Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2024 – 01:58 am BST

PDB ID	:	8P4V
Title	:	80S yeast ribosome in complex with HaterumaimideQ
Authors	:	Terrosu, S.; Yusupov, M.
Deposited on	:	2023-05-23
Resolution	:	3.16 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

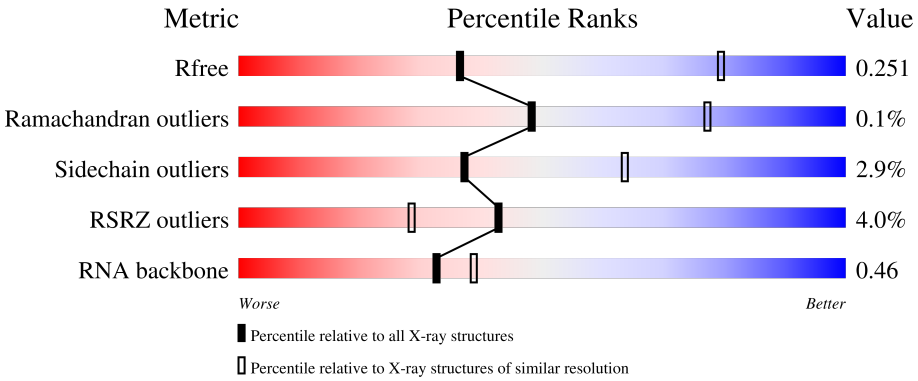
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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}	164625	2168 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)
RNA backbone	3690	1016 (3.42-2.90)

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

Mol	Chain	Length	Quality of chain
1	1	3396	% 74% 19% 7%
1	AR	3396	% 73% 19% 7%
2	3	121	87% 13%
2	AS	121	83% 16%
3	4	158	78% 22%

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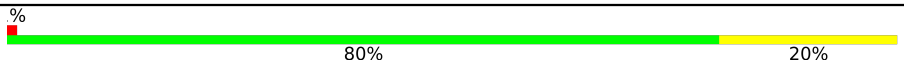
