 3	0	0
86	A	33	Total 33	O 33	0	0
86	M	1	Total 1	O 1	0	0

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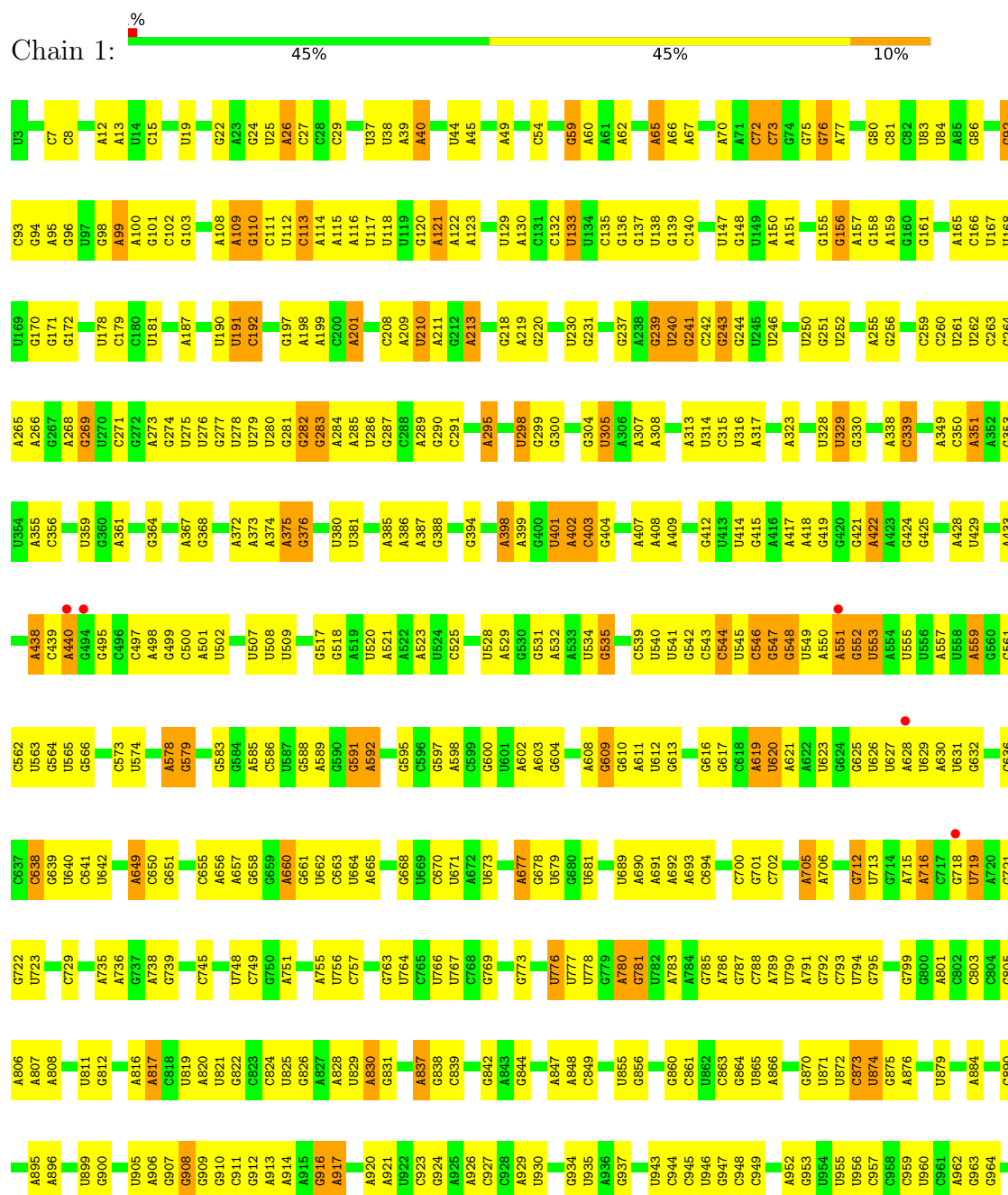
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	sR	23	Total	O	0	0
			23	23		

3 Residue-property plots

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

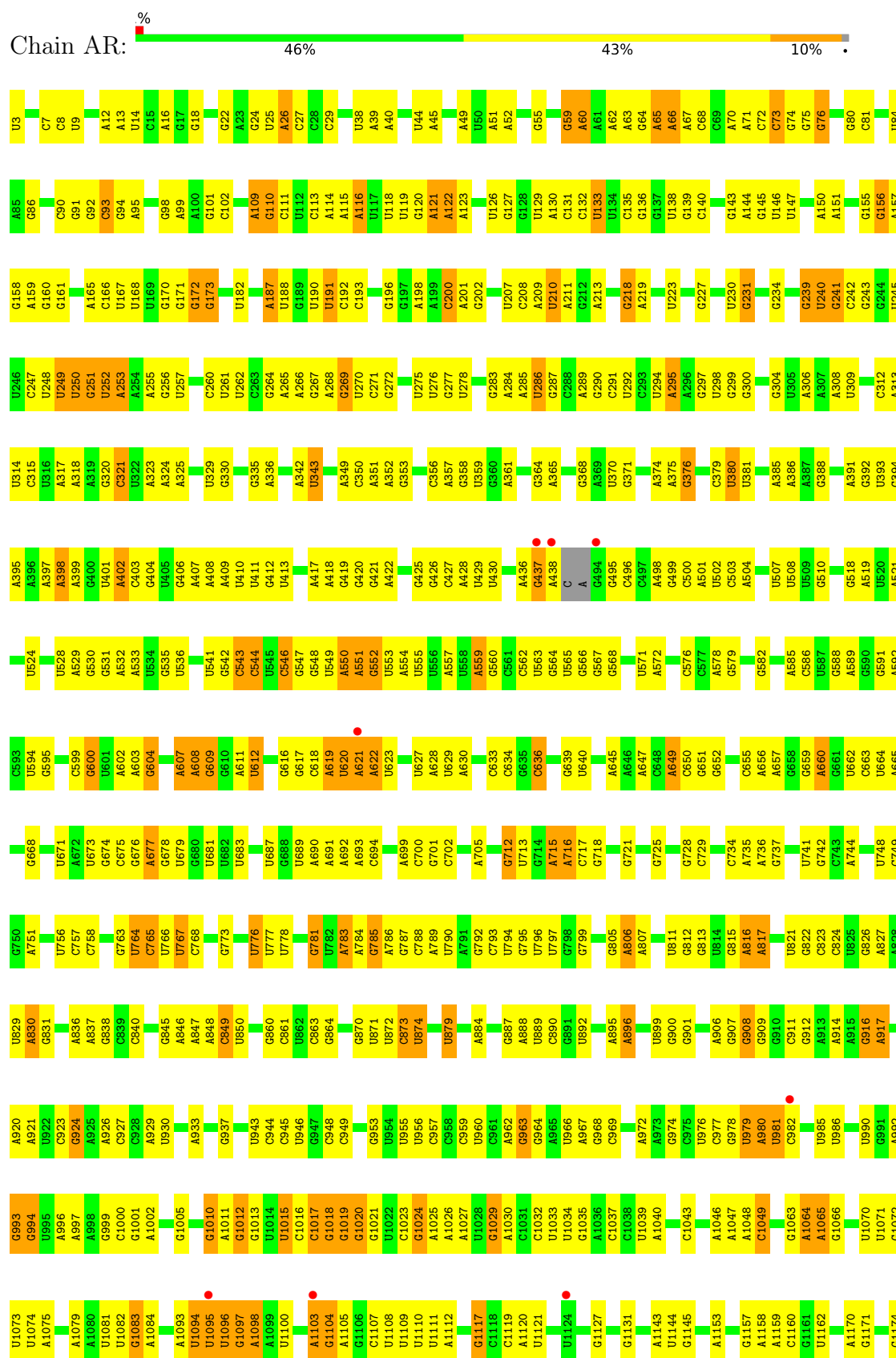
• Molecule 1: 25S ribosomal RNA



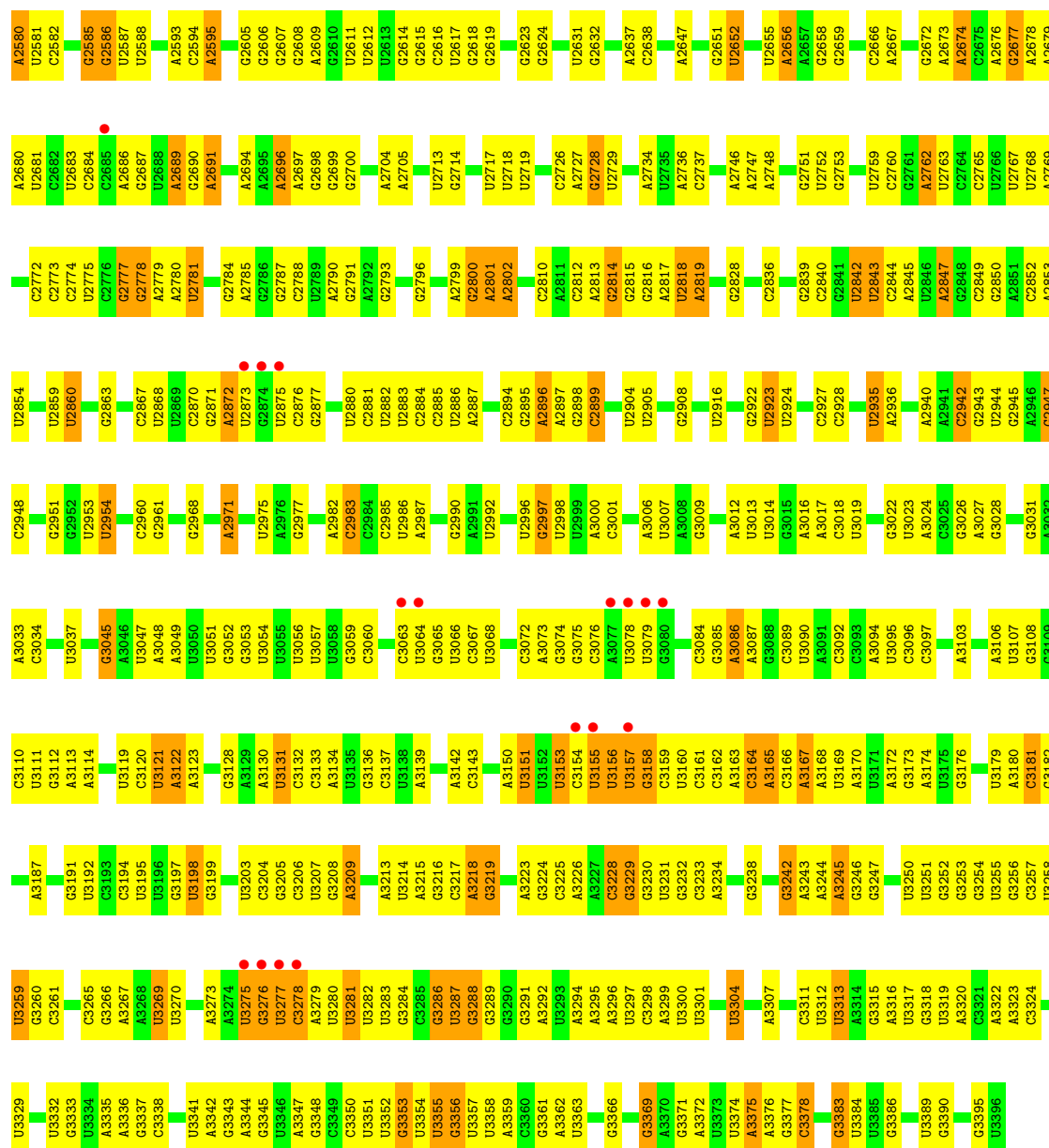
A2138	G968	U1042	C1119	A1203	U1267	G1349	U1450	U1540	A1612	U1686	G1895	U1925	A2138	
A2139	C969	C1043	A1120	A1204	G1268	A1350	G1450	U1540	A1613	U1687	C1826	U1925	A2139	
U2140	A970	U1044	U1121	G1206	U1269	A1351	U1455	G1544	C1614	C1761	C1827	C1926	U2140	
U2141		C1045			A1270	A1352	U1456	U1545	U1615	U1688	U1763	G1927	U2141	
A2144	A973	A1046	U1128	G1209	C1272	G1354	A1460	A1546	G1617	U1695	U1832	G1934	A2144	
A2147	G974	A1047	A1129	U1210	A1273	A1355	A1461	G1547	G1618	A1696	G1893	U1938	A2147	
U2148	C975	A1048	A1130	U1211	A1274	U1356	U1464	U1552	A1619	U1697	U1765	U1939	U2148	
A2149	U976	C1049	G1131	U1212	U1275	U1357	G1464	U1553	A1621	U1768	U1766	G1939	A2149	
G2150	G977	A1057	C1141	A1213	U1276	A1358	G1466	U1554	A1622	C1701	G1767	C1941	G2150	
A2151	U978	U1060	U1144	U1214	U1277	A1369	U1466	U1555	G1623	U1702	G1770	U1942	A2151	
G2152	A980	U1063	U1145	U1215	C1278	G1374	U1470	C1556	G1624	U1703	G1775	G1947	G2152	
U2153	U981	A1064	U1146	A1217	U1280	G1380	U1471	A1559	U1629	C1706	G1776	G1948	U2153	
A2158	C982	A1065	C1146	A1221	G1282	A1381	U1472	G1560	U1630	A1707	G1779	G1949	A2158	
U2159	A983	A1066	A1153	A1222	U1282	G1382	A1473	G1561	C1631	C1708	C1779	U1950	U2159	
G2160	U985	U1071	C1155	A1223	G1285	G1383	A1474	G1562	U1632	C1709	G1780	U1951	G2160	
G2161	A986	U1072	C1156	C1224	A1286	U1384	A1475	C1563	G1634	C1710	C1781	G1952	G2161	
G2162	A992	U1073	C1157	A1225	A1287	C1385	G1476	U1564	G1635	C1711	U1782	G1953	G2162	
C2163	G993	U1074	A1158	G1226	C1292	A1386	A1477	U1565	G1636	G1718	U1785	G1953	C2163	
	G994	A1075	A1159	C1227	C1292	G1389	G1480	U1566	A1637	A1715	U1786	G2093		
	G999	C1076	C1160	G1229	G1295	A1390	A1481	U1567	A1638	U1716	A1787	C2094	G2169	
	G1000	U1077	G1161	G1230	C1296	C1391	A1482	U1568	C1639	U1717	G1788	A2096	U2170	
G1001	A1002	U1081	U1162	A1231	G1297	G1392	G1485	U1570	U1641	G1719	U1789	U2097	U2173	
A1002		U1082		A1232	C1298	G1392	G1486	A1571	U1642	G1720	G1790	C2098	C2174	
A1006		G1083	G1166	G1233	C1298	A1399	G1487	U1572	A1643	U1721	C1793	A2099	U2175	
		A1084	U1168	G1234	A1301	G1400	G1488	C1573	C1644	U1722	U1789	C2100	U2176	
		C1085	A1169	U1235	A1302	G1404	G1488	G1574	G1644	U1723	U1795	C2101	G2177	
G1010		G1086	A1170	G1236	A1303	G1405	G1492	A1575	G1650	A1724	U1796	U2102	A2178	
			G1171	G1237	G1297	U1405	G1493	G1576	A1654	C1725	A1797	U2103	C2179	
G1013		G1090		G1238	G1306	U1408	G1494	C1577	U1654	G1726	U1798	U2104	C2180	
U1014		A1091	C1174	C1239	A1307	G1408	U1494	C1578	C1657	G1727	A1799	C2105	C2181	
U1015		C1092	U1175	A1240	A1308	G1412	U1495	C1579	G1658	G1728	U1800	A2106	G2185	
G1016		A1093	C1176	U1241	U1309	G1412	C1496	A1580	U1659	U1729	U1801	A2107	U2186	
C1017		U1094	G1177	G1242	G1310	G1416	C1497	C1581	C1660	G1730	C1802	U2109	G2187	
G1018		U1095		G1243		G1417	A1498	C1582	G1661	A1731	C1803	G2110	A2188	
G1019		U1096		A1244	G1313	G1418	G1500	A1583	G1662	U1732	A1804	G2111		
U1020		G1097	A1180	A1245	A1317	A1418	G1501	G1586	C1663	G1733	A1805	U2112	U2191	
G1021		A1098	U1181	A1246	A1318	A1419	C1502	A1587	G1664	G1734	U1806	U2113	C2192	
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• Molecule 1: 25S ribosomal RNA

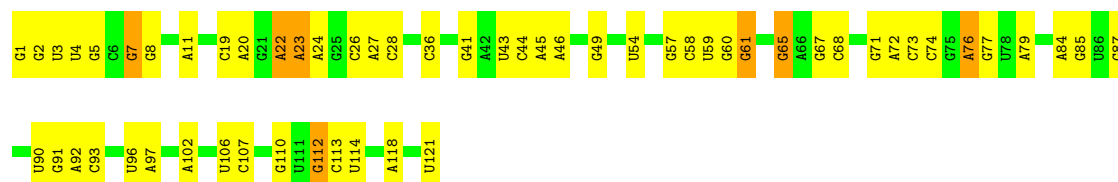






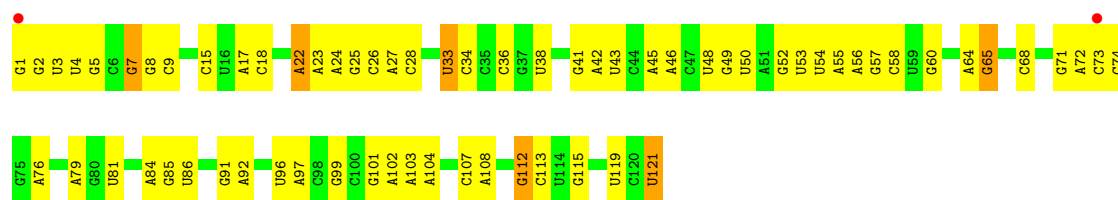
• Molecule 2: 5S ribosomal RNA

Chain 3: 53% 41% 6%



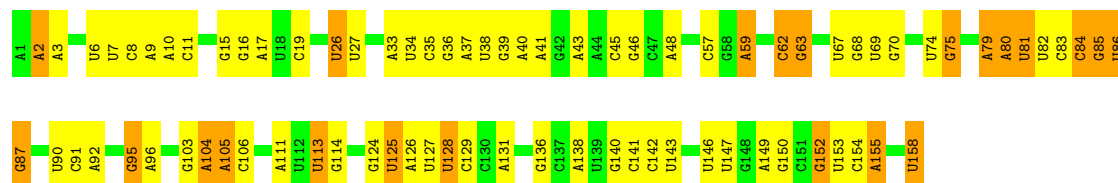
• Molecule 2: 5S ribosomal RNA

Chain AS: 2% 45% 50% 5%



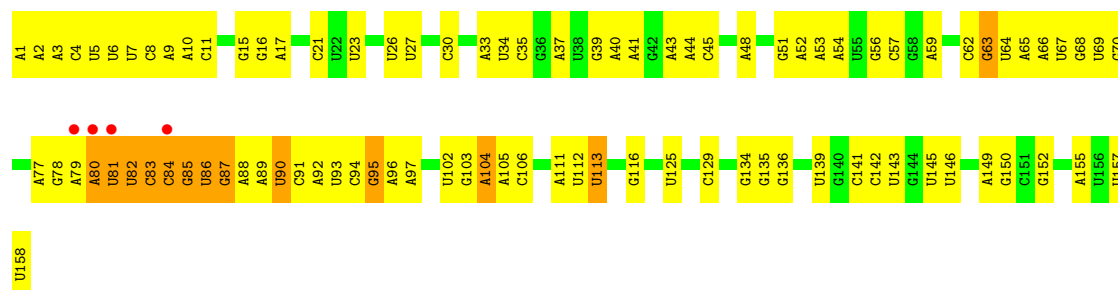
• Molecule 3: 5.8 ribosomal RNA

Chain 4: 49% 37% 14%



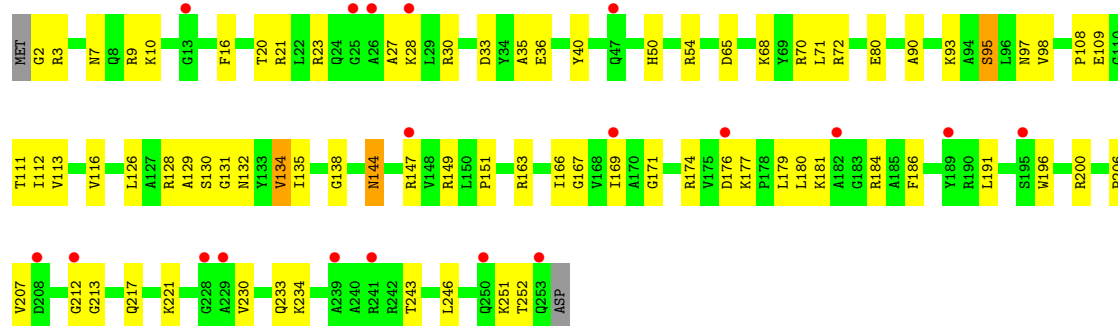
• Molecule 3: 5.8 ribosomal RNA

Chain AT: 3% 41% 51% 8%



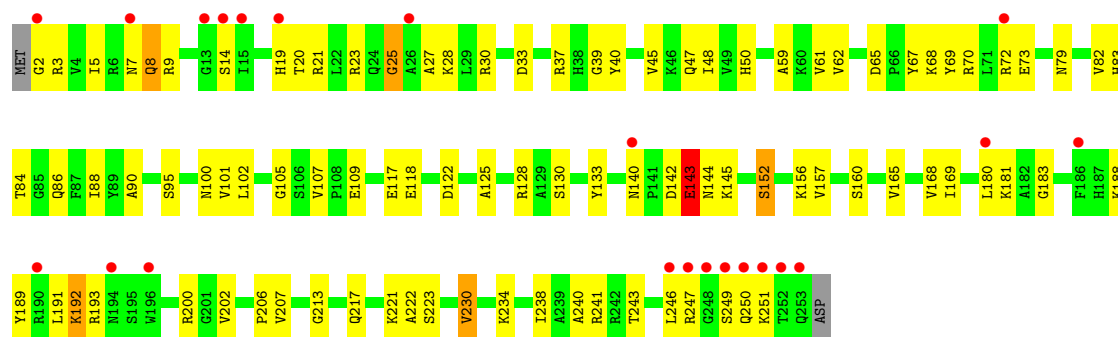
• Molecule 4: 60S ribosomal protein L2-A

Chain j: 7% 69% 29% ..



• Molecule 4: 60S ribosomal protein L2-A

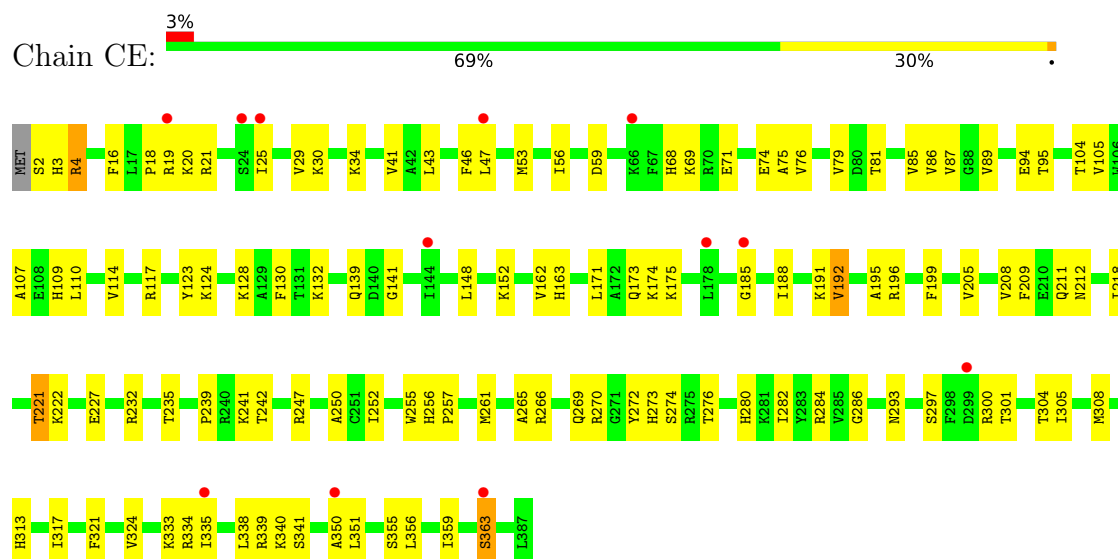
Chain CD: 9% 62% 35% ..



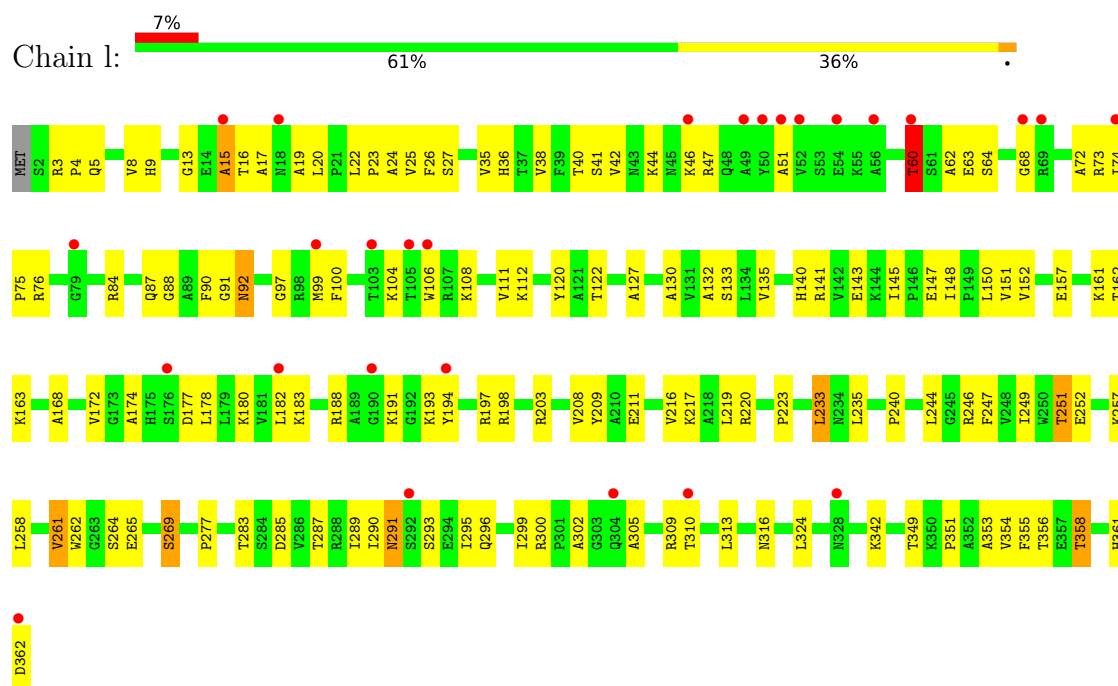
• Molecule 5: 60S ribosomal protein L3



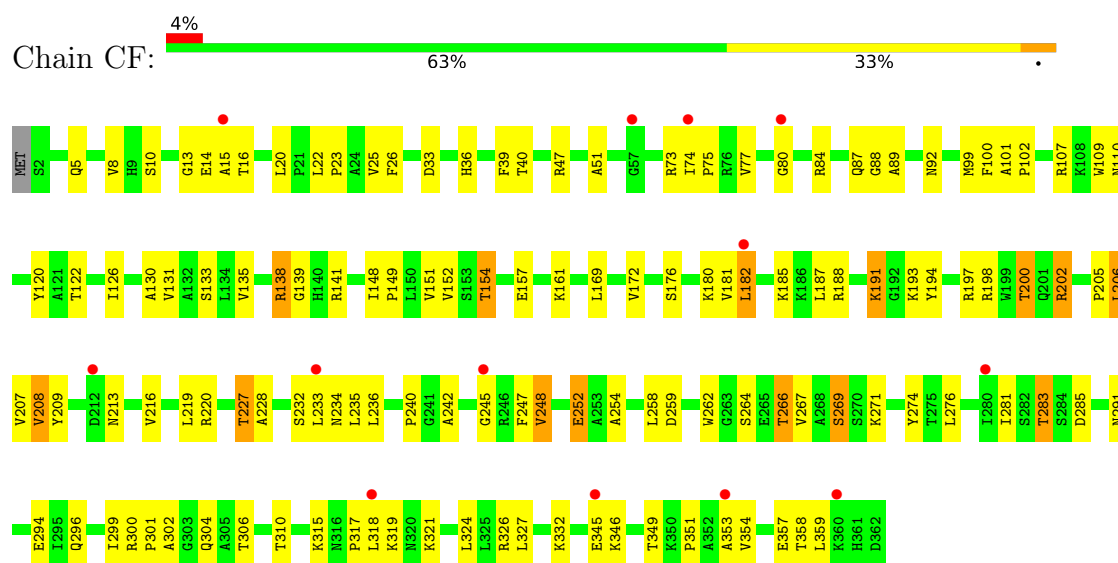
• Molecule 5: 60S ribosomal protein L3



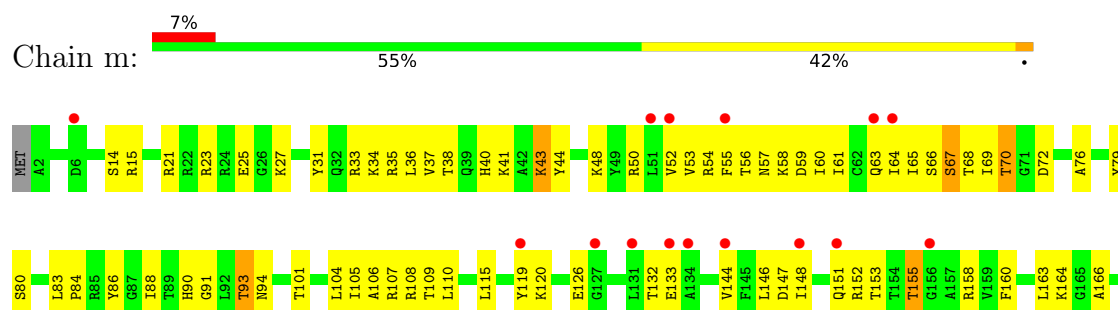
• Molecule 6: 60S ribosomal protein L4-A

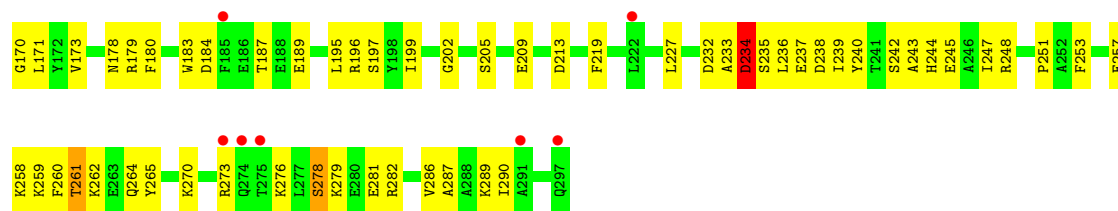


• Molecule 6: 60S ribosomal protein L4-A

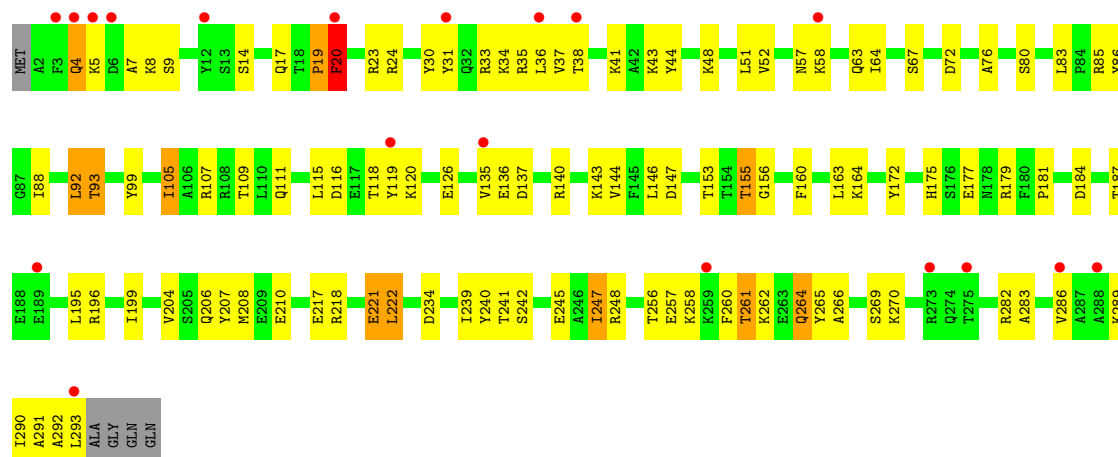


• Molecule 7: 60S ribosomal protein L5

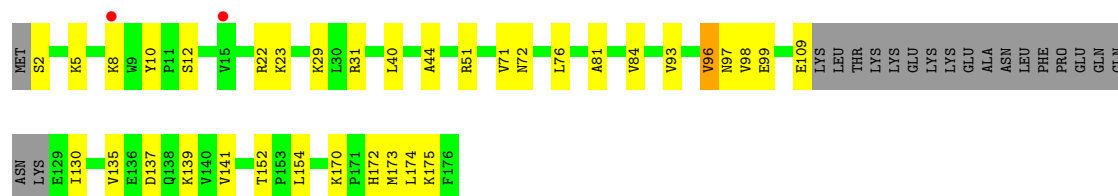




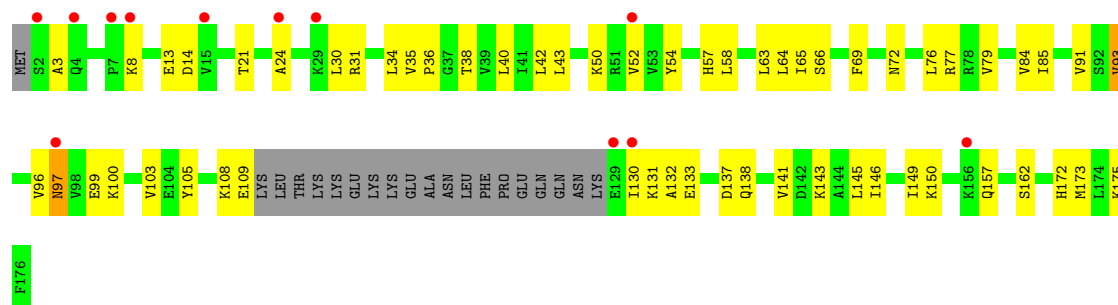
• Molecule 7: 60S ribosomal protein L5



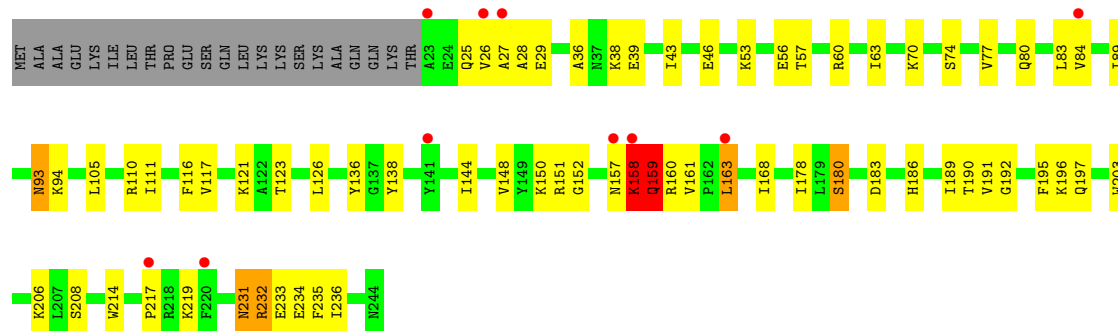
• Molecule 8: 60S ribosomal protein L6-A



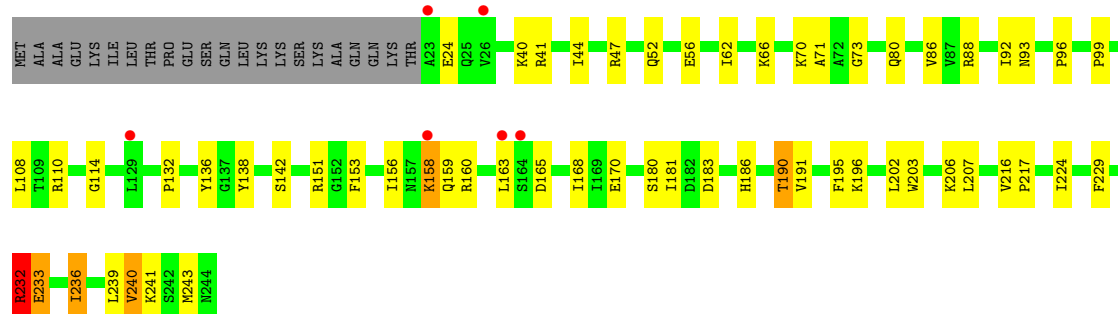
• Molecule 8: 60S ribosomal protein L6-A



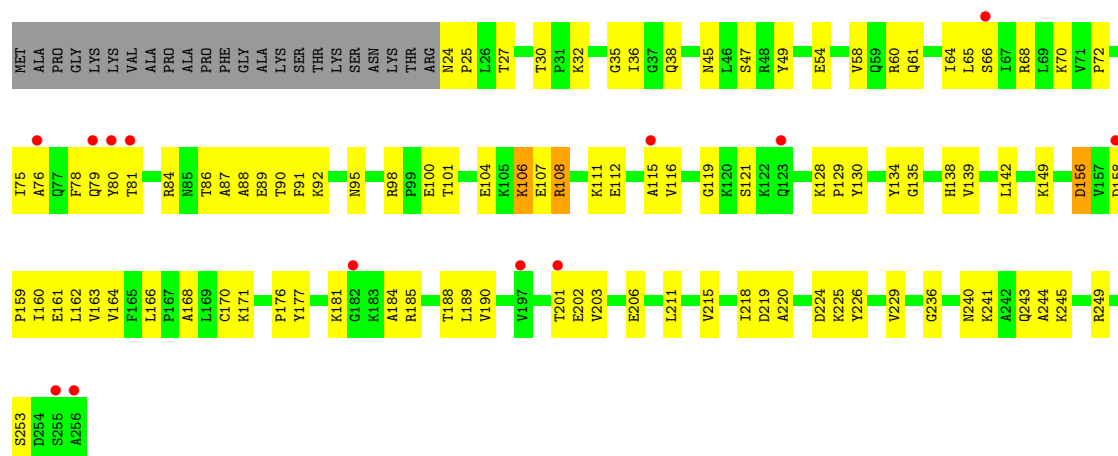
• Molecule 9: 60S ribosomal protein L7-A



• Molecule 9: 60S ribosomal protein L7-A

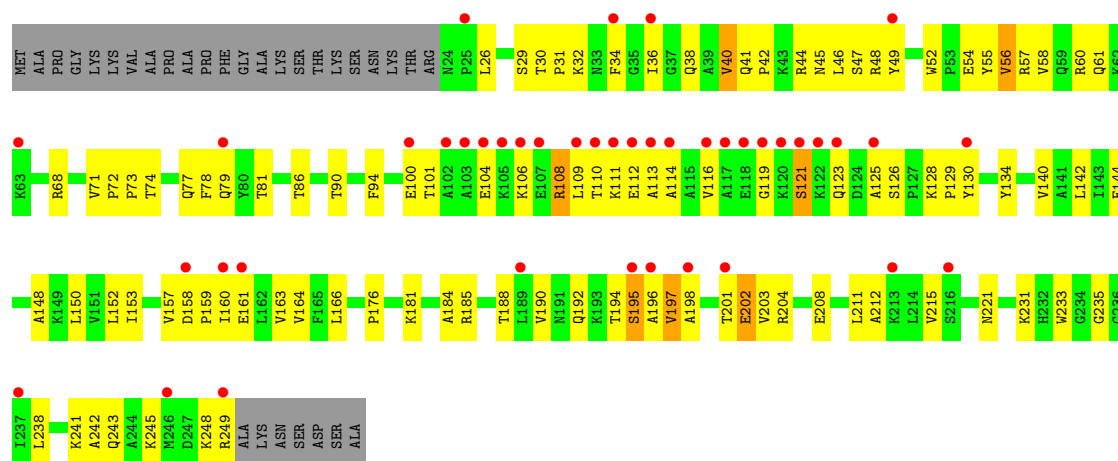


• Molecule 10: 60S ribosomal protein L8-A

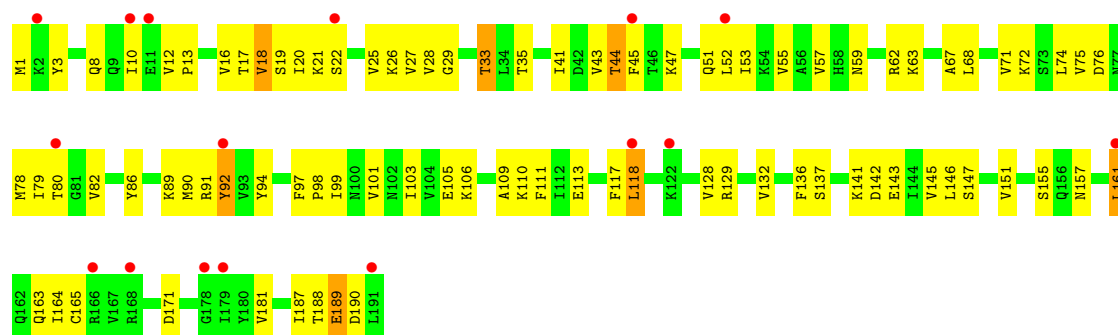


• Molecule 10: 60S ribosomal protein L8-A

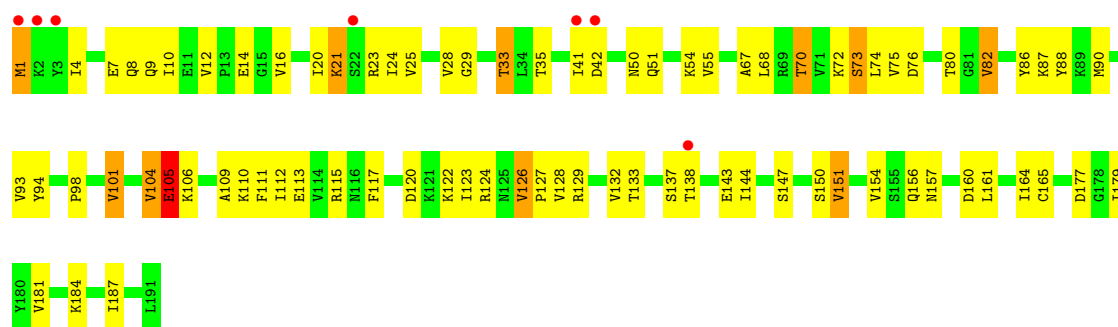




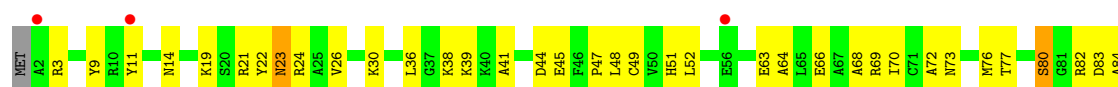
• Molecule 11: 60S ribosomal protein L9-A

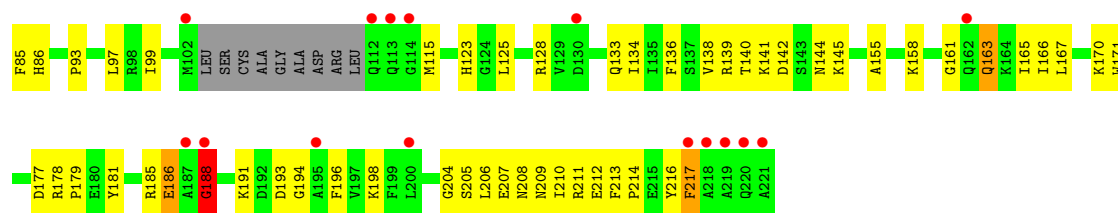


• Molecule 11: 60S ribosomal protein L9-A

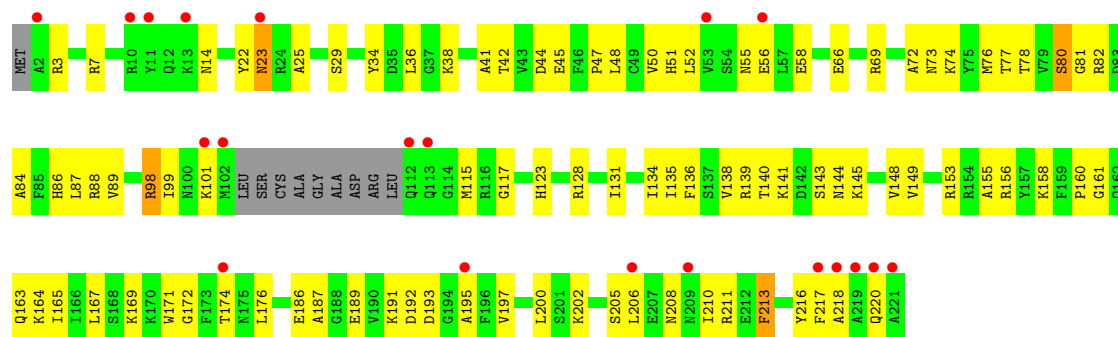


• Molecule 12: 60S ribosomal protein L10

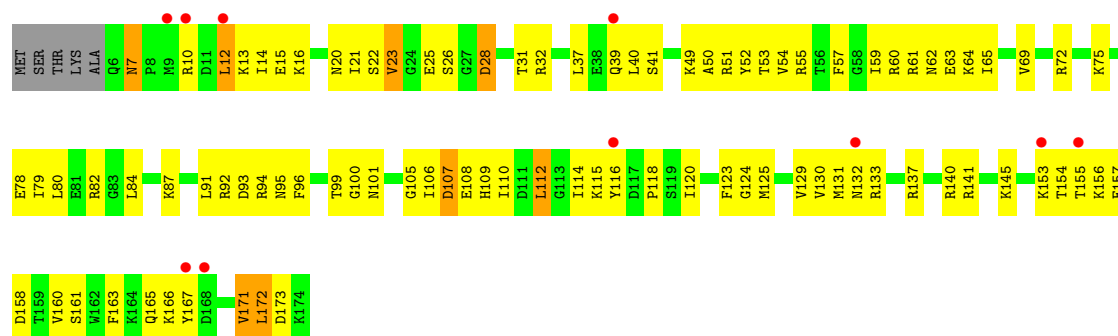
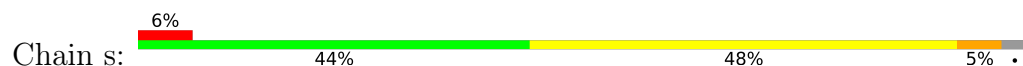




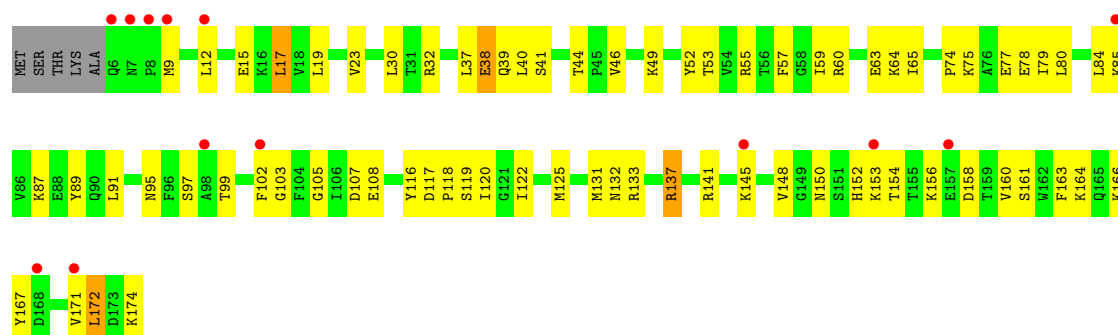
• Molecule 12: 60S ribosomal protein L10



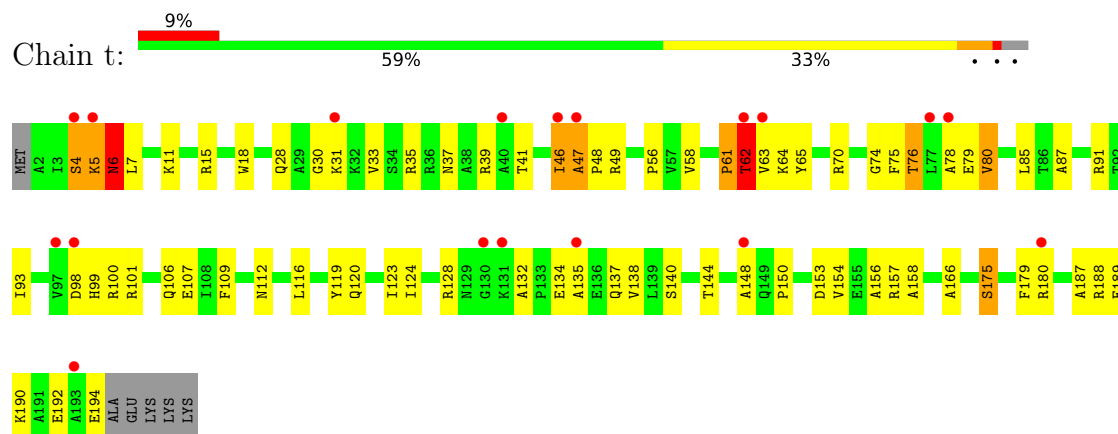
• Molecule 13: Large ribosomal subunit protein uL5B



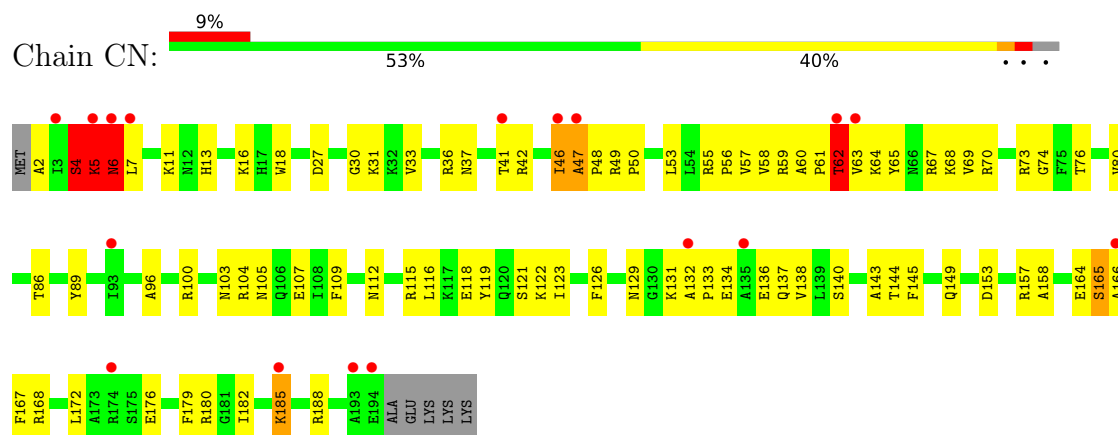
• Molecule 13: Large ribosomal subunit protein uL5B



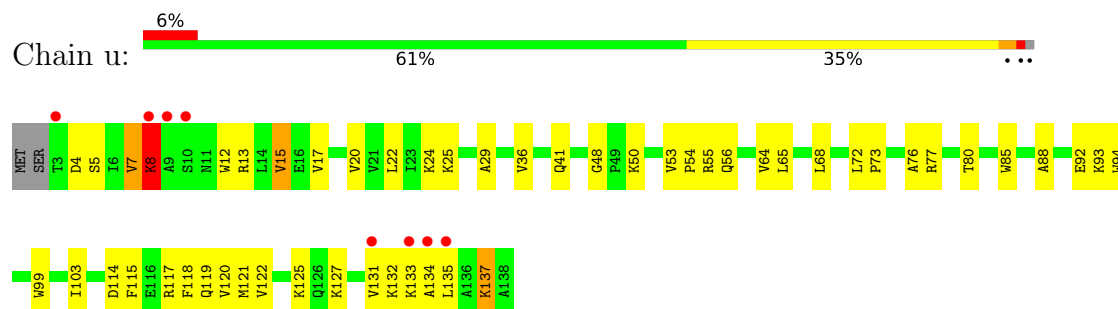
- Molecule 14: 60S ribosomal protein L13-A



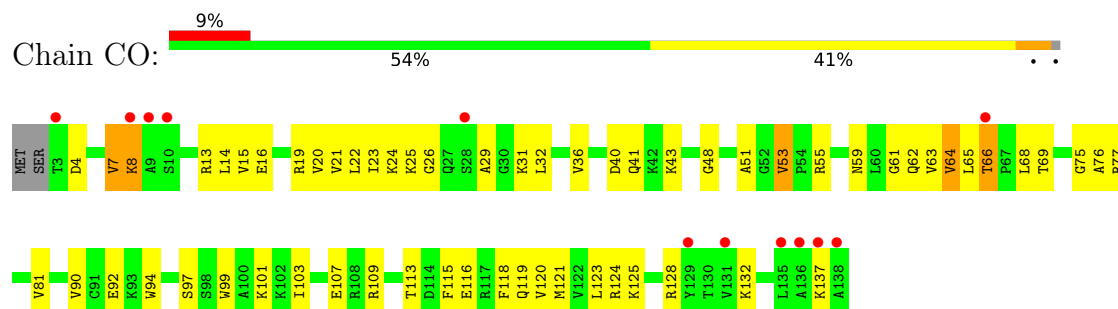
- Molecule 14: 60S ribosomal protein L13-A



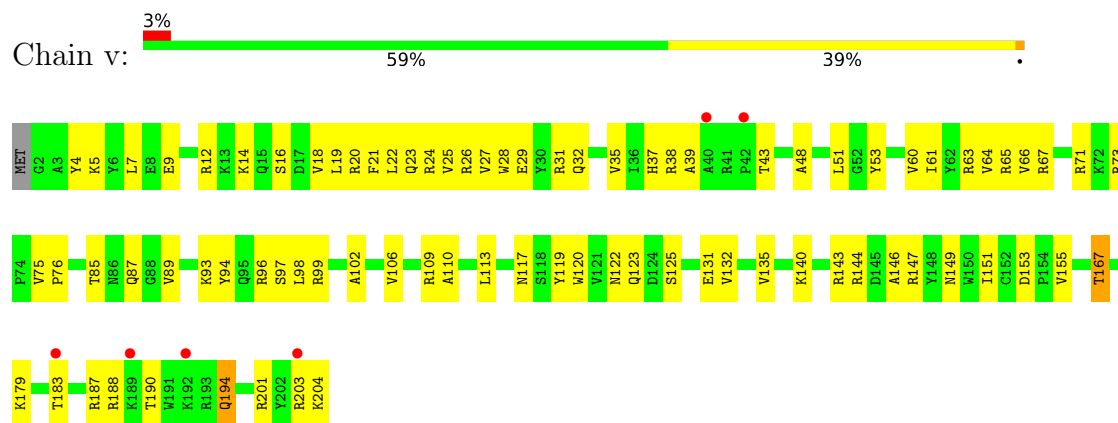
- Molecule 15: 60S ribosomal protein L14-A



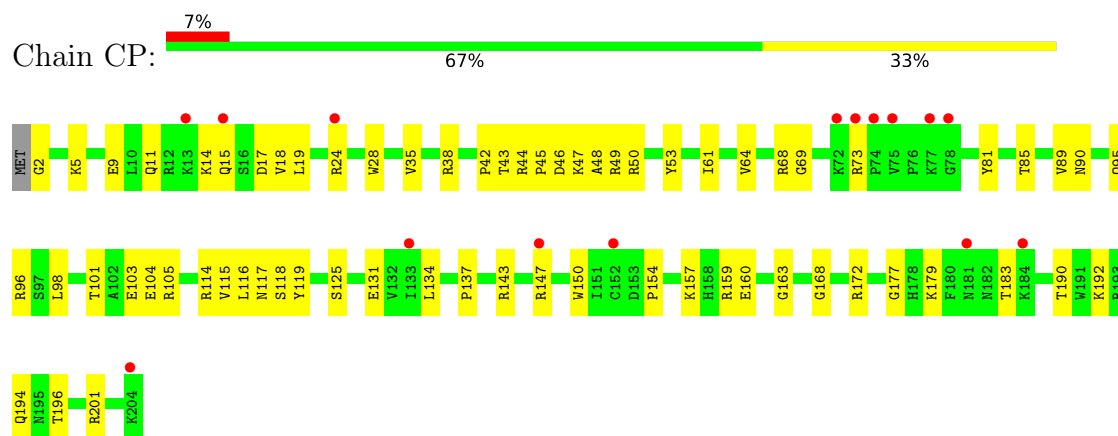
- Molecule 15: 60S ribosomal protein L14-A



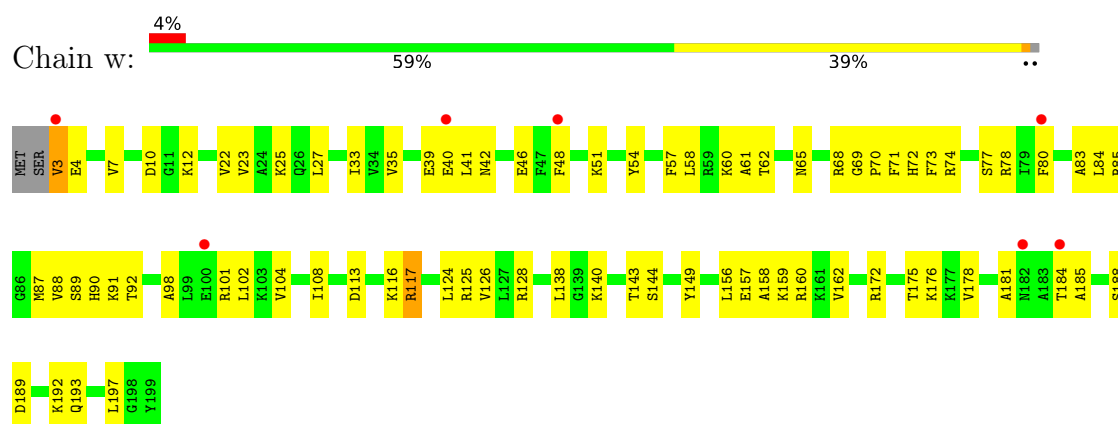
- Molecule 16: 60S ribosomal protein L15-A



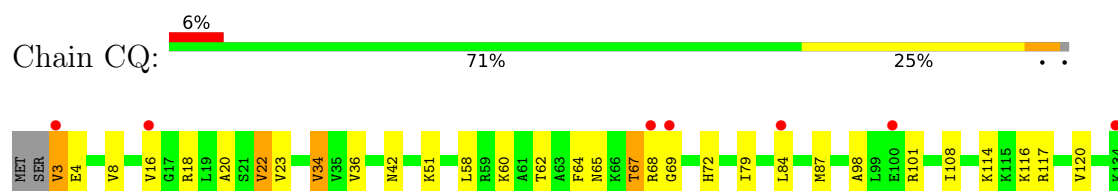
- Molecule 16: 60S ribosomal protein L15-A



- Molecule 17: 60S ribosomal protein L16-A

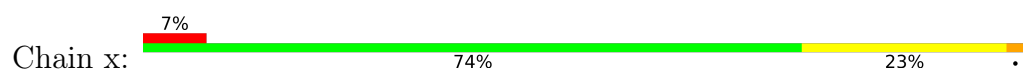


- Molecule 17: 60S ribosomal protein L16-A





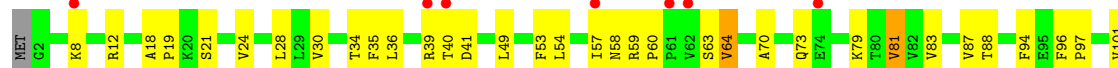
- Molecule 18: 60S ribosomal protein L17-A



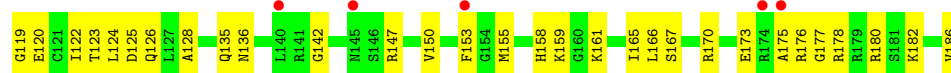
- Molecule 18: 60S ribosomal protein L17-A



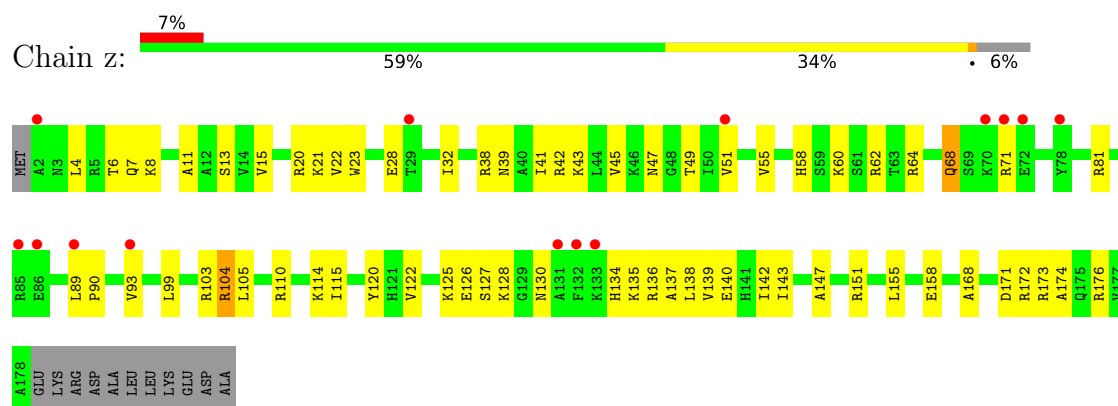
- Molecule 19: 60S ribosomal protein L18-A



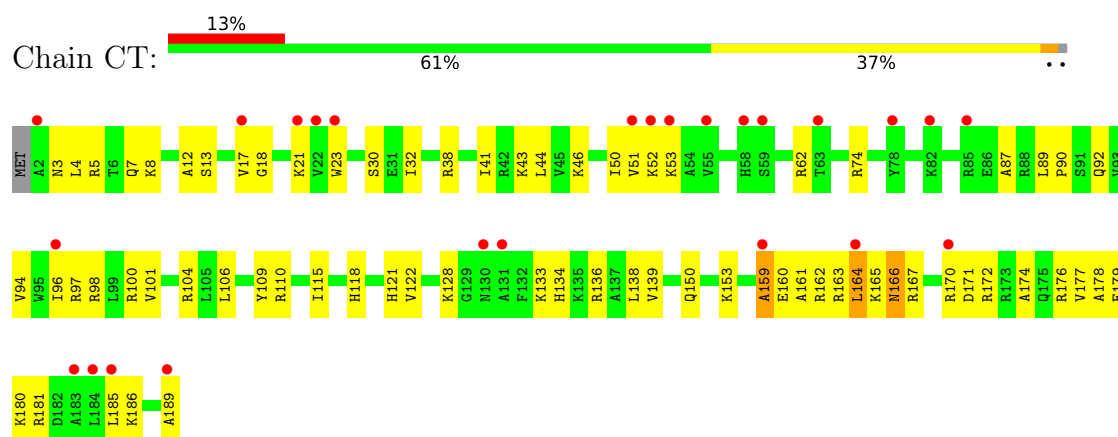
- Molecule 19: 60S ribosomal protein L18-A



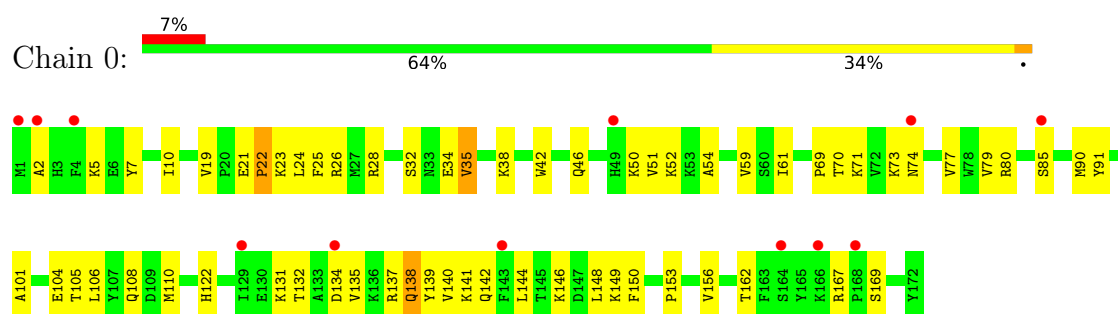
- Molecule 20: 60S ribosomal protein L19-A