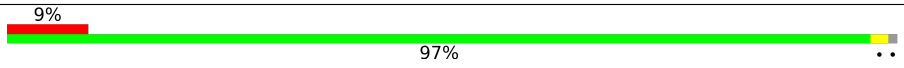
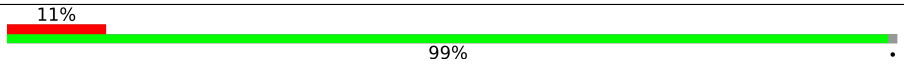
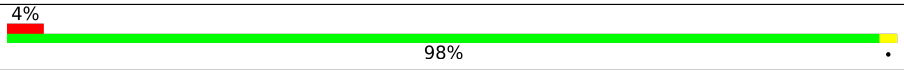
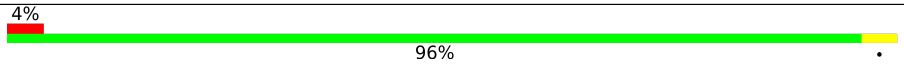
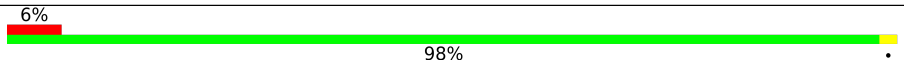
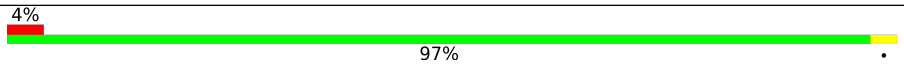
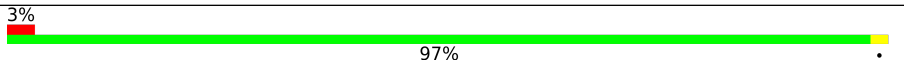
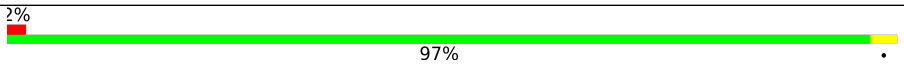
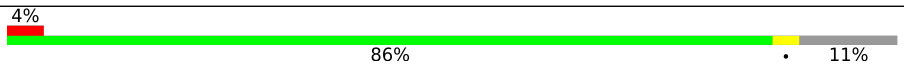
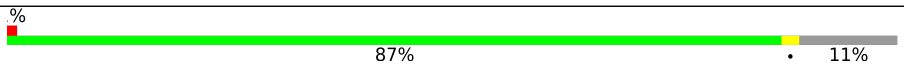
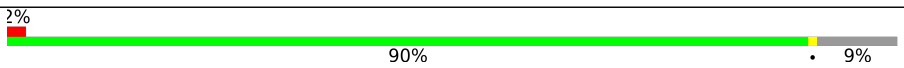
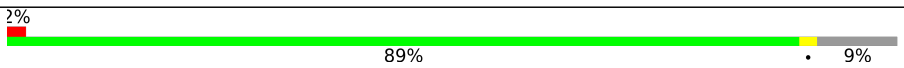
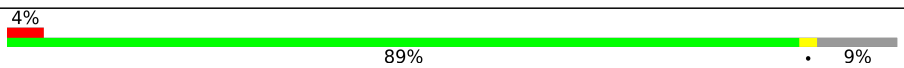
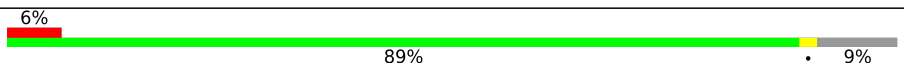
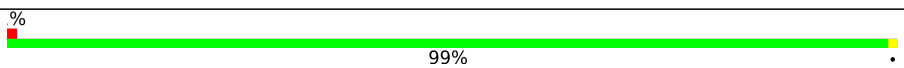
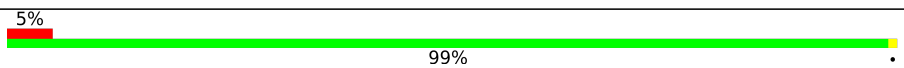
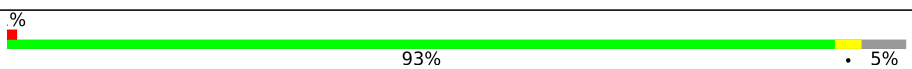
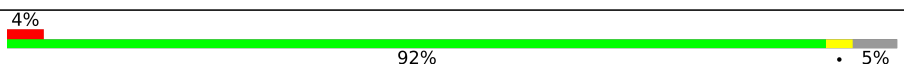
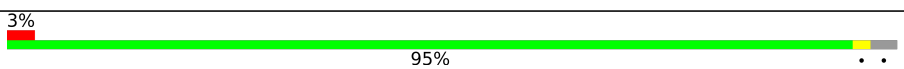
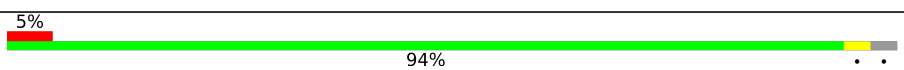