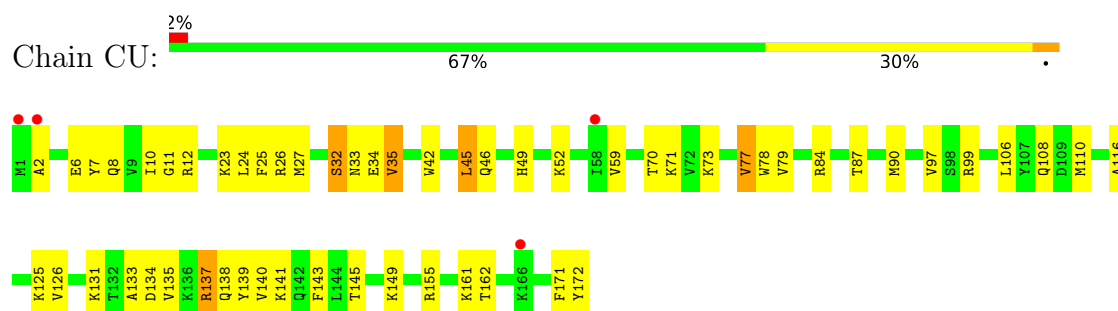
- Molecule 20: 60S ribosomal protein L19-A



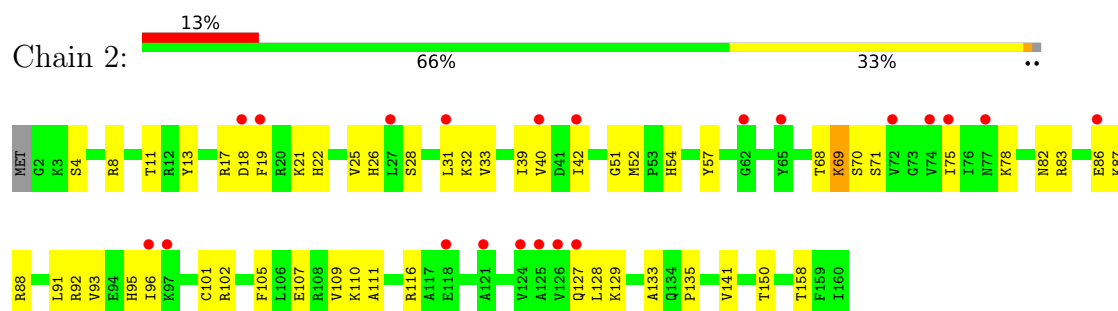
- Molecule 21: 60S ribosomal protein L20-A



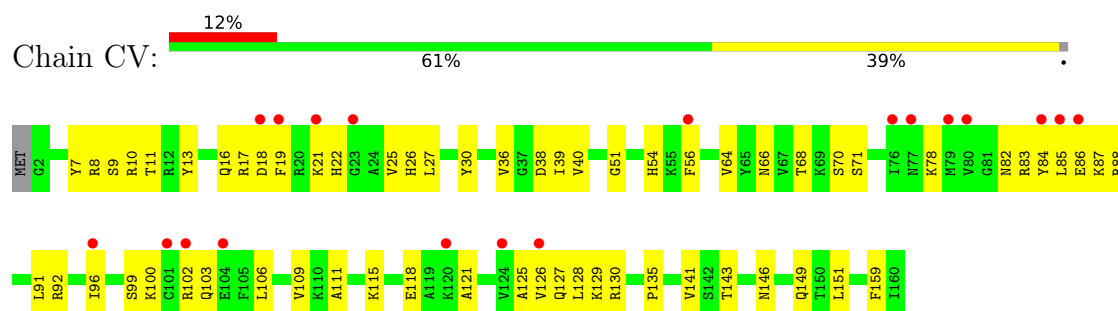
- Molecule 21: 60S ribosomal protein L20-A



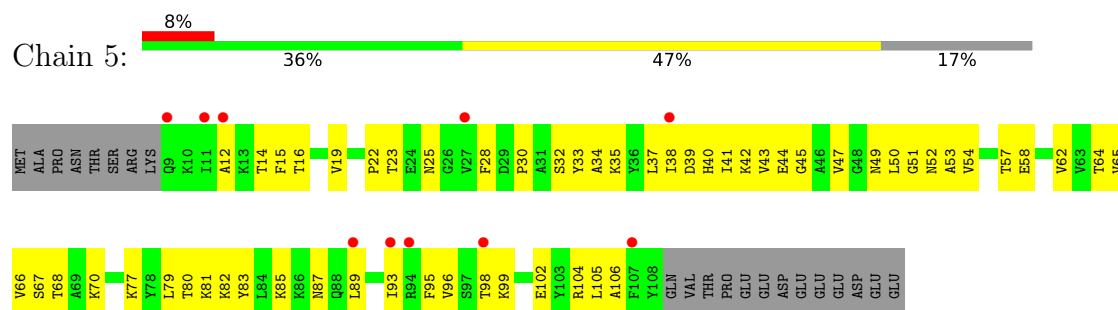
- Molecule 22: 60S ribosomal protein L21-A



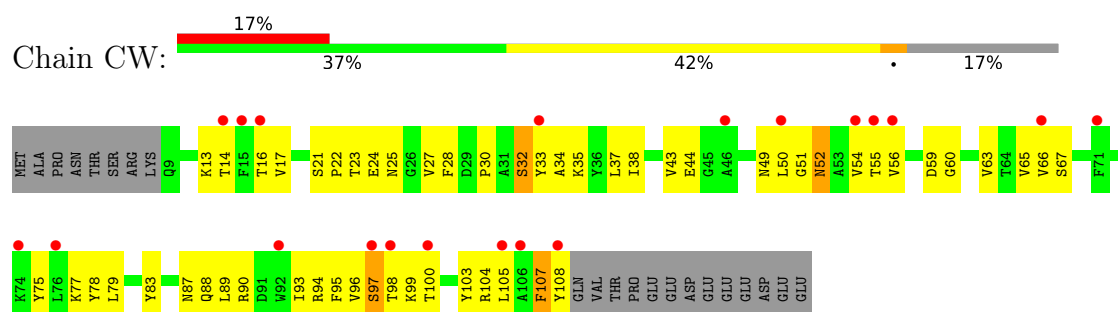
- Molecule 22: 60S ribosomal protein L21-A



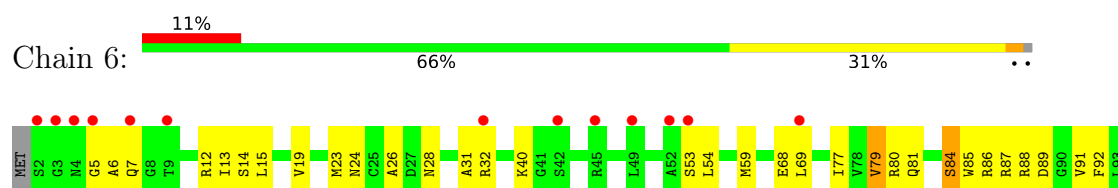
- Molecule 23: 60S ribosomal protein L22-A



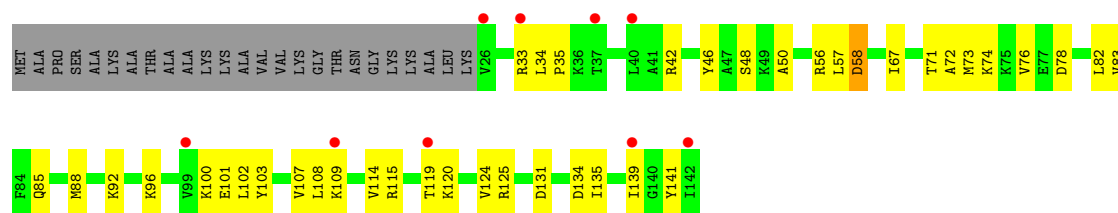
- Molecule 23: 60S ribosomal protein L22-A



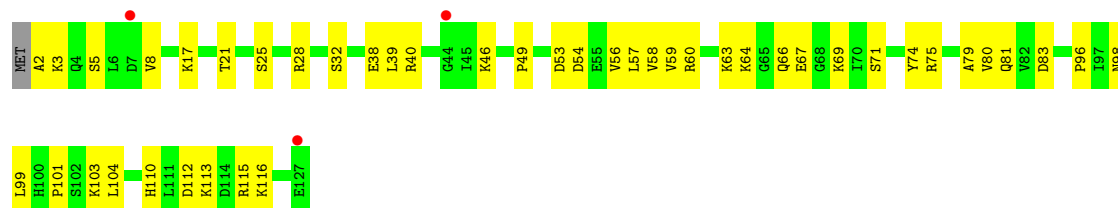
- Molecule 24: 60S ribosomal protein L23-A



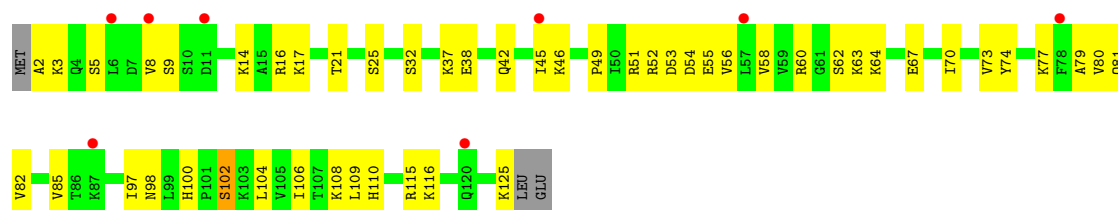




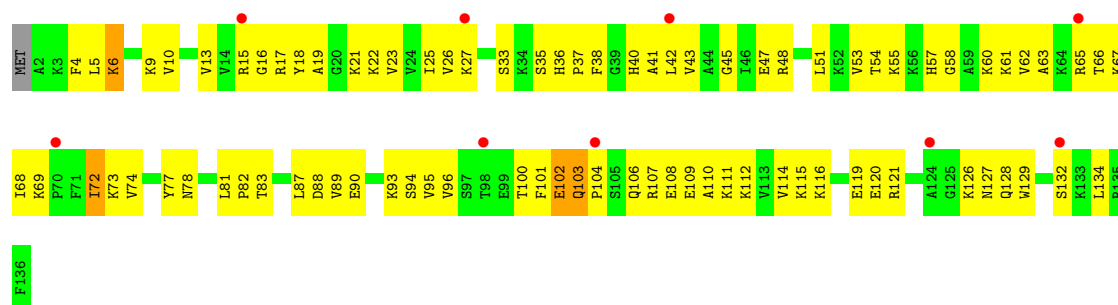
• Molecule 27: 60S ribosomal protein L26-A



• Molecule 27: 60S ribosomal protein L26-A

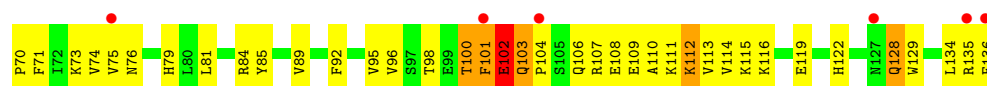


• Molecule 28: 60S ribosomal protein L27-A

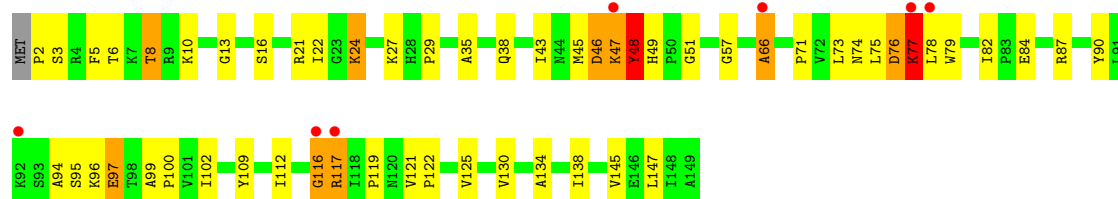


• Molecule 28: 60S ribosomal protein L27-A

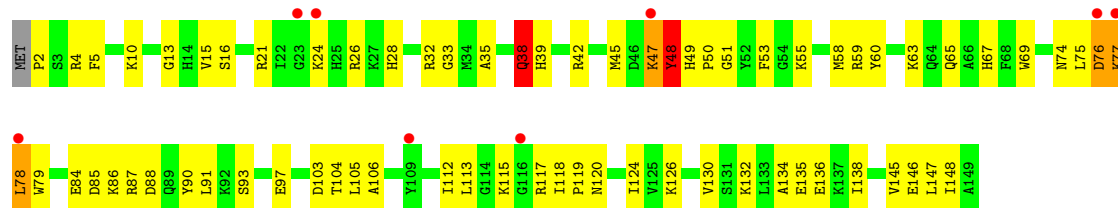




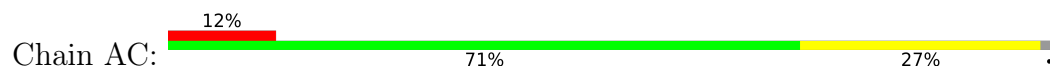
- Molecule 29: 60S ribosomal protein L28



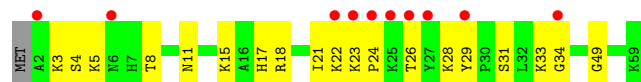
- Molecule 29: 60S ribosomal protein L28



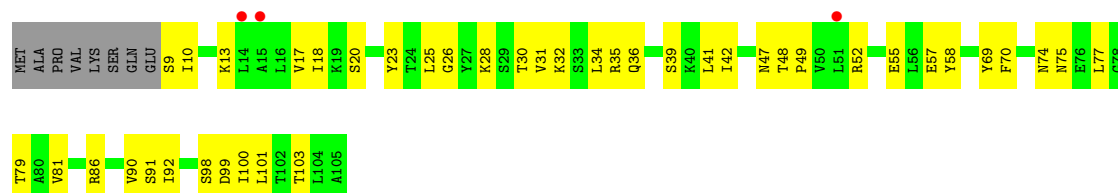
- Molecule 30: 60S ribosomal protein L29



- Molecule 30: 60S ribosomal protein L29

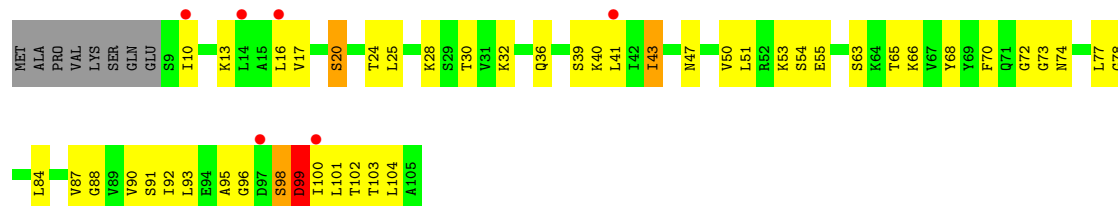


- Molecule 31: 60S ribosomal protein L30



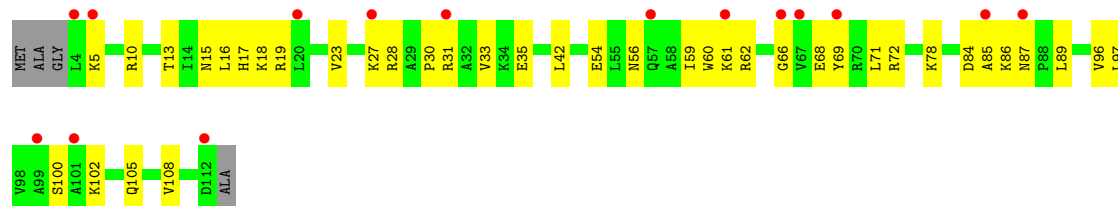
- Molecule 31: 60S ribosomal protein L30

Chain DE: 



- Molecule 32: 60S ribosomal protein L31-A

Chain AE: 



- Molecule 32: 60S ribosomal protein L31-A

Chain DF: 



- Molecule 33: 60S ribosomal protein L32

Chain AF: 



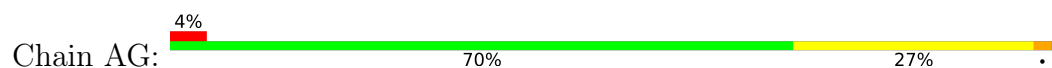
- Molecule 33: 60S ribosomal protein L32

Chain DG: 





- Molecule 34: 60S ribosomal protein L33-A



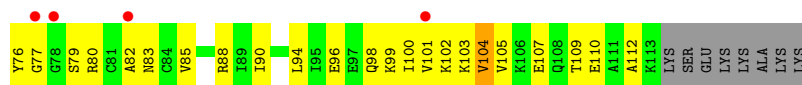
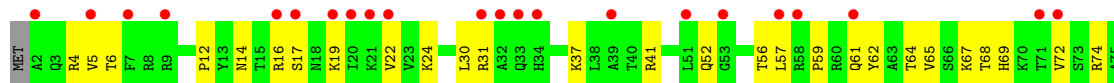
- Molecule 34: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L34-A



- Molecule 35: 60S ribosomal protein L34-A

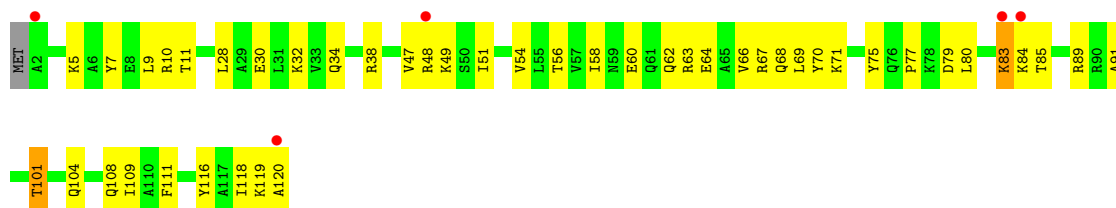


- Molecule 36: 60S ribosomal protein L35-A





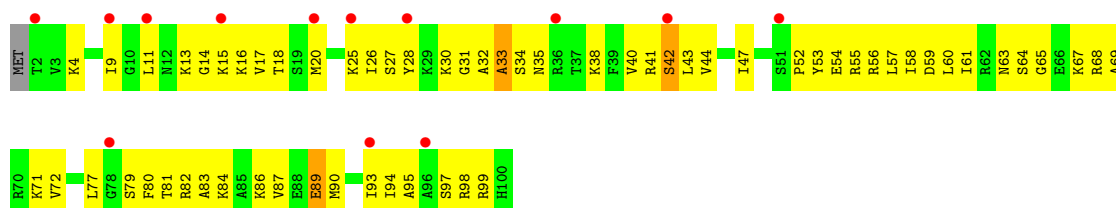
- Molecule 36: 60S ribosomal protein L35-A



- Molecule 37: 60S ribosomal protein L36-A



- Molecule 37: 60S ribosomal protein L36-A



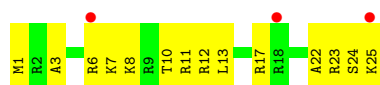
- Molecule 38: 60S ribosomal protein L37-A



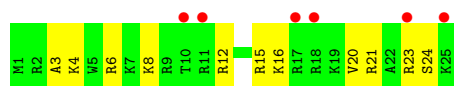
- Molecule 38: 60S ribosomal protein L37-A



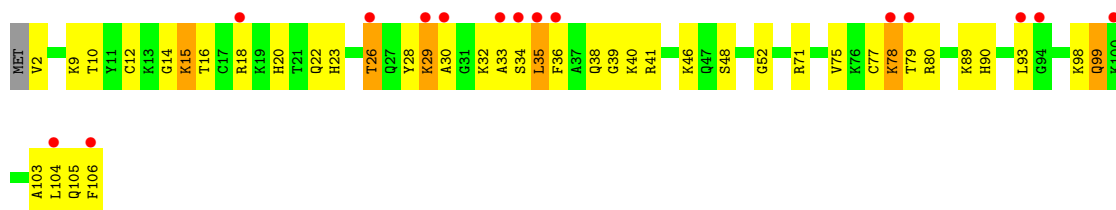
- Molecule 42: Large ribosomal subunit protein eL41B



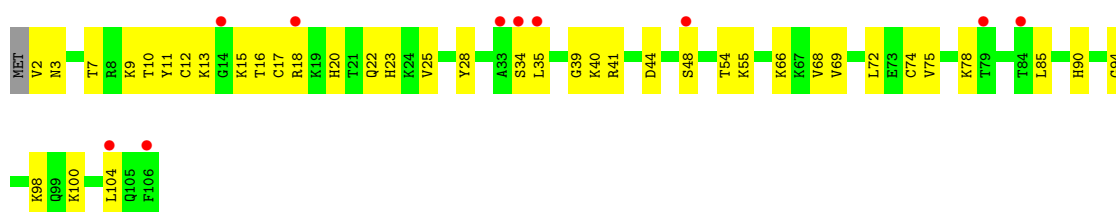
- Molecule 42: Large ribosomal subunit protein eL41B



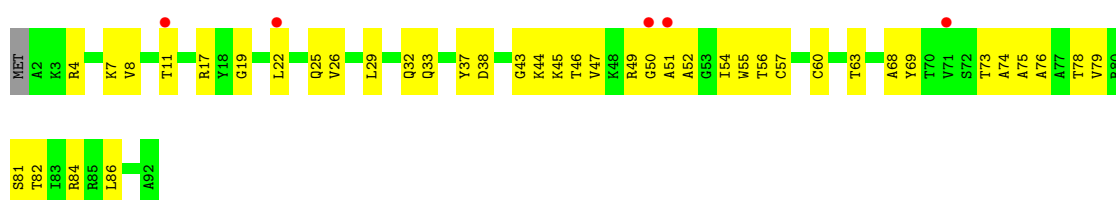
- Molecule 43: 60S ribosomal protein L42-A



- Molecule 43: 60S ribosomal protein L42-A

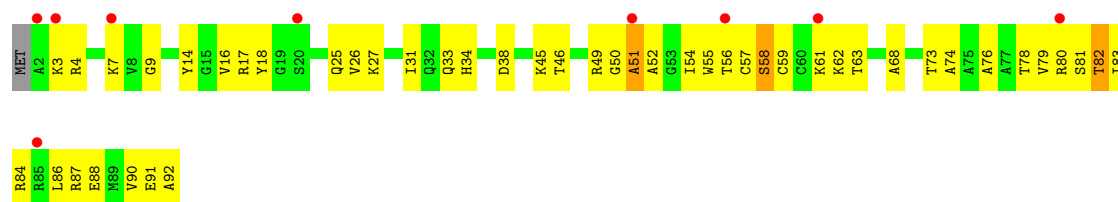


- Molecule 44: 60S ribosomal protein L43-A

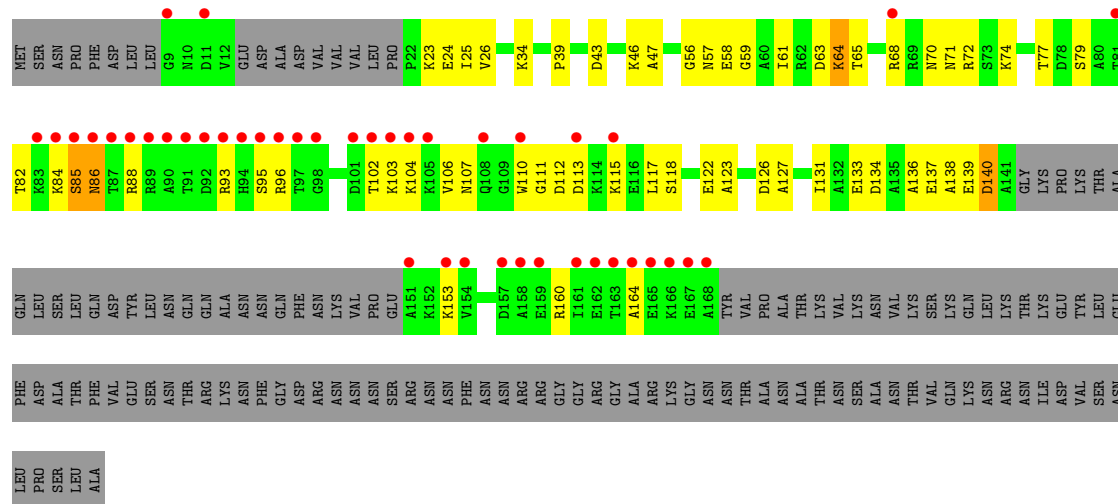
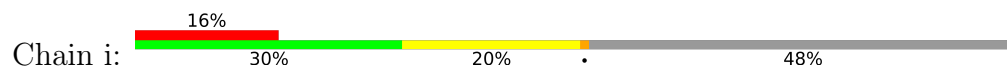


- Molecule 44: 60S ribosomal protein L43-A

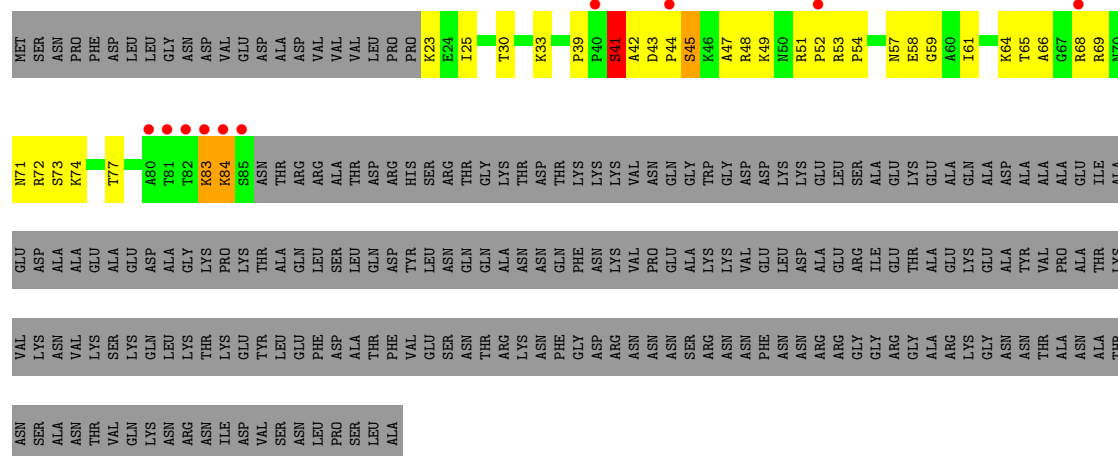




• Molecule 45: Suppressor protein STM1



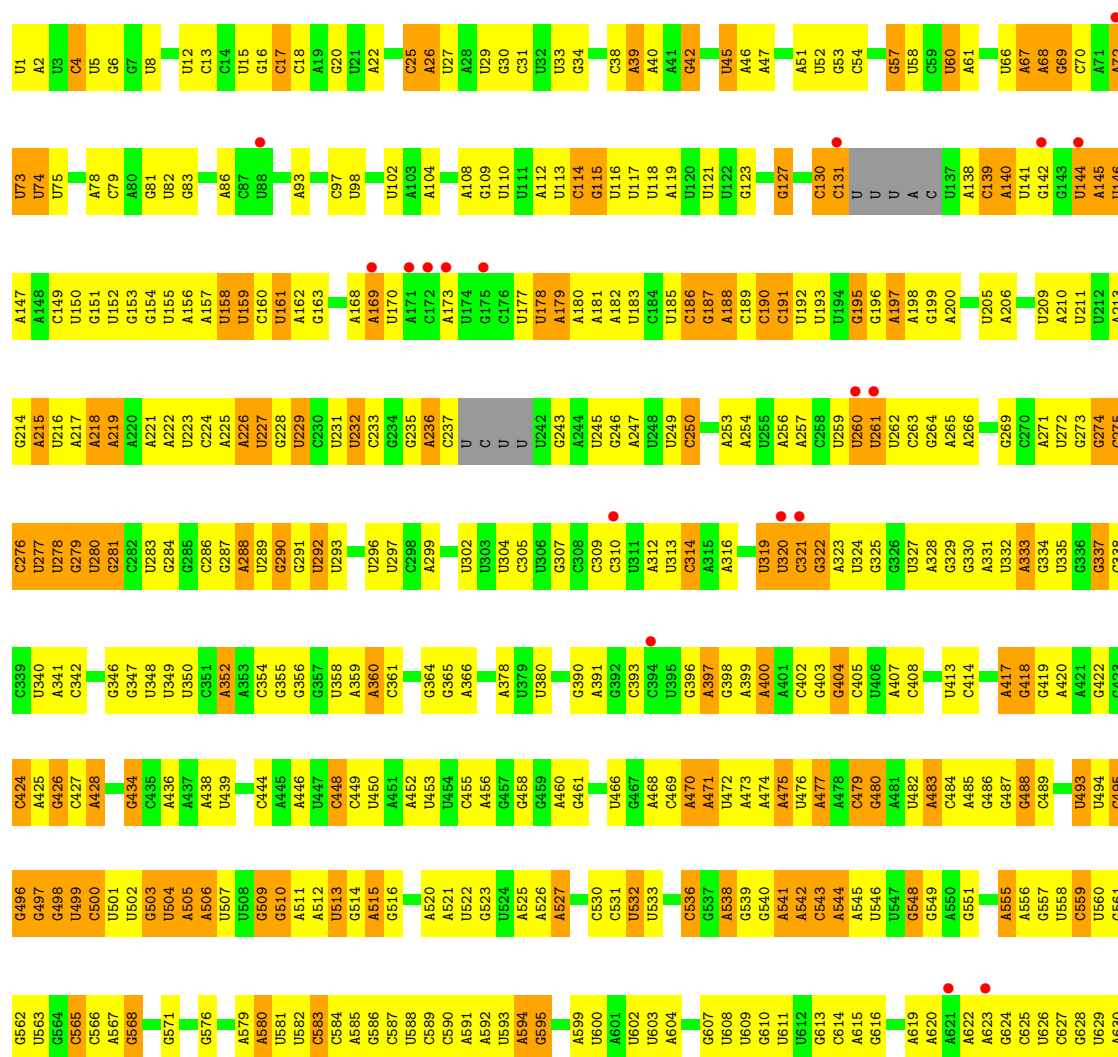
• Molecule 45: Suppressor protein STM1



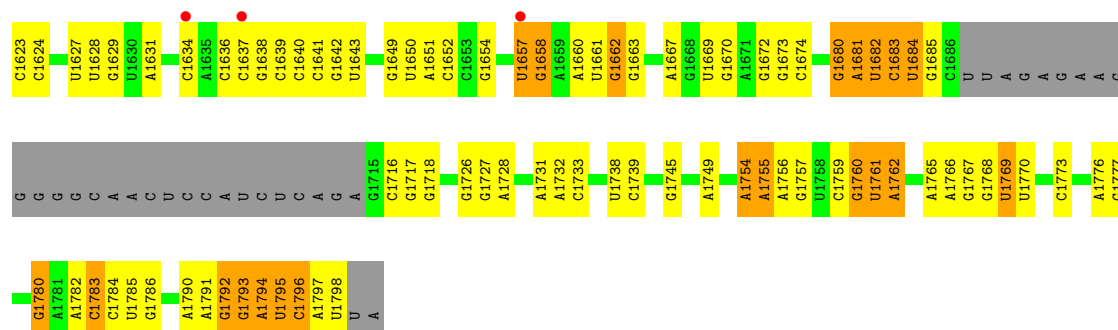
• Molecule 46: 60S acidic ribosomal protein P0



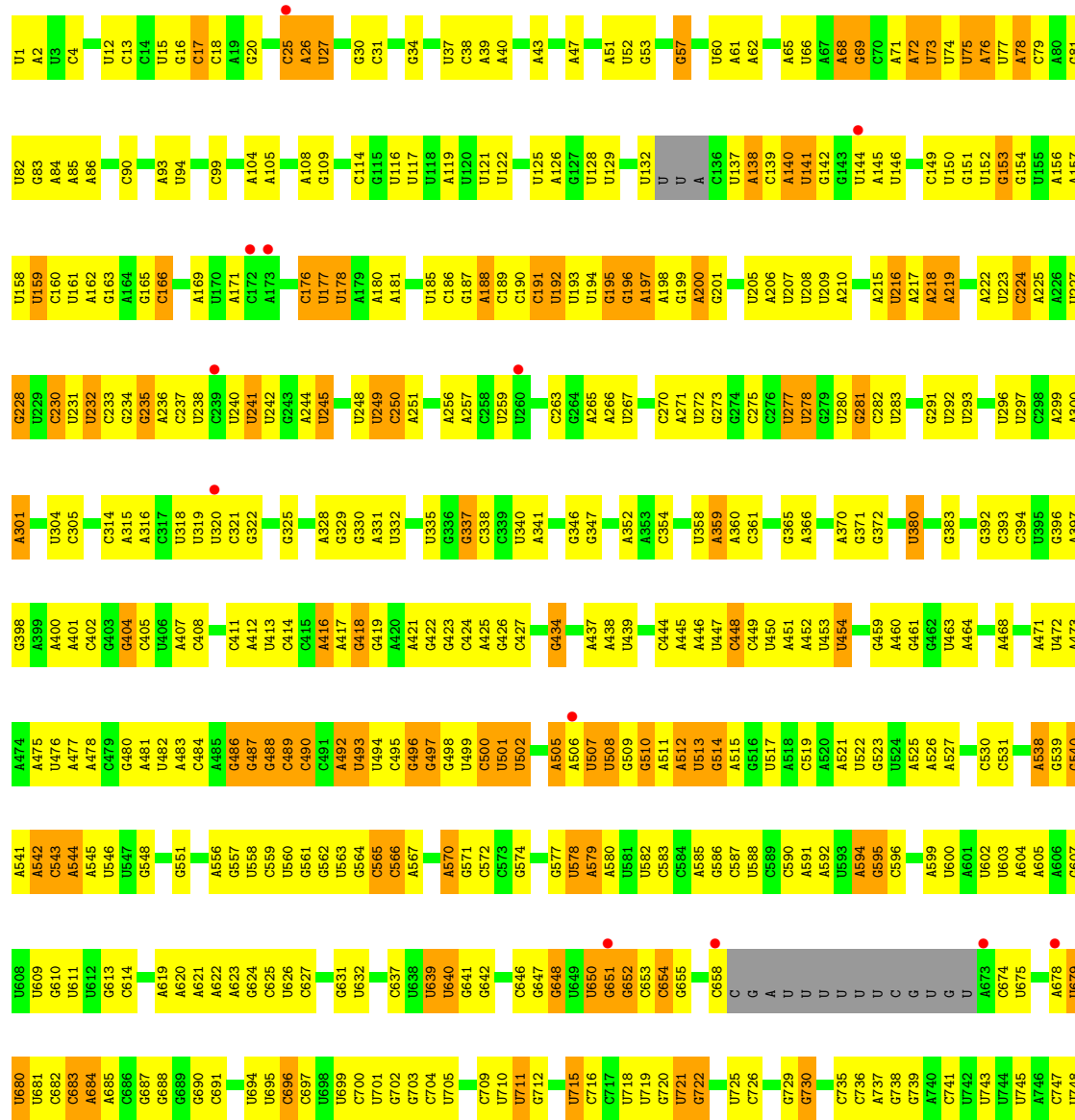
- Molecule 47: 16S ribosomal RNA



A1559	G1428	U1361	C1284	G1213	U1058	G980	U836	U764	U698	G631
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U1564	U1430	G1363	U1290	A1217	A1061	A906	U838	U766	C700	G633
C1565	G1433	C1364	G1291	A1218	A1062	U912	U839	U767	U701	G634
U1566	U1434	C1365	G1292	G1219	U1063	G913	U840	C768	G702	A635
U1567	G1435	U1366	U1293	A1220	G1064	G914	U841	G771	G703	A636
C1568	U1436	G1367	G1294	A1221	A1065	A915	U842	G772	C704	C637
A1569	U1437	U1370	G1297	A1223	U1066	A916	A844	G773	U705	U638
A1570	G1438	U1371	U1298	A1224	C1067	U917	G845	A774	A706	U639
C1571	C1439	U1372	G1299	C1148	C1068	U918	A846	G775	C707	U640
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A1573	C1441	U1376	A1301	G1150	C1070	A920	C849	G777	G709	G642
G1574	U1442	U1377	U1302	A1151	U1071	U921	A850	U778	U710	G646
G1575	U1443	U1378	U1303	A1157	C1072	G922	U851	U781	U711	G647
U1576	A1444	C1379	U1304	C1158	U1073	U923	U852	U782	A713	G648
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A1578	A1446	U1381	U1314	A1160	C1078	G925	U854	C784	U715	U650
U1579	U1449	U1382	U1315	C1161	U1079	A926	A855	U785	C716	G651
C1580	U1450	G1383	G1316	C1162	U1080	C927	A856	C786	C717	G654
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A1586	C1456	U1390	A1321	C1167	U1085	U932	A863	A791	G722	C
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U1608	A1479	G1409	A1344	C1192	G1112	G954	U887	G815	C741	U
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A1611	C1481	A1411	A1346	C1194	G1114	U959	U889	C818	U743	U
U1612	A1482	G1412	U1347	U1195	U1115	U960	C890	C819	U744	U
U1613	G1483	U1413	G1349	A1196	U1116	G961	A891	U820	A745	U
A1614	C1484	U1414	U1350	C1197	U1117	A966	A892	U821	G747	U
C1615	U1485	G1415	G1351	G1198	C1121	U967	U893	U822	U748	U
G1616	A1486	G1416	G1352	U1199	G1130	U968	U894	G823	U749	U
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C1618	G1488	G1418	G1354	C1201	U1049	C969	U896	U830	A754	U
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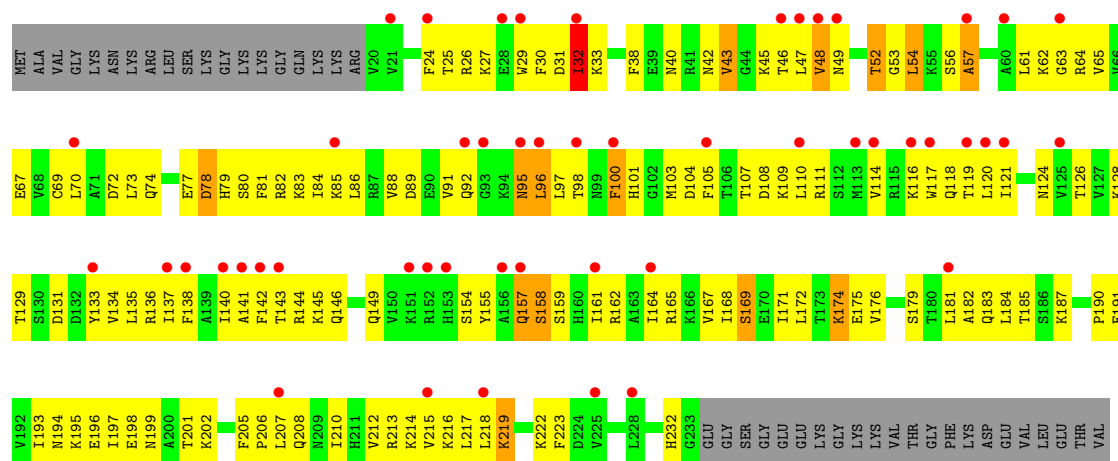


• Molecule 47: 16S ribosomal RNA

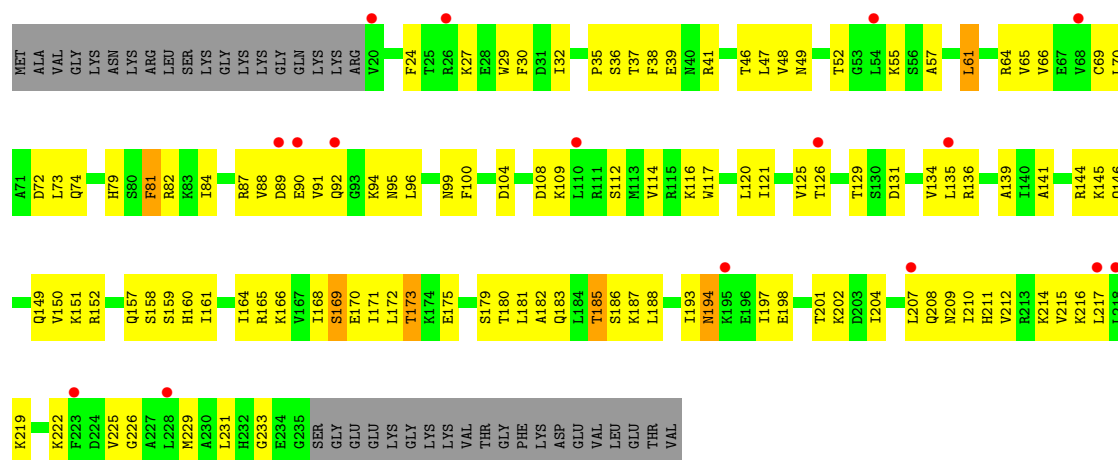


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U1650	G1575	U1513	G1448	A1382	A1319	A1242	C1173	U1099	A1027	A955	A959	G823	A754
A1651	U1579	A1514	U1449	G1383	A1240	A1243	U1174	G1100	C1028	C956	A891	G824	A755
G1652	U1580	A1515	A1450	A1384	A1321	G1244	U1175	G1101	U1029	G957	U893	U825	A756
C1653	G1581	U1517	U1452	G1385	A1322	G1245	C1177	U1102	A1030	U958	G895	U826	A757
G1654	U1582	C1518	G1453	A1388	G1324	C1246	G1178	U1103	A1031	U959	U896	C827	U757
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U1660	U1590	A1524	C1459	G1330	A1330	C1252	C1180	G1112	G1043	A967	U835	U836	U764
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U1672	U1593	C1528	G1464	C1335	A1335	U1256	C1191	U1120	G1048	U970	U841	U841	A774
G1673	G1594	C1529	C1465	U1400	A1336	U1257	C1192	U1121	G1050	A971	U842	U843	G775
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G1680	U1597	C1533	U1468	C1403	C1339	G1261	C1196	G1127	G1053	C975	U847	U848	A778
A1681	U1598	U1534	A1469	C1404	A1340	U1262	G1198	G1130	U1057	G976	U849	U850	A779
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U1701	A1614	U1550	G1484	A1421	C1355	U1285	U1219	U1146	U1071	A992	U876	U877	A792
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U1703	U1620	U1552	G1486	U1423	A1357	U1287	U1219	G1151	G1073	A1001	U880	U881	A794
U1704	G1621	G1553	A1487	A1424	G1358	G1288	C1216	U1152	C1074	A1002	U882	U883	A795
C1705	C1622	U1554	U1488	A1425	C1359	U1289	A1217	G1153	C1075	A1003	U884	U885	A796
C1706	C1623	U1555	U1489	C1426	A1360	G1291	U1218	U1154	U1078	A1004	U886	U887	U800
C1707	C1624	U1556	U1491	U1427	U1361	U1292	A1219	U1155	U1079	U1005	U888	U889	G801
U1708	U1628	A1559	C1493	U1430	U1362	G1294	C1220	G1156	U1080	A1006	U890	U891	G802
C1709	G1629	U1560	C1494	U1432	G1363	G1297	C1221	U1157	A1081	C1006	U892	U893	G803
U1710	C1634	U1561	U1496	G1433	U1364	G1298	A1222	C1158	C1082	U1009	U894	U895	G804
C1711	U1637	C1562	U1497	U1434	G1365	A1300	U1223	U1159	G1085	U1010	U896	U897	U809
G1712	U1638	U1563	G1498	G1435	U1366	U1305	A1224	U1160	A1086	A1013	U898	U899	G810
A1713	U1639	C1564	U1499	A1436	U1367	U1306	U1225	C1161	U1087	U1014	U900	U901	G811
U1714	G1639	U1565	U1437	A1437	A1371	U1311	U1226	C1162	A1087	G1015	U902	U903	G812
G1715	C1640	U1566	G1438	U1438	U1372	A1312	A1227	C1163	A1088	U1016	U904	U905	G813
C1716	U1641	U1567	C1439	G1439	U1373	A1313	U1228	U1164	U1089	U1017	U906	U907	G814
G1717	G1642	A1569	C1440	C1440	A1375	U1314	U1229	U1165	A1091	U1018	U908	U909	G815
G1720		G1572	A1444	U1444	C1376	U1315	G1233	U1166	U1092	U1019	U910	U911	G816
			G1506	G1445	C1379	G1316	A1234	U1167	A1093	A1020	U912	U913	G817
							U1315	U1168	G1094	U1021	U914	U915	G818
								G1170	C1096		U916	U917	G819
											U918	U919	U820

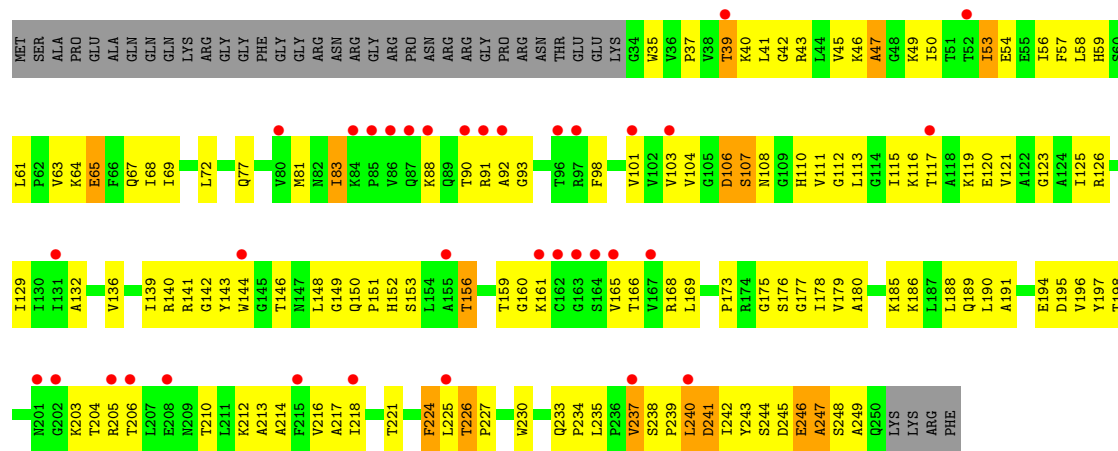




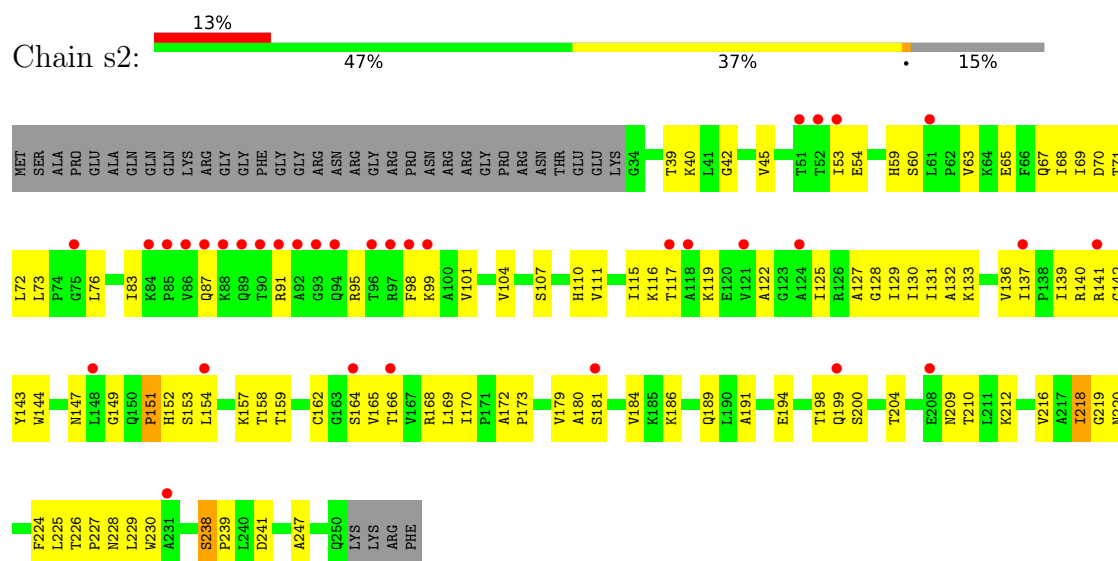
• Molecule 49: 40S ribosomal protein S1-A



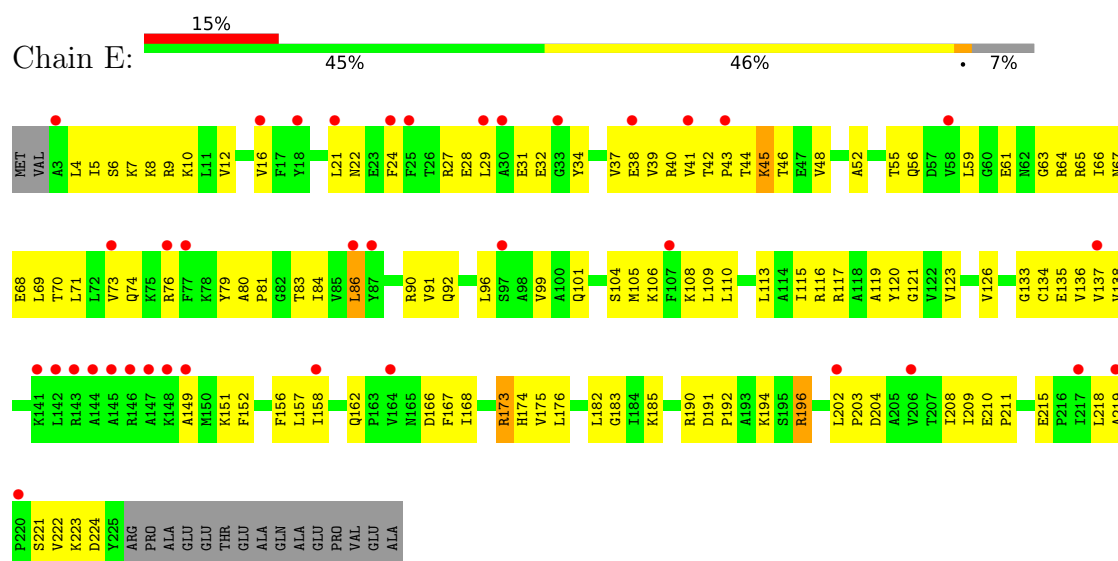
• Molecule 50: 40S ribosomal protein S2



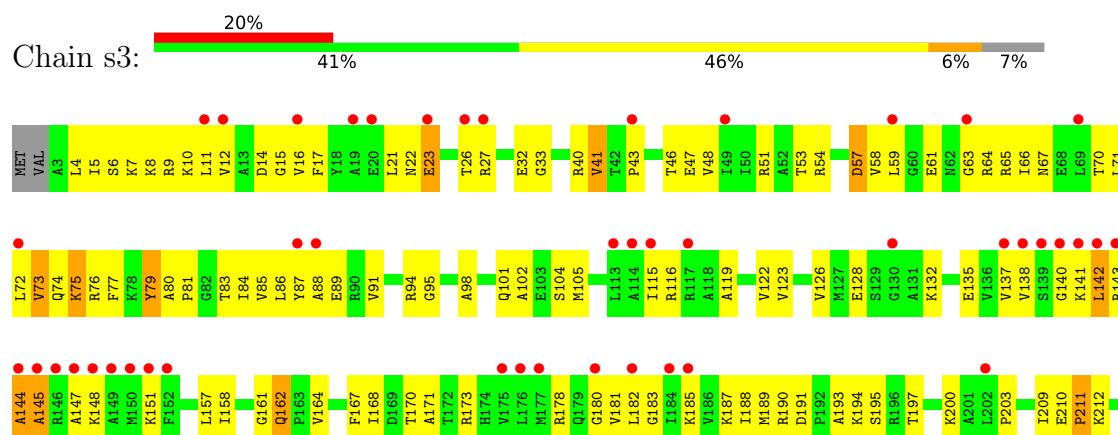
• Molecule 50: 40S ribosomal protein S2

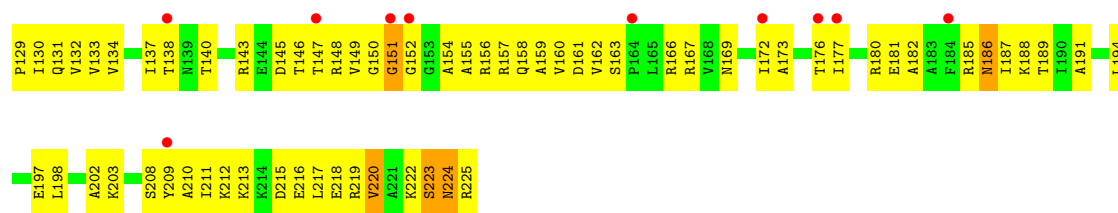


• Molecule 51: Small ribosomal subunit protein uS3

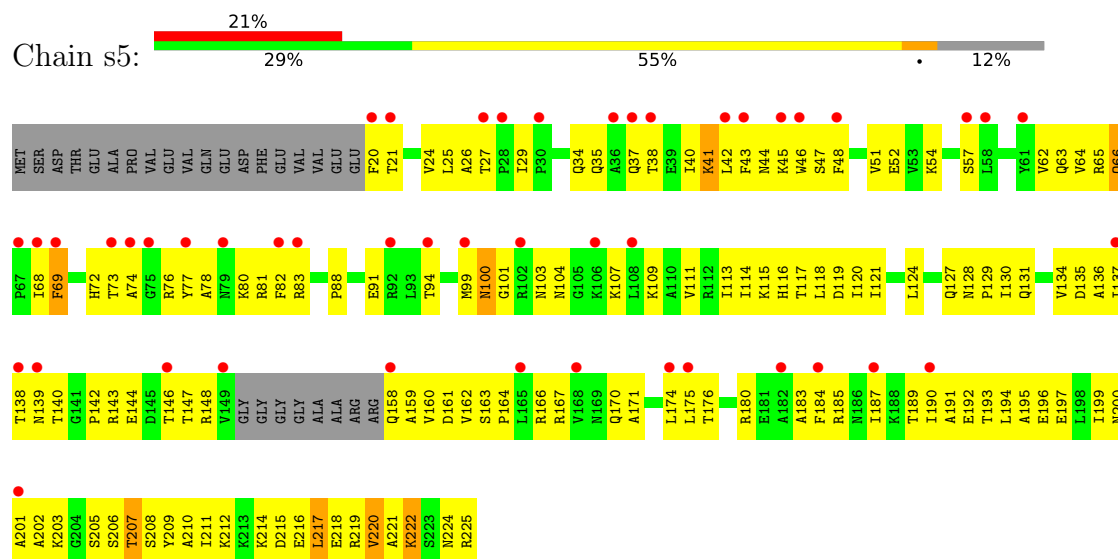


• Molecule 51: Small ribosomal subunit protein uS3

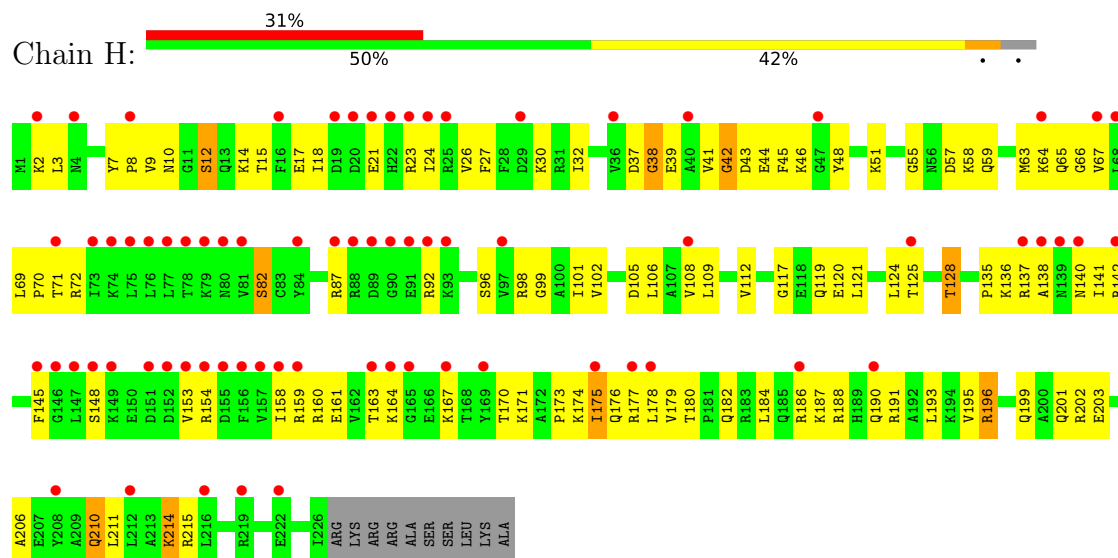




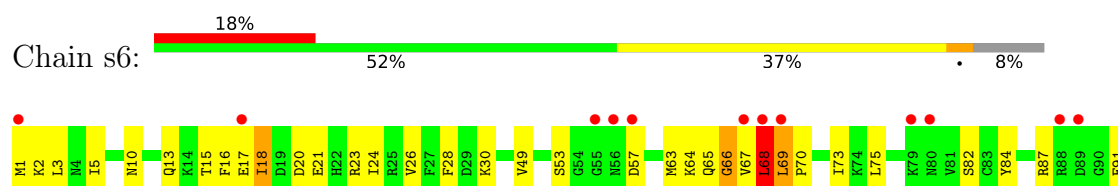
• Molecule 53: 40S ribosomal protein S5

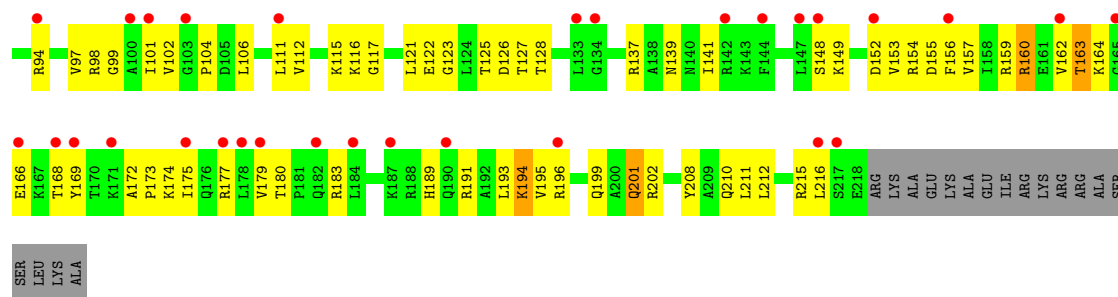


• Molecule 54: 40S ribosomal protein S6-A

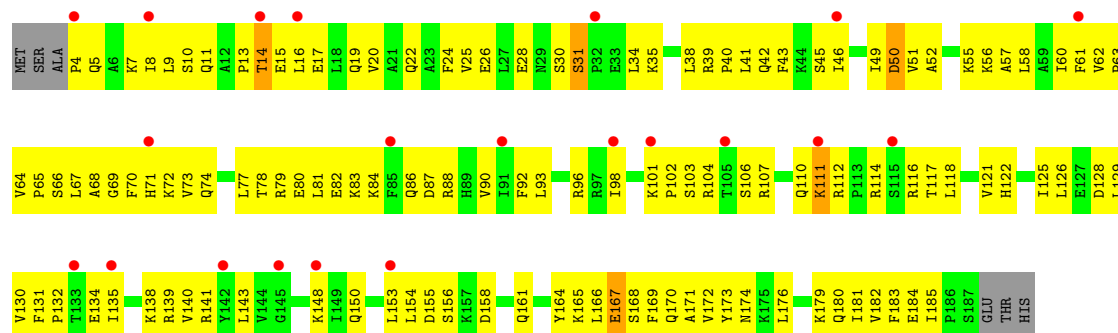


• Molecule 54: 40S ribosomal protein S6-A

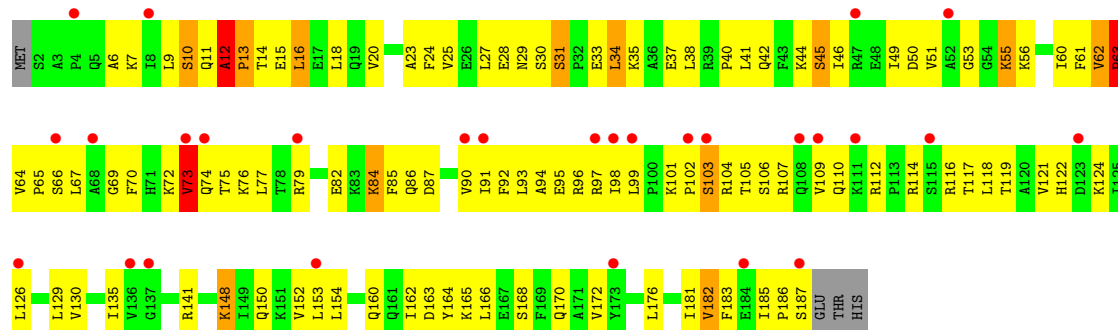




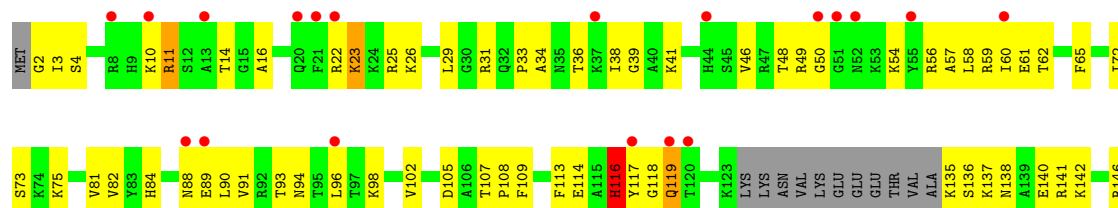
• Molecule 55: 40S ribosomal protein S7-A

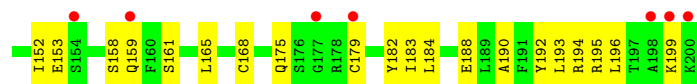


• Molecule 55: 40S ribosomal protein S7-A

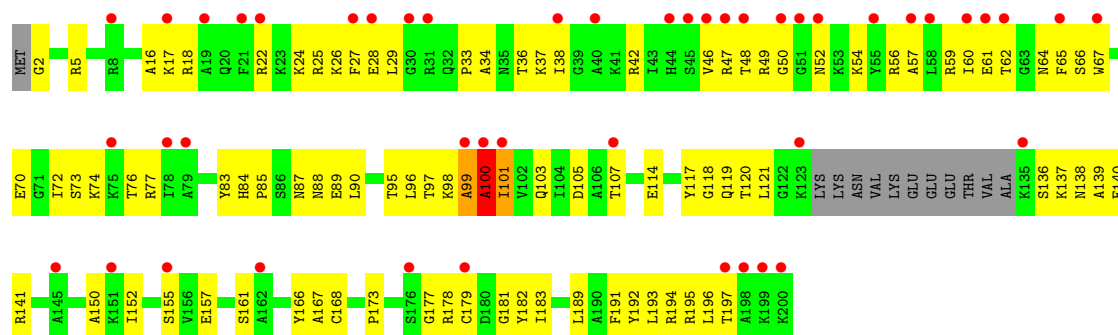


• Molecule 56: 40S ribosomal protein S8-A

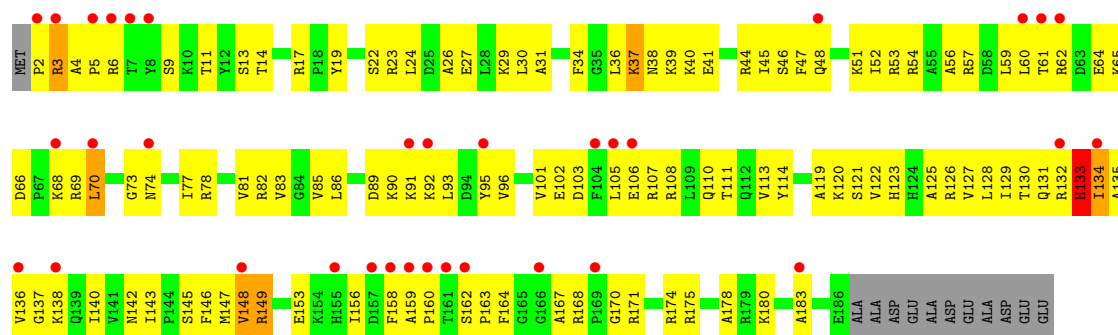




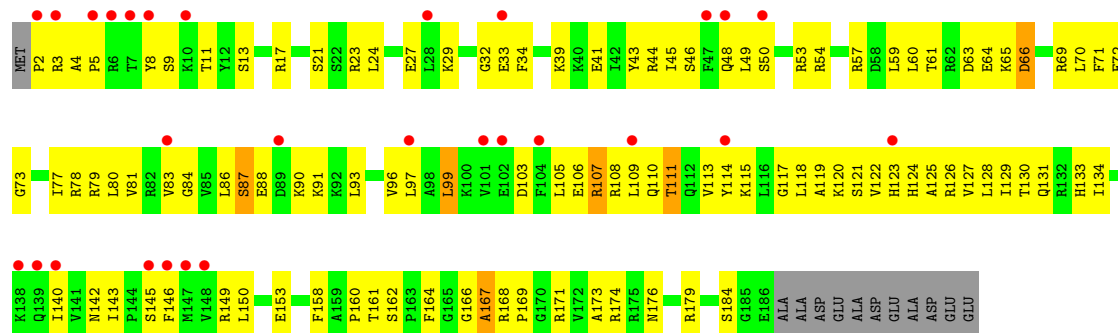
• Molecule 56: 40S ribosomal protein S8-A