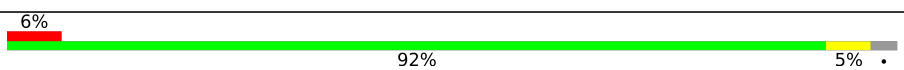
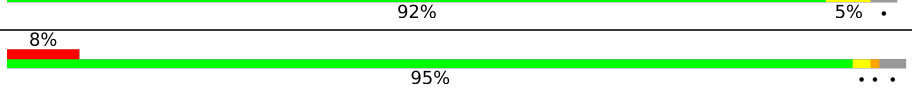
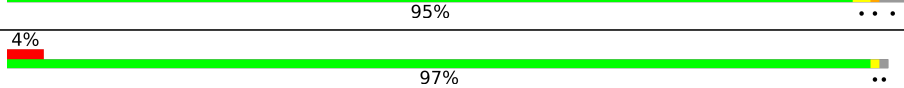
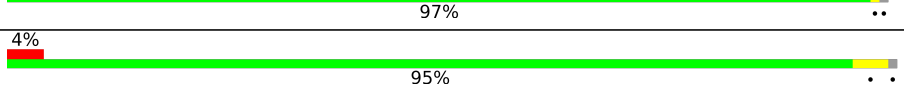
Mol	Chain	Length	Quality of chain
3	AT	158	
4	CD	254	
4	j	254	
5	CE	387	
5	k	387	
6	CF	362	
6	l	362	
7	CG	297	
7	m	297	
8	CH	176	
8	n	176	
9	CI	244	
9	o	244	
10	CJ	256	
10	p	256	
11	CK	191	
11	q	191	
12	CL	221	
12	r	221	
13	CM	174	
13	s	174	
14	CN	199	
14	t	199	
15	CO	138	
15	u	138	

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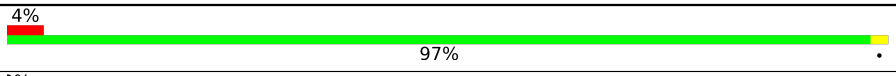
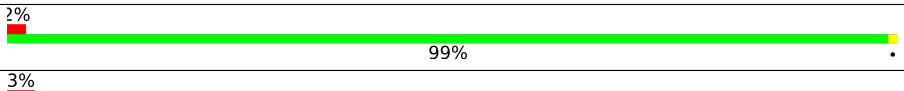
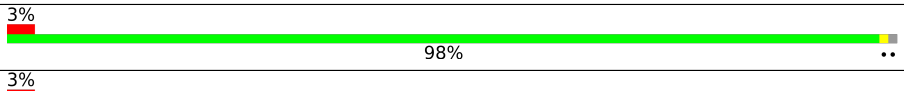
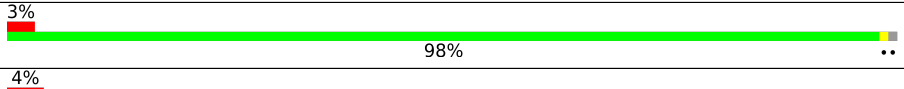
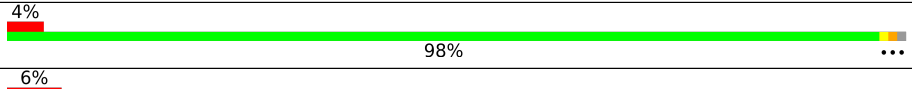
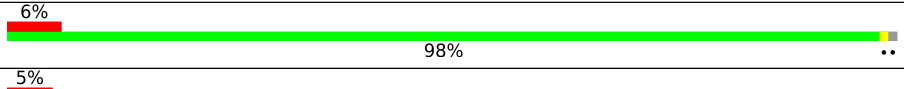
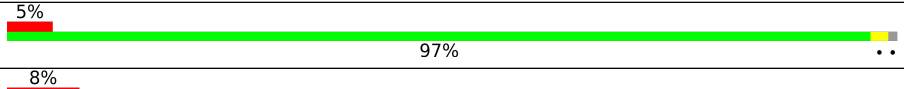
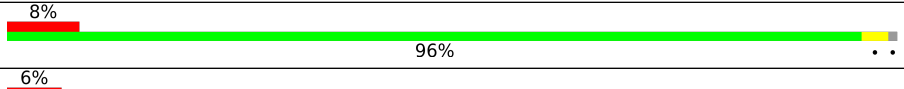
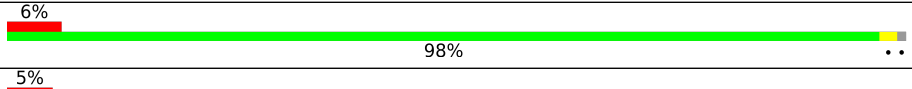
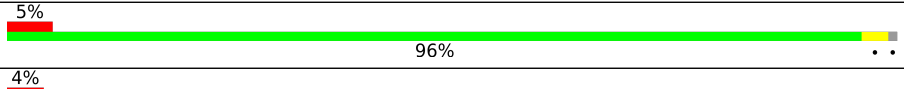
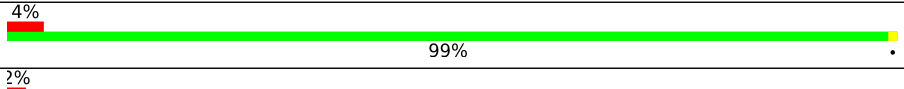
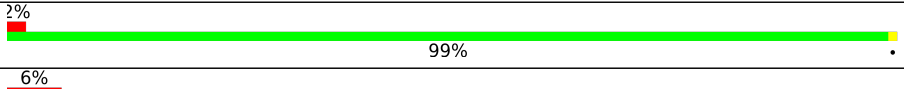
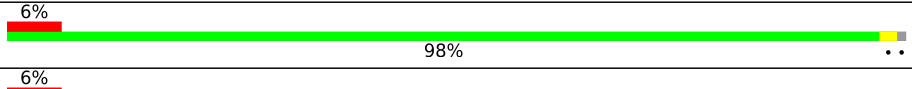
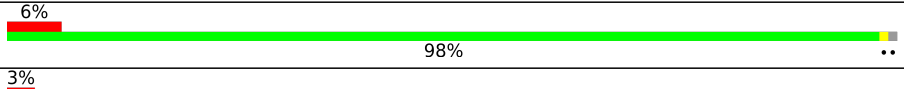
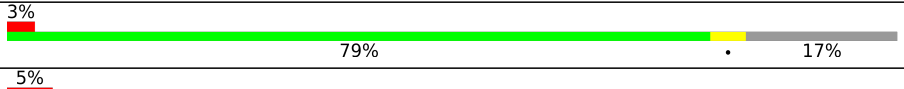
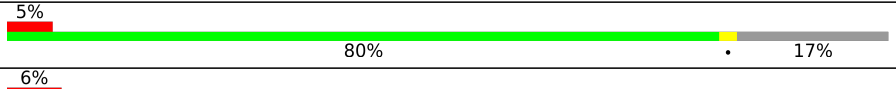
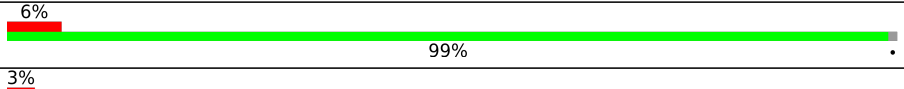
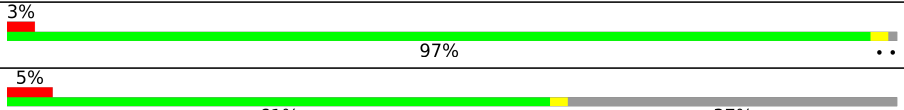
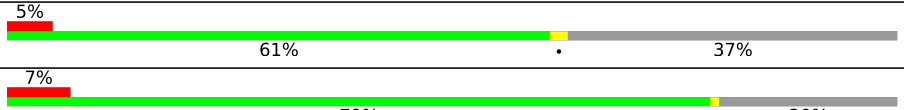
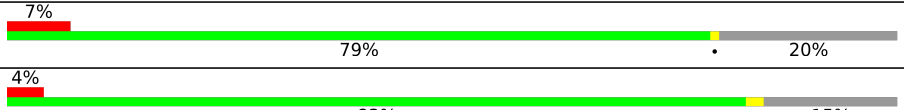
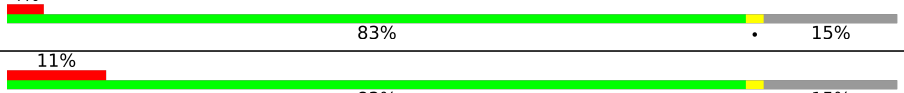
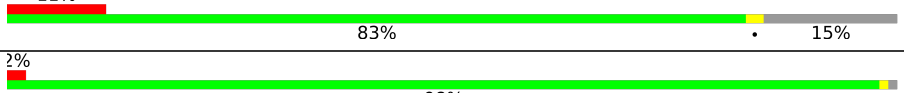
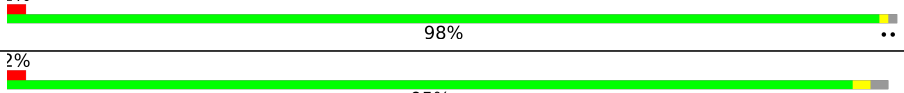
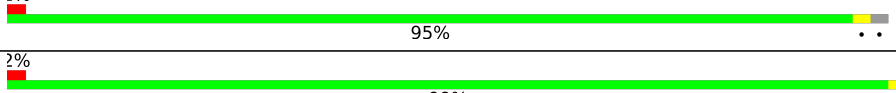
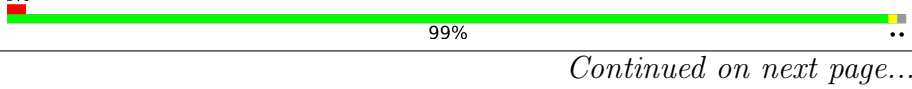
Mol	Chain	Length	Quality of chain
16	CP	204	
16	v	204	
17	CQ	199	
17	w	199	