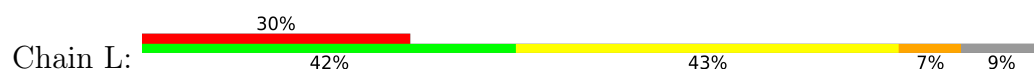
• Molecule 57: 40S ribosomal protein S9-A

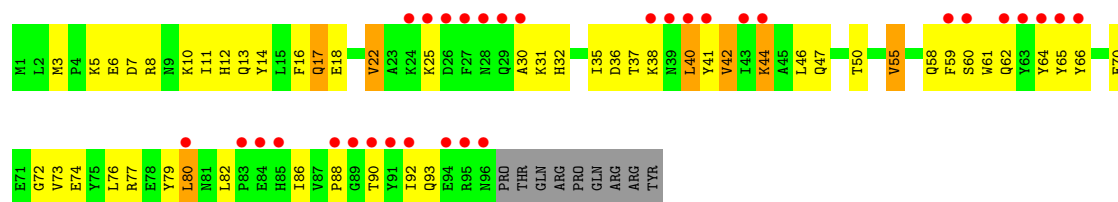


• Molecule 57: 40S ribosomal protein S9-A

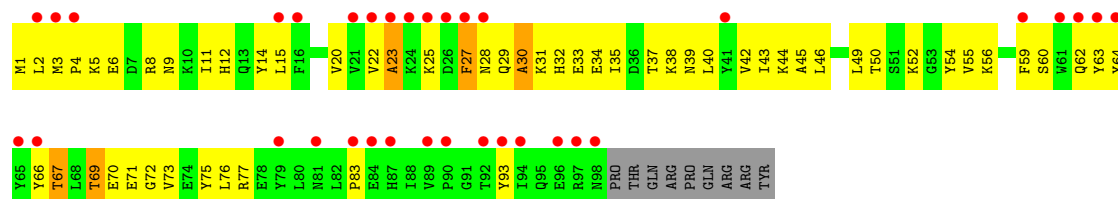


• Molecule 58: 40S ribosomal protein S10-A

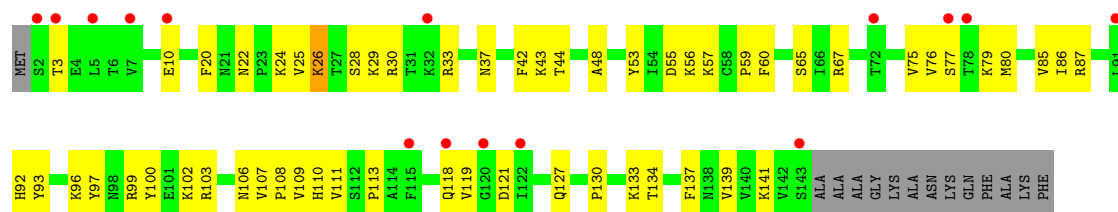




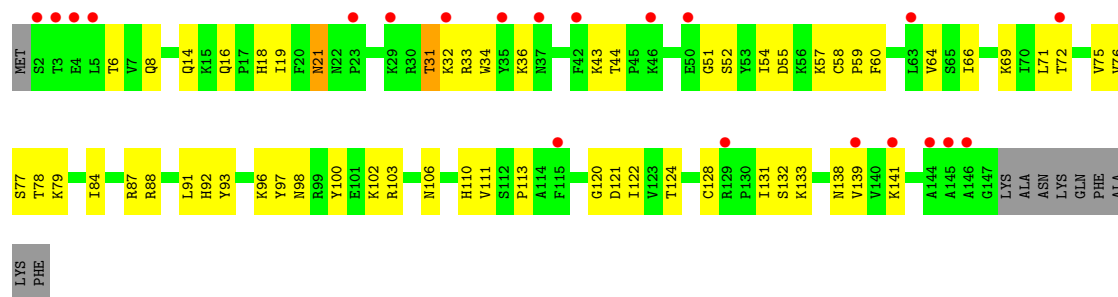
• Molecule 58: 40S ribosomal protein S10-A



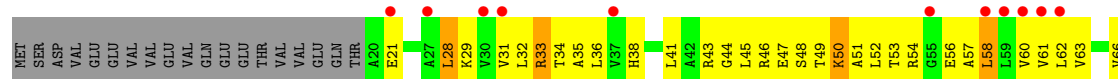
• Molecule 59: 40S ribosomal protein S11-A

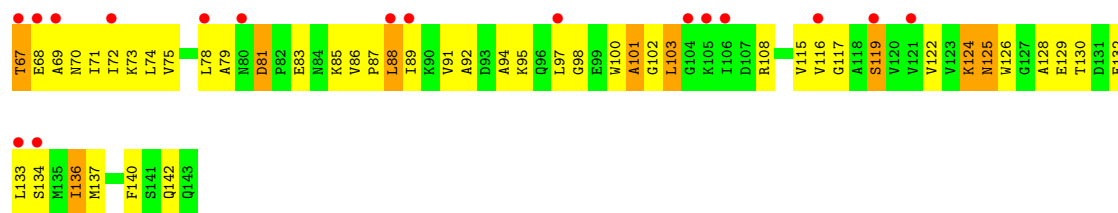


• Molecule 59: 40S ribosomal protein S11-A

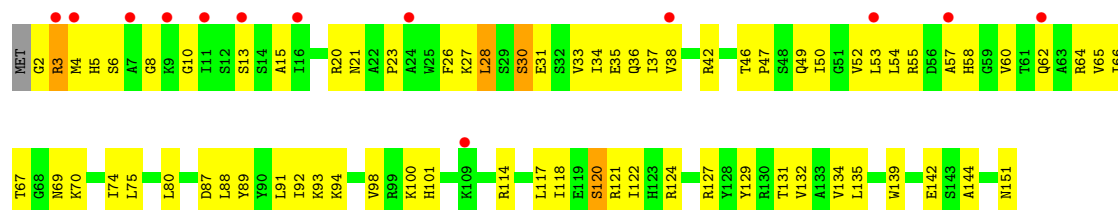


• Molecule 60: 40S ribosomal protein S12

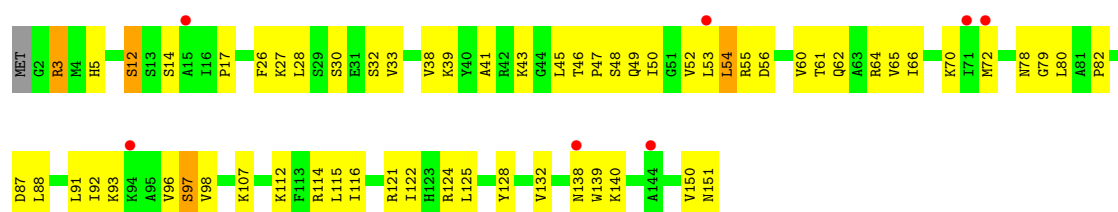




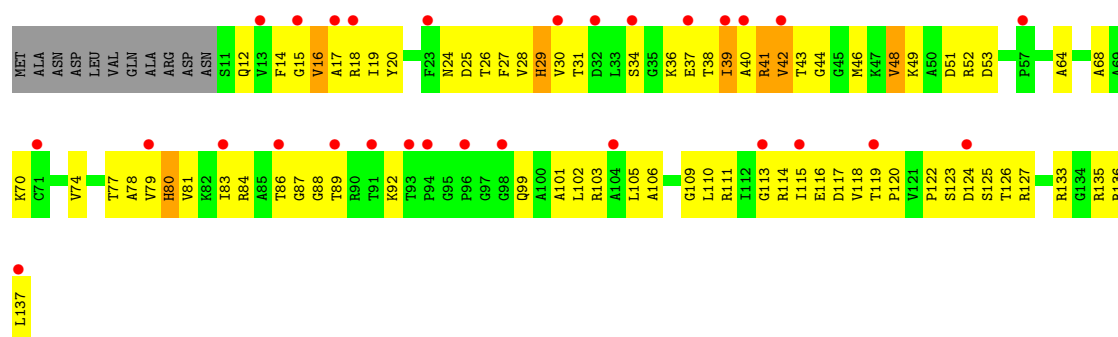
• Molecule 61: 40S ribosomal protein S13



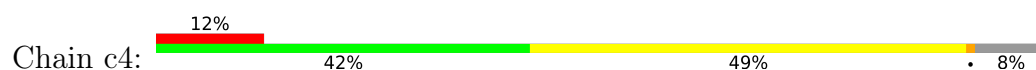
• Molecule 61: 40S ribosomal protein S13



• Molecule 62: 40S ribosomal protein S14-B

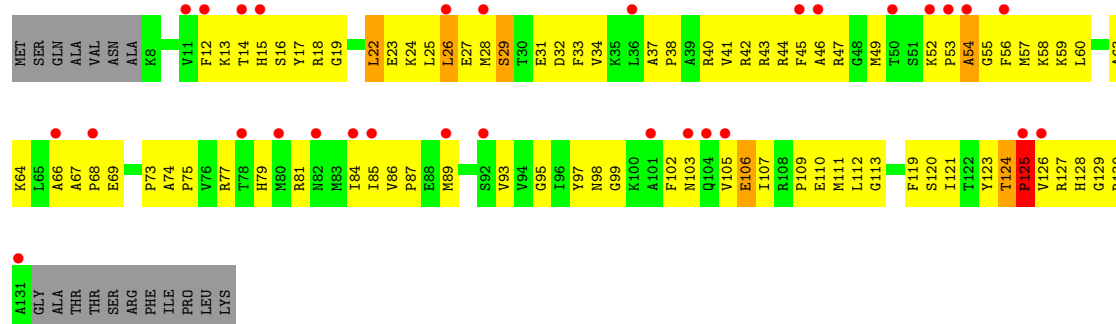


• Molecule 62: 40S ribosomal protein S14-B

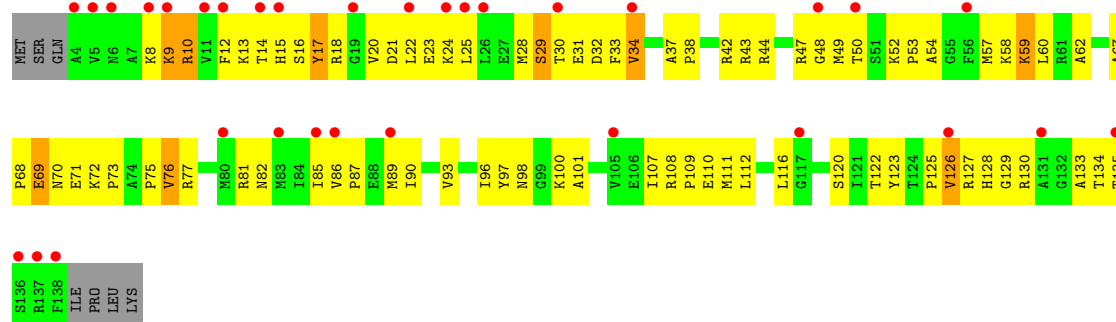
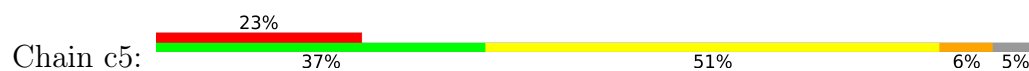




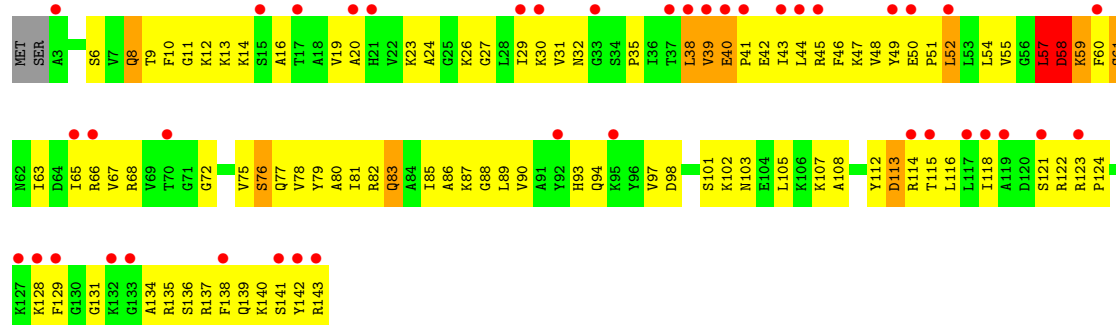
• Molecule 63: 40S ribosomal protein S15



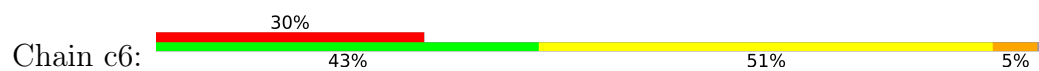
• Molecule 63: 40S ribosomal protein S15

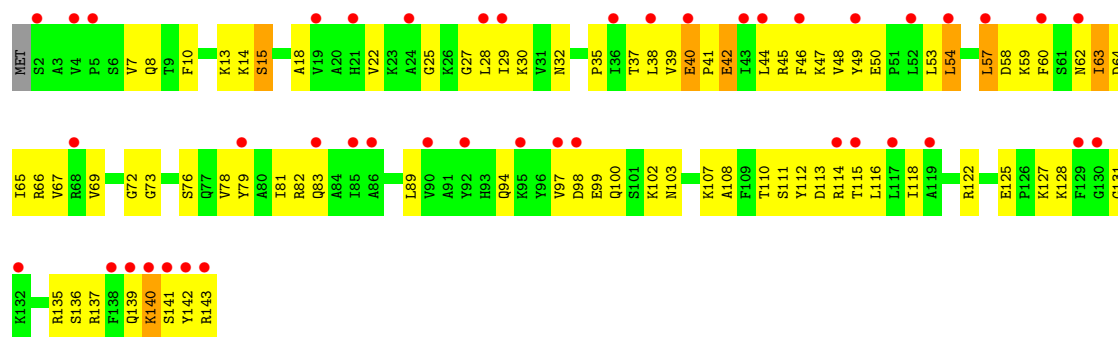


• Molecule 64: 40S ribosomal protein S16-A

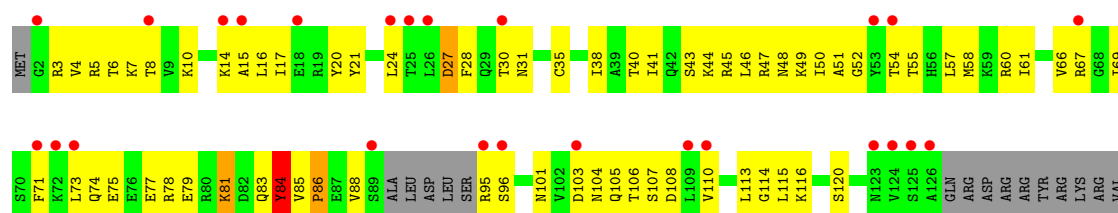


• Molecule 64: 40S ribosomal protein S16-A

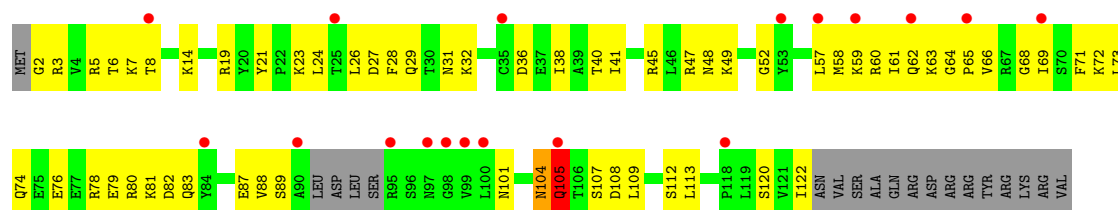




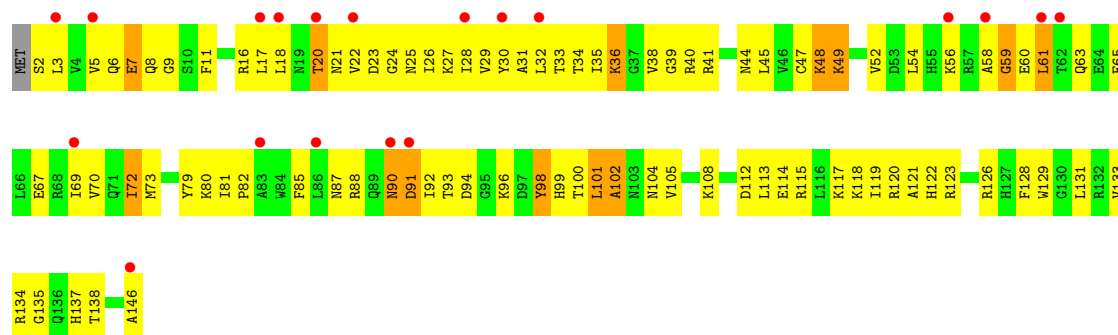
• Molecule 65: 40S ribosomal protein S17-A



• Molecule 65: 40S ribosomal protein S17-A

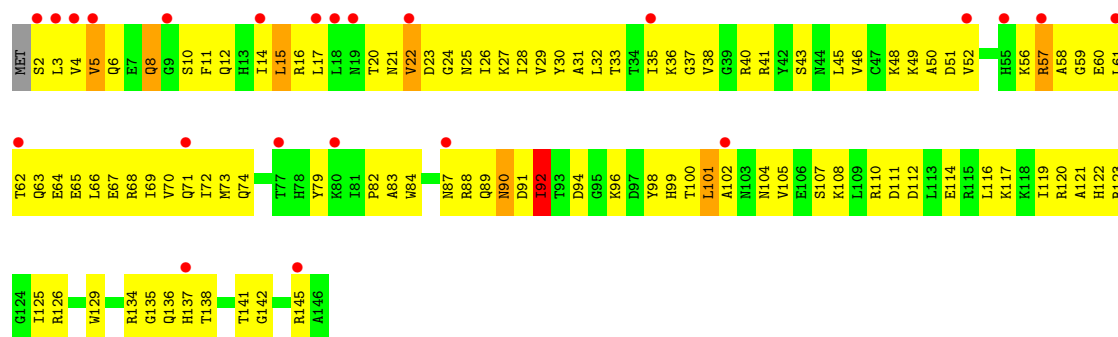


• Molecule 66: 40S ribosomal protein S18-A

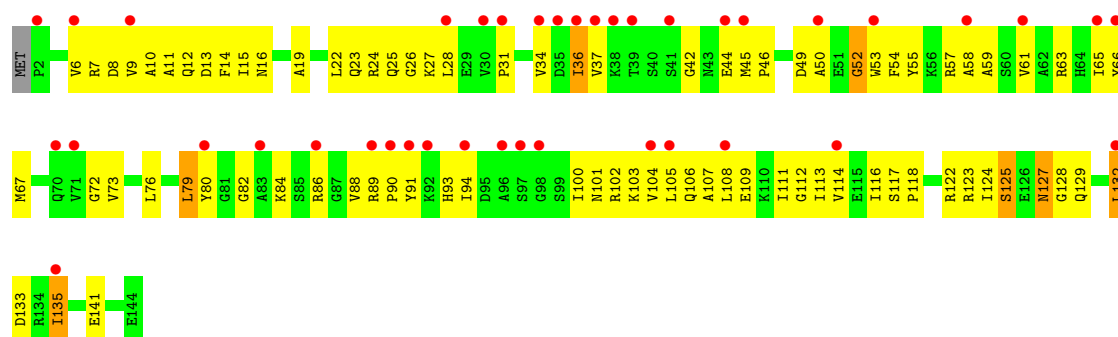
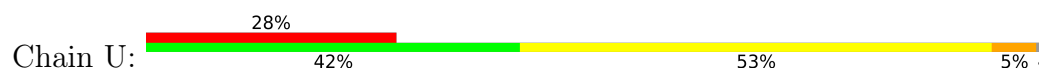


• Molecule 66: 40S ribosomal protein S18-A

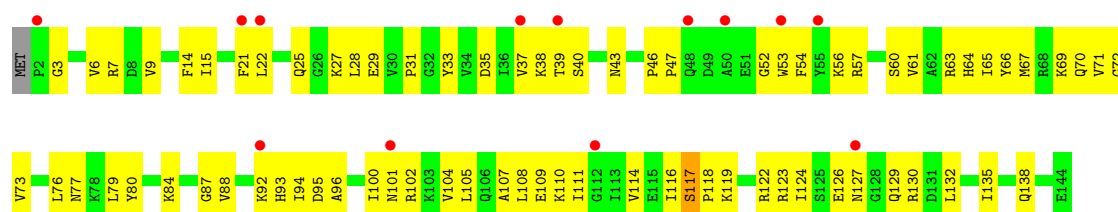




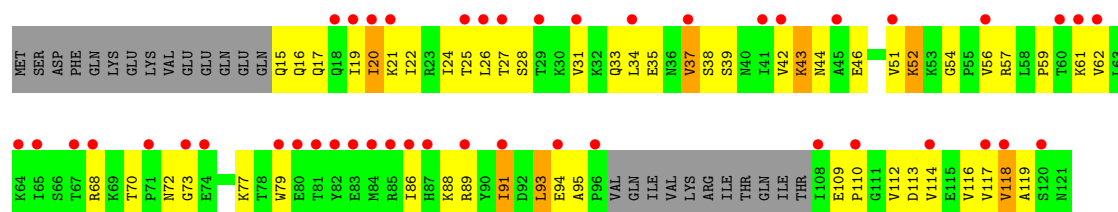
• Molecule 67: 40S ribosomal protein S19-A



• Molecule 67: 40S ribosomal protein S19-A

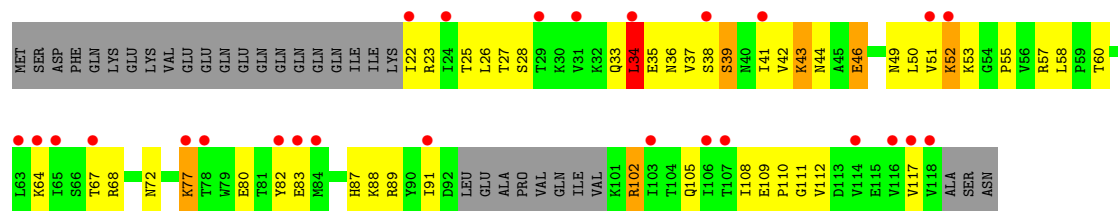


• Molecule 68: Small ribosomal subunit protein uS10



• Molecule 68: Small ribosomal subunit protein uS10

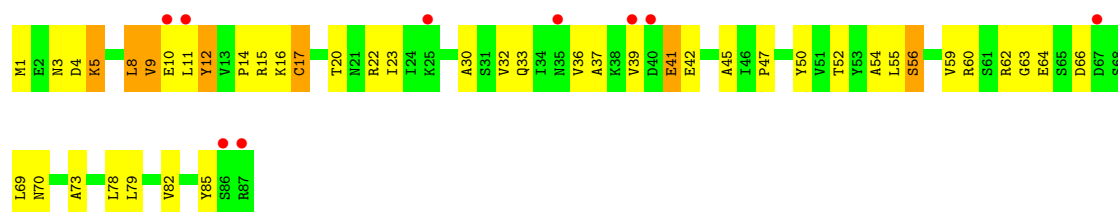




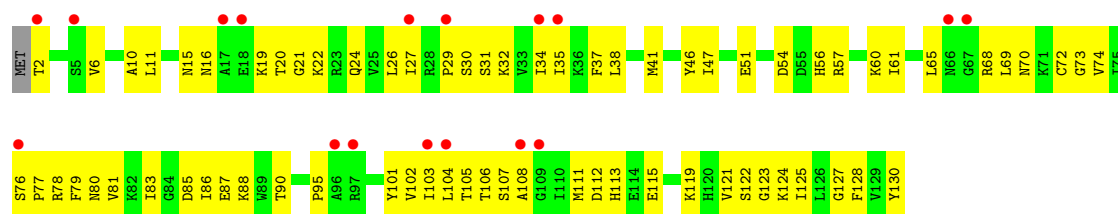
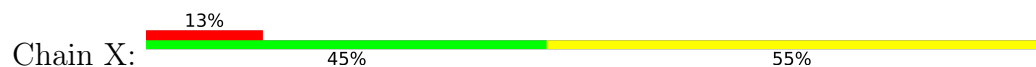
• Molecule 69: 40S ribosomal protein S21-A



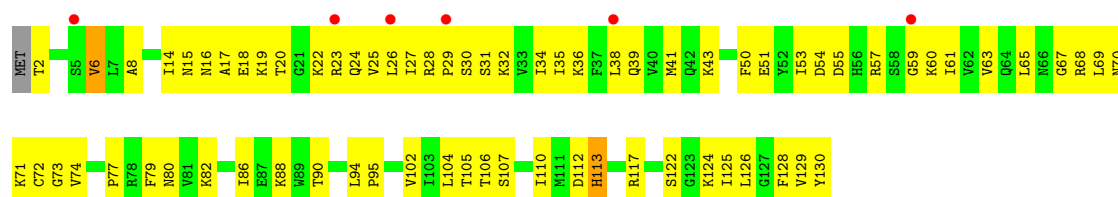
• Molecule 69: 40S ribosomal protein S21-A



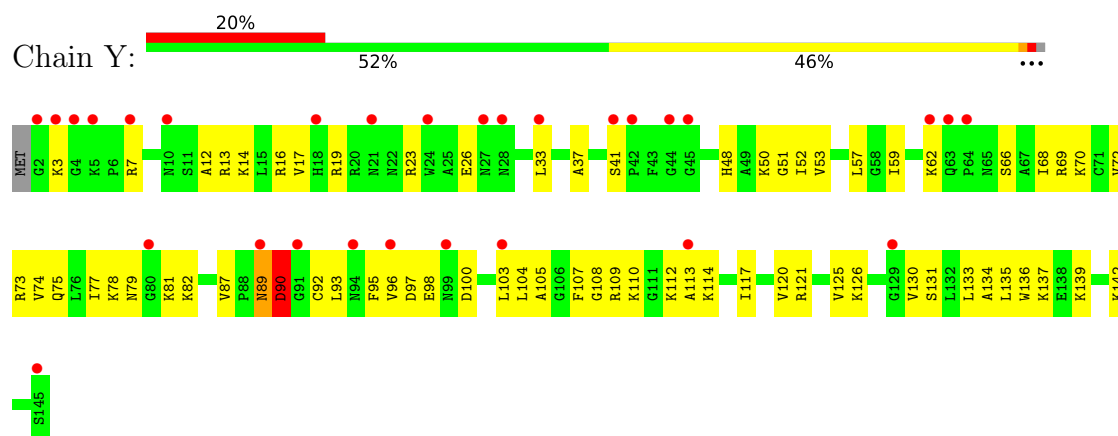
• Molecule 70: 40S ribosomal protein S22-A



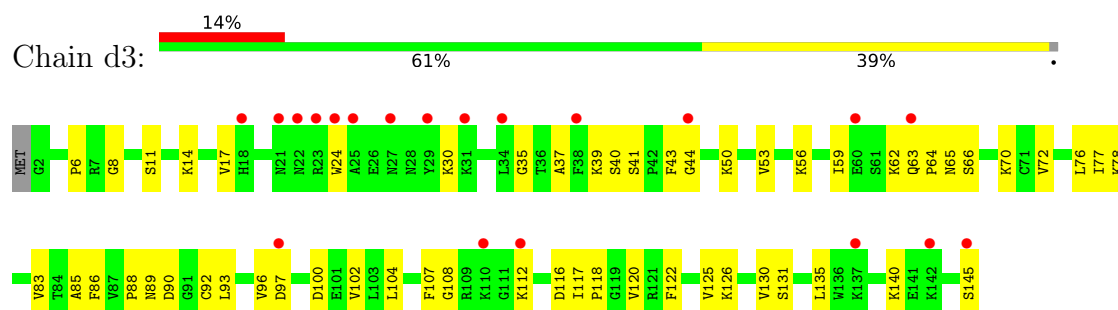
• Molecule 70: 40S ribosomal protein S22-A



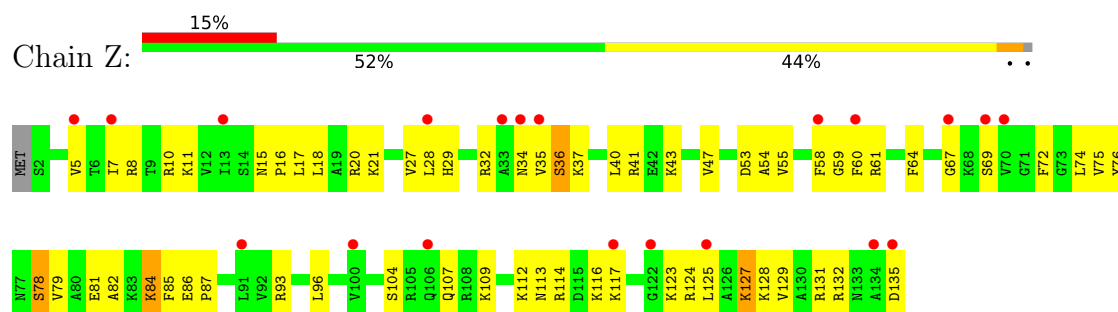
- Molecule 71: 40S ribosomal protein S23-A



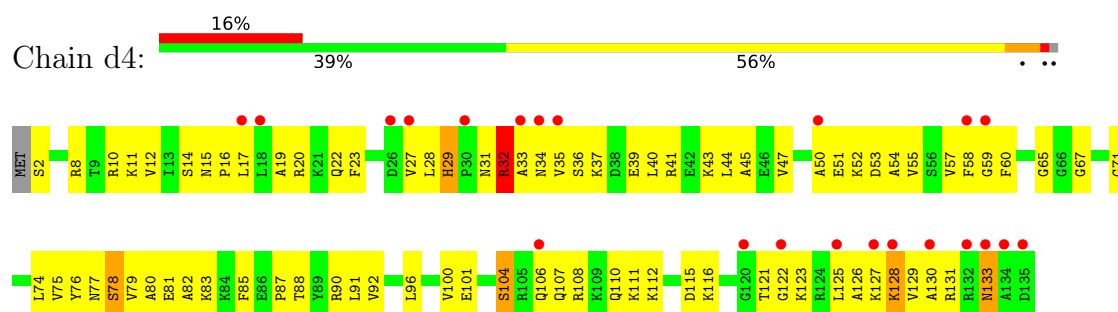
- Molecule 71: 40S ribosomal protein S23-A



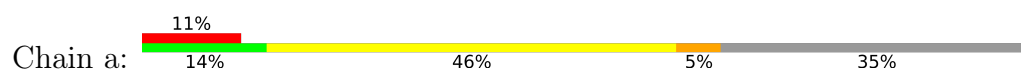
- Molecule 72: 40S ribosomal protein S24-A

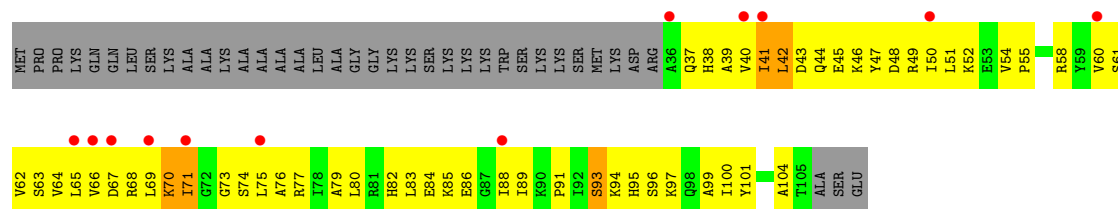


- Molecule 72: 40S ribosomal protein S24-A

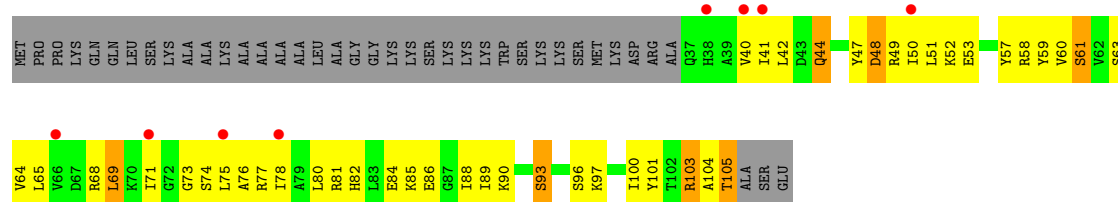
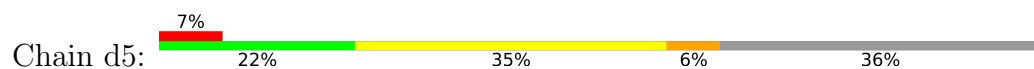


- Molecule 73: 40S ribosomal protein S25-A

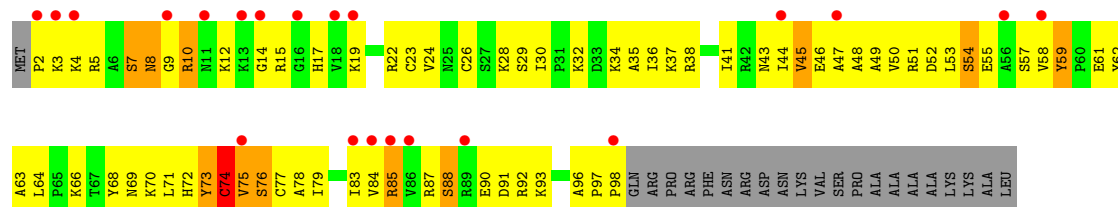
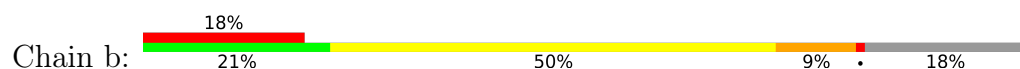




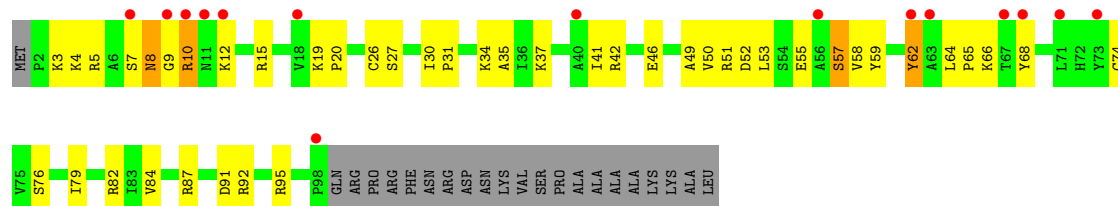
• Molecule 73: 40S ribosomal protein S25-A



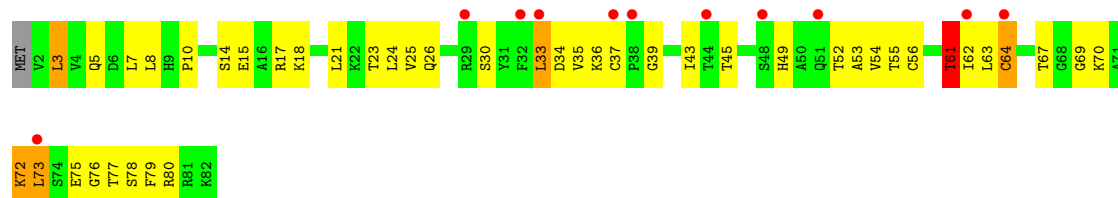
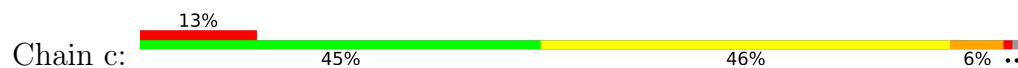
• Molecule 74: Small ribosomal subunit protein eS26B



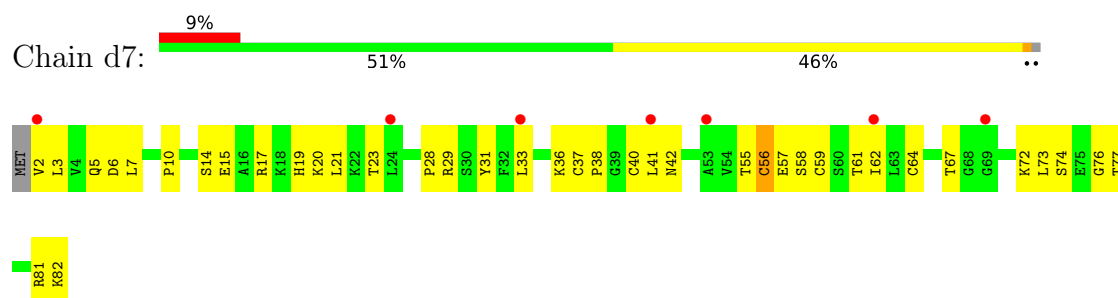
• Molecule 74: Small ribosomal subunit protein eS26B



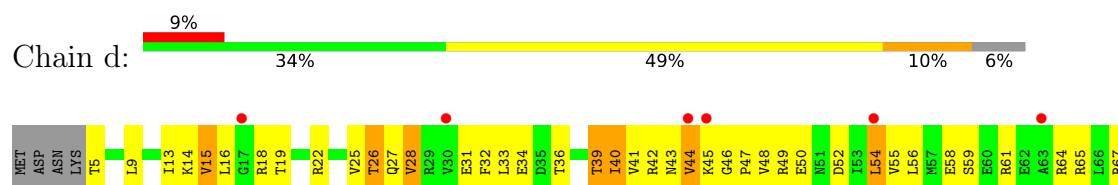
• Molecule 75: 40S ribosomal protein S27-A



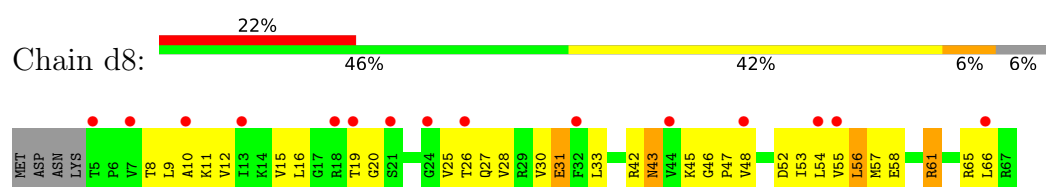
- Molecule 75: 40S ribosomal protein S27-A



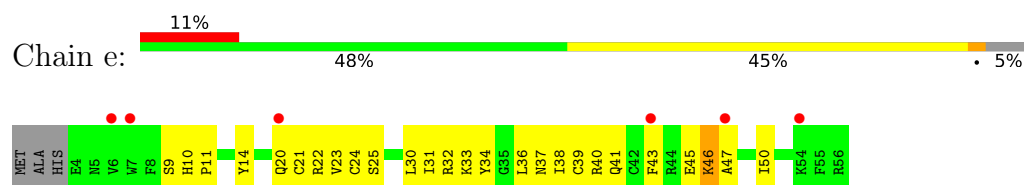
- Molecule 76: 40S ribosomal protein S28-A



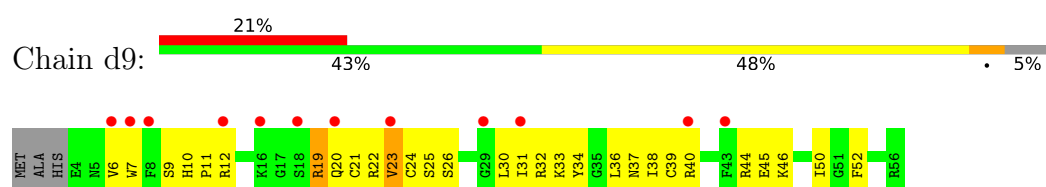
- Molecule 76: 40S ribosomal protein S28-A



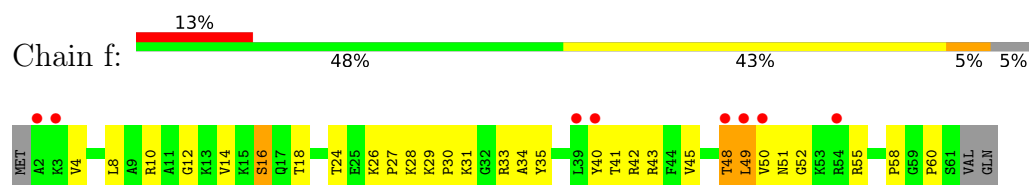
- Molecule 77: Small ribosomal subunit protein uS14A



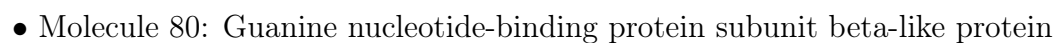
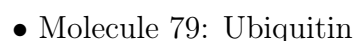
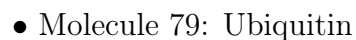
- Molecule 77: Small ribosomal subunit protein uS14A



- Molecule 78: 40S ribosomal protein S30-A

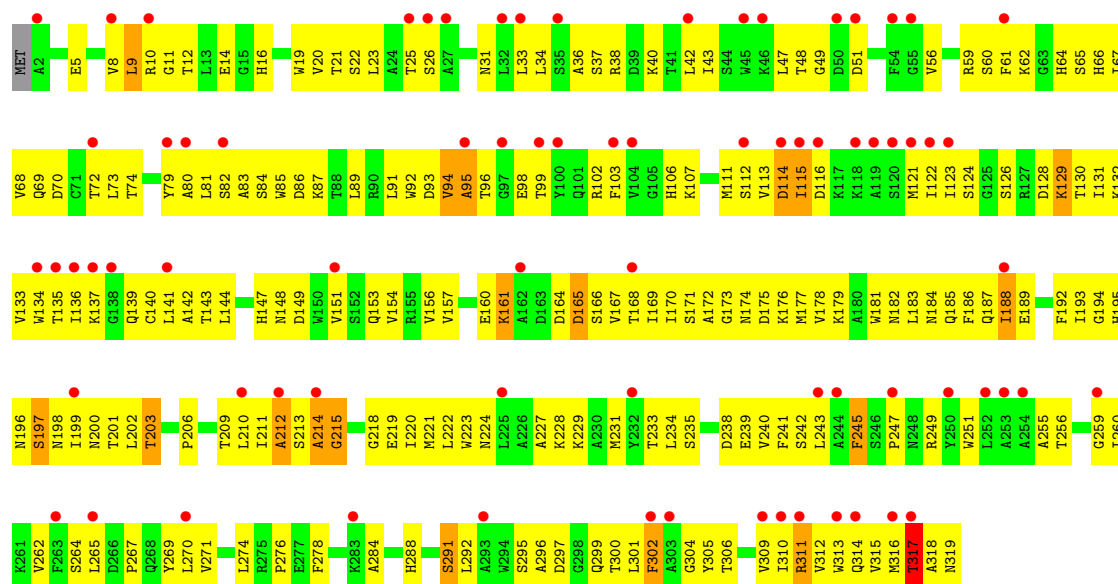


- Molecule 78: 40S ribosomal protein S30-A





● Molecule 80: Guanine nucleotide-binding protein subunit beta-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	303.81Å 287.52Å 435.86Å 90.00° 98.94° 90.00°	Depositor
Resolution (Å)	143.00 – 2.90 143.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (143.00-2.90) 90.3 (143.00-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.14487	Depositor
R, R_{free}	0.214 , (Not available) 0.214 , 0.237	Depositor DCC
R_{free} test set	25000 reflections (1.55%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	405377	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.16	0/75394	0.39	1/117545 (0.0%)
1	AR	0.16	0/74945	0.39	0/116844
2	3	0.14	0/2883	0.34	0/4491
2	AS	0.14	0/2883	0.36	0/4491
3	4	0.15	0/3746	0.39	0/5832
3	AT	0.14	0/3746	0.37	0/5832
4	CD	0.21	0/1948	0.55	0/2617
4	j	0.20	0/1948	0.56	0/2617
5	CE	0.20	0/3146	0.58	2/4228 (0.0%)
5	k	0.22	0/3146	0.61	6/4228 (0.1%)
6	CF	0.43	2/2800 (0.1%)	0.59	2/3790 (0.1%)
6	l	0.23	0/2800	0.60	0/3790
7	CG	0.21	0/2398	0.58	2/3235 (0.1%)
7	m	0.27	0/2425	0.73	2/3271 (0.1%)
8	CH	0.18	0/1260	0.57	0/1694
8	n	0.20	0/1260	0.51	0/1694
9	CI	0.19	0/1821	0.54	0/2451
9	o	0.24	0/1821	0.63	4/2451 (0.2%)
10	CJ	0.24	0/1789	0.64	0/2418
10	p	0.24	0/1836	0.61	0/2481
11	CK	0.19	0/1539	0.53	0/2073
11	q	0.27	0/1539	0.66	0/2073
12	CL	0.34	1/1741 (0.1%)	0.64	5/2335 (0.2%)
12	r	0.23	0/1741	0.68	7/2335 (0.3%)
13	CM	0.24	0/1374	0.63	0/1842
13	s	0.31	0/1374	0.83	4/1842 (0.2%)
14	CN	0.28	0/1568	0.76	6/2106 (0.3%)
14	t	0.25	0/1568	0.72	4/2106 (0.2%)
15	CO	0.27	0/1068	0.60	2/1438 (0.1%)
15	u	0.25	0/1068	0.61	3/1438 (0.2%)
16	CP	0.16	0/1757	0.43	0/2354
16	v	0.21	0/1757	0.54	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CQ	0.19	0/1585	0.46	0/2128
17	w	0.21	0/1585	0.52	0/2128
18	CR	0.18	0/1250	0.52	0/1683
18	x	0.20	0/1443	0.55	0/1944
19	CS	0.19	0/1465	0.57	0/1965
19	y	0.22	0/1465	0.59	2/1965 (0.1%)
20	CT	0.18	0/1538	0.52	0/2050
20	z	0.24	0/1449	0.57	0/1932
21	0	0.25	0/1481	0.56	0/1990
21	CU	0.18	0/1481	0.45	0/1990
22	2	0.22	0/1300	0.55	0/1743
22	CV	0.21	0/1300	0.53	0/1743
23	5	0.48	0/812	0.74	0/1099
23	CW	0.30	0/812	0.75	0/1099
24	6	0.23	0/1018	0.56	0/1369
24	CX	0.20	0/1018	0.48	0/1369
25	7	0.22	0/545	0.48	0/724
25	CY	0.21	0/780	0.52	0/1049
26	8	0.21	0/979	0.58	0/1321
26	CZ	0.23	0/952	0.56	0/1285
27	9	0.22	0/1004	0.60	0/1341
27	DA	0.18	0/987	0.52	0/1318
28	AA	0.40	1/1118 (0.1%)	0.74	2/1497 (0.1%)
28	DB	0.32	0/1118	0.74	3/1497 (0.2%)
29	AB	0.32	0/1204	0.96	14/1612 (0.9%)
29	DC	0.29	0/1204	0.86	10/1612 (0.6%)
30	AC	0.22	0/473	0.62	0/629
30	DD	0.20	0/473	0.71	0/629
31	AD	0.22	0/751	0.54	1/1008 (0.1%)
31	DE	0.20	0/751	0.52	0/1008
32	AE	0.21	0/890	0.48	0/1196
32	DF	0.19	0/890	0.55	0/1196
33	AF	0.16	0/1041	0.48	0/1394
33	DG	0.19	0/1041	0.51	0/1394
34	AG	0.20	0/862	0.55	0/1161
34	DH	0.19	0/868	0.51	0/1168
35	AH	0.27	0/881	0.59	0/1178
35	DI	0.22	0/890	0.59	0/1189
36	AI	0.21	0/978	0.52	0/1301
36	DJ	0.27	0/978	0.54	0/1301
37	AJ	0.24	0/745	0.58	0/991
37	DK	0.27	0/778	0.66	0/1034
38	AK	0.19	0/696	0.60	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DL	0.19	0/691	0.52	0/916
39	AL	0.22	0/618	0.60	0/826
39	DM	0.29	0/618	0.71	3/826 (0.4%)
40	AM	0.19	0/443	0.59	0/588
40	DN	0.19	0/443	0.57	0/588
41	AN	0.22	0/423	0.54	0/562
41	DO	0.22	0/423	0.58	0/562
42	AO	0.19	0/234	0.52	0/300
42	DP	0.18	0/234	0.51	0/300
43	AP	0.32	0/860	0.86	3/1136 (0.3%)
43	DQ	0.18	0/860	0.49	0/1136
44	AQ	0.21	0/701	0.67	0/934
44	DR	0.21	0/701	0.67	0/934
45	i	0.28	0/1024	0.71	0/1374
45	sM	0.26	0/480	0.77	2/642 (0.3%)
46	p0	0.34	0/1007	0.73	2/1355 (0.1%)
47	A	0.17	0/41494	0.41	0/64649
47	sR	0.16	0/42490	0.40	1/66207 (0.0%)
48	B	0.38	0/1602	0.86	2/2196 (0.1%)
48	s0	0.31	0/1623	0.81	2/2222 (0.1%)
49	C	0.45	0/1735	1.01	6/2335 (0.3%)
49	s1	0.25	0/1748	0.66	0/2352
50	D	0.35	0/1665	0.77	2/2263 (0.1%)
50	s2	0.23	0/1665	0.65	1/2263 (0.0%)
51	E	0.33	0/1759	0.71	0/2368
51	s3	0.44	1/1759 (0.1%)	0.76	3/2368 (0.1%)
52	F	0.33	0/2109	0.70	0/2839
52	s4	0.22	0/2109	0.59	0/2839
53	G	0.41	0/1629	0.97	7/2202 (0.3%)
53	s5	0.43	0/1580	0.89	2/2137 (0.1%)
54	H	0.24	0/1823	0.73	4/2439 (0.2%)
54	s6	0.25	0/1779	0.65	4/2379 (0.2%)
55	I	0.46	0/1506	0.91	1/2028 (0.0%)
55	s7	0.39	0/1516	1.04	8/2043 (0.4%)
56	J	0.23	0/1514	0.69	1/2021 (0.0%)
56	s8	0.24	0/1514	0.71	5/2021 (0.2%)
57	K	0.33	0/1519	0.82	4/2035 (0.2%)
57	s9	0.27	0/1519	0.68	1/2035 (0.0%)
58	L	0.28	0/789	0.72	0/1067
58	c0	0.26	0/776	0.75	2/1047 (0.2%)
59	M	0.21	0/1175	0.58	0/1584
59	c1	0.21	0/1194	0.55	0/1610
60	N	0.35	0/898	0.95	2/1220 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	O	0.28	0/1215	0.66	0/1638
61	c3	0.23	0/1215	0.55	0/1638
62	P	0.40	0/901	0.94	3/1217 (0.2%)
62	c4	0.34	0/950	0.77	0/1275
63	Q	0.88	9/998 (0.9%)	1.03	9/1341 (0.7%)
63	c5	0.34	0/1060	0.92	7/1426 (0.5%)
64	R	0.28	0/1125	0.80	4/1510 (0.3%)
64	c6	0.26	0/1131	0.75	0/1518
65	S	0.39	0/935	0.91	4/1254 (0.3%)
65	c7	0.25	0/914	0.71	2/1224 (0.2%)
66	T	0.30	0/1211	0.82	4/1628 (0.2%)
66	c8	0.28	0/1211	0.75	0/1628
67	U	0.38	0/1130	0.86	2/1517 (0.1%)
67	c9	0.25	0/1130	0.58	0/1517
68	V	0.30	0/774	0.76	0/1044
68	d0	0.25	0/723	0.78	0/974
69	W	0.32	0/693	0.77	2/935 (0.2%)
69	d1	0.26	0/693	0.72	3/935 (0.3%)
70	X	0.28	0/1038	0.68	0/1395
70	d2	0.22	0/1038	0.61	2/1395 (0.1%)
71	Y	0.24	0/1139	0.74	2/1518 (0.1%)
71	d3	0.19	0/1139	0.61	0/1518
72	Z	0.32	0/1087	0.72	1/1449 (0.1%)
72	d4	0.26	0/1087	0.81	4/1449 (0.3%)
73	a	0.36	0/571	0.93	0/768
73	d5	0.30	0/566	0.75	0/761
74	b	0.40	0/782	0.95	3/1047 (0.3%)
74	d6	0.31	0/782	0.96	6/1047 (0.6%)
75	c	0.26	0/620	0.91	2/838 (0.2%)
75	d7	0.20	0/620	0.66	0/838
76	d	0.27	0/499	0.67	0/670
76	d8	0.22	0/499	0.72	0/670
77	d9	0.25	0/452	0.71	2/600 (0.3%)
77	e	0.20	0/452	0.58	0/600
78	e0	0.27	0/499	0.79	0/665
78	f	0.26	0/483	0.71	0/643
79	e1	0.22	0/250	0.94	0/346
79	g	0.36	0/577	0.91	0/770
80	Rb	0.32	0/2495	0.76	4/3395 (0.1%)
80	h	0.30	0/2490	0.79	1/3389 (0.0%)
All	All	0.22	14/426391 (0.0%)	0.53	217/626187 (0.0%)

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
4	CD	0	3
5	CE	0	2
5	k	0	4
6	CF	0	4
6	l	0	5
7	CG	0	7
7	m	0	4
8	CH	0	1
9	CI	0	4
9	o	0	5
10	CJ	0	5
10	p	0	1
11	CK	0	2
11	q	0	2
12	CL	0	2
12	r	0	3
13	CM	0	2
13	s	0	3
14	CN	0	9
14	t	0	8
15	CO	0	2
15	u	0	2
19	CS	0	1
20	CT	0	1
21	0	0	1
21	CU	0	1
22	CV	0	1
23	CW	0	3
25	CY	0	1
28	AA	0	1
28	DB	0	2
29	AB	0	3
29	DC	0	2
30	AC	0	1
31	DE	0	1
32	DF	0	1
33	AF	0	2
33	DG	0	1
34	AG	0	1
34	DH	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
35	AH	0	1
35	DI	0	1
36	AI	0	2
36	DJ	0	1
37	DK	0	2
38	AK	0	2
39	AL	0	2
39	DM	0	1
40	DN	0	1
43	AP	0	1
44	DR	0	1
45	i	0	4
45	sM	0	2
47	A	0	1
48	B	0	6
48	s0	0	5
49	C	0	11
49	s1	0	1
50	D	0	3
50	s2	0	1
51	E	0	2
51	s3	0	14
52	F	0	3
52	s4	0	2
53	G	0	4
53	s5	0	1
54	H	0	4
54	s6	0	2
55	I	0	3
55	s7	0	9
56	J	0	3
56	s8	0	2
57	K	0	5
57	s9	0	4
58	L	0	6
58	c0	0	4
59	M	0	1
59	c1	0	1
60	N	0	12
61	c3	0	1
62	P	0	2
62	c4	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	Q	0	4
63	c5	0	3
64	R	0	5
64	c6	0	6
65	S	0	3
65	c7	0	1
66	T	0	6
66	c8	0	4
67	U	0	3
68	V	0	6
68	d0	0	4
69	d1	0	1
70	X	0	1
70	d2	0	1
71	Y	0	2
71	d3	0	1
72	Z	0	1
72	d4	0	3
73	a	0	2
73	d5	0	2
74	b	0	7
74	d6	0	1
75	c	0	4
75	d7	0	1
76	d	0	2
76	d8	0	1
78	e0	0	4
78	f	0	1
79	e1	0	7
79	g	0	2
80	Rb	0	6
80	h	0	3
All	All	0	342

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CF	101	ALA	C-O	18.30	1.32	1.23
12	CL	213	PHE	C-O	10.30	1.29	1.23
63	Q	68	PRO	CG-CD	-9.94	1.17	1.50
63	Q	68	PRO	C-N	9.20	1.46	1.33
51	s3	211	PRO	N-CA	8.86	1.58	1.47

The worst 5 of 217 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	s7	63	PRO	CA-C-N	14.42	147.65	121.70
55	s7	63	PRO	C-N-CA	14.42	147.65	121.70
29	AB	48	TYR	CA-C-N	-11.31	110.04	122.59
29	AB	48	TYR	C-N-CA	-11.31	110.04	122.59
43	AP	29	LYS	CA-C-N	9.66	139.85	122.46

There are no chirality outliers.