18	CR	184	
18	x	184	
19	CS	186	
19	y	186	
20	CT	189	
20	z	189	
21	0	172	
21	CU	172	
22	2	160	
22	CV	160	
23	5	121	
23	CW	121	
24	6	137	
24	CX	137	
25	7	155	
25	CY	155	
26	8	142	
26	CZ	142	
27	9	127	
27	DA	127	
28	AA	136	

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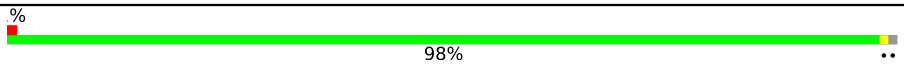
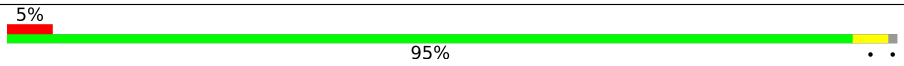
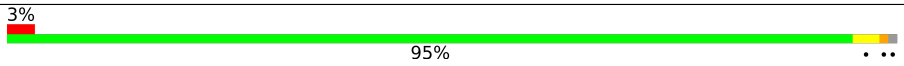
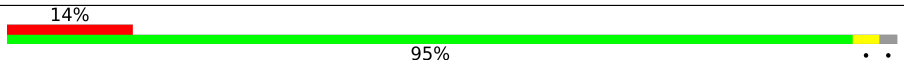
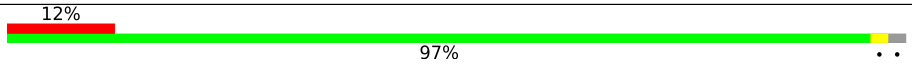
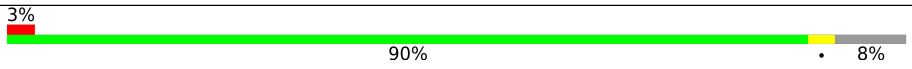
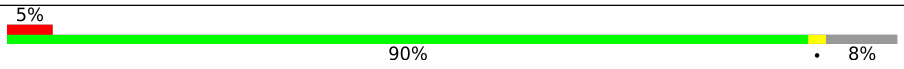
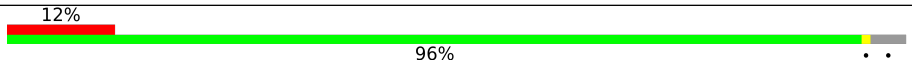
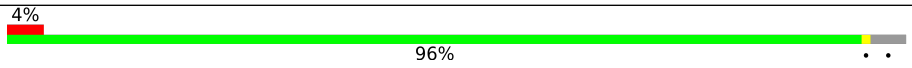
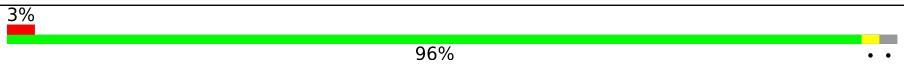
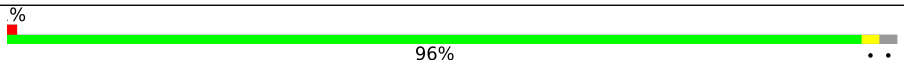
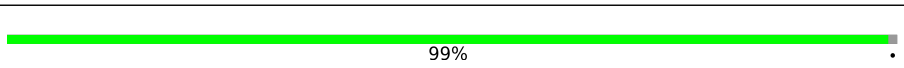
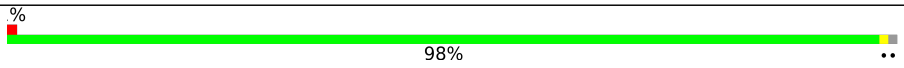