5 of 342 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	k	172	ALA	Peptide
5	k	173	GLN	Peptide
5	k	346	THR	Peptide
5	k	349	LYS	Peptide
6	l	13	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	67355	0	33847	1446	1
1	AR	66954	0	33647	1481	1
2	3	2579	0	1303	58	0
2	AS	2579	0	1304	57	0
3	4	3353	0	1695	72	1
3	AT	3353	0	1695	85	0
4	CD	1914	0	1981	87	0
4	j	1914	0	1981	68	0
5	CE	3075	0	3142	93	0
5	k	3075	0	3142	125	0
6	CF	2748	0	2859	94	0
6	l	2748	0	2859	115	0
7	CG	2348	0	2301	105	2
7	m	2375	0	2325	129	0
8	CH	1239	0	1326	43	0
8	n	1239	0	1326	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	CI	1784	0	1862	42	0
9	o	1784	0	1862	62	0
10	CJ	1757	0	1834	99	1
10	p	1804	0	1877	92	0
11	CK	1518	0	1587	62	1
11	q	1518	0	1587	86	0
12	CL	1705	0	1736	81	0
12	r	1705	0	1736	73	0
13	CM	1353	0	1383	59	1
13	s	1353	0	1383	96	0
14	CN	1543	0	1608	89	0
14	t	1543	0	1608	83	0
15	CO	1053	0	1149	49	0
15	u	1053	0	1149	47	0
16	CP	1720	0	1779	55	0
16	v	1720	0	1779	80	0
17	CQ	1555	0	1659	40	0
17	w	1555	0	1659	61	0
18	CR	1227	0	1236	47	0
18	x	1420	0	1437	31	0
19	CS	1441	0	1543	49	0
19	y	1441	0	1543	57	0
20	CT	1521	0	1617	62	0
20	z	1432	0	1526	62	0
21	0	1445	0	1487	47	0
21	CU	1445	0	1487	42	0
22	2	1276	0	1323	47	0
22	CV	1276	0	1323	54	0
23	5	796	0	812	59	0
23	CW	796	0	812	55	0
24	6	1003	0	1048	36	0
24	CX	1003	0	1048	29	0
25	7	533	0	560	14	0
25	CY	769	0	685	12	0
26	8	964	0	1025	48	0
26	CZ	937	0	994	38	0
27	9	993	0	1081	31	0
27	DA	976	0	1064	35	0
28	AA	1092	0	1155	86	0
28	DB	1092	0	1155	80	0
29	AB	1173	0	1215	52	0
29	DC	1173	0	1215	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	AC	462	0	491	17	0
30	DD	462	0	491	19	0
31	AD	743	0	797	36	0
31	DE	743	0	797	49	0
32	AE	876	0	912	31	0
32	DF	876	0	912	23	0
33	AF	1020	0	1090	28	0
33	DG	1020	0	1090	26	0
34	AG	844	0	869	26	0
34	DH	850	0	880	28	0
35	AH	871	0	928	50	0
35	DI	880	0	944	48	0
36	AI	969	0	1078	46	0
36	DJ	969	0	1078	47	0
37	AJ	739	0	816	43	0
37	DK	771	0	849	68	0
38	AK	681	0	683	33	0
38	DL	676	0	678	25	0
39	AL	612	0	682	30	0
39	DM	612	0	682	35	0
40	AM	436	0	475	22	0
40	DN	436	0	475	19	0
41	AN	417	0	455	19	0
41	DO	417	0	455	19	1
42	AO	233	0	284	12	0
42	DP	233	0	284	10	0
43	AP	847	0	914	38	0
43	DQ	847	0	914	31	0
44	AQ	694	0	734	41	0
44	DR	694	0	734	39	0
45	i	1017	0	958	63	0
45	sM	475	0	492	34	0
46	p0	992	0	1001	59	0
47	A	37101	0	18669	1231	1
47	sR	37990	0	19115	1107	1
48	B	1562	0	1539	155	0
48	s0	1583	0	1578	148	0
49	C	1709	0	1784	197	0
49	s1	1722	0	1793	124	0
50	D	1635	0	1723	151	0
50	s2	1635	0	1723	87	0
51	E	1734	0	1817	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	s3	1734	0	1817	119	0
52	F	2068	0	2154	133	0
52	s4	2068	0	2154	93	0
53	G	1609	0	1675	171	0
53	s5	1561	0	1626	191	0
54	H	1799	0	1879	102	0
54	s6	1755	0	1846	99	0
55	I	1481	0	1572	135	0
55	s7	1491	0	1578	133	0
56	J	1489	0	1525	87	0
56	s8	1489	0	1525	85	0
57	K	1494	0	1573	127	0
57	s9	1494	0	1573	131	0
58	L	772	0	727	51	0
58	c0	761	0	698	56	0
59	M	1149	0	1215	53	0
59	c1	1168	0	1233	49	0
60	N	890	0	887	95	0
61	O	1192	0	1255	70	0
61	c3	1192	0	1255	54	0
62	P	891	0	883	91	0
62	c4	940	0	976	64	0
63	Q	977	0	1002	88	0
63	c5	1039	0	1050	80	0
64	R	1105	0	1166	102	0
64	c6	1111	0	1171	73	0
65	S	926	0	930	80	0
65	c7	906	0	909	66	0
66	T	1192	0	1222	112	0
66	c8	1192	0	1222	109	1
67	U	1112	0	1124	91	0
67	c9	1112	0	1124	81	0
68	V	765	0	809	66	0
68	d0	715	0	767	53	0
69	W	684	0	672	55	0
69	d1	684	0	672	51	0
70	X	1021	0	1060	78	0
70	d2	1021	0	1060	60	0
71	Y	1121	0	1196	62	0
71	d3	1121	0	1196	42	0
72	Z	1073	0	1132	75	0
72	d4	1073	0	1132	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	a	563	0	603	70	0
73	d5	558	0	598	59	0
74	b	769	0	815	96	0
74	d6	769	0	814	51	0
75	c	610	0	633	41	0
75	d7	610	0	633	31	0
76	d	497	0	535	45	0
76	d8	497	0	535	27	0
77	d9	442	0	428	26	0
77	e	442	0	428	22	0
78	e0	491	0	542	40	0
78	f	475	0	525	31	0
79	e1	251	0	115	5	0
79	g	566	0	602	37	0
80	Rb	2442	0	2392	227	0
80	h	2437	0	2386	210	0
81	1	1988	0	0	201	0
81	3	77	0	0	3	0
81	4	105	0	0	6	0
81	A	832	0	0	93	0
81	AC	7	0	0	1	0
81	AG	7	0	0	1	0
81	AK	7	0	0	2	0
81	AP	7	0	0	1	0
81	AR	2125	0	0	242	0
81	AS	70	0	0	7	0
81	AT	98	0	0	4	0
81	CE	14	0	0	1	0
81	CG	20	0	0	2	0
81	CK	7	0	0	1	1
81	CL	21	0	0	5	0
81	CP	14	0	0	0	0
81	CQ	7	0	0	0	0
81	CS	7	0	0	1	0
81	CX	14	0	0	3	0
81	DD	7	0	0	2	0
81	DK	7	0	0	2	0
81	DL	7	0	0	2	0
81	DQ	7	0	0	1	0
81	J	7	0	0	1	0
81	O	7	0	0	1	0
81	Q	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	S	7	0	0	0	0
81	T	7	0	0	0	1
81	U	7	0	0	0	0
81	c3	7	0	0	1	0
81	c5	7	0	0	1	0
81	c8	7	0	0	0	0
81	d0	7	0	0	1	0
81	e	7	0	0	1	0
81	k	7	0	0	2	0
81	l	7	0	0	2	0
81	r	7	0	0	0	0
81	s1	7	0	0	3	0
81	s4	7	0	0	1	0
81	s8	7	0	0	1	0
81	sR	979	0	0	114	0
81	v	7	0	0	2	0
81	x	7	0	0	1	0
81	z	14	0	0	1	0
82	1	476	0	0	0	0
82	3	11	0	0	0	0
82	4	20	0	0	0	0
82	6	3	0	0	0	0
82	A	132	0	0	0	0
82	AB	5	0	0	0	0
82	AF	4	0	0	0	0
82	AG	2	0	0	0	0
82	AK	1	0	0	0	0
82	AR	519	0	0	0	0
82	AS	20	0	0	0	0
82	AT	17	0	0	0	0
82	CD	3	0	0	0	0
82	CE	6	0	0	0	0
82	CF	2	0	0	0	0
82	CG	1	0	0	0	0
82	CI	3	0	0	0	0
82	CK	1	0	0	0	0
82	CL	1	0	0	0	0
82	CM	2	0	0	0	0
82	CO	1	0	0	0	0
82	CP	3	0	0	0	0
82	CQ	4	0	0	0	0
82	CR	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	CU	1	0	0	0	0
82	CX	1	0	0	0	0
82	CY	1	0	0	0	0
82	DA	2	0	0	0	0
82	DC	3	0	0	0	0
82	DF	1	0	0	0	0
82	DH	2	0	0	0	0
82	DI	1	0	0	0	0
82	DL	1	0	0	0	0
82	DO	1	0	0	0	0
82	DP	1	0	0	0	0
82	DQ	2	0	0	0	0
82	F	1	0	0	0	0
82	H	1	0	0	0	0
82	O	1	0	0	0	0
82	P	1	0	0	0	0
82	X	1	0	0	0	0
82	Y	1	0	0	0	0
82	b	1	0	0	0	0
82	c1	1	0	0	0	0
82	c4	2	0	0	0	0
82	c6	2	0	0	0	0
82	c8	1	0	0	0	0
82	c9	1	0	0	0	0
82	d3	4	0	0	0	0
82	d4	3	0	0	0	0
82	d6	2	0	0	0	0
82	d9	1	0	0	0	0
82	j	3	0	0	0	0
82	k	1	0	0	0	0
82	l	3	0	0	0	0
82	n	1	0	0	0	0
82	o	1	0	0	0	0
82	r	3	0	0	0	0
82	s	1	0	0	0	0
82	s1	1	0	0	0	0
82	s2	1	0	0	0	0
82	s4	1	0	0	0	0
82	s8	2	0	0	0	0
82	s9	1	0	0	0	0
82	sM	2	0	0	0	0
82	sR	144	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	t	3	0	0	0	0
82	v	3	0	0	0	0
82	w	1	0	0	0	0
82	x	8	0	0	0	0
82	z	1	0	0	0	0
83	1	10	0	19	3	0
83	AR	10	0	19	2	0
84	1	26	0	0	2	0
84	AR	26	0	0	1	0
85	AH	1	0	0	0	0
85	AK	1	0	0	0	0
85	AN	1	0	0	0	0
85	AP	1	0	0	0	0
85	AQ	1	0	0	0	0
85	DI	1	0	0	0	0
85	DL	1	0	0	0	0
85	DO	1	0	0	0	0
85	DQ	1	0	0	0	0
85	DR	1	0	0	0	0
85	b	1	0	0	0	0
85	c	1	0	0	0	0
85	d6	1	0	0	0	0
85	d7	1	0	0	0	0
85	d9	1	0	0	0	0
85	e	1	0	0	0	0
85	e1	1	0	0	0	0
85	g	1	0	0	0	0
86	1	53	0	0	5	0
86	A	33	0	0	0	0
86	AE	1	0	0	0	0
86	AF	3	0	0	0	0
86	AR	82	0	0	1	0
86	AT	3	0	0	0	0
86	CP	2	0	0	0	0
86	CR	1	0	0	0	0
86	DG	3	0	0	0	0
86	M	1	0	0	1	0
86	j	1	0	0	0	0
86	sR	23	0	0	0	0
All	All	405377	0	293888	13509	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 13509 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:s5:218:GLU:H	53:s5:219:ARG:NH1	1.35	1.25
66:c8:45:LEU:HA	66:c8:48:LYS:HG3	1.28	1.15
47:A:568:G:H4'	71:Y:90:ASP:HB2	1.27	1.14
80:Rb:81:LEU:HD12	80:Rb:122:ILE:HD13	1.26	1.12
48:B:22:THR:HG22	48:B:169:SER:CB	1.80	1.11

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1242:G:O6	7:CG:206:GLN:NE2[2_746]	2.10	0.10
7:CG:217:GLU:OE2	41:DO:83:LYS:NZ[2_756]	2.12	0.08
10:CJ:111:LYS:NZ	47:sR:823:G:O2'[2_656]	2.12	0.08
11:CK:14:GLU:OE2	66:c8:79:TYR:OH[2_746]	2.14	0.06
1:1:3195:U:OP1	81:T:201:OHX:N1[2_545]	2.16	0.04

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	250/254 (98%)	248 (99%)	2 (1%)	0	100	100
4	j	250/254 (98%)	250 (100%)	0	0	100	100
5	CE	384/387 (99%)	379 (99%)	5 (1%)	0	100	100
5	k	384/387 (99%)	377 (98%)	7 (2%)	0	100	100
6	CF	359/362 (99%)	356 (99%)	3 (1%)	0	100	100
6	l	359/362 (99%)	355 (99%)	4 (1%)	0	100	100
7	CG	290/297 (98%)	286 (99%)	4 (1%)	0	100	100
7	m	294/297 (99%)	287 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CH	152/176 (86%)	151 (99%)	1 (1%)	0	100	100
8	n	152/176 (86%)	152 (100%)	0	0	100	100
9	CI	220/244 (90%)	218 (99%)	2 (1%)	0	100	100
9	o	220/244 (90%)	215 (98%)	5 (2%)	0	100	100
10	CJ	224/256 (88%)	224 (100%)	0	0	100	100
10	p	231/256 (90%)	231 (100%)	0	0	100	100
11	CK	189/191 (99%)	188 (100%)	1 (0%)	0	100	100
11	q	189/191 (99%)	188 (100%)	1 (0%)	0	100	100
12	CL	207/221 (94%)	204 (99%)	3 (1%)	0	100	100
12	r	207/221 (94%)	202 (98%)	5 (2%)	0	100	100
13	CM	167/174 (96%)	160 (96%)	7 (4%)	0	100	100
13	s	167/174 (96%)	163 (98%)	4 (2%)	0	100	100
14	CN	191/199 (96%)	179 (94%)	12 (6%)	0	100	100
14	t	191/199 (96%)	185 (97%)	6 (3%)	0	100	100
15	CO	134/138 (97%)	132 (98%)	2 (2%)	0	100	100
15	u	134/138 (97%)	132 (98%)	2 (2%)	0	100	100
16	CP	201/204 (98%)	201 (100%)	0	0	100	100
16	v	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
17	CQ	195/199 (98%)	195 (100%)	0	0	100	100
17	w	195/199 (98%)	195 (100%)	0	0	100	100
18	CR	153/184 (83%)	153 (100%)	0	0	100	100
18	x	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
19	CS	183/186 (98%)	183 (100%)	0	0	100	100
19	y	183/186 (98%)	182 (100%)	1 (0%)	0	100	100
20	CT	186/189 (98%)	184 (99%)	2 (1%)	0	100	100
20	z	175/189 (93%)	175 (100%)	0	0	100	100
21	0	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
21	CU	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
22	2	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
22	CV	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
23	5	98/121 (81%)	98 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	CW	98/121 (81%)	97 (99%)	1 (1%)	0	100	100
24	6	134/137 (98%)	133 (99%)	1 (1%)	0	100	100
24	CX	134/137 (98%)	134 (100%)	0	0	100	100
25	7	63/155 (41%)	63 (100%)	0	0	100	100
25	CY	107/155 (69%)	106 (99%)	1 (1%)	0	100	100
26	8	119/142 (84%)	119 (100%)	0	0	100	100
26	CZ	115/142 (81%)	115 (100%)	0	0	100	100
27	9	124/127 (98%)	124 (100%)	0	0	100	100
27	DA	122/127 (96%)	122 (100%)	0	0	100	100
28	AA	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
28	DB	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
29	AB	146/149 (98%)	140 (96%)	6 (4%)	0	100	100
29	DC	146/149 (98%)	141 (97%)	5 (3%)	0	100	100
30	AC	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
30	DD	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
31	AD	95/105 (90%)	95 (100%)	0	0	100	100
31	DE	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
32	AE	107/113 (95%)	103 (96%)	4 (4%)	0	100	100
32	DF	107/113 (95%)	107 (100%)	0	0	100	100
33	AF	125/130 (96%)	125 (100%)	0	0	100	100
33	DG	125/130 (96%)	125 (100%)	0	0	100	100
34	AG	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
34	DH	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
35	AH	109/121 (90%)	108 (99%)	0	1 (1%)	14	41
35	DI	110/121 (91%)	110 (100%)	0	0	100	100
36	AI	117/120 (98%)	117 (100%)	0	0	100	100
36	DJ	117/120 (98%)	117 (100%)	0	0	100	100
37	AJ	94/100 (94%)	93 (99%)	1 (1%)	0	100	100
37	DK	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
38	AK	85/88 (97%)	85 (100%)	0	0	100	100
38	DL	84/88 (96%)	84 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	AL	75/78 (96%)	75 (100%)	0	0	100	100
39	DM	75/78 (96%)	75 (100%)	0	0	100	100
40	AM	48/51 (94%)	48 (100%)	0	0	100	100
40	DN	48/51 (94%)	48 (100%)	0	0	100	100
41	AN	50/128 (39%)	50 (100%)	0	0	100	100
41	DO	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
42	AO	23/25 (92%)	23 (100%)	0	0	100	100
42	DP	23/25 (92%)	23 (100%)	0	0	100	100
43	AP	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
43	DQ	103/106 (97%)	103 (100%)	0	0	100	100
44	AQ	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
44	DR	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
45	i	136/273 (50%)	135 (99%)	1 (1%)	0	100	100
45	sM	61/273 (22%)	57 (93%)	4 (7%)	0	100	100
46	p0	122/312 (39%)	121 (99%)	1 (1%)	0	100	100
48	B	204/252 (81%)	198 (97%)	6 (3%)	0	100	100
48	s0	204/252 (81%)	196 (96%)	8 (4%)	0	100	100
49	C	212/255 (83%)	207 (98%)	5 (2%)	0	100	100
49	s1	214/255 (84%)	213 (100%)	1 (0%)	0	100	100
50	D	215/254 (85%)	211 (98%)	3 (1%)	1 (0%)	24	54
50	s2	215/254 (85%)	213 (99%)	2 (1%)	0	100	100
51	E	221/240 (92%)	221 (100%)	0	0	100	100
51	s3	221/240 (92%)	214 (97%)	7 (3%)	0	100	100
52	F	258/261 (99%)	257 (100%)	1 (0%)	0	100	100
52	s4	258/261 (99%)	257 (100%)	1 (0%)	0	100	100
53	G	204/225 (91%)	197 (97%)	7 (3%)	0	100	100
53	s5	194/225 (86%)	190 (98%)	4 (2%)	0	100	100
54	H	224/236 (95%)	216 (96%)	8 (4%)	0	100	100
54	s6	216/236 (92%)	210 (97%)	6 (3%)	0	100	100
55	I	182/190 (96%)	180 (99%)	1 (0%)	1 (0%)	24	54
55	s7	184/190 (97%)	180 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	J	184/200 (92%)	178 (97%)	6 (3%)	0	100	100
56	s8	184/200 (92%)	181 (98%)	3 (2%)	0	100	100
57	K	183/197 (93%)	179 (98%)	4 (2%)	0	100	100
57	s9	183/197 (93%)	178 (97%)	5 (3%)	0	100	100
58	L	94/105 (90%)	91 (97%)	3 (3%)	0	100	100
58	c0	92/105 (88%)	88 (96%)	4 (4%)	0	100	100
59	M	140/156 (90%)	140 (100%)	0	0	100	100
59	c1	144/156 (92%)	142 (99%)	2 (1%)	0	100	100
60	N	122/143 (85%)	117 (96%)	5 (4%)	0	100	100
61	O	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
61	c3	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
62	P	125/138 (91%)	123 (98%)	1 (1%)	1 (1%)	16	44
62	c4	123/138 (89%)	122 (99%)	1 (1%)	0	100	100
63	Q	122/142 (86%)	114 (93%)	8 (7%)	0	100	100
63	c5	133/142 (94%)	126 (95%)	7 (5%)	0	100	100
64	R	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
64	c6	140/143 (98%)	140 (100%)	0	0	100	100
65	S	116/136 (85%)	112 (97%)	4 (3%)	0	100	100
65	c7	113/136 (83%)	111 (98%)	2 (2%)	0	100	100
66	T	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
66	c8	143/146 (98%)	137 (96%)	4 (3%)	2 (1%)	9	30
67	U	141/144 (98%)	141 (100%)	0	0	100	100
67	c9	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
68	V	92/121 (76%)	90 (98%)	2 (2%)	0	100	100
68	d0	85/121 (70%)	85 (100%)	0	0	100	100
69	W	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
69	d1	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
70	X	127/130 (98%)	127 (100%)	0	0	100	100
70	d2	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
71	Y	142/145 (98%)	132 (93%)	10 (7%)	0	100	100
71	d3	142/145 (98%)	138 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Z	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
72	d4	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
73	a	68/108 (63%)	64 (94%)	4 (6%)	0	100	100
73	d5	67/108 (62%)	66 (98%)	1 (2%)	0	100	100
74	b	95/119 (80%)	88 (93%)	7 (7%)	0	100	100
74	d6	95/119 (80%)	90 (95%)	5 (5%)	0	100	100
75	c	79/82 (96%)	78 (99%)	1 (1%)	0	100	100
75	d7	79/82 (96%)	79 (100%)	0	0	100	100
76	d	61/67 (91%)	61 (100%)	0	0	100	100
76	d8	61/67 (91%)	61 (100%)	0	0	100	100
77	d9	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
77	e	51/56 (91%)	51 (100%)	0	0	100	100
78	e0	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
78	f	58/63 (92%)	58 (100%)	0	0	100	100
79	e1	49/152 (32%)	48 (98%)	1 (2%)	0	100	100
79	g	69/152 (45%)	65 (94%)	3 (4%)	1 (1%)	9	30
80	Rb	316/319 (99%)	311 (98%)	5 (2%)	0	100	100
80	h	316/319 (99%)	310 (98%)	6 (2%)	0	100	100
All	All	21957/24477 (90%)	21604 (98%)	346 (2%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
50	D	107	SER
55	I	111	LYS
62	P	42	VAL
66	c8	14	ILE
66	c8	92	ILE

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	193/196 (98%)	185 (96%)	8 (4%)	27	61
4	j	193/196 (98%)	189 (98%)	4 (2%)	47	77
5	CE	319/323 (99%)	306 (96%)	13 (4%)	27	61
5	k	319/323 (99%)	299 (94%)	20 (6%)	16	45
6	CF	288/289 (100%)	266 (92%)	22 (8%)	12	36
6	l	288/289 (100%)	273 (95%)	15 (5%)	21	52
7	CG	242/245 (99%)	229 (95%)	13 (5%)	20	51
7	m	244/245 (100%)	235 (96%)	9 (4%)	30	64
8	CH	134/153 (88%)	126 (94%)	8 (6%)	17	47
8	n	134/153 (88%)	129 (96%)	5 (4%)	30	64
9	CI	186/205 (91%)	175 (94%)	11 (6%)	18	48
9	o	186/205 (91%)	183 (98%)	3 (2%)	55	83
10	CJ	182/208 (88%)	175 (96%)	7 (4%)	29	64
10	p	187/208 (90%)	183 (98%)	4 (2%)	47	77
11	CK	171/171 (100%)	156 (91%)	15 (9%)	9	29
11	q	171/171 (100%)	162 (95%)	9 (5%)	20	52
12	CL	177/187 (95%)	172 (97%)	5 (3%)	38	72
12	r	177/187 (95%)	175 (99%)	2 (1%)	65	88
13	CM	147/151 (97%)	139 (95%)	8 (5%)	20	51
13	s	147/151 (97%)	141 (96%)	6 (4%)	27	61
14	CN	154/159 (97%)	147 (96%)	7 (4%)	24	58
14	t	154/159 (97%)	149 (97%)	5 (3%)	34	68
15	CO	107/109 (98%)	102 (95%)	5 (5%)	23	56
15	u	107/109 (98%)	104 (97%)	3 (3%)	38	72
16	CP	175/176 (99%)	175 (100%)	0	100	100
16	v	175/176 (99%)	170 (97%)	5 (3%)	37	71
17	CQ	160/162 (99%)	151 (94%)	9 (6%)	19	50
17	w	160/162 (99%)	154 (96%)	6 (4%)	29	64
18	CR	125/146 (86%)	118 (94%)	7 (6%)	19	50
18	x	140/146 (96%)	133 (95%)	7 (5%)	22	53
19	CS	150/151 (99%)	142 (95%)	8 (5%)	20	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	y	150/151 (99%)	144 (96%)	6 (4%)	28	62
20	CT	153/154 (99%)	149 (97%)	4 (3%)	40	73
20	z	144/154 (94%)	140 (97%)	4 (3%)	38	72
21	0	156/156 (100%)	149 (96%)	7 (4%)	24	58
21	CU	156/156 (100%)	144 (92%)	12 (8%)	12	35
22	2	136/137 (99%)	132 (97%)	4 (3%)	37	71
22	CV	136/137 (99%)	133 (98%)	3 (2%)	45	77
23	5	87/107 (81%)	85 (98%)	2 (2%)	44	76
23	CW	87/107 (81%)	83 (95%)	4 (5%)	24	57
24	6	104/105 (99%)	99 (95%)	5 (5%)	23	55
24	CX	104/105 (99%)	99 (95%)	5 (5%)	23	55
25	7	56/129 (43%)	55 (98%)	1 (2%)	51	80
25	CY	57/129 (44%)	57 (100%)	0	100	100
26	8	104/118 (88%)	102 (98%)	2 (2%)	50	79
26	CZ	102/118 (86%)	101 (99%)	1 (1%)	68	89
27	9	109/110 (99%)	106 (97%)	3 (3%)	38	72
27	DA	107/110 (97%)	102 (95%)	5 (5%)	23	56
28	AA	115/116 (99%)	112 (97%)	3 (3%)	40	73
28	DB	115/116 (99%)	108 (94%)	7 (6%)	17	46
29	AB	118/119 (99%)	111 (94%)	7 (6%)	18	48
29	DC	118/119 (99%)	113 (96%)	5 (4%)	26	60
30	AC	46/47 (98%)	46 (100%)	0	100	100
30	DD	46/47 (98%)	44 (96%)	2 (4%)	26	60
31	AD	81/88 (92%)	80 (99%)	1 (1%)	63	86
31	DE	81/88 (92%)	76 (94%)	5 (6%)	16	46
32	AE	92/97 (95%)	90 (98%)	2 (2%)	45	77
32	DF	92/97 (95%)	90 (98%)	2 (2%)	45	77
33	AF	109/111 (98%)	108 (99%)	1 (1%)	70	90
33	DG	109/111 (98%)	105 (96%)	4 (4%)	30	64
34	AG	89/91 (98%)	87 (98%)	2 (2%)	45	77
34	DH	90/91 (99%)	84 (93%)	6 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	AH	94/103 (91%)	93 (99%)	1 (1%)	65	88
35	DI	95/103 (92%)	94 (99%)	1 (1%)	65	88
36	AI	104/105 (99%)	103 (99%)	1 (1%)	68	89
36	DJ	104/105 (99%)	100 (96%)	4 (4%)	29	64
37	AJ	78/82 (95%)	77 (99%)	1 (1%)	61	86
37	DK	81/82 (99%)	79 (98%)	2 (2%)	42	74
38	AK	70/71 (99%)	69 (99%)	1 (1%)	59	85
38	DL	70/71 (99%)	67 (96%)	3 (4%)	26	60
39	AL	68/69 (99%)	62 (91%)	6 (9%)	9	29
39	DM	68/69 (99%)	66 (97%)	2 (3%)	37	71
40	AM	45/46 (98%)	43 (96%)	2 (4%)	25	59
40	DN	45/46 (98%)	45 (100%)	0	100	100
41	AN	47/116 (40%)	47 (100%)	0	100	100
41	DO	47/116 (40%)	46 (98%)	1 (2%)	47	77
42	AO	23/23 (100%)	22 (96%)	1 (4%)	26	60
42	DP	23/23 (100%)	22 (96%)	1 (4%)	26	60
43	AP	90/91 (99%)	82 (91%)	8 (9%)	9	28
43	DQ	90/91 (99%)	87 (97%)	3 (3%)	33	67
44	AQ	71/72 (99%)	69 (97%)	2 (3%)	38	72
44	DR	71/72 (99%)	66 (93%)	5 (7%)	14	40
45	i	96/228 (42%)	91 (95%)	5 (5%)	21	52
45	sM	54/228 (24%)	50 (93%)	4 (7%)	13	38
46	p0	105/254 (41%)	100 (95%)	5 (5%)	23	55
48	B	160/210 (76%)	150 (94%)	10 (6%)	16	45
48	s0	165/210 (79%)	157 (95%)	8 (5%)	23	55
49	C	191/224 (85%)	183 (96%)	8 (4%)	26	60
49	s1	192/224 (86%)	183 (95%)	9 (5%)	23	56
50	D	176/205 (86%)	164 (93%)	12 (7%)	14	42
50	s2	176/205 (86%)	167 (95%)	9 (5%)	21	53
51	E	182/195 (93%)	177 (97%)	5 (3%)	39	73
51	s3	182/195 (93%)	174 (96%)	8 (4%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	F	221/222 (100%)	213 (96%)	8 (4%)	31	65
52	s4	221/222 (100%)	210 (95%)	11 (5%)	22	53
53	G	173/191 (91%)	166 (96%)	7 (4%)	28	62
53	s5	171/191 (90%)	164 (96%)	7 (4%)	27	61
54	H	188/201 (94%)	178 (95%)	10 (5%)	20	52
54	s6	187/201 (93%)	180 (96%)	7 (4%)	30	64
55	I	165/170 (97%)	161 (98%)	4 (2%)	43	75
55	s7	165/170 (97%)	156 (94%)	9 (6%)	19	50
56	J	150/161 (93%)	146 (97%)	4 (3%)	39	73
56	s8	150/161 (93%)	148 (99%)	2 (1%)	61	86
57	K	158/166 (95%)	149 (94%)	9 (6%)	18	49
57	s9	158/166 (95%)	155 (98%)	3 (2%)	50	79
58	L	77/98 (79%)	72 (94%)	5 (6%)	15	44
58	c0	73/98 (74%)	67 (92%)	6 (8%)	10	32
59	M	129/137 (94%)	128 (99%)	1 (1%)	73	90
59	c1	129/137 (94%)	124 (96%)	5 (4%)	28	63
60	N	88/119 (74%)	83 (94%)	5 (6%)	18	49
61	O	127/128 (99%)	123 (97%)	4 (3%)	35	69
61	c3	127/128 (99%)	123 (97%)	4 (3%)	35	69
62	P	81/105 (77%)	73 (90%)	8 (10%)	7	24
62	c4	96/105 (91%)	94 (98%)	2 (2%)	47	77
63	Q	101/118 (86%)	98 (97%)	3 (3%)	36	70
63	c5	103/118 (87%)	96 (93%)	7 (7%)	14	42
64	R	117/119 (98%)	104 (89%)	13 (11%)	6	20
64	c6	118/119 (99%)	114 (97%)	4 (3%)	32	66
65	S	94/124 (76%)	92 (98%)	2 (2%)	47	77
65	c7	92/124 (74%)	87 (95%)	5 (5%)	20	51
66	T	128/129 (99%)	120 (94%)	8 (6%)	16	45
66	c8	128/129 (99%)	123 (96%)	5 (4%)	28	63
67	U	115/116 (99%)	109 (95%)	6 (5%)	21	52
67	c9	115/116 (99%)	114 (99%)	1 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	V	89/114 (78%)	82 (92%)	7 (8%)	11	34
68	d0	84/114 (74%)	78 (93%)	6 (7%)	13	40
69	W	74/74 (100%)	69 (93%)	5 (7%)	14	42
69	d1	74/74 (100%)	70 (95%)	4 (5%)	20	51
70	X	110/111 (99%)	109 (99%)	1 (1%)	70	90
70	d2	110/111 (99%)	107 (97%)	3 (3%)	39	73
71	Y	119/120 (99%)	115 (97%)	4 (3%)	32	66
71	d3	119/120 (99%)	115 (97%)	4 (3%)	32	66
72	Z	112/113 (99%)	110 (98%)	2 (2%)	51	80
72	d4	112/113 (99%)	103 (92%)	9 (8%)	11	34
73	a	61/89 (68%)	57 (93%)	4 (7%)	15	43
73	d5	61/89 (68%)	56 (92%)	5 (8%)	10	32
74	b	83/100 (83%)	76 (92%)	7 (8%)	10	31
74	d6	83/100 (83%)	80 (96%)	3 (4%)	31	65
75	c	70/71 (99%)	65 (93%)	5 (7%)	13	40
75	d7	70/71 (99%)	68 (97%)	2 (3%)	37	71
76	d	56/60 (93%)	46 (82%)	10 (18%)	2	6
76	d8	56/60 (93%)	50 (89%)	6 (11%)	6	22
77	d9	47/49 (96%)	45 (96%)	2 (4%)	26	60
77	e	47/49 (96%)	44 (94%)	3 (6%)	16	44
78	e0	53/54 (98%)	52 (98%)	1 (2%)	50	79
78	f	51/54 (94%)	48 (94%)	3 (6%)	18	48
79	g	62/135 (46%)	57 (92%)	5 (8%)	11	33
80	Rb	260/262 (99%)	241 (93%)	19 (7%)	13	38
80	h	259/262 (99%)	243 (94%)	16 (6%)	16	46
All	All	18471/20424 (90%)	17668 (96%)	803 (4%)	26	60

5 of 803 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	F	217	THR
72	Z	84	LYS
76	d8	66	LEU

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Mol	Chain	Res	Type
54	H	119	GLN
52	F	206	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 310 such sidechains are listed below:

Mol	Chain	Res	Type
75	c	5	GLN
65	c7	101	ASN
80	h	4	ASN
53	s5	34	GLN
70	d2	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3149 (99%)	574 (18%)	43 (1%)
1	AR	3125/3149 (99%)	559 (17%)	45 (1%)
2	3	120/121 (99%)	12 (10%)	0
2	AS	120/121 (99%)	18 (15%)	1 (0%)
3	4	157/158 (99%)	32 (20%)	2 (1%)
3	AT	157/158 (99%)	30 (19%)	1 (0%)
47	A	1735/1800 (96%)	442 (25%)	38 (2%)
47	sR	1780/1800 (98%)	429 (24%)	0
All	All	10339/10456 (98%)	2096 (20%)	130 (1%)

5 of 2096 RNA backbone outliers are listed below:

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

5 of 130 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	A	1051	G
47	A	1244	A
1	AR	588	G

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Mol	Chain	Res	Type
1	AR	550	A
47	A	1370	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2428 ligands modelled in this entry, 1482 are monoatomic - leaving 946 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	$\# Z > 2$
81	OHX	AR	3564	-	0,6,6	-	-	-		
81	OHX	sR	1954	-	0,6,6	-	-	-		
81	OHX	AR	3441	-	0,6,6	-	-	-		
81	OHX	sR	2000	-	0,6,6	-	-	-		
81	OHX	A	1907	-	0,6,6	-	-	-		
81	OHX	CP	303	-	0,6,6	-	-	-		
81	OHX	1	3604	-	0,6,6	-	-	-		
81	OHX	AR	4201	-	0,6,6	-	-	-		
81	OHX	A	1903	-	0,6,6	-	-	-		
81	OHX	A	2133	-	0,6,6	-	-	-		
84	XBI	AR	4222	-	28,28,28	0.70	1 (3%)	37,45,45	1.93	7 (18%)
81	OHX	sR	1976	-	0,6,6	-	-	-		
81	OHX	A	1963	-	0,6,6	-	-	-		
81	OHX	sR	1996	-	0,6,6	-	-	-		
81	OHX	AR	3608	-	0,6,6	-	-	-		
81	OHX	1	3512	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	AR	3459	-	0,6,6	-	-	-		
81	OHX	A	1901	-	0,6,6	-	-	-		
81	OHX	1	3493	-	0,6,6	-	-	-		
81	OHX	1	3486	-	0,6,6	-	-	-		
81	OHX	AR	3464	-	0,6,6	-	-	-		
81	OHX	AR	3473	-	0,6,6	-	-	-		
81	OHX	AR	3673	-	0,6,6	-	-	-		
81	OHX	A	2113	-	0,6,6	-	-	-		
81	OHX	sR	1917	-	0,6,6	-	-	-		
81	OHX	1	3583	-	0,6,6	-	-	-		
81	OHX	AR	3543	-	0,6,6	-	-	-		
81	OHX	AR	3603	-	0,6,6	-	-	-		
81	OHX	A	1959	-	0,6,6	-	-	-		
81	OHX	CX	202	-	0,6,6	-	-	-		
81	OHX	sR	1969	-	0,6,6	-	-	-		
81	OHX	AR	3482	-	0,6,6	-	-	-		
81	OHX	A	1935	-	0,6,6	-	-	-		
81	OHX	1	4117	-	0,6,6	-	-	-		
81	OHX	1	4110	-	0,6,6	-	-	-		
81	OHX	1	3413	-	0,6,6	-	-	-		
81	OHX	AR	3596	-	0,6,6	-	-	-		
81	OHX	AR	3524	-	0,6,6	-	-	-		
81	OHX	1	4088	-	0,6,6	-	-	-		
81	OHX	1	4101	-	0,6,6	-	-	-		
81	OHX	1	3508	-	0,6,6	-	-	-		
81	OHX	1	4121	-	0,6,6	-	-	-		
81	OHX	1	3421	-	0,6,6	-	-	-		
81	OHX	AR	3456	-	0,6,6	-	-	-		
81	OHX	AR	3454	-	0,6,6	-	-	-		
81	OHX	sR	1977	-	0,6,6	-	-	-		
81	OHX	1	3446	-	0,6,6	-	-	-		
81	OHX	AR	3595	-	0,6,6	-	-	-		
81	OHX	sR	1940	-	0,6,6	-	-	-		
81	OHX	sR	1950[B]	-	0,6,6	-	-	-		
81	OHX	1	3584	-	0,6,6	-	-	-		
81	OHX	AR	3588	-	0,6,6	-	-	-		
81	OHX	1	3617	-	0,6,6	-	-	-		
81	OHX	1	4089	-	0,6,6	-	-	-		
81	OHX	AR	3586	-	0,6,6	-	-	-		
81	OHX	1	3585	-	0,6,6	-	-	-		
81	OHX	AS	3504	-	0,6,6	-	-	-		
81	OHX	AR	3469	-	0,6,6	-	-	-		
81	OHX	1	3441	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	AR	3527	-	0,6,6	-	-	-		
81	OHX	AR	3620	-	0,6,6	-	-	-		
81	OHX	sR	2006	-	0,6,6	-	-	-		
81	OHX	sR	1909	-	0,6,6	-	-	-		
81	OHX	sR	1972	-	0,6,6	-	-	-		
81	OHX	A	1939	-	0,6,6	-	-	-		
81	OHX	1	3411	-	0,6,6	-	-	-		
81	OHX	AR	3627	-	0,6,6	-	-	-		
81	OHX	1	3514	-	0,6,6	-	-	-		
81	OHX	A	1936	-	0,6,6	-	-	-		
81	OHX	T	201	-	0,6,6	-	-	-		
81	OHX	AR	3600	-	0,6,6	-	-	-		
81	OHX	AS	3503	-	0,6,6	-	-	-		
81	OHX	1	3575	-	0,6,6	-	-	-		
81	OHX	A	2120	-	0,6,6	-	-	-		
81	OHX	1	4141	-	0,6,6	-	-	-		
81	OHX	AR	3401	-	0,6,6	-	-	-		
81	OHX	AR	3669	-	0,6,6	-	-	-		
81	OHX	AR	3432	-	0,6,6	-	-	-		
81	OHX	A	1960	-	0,6,6	-	-	-		
81	OHX	AR	3602	-	0,6,6	-	-	-		
81	OHX	AR	3628	-	0,6,6	-	-	-		
81	OHX	1	3567	-	0,6,6	-	-	-		
81	OHX	sR	1929	-	0,6,6	-	-	-		
81	OHX	AR	3438	-	0,6,6	-	-	-		
81	OHX	A	1940	-	0,6,6	-	-	-		
81	OHX	sR	1905	-	0,6,6	-	-	-		
81	OHX	AR	3501	-	0,6,6	-	-	-		
81	OHX	1	3531	-	0,6,6	-	-	-		
81	OHX	AR	3638	-	0,6,6	-	-	-		
81	OHX	AR	3484	-	0,6,6	-	-	-		
81	OHX	AR	3666	-	0,6,6	-	-	-		
81	OHX	1	3525	-	0,6,6	-	-	-		
81	OHX	AT	214	-	0,6,6	-	-	-		
81	OHX	A	2108	-	0,6,6	-	-	-		
81	OHX	AR	3445	-	0,6,6	-	-	-		
81	OHX	A	1958	-	0,6,6	-	-	-		
81	OHX	sR	1907	-	0,6,6	-	-	-		
81	OHX	sR	2016	-	0,6,6	-	-	-		
81	OHX	1	3577	-	0,6,6	-	-	-		
81	OHX	sR	1937	-	0,6,6	-	-	-		
81	OHX	1	3428	-	0,6,6	-	-	-		
81	OHX	1	4076	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	AR	3449	-	0,6,6	-	-	-		
81	OHX	AR	3581	-	0,6,6	-	-	-		
81	OHX	AR	3403	-	0,6,6	-	-	-		
81	OHX	sR	2011	-	0,6,6	-	-	-		
81	OHX	sR	1961	-	0,6,6	-	-	-		
81	OHX	4	210	-	0,6,6	-	-	-		
81	OHX	A	2144	-	0,6,6	-	-	-		
81	OHX	AR	3521	-	0,6,6	-	-	-		
81	OHX	A	2139	-	0,6,6	-	-	-		
81	OHX	AR	3577	-	0,6,6	-	-	-		
81	OHX	AR	3649	-	0,6,6	-	-	-		
81	OHX	DK	201	-	0,6,6	-	-	-		
81	OHX	AR	3625	-	0,6,6	-	-	-		
81	OHX	AT	215	-	0,6,6	-	-	-		
81	OHX	AR	3460	-	0,6,6	-	-	-		
81	OHX	AR	3613	-	0,6,6	-	-	-		
81	OHX	1	3491	-	0,6,6	-	-	-		
81	OHX	AR	3569	-	0,6,6	-	-	-		
81	OHX	sR	1994	-	0,6,6	-	-	-		
81	OHX	1	3601	-	0,6,6	-	-	-		
81	OHX	c8	201	-	0,6,6	-	-	-		
81	OHX	1	3437	-	0,6,6	-	-	-		
81	OHX	A	1942	-	0,6,6	-	-	-		
81	OHX	AR	3478[A]	-	0,6,6	-	-	-		
81	OHX	AR	3516	-	0,6,6	-	-	-		
81	OHX	AR	4196	-	0,6,6	-	-	-		
81	OHX	1	3603	-	0,6,6	-	-	-		
81	OHX	1	4094	-	0,6,6	-	-	-		
81	OHX	J	301	-	0,6,6	-	-	-		
81	OHX	1	3404	-	0,6,6	-	-	-		
81	OHX	1	3424	-	0,6,6	-	-	-		
81	OHX	S	201	-	0,6,6	-	-	-		
81	OHX	AR	3435	-	0,6,6	-	-	-		
81	OHX	AR	3671	-	0,6,6	-	-	-		
81	OHX	1	3548	-	0,6,6	-	-	-		
81	OHX	AR	3610	-	0,6,6	-	-	-		
81	OHX	1	4071	-	0,6,6	-	-	-		
81	OHX	AR	3406	-	0,6,6	-	-	-		
81	OHX	AR	3412	-	0,6,6	-	-	-		
81	OHX	A	2127	-	0,6,6	-	-	-		
81	OHX	4	211	-	0,6,6	-	-	-		
81	OHX	1	3410	-	0,6,6	-	-	-		
81	OHX	1	3481	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	1	3401	-	0,6,6	-	-	-		
81	OHX	AR	3513	-	0,6,6	-	-	-		
81	OHX	A	1923	-	0,6,6	-	-	-		
81	OHX	A	2119	-	0,6,6	-	-	-		
81	OHX	AR	3644	-	0,6,6	-	-	-		
81	OHX	1	3602	-	0,6,6	-	-	-		
81	OHX	A	2136	-	0,6,6	-	-	-		
81	OHX	1	3438	-	0,6,6	-	-	-		
81	OHX	AR	3425	-	0,6,6	-	-	-		
81	OHX	sR	1916[A]	-	0,6,6	-	-	-		
81	OHX	1	3472	-	0,6,6	-	-	-		
81	OHX	sR	1927	-	0,6,6	-	-	-		
81	OHX	AR	3458	-	0,6,6	-	-	-		
81	OHX	1	3492	-	0,6,6	-	-	-		
81	OHX	AR	3616	-	0,6,6	-	-	-		
81	OHX	4	208	-	0,6,6	-	-	-		
81	OHX	AR	3415	-	0,6,6	-	-	-		
81	OHX	AR	3622	-	0,6,6	-	-	-		
81	OHX	1	3454	-	0,6,6	-	-	-		
81	OHX	A	1914	-	0,6,6	-	-	-		
81	OHX	AR	3652	-	0,6,6	-	-	-		
81	OHX	AR	3678	-	0,6,6	-	-	-		
81	OHX	sR	1962	-	0,6,6	-	-	-		
81	OHX	AR	3427	-	0,6,6	-	-	-		
81	OHX	A	2126	-	0,6,6	-	-	-		
81	OHX	AR	3641	-	0,6,6	-	-	-		
81	OHX	sR	2018	-	0,5,6	-	-	-		
81	OHX	1	3521	-	0,6,6	-	-	-		
81	OHX	1	3565	-	0,6,6	-	-	-		
81	OHX	sR	1998	-	0,6,6	-	-	-		
81	OHX	sR	1926	-	0,6,6	-	-	-		
81	OHX	AR	3637	-	0,6,6	-	-	-		
81	OHX	1	3526	-	0,6,6	-	-	-		
81	OHX	A	2107	-	0,6,6	-	-	-		
81	OHX	AR	3552	-	0,6,6	-	-	-		
81	OHX	sR	1938	-	0,6,6	-	-	-		
81	OHX	AR	3497	-	0,6,6	-	-	-		
81	OHX	sR	2024	-	0,6,6	-	-	-		
81	OHX	AR	3606	-	0,6,6	-	-	-		
81	OHX	1	4124	-	0,6,6	-	-	-		
81	OHX	AR	3550	-	0,6,6	-	-	-		
81	OHX	AR	3654	-	0,6,6	-	-	-		
81	OHX	1	3546	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	DD	101	-	0,6,6	-	-	-		
81	OHX	sR	1918	-	0,6,6	-	-	-		
81	OHX	sR	2023	-	0,6,6	-	-	-		
81	OHX	AR	3542	-	0,6,6	-	-	-		
81	OHX	AR	3526	-	0,6,6	-	-	-		
81	OHX	1	3541	-	0,6,6	-	-	-		
81	OHX	AP	502	-	0,6,6	-	-	-		
81	OHX	AR	3478[B]	-	0,6,6	-	-	-		
81	OHX	AS	3508	-	0,6,6	-	-	-		
81	OHX	AR	3494	-	0,6,6	-	-	-		
81	OHX	A	1952	-	0,6,6	-	-	-		
81	OHX	1	3426	-	0,6,6	-	-	-		
81	OHX	A	1962	-	0,6,6	-	-	-		
81	OHX	sR	1989	-	0,6,6	-	-	-		
81	OHX	AR	3572	-	0,6,6	-	-	-		
81	OHX	A	1968	-	0,6,6	-	-	-		
81	OHX	AR	3632	-	0,6,6	-	-	-		
81	OHX	1	3445	-	0,6,6	-	-	-		
81	OHX	A	1965	-	0,6,6	-	-	-		
81	OHX	sR	1915	-	0,6,6	-	-	-		
81	OHX	AR	3607	-	0,6,6	-	-	-		
81	OHX	1	3482[A]	-	0,6,6	-	-	-		
81	OHX	sR	2019	-	0,6,6	-	-	-		
81	OHX	A	1927	-	0,6,6	-	-	-		
81	OHX	1	3442	-	0,6,6	-	-	-		
81	OHX	U	201	-	0,6,6	-	-	-		
81	OHX	1	3555	-	0,6,6	-	-	-		
81	OHX	3	206	-	0,6,6	-	-	-		
81	OHX	AR	3461	-	0,6,6	-	-	-		
81	OHX	4	207	-	0,6,6	-	-	-		
81	OHX	1	3403	-	0,6,6	-	-	-		
81	OHX	AR	3560	-	0,6,6	-	-	-		
81	OHX	A	1957	-	0,6,6	-	-	-		
81	OHX	AR	3487	-	0,6,6	-	-	-		
81	OHX	sR	2020	-	0,6,6	-	-	-		
81	OHX	AR	4197	-	0,6,6	-	-	-		
81	OHX	1	3564	-	0,6,6	-	-	-		
81	OHX	1	3616	-	0,6,6	-	-	-		
81	OHX	1	3457	-	0,6,6	-	-	-		
81	OHX	1	4098	-	0,6,6	-	-	-		
81	OHX	AR	3668	-	0,6,6	-	-	-		
81	OHX	sR	1990	-	0,6,6	-	-	-		
81	OHX	1	3595	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	A	1906	-	0,6,6	-	-	-		
81	OHX	AR	3684	-	0,6,6	-	-	-		
81	OHX	1	4133	-	0,6,6	-	-	-		
81	OHX	1	4116	-	0,6,6	-	-	-		
81	OHX	1	3586	-	0,6,6	-	-	-		
81	OHX	AR	3522	-	0,6,6	-	-	-		
81	OHX	sR	1992	-	0,6,6	-	-	-		
81	OHX	sR	2028	-	0,6,6	-	-	-		
81	OHX	AR	3402	-	0,6,6	-	-	-		
81	OHX	AR	3631	-	0,6,6	-	-	-		
81	OHX	1	3469	-	0,6,6	-	-	-		
81	OHX	sR	2027	-	0,6,6	-	-	-		
81	OHX	AR	3570	-	0,6,6	-	-	-		
81	OHX	A	1950	-	0,6,6	-	-	-		
81	OHX	AR	3565	-	0,6,6	-	-	-		
81	OHX	A	1913	-	0,6,6	-	-	-		
81	OHX	1	4099	-	0,6,6	-	-	-		
81	OHX	1	3576	-	0,6,6	-	-	-		
81	OHX	1	3600	-	0,6,6	-	-	-		
81	OHX	AR	3520	-	0,6,6	-	-	-		
81	OHX	AR	3686	-	0,6,6	-	-	-		
81	OHX	A	1969	-	0,6,6	-	-	-		
81	OHX	1	4142	-	0,6,6	-	-	-		
81	OHX	1	3610	-	0,6,6	-	-	-		
81	OHX	A	2140	-	0,6,6	-	-	-		
81	OHX	1	3474	-	0,6,6	-	-	-		
81	OHX	1	3596	-	0,6,6	-	-	-		
81	OHX	CL	302[B]	-	0,6,6	-	-	-		
81	OHX	sR	2021	-	0,6,6	-	-	-		
81	OHX	AR	3437	-	0,6,6	-	-	-		
81	OHX	AR	3576	-	0,6,6	-	-	-		
81	OHX	1	3435	-	0,6,6	-	-	-		
81	OHX	1	3407	-	0,6,6	-	-	-		
81	OHX	1	3607	-	0,6,6	-	-	-		
81	OHX	A	1972	-	0,6,6	-	-	-		
81	OHX	AR	3507	-	0,6,6	-	-	-		
81	OHX	3	203	-	0,6,6	-	-	-		
81	OHX	sR	1936	-	0,6,6	-	-	-		
81	OHX	1	3415	-	0,6,6	-	-	-		
81	OHX	1	3423	-	0,6,6	-	-	-		
81	OHX	AR	3405	-	0,6,6	-	-	-		
81	OHX	AR	3663	-	0,6,6	-	-	-		
81	OHX	4	214	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	3	220	-	0,6,6	-	-	-		
81	OHX	AR	3685	-	0,6,6	-	-	-		
81	OHX	4	204	-	0,6,6	-	-	-		
81	OHX	AR	3407	-	0,6,6	-	-	-		
81	OHX	AR	3551	-	0,6,6	-	-	-		
81	OHX	A	2114	-	0,6,6	-	-	-		
81	OHX	1	3478	-	0,6,6	-	-	-		
81	OHX	AR	3655	-	0,6,6	-	-	-		
81	OHX	A	1908	-	0,6,6	-	-	-		
81	OHX	A	2110	-	0,6,6	-	-	-		
81	OHX	AR	3448	-	0,6,6	-	-	-		
81	OHX	A	2118	-	0,6,6	-	-	-		
81	OHX	1	4126	-	0,6,6	-	-	-		
81	OHX	1	3459	-	0,6,6	-	-	-		
81	OHX	1	3473	-	0,6,6	-	-	-		
81	OHX	AR	3451	-	0,6,6	-	-	-		
81	OHX	AR	3506	-	0,6,6	-	-	-		
81	OHX	1	3422	-	0,6,6	-	-	-		
81	OHX	1	3613	-	0,6,6	-	-	-		
81	OHX	1	3482[B]	-	0,6,6	-	-	-		
81	OHX	AR	3491	-	0,6,6	-	-	-		
81	OHX	A	2111	-	0,6,6	-	-	-		
81	OHX	A	2115	-	0,6,6	-	-	-		
83	SPD	AR	4206	-	9,9,9	0.32	0	8,8,8	0.89	0
81	OHX	AR	4202	-	0,6,6	-	-	-		
81	OHX	1	3594	-	0,6,6	-	-	-		
81	OHX	A	1932	-	0,6,6	-	-	-		
81	OHX	1	3552	-	0,6,6	-	-	-		
81	OHX	1	3450	-	0,6,6	-	-	-		
81	OHX	AR	4198	-	0,6,6	-	-	-		
81	OHX	s4	301	-	0,6,6	-	-	-		
81	OHX	1	3606	-	0,6,6	-	-	-		
81	OHX	sR	1947	-	0,6,6	-	-	-		
81	OHX	A	1916	-	0,6,6	-	-	-		
81	OHX	A	1922	-	0,6,6	-	-	-		
81	OHX	sR	2004	-	0,6,6	-	-	-		
81	OHX	AR	3475	-	0,6,6	-	-	-		
81	OHX	AR	3477	-	0,6,6	-	-	-		
81	OHX	CL	301	-	0,6,6	-	-	-		
81	OHX	AS	3505	-	0,6,6	-	-	-		
81	OHX	1	4114	-	0,6,6	-	-	-		
81	OHX	1	3494	-	0,6,6	-	-	-		
81	OHX	1	4143	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	1	3449	-	0,6,6	-	-	-		
81	OHX	1	3558	-	0,6,6	-	-	-		
81	OHX	AR	3612	-	0,6,6	-	-	-		
81	OHX	AR	3583	-	0,6,6	-	-	-		
81	OHX	AR	3485	-	0,6,6	-	-	-		
81	OHX	AT	207	-	0,6,6	-	-	-		
81	OHX	AR	4199	-	0,6,6	-	-	-		
81	OHX	1	3551	-	0,6,6	-	-	-		
81	OHX	AG	202	-	0,6,6	-	-	-		
81	OHX	1	4102	-	0,6,6	-	-	-		
81	OHX	AR	3431	-	0,6,6	-	-	-		
81	OHX	1	3520	-	0,6,6	-	-	-		
81	OHX	AS	3507	-	0,6,6	-	-	-		
81	OHX	A	2123	-	0,6,6	-	-	-		
81	OHX	AR	3503	-	0,6,6	-	-	-		
81	OHX	1	3456	-	0,6,6	-	-	-		
81	OHX	1	3532	-	0,6,6	-	-	-		
81	OHX	AR	3624	-	0,6,6	-	-	-		
81	OHX	A	1948	81	0,6,6	-	-	-		
81	OHX	4	206	-	0,6,6	-	-	-		
81	OHX	AR	3457	-	0,6,6	-	-	-		
81	OHX	AR	3531	-	0,6,6	-	-	-		
81	OHX	3	202	-	0,6,6	-	-	-		
81	OHX	AR	3614	-	0,6,6	-	-	-		
81	OHX	AR	3587	-	0,6,6	-	-	-		
81	OHX	sR	2013	-	0,6,6	-	-	-		
81	OHX	1	3554	-	0,6,6	-	-	-		
81	OHX	AR	3557	-	0,6,6	-	-	-		
81	OHX	AR	3416	-	0,6,6	-	-	-		
81	OHX	1	3599	-	0,6,6	-	-	-		
81	OHX	3	201	-	0,6,6	-	-	-		
81	OHX	CG	301	-	0,5,6	-	-	-		
81	OHX	AR	4203	-	0,6,6	-	-	-		
81	OHX	1	3615	-	0,6,6	-	-	-		
81	OHX	sR	1931	-	0,6,6	-	-	-		
81	OHX	1	3414	-	0,6,6	-	-	-		
81	OHX	AR	3466	-	0,6,6	-	-	-		
81	OHX	A	1920	-	0,6,6	-	-	-		
81	OHX	1	3506	-	0,6,6	-	-	-		
81	OHX	sR	1983	-	0,6,6	-	-	-		
81	OHX	1	3518	-	0,6,6	-	-	-		
81	OHX	sR	1968	-	0,6,6	-	-	-		
81	OHX	AT	209	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	AR	3467	-	0,6,6	-	-	-		
81	OHX	1	3571	-	0,6,6	-	-	-		
81	OHX	AR	3592	-	0,5,6	-	-	-		
81	OHX	1	3490	-	0,6,6	-	-	-		
81	OHX	CP	301	-	0,6,6	-	-	-		
81	OHX	O	201	-	0,6,6	-	-	-		
81	OHX	AR	3635	-	0,6,6	-	-	-		
81	OHX	1	3488	-	0,6,6	-	-	-		
81	OHX	sR	1973	-	0,6,6	-	-	-		
81	OHX	AC	101	-	0,6,6	-	-	-		
81	OHX	AR	3657	-	0,6,6	-	-	-		
81	OHX	1	3484	-	0,6,6	-	-	-		
81	OHX	1	3408	-	0,6,6	-	-	-		
81	OHX	1	3483	-	0,6,6	-	-	-		
81	OHX	A	1956	-	0,6,6	-	-	-		
81	OHX	A	2105	-	0,6,6	-	-	-		
81	OHX	A	2143	81	0,5,6	-	-	-		
81	OHX	sR	2009	-	0,6,6	-	-	-		
81	OHX	1	3517	-	0,6,6	-	-	-		
81	OHX	c3	201	-	0,6,6	-	-	-		
81	OHX	4	213	-	0,6,6	-	-	-		
81	OHX	AR	3468	-	0,6,6	-	-	-		
81	OHX	4	235	-	0,6,6	-	-	-		
81	OHX	AR	3440	-	0,6,6	-	-	-		
81	OHX	A	2130	-	0,6,6	-	-	-		
81	OHX	AR	3500	-	0,6,6	-	-	-		
81	OHX	AR	3549	-	0,6,6	-	-	-		
81	OHX	sR	1997	-	0,6,6	-	-	-		
81	OHX	sR	2170	-	0,6,6	-	-	-		
81	OHX	1	4104	-	0,6,6	-	-	-		
81	OHX	AR	3423	-	0,6,6	-	-	-		
81	OHX	1	3611	-	0,6,6	-	-	-		
81	OHX	AR	3650	-	0,6,6	-	-	-		
81	OHX	AR	3517	-	0,6,6	-	-	-		
81	OHX	sR	1930	-	0,6,6	-	-	-		
81	OHX	A	1954	-	0,6,6	-	-	-		
81	OHX	1	3462	-	0,6,6	-	-	-		
81	OHX	1	3591	-	0,6,6	-	-	-		
81	OHX	1	3528	-	0,6,6	-	-	-		
81	OHX	A	1934	-	0,6,6	-	-	-		
81	OHX	A	1973	-	0,6,6	-	-	-		
81	OHX	AR	3426	-	0,6,6	-	-	-		
81	OHX	AR	3444	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	AR	3510	-	0,6,6	-	-	-		
81	OHX	AR	3429	-	0,6,6	-	-	-		
81	OHX	1	3416	-	0,6,6	-	-	-		
81	OHX	AR	3463	-	0,6,6	-	-	-		
81	OHX	AR	3566	-	0,6,6	-	-	-		
81	OHX	1	4105	-	0,5,6	-	-	-		
81	OHX	AR	3509	-	0,6,6	-	-	-		
81	OHX	A	1931	-	0,6,6	-	-	-		
81	OHX	AR	3554	-	0,6,6	-	-	-		
81	OHX	AR	3528	-	0,6,6	-	-	-		
81	OHX	AR	3599	-	0,6,6	-	-	-		
81	OHX	AR	3601	-	0,6,6	-	-	-		
81	OHX	sR	1908	-	0,6,6	-	-	-		
81	OHX	1	4091	-	0,6,6	-	-	-		
81	OHX	A	2100	-	0,6,6	-	-	-		
81	OHX	AR	3447	-	0,6,6	-	-	-		
81	OHX	AR	3540	-	0,6,6	-	-	-		
81	OHX	1	3608[A]	-	0,6,6	-	-	-		
81	OHX	AR	3615	-	0,6,6	-	-	-		
81	OHX	A	1912	-	0,6,6	-	-	-		
81	OHX	s1	301	-	0,6,6	-	-	-		
81	OHX	AR	3443	-	0,6,6	-	-	-		
81	OHX	sR	1987	-	0,6,6	-	-	-		
81	OHX	AR	3417	-	0,6,6	-	-	-		
81	OHX	sR	1971	-	0,6,6	-	-	-		
81	OHX	1	3574	-	0,6,6	-	-	-		
81	OHX	sR	1974	-	0,6,6	-	-	-		
81	OHX	c5	201	-	0,6,6	-	-	-		
81	OHX	1	3519[A]	-	0,6,6	-	-	-		
81	OHX	AR	3489	-	0,6,6	-	-	-		
81	OHX	A	2129	-	0,6,6	-	-	-		
81	OHX	AR	3648	-	0,6,6	-	-	-		
81	OHX	AR	3679	-	0,6,6	-	-	-		
81	OHX	1	3475	-	0,6,6	-	-	-		
81	OHX	1	3573	-	0,6,6	-	-	-		
81	OHX	A	1905	-	0,6,6	-	-	-		
81	OHX	sR	1921	-	0,6,6	-	-	-		
81	OHX	AR	3408	-	0,6,6	-	-	-		
81	OHX	AR	3439	-	0,6,6	-	-	-		
81	OHX	AR	3626	-	0,6,6	-	-	-		
81	OHX	1	3538	-	0,6,6	-	-	-		
81	OHX	1	3487	-	0,6,6	-	-	-		
81	OHX	1	4137	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	AR	3488	-	0,6,6	-	-	-		
81	OHX	sR	1913	-	0,6,6	-	-	-		
81	OHX	AR	3529	-	0,6,6	-	-	-		
81	OHX	sR	1970	-	0,6,6	-	-	-		
81	OHX	3	221	-	0,6,6	-	-	-		
81	OHX	AR	3683	-	0,6,6	-	-	-		
81	OHX	1	4118	-	0,6,6	-	-	-		
81	OHX	AR	3682	-	0,6,6	-	-	-		
81	OHX	AR	3617	-	0,6,6	-	-	-		
81	OHX	1	3500	-	0,6,6	-	-	-		
81	OHX	sR	1903	-	0,6,6	-	-	-		
81	OHX	sR	1925	-	0,6,6	-	-	-		
81	OHX	AR	3544	-	0,6,6	-	-	-		
81	OHX	AR	3496	-	0,6,6	-	-	-		
81	OHX	1	4120	-	0,5,6	-	-	-		
81	OHX	AS	3501	-	0,6,6	-	-	-		
81	OHX	1	3464	-	0,6,6	-	-	-		
81	OHX	AR	3558	-	0,6,6	-	-	-		
81	OHX	AR	3502	-	0,6,6	-	-	-		
81	OHX	1	4119	-	0,6,6	-	-	-		
81	OHX	1	4123	-	0,6,6	-	-	-		
81	OHX	3	222	-	0,6,6	-	-	-		
81	OHX	1	4090	-	0,5,6	-	-	-		
81	OHX	AS	3510	-	0,6,6	-	-	-		
81	OHX	1	3477	-	0,6,6	-	-	-		
81	OHX	1	3429	-	0,6,6	-	-	-		
81	OHX	1	3510	-	0,6,6	-	-	-		
81	OHX	1	3432	-	0,6,6	-	-	-		
81	OHX	AR	3480	-	0,6,6	-	-	-		
81	OHX	AS	3509	-	0,6,6	-	-	-		
81	OHX	1	3466	-	0,6,6	-	-	-		
81	OHX	sR	1999	-	0,6,6	-	-	-		
81	OHX	AR	3636	-	0,6,6	-	-	-		
81	OHX	1	3542	-	0,6,6	-	-	-		
81	OHX	A	2125	-	0,6,6	-	-	-		
81	OHX	sR	2012	-	0,6,6	-	-	-		
81	OHX	1	3507	-	0,6,6	-	-	-		
81	OHX	1	3549	-	0,6,6	-	-	-		
81	OHX	1	3540	-	0,6,6	-	-	-		
81	OHX	k	402	-	0,6,6	-	-	-		
81	OHX	1	3412	-	0,6,6	-	-	-		
81	OHX	1	3592	-	0,6,6	-	-	-		
81	OHX	AR	3674	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	A	1925	-	0,6,6	-	-	-		
81	OHX	AR	3462	-	0,6,6	-	-	-		
81	OHX	AR	3422	-	0,6,6	-	-	-		
81	OHX	e	102	-	0,6,6	-	-	-		
81	OHX	sR	2171	-	0,6,6	-	-	-		
81	OHX	1	3485[A]	-	0,6,6	-	-	-		
81	OHX	A	1902	-	0,6,6	-	-	-		
81	OHX	DQ	502	-	0,6,6	-	-	-		
81	OHX	AR	3643	-	0,6,6	-	-	-		
81	OHX	1	4100	-	0,6,6	-	-	-		
81	OHX	sR	1984	-	0,6,6	-	-	-		
81	OHX	1	3608[B]	-	0,6,6	-	-	-		
81	OHX	sR	1932	-	0,6,6	-	-	-		
81	OHX	1	3556	-	0,6,6	-	-	-		
81	OHX	A	2134	-	0,6,6	-	-	-		
81	OHX	1	4115	-	0,6,6	-	-	-		
81	OHX	AR	3582	-	0,6,6	-	-	-		
81	OHX	A	1919	-	0,6,6	-	-	-		
81	OHX	AR	3409	-	0,6,6	-	-	-		
81	OHX	AR	3562	-	0,6,6	-	-	-		
81	OHX	1	3451	-	0,6,6	-	-	-		
81	OHX	1	3523	-	0,6,6	-	-	-		
81	OHX	1	3519[B]	-	0,6,6	-	-	-		
81	OHX	AR	3471	-	0,6,6	-	-	-		
81	OHX	1	4072	-	0,6,6	-	-	-		
81	OHX	AR	3647	-	0,6,6	-	-	-		
81	OHX	AR	3561	-	0,6,6	-	-	-		
81	OHX	AR	3515	-	0,6,6	-	-	-		
81	OHX	AR	3530	-	0,6,6	-	-	-		
81	OHX	A	2121	-	0,6,6	-	-	-		
81	OHX	sR	1916[B]	-	0,6,6	-	-	-		
81	OHX	AR	3664	-	0,6,6	-	-	-		
81	OHX	1	3503	-	0,6,6	-	-	-		
81	OHX	3	205	-	0,6,6	-	-	-		
81	OHX	AR	3523	-	0,6,6	-	-	-		
81	OHX	sR	1941	-	0,6,6	-	-	-		
81	OHX	1	3550	-	0,6,6	-	-	-		
81	OHX	1	3460	-	0,6,6	-	-	-		
81	OHX	1	3570	-	0,6,6	-	-	-		
81	OHX	sR	1975	-	0,6,6	-	-	-		
81	OHX	sR	2174	-	0,6,6	-	-	-		
81	OHX	sR	1982	-	0,6,6	-	-	-		
81	OHX	1	3569	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	1	3496	-	0,6,6	-	-	-		
81	OHX	AR	3433	-	0,6,6	-	-	-		
81	OHX	d0	201	-	0,6,6	-	-	-		
81	OHX	AT	208	-	0,6,6	-	-	-		
81	OHX	A	1926	-	0,6,6	-	-	-		
81	OHX	sR	1988	-	0,6,6	-	-	-		
81	OHX	AR	3578	-	0,6,6	-	-	-		
81	OHX	1	4140	-	0,6,6	-	-	-		
81	OHX	AR	4175	-	0,6,6	-	-	-		
81	OHX	1	3566	-	0,6,6	-	-	-		
81	OHX	1	4075	-	0,6,6	-	-	-		
81	OHX	1	3467[A]	-	0,5,6	-	-	-		
81	OHX	AR	3532	-	0,6,6	-	-	-		
81	OHX	1	3505	-	0,6,6	-	-	-		
81	OHX	AR	3662	-	0,6,6	-	-	-		
81	OHX	A	2116	-	0,6,6	-	-	-		
81	OHX	AR	3681	-	0,6,6	-	-	-		
81	OHX	A	1924	-	0,6,6	-	-	-		
81	OHX	sR	1944	-	0,6,6	-	-	-		
81	OHX	1	4139	-	0,6,6	-	-	-		
81	OHX	AR	3589	-	0,5,6	-	-	-		
81	OHX	1	3489	-	0,6,6	-	-	-		
81	OHX	A	1971	-	0,6,6	-	-	-		
81	OHX	Q	201	-	0,6,6	-	-	-		
81	OHX	1	4128	-	0,6,6	-	-	-		
81	OHX	1	3547	-	0,6,6	-	-	-		
81	OHX	CG	303	-	0,6,6	-	-	-		
81	OHX	A	2103	-	0,6,6	-	-	-		
81	OHX	sR	1901	-	0,6,6	-	-	-		
81	OHX	1	3597	-	0,6,6	-	-	-		
81	OHX	1	3443	-	0,6,6	-	-	-		
81	OHX	sR	1953	-	0,6,6	-	-	-		
81	OHX	AR	3420	-	0,6,6	-	-	-		
81	OHX	AR	3465	-	0,6,6	-	-	-		
81	OHX	AR	3545	-	0,6,6	-	-	-		
81	OHX	AR	3553	-	0,6,6	-	-	-		
81	OHX	AR	3621	-	0,6,6	-	-	-		
81	OHX	A	1975	-	0,6,6	-	-	-		
81	OHX	AT	203	-	0,6,6	-	-	-		
81	OHX	A	1921	-	0,6,6	-	-	-		
81	OHX	1	4108	-	0,6,6	-	-	-		
81	OHX	sR	2175	-	0,6,6	-	-	-		
81	OHX	1	4122	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	AR	3618	-	0,6,6	-	-	-		
81	OHX	A	1915	-	0,6,6	-	-	-		
81	OHX	1	3535[A]	-	0,6,6	-	-	-		
81	OHX	AR	3499	-	0,6,6	-	-	-		
81	OHX	AR	3504	-	0,6,6	-	-	-		
81	OHX	AR	4200	-	0,6,6	-	-	-		
81	OHX	sR	2001	-	0,6,6	-	-	-		
81	OHX	sR	1950[A]	-	0,6,6	-	-	-		
81	OHX	1	3485[B]	-	0,6,6	-	-	-		
81	OHX	AR	3619	-	0,6,6	-	-	-		
81	OHX	AR	3453	-	0,6,6	-	-	-		
81	OHX	1	4093	-	0,6,6	-	-	-		
81	OHX	sR	2015	-	0,6,6	-	-	-		
81	OHX	1	4136	-	0,6,6	-	-	-		
81	OHX	A	2112	-	0,6,6	-	-	-		
81	OHX	AR	3538	-	0,6,6	-	-	-		
81	OHX	1	3524	-	0,6,6	-	-	-		
81	OHX	AR	3605	-	0,6,6	-	-	-		
81	OHX	1	3533	-	0,6,6	-	-	-		
81	OHX	AR	3430	-	0,6,6	-	-	-		
81	OHX	AS	3530	-	0,6,6	-	-	-		
81	OHX	1	3515	-	0,6,6	-	-	-		
81	OHX	1	3530	-	0,6,6	-	-	-		
81	OHX	AR	3672	-	0,6,6	-	-	-		
81	OHX	sR	1952	-	0,6,6	-	-	-		
81	OHX	AR	3414	-	0,6,6	-	-	-		
81	OHX	1	3497	-	0,6,6	-	-	-		
81	OHX	1	4131	-	0,6,6	-	-	-		
81	OHX	A	2104	-	0,6,6	-	-	-		
81	OHX	sR	1948	-	0,6,6	-	-	-		
81	OHX	1	3588	-	0,6,6	-	-	-		
81	OHX	l	402	-	0,6,6	-	-	-		
81	OHX	sR	2177	-	0,6,6	-	-	-		
81	OHX	1	4112	-	0,6,6	-	-	-		
81	OHX	A	1944	-	0,6,6	-	-	-		
81	OHX	x	209	-	0,6,6	-	-	-		
81	OHX	AR	3591	-	0,6,6	-	-	-		
81	OHX	1	3406	-	0,6,6	-	-	-		
81	OHX	A	1904	-	0,6,6	-	-	-		
81	OHX	AR	3498	-	0,6,6	-	-	-		
81	OHX	AR	3568	-	0,6,6	-	-	-		
81	OHX	AR	3594	-	0,6,6	-	-	-		
81	OHX	sR	1993	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	AR	3424	-	0,6,6	-	-	-		
81	OHX	AR	3574	-	0,6,6	-	-	-		
81	OHX	AR	3495	-	0,6,6	-	-	-		
81	OHX	AR	3659	-	0,6,6	-	-	-		
81	OHX	1	4103	-	0,6,6	-	-	-		
81	OHX	1	4106	-	0,6,6	-	-	-		
81	OHX	A	1967	-	0,6,6	-	-	-		
81	OHX	1	4087	-	0,6,6	-	-	-		
81	OHX	A	1910	-	0,6,6	-	-	-		
81	OHX	sR	1978	-	0,6,6	-	-	-		
81	OHX	z	201	-	0,6,6	-	-	-		
81	OHX	sR	1923	-	0,6,6	-	-	-		
81	OHX	A	1941	-	0,6,6	-	-	-		
81	OHX	AR	4179	-	0,6,6	-	-	-		
81	OHX	sR	1963	-	0,6,6	-	-	-		
81	OHX	AR	3645	-	0,6,6	-	-	-		
81	OHX	sR	1991	-	0,6,6	-	-	-		
81	OHX	1	3458	-	0,6,6	-	-	-		
81	OHX	A	2122	-	0,6,6	-	-	-		
81	OHX	A	2135	-	0,6,6	-	-	-		
81	OHX	1	3572	-	0,6,6	-	-	-		
81	OHX	1	3467[B]	-	0,5,6	-	-	-		
81	OHX	AR	3593	-	0,6,6	-	-	-		
81	OHX	1	3463	-	0,6,6	-	-	-		
81	OHX	sR	1922	-	0,6,6	-	-	-		
81	OHX	sR	1933	-	0,6,6	-	-	-		
81	OHX	1	3545	-	0,6,6	-	-	-		
81	OHX	AR	3525	-	0,6,6	-	-	-		
81	OHX	1	3461	-	0,6,6	-	-	-		
81	OHX	AR	3536	-	0,6,6	-	-	-		
81	OHX	AR	3573	-	0,6,6	-	-	-		
81	OHX	sR	1914	-	0,6,6	-	-	-		
81	OHX	1	3448	-	0,6,6	-	-	-		
81	OHX	AR	3639	-	0,6,6	-	-	-		
81	OHX	CX	201	-	0,6,6	-	-	-		
81	OHX	AR	3534	-	0,6,6	-	-	-		
81	OHX	A	1943	-	0,6,6	-	-	-		
81	OHX	sR	1958	-	0,6,6	-	-	-		
81	OHX	AR	3476	-	0,6,6	-	-	-		
81	OHX	AR	3533	-	0,6,6	-	-	-		
81	OHX	A	1945	-	0,6,6	-	-	-		
81	OHX	4	202	-	0,6,6	-	-	-		
81	OHX	sR	2026	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	1	3561	-	0,6,6	-	-	-		
81	OHX	4	205	-	0,6,6	-	-	-		
81	OHX	AR	3651	-	0,6,6	-	-	-		
81	OHX	sR	1949	-	0,6,6	-	-	-		
81	OHX	4	201	-	0,6,6	-	-	-		
81	OHX	AR	3556	-	0,6,6	-	-	-		
81	OHX	1	3535[B]	-	0,6,6	-	-	-		
81	OHX	sR	1955	-	0,6,6	-	-	-		
81	OHX	1	3614	-	0,6,6	-	-	-		
81	OHX	r	304	-	0,6,6	-	-	-		
81	OHX	1	3430	-	0,6,6	-	-	-		
81	OHX	AR	3511[A]	-	0,6,6	-	-	-		
81	OHX	AT	213	-	0,6,6	-	-	-		
81	OHX	A	1928	-	0,6,6	-	-	-		
81	OHX	sR	1951	-	0,6,6	-	-	-		
81	OHX	sR	2168	-	0,6,6	-	-	-		
81	OHX	A	1933	-	0,6,6	-	-	-		
84	XBI	1	4157	-	28,28,28	0.60	2 (7%)	37,45,45	2.19	7 (18%)
81	OHX	sR	1957	-	0,6,6	-	-	-		
81	OHX	3	219	-	0,6,6	-	-	-		
81	OHX	sR	2008	-	0,6,6	-	-	-		
81	OHX	1	3418	-	0,6,6	-	-	-		
81	OHX	1	3529	-	0,6,6	-	-	-		
81	OHX	A	1946	-	0,6,6	-	-	-		
81	OHX	sR	1945	-	0,6,6	-	-	-		
81	OHX	sR	2176	-	0,6,6	-	-	-		
81	OHX	AR	3535	-	0,6,6	-	-	-		
81	OHX	AR	3479	-	0,6,6	-	-	-		
81	OHX	sR	1911	-	0,6,6	-	-	-		
81	OHX	1	4109	-	0,6,6	-	-	-		
81	OHX	sR	2178	-	0,6,6	-	-	-		
81	OHX	AR	3642	-	0,6,6	-	-	-		
81	OHX	AR	3687[A]	-	0,6,6	-	-	-		
81	OHX	1	3452	-	0,6,6	-	-	-		
81	OHX	AR	3541	-	0,6,6	-	-	-		
81	OHX	AR	3623	-	0,6,6	-	-	-		
81	OHX	sR	2017	-	0,6,6	-	-	-		
81	OHX	sR	1979	-	0,6,6	-	-	-		
81	OHX	1	3589	-	0,6,6	-	-	-		
81	OHX	AR	3518	-	0,6,6	-	-	-		
81	OHX	A	2109	-	0,6,6	-	-	-		
81	OHX	AT	206	-	0,6,6	-	-	-		
81	OHX	1	3440	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	3	204	-	0,6,6	-	-	-		
81	OHX	AR	3571	-	0,6,6	-	-	-		
81	OHX	AR	3661	-	0,6,6	-	-	-		
81	OHX	AT	216	-	0,6,6	-	-	-		
81	OHX	AR	3537	-	0,6,6	-	-	-		
81	OHX	sR	1928	-	0,6,6	-	-	-		
81	OHX	AR	3434	-	0,6,6	-	-	-		
81	OHX	1	3409	-	0,6,6	-	-	-		
81	OHX	1	3581	-	0,6,6	-	-	-		
81	OHX	1	3417	-	0,6,6	-	-	-		
81	OHX	1	3444	-	0,6,6	-	-	-		
81	OHX	A	2145	-	0,6,6	-	-	-		
81	OHX	AR	3472	-	0,6,6	-	-	-		
81	OHX	sR	1965	-	0,6,6	-	-	-		
81	OHX	1	4129	-	0,6,6	-	-	-		
81	OHX	A	2138	-	0,6,6	-	-	-		
81	OHX	1	3559	-	0,6,6	-	-	-		
81	OHX	1	3580	-	0,6,6	-	-	-		
81	OHX	1	3480	-	0,6,6	-	-	-		
81	OHX	1	4111	-	0,6,6	-	-	-		
81	OHX	sR	1906	-	0,6,6	-	-	-		
81	OHX	AT	201	-	0,6,6	-	-	-		
81	OHX	sR	2173	-	0,6,6	-	-	-		
81	OHX	1	3527	-	0,6,6	-	-	-		
81	OHX	1	4138	-	0,6,6	-	-	-		
81	OHX	1	4097	-	0,6,6	-	-	-		
81	OHX	1	3499	-	0,6,6	-	-	-		
81	OHX	AR	3413	-	0,6,6	-	-	-		
81	OHX	1	3447	-	0,6,6	-	-	-		
81	OHX	AR	3539	-	0,6,6	-	-	-		
81	OHX	AR	3563	-	0,6,6	-	-	-		
81	OHX	sR	1919	-	0,6,6	-	-	-		
81	OHX	DL	102	-	0,6,6	-	-	-		
81	OHX	AT	211	-	0,6,6	-	-	-		
81	OHX	1	3534	-	0,6,6	-	-	-		
81	OHX	1	3427	-	0,6,6	-	-	-		
81	OHX	1	3405	-	0,6,6	-	-	-		
81	OHX	AR	3508	-	0,6,6	-	-	-		
81	OHX	AR	3421	-	0,6,6	-	-	-		
81	OHX	AR	3492	-	0,6,6	-	-	-		
81	OHX	AR	3580	-	0,6,6	-	-	-		
81	OHX	z	203	-	0,6,6	-	-	-		
81	OHX	1	3568	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	1	3553	-	0,6,6	-	-	-		
81	OHX	1	3578	-	0,6,6	-	-	-		
81	OHX	AR	3590	-	0,6,6	-	-	-		
81	OHX	A	1911	-	0,6,6	-	-	-		
81	OHX	3	218	-	0,6,6	-	-	-		
81	OHX	AR	3670	-	0,6,6	-	-	-		
81	OHX	A	1929	-	0,6,6	-	-	-		
81	OHX	1	3522	-	0,6,6	-	-	-		
81	OHX	1	3439	-	0,6,6	-	-	-		
81	OHX	AR	3646	-	0,6,6	-	-	-		
81	OHX	A	1937	-	0,6,6	-	-	-		
81	OHX	sR	2014	-	0,6,6	-	-	-		
81	OHX	AR	3442	-	0,6,6	-	-	-		
81	OHX	sR	1939	-	0,6,6	-	-	-		
81	OHX	4	215	-	0,6,6	-	-	-		
81	OHX	sR	2005	-	0,6,6	-	-	-		
81	OHX	1	3582	-	0,6,6	-	-	-		
81	OHX	1	3562	-	0,6,6	-	-	-		
81	OHX	AR	3474	-	0,6,6	-	-	-		
81	OHX	AR	3667	-	0,6,6	-	-	-		
81	OHX	AT	202	-	0,6,6	-	-	-		
81	OHX	1	4127	-	0,6,6	-	-	-		
81	OHX	1	3431	-	0,6,6	-	-	-		
81	OHX	1	3455	-	0,6,6	-	-	-		
81	OHX	1	3468	-	0,6,6	-	-	-		
81	OHX	1	3471	-	0,6,6	-	-	-		
81	OHX	AR	3411	-	0,6,6	-	-	-		
81	OHX	sR	1943	-	0,6,6	-	-	-		
81	OHX	AR	3452	-	0,6,6	-	-	-		
81	OHX	CQ	202	-	0,6,6	-	-	-		
81	OHX	AR	3511[B]	-	0,6,6	-	-	-		
81	OHX	AR	3656	-	0,6,6	-	-	-		
81	OHX	AR	3634	-	0,6,6	-	-	-		
81	OHX	AR	3660	-	0,6,6	-	-	-		
81	OHX	A	1961	-	0,6,6	-	-	-		
81	OHX	A	1938	-	0,6,6	-	-	-		
81	OHX	AK	103	-	0,6,6	-	-	-		
81	OHX	1	3516	-	0,6,6	-	-	-		
81	OHX	1	4113	-	0,6,6	-	-	-		
81	OHX	1	4095	-	0,6,6	-	-	-		
81	OHX	CG	302	-	0,6,6	-	-	-		
81	OHX	1	4135	-	0,6,6	-	-	-		
81	OHX	AR	3687[B]	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	AR	3658	-	0,6,6	-	-	-		
81	OHX	1	3598	-	0,6,6	-	-	-		
81	OHX	sR	1964	-	0,6,6	-	-	-		
81	OHX	1	3453	-	0,6,6	-	-	-		
81	OHX	1	4132	-	0,6,6	-	-	-		
81	OHX	1	3560	-	0,6,6	-	-	-		
81	OHX	sR	1956	-	0,6,6	-	-	-		
81	OHX	AR	3470	-	0,6,6	-	-	-		
81	OHX	A	1949	-	0,6,6	-	-	-		
81	OHX	CE	404	-	0,6,6	-	-	-		
81	OHX	sR	2022	-	0,6,6	-	-	-		
81	OHX	1	3536	-	0,6,6	-	-	-		
81	OHX	v	301	-	0,6,6	-	-	-		
81	OHX	A	1974	-	0,6,6	-	-	-		
81	OHX	1	3557	-	0,6,6	-	-	-		
81	OHX	1	3511	-	0,6,6	-	-	-		
81	OHX	AR	3579	-	0,6,6	-	-	-		
81	OHX	CE	403	-	0,6,6	-	-	-		
81	OHX	sR	1980	-	0,6,6	-	-	-		
81	OHX	AR	3505	-	0,6,6	-	-	-		
81	OHX	A	1966	-	0,6,6	-	-	-		
81	OHX	AR	3419	-	0,6,6	-	-	-		
81	OHX	AR	3514	-	0,6,6	-	-	-		
81	OHX	AR	3598	-	0,6,6	-	-	-		
81	OHX	1	3420	-	0,6,6	-	-	-		
81	OHX	A	1947	-	0,6,6	-	-	-		
81	OHX	A	2132	-	0,6,6	-	-	-		
81	OHX	AR	3609	-	0,6,6	-	-	-		
81	OHX	A	2131	-	0,6,6	-	-	-		
81	OHX	1	4125	-	0,6,6	-	-	-		
81	OHX	A	2137	-	0,6,6	-	-	-		
81	OHX	AR	3675	-	0,6,6	-	-	-		
81	OHX	4	212	-	0,6,6	-	-	-		
81	OHX	AR	3450	-	0,6,6	-	-	-		
81	OHX	sR	1934	-	0,6,6	-	-	-		
81	OHX	A	1953	-	0,6,6	-	-	-		
81	OHX	CL	302[A]	-	0,6,6	-	-	-		
81	OHX	AR	3567	-	0,6,6	-	-	-		
81	OHX	1	3590	-	0,6,6	-	-	-		
81	OHX	AR	3640	-	0,6,6	-	-	-		
81	OHX	A	1964	-	0,6,6	-	-	-		
81	OHX	1	3504	-	0,6,6	-	-	-		
81	OHX	1	3587	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	AR	3493	-	0,6,6	-	-	-		
81	OHX	A	1909	-	0,6,6	-	-	-		
81	OHX	AR	3455	-	0,6,6	-	-	-		
81	OHX	1	3501	-	0,6,6	-	-	-		
81	OHX	AR	3630	-	0,6,6	-	-	-		
81	OHX	sR	1942	-	0,6,6	-	-	-		
81	OHX	1	3502	-	0,6,6	-	-	-		
81	OHX	CS	201	-	0,6,6	-	-	-		
81	OHX	1	3433	-	0,6,6	-	-	-		
81	OHX	A	1917	-	0,6,6	-	-	-		
81	OHX	A	2124	-	0,6,6	-	-	-		
81	OHX	sR	1995	-	0,6,6	-	-	-		
81	OHX	1	3605	-	0,6,6	-	-	-		
81	OHX	1	4096	-	0,6,6	-	-	-		
81	OHX	A	1970	-	0,6,6	-	-	-		
81	OHX	sR	1920	-	0,6,6	-	-	-		
81	OHX	AR	3548	-	0,6,6	-	-	-		
81	OHX	AR	3483	-	0,6,6	-	-	-		
81	OHX	sR	1959	-	0,6,6	-	-	-		
81	OHX	1	3434	-	0,6,6	-	-	-		
81	OHX	sR	1924	-	0,6,6	-	-	-		
81	OHX	AR	3486	-	0,6,6	-	-	-		
81	OHX	AR	3653	-	0,6,6	-	-	-		
81	OHX	AR	3481	-	0,6,6	-	-	-		
81	OHX	AR	3688	-	0,6,6	-	-	-		
81	OHX	sR	2002	-	0,6,6	-	-	-		
81	OHX	sR	1960	-	0,6,6	-	-	-		
81	OHX	1	3612	-	0,6,6	-	-	-		
81	OHX	sR	1904	-	0,6,6	-	-	-		
81	OHX	A	2141	-	0,6,6	-	-	-		
81	OHX	AR	3559	-	0,6,6	-	-	-		
81	OHX	AR	3546	-	0,6,6	-	-	-		
83	SPD	1	4144	-	9,9,9	0.32	0	8,8,8	1.07	0
81	OHX	AR	3665	-	0,6,6	-	-	-		
81	OHX	AR	4205	-	0,5,6	-	-	-		
81	OHX	1	4092	-	0,6,6	-	-	-		
81	OHX	AR	3629	-	0,6,6	-	-	-		
81	OHX	AR	3633	-	0,6,6	-	-	-		
81	OHX	sR	1981	-	0,6,6	-	-	-		
81	OHX	AR	3676	-	0,6,6	-	-	-		
81	OHX	1	3495	-	0,6,6	-	-	-		
81	OHX	AR	3446	-	0,6,6	-	-	-		
81	OHX	AR	3575	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
81	OHX	AR	3428	-	0,6,6	-	-	-		
81	OHX	A	2117	-	0,6,6	-	-	-		
81	OHX	1	3470	-	0,6,6	-	-	-		
81	OHX	1	4068	-	0,6,6	-	-	-		
81	OHX	AR	3604	-	0,6,6	-	-	-		
81	OHX	1	3513	-	0,6,6	-	-	-		
81	OHX	AR	3519	-	0,6,6	-	-	-		
81	OHX	A	1918	-	0,6,6	-	-	-		
81	OHX	A	2106	-	0,6,6	-	-	-		
81	OHX	AR	3512	-	0,6,6	-	-	-		
81	OHX	1	3539	-	0,6,6	-	-	-		
81	OHX	1	3419	-	0,6,6	-	-	-		
81	OHX	AR	3584	-	0,6,6	-	-	-		
81	OHX	A	2142	-	0,6,6	-	-	-		
81	OHX	A	1930	-	0,6,6	-	-	-		
81	OHX	1	3465	-	0,6,6	-	-	-		
81	OHX	1	3593	-	0,6,6	-	-	-		
81	OHX	sR	2172	-	0,6,6	-	-	-		
81	OHX	1	4107	-	0,6,6	-	-	-		
81	OHX	AR	3410	-	0,6,6	-	-	-		
81	OHX	1	3609	-	0,6,6	-	-	-		
81	OHX	sR	1966	-	0,6,6	-	-	-		
81	OHX	sR	1985	-	0,6,6	-	-	-		
81	OHX	AR	3547	-	0,6,6	-	-	-		
81	OHX	sR	2025	-	0,6,6	-	-	-		
81	OHX	1	3543	-	0,6,6	-	-	-		
81	OHX	sR	1967	-	0,6,6	-	-	-		
81	OHX	sR	1910	-	0,6,6	-	-	-		
81	OHX	1	4134	-	0,4,6	-	-	-		
81	OHX	1	3425	-	0,6,6	-	-	-		
81	OHX	AR	4195	-	0,6,6	-	-	-		
81	OHX	AR	3490	-	0,6,6	-	-	-		
81	OHX	AS	3506	-	0,6,6	-	-	-		
81	OHX	AT	210	-	0,6,6	-	-	-		
81	OHX	1	3476	-	0,6,6	-	-	-		
81	OHX	1	3436	-	0,6,6	-	-	-		
81	OHX	AR	3677	-	0,6,6	-	-	-		
81	OHX	1	3402	-	0,6,6	-	-	-		
81	OHX	A	1951	-	0,6,6	-	-	-		
81	OHX	AR	3611	-	0,6,6	-	-	-		
81	OHX	1	4130	-	0,6,6	-	-	-		
81	OHX	AT	212	-	0,6,6	-	-	-		
81	OHX	sR	1946	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OHX	sR	1986	-	0,6,6	-	-	-		
81	OHX	1	3537	-	0,6,6	-	-	-		
81	OHX	AR	3597	-	0,6,6	-	-	-		
81	OHX	1	3509	-	0,6,6	-	-	-		
81	OHX	A	2128	-	0,6,6	-	-	-		
81	OHX	CK	201	-	0,6,6	-	-	-		
81	OHX	1	3544	-	0,6,6	-	-	-		
81	OHX	4	209	-	0,6,6	-	-	-		
81	OHX	sR	2010	-	0,6,6	-	-	-		
81	OHX	AR	3585	-	0,6,6	-	-	-		
81	OHX	AR	4204	-	0,6,6	-	-	-		
81	OHX	sR	2007	-	0,6,6	-	-	-		
81	OHX	sR	2003	-	0,6,6	-	-	-		
81	OHX	AR	3436	-	0,6,6	-	-	-		
81	OHX	sR	2169	-	0,6,6	-	-	-		
81	OHX	AR	3680	-	0,6,6	-	-	-		
81	OHX	A	1955	-	0,6,6	-	-	-		
81	OHX	1	3498	-	0,6,6	-	-	-		
81	OHX	AR	3404	-	0,6,6	-	-	-		
81	OHX	1	3579	-	0,6,6	-	-	-		
81	OHX	AR	3555	-	0,6,6	-	-	-		
81	OHX	sR	1935	-	0,6,6	-	-	-		
81	OHX	sR	1912	-	0,6,6	-	-	-		
81	OHX	1	3563	-	0,6,6	-	-	-		
81	OHX	1	3479	-	0,6,6	-	-	-		
81	OHX	s8	302	-	0,6,6	-	-	-		
81	OHX	AR	3418	-	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
83	SPD	1	4144	-	-	0/7/7/7	-
84	XBI	1	4157	-	-	0/8/60/60	0/3/3/3
83	SPD	AR	4206	-	-	0/7/7/7	-
84	XBI	AR	4222	-	-	2/8/60/60	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	AR	4222	XBI	C1-C10	-2.74	1.52	1.56
84	1	4157	XBI	C5-C10	2.03	1.59	1.56
84	1	4157	XBI	C1-C10	-2.02	1.53	1.56