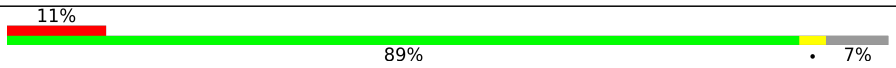
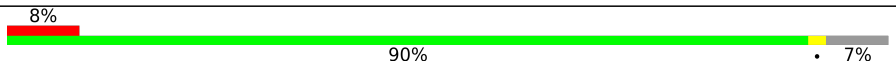
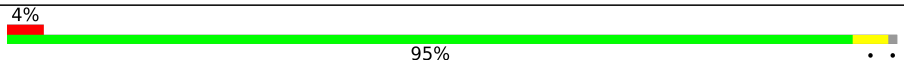
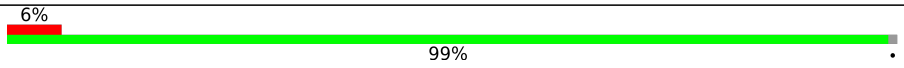
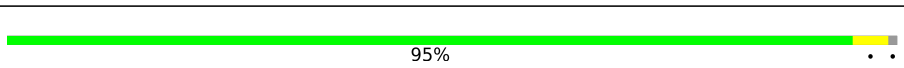
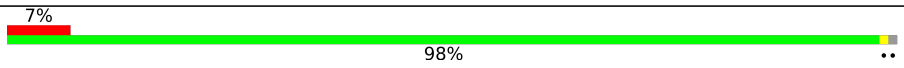
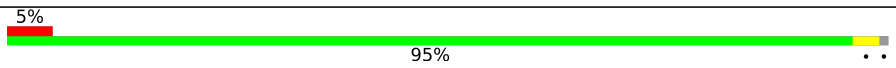
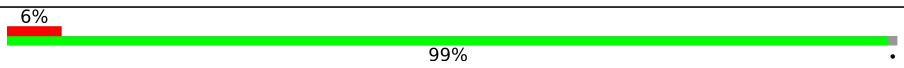
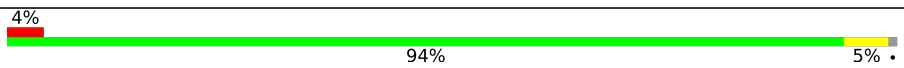
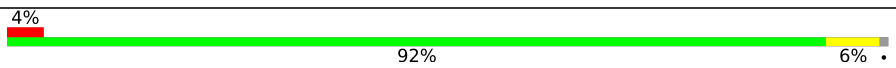
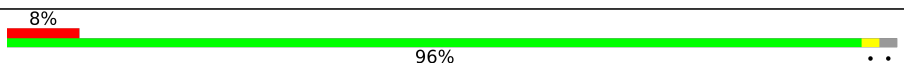
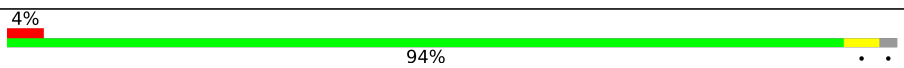
Mol	Chain	Length	Quality of chain
28	DB	136	
29	AB	149	
29	DC	149	
30	AC	59	
30	DD	59	
31	AD	105	
31	DE	105	
32	AE	113	
32	DF	113	
33	AF	130	
33	DG	130	
34	AG	107	
34	DH	107	
35	AH	121	
35	DI	121	
36	AI	120	
36	DJ	120	
37	AJ	100	
37	DK	100	
38	AK	88	
38	DL	88	
39	AL	78	
39	DM	78	
40	AM	51	
40	DN	51	