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	1	4157	XBI	C1-C10-C5	-9.31	106.84	116.76
84	AR	4222	XBI	C1-C10-C5	-7.16	109.14	116.76
84	1	4157	XBI	C21-C1-C2	-4.57	100.89	109.41
84	AR	4222	XBI	C21-C1-C2	-4.17	101.63	109.41
84	1	4157	XBI	C-C1-C21	-4.04	101.99	107.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	AR	4222	XBI	C6-C13-C14-O3
84	AR	4222	XBI	C6-C13-C14-C15

There are no ring outliers.

520 monomers are involved in 722 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	sR	1954	OHX	2	0
81	sR	2000	OHX	1	0
81	A	1907	OHX	2	0
81	1	3604	OHX	1	0
81	AR	4201	OHX	1	0
84	AR	4222	XBI	1	0
81	sR	1976	OHX	1	0
81	sR	1996	OHX	1	0
81	A	1901	OHX	1	0
81	1	3493	OHX	2	0
81	1	3486	OHX	1	0
81	AR	3464	OHX	2	0
81	AR	3473	OHX	1	0
81	sR	1917	OHX	1	0
81	AR	3603	OHX	3	0
81	CX	202	OHX	3	0
81	sR	1969	OHX	2	0
81	1	4117	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	1	4110	OHX	2	0
81	1	3413	OHX	1	0
81	AR	3596	OHX	1	0
81	AR	3524	OHX	1	0
81	1	4088	OHX	1	0
81	1	4101	OHX	1	0
81	1	3508	OHX	1	0
81	AR	3456	OHX	3	0
81	AR	3454	OHX	2	0
81	sR	1977	OHX	2	0
81	1	3446	OHX	1	0
81	sR	1940	OHX	2	0
81	sR	1950[B]	OHX	2	0
81	AR	3588	OHX	2	0
81	1	4089	OHX	1	0
81	AR	3586	OHX	1	0
81	AR	3469	OHX	2	0
81	1	3441	OHX	1	0
81	AR	3527	OHX	1	0
81	sR	1972	OHX	1	0
81	A	1939	OHX	1	0
81	T	201	OHX	0	1
81	A	2120	OHX	1	0
81	AR	3401	OHX	2	0
81	AR	3432	OHX	1	0
81	A	1960	OHX	2	0
81	AR	3602	OHX	1	0
81	1	3567	OHX	2	0
81	sR	1929	OHX	1	0
81	AR	3438	OHX	2	0
81	A	2108	OHX	1	0
81	A	1958	OHX	2	0
81	sR	1907	OHX	1	0
81	1	3577	OHX	1	0
81	1	4076	OHX	3	0
81	AR	3449	OHX	1	0
81	AR	3521	OHX	1	0
81	A	2139	OHX	1	0
81	DK	201	OHX	2	0
81	sR	1994	OHX	1	0
81	1	3601	OHX	1	0
81	1	3437	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	A	1942	OHX	1	0
81	AR	3478[A]	OHX	2	0
81	AR	3516	OHX	1	0
81	AR	4196	OHX	1	0
81	1	3603	OHX	1	0
81	1	4094	OHX	2	0
81	J	301	OHX	1	0
81	1	3404	OHX	3	0
81	AR	3435	OHX	1	0
81	AR	3671	OHX	4	0
81	AR	3610	OHX	1	0
81	1	4071	OHX	1	0
81	AR	3406	OHX	3	0
81	AR	3412	OHX	2	0
81	A	2127	OHX	1	0
81	1	3401	OHX	1	0
81	A	2119	OHX	1	0
81	AR	3644	OHX	1	0
81	1	3602	OHX	1	0
81	1	3438	OHX	1	0
81	AR	3425	OHX	4	0
81	sR	1927	OHX	1	0
81	1	3492	OHX	1	0
81	AR	3616	OHX	1	0
81	4	208	OHX	1	0
81	AR	3622	OHX	1	0
81	AR	3427	OHX	1	0
81	A	2126	OHX	1	0
81	AR	3641	OHX	1	0
81	sR	2018	OHX	1	0
81	1	3565	OHX	1	0
81	sR	1926	OHX	1	0
81	AR	3637	OHX	1	0
81	A	2107	OHX	1	0
81	AR	3552	OHX	1	0
81	sR	1938	OHX	1	0
81	AR	3606	OHX	1	0
81	AR	3550	OHX	1	0
81	AR	3654	OHX	1	0
81	DD	101	OHX	2	0
81	AR	3526	OHX	1	0
81	AP	502	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	AR	3478[B]	OHX	5	0
81	1	3426	OHX	1	0
81	sR	1989	OHX	1	0
81	1	3445	OHX	1	0
81	A	1965	OHX	1	0
81	sR	1915	OHX	1	0
81	1	3482[A]	OHX	1	0
81	sR	2019	OHX	1	0
81	A	1927	OHX	2	0
81	1	3442	OHX	1	0
81	AR	3461	OHX	1	0
81	4	207	OHX	1	0
81	1	3403	OHX	1	0
81	sR	2020	OHX	1	0
81	AR	4197	OHX	1	0
81	1	3616	OHX	1	0
81	1	3457	OHX	1	0
81	1	4098	OHX	2	0
81	AR	3668	OHX	2	0
81	sR	1990	OHX	1	0
81	1	3595	OHX	2	0
81	A	1906	OHX	2	0
81	AR	3684	OHX	1	0
81	1	4116	OHX	1	0
81	AR	3402	OHX	1	0
81	A	1950	OHX	1	0
81	AR	3565	OHX	1	0
81	1	4099	OHX	1	0
81	1	3600	OHX	2	0
81	AR	3520	OHX	1	0
81	AR	3686	OHX	1	0
81	A	1969	OHX	1	0
81	1	4142	OHX	1	0
81	1	3610	OHX	1	0
81	A	2140	OHX	1	0
81	1	3474	OHX	1	0
81	1	3596	OHX	1	0
81	CL	302[B]	OHX	1	0
81	AR	3437	OHX	1	0
81	1	3435	OHX	1	0
81	A	1972	OHX	1	0
81	AR	3507	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	sR	1936	OHX	1	0
81	1	3423	OHX	1	0
81	4	204	OHX	2	0
81	AR	3407	OHX	2	0
81	AR	3551	OHX	1	0
81	A	2114	OHX	1	0
81	A	1908	OHX	2	0
81	A	2110	OHX	1	0
81	AR	3448	OHX	2	0
81	1	4126	OHX	1	0
81	1	3459	OHX	1	0
81	AR	3451	OHX	1	0
81	AR	3506	OHX	1	0
81	1	3613	OHX	1	0
81	AR	3491	OHX	1	0
81	A	2111	OHX	2	0
83	AR	4206	SPD	2	0
81	AR	4202	OHX	2	0
81	1	3552	OHX	1	0
81	s4	301	OHX	1	0
81	1	3606	OHX	1	0
81	A	1916	OHX	1	0
81	A	1922	OHX	1	0
81	sR	2004	OHX	1	0
81	AR	3475	OHX	1	0
81	CL	301	OHX	4	0
81	AS	3505	OHX	2	0
81	1	4114	OHX	1	0
81	1	3494	OHX	1	0
81	1	4143	OHX	1	0
81	1	3558	OHX	1	0
81	AR	3612	OHX	1	0
81	AR	3583	OHX	1	0
81	AR	3485	OHX	1	0
81	AR	4199	OHX	2	0
81	AG	202	OHX	1	0
81	1	4102	OHX	1	0
81	AR	3431	OHX	1	0
81	A	2123	OHX	3	0
81	AR	3503	OHX	1	0
81	AR	3624	OHX	1	0
81	AR	3457	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	AR	3531	OHX	1	0
81	sR	2013	OHX	1	0
81	1	3554	OHX	2	0
81	AR	3416	OHX	1	0
81	1	3599	OHX	1	0
81	3	201	OHX	1	0
81	CG	301	OHX	1	0
81	1	3615	OHX	1	0
81	sR	1931	OHX	2	0
81	1	3506	OHX	1	0
81	1	3518	OHX	1	0
81	AR	3467	OHX	1	0
81	AR	3592	OHX	1	0
81	O	201	OHX	1	0
81	AC	101	OHX	1	0
81	1	3408	OHX	1	0
81	A	1956	OHX	1	0
81	A	2105	OHX	2	0
81	A	2143	OHX	1	0
81	sR	2009	OHX	2	0
81	1	3517	OHX	1	0
81	c3	201	OHX	1	0
81	4	235	OHX	1	0
81	AR	3440	OHX	1	0
81	A	2130	OHX	1	0
81	AR	3549	OHX	1	0
81	AR	3423	OHX	2	0
81	sR	1930	OHX	3	0
81	A	1973	OHX	2	0
81	AR	3426	OHX	2	0
81	AR	3444	OHX	1	0
81	1	3416	OHX	1	0
81	AR	3463	OHX	1	0
81	1	4105	OHX	4	0
81	A	1931	OHX	1	0
81	AR	3554	OHX	3	0
81	AR	3528	OHX	1	0
81	AR	3601	OHX	3	0
81	1	4091	OHX	2	0
81	A	2100	OHX	2	0
81	1	3608[A]	OHX	2	0
81	s1	301	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	sR	1987	OHX	1	0
81	AR	3417	OHX	1	0
81	sR	1971	OHX	1	0
81	sR	1974	OHX	3	0
81	c5	201	OHX	1	0
81	1	3519[A]	OHX	1	0
81	AR	3489	OHX	1	0
81	A	2129	OHX	1	0
81	AR	3648	OHX	3	0
81	AR	3408	OHX	3	0
81	1	3487	OHX	1	0
81	1	4137	OHX	1	0
81	sR	1913	OHX	3	0
81	AR	3529	OHX	1	0
81	AR	3683	OHX	1	0
81	1	3500	OHX	1	0
81	sR	1903	OHX	3	0
81	AR	3496	OHX	1	0
81	1	4120	OHX	3	0
81	AS	3501	OHX	4	0
81	AR	3502	OHX	4	0
81	1	4123	OHX	1	0
81	1	4090	OHX	5	0
81	1	3477	OHX	2	0
81	1	3432	OHX	2	0
81	AR	3636	OHX	2	0
81	A	2125	OHX	3	0
81	sR	2012	OHX	1	0
81	k	402	OHX	2	0
81	1	3412	OHX	1	0
81	AR	3462	OHX	2	0
81	e	102	OHX	1	0
81	1	3485[A]	OHX	1	0
81	DQ	502	OHX	1	0
81	1	4100	OHX	2	0
81	1	3608[B]	OHX	2	0
81	sR	1932	OHX	1	0
81	A	2134	OHX	2	0
81	AR	3562	OHX	1	0
81	1	3451	OHX	1	0
81	AR	3647	OHX	1	0
81	AR	3515	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	AR	3530	OHX	1	0
81	A	2121	OHX	1	0
81	sR	1916[B]	OHX	2	0
81	AR	3664	OHX	2	0
81	1	3503	OHX	1	0
81	AR	3523	OHX	1	0
81	1	3460	OHX	1	0
81	sR	1975	OHX	1	0
81	AR	3433	OHX	1	0
81	d0	201	OHX	1	0
81	sR	1988	OHX	1	0
81	1	4140	OHX	1	0
81	AR	4175	OHX	2	0
81	1	3566	OHX	1	0
81	1	4075	OHX	1	0
81	1	3467[A]	OHX	1	0
81	AR	3662	OHX	1	0
81	A	2116	OHX	2	0
81	AR	3681	OHX	1	0
81	1	4139	OHX	3	0
81	AR	3589	OHX	1	0
81	A	1971	OHX	2	0
81	1	4128	OHX	1	0
81	1	3547	OHX	1	0
81	A	2103	OHX	1	0
81	sR	1901	OHX	1	0
81	AR	3420	OHX	2	0
81	AR	3545	OHX	2	0
81	AR	3553	OHX	1	0
81	AR	3621	OHX	1	0
81	AT	203	OHX	1	0
81	1	4108	OHX	2	0
81	sR	2175	OHX	1	0
81	1	4122	OHX	1	0
81	AR	3618	OHX	1	0
81	AR	4200	OHX	1	0
81	sR	2001	OHX	1	0
81	sR	1950[A]	OHX	2	0
81	AR	3619	OHX	1	0
81	1	4093	OHX	1	0
81	sR	2015	OHX	1	0
81	A	2112	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	AR	3538	OHX	1	0
81	1	3524	OHX	1	0
81	1	3533	OHX	1	0
81	AR	3414	OHX	1	0
81	A	2104	OHX	1	0
81	sR	1948	OHX	1	0
81	l	402	OHX	2	0
81	1	4112	OHX	1	0
81	A	1944	OHX	1	0
81	x	209	OHX	1	0
81	1	3406	OHX	2	0
81	AR	3498	OHX	1	0
81	AR	3568	OHX	2	0
81	AR	3594	OHX	1	0
81	AR	3574	OHX	2	0
81	AR	3495	OHX	1	0
81	1	4103	OHX	1	0
81	1	4106	OHX	2	0
81	A	1967	OHX	1	0
81	A	1910	OHX	2	0
81	sR	1978	OHX	1	0
81	sR	1923	OHX	2	0
81	AR	4179	OHX	1	0
81	AR	3645	OHX	1	0
81	A	2135	OHX	1	0
81	sR	1922	OHX	2	0
81	sR	1933	OHX	1	0
81	1	3545	OHX	1	0
81	AR	3525	OHX	1	0
81	1	3448	OHX	1	0
81	AR	3639	OHX	2	0
81	AR	3534	OHX	1	0
81	sR	1958	OHX	3	0
81	AR	3476	OHX	1	0
81	sR	1949	OHX	1	0
81	AR	3556	OHX	1	0
81	sR	1955	OHX	1	0
81	1	3430	OHX	3	0
81	A	1928	OHX	1	0
81	sR	1951	OHX	1	0
81	A	1933	OHX	1	0
84	1	4157	XBI	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	sR	1957	OHX	1	0
81	3	219	OHX	1	0
81	sR	2008	OHX	1	0
81	1	3418	OHX	1	0
81	1	3529	OHX	1	0
81	A	1946	OHX	1	0
81	AR	3535	OHX	1	0
81	sR	2178	OHX	2	0
81	AR	3687[A]	OHX	1	0
81	1	3452	OHX	1	0
81	AR	3541	OHX	1	0
81	AR	3623	OHX	1	0
81	sR	1979	OHX	1	0
81	AR	3518	OHX	2	0
81	1	3440	OHX	1	0
81	3	204	OHX	1	0
81	AR	3537	OHX	1	0
81	sR	1928	OHX	1	0
81	AR	3434	OHX	1	0
81	1	3409	OHX	2	0
81	1	3581	OHX	1	0
81	AR	3472	OHX	2	0
81	sR	1965	OHX	2	0
81	1	4129	OHX	2	0
81	A	2138	OHX	3	0
81	sR	1906	OHX	1	0
81	AT	201	OHX	1	0
81	1	3527	OHX	1	0
81	1	4097	OHX	2	0
81	1	3499	OHX	1	0
81	1	3447	OHX	2	0
81	AR	3539	OHX	4	0
81	DL	102	OHX	2	0
81	1	3534	OHX	1	0
81	1	3427	OHX	1	0
81	AR	3508	OHX	2	0
81	AR	3492	OHX	1	0
81	AR	3580	OHX	2	0
81	z	203	OHX	1	0
81	1	3553	OHX	1	0
81	A	1929	OHX	1	0
81	1	3439	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	AR	3646	OHX	1	0
81	A	1937	OHX	1	0
81	sR	2014	OHX	1	0
81	4	215	OHX	1	0
81	sR	2005	OHX	1	0
81	1	3582	OHX	1	0
81	1	3562	OHX	2	0
81	AR	3474	OHX	1	0
81	AR	3667	OHX	3	0
81	AT	202	OHX	1	0
81	1	4127	OHX	1	0
81	1	3455	OHX	2	0
81	1	3468	OHX	1	0
81	AR	3411	OHX	1	0
81	AR	3452	OHX	2	0
81	AR	3511[B]	OHX	1	0
81	AR	3656	OHX	2	0
81	AR	3634	OHX	1	0
81	A	1961	OHX	1	0
81	AK	103	OHX	2	0
81	1	3516	OHX	1	0
81	1	4113	OHX	3	0
81	1	4095	OHX	3	0
81	CG	302	OHX	1	0
81	1	4135	OHX	1	0
81	AR	3687[B]	OHX	1	0
81	1	3598	OHX	1	0
81	sR	1964	OHX	2	0
81	1	4132	OHX	1	0
81	A	1949	OHX	1	0
81	sR	2022	OHX	4	0
81	1	3536	OHX	1	0
81	v	301	OHX	2	0
81	1	3557	OHX	1	0
81	1	3511	OHX	1	0
81	AR	3579	OHX	2	0
81	CE	403	OHX	1	0
81	sR	1980	OHX	1	0
81	AR	3505	OHX	1	0
81	AR	3419	OHX	2	0
81	AR	3514	OHX	2	0
81	AR	3598	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	1	3420	OHX	1	0
81	A	1947	OHX	1	0
81	A	2132	OHX	3	0
81	AR	3609	OHX	1	0
81	A	2131	OHX	1	0
81	A	2137	OHX	2	0
81	AR	3675	OHX	1	0
81	sR	1934	OHX	2	0
81	1	3590	OHX	1	0
81	1	3504	OHX	2	0
81	1	3587	OHX	2	0
81	A	1909	OHX	1	0
81	AR	3455	OHX	1	0
81	1	3501	OHX	1	0
81	AR	3630	OHX	1	0
81	1	3502	OHX	1	0
81	CS	201	OHX	1	0
81	1	3433	OHX	1	0
81	A	1917	OHX	1	0
81	A	2124	OHX	2	0
81	sR	1995	OHX	3	0
81	1	3605	OHX	2	0
81	A	1970	OHX	1	0
81	sR	1920	OHX	1	0
81	AR	3483	OHX	2	0
81	sR	1959	OHX	1	0
81	1	3434	OHX	1	0
81	sR	1924	OHX	1	0
81	AR	3486	OHX	1	0
81	AR	3688	OHX	1	0
81	sR	2002	OHX	1	0
81	sR	1960	OHX	1	0
81	1	3612	OHX	3	0
81	AR	3559	OHX	2	0
81	AR	3546	OHX	1	0
83	1	4144	SPD	3	0
81	AR	4205	OHX	1	0
81	1	4092	OHX	1	0
81	AR	3633	OHX	1	0
81	sR	1981	OHX	1	0
81	AR	3676	OHX	1	0
81	AR	3446	OHX	2	0

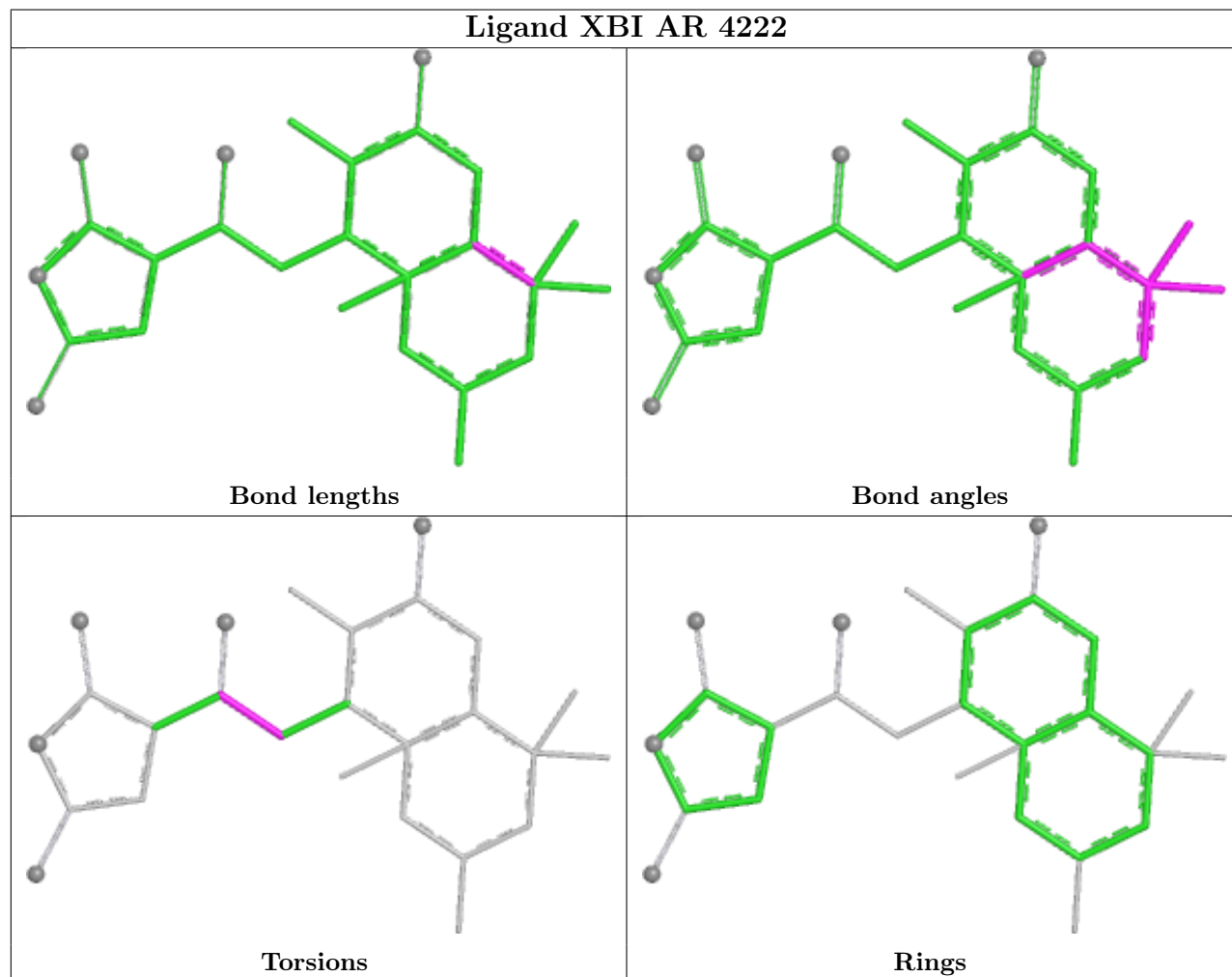
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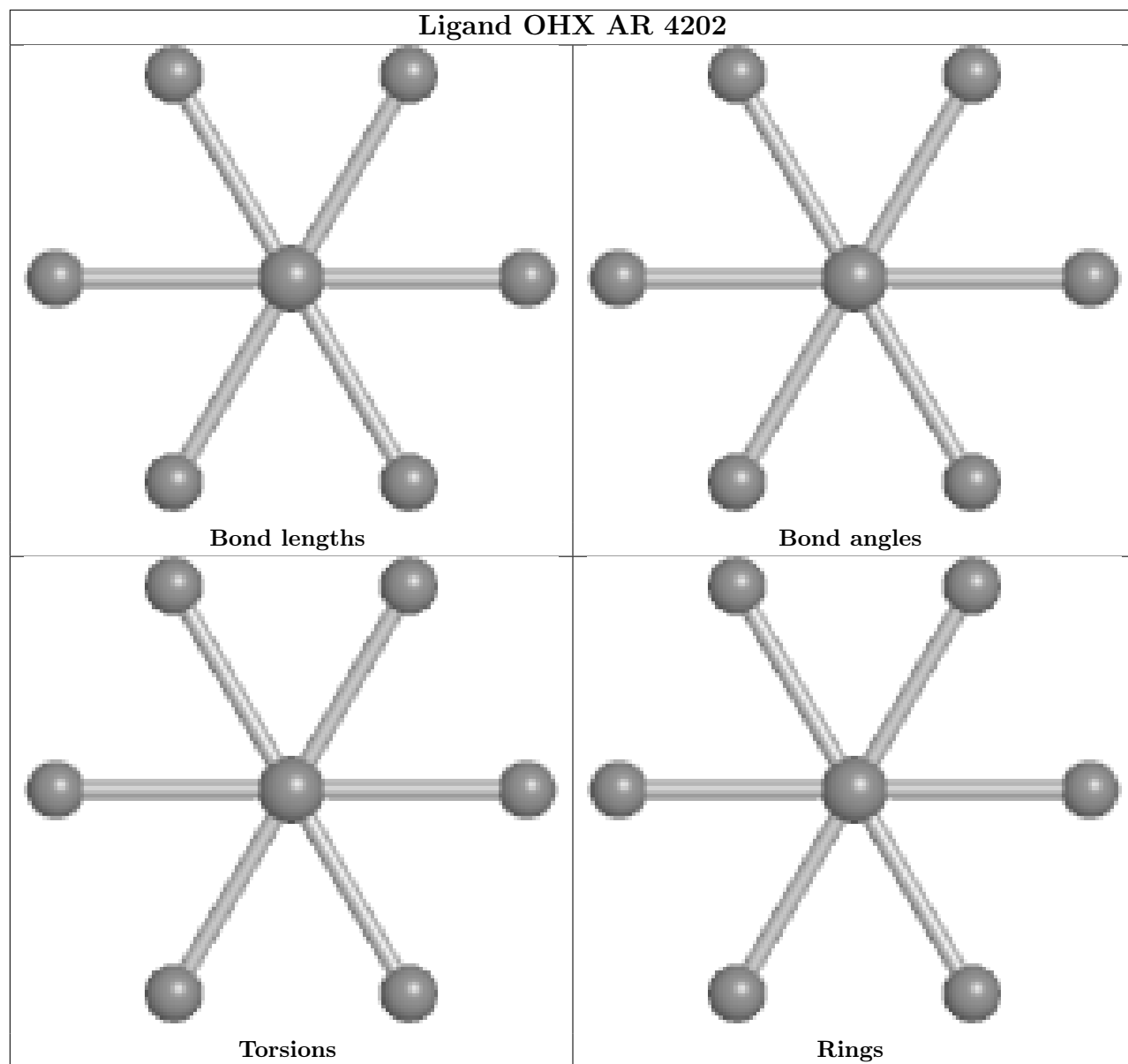
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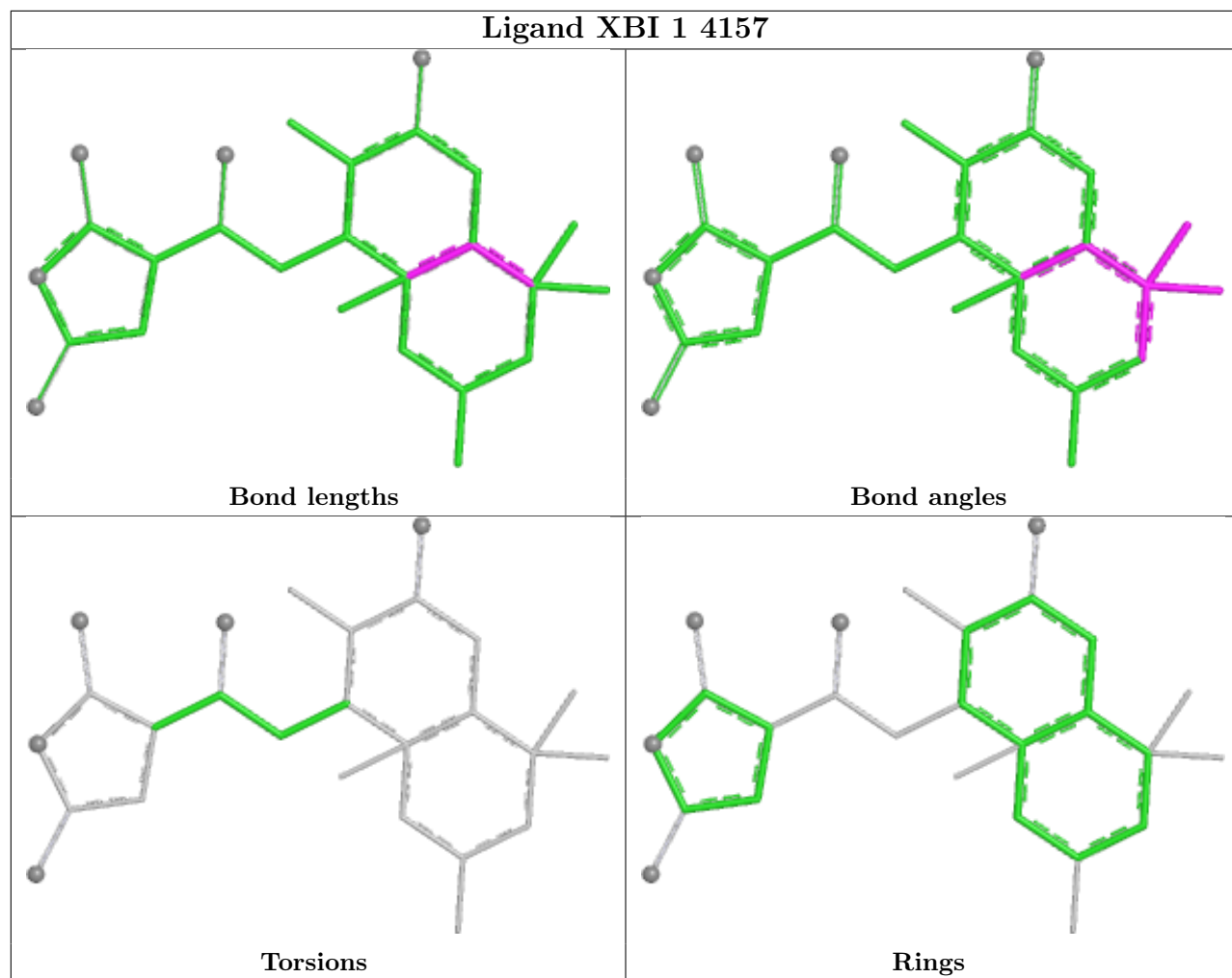
Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	AR	3428	OHX	1	0
81	A	2117	OHX	1	0
81	1	3470	OHX	1	0
81	1	4068	OHX	2	0
81	AR	3604	OHX	1	0
81	AR	3519	OHX	1	0
81	A	1918	OHX	1	0
81	A	2106	OHX	1	0
81	1	3539	OHX	1	0
81	1	3419	OHX	1	0
81	A	1930	OHX	1	0
81	1	4107	OHX	2	0
81	AR	3410	OHX	2	0
81	1	3609	OHX	1	0
81	AR	3547	OHX	1	0
81	sR	2025	OHX	2	0
81	1	3543	OHX	1	0
81	sR	1967	OHX	1	0
81	sR	1910	OHX	2	0
81	1	4134	OHX	1	0
81	AS	3506	OHX	1	0
81	AR	3677	OHX	1	0
81	A	1951	OHX	1	0
81	1	4130	OHX	1	0
81	AT	212	OHX	1	0
81	sR	1946	OHX	1	0
81	sR	1986	OHX	1	0
81	1	3537	OHX	1	0
81	1	3509	OHX	1	0
81	CK	201	OHX	1	1
81	1	3544	OHX	1	0
81	sR	2007	OHX	3	0
81	AR	3436	OHX	1	0
81	sR	2169	OHX	1	0
81	AR	3404	OHX	1	0
81	AR	3555	OHX	1	0
81	sR	1935	OHX	1	0
81	sR	1912	OHX	1	0
81	s8	302	OHX	1	0
81	AR	3418	OHX	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	3
1	AR	1
58	c0	1
47	A	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1955:U	O3'	2093:A	P	26.04
1	AR	1955:U	O3'	2093:A	P	23.44
1	1	2445:A	O3'	2501:U	P	15.18
1	1	440:A	O3'	494:G	P	12.11
1	c0	84:GLU	C	87:HIS	N	8.58

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	3149/3149 (100%)	-0.01	35 (1%) 78 71	42, 64, 172, 261	0
1	AR	3130/3149 (99%)	-0.01	46 (1%) 72 64	42, 61, 152, 267	0
2	3	121/121 (100%)	-0.27	0 100 100	48, 75, 93, 135	0
2	AS	121/121 (100%)	-0.21	2 (1%) 69 61	46, 63, 79, 140	0
3	4	158/158 (100%)	-0.11	0 100 100	49, 65, 122, 208	0
3	AT	158/158 (100%)	-0.01	4 (2%) 58 48	50, 69, 137, 200	0
4	CD	252/254 (99%)	0.79	22 (8%) 16 13	43, 65, 89, 158	0
4	j	252/254 (99%)	0.77	19 (7%) 20 16	44, 65, 88, 138	0
5	CE	386/387 (99%)	0.40	12 (3%) 51 42	42, 56, 82, 140	0
5	k	386/387 (99%)	0.63	21 (5%) 31 24	45, 65, 93, 152	0
6	CF	361/362 (99%)	0.53	13 (3%) 46 38	41, 64, 92, 129	0
6	l	361/362 (99%)	0.56	27 (7%) 20 16	42, 61, 94, 143	0
7	CG	292/297 (98%)	0.52	19 (6%) 25 20	50, 69, 111, 165	0
7	m	296/297 (99%)	0.68	22 (7%) 20 17	55, 83, 133, 174	0
8	CH	156/176 (88%)	0.60	12 (7%) 19 16	48, 66, 103, 152	0
8	n	156/176 (88%)	0.40	2 (1%) 75 67	48, 64, 99, 136	0
9	CI	222/244 (90%)	0.40	6 (2%) 56 47	45, 56, 100, 175	0
9	o	222/244 (90%)	0.37	10 (4%) 38 30	46, 58, 103, 167	0
10	CJ	226/256 (88%)	1.23	42 (18%) 3 3	66, 95, 135, 157	0
10	p	233/256 (91%)	0.80	13 (5%) 30 23	59, 85, 144, 180	0
11	CK	191/191 (100%)	0.37	7 (3%) 45 37	48, 63, 97, 172	0
11	q	191/191 (100%)	0.69	16 (8%) 17 14	52, 75, 108, 169	0
12	CL	211/221 (95%)	0.74	20 (9%) 14 11	45, 67, 104, 151	0
12	r	211/221 (95%)	0.67	18 (8%) 16 14	47, 66, 119, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CM	169/174 (97%)	0.71	13 (7%) 19 16	52, 73, 102, 134	0
13	s	169/174 (97%)	0.72	10 (5%) 28 22	64, 88, 116, 159	0
14	CN	193/199 (96%)	0.74	17 (8%) 15 13	44, 74, 128, 176	0
14	t	193/199 (96%)	0.64	18 (9%) 14 12	44, 70, 120, 170	0
15	CO	136/138 (98%)	0.50	12 (8%) 15 13	49, 62, 93, 136	0
15	u	136/138 (98%)	0.46	8 (5%) 28 22	51, 67, 97, 143	0
16	CP	203/204 (99%)	0.87	15 (7%) 20 17	44, 68, 86, 99	0
16	v	203/204 (99%)	0.64	6 (2%) 52 43	43, 62, 78, 94	0
17	CQ	197/199 (98%)	0.37	11 (5%) 30 23	42, 51, 91, 145	0
17	w	197/199 (98%)	0.38	7 (3%) 46 38	45, 57, 88, 129	0
18	CR	155/184 (84%)	0.34	4 (2%) 57 48	42, 56, 75, 147	0
18	x	183/184 (99%)	0.53	12 (6%) 24 19	44, 59, 139, 174	0
19	CS	185/186 (99%)	0.40	6 (3%) 50 41	46, 64, 85, 105	0
19	y	185/186 (99%)	0.67	19 (10%) 12 10	46, 60, 77, 107	0
20	CT	188/189 (99%)	0.87	25 (13%) 7 6	51, 76, 151, 201	0
20	z	177/189 (93%)	0.81	14 (7%) 18 15	59, 80, 137, 166	0
21	0	172/172 (100%)	0.51	12 (6%) 22 18	49, 63, 94, 160	0
21	CU	172/172 (100%)	0.28	4 (2%) 61 52	46, 58, 84, 124	0
22	2	159/160 (99%)	0.94	21 (13%) 7 6	46, 65, 114, 157	0
22	CV	159/160 (99%)	0.77	19 (11%) 9 7	45, 59, 113, 181	0
23	5	100/121 (82%)	0.98	10 (10%) 12 10	82, 114, 148, 169	0
23	CW	100/121 (82%)	1.15	20 (20%) 3 2	76, 103, 152, 166	0
24	6	136/137 (99%)	0.80	15 (11%) 10 9	46, 65, 101, 133	0
24	CX	136/137 (99%)	0.53	9 (6%) 24 19	43, 56, 89, 145	0
25	7	65/155 (41%)	0.82	8 (12%) 8 7	58, 71, 99, 156	0
25	CY	111/155 (71%)	0.83	10 (9%) 15 13	48, 77, 130, 146	0
26	8	121/142 (85%)	0.67	13 (10%) 11 9	56, 75, 108, 147	0
26	CZ	117/142 (82%)	0.70	9 (7%) 19 16	55, 79, 104, 131	0
27	9	126/127 (99%)	0.49	3 (2%) 59 50	47, 68, 96, 124	0
27	DA	124/127 (97%)	0.69	8 (6%) 25 20	48, 72, 97, 150	0
28	AA	135/136 (99%)	0.76	9 (6%) 24 19	77, 100, 132, 176	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	DB	135/136 (99%)	1.10	13 (9%)	13 11	76, 107, 148, 162	0
29	AB	148/149 (99%)	0.59	7 (4%)	36 28	42, 61, 93, 134	0
29	DC	148/149 (99%)	0.50	8 (5%)	31 24	42, 62, 95, 133	0
30	AC	58/59 (98%)	0.73	7 (12%)	8 7	45, 69, 128, 143	0
30	DD	58/59 (98%)	0.82	10 (17%)	4 3	44, 66, 110, 141	0
31	AD	97/105 (92%)	0.54	3 (3%)	51 42	73, 98, 134, 147	0
31	DE	97/105 (92%)	0.78	6 (6%)	26 21	74, 95, 132, 156	0
32	AE	109/113 (96%)	1.00	15 (13%)	6 5	54, 78, 137, 166	0
32	DF	109/113 (96%)	0.52	4 (3%)	45 37	48, 66, 144, 175	0
33	AF	127/130 (97%)	0.50	5 (3%)	43 35	43, 54, 74, 140	0
33	DG	127/130 (97%)	0.40	5 (3%)	43 35	42, 57, 82, 125	0
34	AG	106/107 (99%)	0.36	4 (3%)	44 36	45, 55, 73, 89	0
34	DH	106/107 (99%)	0.53	8 (7%)	20 16	44, 54, 82, 124	0
35	AH	111/121 (91%)	1.05	14 (12%)	8 6	53, 79, 123, 171	0
35	DI	112/121 (92%)	1.18	26 (23%)	2 2	54, 78, 140, 163	0
36	AI	119/120 (99%)	0.71	9 (7%)	20 16	51, 75, 99, 126	0
36	DJ	119/120 (99%)	0.74	5 (4%)	40 32	59, 81, 109, 126	0
37	AJ	96/100 (96%)	0.74	5 (5%)	33 26	59, 77, 112, 127	0
37	DK	99/100 (99%)	1.08	13 (13%)	7 6	67, 85, 141, 167	0
38	AK	87/88 (98%)	0.59	7 (8%)	18 15	44, 57, 76, 153	0
38	DL	86/88 (97%)	0.58	4 (4%)	36 28	44, 59, 93, 117	0
39	AL	77/78 (98%)	0.89	5 (6%)	25 20	68, 104, 135, 159	0
39	DM	77/78 (98%)	0.95	8 (10%)	11 10	73, 102, 142, 150	0
40	AM	50/51 (98%)	0.94	9 (18%)	3 3	46, 66, 81, 101	0
40	DN	50/51 (98%)	0.78	5 (10%)	12 10	49, 67, 84, 93	0
41	AN	52/128 (40%)	0.48	4 (7%)	19 16	52, 68, 98, 136	0
41	DO	52/128 (40%)	0.28	3 (5%)	29 22	45, 55, 82, 113	0
42	AO	25/25 (100%)	1.15	3 (12%)	9 7	58, 72, 87, 96	0
42	DP	25/25 (100%)	1.05	6 (24%)	2 1	52, 65, 82, 99	0
43	AP	105/106 (99%)	0.74	15 (14%)	6 5	44, 65, 105, 154	0
43	DQ	105/106 (99%)	0.63	10 (9%)	14 11	45, 64, 99, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AQ	91/92 (98%)	0.72	5 (5%) 30 24	51, 72, 104, 130	0
44	DR	91/92 (98%)	0.69	9 (9%) 13 11	45, 71, 101, 128	0
45	i	142/273 (52%)	1.52	43 (30%) 1 1	54, 108, 165, 189	0
45	sM	63/273 (23%)	1.21	10 (15%) 5 4	49, 113, 154, 172	0
46	p0	126/312 (40%)	1.26	30 (23%) 2 2	83, 121, 151, 164	0
47	A	1741/1800 (96%)	0.25	39 (2%) 62 53	60, 94, 198, 266	0
47	sR	1783/1800 (99%)	0.19	44 (2%) 58 48	48, 86, 204, 258	0
48	B	206/252 (81%)	1.41	53 (25%) 1 1	94, 123, 157, 175	0
48	s0	206/252 (81%)	1.07	28 (13%) 7 5	71, 104, 140, 166	0
49	C	214/255 (83%)	1.41	50 (23%) 2 2	88, 139, 176, 208	0
49	s1	216/255 (84%)	0.69	16 (7%) 20 17	62, 92, 127, 173	0
50	D	217/254 (85%)	1.18	35 (16%) 4 4	74, 100, 139, 161	0
50	s2	217/254 (85%)	1.15	34 (15%) 5 4	60, 86, 125, 150	0
51	E	223/240 (92%)	1.10	37 (16%) 4 3	76, 105, 151, 190	0
51	s3	223/240 (92%)	1.34	48 (21%) 2 2	79, 118, 157, 179	0
52	F	260/261 (99%)	1.24	47 (18%) 3 3	71, 99, 135, 156	0
52	s4	260/261 (99%)	0.92	22 (8%) 16 14	59, 86, 117, 165	0
53	G	206/225 (91%)	1.19	37 (17%) 3 3	85, 127, 162, 184	0
53	s5	198/225 (88%)	1.45	47 (23%) 2 2	79, 117, 155, 187	0
54	H	226/236 (95%)	1.70	73 (32%) 1 1	62, 106, 150, 167	0
54	s6	218/236 (92%)	1.16	42 (19%) 3 2	59, 89, 132, 167	0
55	I	184/190 (96%)	1.11	21 (11%) 10 8	81, 127, 165, 181	0
55	s7	186/190 (97%)	1.23	28 (15%) 5 4	67, 115, 162, 187	0
56	J	188/200 (94%)	1.06	26 (13%) 6 5	61, 85, 125, 161	0
56	s8	188/200 (94%)	1.47	46 (24%) 2 1	54, 82, 137, 160	0
57	K	185/197 (93%)	1.21	34 (18%) 3 3	76, 107, 162, 208	0
57	s9	185/197 (93%)	1.05	28 (15%) 5 4	63, 90, 137, 169	0
58	L	96/105 (91%)	1.48	32 (33%) 1 1	75, 117, 166, 171	0
58	c0	96/105 (91%)	1.64	34 (35%) 1 1	100, 135, 173, 187	0
59	M	142/156 (91%)	0.86	15 (10%) 11 9	62, 82, 122, 162	0
59	c1	146/156 (93%)	1.06	21 (14%) 6 5	53, 79, 143, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
60	N	124/143 (86%)	1.32	28 (22%)	2	2	117, 157, 185, 202	0
61	O	150/151 (99%)	0.88	13 (8%)	16	13	64, 102, 130, 150	0
61	c3	150/151 (99%)	0.68	7 (4%)	36	28	59, 88, 115, 143	0
62	P	127/138 (92%)	1.60	29 (22%)	2	2	68, 135, 165, 189	0
62	c4	127/138 (92%)	0.99	17 (13%)	7	5	58, 96, 127, 165	0
63	Q	124/142 (87%)	1.36	30 (24%)	2	1	78, 102, 158, 195	0
63	c5	135/142 (95%)	1.41	32 (23%)	2	2	84, 116, 163, 181	0
64	R	141/143 (98%)	1.54	41 (29%)	1	1	80, 113, 139, 169	0
64	c6	142/143 (99%)	1.82	43 (30%)	1	1	66, 112, 155, 176	0
65	S	120/136 (88%)	1.28	25 (20%)	2	2	77, 124, 162, 183	0
65	c7	117/136 (86%)	1.09	18 (15%)	5	4	74, 110, 153, 198	0
66	T	145/146 (99%)	0.99	19 (13%)	7	6	67, 113, 158, 173	0
66	c8	145/146 (99%)	1.11	23 (15%)	5	4	79, 110, 154, 173	0
67	U	143/144 (99%)	1.50	40 (27%)	1	1	80, 114, 147, 173	0
67	c9	143/144 (99%)	0.91	13 (9%)	15	12	72, 105, 138, 181	0
68	V	96/121 (79%)	2.15	45 (46%)	0	0	71, 116, 155, 164	0
68	d0	89/121 (73%)	1.57	26 (29%)	1	1	67, 116, 163, 173	0
69	W	87/87 (100%)	1.12	13 (14%)	5	4	83, 113, 146, 175	0
69	d1	87/87 (100%)	1.01	9 (10%)	12	10	66, 93, 123, 155	0
70	X	129/130 (99%)	1.00	17 (13%)	7	6	71, 96, 116, 132	0
70	d2	129/130 (99%)	0.85	6 (4%)	36	28	56, 76, 94, 109	0
71	Y	144/145 (99%)	1.30	29 (20%)	3	2	60, 80, 115, 143	0
71	d3	144/145 (99%)	0.98	20 (13%)	6	5	51, 68, 89, 135	0
72	Z	134/135 (99%)	1.11	20 (14%)	5	4	69, 113, 151, 174	0
72	d4	134/135 (99%)	1.02	22 (16%)	4	3	62, 93, 135, 177	0
73	a	70/108 (64%)	1.24	12 (17%)	4	3	106, 141, 171, 181	0
73	d5	69/108 (63%)	1.21	8 (11%)	9	8	96, 133, 168, 187	0
74	b	97/119 (81%)	1.41	21 (21%)	2	2	78, 108, 171, 186	0
74	d6	97/119 (81%)	0.91	15 (15%)	5	4	54, 76, 134, 150	0
75	c	81/82 (98%)	1.05	11 (13%)	7	5	81, 114, 161, 183	0
75	d7	81/82 (98%)	0.83	7 (8%)	16	13	59, 96, 159, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	d	63/67 (94%)	1.20	6 (9%) 14 11	89, 140, 163, 180	0
76	d8	63/67 (94%)	1.53	15 (23%) 2 2	98, 133, 167, 192	0
77	d9	53/56 (94%)	1.39	12 (22%) 2 2	78, 93, 137, 161	0
77	e	53/56 (94%)	0.93	6 (11%) 10 9	71, 90, 110, 163	0
78	e0	62/63 (98%)	1.09	9 (14%) 6 4	60, 97, 155, 171	0
78	f	60/63 (95%)	1.01	8 (13%) 7 6	67, 112, 157, 176	0
79	e1	51/152 (33%)	1.96	23 (45%) 0 0	121, 163, 186, 196	0
79	g	71/152 (46%)	1.44	19 (26%) 1 1	97, 150, 181, 218	0
80	Rb	318/319 (99%)	1.33	75 (23%) 2 2	91, 134, 165, 194	0
80	h	318/319 (99%)	1.44	75 (23%) 2 2	84, 123, 162, 199	0
All	All	32652/34933 (93%)	0.64	2942 (9%) 15 13	41, 80, 154, 267	0

The worst 5 of 2942 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	r	112	GLN	9.2
64	c6	141	SER	8.9
45	i	88	ARG	8.7
50	s2	92	ALA	8.5
54	H	79	LYS	8.5

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
82	MG	A	2086	1/1	0.26	0.27	128,128,128,128	0
82	MG	sR	2131	1/1	0.40	0.26	90,90,90,90	0
82	MG	1	3962	1/1	0.45	0.26	107,107,107,107	0
82	MG	A	2020	1/1	0.45	0.25	104,104,104,104	0
82	MG	1	4016	1/1	0.48	0.27	89,89,89,89	0
82	MG	A	2051	1/1	0.48	0.27	97,97,97,97	0
82	MG	A	2072	1/1	0.49	0.39	109,109,109,109	0
82	MG	1	3683	1/1	0.50	0.37	79,79,79,79	0
82	MG	AR	3768	1/1	0.51	0.64	104,104,104,104	0
81	OHX	1	3582	7/7	0.51	0.24	260,263,270,343	0
82	MG	1	4057	1/1	0.52	0.30	89,89,89,89	0
81	OHX	4	214	7/7	0.53	0.17	208,216,218,304	0
82	MG	AR	4034	1/1	0.55	0.15	117,117,117,117	0
82	MG	A	2036	1/1	0.55	0.36	85,85,85,85	0
82	MG	AS	3525	1/1	0.56	0.21	87,87,87,87	0
82	MG	A	2085	1/1	0.58	0.19	102,102,102,102	0
82	MG	AR	4115	1/1	0.58	0.12	86,86,86,86	0
82	MG	1	4015	1/1	0.58	0.36	87,87,87,87	0
82	MG	AR	3715	1/1	0.59	0.34	93,93,93,93	0
82	MG	AR	3994	1/1	0.60	0.13	85,85,85,85	0
82	MG	sR	2161	1/1	0.61	0.33	87,87,87,87	0
82	MG	sR	2121	1/1	0.62	0.26	98,98,98,98	0
81	OHX	AR	4195	7/7	0.62	0.16	253,261,266,349	0
82	MG	A	2076	1/1	0.62	0.19	91,91,91,91	0
82	MG	1	3973	1/1	0.63	0.20	79,79,79,79	0
82	MG	1	4070	1/1	0.63	0.35	91,91,91,91	0
81	OHX	AR	3634	7/7	0.63	0.18	237,250,262,351	0
81	OHX	1	4133	7/7	0.63	0.16	232,246,250,329	0
82	MG	A	2008	1/1	0.63	0.37	102,102,102,102	0
81	OHX	4	202	7/7	0.64	0.17	225,236,247,324	0
82	MG	AR	3755	1/1	0.64	0.39	88,88,88,88	0
82	MG	d4	202	1/1	0.64	0.20	92,92,92,92	0
82	MG	A	2087	1/1	0.65	0.24	100,100,100,100	0
82	MG	1	3948	1/1	0.66	0.23	79,79,79,79	0
82	MG	sR	2119	1/1	0.66	0.17	97,97,97,97	0
81	OHX	AR	3630	7/7	0.66	0.23	176,186,198,288	0
82	MG	AR	3922	1/1	0.66	0.35	82,82,82,82	0
81	OHX	1	3602	7/7	0.66	0.20	265,272,280,365	0
82	MG	1	3764	1/1	0.66	0.40	102,102,102,102	0
82	MG	1	3711	1/1	0.67	0.32	81,81,81,81	0
82	MG	AR	3960	1/1	0.67	0.19	83,83,83,83	0
81	OHX	sR	1986	7/7	0.67	0.16	201,206,214,287	0
82	MG	A	2045	1/1	0.67	0.29	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
82	MG	AR	3740	1/1	0.67	0.39	64,64,64,64	0
82	MG	A	2063	1/1	0.67	0.28	72,72,72,72	0
81	OHX	sR	2023	7/7	0.67	0.17	216,226,238,304	0
81	OHX	AR	3681	7/7	0.67	0.17	203,212,225,308	0
82	MG	AR	4020	1/1	0.68	0.26	79,79,79,79	0
82	MG	AR	3769	1/1	0.68	0.40	85,85,85,85	0
82	MG	AR	4051	1/1	0.68	0.16	96,96,96,96	0
82	MG	1	3949	1/1	0.68	0.38	78,78,78,78	0
82	MG	sR	2104	1/1	0.68	0.17	84,84,84,84	0
81	OHX	sR	2169	7/7	0.69	0.16	183,189,200,280	0
82	MG	1	3736	1/1	0.69	0.32	63,63,63,63	0
81	OHX	1	3501	7/7	0.69	0.18	159,167,177,262	0
82	MG	sR	2150	1/1	0.69	0.18	73,73,73,73	0
82	MG	b	202	1/1	0.69	0.23	87,87,87,87	0
82	MG	A	2001	1/1	0.69	0.46	71,71,71,71	0
81	OHX	1	3611	7/7	0.70	0.17	218,226,239,311	0
81	OHX	sR	2168	7/7	0.70	0.17	228,237,241,321	0
81	OHX	AR	3638	7/7	0.70	0.22	163,176,191,270	0
82	MG	AR	4112	1/1	0.70	0.30	79,79,79,79	0
82	MG	1	3860	1/1	0.70	0.31	65,65,65,65	0
82	MG	AR	3971	1/1	0.70	0.38	84,84,84,84	0
81	OHX	AR	3674	7/7	0.70	0.19	210,218,232,310	0
82	MG	AR	4013	1/1	0.70	0.42	82,82,82,82	0
82	MG	c6	202	1/1	0.70	0.27	94,94,94,94	0
82	MG	A	2012	1/1	0.70	0.29	68,68,68,68	0
81	OHX	1	3613	7/7	0.71	0.15	192,202,210,278	0
82	MG	AR	3919	1/1	0.71	0.29	84,84,84,84	0
81	OHX	1	3598	7/7	0.71	0.16	206,211,229,307	0
82	MG	1	4151	1/1	0.71	0.39	89,89,89,89	0
82	MG	AR	3962	1/1	0.71	0.36	92,92,92,92	0
82	MG	sR	2147	1/1	0.71	0.30	81,81,81,81	0
81	OHX	1	3555	7/7	0.71	0.18	193,201,210,295	0
81	OHX	sR	2001	7/7	0.71	0.18	182,189,199,265	0
82	MG	s9	201	1/1	0.71	0.41	79,79,79,79	0
81	OHX	AR	3673	7/7	0.71	0.13	211,212,225,296	0
81	OHX	1	3552	7/7	0.71	0.23	170,177,189,266	0
81	OHX	AR	3663	7/7	0.72	0.14	210,217,230,302	0
82	MG	AR	3942	1/1	0.72	0.14	76,76,76,76	0
82	MG	1	4006	1/1	0.72	0.38	93,93,93,93	0
81	OHX	1	3615	7/7	0.72	0.19	228,238,250,339	0
82	MG	6	202	1/1	0.72	0.32	96,96,96,96	0
82	MG	A	2027	1/1	0.72	0.21	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	AR	3653	7/7	0.72	0.17	227,234,240,302	0
82	MG	A	2095	1/1	0.72	0.32	76,76,76,76	0
82	MG	AR	4140	1/1	0.72	0.19	50,50,50,50	0
82	MG	sR	2042	1/1	0.72	0.37	80,80,80,80	0
82	MG	sR	2114	1/1	0.73	0.19	63,63,63,63	0
82	MG	4	228	1/1	0.73	0.16	67,67,67,67	0
81	OHX	1	3584	7/7	0.73	0.15	184,203,208,281	0
81	OHX	AR	3683	7/7	0.73	0.20	209,223,235,333	0
82	MG	1	4017	1/1	0.73	0.32	77,77,77,77	0
81	OHX	x	209	7/7	0.73	0.12	218,231,243,322	0
82	MG	AR	3764	1/1	0.73	0.27	80,80,80,80	0
81	OHX	1	3599	7/7	0.73	0.18	205,206,217,309	0
82	MG	A	2062	1/1	0.73	0.11	82,82,82,82	0
82	MG	1	3626	1/1	0.73	0.24	70,70,70,70	0
82	MG	AR	4022	1/1	0.74	0.17	74,74,74,74	0
82	MG	1	3754	1/1	0.74	0.30	64,64,64,64	0
82	MG	AR	4050	1/1	0.74	0.33	72,72,72,72	0
82	MG	AR	3772	1/1	0.74	0.14	70,70,70,70	0
82	MG	AR	3836	1/1	0.74	0.16	63,63,63,63	0
82	MG	AR	3864	1/1	0.74	0.25	58,58,58,58	0
81	OHX	1	3610	7/7	0.74	0.13	253,257,270,345	0
82	MG	AR	4161	1/1	0.74	0.30	67,67,67,67	0
82	MG	AS	3517	1/1	0.74	0.18	79,79,79,79	0
82	MG	t	202	1/1	0.74	0.25	86,86,86,86	0
82	MG	CO	201	1/1	0.74	0.20	67,67,67,67	0
82	MG	A	1998	1/1	0.74	0.31	74,74,74,74	0
82	MG	1	3814	1/1	0.74	0.29	80,80,80,80	0
81	OHX	1	3601	7/7	0.74	0.22	156,165,176,261	0
81	OHX	AR	3661	7/7	0.74	0.18	189,196,210,290	0
82	MG	sR	2145	1/1	0.74	0.14	99,99,99,99	0
82	MG	AR	3748	1/1	0.74	0.31	63,63,63,63	0
82	MG	1	4051	1/1	0.74	0.27	85,85,85,85	0
82	MG	AR	4010	1/1	0.74	0.31	57,57,57,57	0
82	MG	A	2039	1/1	0.74	0.13	92,92,92,92	0
81	OHX	sR	2026	7/7	0.74	0.16	211,218,223,298	0
81	OHX	AT	215	7/7	0.74	0.15	189,196,203,292	0
82	MG	AR	3886	1/1	0.75	0.20	75,75,75,75	0
81	OHX	sR	1999	7/7	0.75	0.19	188,194,204,274	0
82	MG	1	3872	1/1	0.75	0.22	66,66,66,66	0
82	MG	1	3628	1/1	0.75	0.30	68,68,68,68	0
82	MG	AR	4104	1/1	0.75	0.28	88,88,88,88	0
82	MG	AR	3952	1/1	0.75	0.48	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	OHX	3	222	7/7	0.75	0.12	222,231,235,310	0
82	MG	AR	4129	1/1	0.75	0.18	77,77,77,77	0
82	MG	A	2047	1/1	0.75	0.31	91,91,91,91	0
81	OHX	AR	4197	7/7	0.75	0.11	227,239,243,309	0
81	OHX	AS	3510	7/7	0.75	0.19	192,197,211,275	0
81	OHX	1	3569	7/7	0.75	0.16	178,185,195,273	0
82	MG	AS	3519	1/1	0.75	0.28	73,73,73,73	0
82	MG	s8	301	1/1	0.75	0.55	117,117,117,117	0
82	MG	AR	3786	1/1	0.75	0.30	66,66,66,66	0
81	OHX	AR	3684	7/7	0.75	0.12	203,215,220,304	0
81	OHX	sR	2177	7/7	0.75	0.12	208,210,216,292	0
82	MG	sR	2098	1/1	0.76	0.12	73,73,73,73	0
81	OHX	sR	2020	7/7	0.76	0.14	198,206,212,285	0
82	MG	AR	3923	1/1	0.76	0.26	85,85,85,85	0
82	MG	AT	205	1/1	0.76	0.41	68,68,68,68	0
81	OHX	AR	3640	7/7	0.76	0.17	198,204,219,298	0
82	MG	sR	2124	1/1	0.76	0.40	82,82,82,82	0
82	MG	1	3992	1/1	0.76	0.50	102,102,102,102	0
82	MG	1	3841	1/1	0.76	0.25	76,76,76,76	0
82	MG	1	3844	1/1	0.76	0.22	72,72,72,72	0
81	OHX	sR	2025	7/7	0.76	0.13	209,214,224,303	0
82	MG	AR	3861	1/1	0.76	0.33	48,48,48,48	0
82	MG	1	3620	1/1	0.76	0.26	72,72,72,72	0
81	OHX	AR	3672	7/7	0.76	0.13	215,220,235,315	0
82	MG	1	3755	1/1	0.76	0.23	65,65,65,65	0
82	MG	A	2040	1/1	0.76	0.28	82,82,82,82	0
81	OHX	d0	201	7/7	0.77	0.15	212,218,221,290	0
81	OHX	AR	3679	7/7	0.77	0.12	230,233,251,317	0
81	OHX	AR	4202	7/7	0.77	0.61	70,70,72,87	7
82	MG	1	4025	1/1	0.77	0.15	73,73,73,73	0
81	OHX	AR	3668	7/7	0.77	0.15	182,189,194,282	0
82	MG	A	2088	1/1	0.77	0.32	81,81,81,81	0
82	MG	CI	302	1/1	0.77	0.27	58,58,58,58	0
82	MG	Y	201	1/1	0.77	0.23	79,79,79,79	0
82	MG	1	3871	1/1	0.77	0.33	68,68,68,68	0
82	MG	AR	3809	1/1	0.77	0.27	61,61,61,61	0
81	OHX	AT	212	7/7	0.77	0.18	170,188,191,275	0
82	MG	A	2004	1/1	0.77	0.22	74,74,74,74	0
82	MG	sR	2109	1/1	0.77	0.28	75,75,75,75	0
82	MG	1	3688	1/1	0.77	0.20	66,66,66,66	0
81	OHX	1	3556	7/7	0.77	0.17	191,200,207,290	0
82	MG	AR	3865	1/1	0.77	0.41	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	OHX	A	2121	7/7	0.77	0.18	231,237,244,321	0
82	MG	AR	4058	1/1	0.77	0.32	87,87,87,87	0
82	MG	sR	2144	1/1	0.77	0.26	85,85,85,85	0
82	MG	A	2038	1/1	0.77	0.20	76,76,76,76	0
82	MG	AR	4097	1/1	0.77	0.41	82,82,82,82	0
81	OHX	1	3578	7/7	0.77	0.11	231,240,248,308	0
82	MG	1	3984	1/1	0.77	0.29	66,66,66,66	0
81	OHX	sR	2176	7/7	0.77	0.18	168,172,175,207	7
82	MG	AR	4124	1/1	0.77	0.29	106,106,106,106	0
82	MG	AR	3935	1/1	0.77	0.25	65,65,65,65	0
81	OHX	AR	3631	7/7	0.77	0.14	200,210,222,306	0
82	MG	AR	3904	1/1	0.78	0.24	71,71,71,71	0
82	MG	4	225	1/1	0.78	0.25	70,70,70,70	0
82	MG	CE	408	1/1	0.78	0.34	78,78,78,78	0
82	MG	CF	402	1/1	0.78	0.27	84,84,84,84	0
82	MG	1	3894	1/1	0.78	0.20	66,66,66,66	0
82	MG	1	3896	1/1	0.78	0.21	81,81,81,81	0
82	MG	x	202	1/1	0.78	0.41	93,93,93,93	0
82	MG	AR	4057	1/1	0.78	0.20	83,83,83,83	0
82	MG	sR	2059	1/1	0.78	0.12	62,62,62,62	0
82	MG	sR	2092	1/1	0.78	0.40	83,83,83,83	0
82	MG	sR	2093	1/1	0.78	0.26	83,83,83,83	0
82	MG	AR	3782	1/1	0.78	0.30	70,70,70,70	0
82	MG	AR	4075	1/1	0.78	0.20	82,82,82,82	0
82	MG	1	4039	1/1	0.78	0.47	64,64,64,64	0
82	MG	AR	3958	1/1	0.78	0.19	71,71,71,71	0
82	MG	A	2023	1/1	0.78	0.15	71,71,71,71	0
82	MG	AR	4111	1/1	0.78	0.22	77,77,77,77	0
82	MG	AR	3700	1/1	0.78	0.29	69,69,69,69	0
82	MG	1	3928	1/1	0.78	0.32	83,83,83,83	0
82	MG	sR	2141	1/1	0.78	0.11	85,85,85,85	0
82	MG	AR	4119	1/1	0.78	0.34	83,83,83,83	0
82	MG	1	3832	1/1	0.78	0.30	54,54,54,54	0
82	MG	AR	3976	1/1	0.78	0.18	60,60,60,60	0
82	MG	sR	2148	1/1	0.78	0.16	69,69,69,69	0
81	OHX	AR	4200	7/7	0.78	0.14	175,176,186,273	0
82	MG	sR	2154	1/1	0.78	0.29	88,88,88,88	0
82	MG	AR	3996	1/1	0.78	0.19	80,80,80,80	0
82	MG	AR	4162	1/1	0.78	0.45	79,79,79,79	0
82	MG	AR	4166	1/1	0.78	0.37	83,83,83,83	0
82	MG	AR	3750	1/1	0.78	0.25	76,76,76,76	0
81	OHX	AR	4201	7/7	0.78	0.14	192,200,208,288	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	4049	1/1	0.79	0.25	76,76,76,76	0
82	MG	AR	3900	1/1	0.79	0.22	79,79,79,79	0
82	MG	sR	2035	1/1	0.79	0.27	69,69,69,69	0
81	OHX	sR	2175	7/7	0.79	0.23	142,149,152,168	7
82	MG	AR	4131	1/1	0.79	0.15	82,82,82,82	0
82	MG	AR	3914	1/1	0.79	0.27	59,59,59,59	0
81	OHX	1	3548	7/7	0.79	0.14	197,201,205,291	0
82	MG	1	4059	1/1	0.79	0.17	79,79,79,79	0
82	MG	AR	4041	1/1	0.79	0.29	70,70,70,70	0
82	MG	AS	3502	1/1	0.79	0.20	88,88,88,88	0
81	OHX	1	3562	7/7	0.79	0.12	216,222,234,324	0
81	OHX	c3	201	7/7	0.79	0.13	203,210,217,273	0
82	MG	1	3993	1/1	0.79	0.15	91,91,91,91	0
82	MG	A	2048	1/1	0.79	0.25	79,79,79,79	0
82	MG	sR	2130	1/1	0.79	0.21	74,74,74,74	0
82	MG	AS	3526	1/1	0.79	0.16	73,73,73,73	0
82	MG	sR	2133	1/1	0.79	0.37	97,97,97,97	0
82	MG	A	2053	1/1	0.79	0.29	80,80,80,80	0
82	MG	sR	2142	1/1	0.79	0.17	105,105,105,105	0
81	OHX	A	1962	7/7	0.79	0.15	200,202,209,267	0
81	OHX	A	1966	7/7	0.79	0.15	201,205,214,291	0
82	MG	A	2069	1/1	0.79	0.18	75,75,75,75	0
81	OHX	1	3617	7/7	0.79	0.16	179,186,195,267	0
81	OHX	1	3585	7/7	0.79	0.12	239,243,249,307	0
82	MG	CM	202	1/1	0.79	0.27	74,74,74,74	0
81	OHX	AR	3677	7/7	0.79	0.13	186,195,207,294	0
82	MG	sR	2167	1/1	0.79	0.20	64,64,64,64	0
82	MG	DP	101	1/1	0.79	0.34	66,66,66,66	0
82	MG	1	4026	1/1	0.79	0.21	72,72,72,72	0
82	MG	1	3953	1/1	0.79	0.16	64,64,64,64	0
82	MG	A	2096	1/1	0.79	0.40	82,82,82,82	0
82	MG	A	2059	1/1	0.80	0.14	65,65,65,65	0
82	MG	1	4082	1/1	0.80	0.32	86,86,86,86	0
82	MG	1	3642	1/1	0.80	0.17	64,64,64,64	0
82	MG	AR	4133	1/1	0.80	0.41	57,57,57,57	0
82	MG	1	3930	1/1	0.80	0.22	72,72,72,72	0
82	MG	AR	4153	1/1	0.80	0.20	58,58,58,58	0
82	MG	AR	3928	1/1	0.80	0.38	74,74,74,74	0
82	MG	1	3935	1/1	0.80	0.20	73,73,73,73	0
82	MG	s	300	1/1	0.80	0.12	100,100,100,100	0
81	OHX	AT	203	7/7	0.80	0.15	179,183,187,270	0
82	MG	AR	3953	1/1	0.80	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	sR	2024	7/7	0.80	0.14	210,223,227,300	0
82	MG	A	2099	1/1	0.80	0.29	76,76,76,76	0
82	MG	1	3709	1/1	0.80	0.19	53,53,53,53	0
82	MG	AF	202	1/1	0.80	0.21	59,59,59,59	0
82	MG	sR	2033	1/1	0.80	0.40	76,76,76,76	0
81	OHX	1	3593	7/7	0.80	0.13	193,199,208,280	0
82	MG	AT	224	1/1	0.80	0.14	79,79,79,79	0
82	MG	1	3966	1/1	0.80	0.38	84,84,84,84	0
82	MG	AR	3977	1/1	0.80	0.11	78,78,78,78	0
82	MG	1	3731	1/1	0.80	0.36	50,50,50,50	0
81	OHX	1	402	7/7	0.80	0.11	203,213,227,297	0
82	MG	1	3987	1/1	0.80	0.21	85,85,85,85	0
81	OHX	sR	2027	7/7	0.80	0.13	221,223,232,292	0
82	MG	sR	2112	1/1	0.80	0.37	136,136,136,136	0
82	MG	A	1985	1/1	0.80	0.33	66,66,66,66	0
81	OHX	AR	4196	7/7	0.80	0.20	153,165,179,262	0
81	OHX	AR	3641	7/7	0.80	0.15	176,184,188,269	0
81	OHX	sR	2172	7/7	0.80	0.11	235,239,246,293	0
82	MG	1	3821	1/1	0.80	0.22	65,65,65,65	0
81	OHX	A	1968	7/7	0.80	0.11	236,237,247,292	0
82	MG	1	4020	1/1	0.80	0.34	88,88,88,88	0
82	MG	sR	2136	1/1	0.80	0.17	85,85,85,85	0
82	MG	AR	3801	1/1	0.80	0.36	51,51,51,51	0
82	MG	1	4024	1/1	0.80	0.18	80,80,80,80	0
82	MG	A	2031	1/1	0.80	0.14	76,76,76,76	0
81	OHX	AR	4198	7/7	0.80	0.17	181,191,191,280	0
81	OHX	1	4124	7/7	0.80	0.12	192,199,210,281	0
81	OHX	1	3600	7/7	0.80	0.11	190,198,211,281	0
82	MG	sR	2149	1/1	0.80	0.19	71,71,71,71	0
82	MG	1	3867	1/1	0.80	0.42	85,85,85,85	0
82	MG	sR	2153	1/1	0.80	0.26	103,103,103,103	0
82	MG	A	2042	1/1	0.80	0.13	80,80,80,80	0
81	OHX	1	3597	7/7	0.80	0.15	182,190,204,279	0
81	OHX	sR	2018	6/7	0.80	0.16	204,205,213,301	0
81	OHX	sR	2019	7/7	0.80	0.11	224,227,232,312	0
82	MG	AR	4120	1/1	0.80	0.29	63,63,63,63	0
81	OHX	1	3564	7/7	0.80	0.13	199,200,207,274	0
82	MG	A	2058	1/1	0.80	0.13	92,92,92,92	0
82	MG	1	3952	1/1	0.81	0.19	71,71,71,71	0
81	OHX	3	206	7/7	0.81	0.12	201,204,208,274	0
82	MG	1	4023	1/1	0.81	0.41	72,72,72,72	0
82	MG	1	3958	1/1	0.81	0.18	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AR	3797	1/1	0.81	0.29	45,45,45,45	0
81	OHX	AR	3686	7/7	0.81	0.12	195,201,208,299	0
82	MG	sR	2060	1/1	0.81	0.30	93,93,93,93	0
82	MG	sR	2082	1/1	0.81	0.39	68,68,68,68	0
82	MG	sR	2086	1/1	0.81	0.16	78,78,78,78	0
82	MG	z	202	1/1	0.81	0.21	73,73,73,73	0
82	MG	AR	3832	1/1	0.81	0.29	43,43,43,43	0
82	MG	AR	4128	1/1	0.81	0.22	70,70,70,70	0
81	OHX	1	3595	7/7	0.81	0.19	148,155,166,240	0
82	MG	AR	3980	1/1	0.81	0.23	67,67,67,67	0
82	MG	A	2033	1/1	0.81	0.31	82,82,82,82	0
82	MG	AB	205	1/1	0.81	0.31	81,81,81,81	0
82	MG	1	3819	1/1	0.81	0.23	60,60,60,60	0
82	MG	AR	4150	1/1	0.81	0.29	80,80,80,80	0
82	MG	sR	2123	1/1	0.81	0.16	97,97,97,97	0
82	MG	AR	3999	1/1	0.81	0.16	57,57,57,57	0
82	MG	1	4042	1/1	0.81	0.25	58,58,58,58	0
81	OHX	1	3583	7/7	0.81	0.16	144,150,161,234	0
82	MG	AR	3718	1/1	0.81	0.12	89,89,89,89	0
82	MG	AR	4184	1/1	0.81	0.26	77,77,77,77	0
82	MG	1	3902	1/1	0.81	0.44	74,74,74,74	0
82	MG	AS	3514	1/1	0.81	0.58	130,130,130,130	0
82	MG	AR	4025	1/1	0.81	0.26	78,78,78,78	0
82	MG	AR	4026	1/1	0.81	0.17	82,82,82,82	0
82	MG	AR	3910	1/1	0.81	0.25	55,55,55,55	0
81	OHX	sR	2013	7/7	0.81	0.12	212,219,229,298	0
82	MG	AR	4049	1/1	0.81	0.25	74,74,74,74	0
82	MG	AT	222	1/1	0.81	0.17	89,89,89,89	0
82	MG	sR	2152	1/1	0.81	0.21	67,67,67,67	0
82	MG	1	3840	1/1	0.81	0.15	71,71,71,71	0
82	MG	AT	229	1/1	0.81	0.40	75,75,75,75	0
82	MG	sR	2155	1/1	0.81	0.28	80,80,80,80	0
81	OHX	AR	3667	7/7	0.81	0.14	182,187,205,273	0
82	MG	AR	3756	1/1	0.81	0.20	59,59,59,59	0
81	OHX	AT	202	7/7	0.81	0.16	174,186,188,275	0
81	OHX	A	1970	7/7	0.81	0.11	207,215,226,295	0
82	MG	AR	4084	1/1	0.81	0.37	86,86,86,86	0
82	MG	DC	203	1/1	0.81	0.34	78,78,78,78	0
82	MG	AR	4074	1/1	0.82	0.10	75,75,75,75	0
81	OHX	AR	3502	7/7	0.82	0.20	110,127,129,205	0
82	MG	AR	3738	1/1	0.82	0.24	54,54,54,54	0
82	MG	1	4045	1/1	0.82	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	3	221	7/7	0.82	0.12	198,202,208,290	0
82	MG	1	3865	1/1	0.82	0.17	84,84,84,84	0
82	MG	sR	2068	1/1	0.82	0.24	76,76,76,76	0
82	MG	sR	2081	1/1	0.82	0.25	56,56,56,56	0
82	MG	1	4054	1/1	0.82	0.34	75,75,75,75	0
81	OHX	1	3575	7/7	0.82	0.12	183,192,202,270	0
82	MG	sR	2089	1/1	0.82	0.21	78,78,78,78	0
82	MG	AR	3956	1/1	0.82	0.18	82,82,82,82	0
82	MG	AR	3763	1/1	0.82	0.29	68,68,68,68	0
82	MG	AR	4122	1/1	0.82	0.26	73,73,73,73	0
81	OHX	sR	2008	7/7	0.82	0.13	176,179,194,261	0
81	OHX	1	3612	7/7	0.82	0.13	170,172,178,260	0
82	MG	1	3891	1/1	0.82	0.28	63,63,63,63	0
81	OHX	4	213	7/7	0.82	0.13	156,161,172,257	0
82	MG	3	208	1/1	0.82	0.17	65,65,65,65	0
82	MG	3	212	1/1	0.82	0.28	66,66,66,66	0
82	MG	AR	3988	1/1	0.82	0.10	61,61,61,61	0
82	MG	AR	3990	1/1	0.82	0.10	75,75,75,75	0
82	MG	4	216	1/1	0.82	0.36	77,77,77,77	0
82	MG	1	4002	1/1	0.82	0.14	70,70,70,70	0
82	MG	4	226	1/1	0.82	0.16	55,55,55,55	0
82	MG	AR	3817	1/1	0.82	0.38	54,54,54,54	0
81	OHX	CG	303	7/7	0.82	0.12	198,206,217,289	0
82	MG	4	234	1/1	0.82	0.34	62,62,62,62	0
81	OHX	DK	201	7/7	0.82	0.13	220,222,242,324	0
82	MG	1	3781	1/1	0.82	0.43	57,57,57,57	0
82	MG	sR	2146	1/1	0.82	0.17	69,69,69,69	0
81	OHX	1	4131	7/7	0.82	0.14	170,172,182,255	0
82	MG	AR	4027	1/1	0.82	0.14	58,58,58,58	0
82	MG	AR	3867	1/1	0.82	0.32	55,55,55,55	0
81	OHX	1	3603	7/7	0.82	0.12	201,203,218,286	0
82	MG	AR	4042	1/1	0.82	0.11	74,74,74,74	0
81	OHX	AR	3649	7/7	0.82	0.15	187,199,208,291	0
81	OHX	1	3594	7/7	0.82	0.11	206,219,228,293	0
82	MG	A	2093	1/1	0.82	0.47	83,83,83,83	0
82	MG	1	3672	1/1	0.82	0.39	79,79,79,79	0
81	OHX	AR	3658	7/7	0.82	0.13	189,194,204,272	0
82	MG	1	3957	1/1	0.82	0.12	82,82,82,82	0
82	MG	A	2101	1/1	0.82	0.18	68,68,68,68	0
82	MG	A	2102	1/1	0.82	0.23	79,79,79,79	0
82	MG	AR	4069	1/1	0.82	0.32	83,83,83,83	0
81	OHX	1	3544	7/7	0.83	0.12	182,185,193,271	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
82	MG	AR	4000	1/1	0.83	0.30	80,80,80,80	0
82	MG	1	3932	1/1	0.83	0.09	91,91,91,91	0
82	MG	AR	3785	1/1	0.83	0.43	54,54,54,54	0
82	MG	1	3761	1/1	0.83	0.29	55,55,55,55	0
82	MG	1	4065	1/1	0.83	0.41	58,58,58,58	0
81	OHX	AR	3671	7/7	0.83	0.12	160,174,185,264	0
82	MG	1	3765	1/1	0.83	0.32	60,60,60,60	0
81	OHX	sR	2007	7/7	0.83	0.16	165,174,186,246	0
82	MG	1	4155	1/1	0.83	0.29	65,65,65,65	0
82	MG	1	3788	1/1	0.83	0.19	60,60,60,60	0
82	MG	AR	3838	1/1	0.83	0.44	60,60,60,60	0
82	MG	1	3797	1/1	0.83	0.27	65,65,65,65	0
81	OHX	AR	3575	7/7	0.83	0.17	156,163,167,254	0
82	MG	A	1989	1/1	0.83	0.25	70,70,70,70	0
82	MG	sR	2084	1/1	0.83	0.20	80,80,80,80	0
82	MG	1	3959	1/1	0.83	0.17	58,58,58,58	0
82	MG	A	2000	1/1	0.83	0.26	72,72,72,72	0
82	MG	1	3817	1/1	0.83	0.15	69,69,69,69	0
81	OHX	AR	3598	7/7	0.83	0.15	150,164,177,245	0
82	MG	AR	4061	1/1	0.83	0.21	78,78,78,78	0
81	OHX	AR	3599	7/7	0.83	0.12	163,169,186,260	0
82	MG	A	2018	1/1	0.83	0.23	85,85,85,85	0
82	MG	AR	3903	1/1	0.83	0.30	76,76,76,76	0
82	MG	1	3822	1/1	0.83	0.22	54,54,54,54	0
82	MG	sR	2118	1/1	0.83	0.12	93,93,93,93	0
81	OHX	1	3561	7/7	0.83	0.19	142,151,163,225	0
81	OHX	1	4122	7/7	0.83	0.16	127,143,153,230	0
82	MG	1	3634	1/1	0.83	0.36	69,69,69,69	0
81	OHX	AR	3680	7/7	0.83	0.10	219,228,232,300	0
82	MG	1	4003	1/1	0.83	0.18	62,62,62,62	0
82	MG	AR	3924	1/1	0.83	0.26	69,69,69,69	0
82	MG	1	3852	1/1	0.83	0.19	65,65,65,65	0
82	MG	1	3859	1/1	0.83	0.28	59,59,59,59	0
82	MG	AR	3706	1/1	0.83	0.28	66,66,66,66	0
82	MG	1	3645	1/1	0.83	0.37	65,65,65,65	0
81	OHX	1	3566	7/7	0.83	0.15	180,184,195,265	0
82	MG	AR	3955	1/1	0.83	0.14	63,63,63,63	0
82	MG	AR	3727	1/1	0.83	0.20	41,41,41,41	0
81	OHX	AR	3682	7/7	0.83	0.11	204,209,218,283	0
81	OHX	A	2130	7/7	0.83	0.12	187,188,201,269	0
82	MG	1	3705	1/1	0.83	0.15	80,80,80,80	0
82	MG	1	3888	1/1	0.83	0.38	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	A	2068	1/1	0.83	0.24	77,77,77,77	0
82	MG	AR	3751	1/1	0.83	0.17	48,48,48,48	0
81	OHX	A	2134	7/7	0.83	0.12	215,218,228,290	0
82	MG	AR	3978	1/1	0.83	0.19	75,75,75,75	0
81	OHX	A	2135	7/7	0.83	0.10	222,229,241,301	0
81	OHX	sR	1979	7/7	0.83	0.11	198,203,212,286	0
82	MG	s4	302	1/1	0.83	0.17	73,73,73,73	0
81	OHX	sR	2171	7/7	0.83	0.14	191,200,205,281	0
82	MG	1	3918	1/1	0.83	0.39	78,78,78,78	0
82	MG	A	2092	1/1	0.83	0.32	76,76,76,76	0
81	OHX	1	4129	7/7	0.83	0.12	179,190,201,285	0
82	MG	CE	407	1/1	0.84	0.29	59,59,59,59	0
82	MG	A	2098	1/1	0.84	0.19	85,85,85,85	0
81	OHX	A	1944	7/7	0.84	0.15	180,182,186,246	0
82	MG	1	3846	1/1	0.84	0.36	74,74,74,74	0
82	MG	1	4046	1/1	0.84	0.27	61,61,61,61	0
81	OHX	sR	2005	7/7	0.84	0.13	189,193,197,268	0
82	MG	AR	3747	1/1	0.84	0.13	69,69,69,69	0
82	MG	AR	4064	1/1	0.84	0.13	64,64,64,64	0
82	MG	1	3853	1/1	0.84	0.22	84,84,84,84	0
82	MG	A	1979	1/1	0.84	0.13	70,70,70,70	0
82	MG	sR	2051	1/1	0.84	0.24	63,63,63,63	0
82	MG	sR	2055	1/1	0.84	0.26	76,76,76,76	0
82	MG	AR	4072	1/1	0.84	0.07	65,65,65,65	0
82	MG	1	3651	1/1	0.84	0.25	61,61,61,61	0
82	MG	A	1990	1/1	0.84	0.19	62,62,62,62	0
82	MG	A	1991	1/1	0.84	0.31	69,69,69,69	0
81	OHX	A	2145	7/7	0.84	0.14	183,192,199,274	0
82	MG	AR	3947	1/1	0.84	0.22	73,73,73,73	0
81	OHX	J	301	7/7	0.84	0.10	227,233,241,307	0
82	MG	1	3866	1/1	0.84	0.31	76,76,76,76	0
82	MG	1	3967	1/1	0.84	0.31	72,72,72,72	0
82	MG	1	3970	1/1	0.84	0.12	81,81,81,81	0
82	MG	sR	2095	1/1	0.84	0.23	76,76,76,76	0
82	MG	1	3770	1/1	0.84	0.17	63,63,63,63	0
82	MG	1	3978	1/1	0.84	0.20	64,64,64,64	0
82	MG	1	3771	1/1	0.84	0.25	65,65,65,65	0
82	MG	A	2026	1/1	0.84	0.10	88,88,88,88	0
82	MG	AR	4121	1/1	0.84	0.15	93,93,93,93	0
82	MG	A	2030	1/1	0.84	0.25	76,76,76,76	0
82	MG	AR	3965	1/1	0.84	0.20	64,64,64,64	0
82	MG	AR	3773	1/1	0.84	0.29	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AR	4126	1/1	0.84	0.15	59,59,59,59	0
81	OHX	sR	1963	7/7	0.84	0.16	155,158,167,227	0
82	MG	1	3692	1/1	0.84	0.38	88,88,88,88	0
81	OHX	sR	2016	7/7	0.84	0.15	141,147,167,229	0
82	MG	1	3804	1/1	0.84	0.41	55,55,55,55	0
82	MG	sR	2134	1/1	0.84	0.11	62,62,62,62	0
82	MG	AR	4139	1/1	0.84	0.37	63,63,63,63	0
82	MG	A	2046	1/1	0.84	0.16	78,78,78,78	0
82	MG	1	3895	1/1	0.84	0.30	91,91,91,91	0
82	MG	4	231	1/1	0.84	0.25	73,73,73,73	0
82	MG	AR	4152	1/1	0.84	0.44	64,64,64,64	0
82	MG	AR	3815	1/1	0.84	0.24	53,53,53,53	0
82	MG	4	232	1/1	0.84	0.11	55,55,55,55	0
82	MG	AR	3830	1/1	0.84	0.29	64,64,64,64	0
82	MG	1	3707	1/1	0.84	0.26	77,77,77,77	0
82	MG	n	201	1/1	0.84	0.13	71,71,71,71	0
82	MG	AR	4188	1/1	0.84	0.26	68,68,68,68	0
82	MG	1	3899	1/1	0.84	0.09	119,119,119,119	0
82	MG	1	3621	1/1	0.84	0.24	69,69,69,69	0
81	OHX	z	203	7/7	0.84	0.12	130,132,137,165	7
82	MG	sR	2160	1/1	0.84	0.35	69,69,69,69	0
82	MG	1	3922	1/1	0.84	0.20	52,52,52,52	0
82	MG	1	3730	1/1	0.84	0.27	43,43,43,43	0
81	OHX	AG	202	7/7	0.84	0.17	155,169,173,243	0
81	OHX	AR	3647	7/7	0.84	0.12	171,177,186,255	0
82	MG	1	3744	1/1	0.84	0.31	54,54,54,54	0
82	MG	1	4032	1/1	0.84	0.23	47,47,47,47	0
82	MG	1	3746	1/1	0.84	0.26	70,70,70,70	0
82	MG	AR	3775	1/1	0.85	0.09	45,45,45,45	0
82	MG	AR	3983	1/1	0.85	0.41	86,86,86,86	0
82	MG	1	3718	1/1	0.85	0.31	42,42,42,42	0
82	MG	1	3720	1/1	0.85	0.17	54,54,54,54	0
82	MG	1	3725	1/1	0.85	0.35	62,62,62,62	0
82	MG	4	220	1/1	0.85	0.30	70,70,70,70	0
81	OHX	sR	2173	7/7	0.85	0.20	130,137,142,166	7
81	OHX	1	3588	7/7	0.85	0.14	172,176,188,262	0
82	MG	AR	4008	1/1	0.85	0.18	68,68,68,68	0
81	OHX	sR	2004	7/7	0.85	0.13	194,196,202,266	0
82	MG	4	230	1/1	0.85	0.16	85,85,85,85	0
82	MG	1	3739	1/1	0.85	0.20	41,41,41,41	0
81	OHX	1	3589	7/7	0.85	0.19	155,161,167,248	0
81	OHX	AR	3637	7/7	0.85	0.15	164,171,187,255	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
82	MG	j	301	1/1	0.85	0.41	64,64,64,64	0
82	MG	AR	3846	1/1	0.85	0.29	51,51,51,51	0
82	MG	AR	4030	1/1	0.85	0.14	63,63,63,63	0
81	OHX	AR	3542	7/7	0.85	0.15	138,138,149,217	0
81	OHX	A	2127	7/7	0.85	0.13	181,182,190,256	0
81	OHX	AR	3670	7/7	0.85	0.11	160,172,179,249	0
82	MG	AR	4044	1/1	0.85	0.21	75,75,75,75	0
82	MG	sR	2070	1/1	0.85	0.27	70,70,70,70	0
81	OHX	A	2131	7/7	0.85	0.13	183,192,199,259	0
82	MG	AR	3869	1/1	0.85	0.35	51,51,51,51	0
81	OHX	1	4136	7/7	0.85	0.10	184,188,198,268	0
82	MG	AR	3889	1/1	0.85	0.36	61,61,61,61	0
82	MG	1	3630	1/1	0.85	0.28	52,52,52,52	0
82	MG	A	1996	1/1	0.85	0.23	69,69,69,69	0
81	OHX	AR	3578	7/7	0.85	0.14	162,168,181,251	0
82	MG	AF	201	1/1	0.85	0.28	57,57,57,57	0
82	MG	AR	4067	1/1	0.85	0.05	126,126,126,126	0
82	MG	A	2002	1/1	0.85	0.33	75,75,75,75	0
82	MG	sR	2105	1/1	0.85	0.22	67,67,67,67	0
82	MG	AR	3908	1/1	0.85	0.15	61,61,61,61	0
82	MG	1	3905	1/1	0.85	0.12	62,62,62,62	0
82	MG	1	3909	1/1	0.85	0.38	71,71,71,71	0
82	MG	AR	3917	1/1	0.85	0.37	79,79,79,79	0
82	MG	AR	4078	1/1	0.85	0.23	51,51,51,51	0
81	OHX	sR	2021	7/7	0.85	0.16	185,191,209,289	0
82	MG	AR	3921	1/1	0.85	0.14	57,57,57,57	0
82	MG	AR	3710	1/1	0.85	0.15	53,53,53,53	0
81	OHX	sR	2022	7/7	0.85	0.10	215,220,227,303	0
81	OHX	A	2140	7/7	0.85	0.15	172,177,180,248	0
82	MG	1	4040	1/1	0.85	0.35	60,60,60,60	0
82	MG	AR	3732	1/1	0.85	0.27	80,80,80,80	0
82	MG	AR	3936	1/1	0.85	0.17	54,54,54,54	0
81	OHX	A	2141	7/7	0.85	0.09	256,257,259,308	0
82	MG	1	3931	1/1	0.85	0.58	79,79,79,79	0
82	MG	1	3677	1/1	0.85	0.16	58,58,58,58	0
81	OHX	1	3567	7/7	0.85	0.17	157,164,168,250	0
81	OHX	1	3574	7/7	0.85	0.11	177,182,197,271	0
82	MG	1	3690	1/1	0.85	0.38	76,76,76,76	0
81	OHX	O	201	7/7	0.85	0.10	217,222,232,288	0
82	MG	1	3700	1/1	0.85	0.28	58,58,58,58	0
81	OHX	AR	3614	7/7	0.85	0.13	176,179,190,252	0
82	MG	A	2057	1/1	0.85	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	A	1952	7/7	0.85	0.14	186,189,203,261	0
82	MG	AR	4145	1/1	0.85	0.33	61,61,61,61	0
82	MG	AR	4147	1/1	0.85	0.27	46,46,46,46	0
82	MG	AR	3969	1/1	0.85	0.23	62,62,62,62	0
82	MG	A	2064	1/1	0.85	0.15	84,84,84,84	0
82	MG	1	3842	1/1	0.85	0.13	55,55,55,55	0
82	MG	1	4145	1/1	0.85	0.23	47,47,47,47	0
81	OHX	A	1961	7/7	0.85	0.10	200,208,216,276	0
81	OHX	1	3614	7/7	0.85	0.13	161,164,180,256	0
82	MG	c6	201	1/1	0.85	0.23	81,81,81,81	0
82	MG	A	2081	1/1	0.85	0.27	74,74,74,74	0
82	MG	AR	4164	1/1	0.85	0.38	67,67,67,67	0
82	MG	1	4031	1/1	0.86	0.20	62,62,62,62	0
82	MG	AR	4189	1/1	0.86	0.16	63,63,63,63	0
82	MG	AR	4191	1/1	0.86	0.17	70,70,70,70	0
82	MG	AK	101	1/1	0.86	0.33	61,61,61,61	0
81	OHX	AR	3655	7/7	0.86	0.14	164,171,184,253	0
81	OHX	AR	3596	7/7	0.86	0.12	174,182,189,261	0
82	MG	1	3836	1/1	0.86	0.14	56,56,56,56	0
81	OHX	1	3607	7/7	0.86	0.12	191,204,216,298	0
82	MG	AR	3905	1/1	0.86	0.26	72,72,72,72	0
81	OHX	sR	1991	7/7	0.86	0.13	151,154,162,226	0
82	MG	AT	219	1/1	0.86	0.23	64,64,64,64	0
81	OHX	sR	1997	7/7	0.86	0.14	174,182,193,256	0
82	MG	1	3732	1/1	0.86	0.30	42,42,42,42	0
82	MG	AT	227	1/1	0.86	0.23	72,72,72,72	0
82	MG	AR	4045	1/1	0.86	0.18	41,41,41,41	0
82	MG	AR	4046	1/1	0.86	0.40	80,80,80,80	0
81	OHX	1	3560	7/7	0.86	0.14	158,166,170,244	0
81	OHX	AR	3664	7/7	0.86	0.11	205,214,221,289	0
81	OHX	sR	2003	7/7	0.86	0.14	180,183,191,250	0
82	MG	sR	2043	1/1	0.86	0.26	72,72,72,72	0
82	MG	CM	201	1/1	0.86	0.31	77,77,77,77	0
82	MG	AR	4052	1/1	0.86	0.17	55,55,55,55	0
81	OHX	AR	3650	7/7	0.86	0.12	160,168,186,257	0
82	MG	CR	203	1/1	0.86	0.22	55,55,55,55	0
82	MG	CY	201	1/1	0.86	0.10	108,108,108,108	0
82	MG	1	3663	1/1	0.86	0.25	63,63,63,63	0
82	MG	sR	2074	1/1	0.86	0.18	49,49,49,49	0
81	OHX	A	2136	7/7	0.86	0.14	192,198,203,267	0
82	MG	AR	4063	1/1	0.86	0.12	52,52,52,52	0
81	OHX	A	1964	7/7	0.86	0.11	187,193,208,266	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	A	1988	1/1	0.86	0.33	80,80,80,80	0
82	MG	1	3762	1/1	0.86	0.39	53,53,53,53	0
81	OHX	AR	3633	7/7	0.86	0.13	160,165,175,247	0
81	OHX	sR	2010	7/7	0.86	0.14	145,153,156,232	0
82	MG	AR	3946	1/1	0.86	0.23	80,80,80,80	0
82	MG	1	3875	1/1	0.86	0.32	70,70,70,70	0
82	MG	1	3986	1/1	0.86	0.23	64,64,64,64	0
82	MG	AR	3770	1/1	0.86	0.35	41,41,41,41	0
82	MG	AR	4095	1/1	0.86	0.17	59,59,59,59	0
82	MG	sR	2110	1/1	0.86	0.17	80,80,80,80	0
82	MG	3	217	1/1	0.86	0.17	61,61,61,61	0
82	MG	A	2006	1/1	0.86	0.31	59,59,59,59	0
82	MG	A	2007	1/1	0.86	0.23	71,71,71,71	0
82	MG	1	3879	1/1	0.86	0.10	56,56,56,56	0
81	OHX	sR	2012	7/7	0.86	0.11	220,227,229,273	0
81	OHX	AR	3654	7/7	0.86	0.14	161,165,184,259	0
82	MG	AR	3961	1/1	0.86	0.27	81,81,81,81	0
82	MG	sR	2129	1/1	0.86	0.24	81,81,81,81	0
82	MG	1	3697	1/1	0.86	0.38	62,62,62,62	0
82	MG	AR	3963	1/1	0.86	0.25	57,57,57,57	0
82	MG	AR	3964	1/1	0.86	0.17	72,72,72,72	0
81	OHX	CG	302	7/7	0.86	0.10	215,218,224,290	0
82	MG	1	4004	1/1	0.86	0.30	72,72,72,72	0
82	MG	AR	4125	1/1	0.86	0.26	94,94,94,94	0
82	MG	AR	3970	1/1	0.86	0.08	73,73,73,73	0
82	MG	1	3794	1/1	0.86	0.37	56,56,56,56	0
82	MG	AR	3807	1/1	0.86	0.29	68,68,68,68	0
82	MG	1	4009	1/1	0.86	0.16	58,58,58,58	0
82	MG	1	3897	1/1	0.86	0.15	76,76,76,76	0
82	MG	1	3702	1/1	0.86	0.18	68,68,68,68	0
82	MG	AR	3825	1/1	0.86	0.38	70,70,70,70	0
82	MG	AR	4141	1/1	0.86	0.19	48,48,48,48	0
82	MG	AR	4142	1/1	0.86	0.17	46,46,46,46	0
82	MG	AR	3985	1/1	0.86	0.20	72,72,72,72	0
82	MG	A	2052	1/1	0.86	0.23	60,60,60,60	0
82	MG	1	3798	1/1	0.86	0.34	56,56,56,56	0
82	MG	sR	2156	1/1	0.86	0.38	71,71,71,71	0
82	MG	1	4018	1/1	0.86	0.16	79,79,79,79	0
81	OHX	s8	302	7/7	0.86	0.10	216,223,229,295	0
82	MG	1	4022	1/1	0.86	0.21	55,55,55,55	0
81	OHX	A	1975	7/7	0.86	0.12	168,174,180,242	0
81	OHX	c5	201	7/7	0.86	0.10	194,202,210,264	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	6	203	1/1	0.86	0.39	66,66,66,66	0
81	OHX	U	201	7/7	0.86	0.12	218,223,227,290	0
82	MG	AR	4171	1/1	0.86	0.29	73,73,73,73	0
82	MG	1	3712	1/1	0.86	0.17	69,69,69,69	0
82	MG	d6	203	1/1	0.86	0.18	65,65,65,65	0
85	ZN	d7	101	1/1	0.86	0.15	202,202,202,202	0
82	MG	AR	3776	1/1	0.87	0.27	44,44,44,44	0
82	MG	AR	3781	1/1	0.87	0.28	42,42,42,42	0
81	OHX	sR	1989	7/7	0.87	0.12	157,158,163,241	0
82	MG	1	4037	1/1	0.87	0.30	42,42,42,42	0
82	MG	A	2024	1/1	0.87	0.15	67,67,67,67	0
81	OHX	A	1939	7/7	0.87	0.14	142,148,155,215	0
81	OHX	sR	1996	7/7	0.87	0.12	175,178,191,258	0
81	OHX	AR	3526	7/7	0.87	0.15	130,139,147,217	0
82	MG	1	3748	1/1	0.87	0.31	77,77,77,77	0
82	MG	1	3750	1/1	0.87	0.32	49,49,49,49	0
81	OHX	AR	3656	7/7	0.87	0.09	196,208,215,276	0
82	MG	A	2037	1/1	0.87	0.21	76,76,76,76	0
82	MG	AR	3816	1/1	0.87	0.29	52,52,52,52	0
82	MG	1	3903	1/1	0.87	0.21	83,83,83,83	0
81	OHX	A	1955	7/7	0.87	0.15	137,151,156,198	0
82	MG	AR	3829	1/1	0.87	0.38	50,50,50,50	0
81	OHX	1	3592	7/7	0.87	0.15	165,171,180,243	0
82	MG	1	4058	1/1	0.87	0.17	56,56,56,56	0
82	MG	1	3915	1/1	0.87	0.20	68,68,68,68	0
81	OHX	AR	3660	7/7	0.87	0.12	166,170,179,256	0
82	MG	AR	4076	1/1	0.87	0.23	75,75,75,75	0
82	MG	1	3919	1/1	0.87	0.14	55,55,55,55	0
82	MG	AR	4079	1/1	0.87	0.16	84,84,84,84	0
82	MG	A	2055	1/1	0.87	0.09	76,76,76,76	0
82	MG	1	3920	1/1	0.87	0.22	57,57,57,57	0
82	MG	AR	3863	1/1	0.87	0.32	43,43,43,43	0
82	MG	1	4083	1/1	0.87	0.24	68,68,68,68	0
81	OHX	1	3520	7/7	0.87	0.14	153,155,158,235	0
82	MG	1	4147	1/1	0.87	0.14	107,107,107,107	0
82	MG	1	3923	1/1	0.87	0.27	55,55,55,55	0
82	MG	A	2066	1/1	0.87	0.26	72,72,72,72	0
82	MG	A	2067	1/1	0.87	0.10	58,58,58,58	0
82	MG	AR	3873	1/1	0.87	0.16	82,82,82,82	0
82	MG	AR	4118	1/1	0.87	0.12	53,53,53,53	0
82	MG	AR	3877	1/1	0.87	0.27	69,69,69,69	0
82	MG	1	4152	1/1	0.87	0.18	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	AR	4175	7/7	0.87	0.12	147,156,162,237	0
82	MG	1	3631	1/1	0.87	0.14	64,64,64,64	0
82	MG	AR	4123	1/1	0.87	0.21	73,73,73,73	0
82	MG	AR	3902	1/1	0.87	0.15	60,60,60,60	0
82	MG	1	3633	1/1	0.87	0.26	48,48,48,48	0
81	OHX	1	3609	7/7	0.87	0.12	179,189,199,272	0
82	MG	1	3636	1/1	0.87	0.32	72,72,72,72	0
82	MG	1	3936	1/1	0.87	0.32	80,80,80,80	0
82	MG	AR	3909	1/1	0.87	0.38	72,72,72,72	0
82	MG	A	2097	1/1	0.87	0.29	71,71,71,71	0
82	MG	AR	4132	1/1	0.87	0.24	64,64,64,64	0
82	MG	1	3937	1/1	0.87	0.21	80,80,80,80	0
82	MG	AR	4135	1/1	0.87	0.34	71,71,71,71	0
82	MG	AR	4137	1/1	0.87	0.34	68,68,68,68	0
82	MG	AR	3913	1/1	0.87	0.25	65,65,65,65	0
82	MG	1	3789	1/1	0.87	0.24	46,46,46,46	0
81	OHX	sR	2009	7/7	0.87	0.10	171,184,192,262	0
81	OHX	1	4134	5/7	0.87	0.14	140,143,147,230	0
81	OHX	sR	2011	7/7	0.87	0.12	158,165,181,241	0
82	MG	1	3653	1/1	0.87	0.51	70,70,70,70	0
82	MG	sR	2045	1/1	0.87	0.17	63,63,63,63	0
81	OHX	A	1974	7/7	0.87	0.11	189,199,205,256	0
82	MG	1	3666	1/1	0.87	0.28	68,68,68,68	0
81	OHX	AR	3665	7/7	0.87	0.11	170,178,190,267	0
81	OHX	1	4135	7/7	0.87	0.15	176,180,189,262	0
81	OHX	AR	3642	7/7	0.87	0.12	147,154,160,244	0
82	MG	t	203	1/1	0.87	0.15	56,56,56,56	0
82	MG	1	3827	1/1	0.87	0.11	79,79,79,79	0
82	MG	1	3971	1/1	0.87	0.20	70,70,70,70	0
81	OHX	AR	3669	7/7	0.87	0.11	225,234,239,295	0
82	MG	1	3975	1/1	0.87	0.25	67,67,67,67	0
82	MG	AR	3954	1/1	0.87	0.18	60,60,60,60	0
82	MG	AB	201	1/1	0.87	0.28	66,66,66,66	0
82	MG	1	3834	1/1	0.87	0.26	68,68,68,68	0
82	MG	1	3980	1/1	0.87	0.21	62,62,62,62	0
81	OHX	AR	3643	7/7	0.87	0.13	180,191,201,267	0
81	OHX	AR	4203	7/7	0.87	0.12	163,179,185,271	0
82	MG	AR	3692	1/1	0.87	0.10	51,51,51,51	0
82	MG	1	3695	1/1	0.87	0.25	64,64,64,64	0
82	MG	1	3988	1/1	0.87	0.14	74,74,74,74	0
82	MG	AR	3708	1/1	0.87	0.28	64,64,64,64	0
82	MG	AR	3966	1/1	0.87	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AT	223	1/1	0.87	0.21	79,79,79,79	0
81	OHX	AR	4204	7/7	0.87	0.33	135,141,143,170	7
82	MG	AT	226	1/1	0.87	0.33	66,66,66,66	0
81	OHX	1	3559	7/7	0.87	0.14	143,146,159,226	0
82	MG	AR	3716	1/1	0.87	0.31	71,71,71,71	0
82	MG	CE	401	1/1	0.87	0.07	47,47,47,47	0
82	MG	sR	2127	1/1	0.87	0.15	60,60,60,60	0
82	MG	sR	2128	1/1	0.87	0.28	72,72,72,72	0
82	MG	AR	3972	1/1	0.87	0.33	59,59,59,59	0
82	MG	AR	3717	1/1	0.87	0.31	63,63,63,63	0
81	OHX	AS	3530	7/7	0.87	0.15	194,201,206,302	0
82	MG	AR	3721	1/1	0.87	0.15	62,62,62,62	0
82	MG	1	3847	1/1	0.87	0.14	58,58,58,58	0
82	MG	1	3850	1/1	0.87	0.29	52,52,52,52	0
82	MG	sR	2139	1/1	0.87	0.11	70,70,70,70	0
81	OHX	AR	3648	7/7	0.87	0.12	172,173,181,270	0
82	MG	CR	201	1/1	0.87	0.34	45,45,45,45	0
81	OHX	A	2142	7/7	0.87	0.19	138,141,146,174	7
82	MG	1	4012	1/1	0.87	0.26	68,68,68,68	0
82	MG	AR	3993	1/1	0.87	0.24	77,77,77,77	0
82	MG	DI	201	1/1	0.87	0.32	62,62,62,62	0
82	MG	1	4013	1/1	0.87	0.32	67,67,67,67	0
82	MG	1	4014	1/1	0.87	0.24	83,83,83,83	0
82	MG	A	1982	1/1	0.87	0.25	67,67,67,67	0
81	OHX	1	4142	7/7	0.87	0.11	191,205,217,301	0
81	OHX	sR	2028	7/7	0.87	0.11	182,188,196,261	0
82	MG	AR	4003	1/1	0.87	0.12	65,65,65,65	0
81	OHX	AR	3618	7/7	0.87	0.12	158,160,174,238	0
82	MG	AR	3762	1/1	0.87	0.12	69,69,69,69	0
81	OHX	AR	3652	7/7	0.87	0.11	173,180,185,267	0
81	OHX	AR	3678	7/7	0.87	0.10	222,226,233,281	0
82	MG	sR	2164	1/1	0.87	0.13	61,61,61,61	0
82	MG	AR	3765	1/1	0.87	0.20	51,51,51,51	0
82	MG	1	3724	1/1	0.87	0.31	42,42,42,42	0
81	OHX	1	3525	7/7	0.87	0.13	143,145,158,222	0
81	OHX	CK	201	7/7	0.87	0.11	172,177,183,260	0
82	MG	1	3876	1/1	0.87	0.21	71,71,71,71	0
81	OHX	sR	1980	7/7	0.87	0.14	144,150,167,240	0
82	MG	d3	201	1/1	0.87	0.31	70,70,70,70	0
81	OHX	1	3590	7/7	0.87	0.15	165,170,179,249	0
82	MG	d6	201	1/1	0.87	0.29	63,63,63,63	0
82	MG	A	2010	1/1	0.87	0.36	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	A	2011	1/1	0.87	0.27	59,59,59,59	0
82	MG	AR	3824	1/1	0.88	0.33	54,54,54,54	0
82	MG	AR	4172	1/1	0.88	0.11	56,56,56,56	0
82	MG	AR	4177	1/1	0.88	0.22	60,60,60,60	0
82	MG	AR	3997	1/1	0.88	0.34	66,66,66,66	0
82	MG	AR	4187	1/1	0.88	0.18	41,41,41,41	0
81	OHX	AR	3635	7/7	0.88	0.11	171,180,187,257	0
82	MG	AR	3827	1/1	0.88	0.35	51,51,51,51	0
81	OHX	1	3543	7/7	0.88	0.18	148,158,165,249	0
82	MG	AR	4192	1/1	0.88	0.17	45,45,45,45	0
81	OHX	1	3554	7/7	0.88	0.14	165,169,174,256	0
82	MG	1	3743	1/1	0.88	0.24	55,55,55,55	0
81	OHX	sR	2006	7/7	0.88	0.11	181,190,204,266	0
82	MG	AR	4016	1/1	0.88	0.21	67,67,67,67	0
82	MG	AR	4017	1/1	0.88	0.10	60,60,60,60	0
82	MG	r	301	1/1	0.88	0.23	49,49,49,49	0
82	MG	AR	3844	1/1	0.88	0.29	43,43,43,43	0
82	MG	AT	218	1/1	0.88	0.27	49,49,49,49	0
81	OHX	A	2100	7/7	0.88	0.12	177,179,186,251	0
81	OHX	A	2116	7/7	0.88	0.11	170,177,186,247	0
81	OHX	1	3504	7/7	0.88	0.17	129,134,144,226	0
81	OHX	A	2126	7/7	0.88	0.10	195,199,207,274	0
81	OHX	1	3586	7/7	0.88	0.11	158,166,181,253	0
82	MG	sR	2031	1/1	0.88	0.15	55,55,55,55	0
81	OHX	1	4137	7/7	0.88	0.11	170,175,188,259	0
81	OHX	1	4138	7/7	0.88	0.13	138,138,141,176	7
82	MG	sR	2037	1/1	0.88	0.20	85,85,85,85	0
82	MG	CD	301	1/1	0.88	0.40	62,62,62,62	0
82	MG	1	3650	1/1	0.88	0.27	62,62,62,62	0
81	OHX	A	2132	7/7	0.88	0.12	178,188,192,264	0
82	MG	sR	2050	1/1	0.88	0.28	61,61,61,61	0
82	MG	AR	3884	1/1	0.88	0.19	61,61,61,61	0
81	OHX	A	2133	7/7	0.88	0.11	220,224,229,297	0
82	MG	sR	2056	1/1	0.88	0.22	52,52,52,52	0
82	MG	1	3654	1/1	0.88	0.20	68,68,68,68	0
82	MG	CL	303	1/1	0.88	0.22	43,43,43,43	0
82	MG	sR	2064	1/1	0.88	0.20	73,73,73,73	0
82	MG	1	3778	1/1	0.88	0.36	60,60,60,60	0
81	OHX	1	3605	7/7	0.88	0.12	157,172,185,260	0
82	MG	1	3787	1/1	0.88	0.28	51,51,51,51	0
81	OHX	AR	3675	7/7	0.88	0.17	189,190,204,300	0
82	MG	AR	4060	1/1	0.88	0.30	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	OHX	AR	3587	7/7	0.88	0.13	146,148,152,238	0
82	MG	DA	201	1/1	0.88	0.15	67,67,67,67	0
82	MG	sR	2088	1/1	0.88	0.19	77,77,77,77	0
82	MG	1	3913	1/1	0.88	0.31	76,76,76,76	0
82	MG	sR	2090	1/1	0.88	0.11	73,73,73,73	0
82	MG	1	3790	1/1	0.88	0.29	51,51,51,51	0
82	MG	AR	4065	1/1	0.88	0.18	70,70,70,70	0
81	OHX	AR	3593	7/7	0.88	0.15	135,141,151,207	0
82	MG	sR	2096	1/1	0.88	0.23	60,60,60,60	0
81	OHX	CE	404	7/7	0.88	0.09	195,201,214,284	0
81	OHX	1	3579	7/7	0.88	0.12	149,158,165,224	0