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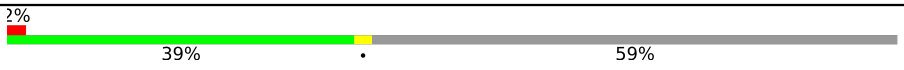
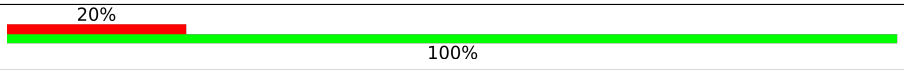
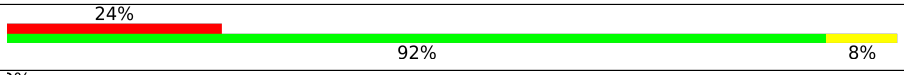
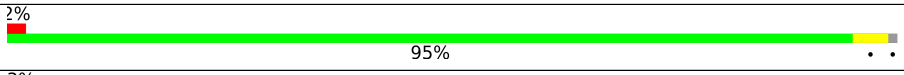
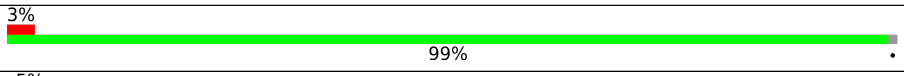
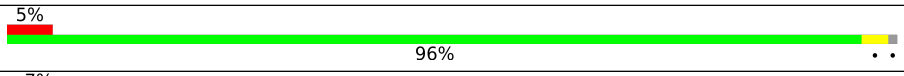
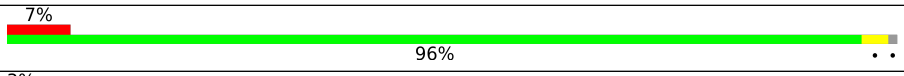
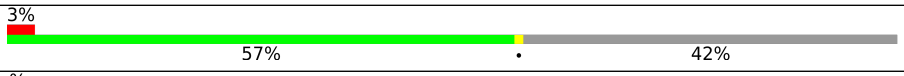
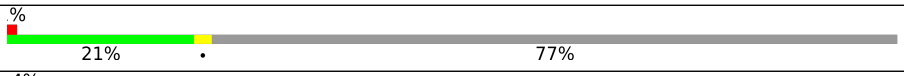
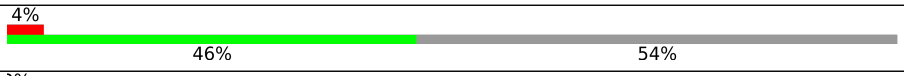
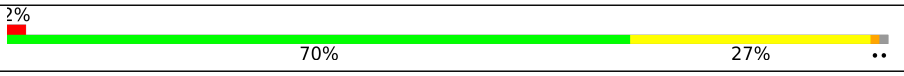
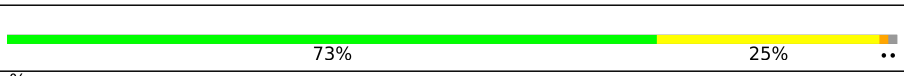
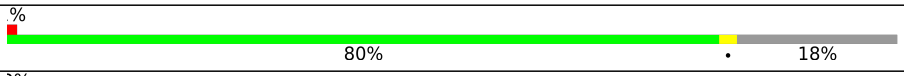
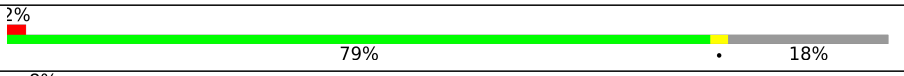
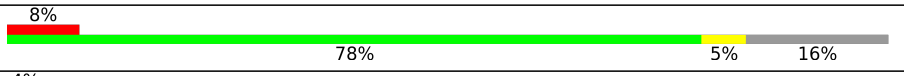
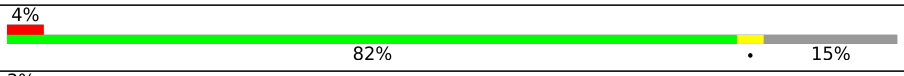
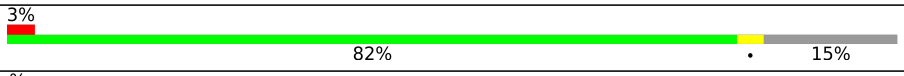
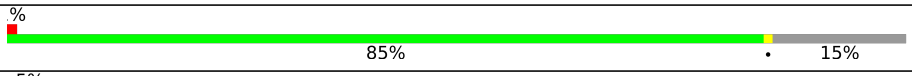
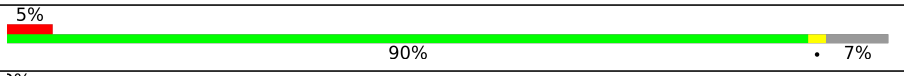