81	OHX	1	4105	6/7	0.88	0.17	111,116,120,186	0
81	OHX	1	3608[A]	7/7	0.88	0.20	132,135,141,177	7
82	MG	1	3924	1/1	0.88	0.11	72,72,72,72	0
82	MG	AR	3733	1/1	0.88	0.10	62,62,62,62	0
82	MG	1	3815	1/1	0.88	0.34	71,71,71,71	0
82	MG	AR	4080	1/1	0.88	0.16	56,56,56,56	0
81	OHX	AR	3613	7/7	0.88	0.12	147,148,155,235	0
82	MG	AR	3743	1/1	0.88	0.23	41,41,41,41	0
82	MG	AR	3930	1/1	0.88	0.29	61,61,61,61	0
82	MG	AR	3933	1/1	0.88	0.19	41,41,41,41	0
81	OHX	1	4123	7/7	0.88	0.14	170,175,184,263	0
81	OHX	A	1943	7/7	0.88	0.13	181,188,194,253	0
82	MG	AR	4113	1/1	0.88	0.26	73,73,73,73	0
82	MG	1	3934	1/1	0.88	0.29	67,67,67,67	0
81	OHX	sR	1972	7/7	0.88	0.11	158,168,172,227	0
82	MG	1	3824	1/1	0.88	0.21	62,62,62,62	0
82	MG	1	4055	1/1	0.88	0.29	68,68,68,68	0
82	MG	A	2019	1/1	0.88	0.08	70,70,70,70	0
82	MG	AR	3760	1/1	0.88	0.23	43,43,43,43	0
81	OHX	1	3608[B]	7/7	0.88	0.20	132,136,138,169	7
82	MG	1	3943	1/1	0.88	0.13	61,61,61,61	0
82	MG	1	3946	1/1	0.88	0.10	55,55,55,55	0
82	MG	1	3831	1/1	0.88	0.29	80,80,80,80	0
81	OHX	A	1949	7/7	0.88	0.12	189,190,195,258	0
82	MG	1	3951	1/1	0.88	0.18	61,61,61,61	0
81	OHX	AR	3623	7/7	0.88	0.11	166,175,187,245	0
82	MG	A	2034	1/1	0.88	0.11	71,71,71,71	0
81	OHX	AR	3688	7/7	0.88	0.12	173,177,185,281	0
82	MG	1	3839	1/1	0.88	0.20	90,90,90,90	0
81	OHX	AR	3626	7/7	0.88	0.11	148,159,167,245	0
82	MG	1	3715	1/1	0.88	0.36	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AR	4136	1/1	0.88	0.26	41,41,41,41	0
82	MG	AR	3778	1/1	0.88	0.29	76,76,76,76	0
81	OHX	1	4128	7/7	0.88	0.11	145,160,169,252	0
81	OHX	sR	2178	7/7	0.88	0.10	222,230,236,314	0
82	MG	1	3723	1/1	0.88	0.31	44,44,44,44	0
82	MG	sR	2165	1/1	0.88	0.16	66,66,66,66	0
82	MG	sR	2166	1/1	0.88	0.11	58,58,58,58	0
82	MG	3	213	1/1	0.88	0.09	65,65,65,65	0
82	MG	AR	3787	1/1	0.88	0.25	45,45,45,45	0
81	OHX	4	215	7/7	0.88	0.13	165,169,180,262	0
82	MG	s8	303	1/1	0.88	0.17	63,63,63,63	0
81	OHX	1	3580	7/7	0.88	0.14	157,163,168,240	0
82	MG	AR	3806	1/1	0.88	0.32	45,45,45,45	0
82	MG	1	3972	1/1	0.88	0.24	74,74,74,74	0
82	MG	c8	202	1/1	0.88	0.43	79,79,79,79	0
82	MG	AR	4156	1/1	0.88	0.17	52,52,52,52	0
81	OHX	1	3539	7/7	0.88	0.16	142,147,150,225	0
81	OHX	sR	2002	7/7	0.88	0.14	166,168,176,259	0
82	MG	1	3856	1/1	0.88	0.16	48,48,48,48	0
82	MG	1	3979	1/1	0.88	0.15	65,65,65,65	0
82	MG	1	3864	1/1	0.89	0.08	60,60,60,60	0
81	OHX	A	1967	7/7	0.89	0.12	178,182,189,251	0
82	MG	AR	3893	1/1	0.89	0.27	61,61,61,61	0
82	MG	AR	3894	1/1	0.89	0.11	64,64,64,64	0
82	MG	A	2043	1/1	0.89	0.14	76,76,76,76	0
81	OHX	AR	3659	7/7	0.89	0.15	145,151,157,233	0
81	OHX	A	1969	7/7	0.89	0.12	153,155,163,208	0
82	MG	1	3870	1/1	0.89	0.12	74,74,74,74	0
82	MG	1	3622	1/1	0.89	0.19	49,49,49,49	0
82	MG	x	204	1/1	0.89	0.36	57,57,57,57	0
82	MG	x	207	1/1	0.89	0.39	89,89,89,89	0
82	MG	1	3989	1/1	0.89	0.20	68,68,68,68	0
81	OHX	1	3576	7/7	0.89	0.09	191,192,203,265	0
82	MG	A	2056	1/1	0.89	0.10	83,83,83,83	0
82	MG	1	3873	1/1	0.89	0.37	67,67,67,67	0
82	MG	1	3995	1/1	0.89	0.42	50,50,50,50	0
82	MG	AR	3915	1/1	0.89	0.25	71,71,71,71	0
82	MG	1	3997	1/1	0.89	0.20	55,55,55,55	0
82	MG	1	3998	1/1	0.89	0.17	64,64,64,64	0
81	OHX	AR	3537	7/7	0.89	0.12	143,148,158,214	0
81	OHX	1	4132	7/7	0.89	0.09	230,235,238,284	0
81	OHX	AR	3551	7/7	0.89	0.12	143,146,158,232	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AR	3697	1/1	0.89	0.19	45,45,45,45	0
82	MG	AR	3926	1/1	0.89	0.30	69,69,69,69	0
82	MG	A	2070	1/1	0.89	0.15	85,85,85,85	0
82	MG	A	2071	1/1	0.89	0.14	75,75,75,75	0
81	OHX	AR	3554	7/7	0.89	0.15	128,130,137,212	0
82	MG	AR	3701	1/1	0.89	0.19	53,53,53,53	0
82	MG	A	2080	1/1	0.89	0.41	67,67,67,67	0
82	MG	AR	3932	1/1	0.89	0.34	60,60,60,60	0
82	MG	1	3890	1/1	0.89	0.13	50,50,50,50	0
82	MG	1	4010	1/1	0.89	0.21	73,73,73,73	0
82	MG	AR	4144	1/1	0.89	0.25	41,41,41,41	0
81	OHX	AR	3632	7/7	0.89	0.10	180,188,200,270	0
81	OHX	1	4068	7/7	0.89	0.14	135,136,149,221	0
81	OHX	1	3507	7/7	0.89	0.13	118,126,130,190	0
81	OHX	1	3604	7/7	0.89	0.11	204,208,214,287	0
82	MG	AR	3948	1/1	0.89	0.15	68,68,68,68	0
82	MG	AR	4154	1/1	0.89	0.28	70,70,70,70	0
82	MG	1	3769	1/1	0.89	0.27	44,44,44,44	0
82	MG	AR	4158	1/1	0.89	0.33	75,75,75,75	0
82	MG	AR	3720	1/1	0.89	0.16	50,50,50,50	0
81	OHX	AR	3591	7/7	0.89	0.13	131,136,146,219	0
81	OHX	AR	3592	6/7	0.89	0.11	155,161,166,245	0
82	MG	AR	3730	1/1	0.89	0.21	65,65,65,65	0
82	MG	AR	3957	1/1	0.89	0.36	61,61,61,61	0
81	OHX	1	3591	7/7	0.89	0.11	172,176,185,258	0
82	MG	1	4021	1/1	0.89	0.14	71,71,71,71	0
81	OHX	sR	2015	7/7	0.89	0.10	195,203,208,267	0
81	OHX	AR	3595	7/7	0.89	0.10	167,174,180,242	0
81	OHX	CG	301	6/7	0.89	0.10	170,175,188,243	0
82	MG	AR	3744	1/1	0.89	0.32	52,52,52,52	0
82	MG	sR	2048	1/1	0.89	0.20	57,57,57,57	0
82	MG	1	3669	1/1	0.89	0.43	76,76,76,76	0
81	OHX	1	3571	7/7	0.89	0.10	147,153,167,237	0
82	MG	AR	4209	1/1	0.89	0.17	94,94,94,94	0
82	MG	1	4027	1/1	0.89	0.16	42,42,42,42	0
81	OHX	1	4125	7/7	0.89	0.14	123,129,144,227	0
82	MG	1	3680	1/1	0.89	0.18	66,66,66,66	0
82	MG	sR	2061	1/1	0.89	0.28	50,50,50,50	0
82	MG	1	3921	1/1	0.89	0.28	78,78,78,78	0
82	MG	1	4038	1/1	0.89	0.28	56,56,56,56	0
82	MG	1	3681	1/1	0.89	0.18	61,61,61,61	0
82	MG	sR	2073	1/1	0.89	0.25	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
82	MG	AS	3529	1/1	0.89	0.19	63,63,63,63	0
82	MG	sR	2076	1/1	0.89	0.16	68,68,68,68	0
82	MG	sR	2079	1/1	0.89	0.31	51,51,51,51	0
81	OHX	AR	3644	7/7	0.89	0.18	150,158,167,250	0
82	MG	1	3686	1/1	0.89	0.31	42,42,42,42	0
82	MG	1	3926	1/1	0.89	0.18	56,56,56,56	0
82	MG	AT	220	1/1	0.89	0.25	60,60,60,60	0
82	MG	sR	2087	1/1	0.89	0.15	59,59,59,59	0
82	MG	1	3927	1/1	0.89	0.14	76,76,76,76	0
81	OHX	AR	3646	7/7	0.89	0.09	181,187,193,279	0
81	OHX	1	4140	7/7	0.89	0.18	105,106,109,139	7
81	OHX	AR	3600	7/7	0.89	0.14	160,164,173,221	0
81	OHX	AR	3602	7/7	0.89	0.11	166,170,181,235	0
81	OHX	AR	3603	7/7	0.89	0.12	118,134,140,226	0
81	OHX	e	102	7/7	0.89	0.10	202,204,212,283	0
82	MG	1	3825	1/1	0.89	0.20	66,66,66,66	0
82	MG	sR	2102	1/1	0.89	0.17	70,70,70,70	0
82	MG	sR	2103	1/1	0.89	0.11	75,75,75,75	0
82	MG	CE	406	1/1	0.89	0.23	62,62,62,62	0
82	MG	1	4060	1/1	0.89	0.12	52,52,52,52	0
82	MG	1	4062	1/1	0.89	0.24	72,72,72,72	0
82	MG	AR	4006	1/1	0.89	0.14	61,61,61,61	0
81	OHX	A	1950	7/7	0.89	0.11	172,180,185,241	0
81	OHX	AR	3605	7/7	0.89	0.11	160,166,175,238	0
82	MG	sR	2115	1/1	0.89	0.10	71,71,71,71	0
82	MG	sR	2117	1/1	0.89	0.18	62,62,62,62	0
82	MG	1	4074	1/1	0.89	0.28	63,63,63,63	0
82	MG	AR	3795	1/1	0.89	0.34	45,45,45,45	0
82	MG	1	4078	1/1	0.89	0.21	42,42,42,42	0
82	MG	CQ	205	1/1	0.89	0.24	50,50,50,50	0
81	OHX	sR	1976	7/7	0.89	0.10	177,186,196,243	0
82	MG	CR	202	1/1	0.89	0.16	74,74,74,74	0
82	MG	1	3947	1/1	0.89	0.18	71,71,71,71	0
82	MG	CX	203	1/1	0.89	0.31	43,43,43,43	0
82	MG	1	4084	1/1	0.89	0.10	79,79,79,79	0
82	MG	1	4086	1/1	0.89	0.15	91,91,91,91	0
81	OHX	sR	2170	7/7	0.89	0.12	156,166,171,233	0
82	MG	AR	4029	1/1	0.89	0.18	66,66,66,66	0
82	MG	1	3710	1/1	0.89	0.34	44,44,44,44	0
81	OHX	sR	1977	7/7	0.89	0.14	151,156,164,219	0
82	MG	A	1980	1/1	0.89	0.29	69,69,69,69	0
82	MG	AR	4038	1/1	0.89	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	AR	3608	7/7	0.89	0.17	145,149,163,239	0
81	OHX	A	1959	7/7	0.89	0.10	175,177,190,248	0
81	OHX	sR	1984	7/7	0.89	0.11	170,181,186,246	0
81	OHX	1	3551	7/7	0.89	0.13	121,131,149,214	0
81	OHX	1	3563	7/7	0.89	0.12	162,164,175,234	0
82	MG	3	216	1/1	0.89	0.08	81,81,81,81	0
82	MG	1	3960	1/1	0.89	0.20	60,60,60,60	0
82	MG	sR	2151	1/1	0.89	0.24	68,68,68,68	0
82	MG	1	3961	1/1	0.89	0.13	78,78,78,78	0
82	MG	AR	3842	1/1	0.89	0.30	53,53,53,53	0
82	MG	4	217	1/1	0.89	0.35	68,68,68,68	0
81	OHX	AR	3616	7/7	0.89	0.10	184,189,198,274	0
82	MG	AR	3847	1/1	0.89	0.33	52,52,52,52	0
82	MG	AR	3849	1/1	0.89	0.36	47,47,47,47	0
82	MG	AR	3855	1/1	0.89	0.35	54,54,54,54	0
81	OHX	s4	301	7/7	0.89	0.12	188,189,203,267	0
82	MG	1	3726	1/1	0.89	0.31	47,47,47,47	0
82	MG	1	3729	1/1	0.89	0.36	64,64,64,64	0
82	MG	1	3854	1/1	0.89	0.10	70,70,70,70	0
82	MG	AR	4070	1/1	0.89	0.14	61,61,61,61	0
82	MG	AR	3866	1/1	0.89	0.40	51,51,51,51	0
81	OHX	sR	1993	7/7	0.89	0.09	194,197,198,261	0
82	MG	1	3857	1/1	0.89	0.38	63,63,63,63	0
81	OHX	sR	1995	7/7	0.89	0.09	226,229,238,302	0
82	MG	AR	3875	1/1	0.89	0.37	68,68,68,68	0
82	MG	AR	3876	1/1	0.89	0.13	53,53,53,53	0
81	OHX	AR	3617	7/7	0.89	0.12	169,173,184,256	0
82	MG	d3	202	1/1	0.89	0.35	67,67,67,67	0
82	MG	AR	3878	1/1	0.89	0.27	43,43,43,43	0
82	MG	AR	4090	1/1	0.89	0.29	75,75,75,75	0
82	MG	AR	4094	1/1	0.89	0.16	89,89,89,89	0
83	SPD	AR	4206	10/10	0.89	0.20	45,49,50,52	0
82	MG	l	401	1/1	0.89	0.34	47,47,47,47	0
81	OHX	1	3542	7/7	0.90	0.12	144,153,164,222	0
82	MG	AR	4180	1/1	0.90	0.26	66,66,66,66	0
82	MG	AR	3874	1/1	0.90	0.20	62,62,62,62	0
82	MG	AR	4186	1/1	0.90	0.32	69,69,69,69	0
82	MG	AR	4015	1/1	0.90	0.27	70,70,70,70	0
82	MG	1	3892	1/1	0.90	0.30	72,72,72,72	0
82	MG	A	2078	1/1	0.90	0.13	64,64,64,64	0
82	MG	1	3643	1/1	0.90	0.12	53,53,53,53	0
82	MG	AR	3722	1/1	0.90	0.31	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	A	2084	1/1	0.90	0.28	57,57,57,57	0
82	MG	AR	4021	1/1	0.90	0.25	63,63,63,63	0
82	MG	AR	4193	1/1	0.90	0.18	71,71,71,71	0
82	MG	1	4079	1/1	0.90	0.19	64,64,64,64	0
82	MG	AR	3880	1/1	0.90	0.25	53,53,53,53	0
82	MG	1	3982	1/1	0.90	0.21	69,69,69,69	0
81	OHX	A	1954	7/7	0.90	0.11	144,152,166,227	0
82	MG	1	3649	1/1	0.90	0.28	61,61,61,61	0
82	MG	AS	3522	1/1	0.90	0.10	82,82,82,82	0
82	MG	1	3820	1/1	0.90	0.16	45,45,45,45	0
82	MG	AR	4031	1/1	0.90	0.18	56,56,56,56	0
82	MG	AS	3528	1/1	0.90	0.17	56,56,56,56	0
82	MG	AR	4032	1/1	0.90	0.10	54,54,54,54	0
81	OHX	AR	3666	7/7	0.90	0.10	175,178,188,258	0
82	MG	X	201	1/1	0.90	0.11	58,58,58,58	0
82	MG	AR	3896	1/1	0.90	0.26	56,56,56,56	0
82	MG	AR	4039	1/1	0.90	0.17	76,76,76,76	0
82	MG	sR	2030	1/1	0.90	0.19	53,53,53,53	0
82	MG	AR	4040	1/1	0.90	0.45	81,81,81,81	0
82	MG	1	3727	1/1	0.90	0.46	66,66,66,66	0
82	MG	1	4148	1/1	0.90	0.07	111,111,111,111	0
82	MG	AR	4043	1/1	0.90	0.18	109,109,109,109	0
82	MG	1	3823	1/1	0.90	0.10	67,67,67,67	0
81	OHX	AR	3581	7/7	0.90	0.12	144,152,162,228	0
82	MG	1	3906	1/1	0.90	0.12	55,55,55,55	0
82	MG	sR	2046	1/1	0.90	0.29	51,51,51,51	0
82	MG	AR	4047	1/1	0.90	0.30	81,81,81,81	0
82	MG	3	207	1/1	0.90	0.18	61,61,61,61	0
82	MG	CE	402	1/1	0.90	0.28	52,52,52,52	0
82	MG	CE	405	1/1	0.90	0.33	42,42,42,42	0
81	OHX	AR	3651	7/7	0.90	0.12	151,153,166,247	0
82	MG	sR	2057	1/1	0.90	0.31	87,87,87,87	0
82	MG	sR	2058	1/1	0.90	0.12	79,79,79,79	0
81	OHX	1	3572	7/7	0.90	0.09	160,176,182,239	0
82	MG	AR	3757	1/1	0.90	0.23	66,66,66,66	0
82	MG	1	3829	1/1	0.90	0.11	64,64,64,64	0
81	OHX	AR	3588	7/7	0.90	0.13	165,166,172,266	0
81	OHX	AR	3639	7/7	0.90	0.13	142,144,151,243	0
82	MG	sR	2069	1/1	0.90	0.31	62,62,62,62	0
82	MG	4	203	1/1	0.90	0.10	65,65,65,65	0
82	MG	sR	2071	1/1	0.90	0.28	65,65,65,65	0
82	MG	sR	2072	1/1	0.90	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	AR	3589	6/7	0.90	0.16	133,145,147,221	0
82	MG	1	3670	1/1	0.90	0.22	42,42,42,42	0
82	MG	sR	2075	1/1	0.90	0.20	69,69,69,69	0
82	MG	4	219	1/1	0.90	0.23	72,72,72,72	0
82	MG	sR	2078	1/1	0.90	0.18	53,53,53,53	0
82	MG	AR	4066	1/1	0.90	0.12	73,73,73,73	0
81	OHX	AR	3619	7/7	0.90	0.09	173,184,189,237	0
82	MG	AR	4068	1/1	0.90	0.28	69,69,69,69	0
82	MG	CR	205	1/1	0.90	0.14	68,68,68,68	0
81	OHX	1	3506	7/7	0.90	0.14	111,121,143,197	0
81	OHX	sR	1961	7/7	0.90	0.15	127,135,144,201	0
82	MG	AR	3929	1/1	0.90	0.25	49,49,49,49	0
82	MG	DC	202	1/1	0.90	0.21	64,64,64,64	0
81	OHX	1	3570	7/7	0.90	0.08	201,206,212,264	0
82	MG	sR	2091	1/1	0.90	0.19	74,74,74,74	0
82	MG	4	229	1/1	0.90	0.17	68,68,68,68	0
82	MG	AR	3777	1/1	0.90	0.34	54,54,54,54	0
82	MG	AR	3934	1/1	0.90	0.11	50,50,50,50	0
82	MG	1	3752	1/1	0.90	0.07	42,42,42,42	0
81	OHX	CL	302[A]	7/7	0.90	0.29	122,129,137,147	7
82	MG	AR	3937	1/1	0.90	0.23	59,59,59,59	0
82	MG	AR	4088	1/1	0.90	0.13	60,60,60,60	0
81	OHX	CL	302[B]	7/7	0.90	0.29	127,130,140,179	7
82	MG	AR	3944	1/1	0.90	0.23	60,60,60,60	0
81	OHX	AR	4199	7/7	0.90	0.09	174,176,182,262	0
81	OHX	c8	201	7/7	0.90	0.10	168,179,184,232	0
82	MG	AR	4101	1/1	0.90	0.10	69,69,69,69	0
81	OHX	A	1938	7/7	0.90	0.14	139,147,151,222	0
82	MG	AR	3790	1/1	0.90	0.23	49,49,49,49	0
82	MG	sR	2116	1/1	0.90	0.12	78,78,78,78	0
82	MG	1	3618	1/1	0.90	0.27	50,50,50,50	0
82	MG	1	3766	1/1	0.90	0.25	42,42,42,42	0
82	MG	1	3767	1/1	0.90	0.34	51,51,51,51	0
82	MG	sR	2120	1/1	0.90	0.17	65,65,65,65	0
82	MG	AR	4117	1/1	0.90	0.22	47,47,47,47	0
82	MG	AR	3803	1/1	0.90	0.29	45,45,45,45	0
82	MG	1	3696	1/1	0.90	0.19	63,63,63,63	0
82	MG	sR	2125	1/1	0.90	0.08	64,64,64,64	0
82	MG	1	3945	1/1	0.90	0.12	49,49,49,49	0
82	MG	w	201	1/1	0.90	0.27	89,89,89,89	0
82	MG	A	2013	1/1	0.90	0.22	73,73,73,73	0
82	MG	A	2016	1/1	0.90	0.21	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	OHX	sR	2017	7/7	0.90	0.12	163,164,173,262	0
82	MG	sR	2132	1/1	0.90	0.17	68,68,68,68	0
81	OHX	AR	3676	7/7	0.90	0.09	172,178,193,266	0
82	MG	x	206	1/1	0.90	0.28	61,61,61,61	0
82	MG	sR	2135	1/1	0.90	0.32	67,67,67,67	0
82	MG	A	2021	1/1	0.90	0.17	69,69,69,69	0
82	MG	A	2022	1/1	0.90	0.30	64,64,64,64	0
82	MG	sR	2140	1/1	0.90	0.29	66,66,66,66	0
82	MG	AR	3820	1/1	0.90	0.25	51,51,51,51	0
81	OHX	A	1940	7/7	0.90	0.12	163,166,171,231	0
81	OHX	A	1942	7/7	0.90	0.13	145,148,152,220	0
82	MG	AR	3968	1/1	0.90	0.23	66,66,66,66	0
81	OHX	sR	1987	7/7	0.90	0.10	162,169,181,247	0
82	MG	1	3629	1/1	0.90	0.29	64,64,64,64	0
81	OHX	A	2129	7/7	0.90	0.10	172,180,192,257	0
81	OHX	AR	3527	7/7	0.90	0.13	98,105,118,174	0
82	MG	AR	3974	1/1	0.90	0.23	81,81,81,81	0
82	MG	AR	3975	1/1	0.90	0.29	64,64,64,64	0
82	MG	AR	4138	1/1	0.90	0.18	55,55,55,55	0
81	OHX	AR	3594	7/7	0.90	0.11	141,142,148,215	0
82	MG	1	3874	1/1	0.90	0.27	42,42,42,42	0
82	MG	AR	3841	1/1	0.90	0.18	42,42,42,42	0
82	MG	1	3796	1/1	0.90	0.27	45,45,45,45	0
82	MG	A	2044	1/1	0.90	0.20	80,80,80,80	0
81	OHX	AR	3611	7/7	0.90	0.10	154,171,175,231	0
82	MG	AR	3696	1/1	0.90	0.26	66,66,66,66	0
82	MG	AR	4146	1/1	0.90	0.28	42,42,42,42	0
82	MG	AR	3986	1/1	0.90	0.19	56,56,56,56	0
82	MG	A	2049	1/1	0.90	0.12	58,58,58,58	0
82	MG	s1	302	1/1	0.90	0.14	86,86,86,86	0
82	MG	A	2050	1/1	0.90	0.12	81,81,81,81	0
82	MG	1	3878	1/1	0.90	0.16	58,58,58,58	0
82	MG	1	3716	1/1	0.90	0.22	47,47,47,47	0
82	MG	AR	3992	1/1	0.90	0.28	77,77,77,77	0
82	MG	c1	201	1/1	0.90	0.25	68,68,68,68	0
82	MG	1	3880	1/1	0.90	0.26	72,72,72,72	0
82	MG	1	3881	1/1	0.90	0.16	69,69,69,69	0
82	MG	AR	3862	1/1	0.90	0.30	40,40,40,40	0
82	MG	1	3883	1/1	0.90	0.19	60,60,60,60	0
82	MG	1	3887	1/1	0.90	0.28	61,61,61,61	0
82	MG	AR	3711	1/1	0.90	0.29	60,60,60,60	0
81	OHX	AR	3612	7/7	0.90	0.14	134,145,157,232	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AR	4167	1/1	0.90	0.20	51,51,51,51	0
82	MG	1	4064	1/1	0.90	0.32	64,64,64,64	0
82	MG	1	3811	1/1	0.90	0.14	61,61,61,61	0
85	ZN	e1	501	1/1	0.90	0.14	144,144,144,144	0
81	OHX	3	203	7/7	0.91	0.11	144,148,156,216	0
82	MG	A	2082	1/1	0.91	0.36	56,56,56,56	0
81	OHX	sR	1994	7/7	0.91	0.10	162,167,174,232	0
82	MG	1	4066	1/1	0.91	0.35	65,65,65,65	0
82	MG	1	3807	1/1	0.91	0.23	41,41,41,41	0
81	OHX	3	205	7/7	0.91	0.10	152,155,158,210	0
82	MG	AS	3513	1/1	0.91	0.16	62,62,62,62	0
82	MG	A	2090	1/1	0.91	0.10	74,74,74,74	0
82	MG	AR	3725	1/1	0.91	0.24	42,42,42,42	0
82	MG	1	3812	1/1	0.91	0.13	61,61,61,61	0
82	MG	AS	3518	1/1	0.91	0.18	80,80,80,80	0
82	MG	AR	3728	1/1	0.91	0.12	46,46,46,46	0
82	MG	AS	3520	1/1	0.91	0.14	67,67,67,67	0
82	MG	AR	4028	1/1	0.91	0.09	59,59,59,59	0
82	MG	AR	3881	1/1	0.91	0.08	48,48,48,48	0
81	OHX	1	4116	7/7	0.91	0.10	141,152,159,216	0
82	MG	1	3721	1/1	0.91	0.21	46,46,46,46	0
82	MG	A	2151	1/1	0.91	0.08	68,68,68,68	0
82	MG	AR	3888	1/1	0.91	0.30	61,61,61,61	0
82	MG	AT	204	1/1	0.91	0.16	82,82,82,82	0
82	MG	1	3893	1/1	0.91	0.38	65,65,65,65	0
82	MG	AR	3890	1/1	0.91	0.24	86,86,86,86	0
82	MG	AR	3736	1/1	0.91	0.15	60,60,60,60	0
81	OHX	AR	3622	7/7	0.91	0.08	193,195,204,265	0
82	MG	sR	2034	1/1	0.91	0.24	56,56,56,56	0
81	OHX	A	1951	7/7	0.91	0.10	163,167,177,227	0
81	OHX	1	3512	7/7	0.91	0.12	132,137,143,204	0
82	MG	sR	2038	1/1	0.91	0.25	59,59,59,59	0
82	MG	sR	2039	1/1	0.91	0.17	85,85,85,85	0
82	MG	sR	2040	1/1	0.91	0.33	60,60,60,60	0
82	MG	AR	3901	1/1	0.91	0.20	56,56,56,56	0
81	OHX	AR	3597	7/7	0.91	0.12	134,135,145,208	0
82	MG	AR	3745	1/1	0.91	0.23	54,54,54,54	0
82	MG	AT	228	1/1	0.91	0.31	61,61,61,61	0
82	MG	1	3898	1/1	0.91	0.27	46,46,46,46	0
82	MG	1	4150	1/1	0.91	0.24	66,66,66,66	0
82	MG	AR	3906	1/1	0.91	0.20	43,43,43,43	0
82	MG	sR	2054	1/1	0.91	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3657	1/1	0.91	0.32	71,71,71,71	0
82	MG	1	3990	1/1	0.91	0.20	67,67,67,67	0
82	MG	1	3662	1/1	0.91	0.24	54,54,54,54	0
82	MG	AR	4056	1/1	0.91	0.20	59,59,59,59	0
82	MG	AR	3911	1/1	0.91	0.15	64,64,64,64	0
81	OHX	AR	3628	7/7	0.91	0.11	147,151,155,219	0
82	MG	1	3904	1/1	0.91	0.28	67,67,67,67	0
82	MG	sR	2063	1/1	0.91	0.12	59,59,59,59	0
82	MG	AR	3759	1/1	0.91	0.10	80,80,80,80	0
82	MG	sR	2065	1/1	0.91	0.18	57,57,57,57	0
82	MG	sR	2067	1/1	0.91	0.30	48,48,48,48	0
82	MG	AR	4062	1/1	0.91	0.26	53,53,53,53	0
82	MG	3	210	1/1	0.91	0.06	45,45,45,45	0
82	MG	AR	3918	1/1	0.91	0.09	71,71,71,71	0
82	MG	CP	305	1/1	0.91	0.18	66,66,66,66	0
82	MG	1	3996	1/1	0.91	0.17	70,70,70,70	0
81	OHX	AR	3558	7/7	0.91	0.12	151,155,158,217	0
82	MG	1	3826	1/1	0.91	0.21	65,65,65,65	0
82	MG	1	3667	1/1	0.91	0.24	60,60,60,60	0
82	MG	AR	3766	1/1	0.91	0.35	62,62,62,62	0
82	MG	1	3735	1/1	0.91	0.22	46,46,46,46	0
82	MG	AR	3927	1/1	0.91	0.23	49,49,49,49	0
82	MG	sR	2080	1/1	0.91	0.29	69,69,69,69	0
81	OHX	A	1960	7/7	0.91	0.10	190,196,201,255	0
82	MG	1	3916	1/1	0.91	0.17	61,61,61,61	0
82	MG	1	3738	1/1	0.91	0.11	64,64,64,64	0
81	OHX	AR	3574	7/7	0.91	0.12	135,137,141,206	0
82	MG	DO	202	1/1	0.91	0.14	73,73,73,73	0
82	MG	1	3741	1/1	0.91	0.12	52,52,52,52	0
82	MG	sM	302	1/1	0.91	0.12	51,51,51,51	0
82	MG	A	1978	1/1	0.91	0.15	61,61,61,61	0
82	MG	1	3838	1/1	0.91	0.23	75,75,75,75	0
82	MG	1	3671	1/1	0.91	0.26	58,58,58,58	0
82	MG	AR	4086	1/1	0.91	0.10	60,60,60,60	0
82	MG	sR	2094	1/1	0.91	0.11	69,69,69,69	0
81	OHX	1	3577	7/7	0.91	0.11	159,165,171,246	0
82	MG	1	3675	1/1	0.91	0.27	46,46,46,46	0
82	MG	AR	4092	1/1	0.91	0.11	65,65,65,65	0
82	MG	sR	2100	1/1	0.91	0.20	50,50,50,50	0
81	OHX	A	1963	7/7	0.91	0.09	176,182,189,242	0
82	MG	AR	3784	1/1	0.91	0.15	50,50,50,50	0
81	OHX	AR	3601	7/7	0.91	0.13	123,133,142,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AR	4099	1/1	0.91	0.24	123,123,123,123	0
82	MG	sR	2106	1/1	0.91	0.08	63,63,63,63	0
82	MG	1	4019	1/1	0.91	0.07	57,57,57,57	0
82	MG	1	3751	1/1	0.91	0.30	51,51,51,51	0
82	MG	AR	4107	1/1	0.91	0.27	79,79,79,79	0
82	MG	AR	4109	1/1	0.91	0.12	43,43,43,43	0
82	MG	AR	4110	1/1	0.91	0.21	55,55,55,55	0
82	MG	AR	3949	1/1	0.91	0.08	68,68,68,68	0
81	OHX	Q	201	7/7	0.91	0.09	219,224,231,285	0
82	MG	AR	3792	1/1	0.91	0.34	42,42,42,42	0
81	OHX	AP	502	7/7	0.91	0.15	132,140,152,236	0
82	MG	1	3851	1/1	0.91	0.16	70,70,70,70	0
82	MG	AR	3800	1/1	0.91	0.26	42,42,42,42	0
81	OHX	AR	3472	7/7	0.91	0.18	113,115,123,189	0
82	MG	1	3687	1/1	0.91	0.13	45,45,45,45	0
81	OHX	AR	3585	7/7	0.91	0.10	150,160,171,238	0
82	MG	sR	2126	1/1	0.91	0.27	75,75,75,75	0
81	OHX	sR	2014	7/7	0.91	0.10	160,165,174,224	0
82	MG	1	4030	1/1	0.91	0.31	58,58,58,58	0
82	MG	AR	3812	1/1	0.91	0.24	58,58,58,58	0
82	MG	AR	3813	1/1	0.91	0.23	48,48,48,48	0
81	OHX	AR	3685	7/7	0.91	0.11	135,141,158,217	0
82	MG	x	205	1/1	0.91	0.16	50,50,50,50	0
81	OHX	AR	3607	7/7	0.91	0.13	140,148,157,231	0
82	MG	A	2028	1/1	0.91	0.13	97,97,97,97	0
82	MG	AR	3818	1/1	0.91	0.23	41,41,41,41	0
82	MG	1	4036	1/1	0.91	0.33	76,76,76,76	0
82	MG	A	2032	1/1	0.91	0.23	65,65,65,65	0
82	MG	AR	3822	1/1	0.91	0.27	69,69,69,69	0
81	OHX	A	1973	7/7	0.91	0.11	149,151,157,209	0
81	OHX	AR	3586	7/7	0.91	0.11	143,146,155,217	0
81	OHX	1	3550	7/7	0.91	0.09	158,163,171,222	0
81	OHX	AR	3521	7/7	0.91	0.13	94,105,127,178	0
82	MG	AB	202	1/1	0.91	0.16	69,69,69,69	0
82	MG	AB	204	1/1	0.91	0.13	58,58,58,58	0
82	MG	A	2041	1/1	0.91	0.15	96,96,96,96	0
82	MG	AR	3979	1/1	0.91	0.22	76,76,76,76	0
82	MG	1	3777	1/1	0.91	0.18	42,42,42,42	0
82	MG	1	3704	1/1	0.91	0.12	62,62,62,62	0
82	MG	AR	3984	1/1	0.91	0.20	67,67,67,67	0
81	OHX	1	3547	7/7	0.91	0.10	152,157,165,219	0
81	OHX	1	4127	7/7	0.91	0.10	205,209,216,277	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3632	1/1	0.91	0.15	47,47,47,47	0
82	MG	AR	4151	1/1	0.91	0.23	40,40,40,40	0
82	MG	sR	2157	1/1	0.91	0.10	80,80,80,80	0
82	MG	1	4052	1/1	0.91	0.32	70,70,70,70	0
82	MG	1	4053	1/1	0.91	0.27	50,50,50,50	0
82	MG	AR	3848	1/1	0.91	0.22	44,44,44,44	0
81	OHX	AR	3615	7/7	0.91	0.10	165,169,176,235	0
82	MG	A	2054	1/1	0.91	0.22	65,65,65,65	0
82	MG	AR	3995	1/1	0.91	0.18	70,70,70,70	0
82	MG	AR	4159	1/1	0.91	0.12	46,46,46,46	0
82	MG	AR	4160	1/1	0.91	0.29	45,45,45,45	0
82	MG	AR	3852	1/1	0.91	0.27	51,51,51,51	0
81	OHX	AR	3535	7/7	0.91	0.12	110,122,127,191	0
82	MG	AR	3703	1/1	0.91	0.35	41,41,41,41	0
82	MG	1	4056	1/1	0.91	0.26	44,44,44,44	0
82	MG	AR	4002	1/1	0.91	0.14	61,61,61,61	0
82	MG	1	3793	1/1	0.91	0.33	67,67,67,67	0
81	OHX	A	2128	7/7	0.91	0.14	157,161,162,227	0
82	MG	AR	4007	1/1	0.91	0.12	53,53,53,53	0
82	MG	1	3963	1/1	0.91	0.11	71,71,71,71	0
82	MG	d3	204	1/1	0.91	0.27	49,49,49,49	0
82	MG	AR	4009	1/1	0.91	0.08	58,58,58,58	0
82	MG	d4	203	1/1	0.91	0.32	73,73,73,73	0
82	MG	AR	4185	1/1	0.91	0.26	66,66,66,66	0
82	MG	1	3713	1/1	0.91	0.24	52,52,52,52	0
82	MG	d9	102	1/1	0.91	0.11	78,78,78,78	0
82	MG	1	3714	1/1	0.91	0.26	42,42,42,42	0
85	ZN	DI	202	1/1	0.91	0.09	110,110,110,110	0
82	MG	AR	4014	1/1	0.91	0.26	74,74,74,74	0
82	MG	AR	3868	1/1	0.91	0.27	48,48,48,48	0
82	MG	AR	3798	1/1	0.92	0.21	48,48,48,48	0
81	OHX	1	3537	7/7	0.92	0.10	143,146,154,212	0
82	MG	A	2077	1/1	0.92	0.10	76,76,76,76	0
81	OHX	DQ	502	7/7	0.92	0.15	142,151,165,248	0
82	MG	AR	3802	1/1	0.92	0.38	49,49,49,49	0
82	MG	1	3753	1/1	0.92	0.22	61,61,61,61	0
82	MG	AR	4173	1/1	0.92	0.29	59,59,59,59	0
82	MG	4	218	1/1	0.92	0.31	69,69,69,69	0
81	OHX	A	1926	7/7	0.92	0.11	176,177,181,232	0
82	MG	AR	4181	1/1	0.92	0.15	61,61,61,61	0
82	MG	AR	4183	1/1	0.92	0.09	51,51,51,51	0
81	OHX	A	1933	7/7	0.92	0.10	147,151,157,219	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3758	1/1	0.92	0.32	44,44,44,44	0
81	OHX	A	1935	7/7	0.92	0.12	152,158,167,223	0
81	OHX	1	3509	7/7	0.92	0.12	138,139,146,210	0
81	OHX	1	3558	7/7	0.92	0.10	153,158,166,235	0
82	MG	1	3676	1/1	0.92	0.19	43,43,43,43	0
82	MG	AR	4190	1/1	0.92	0.18	76,76,76,76	0
81	OHX	1	3541	7/7	0.92	0.10	137,144,156,203	0
82	MG	1	3679	1/1	0.92	0.23	68,68,68,68	0
82	MG	AR	4001	1/1	0.92	0.22	58,58,58,58	0
82	MG	AR	4194	1/1	0.92	0.11	72,72,72,72	0
81	OHX	AR	3590	7/7	0.92	0.12	147,148,154,218	0
82	MG	F	301	1/1	0.92	0.16	81,81,81,81	0
81	OHX	1	3511	7/7	0.92	0.12	142,148,154,222	0
82	MG	j	303	1/1	0.92	0.10	50,50,50,50	0
81	OHX	1	3487	7/7	0.92	0.13	114,119,125,182	0
82	MG	sR	2029	1/1	0.92	0.28	60,60,60,60	0
82	MG	AR	3828	1/1	0.92	0.38	56,56,56,56	0
82	MG	1	3882	1/1	0.92	0.23	63,63,63,63	0
82	MG	o	301	1/1	0.92	0.18	65,65,65,65	0
82	MG	1	3772	1/1	0.92	0.18	59,59,59,59	0
82	MG	r	303	1/1	0.92	0.14	55,55,55,55	0
82	MG	AS	3523	1/1	0.92	0.09	80,80,80,80	0
82	MG	AR	3837	1/1	0.92	0.24	41,41,41,41	0
82	MG	1	4000	1/1	0.92	0.12	106,106,106,106	0
82	MG	t	201	1/1	0.92	0.08	63,63,63,63	0
82	MG	sR	2041	1/1	0.92	0.30	55,55,55,55	0
82	MG	AR	4019	1/1	0.92	0.08	68,68,68,68	0
82	MG	1	3684	1/1	0.92	0.31	57,57,57,57	0
82	MG	sR	2044	1/1	0.92	0.22	63,63,63,63	0
81	OHX	1	3514	7/7	0.92	0.12	143,150,160,217	0
82	MG	AR	3845	1/1	0.92	0.26	43,43,43,43	0
82	MG	v	304	1/1	0.92	0.32	63,63,63,63	0
82	MG	sR	2049	1/1	0.92	0.15	67,67,67,67	0
82	MG	1	3889	1/1	0.92	0.18	70,70,70,70	0
82	MG	x	201	1/1	0.92	0.20	42,42,42,42	0
82	MG	sR	2052	1/1	0.92	0.20	65,65,65,65	0
82	MG	sR	2053	1/1	0.92	0.16	59,59,59,59	0
82	MG	1	4005	1/1	0.92	0.19	102,102,102,102	0
82	MG	1	3779	1/1	0.92	0.26	49,49,49,49	0
82	MG	1	4008	1/1	0.92	0.09	67,67,67,67	0
81	OHX	sR	1967	7/7	0.92	0.12	149,155,160,214	0
82	MG	1	3782	1/1	0.92	0.35	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
82	MG	1	4011	1/1	0.92	0.31	76,76,76,76	0
82	MG	AT	230	1/1	0.92	0.25	48,48,48,48	0
82	MG	AR	4035	1/1	0.92	0.09	70,70,70,70	0
82	MG	sR	2062	1/1	0.92	0.21	62,62,62,62	0
82	MG	6	201	1/1	0.92	0.33	46,46,46,46	0
82	MG	1	3783	1/1	0.92	0.28	43,43,43,43	0
82	MG	1	3785	1/1	0.92	0.19	42,42,42,42	0
81	OHX	sR	1969	7/7	0.92	0.11	129,131,137,202	0
81	OHX	1	3616	7/7	0.92	0.15	95,107,115,153	0
81	OHX	1	3546	7/7	0.92	0.11	147,149,163,226	0
81	OHX	1	4139	7/7	0.92	0.27	106,108,110,130	7
82	MG	CG	304	1/1	0.92	0.08	63,63,63,63	0
82	MG	CI	301	1/1	0.92	0.14	65,65,65,65	0
81	OHX	1	3516	7/7	0.92	0.10	162,167,172,227	0
82	MG	1	3901	1/1	0.92	0.36	76,76,76,76	0
82	MG	AG	203	1/1	0.92	0.26	62,62,62,62	0
81	OHX	1	4141	7/7	0.92	0.09	169,173,183,222	7
82	MG	1	3698	1/1	0.92	0.23	54,54,54,54	0
82	MG	CP	304	1/1	0.92	0.14	56,56,56,56	0
82	MG	AR	3693	1/1	0.92	0.11	54,54,54,54	0
82	MG	1	3699	1/1	0.92	0.34	60,60,60,60	0
82	MG	AR	4054	1/1	0.92	0.17	53,53,53,53	0
81	OHX	1	3469	7/7	0.92	0.14	88,105,112,161	0
82	MG	AR	3698	1/1	0.92	0.28	62,62,62,62	0
81	OHX	1	4107	7/7	0.92	0.11	110,115,125,171	0
81	OHX	3	204	7/7	0.92	0.11	142,146,150,216	0
82	MG	1	3911	1/1	0.92	0.11	59,59,59,59	0
82	MG	AR	3891	1/1	0.92	0.22	52,52,52,52	0
82	MG	DC	201	1/1	0.92	0.29	74,74,74,74	0
81	OHX	sR	1988	7/7	0.92	0.10	147,165,166,226	0
81	OHX	1	3524	7/7	0.92	0.12	151,156,172,246	0
82	MG	DH	201	1/1	0.92	0.13	59,59,59,59	0
82	MG	AR	3709	1/1	0.92	0.23	62,62,62,62	0
82	MG	AR	3898	1/1	0.92	0.14	68,68,68,68	0
82	MG	sR	2097	1/1	0.92	0.13	74,74,74,74	0
82	MG	1	3813	1/1	0.92	0.23	64,64,64,64	0
82	MG	1	3917	1/1	0.92	0.11	76,76,76,76	0
82	MG	sR	2101	1/1	0.92	0.15	87,87,87,87	0
82	MG	1	4034	1/1	0.92	0.35	52,52,52,52	0
82	MG	1	4035	1/1	0.92	0.34	61,61,61,61	0
82	MG	AR	4071	1/1	0.92	0.14	67,67,67,67	0
81	OHX	AR	3556	7/7	0.92	0.14	116,120,128,188	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	AR	3604	7/7	0.92	0.11	144,149,156,235	0
81	OHX	A	1965	7/7	0.92	0.09	173,176,192,241	0
82	MG	AR	3907	1/1	0.92	0.20	53,53,53,53	0
81	OHX	1	3503	7/7	0.92	0.11	115,129,139,214	0
81	OHX	AR	3561	7/7	0.92	0.14	120,126,133,199	0
82	MG	A	1995	1/1	0.92	0.29	58,58,58,58	0
81	OHX	AR	3562	7/7	0.92	0.13	136,140,150,212	0
82	MG	A	1997	1/1	0.92	0.23	59,59,59,59	0
82	MG	1	3624	1/1	0.92	0.19	45,45,45,45	0
82	MG	AR	4085	1/1	0.92	0.20	66,66,66,66	0
82	MG	AR	3912	1/1	0.92	0.16	72,72,72,72	0
82	MG	AR	4087	1/1	0.92	0.18	44,44,44,44	0
81	OHX	sR	1998	7/7	0.92	0.11	154,160,167,230	0
82	MG	AR	3729	1/1	0.92	0.22	59,59,59,59	0
82	MG	AR	4091	1/1	0.92	0.07	75,75,75,75	0
81	OHX	AR	3609	7/7	0.92	0.13	143,149,156,236	0
81	OHX	AR	3610	7/7	0.92	0.14	125,131,141,202	0
82	MG	1	3929	1/1	0.92	0.13	55,55,55,55	0
81	OHX	A	1972	7/7	0.92	0.09	188,192,196,254	0
82	MG	1	3722	1/1	0.92	0.23	48,48,48,48	0
82	MG	AR	3739	1/1	0.92	0.19	63,63,63,63	0
81	OHX	AR	3563	7/7	0.92	0.12	125,136,151,197	0
82	MG	AR	4105	1/1	0.92	0.16	52,52,52,52	0
82	MG	1	3830	1/1	0.92	0.32	69,69,69,69	0
81	OHX	AR	3568	7/7	0.92	0.11	109,112,122,183	0
81	OHX	AR	3570	7/7	0.92	0.11	135,139,149,221	0
81	OHX	AR	3571	7/7	0.92	0.12	126,131,136,205	0
82	MG	1	3942	1/1	0.92	0.11	54,54,54,54	0
82	MG	A	2025	1/1	0.92	0.19	78,78,78,78	0
81	OHX	AR	3572	7/7	0.92	0.11	130,135,146,206	0
82	MG	sR	2143	1/1	0.92	0.32	76,76,76,76	0
82	MG	1	4063	1/1	0.92	0.10	43,43,43,43	0
82	MG	AR	3752	1/1	0.92	0.15	57,57,57,57	0
82	MG	1	3837	1/1	0.92	0.10	47,47,47,47	0
82	MG	1	3728	1/1	0.92	0.24	45,45,45,45	0
81	OHX	AR	3573	7/7	0.92	0.10	146,154,166,230	0
82	MG	1	4067	1/1	0.92	0.11	54,54,54,54	0
81	OHX	1	3526	7/7	0.92	0.10	155,161,165,229	0
81	OHX	1	3606	7/7	0.92	0.13	143,146,152,218	0
82	MG	1	3950	1/1	0.92	0.35	68,68,68,68	0
82	MG	1	3646	1/1	0.92	0.23	55,55,55,55	0
82	MG	1	4080	1/1	0.92	0.29	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	4081	1/1	0.92	0.10	68,68,68,68	0
82	MG	AR	3951	1/1	0.92	0.38	63,63,63,63	0
82	MG	1	3647	1/1	0.92	0.22	65,65,65,65	0
81	OHX	1	3553	7/7	0.92	0.14	142,147,153,223	0
82	MG	1	3954	1/1	0.92	0.22	68,68,68,68	0
82	MG	sR	2163	1/1	0.92	0.09	70,70,70,70	0
81	OHX	AR	3621	7/7	0.92	0.11	142,147,158,228	0
82	MG	1	3848	1/1	0.92	0.25	62,62,62,62	0
81	OHX	AR	3579	7/7	0.92	0.10	116,122,129,189	0
81	OHX	1	3534	7/7	0.92	0.11	116,124,135,201	0
81	OHX	AR	3584	7/7	0.92	0.09	134,138,153,217	0
82	MG	1	3656	1/1	0.92	0.10	94,94,94,94	0
82	MG	AR	3779	1/1	0.92	0.14	42,42,42,42	0
82	MG	AR	3780	1/1	0.92	0.18	47,47,47,47	0
81	OHX	1	3573	7/7	0.92	0.10	150,156,169,225	0
82	MG	1	3964	1/1	0.92	0.13	60,60,60,60	0
82	MG	c4	2201	1/1	0.92	0.08	74,74,74,74	0
82	MG	c4	2202	1/1	0.92	0.17	57,57,57,57	0
82	MG	AR	3783	1/1	0.92	0.19	65,65,65,65	0
82	MG	AR	3967	1/1	0.92	0.11	66,66,66,66	0
82	MG	1	3855	1/1	0.92	0.15	51,51,51,51	0
82	MG	1	3747	1/1	0.92	0.33	47,47,47,47	0
82	MG	1	3968	1/1	0.92	0.20	76,76,76,76	0
82	MG	A	2060	1/1	0.92	0.20	74,74,74,74	0
82	MG	3	211	1/1	0.92	0.31	45,45,45,45	0
82	MG	AR	3789	1/1	0.92	0.31	44,44,44,44	0
81	OHX	AR	3629	7/7	0.92	0.10	151,153,163,227	0
82	MG	AR	3791	1/1	0.92	0.32	41,41,41,41	0
82	MG	1	3858	1/1	0.92	0.12	47,47,47,47	0
82	MG	AR	3794	1/1	0.92	0.09	55,55,55,55	0
84	XBI	AR	4222	26/26	0.92	0.14	57,61,64,65	0
82	MG	1	3749	1/1	0.92	0.22	48,48,48,48	0
81	OHX	CS	201	7/7	0.92	0.12	143,146,151,232	0
82	MG	AR	4163	1/1	0.92	0.13	51,51,51,51	0
82	MG	AR	3950	1/1	0.93	0.09	45,45,45,45	0
82	MG	sR	1902	1/1	0.93	0.12	69,69,69,69	0
82	MG	1	3689	1/1	0.93	0.25	71,71,71,71	0
82	MG	1	4047	1/1	0.93	0.23	51,51,51,51	0
82	MG	AR	3811	1/1	0.93	0.36	41,41,41,41	0
82	MG	sR	2032	1/1	0.93	0.14	73,73,73,73	0
81	OHX	A	2124	7/7	0.93	0.08	180,185,197,258	0
81	OHX	AR	3517	7/7	0.93	0.11	125,136,143,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AR	3814	1/1	0.93	0.17	53,53,53,53	0
81	OHX	AR	3687[A]	7/7	0.93	0.21	134,135,139,158	7
81	OHX	A	1934	7/7	0.93	0.08	177,179,181,226	0
82	MG	AR	3691	1/1	0.93	0.19	45,45,45,45	0
81	OHX	AR	3687[B]	7/7	0.93	0.21	129,134,139,161	7
82	MG	AR	3819	1/1	0.93	0.34	40,40,40,40	0
81	OHX	AR	3657	7/7	0.93	0.08	207,211,215,269	0
82	MG	AR	3695	1/1	0.93	0.36	58,58,58,58	0
82	MG	CR	204	1/1	0.93	0.31	58,58,58,58	0
81	OHX	1	3545	7/7	0.93	0.09	205,206,211,259	0
81	OHX	AR	3523	7/7	0.93	0.10	142,146,156,214	0
82	MG	AR	4108	1/1	0.93	0.39	63,63,63,63	0
82	MG	1	3868	1/1	0.93	0.28	61,61,61,61	0
82	MG	DA	202	1/1	0.93	0.33	65,65,65,65	0
81	OHX	1	4126	7/7	0.93	0.08	175,185,196,270	0
81	OHX	1	3480	7/7	0.93	0.13	119,127,135,181	0
81	OHX	1	4103	7/7	0.93	0.13	122,126,130,197	0
82	MG	DF	201	1/1	0.93	0.17	63,63,63,63	0
82	MG	1	3706	1/1	0.93	0.11	45,45,45,45	0
82	MG	AR	3834	1/1	0.93	0.27	54,54,54,54	0
82	MG	AR	4116	1/1	0.93	0.14	85,85,85,85	0
81	OHX	1	3587	7/7	0.93	0.11	143,149,157,220	0
82	MG	DQ	504	1/1	0.93	0.23	56,56,56,56	0
81	OHX	1	3517	7/7	0.93	0.10	134,147,152,214	0
82	MG	A	1976	1/1	0.93	0.17	72,72,72,72	0
81	OHX	AR	3636	7/7	0.93	0.09	142,153,161,222	0
81	OHX	AR	3548	7/7	0.93	0.11	125,127,139,193	0
82	MG	AR	3712	1/1	0.93	0.16	46,46,46,46	0
82	MG	AR	3843	1/1	0.93	0.38	52,52,52,52	0
82	MG	sR	2066	1/1	0.93	0.22	46,46,46,46	0
82	MG	A	1983	1/1	0.93	0.15	63,63,63,63	0
82	MG	A	1984	1/1	0.93	0.19	68,68,68,68	0
81	OHX	v	301	7/7	0.93	0.11	128,130,143,200	0
82	MG	A	1986	1/1	0.93	0.17	60,60,60,60	0
82	MG	A	1987	1/1	0.93	0.06	57,57,57,57	0
82	MG	1	4073	1/1	0.93	0.24	69,69,69,69	0
82	MG	1	3969	1/1	0.93	0.11	66,66,66,66	0
82	MG	1	3791	1/1	0.93	0.30	54,54,54,54	0
82	MG	1	3639	1/1	0.93	0.34	62,62,62,62	0
82	MG	A	1993	1/1	0.93	0.34	63,63,63,63	0
82	MG	sR	2077	1/1	0.93	0.39	70,70,70,70	0
82	MG	A	1994	1/1	0.93	0.24	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AR	3987	1/1	0.93	0.17	56,56,56,56	0
82	MG	1	3641	1/1	0.93	0.18	47,47,47,47	0
81	OHX	AR	3552	7/7	0.93	0.12	116,124,133,190	0
82	MG	AR	3724	1/1	0.93	0.30	56,56,56,56	0
82	MG	1	3884	1/1	0.93	0.27	65,65,65,65	0
82	MG	sR	2085	1/1	0.93	0.20	54,54,54,54	0
81	OHX	A	1957	7/7	0.93	0.11	173,174,180,238	0
81	OHX	AR	4205	6/7	0.93	0.11	139,142,146,213	0
82	MG	1	3800	1/1	0.93	0.26	44,44,44,44	0
82	MG	1	3981	1/1	0.93	0.17	54,54,54,54	0
82	MG	AR	3998	1/1	0.93	0.28	63,63,63,63	0
82	MG	1	3803	1/1	0.93	0.29	48,48,48,48	0
81	OHX	AS	3509	7/7	0.93	0.11	129,134,140,197	0
82	MG	AR	3734	1/1	0.93	0.19	41,41,41,41	0
82	MG	AR	3735	1/1	0.93	0.24	51,51,51,51	0
81	OHX	1	3518	7/7	0.93	0.10	134,138,148,204	0
82	MG	AR	4005	1/1	0.93	0.20	41,41,41,41	0
81	OHX	sR	1956	7/7	0.93	0.11	138,142,149,177	0
81	OHX	AR	3555	7/7	0.93	0.10	125,131,136,197	0
81	OHX	1	4118	7/7	0.93	0.09	131,137,141,211	0
81	OHX	sR	1965	7/7	0.93	0.09	122,124,135,187	0
82	MG	1	3991	1/1	0.93	0.09	68,68,68,68	0
81	OHX	sR	1966	7/7	0.93	0.10	123,126,142,203	0
82	MG	1	3816	1/1	0.93	0.15	55,55,55,55	0
82	MG	1	3994	1/1	0.93	0.16	42,42,42,42	0
82	MG	1	3655	1/1	0.93	0.22	42,42,42,42	0
82	MG	sR	2108	1/1	0.93	0.11	73,73,73,73	0
82	MG	1	3900	1/1	0.93	0.26	58,58,58,58	0
81	OHX	1	3528	7/7	0.93	0.10	122,129,133,195	0
82	MG	sR	2111	1/1	0.93	0.08	78,78,78,78	0
82	MG	AR	3754	1/1	0.93	0.19	42,42,42,42	0
81	OHX	AR	3560	7/7	0.93	0.10	146,149,155,217	0
82	MG	1	3658	1/1	0.93	0.18	57,57,57,57	0
82	MG	1	3660	1/1	0.93	0.34	64,64,64,64	0
81	OHX	AR	3645	7/7	0.93	0.10	127,134,149,214	0
82	MG	A	2035	1/1	0.93	0.12	60,60,60,60	0
82	MG	AR	3897	1/1	0.93	0.13	44,44,44,44	0
82	MG	1	3733	1/1	0.93	0.30	45,45,45,45	0
82	MG	AR	3761	1/1	0.93	0.25	44,44,44,44	0
82	MG	1	3907	1/1	0.93	0.09	84,84,84,84	0
82	MG	4	221	1/1	0.93	0.34	46,46,46,46	0
82	MG	AR	4182	1/1	0.93	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3734	1/1	0.93	0.18	43,43,43,43	0
82	MG	AR	4033	1/1	0.93	0.09	58,58,58,58	0
81	OHX	sR	1973	7/7	0.93	0.11	138,142,146,199	0
82	MG	1	3664	1/1	0.93	0.29	60,60,60,60	0
82	MG	AR	4037	1/1	0.93	0.09	57,57,57,57	0
82	MG	1	3914	1/1	0.93	0.23	56,56,56,56	0
82	MG	1	3828	1/1	0.93	0.07	59,59,59,59	0
81	OHX	sR	1975	7/7	0.93	0.13	126,136,142,209	0
81	OHX	1	3532	7/7	0.93	0.10	148,152,158,217	0
81	OHX	3	218	7/7	0.93	0.11	129,140,144,204	0
81	OHX	AR	3494	7/7	0.93	0.09	122,127,138,190	0
82	MG	1	3833	1/1	0.93	0.29	65,65,65,65	0
81	OHX	AR	3564	7/7	0.93	0.08	162,164,168,220	0
82	MG	1	3835	1/1	0.93	0.10	78,78,78,78	0
81	OHX	sR	1981	7/7	0.93	0.11	150,153,160,211	0
82	MG	1	3673	1/1	0.93	0.33	45,45,45,45	0
82	MG	AS	3515	1/1	0.93	0.33	48,48,48,48	0
82	MG	AS	3516	1/1	0.93	0.16	68,68,68,68	0
82	MG	1	3925	1/1	0.93	0.07	68,68,68,68	0
82	MG	A	2061	1/1	0.93	0.18	86,86,86,86	0
82	MG	1	3674	1/1	0.93	0.23	42,42,42,42	0
81	OHX	AR	3620	7/7	0.93	0.09	150,159,167,227	0
82	MG	AR	4053	1/1	0.93	0.16	73,73,73,73	0
81	OHX	sR	1985	7/7	0.93	0.12	129,136,147,202	0
81	OHX	AR	3565	7/7	0.93	0.11	127,134,141,209	0
82	MG	AS	3524	1/1	0.93	0.14	62,62,62,62	0
81	OHX	AR	3567	7/7	0.93	0.10	139,141,150,213	0
81	OHX	1	3508	7/7	0.93	0.10	125,128,134,192	0
82	MG	AR	4059	1/1	0.93	0.23	76,76,76,76	0
82	MG	AR	3788	1/1	0.93	0.30	43,43,43,43	0
82	MG	sR	2159	1/1	0.93	0.13	68,68,68,68	0
82	MG	A	2075	1/1	0.93	0.24	59,59,59,59	0
81	OHX	AR	3569	7/7	0.93	0.09	150,153,164,226	0
82	MG	sR	2162	1/1	0.93	0.09	47,47,47,47	0
81	OHX	sR	1990	7/7	0.93	0.09	164,170,177,235	0
82	MG	AT	217	1/1	0.93	0.16	49,49,49,49	0
82	MG	x	203	1/1	0.93	0.23	50,50,50,50	0
82	MG	AR	3931	1/1	0.93	0.10	61,61,61,61	0
82	MG	1	3756	1/1	0.93	0.22	63,63,63,63	0
82	MG	AT	221	1/1	0.93	0.23	63,63,63,63	0
81	OHX	AR	3627	7/7	0.93	0.10	125,130,138,199	0
82	MG	1	3759	1/1	0.93	0.32	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AR	3796	1/1	0.93	0.23	57,57,57,57	0
82	MG	AT	225	1/1	0.93	0.12	51,51,51,51	0
82	MG	A	2089	1/1	0.93	0.05	65,65,65,65	0
82	MG	1	3938	1/1	0.93	0.31	70,70,70,70	0
82	MG	A	2091	1/1	0.93	0.26	61,61,61,61	0
82	MG	1	3939	1/1	0.93	0.17	69,69,69,69	0
82	MG	AR	3941	1/1	0.93	0.07	47,47,47,47	0
82	MG	A	2094	1/1	0.93	0.39	76,76,76,76	0
82	MG	c9	201	1/1	0.93	0.06	74,74,74,74	0
81	OHX	sR	1992	7/7	0.93	0.09	156,167,174,233	0
82	MG	AR	3943	1/1	0.93	0.20	52,52,52,52	0
81	OHX	A	2120	7/7	0.93	0.10	155,159,163,211	0
82	MG	d4	201	1/1	0.93	0.13	64,64,64,64	0
82	MG	CD	303	1/1	0.93	0.22	64,64,64,64	0
82	MG	1	3944	1/1	0.93	0.16	43,43,43,43	0
82	MG	1	3763	1/1	0.93	0.28	48,48,48,48	0
82	MG	AR	3805	1/1	0.93	0.11	45,45,45,45	0
81	OHX	A	1923	7/7	0.93	0.10	140,145,150,200	0
82	MG	AR	4081	1/1	0.93	0.09	61,61,61,61	0
84	XBI	1	4157	26/26	0.93	0.13	50,53,56,58	0
82	MG	O	202	1/1	0.93	0.22	71,71,71,71	0
82	MG	P	201	1/1	0.93	0.07	69,69,69,69	0
82	MG	AR	4083	1/1	0.93	0.18	69,69,69,69	0
82	MG	CF	401	1/1	0.93	0.17	62,62,62,62	0
81	OHX	A	1956	7/7	0.94	0.09	171,176,182,233	0
81	OHX	sR	2174	7/7	0.94	0.26	101,103,104,133	7
81	OHX	sR	1971	7/7	0.94	0.09	137,143,151,206	0
81	OHX	AR	3662	7/7	0.94	0.08	183,190,194,244	0
82	MG	1	3773	1/1	0.94	0.37	51,51,51,51	0
82	MG	AR	4114	1/1	0.94	0.08	69,69,69,69	0
81	OHX	AR	3544	7/7	0.94	0.11	122,129,135,206	0
82	MG	sR	2047	1/1	0.94	0.28	60,60,60,60	0
82	MG	DH	202	1/1	0.94	0.07	57,57,57,57	0
82	MG	AR	3699	1/1	0.94	0.29	47,47,47,47	0
81	OHX	AR	3546	7/7	0.94	0.11	125,129,141,215	0
82	MG	AR	3973	1/1	0.94	0.23	57,57,57,57	0
82	MG	1	4061	1/1	0.94	0.14	59,59,59,59	0
82	MG	AR	3702	1/1	0.94	0.14	42,42,42,42	0
82	MG	AR	3833	1/1	0.94	0.26	59,59,59,59	0
82	MG	1	3694	1/1	0.94	0.18	45,45,45,45	0
82	MG	AR	3705	1/1	0.94	0.07	70,70,70,70	0
81	OHX	AS	3506	7/7	0.94	0.12	114,116,127,186	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3965	1/1	0.94	0.40	64,64,64,64	0
81	OHX	4	211	7/7	0.94	0.09	141,146,157,207	0
82	MG	AR	4127	1/1	0.94	0.37	75,75,75,75	0
81	OHX	sR	1978	7/7	0.94	0.11	110,114,122,186	0
82	MG	1	3784	1/1	0.94	0.20	40,40,40,40	0
82	MG	1	4069	1/1	0.94	0.32	59,59,59,59	0
81	OHX	1	3510	7/7	0.94	0.10	130,137,145,214	0
81	OHX	1	3533	7/7	0.94	0.12	140,143,144,215	0
81	OHX	1	4108	7/7	0.94	0.09	108,124,125,191	0
82	MG	AR	3991	1/1	0.94	0.22	44,44,44,44	0
82	MG	1	4077	1/1	0.94	0.16	59,59,59,59	0
81	OHX	sR	1982	7/7	0.94	0.10	151,153,164,216	0
82	MG	AR	3851	1/1	0.94	0.30	54,54,54,54	0
82	MG	1	3703	1/1	0.94	0.18	52,52,52,52	0
82	MG	AR	3854	1/1	0.94	0.20	48,48,48,48	0
81	OHX	1	4114	7/7	0.94	0.10	123,127,131,192	0
82	MG	AR	3858	1/1	0.94	0.43	59,59,59,59	0
82	MG	1	3976	1/1	0.94	0.14	46,46,46,46	0
82	MG	1	3977	1/1	0.94	0.33	79,79,79,79	0
82	MG	A	2003	1/1	0.94	0.15	57,57,57,57	0
82	MG	AR	3726	1/1	0.94	0.20	58,58,58,58	0
82	MG	A	2005	1/1	0.94	0.28	88,88,88,88	0
82	MG	AR	4149	1/1	0.94	0.28	66,66,66,66	0
82	MG	1	3885	1/1	0.94	0.06	59,59,59,59	0
82	MG	1	3886	1/1	0.94	0.22	61,61,61,61	0
82	MG	A	2009	1/1	0.94	0.32	68,68,68,68	0
81	OHX	AT	209	7/7	0.94	0.11	110,113,119,178	0
81	OHX	AT	211	7/7	0.94	0.10	124,129,140,198	0
82	MG	1	3623	1/1	0.94	0.12	46,46,46,46	0
81	OHX	1	3491	7/7	0.94	0.11	119,122,125,182	0
82	MG	AR	4157	1/1	0.94	0.32	43,43,43,43	0
82	MG	1	3625	1/1	0.94	0.19	44,44,44,44	0
82	MG	1	3799	1/1	0.94	0.16	73,73,73,73	0
82	MG	AR	4012	1/1	0.94	0.07	63,63,63,63	0
81	OHX	AT	213	7/7	0.94	0.09	128,130,144,205	0
81	OHX	AR	3557	7/7	0.94	0.09	139,143,148,202	0
81	OHX	AT	216	7/7	0.94	0.08	151,156,166,230	0
82	MG	1	3805	1/1	0.94	0.32	43,43,43,43	0
82	MG	AR	4165	1/1	0.94	0.11	55,55,55,55	0
81	OHX	1	4117	7/7	0.94	0.11	119,123,138,185	0
82	MG	1	3808	1/1	0.94	0.28	45,45,45,45	0
82	MG	AR	4169	1/1	0.94	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	OHX	1	3581	7/7	0.94	0.09	154,159,169,227	0
81	OHX	1	4120	6/7	0.94	0.11	117,126,129,186	0
82	MG	AR	3887	1/1	0.94	0.17	53,53,53,53	0
82	MG	AR	4023	1/1	0.94	0.09	65,65,65,65	0
82	MG	3	214	1/1	0.94	0.19	56,56,56,56	0
82	MG	AR	3749	1/1	0.94	0.17	69,69,69,69	0
82	MG	3	215	1/1	0.94	0.21	72,72,72,72	0
81	OHX	1	3536	7/7	0.94	0.10	112,113,115,177	0
82	MG	AR	3892	1/1	0.94	0.22	72,72,72,72	0
82	MG	1	3719	1/1	0.94	0.36	42,42,42,42	0
82	MG	AR	3753	1/1	0.94	0.10	92,92,92,92	0
81	OHX	A	2119	7/7	0.94	0.10	136,144,151,212	0
82	MG	1	3999	1/1	0.94	0.11	82,82,82,82	0
81	OHX	AR	3442	7/7	0.94	0.17	74,92,100,120	0
81	OHX	1	3468	7/7	0.94	0.13	106,115,118,170	0
82	MG	AR	4036	1/1	0.94	0.18	57,57,57,57	0
82	MG	AR	3758	1/1	0.94	0.22	66,66,66,66	0
82	MG	1	3640	1/1	0.94	0.16	45,45,45,45	0
81	OHX	A	2122	7/7	0.94	0.09	137,140,147,192	0
81	OHX	1	3521	7/7	0.94	0.11	120,124,138,185	0
82	MG	AR	4217	1/1	0.94	0.11	59,59,59,59	0
82	MG	4	223	1/1	0.94	0.26	59,59,59,59	0
82	MG	AS	3511	1/1	0.94	0.23	51,51,51,51	0
82	MG	AS	3512	1/1	0.94	0.09	44,44,44,44	0
81	OHX	1	3522	7/7	0.94	0.09	136,144,147,198	0
82	MG	1	3644	1/1	0.94	0.20	65,65,65,65	0
81	OHX	AR	3506	7/7	0.94	0.13	106,112,116,176	0
81	OHX	DL	102	7/7	0.94	0.11	109,115,118,170	0
82	MG	AR	3767	1/1	0.94	0.11	71,71,71,71	0
81	OHX	AR	3509	7/7	0.94	0.15	97,109,117,183	0
81	OHX	A	1919	7/7	0.94	0.10	149,154,156,198	0
81	OHX	AR	3513	7/7	0.94	0.09	163,166,168,202	0
82	MG	4	233	1/1	0.94	0.13	60,60,60,60	0
81	OHX	A	1924	7/7	0.94	0.10	124,128,137,191	0
82	MG	AR	3916	1/1	0.94	0.22	50,50,50,50	0
81	OHX	AR	3514	7/7	0.94	0.12	98,105,111,169	0
81	OHX	A	1932	7/7	0.94	0.09	139,145,150,193	0
81	OHX	AR	3515	7/7	0.94	0.09	119,132,140,200	0
82	MG	AR	3920	1/1	0.94	0.12	46,46,46,46	0
82	MG	1	403	1/1	0.94	0.08	64,64,64,64	0
82	MG	1	404	1/1	0.94	0.11	52,52,52,52	0
81	OHX	1	3513	7/7	0.94	0.09	145,148,154,212	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	A	2073	1/1	0.94	0.12	57,57,57,57	0
81	OHX	A	2139	7/7	0.94	0.08	145,150,156,218	0
81	OHX	1	3474	7/7	0.94	0.10	107,110,117,164	0
81	OHX	A	1936	7/7	0.94	0.09	185,191,197,241	0
81	OHX	1	3515	7/7	0.94	0.09	127,134,148,204	0
82	MG	A	2079	1/1	0.94	0.40	52,52,52,52	0
82	MG	1	3745	1/1	0.94	0.36	49,49,49,49	0
81	OHX	A	2144	7/7	0.94	0.09	137,140,144,186	0
81	OHX	AR	3576	7/7	0.94	0.10	149,152,154,191	0
81	OHX	1	3527	7/7	0.94	0.10	125,130,134,195	0
81	OHX	1	3490	7/7	0.94	0.12	108,116,121,183	0
82	MG	1	4028	1/1	0.94	0.20	58,58,58,58	0
82	MG	1	3843	1/1	0.94	0.17	49,49,49,49	0
82	MG	AR	4073	1/1	0.94	0.11	76,76,76,76	0
82	MG	1	3668	1/1	0.94	0.12	58,58,58,58	0
81	OHX	AR	3532	7/7	0.94	0.10	129,134,143,202	0
82	MG	1	4033	1/1	0.94	0.31	44,44,44,44	0
81	OHX	S	201	7/7	0.94	0.10	180,182,185,246	0
81	OHX	AR	3582	7/7	0.94	0.10	120,125,133,192	0
82	MG	s2	301	1/1	0.94	0.10	91,91,91,91	0
81	OHX	AR	3583	7/7	0.94	0.08	146,151,155,213	0
82	MG	AR	3945	1/1	0.94	0.06	47,47,47,47	0
81	OHX	sR	1901	7/7	0.94	0.11	140,141,145,214	0
81	OHX	sR	1941	7/7	0.94	0.10	145,147,151,189	0
81	OHX	sR	1951	7/7	0.94	0.10	124,128,135,184	0
81	OHX	1	3529	7/7	0.94	0.11	125,127,138,197	0
82	MG	AR	3804	1/1	0.94	0.33	55,55,55,55	0
81	OHX	sR	1957	7/7	0.94	0.12	158,160,162,200	0
82	MG	AB	203	1/1	0.94	0.24	56,56,56,56	0
82	MG	CK	202	1/1	0.94	0.30	72,72,72,72	0
81	OHX	AR	3536	7/7	0.94	0.09	129,135,148,191	0
81	OHX	4	208	7/7	0.94	0.09	141,149,157,218	0
82	MG	AR	4093	1/1	0.94	0.17	58,58,58,58	0
82	MG	AR	3810	1/1	0.94	0.23	47,47,47,47	0
81	OHX	A	1953	7/7	0.94	0.08	205,206,211,241	0
82	MG	AR	4096	1/1	0.94	0.29	55,55,55,55	0
82	MG	CQ	201	1/1	0.94	0.13	80,80,80,80	0
81	OHX	4	210	7/7	0.94	0.10	120,122,136,195	0
82	MG	AF	203	1/1	0.94	0.09	50,50,50,50	0
81	OHX	AR	3625	7/7	0.94	0.08	198,200,207,262	0
82	MG	1	3863	1/1	0.94	0.21	74,74,74,74	0
82	MG	AR	3689	1/1	0.94	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AR	4106	1/1	0.94	0.12	65,65,65,65	0
82	MG	CU	201	1/1	0.94	0.18	71,71,71,71	0
85	ZN	c	101	1/1	0.94	0.11	164,164,164,164	0
82	MG	AR	3690	1/1	0.94	0.10	44,44,44,44	0
82	MG	1	3685	1/1	0.94	0.22	43,43,43,43	0
82	MG	4	227	1/1	0.95	0.06	57,57,57,57	0
81	OHX	AR	3522	7/7	0.95	0.10	99,103,116,162	0
82	MG	A	1981	1/1	0.95	0.24	51,51,51,51	0
81	OHX	4	207	7/7	0.95	0.08	117,119,129,179	0
81	OHX	A	1958	7/7	0.95	0.08	147,156,160,220	0
82	MG	AR	4148	1/1	0.95	0.29	47,47,47,47	0
81	OHX	1	3495	7/7	0.95	0.09	113,123,128,179	0
82	MG	AR	4018	1/1	0.95	0.24	68,68,68,68	0
81	OHX	4	209	7/7	0.95	0.09	119,121,136,210	0
81	OHX	AR	3528	7/7	0.95	0.11	96,98,107,166	0
81	OHX	AT	208	7/7	0.95	0.12	96,102,113,157	0
81	OHX	AR	3624	7/7	0.95	0.08	130,135,141,200	0
81	OHX	sR	1983	7/7	0.95	0.10	120,128,132,182	0
82	MG	k	401	1/1	0.95	0.24	55,55,55,55	0
81	OHX	AT	210	7/7	0.95	0.09	132,133,144,196	0
82	MG	1	3635	1/1	0.95	0.12	65,65,65,65	0
81	OHX	AR	3529	7/7	0.95	0.10	82,92,99,161	0
82	MG	1	3638	1/1	0.95	0.07	47,47,47,47	0
81	OHX	AR	3530	7/7	0.95	0.11	120,126,128,191	0
82	MG	A	1999	1/1	0.95	0.31	74,74,74,74	0
81	OHX	AR	3531	7/7	0.95	0.10	136,140,149,190	0
81	OHX	1	4130	7/7	0.95	0.08	174,176,179,215	0
81	OHX	1	3496	7/7	0.95	0.09	122,129,133,179	0
81	OHX	1	3499	7/7	0.95	0.09	149,157,160,195	0
81	OHX	1	3464	7/7	0.95	0.12	97,102,107,157	0
82	MG	AR	4168	1/1	0.95	0.25	50,50,50,50	0
81	OHX	1	3477	7/7	0.95	0.10	91,101,105,152	0
82	MG	AR	4170	1/1	0.95	0.23	62,62,62,62	0
82	MG	v	302	1/1	0.95	0.08	49,49,49,49	0
82	MG	1	3933	1/1	0.95	0.10	67,67,67,67	0
81	OHX	k	402	7/7	0.95	0.09	125,129,142,193	0
82	MG	AR	4174	1/1	0.95	0.16	55,55,55,55	0
82	MG	AR	4176	1/1	0.95	0.26	56,56,56,56	0
81	OHX	1	3565	7/7	0.95	0.08	187,191,196,227	0
82	MG	A	2015	1/1	0.95	0.23	66,66,66,66	0
82	MG	AR	4178	1/1	0.95	0.13	59,59,59,59	0
82	MG	1	3648	1/1	0.95	0.06	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
82	MG	sR	2083	1/1	0.95	0.26	51,51,51,51	0
81	OHX	CL	301	7/7	0.95	0.10	134,139,146,195	0
82	MG	1	3742	1/1	0.95	0.31	44,44,44,44	0
81	OHX	AR	3547	7/7	0.95	0.10	121,125,137,192	0
81	OHX	1	3466	7/7	0.95	0.11	97,103,113,149	0
81	OHX	CP	303	7/7	0.95	0.09	133,142,146,203	0
81	OHX	AR	3549	7/7	0.95	0.11	118,121,129,194	0
81	OHX	CX	202	7/7	0.95	0.09	135,137,140,211	0
81	OHX	1	3549	7/7	0.95	0.11	121,124,132,198	0
81	OHX	z	201	7/7	0.95	0.13	123,128,131,195	0
81	OHX	1	4115	7/7	0.95	0.09	132,140,144,203	0
82	MG	AR	3793	1/1	0.95	0.20	43,43,43,43	0
81	OHX	A	1908	7/7	0.95	0.12	83,97,105,139	0
82	MG	1	3661	1/1	0.95	0.21	61,61,61,61	0
81	OHX	A	1914	7/7	0.95	0.12	125,128,130,176	0
81	OHX	A	1916	7/7	0.95	0.10	119,123,132,166	0
82	MG	sR	2099	1/1	0.95	0.13	50,50,50,50	0
82	MG	AR	4211	1/1	0.95	0.14	90,90,90,90	0
81	OHX	A	1917	7/7	0.95	0.10	114,118,126,176	0
82	MG	AR	4221	1/1	0.95	0.09	90,90,90,90	0
82	MG	AR	3799	1/1	0.95	0.36	49,49,49,49	0
82	MG	1	3665	1/1	0.95	0.20	49,49,49,49	0
82	MG	1	3956	1/1	0.95	0.15	43,43,43,43	0
82	MG	AF	204	1/1	0.95	0.07	47,47,47,47	0
82	MG	AG	201	1/1	0.95	0.06	50,50,50,50	0
81	OHX	1	3505	7/7	0.95	0.09	135,139,142,204	0
82	MG	AR	3939	1/1	0.95	0.06	68,68,68,68	0
81	OHX	A	1920	7/7	0.95	0.10	135,135,142,179	0
81	OHX	1	3486	7/7	0.95	0.11	105,114,120,180	0
81	OHX	1	3435	7/7	0.95	0.16	81,87,97,132	0
81	OHX	A	1925	7/7	0.95	0.10	137,140,145,189	0
82	MG	AS	3521	1/1	0.95	0.23	51,51,51,51	0
81	OHX	1	3488	7/7	0.95	0.14	103,108,113,164	0
81	OHX	A	1927	7/7	0.95	0.10	128,134,141,204	0
81	OHX	A	1928	7/7	0.95	0.08	141,145,149,200	0
81	OHX	A	1930	7/7	0.95	0.10	131,137,144,202	0
82	MG	1	3768	1/1	0.95	0.32	45,45,45,45	0
81	OHX	A	2143	6/7	0.95	0.09	146,150,156,214	0
81	OHX	A	1931	7/7	0.95	0.10	122,125,133,178	0
81	OHX	AR	3559	7/7	0.95	0.08	123,134,145,201	0
82	MG	1	3678	1/1	0.95	0.27	60,60,60,60	0
81	OHX	AR	3477	7/7	0.95	0.13	94,96,98,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
82	MG	1	3877	1/1	0.95	0.25	60,60,60,60	0
81	OHX	AR	3493	7/7	0.95	0.11	98,105,110,169	0
81	OHX	1	4121	7/7	0.95	0.09	150,157,166,208	0
82	MG	AR	3707	1/1	0.95	0.07	48,48,48,48	0
81	OHX	AR	3499	7/7	0.95	0.10	92,102,118,153	0
82	MG	A	2065	1/1	0.95	0.05	77,77,77,77	0
81	OHX	A	1937	7/7	0.95	0.10	150,154,161,216	0
82	MG	AR	4089	1/1	0.95	0.24	74,74,74,74	0
81	OHX	AR	3500	7/7	0.95	0.12	91,102,111,154	0
81	OHX	1	3538	7/7	0.95	0.08	144,148,155,212	0
82	MG	1	4085	1/1	0.95	0.10	81,81,81,81	0
82	MG	AR	3714	1/1	0.95	0.10	46,46,46,46	0
81	OHX	sR	1920	7/7	0.95	0.12	82,93,104,140	0
81	OHX	sR	1933	7/7	0.95	0.13	94,103,112,146	0
82	MG	AT	231	1/1	0.95	0.10	86,86,86,86	0
81	OHX	sR	1935	7/7	0.95	0.10	119,125,129,170	0
82	MG	1	3983	1/1	0.95	0.12	81,81,81,81	0
82	MG	AR	3719	1/1	0.95	0.23	47,47,47,47	0
82	MG	AR	4100	1/1	0.95	0.11	45,45,45,45	0
82	MG	1	4149	1/1	0.95	0.07	96,96,96,96	0
82	MG	AR	4102	1/1	0.95	0.17	79,79,79,79	0
81	OHX	AR	3566	7/7	0.95	0.09	139,148,153,220	0
82	MG	1	3691	1/1	0.95	0.11	67,67,67,67	0
82	MG	AR	3723	1/1	0.95	0.25	46,46,46,46	0
81	OHX	sR	1942	7/7	0.95	0.12	90,97,102,147	0
82	MG	1	4154	1/1	0.95	0.06	78,78,78,78	0
81	OHX	1	3456	7/7	0.95	0.12	91,93,107,140	0
81	OHX	sR	1953	7/7	0.95	0.09	158,159,163,206	0
82	MG	sR	2158	1/1	0.95	0.18	66,66,66,66	0
82	MG	CI	303	1/1	0.95	0.18	64,64,64,64	0
81	OHX	sR	1954	7/7	0.95	0.09	108,115,120,169	0
81	OHX	AR	3507	7/7	0.95	0.09	133,138,142,184	0
81	OHX	1	3540	7/7	0.95	0.11	125,130,133,194	0
82	MG	AR	3731	1/1	0.95	0.06	64,64,64,64	0
82	MG	AR	3856	1/1	0.95	0.26	45,45,45,45	0
81	OHX	A	1946	7/7	0.95	0.10	161,165,169,204	0
82	MG	AR	3860	1/1	0.95	0.40	41,41,41,41	0
81	OHX	sR	1962	7/7	0.95	0.11	124,130,137,198	0
82	MG	CQ	203	1/1	0.95	0.10	74,74,74,74	0
81	OHX	A	1947	7/7	0.95	0.09	154,158,164,213	0
81	OHX	1	3557	7/7	0.95	0.09	135,136,155,205	0
82	MG	A	2150	1/1	0.95	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	OHX	1	3523	7/7	0.95	0.08	125,125,138,183	0
81	OHX	1	3596	7/7	0.95	0.14	88,99,106,164	0
82	MG	H	301	1/1	0.95	0.06	76,76,76,76	0
81	OHX	sR	1968	7/7	0.95	0.09	120,126,132,180	0
81	OHX	4	201	7/7	0.95	0.10	101,109,112,166	0
82	MG	AR	3741	1/1	0.95	0.28	41,41,41,41	0
82	MG	1	3809	1/1	0.95	0.08	55,55,55,55	0
82	MG	AR	3871	1/1	0.95	0.08	51,51,51,51	0
82	MG	AR	3872	1/1	0.95	0.09	51,51,51,51	0
81	OHX	sR	1970	7/7	0.95	0.10	129,138,148,199	0
82	MG	AR	4130	1/1	0.95	0.12	54,54,54,54	0
82	MG	1	3619	1/1	0.95	0.23	53,53,53,53	0
81	OHX	AS	3505	7/7	0.95	0.11	100,104,122,157	0
81	OHX	1	3470	7/7	0.95	0.12	90,100,102,148	0
82	MG	AR	4004	1/1	0.95	0.27	57,57,57,57	0
82	MG	4	222	1/1	0.95	0.12	40,40,40,40	0
81	OHX	AS	3508	7/7	0.95	0.09	109,114,122,173	0
82	MG	AR	3879	1/1	0.95	0.21	41,41,41,41	0
83	SPD	1	4144	10/10	0.95	0.13	43,43,44,44	0
82	MG	4	224	1/1	0.95	0.08	61,61,61,61	0
82	MG	DQ	503	1/1	0.95	0.12	66,66,66,66	0
81	OHX	sR	1974	7/7	0.95	0.09	123,125,137,187	0
85	ZN	AH	201	1/1	0.95	0.10	147,147,147,147	0
85	ZN	AP	501	1/1	0.95	0.11	103,103,103,103	0
82	MG	sM	301	1/1	0.95	0.08	48,48,48,48	0
82	MG	AR	3883	1/1	0.95	0.06	53,53,53,53	0
82	MG	1	3912	1/1	0.95	0.28	61,61,61,61	0
82	MG	AR	4143	1/1	0.95	0.25	59,59,59,59	0
81	OHX	1	3444	7/7	0.96	0.10	101,113,120,151	0
81	OHX	AR	3545	7/7	0.96	0.09	126,128,135,194	0
81	OHX	A	1941	7/7	0.96	0.10	149,149,156,215	0
82	MG	AR	3938	1/1	0.96	0.10	55,55,55,55	0
82	MG	1	3637	1/1	0.96	0.26	52,52,52,52	0
81	OHX	sR	1964	7/7	0.96	0.09	115,118,119,176	0
82	MG	CQ	204	1/1	0.96	0.36	58,58,58,58	0
81	OHX	1	3451	7/7	0.96	0.14	77,95,103,134	0
81	OHX	r	304	7/7	0.96	0.10	93,100,107,151	0
81	OHX	1	3489	7/7	0.96	0.11	98,100,109,163	0
82	MG	1	4001	1/1	0.96	0.21	67,67,67,67	0
82	MG	r	302	1/1	0.96	0.11	47,47,47,47	0
81	OHX	A	1945	7/7	0.96	0.09	146,148,152,194	0
81	OHX	1	3441	7/7	0.96	0.11	90,94,98,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	AR	3550	7/7	0.96	0.09	127,131,135,184	0
81	OHX	1	3457	7/7	0.96	0.12	93,96,101,133	0
81	OHX	1	3492	7/7	0.96	0.09	128,128,140,191	0
81	OHX	AR	3553	7/7	0.96	0.12	116,121,127,203	0
82	MG	1	3760	1/1	0.96	0.23	60,60,60,60	0
81	OHX	1	3493	7/7	0.96	0.09	124,127,131,190	0
81	OHX	1	3494	7/7	0.96	0.09	104,109,115,158	0
81	OHX	AR	3440	7/7	0.96	0.10	78,87,92,119	0
81	OHX	AR	3441	7/7	0.96	0.12	81,89,90,116	0
81	OHX	1	3473	7/7	0.96	0.09	114,118,123,165	0
82	MG	AR	3959	1/1	0.96	0.13	68,68,68,68	0
82	MG	DL	101	1/1	0.96	0.22	57,57,57,57	0
81	OHX	AR	3449	7/7	0.96	0.12	98,107,116,142	0
81	OHX	AR	3455	7/7	0.96	0.14	83,88,95,134	0
82	MG	AR	3808	1/1	0.96	0.37	50,50,50,50	0
81	OHX	AR	3460	7/7	0.96	0.11	68,83,90,121	0
82	MG	x	208	1/1	0.96	0.32	60,60,60,60	0
81	OHX	1	3459	7/7	0.96	0.11	98,101,105,142	0
81	OHX	AR	3473	7/7	0.96	0.12	82,89,102,133	0
82	MG	A	1977	1/1	0.96	0.26	52,52,52,52	0
82	MG	1	3659	1/1	0.96	0.04	53,53,53,53	0
81	OHX	AR	3474	7/7	0.96	0.11	76,95,98,144	0
81	OHX	AR	3475	7/7	0.96	0.13	82,96,104,132	0
82	MG	1	3775	1/1	0.96	0.21	45,45,45,45	0
82	MG	1	3776	1/1	0.96	0.23	43,43,43,43	0
81	OHX	1	4099	7/7	0.96	0.13	79,91,100,136	0
81	OHX	AR	3479	7/7	0.96	0.10	79,84,99,132	0
81	OHX	AT	201	7/7	0.96	0.09	108,113,117,179	0
82	MG	AR	4134	1/1	0.96	0.25	43,43,43,43	0
82	MG	AR	3821	1/1	0.96	0.21	47,47,47,47	0
81	OHX	AR	3483	7/7	0.96	0.09	97,111,120,172	0
82	MG	AR	3823	1/1	0.96	0.14	40,40,40,40	0
82	MG	1	4029	1/1	0.96	0.14	43,43,43,43	0
81	OHX	AR	3484	7/7	0.96	0.10	85,91,104,141	0
82	MG	A	1992	1/1	0.96	0.20	58,58,58,58	0
82	MG	AR	3826	1/1	0.96	0.27	55,55,55,55	0
82	MG	AR	3982	1/1	0.96	0.17	64,64,64,64	0
81	OHX	AR	3487	7/7	0.96	0.10	91,98,107,148	0
81	OHX	AR	3488	7/7	0.96	0.09	110,119,123,162	0
81	OHX	A	1971	7/7	0.96	0.12	94,97,106,127	0
82	MG	1	3908	1/1	0.96	0.07	65,65,65,65	0
82	MG	AR	3831	1/1	0.96	0.37	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	AR	3492	7/7	0.96	0.09	92,100,112,151	0
81	OHX	1	4101	7/7	0.96	0.09	123,126,129,174	0
81	OHX	1	3568	7/7	0.96	0.11	95,97,103,152	0
82	MG	AR	3835	1/1	0.96	0.25	42,42,42,42	0
81	OHX	AR	3495	7/7	0.96	0.10	97,105,111,178	0
81	OHX	AT	214	7/7	0.96	0.07	146,155,157,209	0
82	MG	1	3792	1/1	0.96	0.29	51,51,51,51	0
82	MG	AR	3839	1/1	0.96	0.31	42,42,42,42	0
82	MG	AR	4155	1/1	0.96	0.26	68,68,68,68	0
82	MG	AR	3840	1/1	0.96	0.25	43,43,43,43	0
81	OHX	A	2113	7/7	0.96	0.09	129,131,138,189	0
82	MG	1	4043	1/1	0.96	0.25	46,46,46,46	0
82	MG	1	4044	1/1	0.96	0.22	58,58,58,58	0
81	OHX	sR	2000	7/7	0.96	0.10	118,122,133,195	0
82	MG	A	2014	1/1	0.96	0.07	74,74,74,74	0
81	OHX	A	2114	7/7	0.96	0.11	116,122,126,171	0
81	OHX	A	2115	7/7	0.96	0.07	137,142,147,192	0
82	MG	A	2017	1/1	0.96	0.15	68,68,68,68	0
82	MG	1	4048	1/1	0.96	0.17	50,50,50,50	0
81	OHX	AR	3496	7/7	0.96	0.10	93,99,103,161	0
81	OHX	A	2117	7/7	0.96	0.11	114,118,126,169	0
82	MG	AR	3850	1/1	0.96	0.29	43,43,43,43	0
82	MG	sR	2107	1/1	0.96	0.07	62,62,62,62	0
81	OHX	1	3497	7/7	0.96	0.10	114,115,125,171	0
82	MG	1	3801	1/1	0.96	0.31	42,42,42,42	0
81	OHX	CE	403	7/7	0.96	0.08	101,107,118,166	0
82	MG	AR	4011	1/1	0.96	0.20	69,69,69,69	0
81	OHX	1	3519[A]	7/7	0.96	0.14	96,101,107,129	7
82	MG	sR	2113	1/1	0.96	0.07	69,69,69,69	0
81	OHX	AR	3501	7/7	0.96	0.11	129,131,133,207	0
82	MG	1	3806	1/1	0.96	0.14	48,48,48,48	0
81	OHX	1	3519[B]	7/7	0.96	0.14	95,99,104,118	7
81	OHX	A	2125	7/7	0.96	0.08	128,131,134,191	0
81	OHX	3	202	7/7	0.96	0.09	119,126,130,177	0
82	MG	1	3810	1/1	0.96	0.18	46,46,46,46	0
81	OHX	1	4109	7/7	0.96	0.11	93,99,103,166	0
81	OHX	1	4110	7/7	0.96	0.10	116,118,124,170	0
82	MG	sR	2122	1/1	0.96	0.05	67,67,67,67	0
81	OHX	AR	3512	7/7	0.96	0.08	111,116,127,177	0
81	OHX	1	4112	7/7	0.96	0.09	123,124,132,190	0
82	MG	1	3693	1/1	0.96	0.22	51,51,51,51	0
82	MG	AR	4024	1/1	0.96	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	OHX	1	4113	7/7	0.96	0.08	107,109,120,176	0
82	MG	AR	3870	1/1	0.96	0.16	44,44,44,44	0
81	OHX	1	3498	7/7	0.96	0.08	136,139,148,194	0
82	MG	1	3818	1/1	0.96	0.08	64,64,64,64	0
82	MG	1	3940	1/1	0.96	0.14	55,55,55,55	0
82	MG	1	3941	1/1	0.96	0.05	51,51,51,51	0
81	OHX	AR	3516	7/7	0.96	0.10	101,112,121,167	0
81	OHX	1	3476	7/7	0.96	0.08	113,114,124,163	0
81	OHX	AR	3519	7/7	0.96	0.10	102,113,116,175	0
81	OHX	AR	3520	7/7	0.96	0.09	118,124,131,186	0
82	MG	sR	2137	1/1	0.96	0.13	90,90,90,90	0
81	OHX	1	3500	7/7	0.96	0.09	158,162,166,215	0
82	MG	AR	4215	1/1	0.96	0.11	52,52,52,52	0
82	MG	1	3701	1/1	0.96	0.36	63,63,63,63	0
81	OHX	A	1911	7/7	0.96	0.10	102,107,116,147	0
81	OHX	1	3463	7/7	0.96	0.10	89,96,104,135	0
81	OHX	A	1915	7/7	0.96	0.09	109,118,128,170	0
82	MG	AR	3885	1/1	0.96	0.11	46,46,46,46	0
81	OHX	1	3502	7/7	0.96	0.14	99,104,114,165	0
81	OHX	AR	3525	7/7	0.96	0.10	103,113,118,173	0
82	MG	1	4146	1/1	0.96	0.10	70,70,70,70	0
81	OHX	4	206	7/7	0.96	0.09	96,100,109,156	0
82	MG	AR	3742	1/1	0.96	0.29	43,43,43,43	0
81	OHX	1	4119	7/7	0.96	0.08	140,143,149,201	0
81	OHX	1	3478	7/7	0.96	0.10	98,101,110,151	0
82	MG	AR	4048	1/1	0.96	0.07	50,50,50,50	0
81	OHX	1	3479	7/7	0.96	0.10	102,105,123,173	0
82	MG	AR	3746	1/1	0.96	0.25	41,41,41,41	0
81	OHX	1	3442	7/7	0.96	0.11	98,101,113,138	0
81	OHX	1	3484	7/7	0.96	0.10	100,108,117,162	0
81	OHX	4	212	7/7	0.96	0.07	145,148,156,217	0
82	MG	AR	3899	1/1	0.96	0.06	64,64,64,64	0
82	MG	AS	3527	1/1	0.96	0.35	53,53,53,53	0
82	MG	AR	4055	1/1	0.96	0.15	61,61,61,61	0
81	OHX	AR	3533	7/7	0.96	0.09	120,128,137,203	0
81	OHX	sR	1911	7/7	0.96	0.12	91,102,107,128	0
81	OHX	A	1929	7/7	0.96	0.09	126,128,134,183	0
82	MG	3	209	1/1	0.96	0.32	55,55,55,55	0
81	OHX	sR	1922	7/7	0.96	0.12	105,110,115,136	0
81	OHX	sR	1923	7/7	0.96	0.10	99,101,105,143	0
81	OHX	sR	1925	7/7	0.96	0.11	98,102,110,145	0
81	OHX	AR	3606	7/7	0.96	0.11	104,105,109,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	sR	1934	7/7	0.96	0.11	77,84,94,140	0
82	MG	1	3845	1/1	0.96	0.18	53,53,53,53	0
81	OHX	1	3465	7/7	0.96	0.13	91,99,105,144	0
81	OHX	1	3530	7/7	0.96	0.08	145,147,152,201	0
81	OHX	1	3531	7/7	0.96	0.11	91,96,102,156	0
81	OHX	sR	1943	7/7	0.96	0.09	121,124,130,174	0
81	OHX	sR	1944	7/7	0.96	0.07	108,113,119,161	0
81	OHX	sR	1945	7/7	0.96	0.08	129,133,137,179	0
81	OHX	sR	1946	7/7	0.96	0.10	109,116,122,172	0
81	OHX	sR	1947	7/7	0.96	0.09	117,124,125,197	0
81	OHX	sR	1950[A]	7/7	0.96	0.21	111,115,118,123	7
82	MG	CD	302	1/1	0.96	0.34	41,41,41,41	0
81	OHX	sR	1950[B]	7/7	0.96	0.21	111,115,123,151	7
81	OHX	AR	3538	7/7	0.96	0.08	125,126,136,181	0
82	MG	AR	3771	1/1	0.96	0.15	64,64,64,64	0
81	OHX	AR	3539	7/7	0.96	0.11	92,100,106,163	0
82	MG	1	3627	1/1	0.96	0.23	58,58,58,58	0
82	MG	AR	3774	1/1	0.96	0.07	49,49,49,49	0
82	MG	AR	3925	1/1	0.96	0.24	62,62,62,62	0
82	MG	A	2147	1/1	0.96	0.07	95,95,95,95	0
82	MG	A	2149	1/1	0.96	0.08	84,84,84,84	0
81	OHX	AR	3540	7/7	0.96	0.10	117,127,135,186	0
82	MG	1	3985	1/1	0.96	0.24	55,55,55,55	0
82	MG	1	3861	1/1	0.96	0.24	53,53,53,53	0
81	OHX	sR	1955	7/7	0.96	0.08	148,152,153,194	0
82	MG	1	3740	1/1	0.96	0.33	60,60,60,60	0
81	OHX	4	235	7/7	0.96	0.10	99,105,113,160	0
81	OHX	AR	3543	7/7	0.96	0.12	107,110,117,174	0
81	OHX	sR	1959	7/7	0.96	0.09	107,115,122,178	0
81	OHX	sR	1960	7/7	0.96	0.08	125,130,137,184	0
81	OHX	1	3485[B]	7/7	0.97	0.25	90,91,95,124	7
81	OHX	1	3440	7/7	0.97	0.09	81,91,97,131	0
81	OHX	A	1918	7/7	0.97	0.07	123,125,129,175	0
81	OHX	A	2123	7/7	0.97	0.08	118,122,124,173	0
81	OHX	3	219	7/7	0.97	0.08	105,109,120,164	0
81	OHX	AR	3443	7/7	0.97	0.11	74,79,88,115	0
81	OHX	AR	3518	7/7	0.97	0.09	117,120,127,169	0
81	OHX	AR	3444	7/7	0.97	0.10	74,79,96,110	0
81	OHX	1	4075	7/7	0.97	0.09	104,108,116,167	0
82	MG	A	2074	1/1	0.97	0.09	71,71,71,71	0
81	OHX	AR	3450	7/7	0.97	0.11	81,81,86,114	0
81	OHX	AR	3451	7/7	0.97	0.10	99,104,111,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3802	1/1	0.97	0.44	43,43,43,43	0
81	OHX	AR	3580	7/7	0.97	0.10	107,110,112,167	0
81	OHX	AR	3452	7/7	0.97	0.11	91,95,101,138	0
82	MG	1	3717	1/1	0.97	0.47	62,62,62,62	0
82	MG	AR	4077	1/1	0.97	0.05	77,77,77,77	0
81	OHX	1	4096	7/7	0.97	0.10	89,91,102,129	0
82	MG	A	2083	1/1	0.97	0.29	51,51,51,51	0
81	OHX	AR	3456	7/7	0.97	0.12	80,88,104,126	0
81	OHX	1	3453	7/7	0.97	0.10	85,94,104,128	0
81	OHX	AR	3463	7/7	0.97	0.12	83,86,98,130	0
82	MG	AR	3981	1/1	0.97	0.17	61,61,61,61	0
82	MG	AR	3882	1/1	0.97	0.24	60,60,60,60	0
81	OHX	A	2138	7/7	0.97	0.08	115,119,122,176	0
81	OHX	AR	3466	7/7	0.97	0.09	95,100,103,137	0
81	OHX	AR	3467	7/7	0.97	0.09	83,87,99,133	0
81	OHX	AR	3471	7/7	0.97	0.09	94,96,101,143	0
82	MG	AR	3694	1/1	0.97	0.08	44,44,44,44	0
82	MG	AR	4207	1/1	0.97	0.07	95,95,95,95	0
81	OHX	1	4100	7/7	0.97	0.09	92,99,103,156	0
82	MG	AR	3989	1/1	0.97	0.16	60,60,60,60	0
82	MG	AR	4214	1/1	0.97	0.16	108,108,108,108	0
81	OHX	AS	3501	7/7	0.97	0.08	92,98,109,149	0
81	OHX	1	3454	7/7	0.97	0.10	90,96,107,139	0
81	OHX	AR	3534	7/7	0.97	0.10	86,89,97,127	0
81	OHX	AS	3507	7/7	0.97	0.09	93,97,100,148	0
82	MG	A	2146	1/1	0.97	0.20	70,70,70,70	0
81	OHX	1	4102	7/7	0.97	0.08	111,117,120,158	0
81	OHX	1	3455	7/7	0.97	0.11	92,99,106,135	0
81	OHX	AR	3476	7/7	0.97	0.10	91,98,104,145	0
81	OHX	T	201	7/7	0.97	0.10	108,113,119,140	0
82	MG	AR	3704	1/1	0.97	0.14	49,49,49,49	0
82	MG	1	3910	1/1	0.97	0.31	55,55,55,55	0
82	MG	AR	4103	1/1	0.97	0.13	56,56,56,56	0
81	OHX	1	4104	7/7	0.97	0.10	91,96,102,148	0
82	MG	1	4156	1/1	0.97	0.05	80,80,80,80	0
81	OHX	AR	3478[A]	7/7	0.97	0.19	72,74,81,81	7
81	OHX	AR	3478[B]	7/7	0.97	0.19	74,74,79,86	7
82	MG	sR	2138	1/1	0.97	0.09	70,70,70,70	0
81	OHX	AR	3541	7/7	0.97	0.08	147,151,156,185	0
81	OHX	1	3422	7/7	0.97	0.16	75,84,90,115	0
81	OHX	AR	3480	7/7	0.97	0.09	88,94,108,150	0
81	OHX	AR	3481	7/7	0.97	0.09	88,91,109,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	1	4106	7/7	0.97	0.13	70,77,89,109	0
81	OHX	sR	1927	7/7	0.97	0.08	102,108,112,148	0
81	OHX	sR	1928	7/7	0.97	0.08	93,96,108,156	0
81	OHX	sR	1932	7/7	0.97	0.09	95,98,107,145	0
82	MG	sR	2036	1/1	0.97	0.23	59,59,59,59	0
81	OHX	1	3472	7/7	0.97	0.08	94,101,110,146	0
81	OHX	AR	3485	7/7	0.97	0.09	90,93,98,139	0
81	OHX	AR	3486	7/7	0.97	0.09	85,91,95,128	0
81	OHX	sR	1936	7/7	0.97	0.09	97,103,109,153	0
81	OHX	sR	1938	7/7	0.97	0.09	98,105,109,148	0
81	OHX	sR	1939	7/7	0.97	0.09	104,109,115,148	0
81	OHX	sR	1940	7/7	0.97	0.09	111,113,121,169	0
81	OHX	1	3436	7/7	0.97	0.11	86,93,100,124	0
81	OHX	1	3458	7/7	0.97	0.11	90,95,106,143	0
81	OHX	AR	3490	7/7	0.97	0.09	90,101,107,164	0
81	OHX	AR	3491	7/7	0.97	0.09	107,108,114,170	0
81	OHX	1	3475	7/7	0.97	0.10	95,100,112,156	0
81	OHX	1	4111	7/7	0.97	0.08	103,110,116,162	0
81	OHX	1	3437	7/7	0.97	0.11	74,83,92,114	0
81	OHX	sR	1948	7/7	0.97	0.09	105,109,114,165	0
82	MG	1	3849	1/1	0.97	0.08	52,52,52,52	0
82	MG	A	2029	1/1	0.97	0.14	54,54,54,54	0
81	OHX	sR	1949	7/7	0.97	0.08	100,107,115,163	0
81	OHX	1	3460	7/7	0.97	0.09	93,95,110,145	0
82	MG	AR	3737	1/1	0.97	0.34	50,50,50,50	0
82	MG	sR	2179	1/1	0.97	0.11	94,94,94,94	0
81	OHX	1	3461	7/7	0.97	0.09	98,102,106,160	0
82	MG	1	3682	1/1	0.97	0.20	62,62,62,62	0
81	OHX	1	3462	7/7	0.97	0.09	102,102,108,138	0
81	OHX	sR	1952	7/7	0.97	0.07	119,126,132,166	0
82	MG	j	302	1/1	0.97	0.11	43,43,43,43	0
81	OHX	1	3449	7/7	0.97	0.10	95,100,107,140	0
81	OHX	1	3481	7/7	0.97	0.07	99,109,113,149	0
81	OHX	CQ	202	7/7	0.97	0.09	83,91,99,147	0
81	OHX	1	3483	7/7	0.97	0.08	123,127,135,185	0
82	MG	AR	3940	1/1	0.97	0.22	52,52,52,52	0
81	OHX	AR	3503	7/7	0.97	0.08	97,105,115,164	0
82	MG	1	3774	1/1	0.97	0.33	46,46,46,46	0
82	MG	1	3862	1/1	0.97	0.12	44,44,44,44	0
82	MG	1	4041	1/1	0.97	0.20	51,51,51,51	0
81	OHX	sR	1958	7/7	0.97	0.09	111,117,120,165	0
81	OHX	AR	3504	7/7	0.97	0.09	89,96,102,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	AR	3505	7/7	0.97	0.09	103,104,113,168	0
81	OHX	1	3450	7/7	0.97	0.09	92,93,100,128	0
82	MG	CP	302	1/1	0.97	0.10	57,57,57,57	0
82	MG	1	3955	1/1	0.97	0.07	54,54,54,54	0
81	OHX	A	1906	7/7	0.97	0.10	100,104,108,133	0
81	OHX	A	1907	7/7	0.97	0.09	117,124,128,154	0
81	OHX	AK	103	7/7	0.97	0.10	86,96,102,129	0
81	OHX	1	3485[A]	7/7	0.97	0.25	90,93,94,96	7
81	OHX	A	1912	7/7	0.97	0.08	108,113,114,155	0
81	OHX	A	1913	7/7	0.97	0.08	117,128,131,173	0
82	MG	AR	3857	1/1	0.97	0.19	49,49,49,49	0
82	MG	1	3786	1/1	0.97	0.36	46,46,46,46	0
82	MG	AR	3859	1/1	0.97	0.34	43,43,43,43	0
85	ZN	DQ	501	1/1	0.97	0.07	136,136,136,136	0
85	ZN	DR	501	1/1	0.97	0.04	85,85,85,85	0
81	OHX	AR	3430	7/7	0.97	0.12	79,86,89,116	0
81	OHX	A	2118	7/7	0.97	0.08	115,120,124,178	0
85	ZN	d9	101	1/1	0.97	0.05	97,97,97,97	0
81	OHX	AR	3432	7/7	0.97	0.14	75,84,88,106	0
81	OHX	1	3425	7/7	0.98	0.09	81,83,89,106	0
81	OHX	1	3426	7/7	0.98	0.09	84,90,99,104	0
82	MG	1	3737	1/1	0.98	0.30	45,45,45,45	0
81	OHX	AR	3433	7/7	0.98	0.11	79,87,100,110	0
81	OHX	AR	3434	7/7	0.98	0.11	82,84,95,103	0
81	OHX	AR	3435	7/7	0.98	0.10	78,84,97,108	0
81	OHX	AR	3497	7/7	0.98	0.06	120,125,130,166	0
81	OHX	AR	3498	7/7	0.98	0.07	105,110,118,151	0
81	OHX	AR	3436	7/7	0.98	0.09	79,86,90,109	0
81	OHX	1	3535[A]	7/7	0.98	0.19	86,89,97,97	7
81	OHX	A	1921	7/7	0.98	0.07	124,128,131,176	0
81	OHX	A	1922	7/7	0.98	0.07	111,119,127,158	0
82	MG	1	3652	1/1	0.98	0.30	52,52,52,52	0
81	OHX	1	3535[B]	7/7	0.98	0.19	84,89,96,108	7
81	OHX	1	3443	7/7	0.98	0.08	83,85,93,125	0
81	OHX	3	220	7/7	0.98	0.08	96,103,115,150	0
81	OHX	A	2137	7/7	0.98	0.07	93,97,103,133	0
82	MG	AR	4082	1/1	0.98	0.06	65,65,65,65	0
81	OHX	1	3427	7/7	0.98	0.08	86,88,98,124	0
81	OHX	AR	3446	7/7	0.98	0.10	76,84,90,101	0
82	MG	1	4050	1/1	0.98	0.29	53,53,53,53	0
81	OHX	AR	3447	7/7	0.98	0.08	82,90,95,120	0
81	OHX	AR	3448	7/7	0.98	0.10	87,93,101,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	AR	3508	7/7	0.98	0.10	77,79,88,110	0
82	MG	AR	4208	1/1	0.98	0.11	82,82,82,82	0
81	OHX	1	3445	7/7	0.98	0.10	92,97,98,138	0
81	OHX	AR	3510	7/7	0.98	0.06	107,110,118,156	0
82	MG	AR	4213	1/1	0.98	0.05	77,77,77,77	0
81	OHX	AR	3511[A]	7/7	0.98	0.12	80,81,85,99	7
81	OHX	AR	3511[B]	7/7	0.98	0.12	83,85,85,111	7
81	OHX	1	3467[A]	6/7	0.98	0.22	69,73,78,79	6
82	MG	AR	4219	1/1	0.98	0.07	43,43,43,43	0
82	MG	AR	4220	1/1	0.98	0.10	50,50,50,50	0
81	OHX	1	3467[B]	6/7	0.98	0.22	75,78,82,112	6
81	OHX	4	205	7/7	0.98	0.09	78,87,91,114	0
81	OHX	AS	3503	7/7	0.98	0.09	83,86,90,116	0
81	OHX	AS	3504	7/7	0.98	0.09	90,94,99,127	0
82	MG	AR	4098	1/1	0.98	0.11	63,63,63,63	0
81	OHX	AR	3577	7/7	0.98	0.08	96,101,111,166	0
81	OHX	AR	3453	7/7	0.98	0.07	84,85,96,120	0
81	OHX	AR	3454	7/7	0.98	0.10	94,95,97,129	0
81	OHX	sR	1915	7/7	0.98	0.10	96,98,102,118	0
82	MG	AR	3895	1/1	0.98	0.16	42,42,42,42	0
81	OHX	sR	1918	7/7	0.98	0.09	84,91,95,122	0
82	MG	1	3869	1/1	0.98	0.06	70,70,70,70	0
81	OHX	1	4097	7/7	0.98	0.09	87,95,98,131	0
81	OHX	sR	1921	7/7	0.98	0.08	92,97,105,143	0
81	OHX	1	3447	7/7	0.98	0.10	74,84,96,119	0
81	OHX	AR	3457	7/7	0.98	0.07	80,86,91,115	0
81	OHX	sR	1924	7/7	0.98	0.07	88,95,101,127	0
81	OHX	AR	3458	7/7	0.98	0.10	79,88,99,129	0
82	MG	1	3974	1/1	0.98	0.08	72,72,72,72	0
81	OHX	sR	1926	7/7	0.98	0.09	93,95,102,139	0
81	OHX	AR	3459	7/7	0.98	0.11	76,81,97,99	0
82	MG	1	3780	1/1	0.98	0.32	46,46,46,46	0
81	OHX	A	1948	7/7	0.98	0.07	110,111,122,152	0
81	OHX	sR	1929	7/7	0.98	0.08	110,116,121,154	0
81	OHX	sR	1930	7/7	0.98	0.07	119,122,127,152	0
81	OHX	sR	1931	7/7	0.98	0.08	90,94,96,127	0
81	OHX	1	3448	7/7	0.98	0.08	81,86,94,116	0
81	OHX	AR	3461	7/7	0.98	0.09	86,95,99,131	0
81	OHX	AT	207	7/7	0.98	0.11	83,86,93,108	0
81	OHX	AR	3524	7/7	0.98	0.08	116,117,121,172	0
81	OHX	AR	3462	7/7	0.98	0.08	89,94,101,131	0
81	OHX	sR	1937	7/7	0.98	0.08	93,94,102,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	1	3429	7/7	0.98	0.09	85,87,97,109	0
82	MG	AR	3713	1/1	0.98	0.10	46,46,46,46	0
81	OHX	AR	3464	7/7	0.98	0.09	82,88,94,113	0
81	OHX	AR	3465	7/7	0.98	0.11	92,94,102,121	0
81	OHX	1	3471	7/7	0.98	0.08	89,96,98,135	0
82	MG	1	3795	1/1	0.98	0.36	50,50,50,50	0
81	OHX	1	3430	7/7	0.98	0.12	78,86,91,106	0
81	OHX	AR	3469	7/7	0.98	0.08	90,97,102,136	0
81	OHX	1	3431	7/7	0.98	0.10	82,83,101,113	0
82	MG	sR	2180	1/1	0.98	0.10	85,85,85,85	0
82	MG	sR	2181	1/1	0.98	0.07	76,76,76,76	0
82	MG	sR	2182	1/1	0.98	0.13	59,59,59,59	0
81	OHX	1	3452	7/7	0.98	0.09	100,102,107,138	0
81	OHX	1	3432	7/7	0.98	0.10	86,89,96,116	0
81	OHX	1	3433	7/7	0.98	0.10	81,86,97,113	0
81	OHX	1	3434	7/7	0.98	0.10	88,91,95,120	0
81	OHX	1	3419	7/7	0.98	0.10	81,84,94,99	0
81	OHX	1	3418	7/7	0.98	0.11	75,86,93,101	0
81	OHX	1	3423	7/7	0.98	0.13	61,79,88,107	0
82	MG	1	3708	1/1	0.98	0.14	43,43,43,43	0
81	OHX	1	3438	7/7	0.98	0.10	86,92,103,133	0
81	OHX	1	3482[A]	7/7	0.98	0.14	84,85,98,101	7
81	OHX	1	3482[B]	7/7	0.98	0.14	88,88,98,111	7
82	MG	1	4007	1/1	0.98	0.15	49,49,49,49	0
81	OHX	1	4143	7/7	0.98	0.10	104,108,111,114	0
81	OHX	AR	3482	7/7	0.98	0.07	83,89,93,122	0
81	OHX	CX	201	7/7	0.98	0.09	88,90,101,126	0
82	MG	d3	203	1/1	0.98	0.28	86,86,86,86	0
81	OHX	3	201	7/7	0.98	0.07	85,87,100,118	0
81	OHX	DD	101	7/7	0.98	0.10	69,79,90,92	0
81	OHX	1	3439	7/7	0.98	0.08	97,99,103,139	0
81	OHX	A	2106	7/7	0.98	0.08	94,98,103,123	0
81	OHX	A	2107	7/7	0.98	0.09	93,102,110,122	0
81	OHX	A	2108	7/7	0.98	0.10	97,99,106,141	0
81	OHX	A	2109	7/7	0.98	0.08	95,100,102,129	0
81	OHX	A	2110	7/7	0.98	0.08	99,100,103,133	0
81	OHX	A	2111	7/7	0.98	0.08	95,101,105,148	0
81	OHX	A	2112	7/7	0.98	0.07	124,127,130,168	0
81	OHX	1	3424	7/7	0.98	0.10	78,85,99,104	0
81	OHX	AR	3413	7/7	0.98	0.11	80,89,92,95	0
81	OHX	A	1901	7/7	0.98	0.12	85,95,98,108	0
81	OHX	A	1903	7/7	0.98	0.10	86,89,99,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	AR	3414	7/7	0.98	0.14	84,85,92,93	0
81	OHX	AR	3416	7/7	0.98	0.11	58,73,82,91	0
81	OHX	AR	3418	7/7	0.98	0.11	65,80,88,89	0
81	OHX	A	1909	7/7	0.98	0.08	94,97,101,130	0
81	OHX	A	1910	7/7	0.98	0.08	101,103,111,142	0
81	OHX	AR	3427	7/7	0.98	0.12	59,81,85,95	0
81	OHX	1	4087	7/7	0.99	0.12	63,68,74,76	0
81	OHX	AR	3428	7/7	0.99	0.07	75,81,87,103	0
81	OHX	AR	3429	7/7	0.99	0.09	75,81,86,102	0
81	OHX	1	4088	7/7	0.99	0.10	64,67,73,75	0
82	MG	AR	3853	1/1	0.99	0.34	49,49,49,49	0
82	MG	A	2148	1/1	0.99	0.10	52,52,52,52	0
81	OHX	AR	3431	7/7	0.99	0.09	80,82,90,90	0
81	OHX	1	4089	7/7	0.99	0.09	76,78,84,85	0
81	OHX	AR	4179	7/7	0.99	0.12	60,67,75,77	0
81	OHX	s1	301	7/7	0.99	0.09	74,82,91,102	0
81	OHX	1	4090	6/7	0.99	0.10	72,79,83,90	0
81	OHX	1	4091	7/7	0.99	0.10	80,85,92,97	0
81	OHX	1	4092	7/7	0.99	0.09	78,81,84,95	0
81	OHX	4	204	7/7	0.99	0.10	69,78,83,83	0
81	OHX	AR	3437	7/7	0.99	0.09	74,83,87,94	0
81	OHX	AR	3438	7/7	0.99	0.09	80,82,89,104	0
81	OHX	AR	3439	7/7	0.99	0.07	91,97,99,123	0
81	OHX	1	4093	7/7	0.99	0.09	80,82,91,92	0
81	OHX	1	4094	7/7	0.99	0.07	80,88,91,96	0
81	OHX	1	4095	7/7	0.99	0.08	90,92,97,125	0
81	OHX	1	3446	7/7	0.99	0.06	92,94,100,129	0
81	OHX	1	3408	7/7	0.99	0.09	72,77,81,81	0
81	OHX	AR	3445	7/7	0.99	0.09	78,81,85,114	0
81	OHX	1	4098	7/7	0.99	0.09	77,81,88,107	0
81	OHX	1	3428	7/7	0.99	0.09	78,83,87,96	0
81	OHX	1	3410	7/7	0.99	0.07	82,83,88,100	0
81	OHX	1	3411	7/7	0.99	0.11	72,75,84,85	0
81	OHX	1	3412	7/7	0.99	0.08	78,79,90,94	0
81	OHX	1	3413	7/7	0.99	0.10	74,75,83,93	0
81	OHX	1	3414	7/7	0.99	0.10	74,80,86,94	0
81	OHX	1	3415	7/7	0.99	0.13	74,81,83,89	0
81	OHX	1	3416	7/7	0.99	0.09	81,82,91,96	0
81	OHX	1	3417	7/7	0.99	0.11	81,82,90,102	0
81	OHX	1	3401	7/7	0.99	0.11	47,52,58,66	0
81	OHX	AT	206	7/7	0.99	0.12	74,80,84,90	0
81	OHX	1	3402	7/7	0.99	0.10	67,68,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	OHX	1	3420	7/7	0.99	0.08	81,82,88,94	0
81	OHX	1	3421	7/7	0.99	0.07	79,84,93,106	0
81	OHX	AC	101	7/7	0.99	0.11	63,79,84,86	0
82	MG	1	4153	1/1	0.99	0.06	59,59,59,59	0
81	OHX	1	3403	7/7	0.99	0.10	48,50,57,66	0
81	OHX	1	3404	7/7	0.99	0.11	71,77,81,85	0
81	OHX	1	3405	7/7	0.99	0.13	70,78,88,96	0
81	OHX	AR	3401	7/7	0.99	0.10	63,64,69,70	0
81	OHX	AR	3402	7/7	0.99	0.12	53,61,66,70	0
81	OHX	AR	3403	7/7	0.99	0.10	54,58,62,67	0
81	OHX	AR	3405	7/7	0.99	0.13	64,71,72,74	0
81	OHX	AR	3468	7/7	0.99	0.07	89,92,97,121	0
81	OHX	sR	1903	7/7	0.99	0.10	63,67,70,78	0
81	OHX	sR	1904	7/7	0.99	0.11	77,86,90,100	0
81	OHX	sR	1905	7/7	0.99	0.11	74,76,82,84	0
81	OHX	sR	1906	7/7	0.99	0.08	82,82,91,100	0
81	OHX	sR	1907	7/7	0.99	0.09	68,84,90,100	0
81	OHX	sR	1908	7/7	0.99	0.08	80,83,86,96	0
81	OHX	sR	1909	7/7	0.99	0.10	77,80,88,97	0
81	OHX	sR	1910	7/7	0.99	0.10	73,82,86,105	0
81	OHX	AR	3406	7/7	0.99	0.09	75,76,81,82	0
81	OHX	sR	1912	7/7	0.99	0.09	73,79,83,94	0
81	OHX	sR	1913	7/7	0.99	0.07	83,86,91,107	0
81	OHX	sR	1914	7/7	0.99	0.08	84,85,89,109	0
81	OHX	AR	3470	7/7	0.99	0.06	97,100,107,139	0
81	OHX	sR	1916[A]	7/7	0.99	0.18	68,71,72,80	7
81	OHX	sR	1916[B]	7/7	0.99	0.18	73,75,81,117	7
81	OHX	sR	1917	7/7	0.99	0.07	82,83,91,110	0
81	OHX	AR	3407	7/7	0.99	0.11	65,67,72,72	0
81	OHX	sR	1919	7/7	0.99	0.07	80,84,94,114	0
81	OHX	AR	3408	7/7	0.99	0.11	77,83,85,88	0
82	MG	1	3757	1/1	0.99	0.13	44,44,44,44	0
81	OHX	AR	3409	7/7	0.99	0.10	62,64,73,75	0
82	MG	AR	4210	1/1	0.99	0.05	41,41,41,41	0
81	OHX	AR	3410	7/7	0.99	0.08	61,62,65,73	0
82	MG	AR	4212	1/1	0.99	0.05	60,60,60,60	0
81	OHX	AR	3411	7/7	0.99	0.12	79,81,90,94	0
81	OHX	AR	3412	7/7	0.99	0.10	72,76,84,85	0
81	OHX	1	3406	7/7	0.99	0.08	78,80,82,83	0
82	MG	AR	4216	1/1	0.99	0.04	44,44,44,44	0
81	OHX	1	4072	7/7	0.99	0.09	73,78,83,87	0
82	MG	AR	4218	1/1	0.99	0.13	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	OHX	AR	3415	7/7	0.99	0.10	75,81,86,95	0
81	OHX	1	3407	7/7	0.99	0.09	71,78,84,86	0
81	OHX	AR	3417	7/7	0.99	0.10	81,82,86,97	0
81	OHX	1	4076	7/7	0.99	0.09	74,76,83,91	0
81	OHX	AR	3419	7/7	0.99	0.07	76,79,86,90	0
81	OHX	AR	3420	7/7	0.99	0.09	76,80,88,95	0
81	OHX	AR	3421	7/7	0.99	0.10	75,83,87,93	0
81	OHX	A	1902	7/7	0.99	0.09	84,85,89,107	0
81	OHX	AR	3422	7/7	0.99	0.06	73,80,84,91	0
81	OHX	A	1904	7/7	0.99	0.08	92,95,99,121	0
81	OHX	A	1905	7/7	0.99	0.08	96,99,105,129	0
81	OHX	AR	3423	7/7	0.99	0.09	78,83,87,89	0
85	ZN	AK	102	1/1	0.99	0.02	54,54,54,54	0
85	ZN	AN	500	1/1	0.99	0.02	59,59,59,59	0
81	OHX	A	2103	7/7	0.99	0.10	73,85,92,95	0
85	ZN	AQ	501	1/1	0.99	0.04	83,83,83,83	0
81	OHX	A	2104	7/7	0.99	0.11	85,88,90,102	0
85	ZN	DL	103	1/1	0.99	0.04	58,58,58,58	0
85	ZN	DO	201	1/1	0.99	0.03	50,50,50,50	0
81	OHX	A	2105	7/7	0.99	0.09	85,88,95,107	0
81	OHX	AR	3424	7/7	0.99	0.11	77,84,92,94	0
85	ZN	b	201	1/1	0.99	0.04	92,92,92,92	0
81	OHX	AR	3425	7/7	0.99	0.10	83,87,89,99	0
85	ZN	e	101	1/1	0.99	0.04	94,94,94,94	0
85	ZN	g	501	1/1	0.99	0.03	136,136,136,136	0
85	ZN	d6	202	1/1	0.99	0.04	66,66,66,66	0
82	MG	v	303	1/1	0.99	0.04	52,52,52,52	0
81	OHX	AR	3489	7/7	0.99	0.10	81,82,91,112	0
81	OHX	AR	3426	7/7	0.99	0.08	78,79,88,94	0
81	OHX	1	3409	7/7	1.00	0.08	73,79,89,89	0
81	OHX	1	4071	7/7	1.00	0.09	64,67,73,74	0
81	OHX	AR	3404	7/7	1.00	0.08	60,66,66,74	0
81	OHX	CP	301	7/7	1.00	0.09	77,77,81,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.