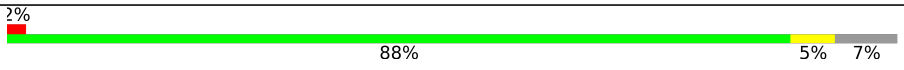
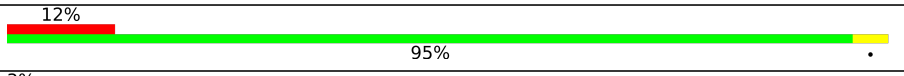
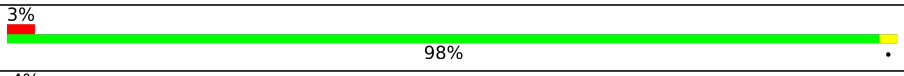
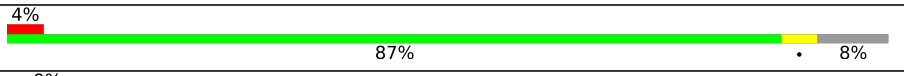
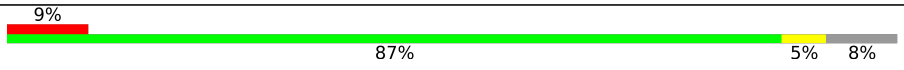
Mol	Chain	Length	Quality of chain
41	AN	128	
41	DO	128	
42	AO	25	
42	DP	25	
43	AP	106	
43	DQ	106	
44	AQ	92	
44	DR	92	
45	i	273	
45	sM	273	
46	p0	311	
47	A	1800	
47	sR	1800	
48	B	252	
48	s0	252	
49	C	255	
49	s1	255	
50	D	254	
50	s2	254	
51	E	240	
51	s3	240	
52	F	261	
52	s4	261	
53	G	225	
53	s5	225	

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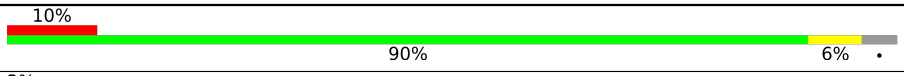
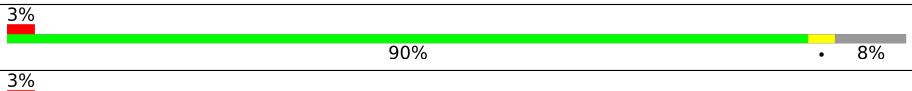
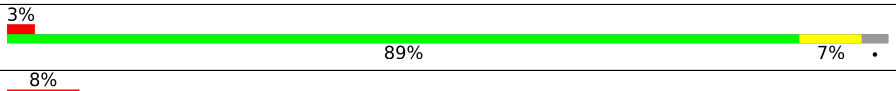
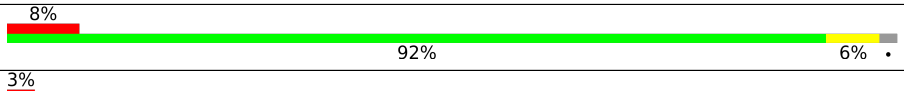
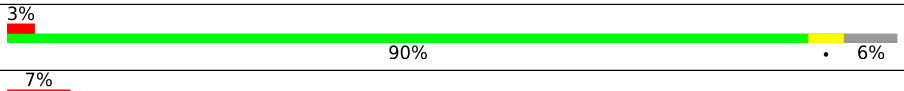
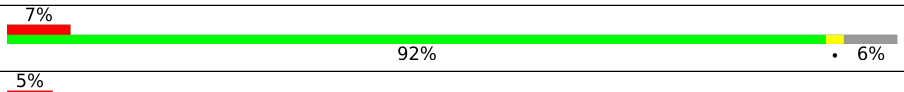
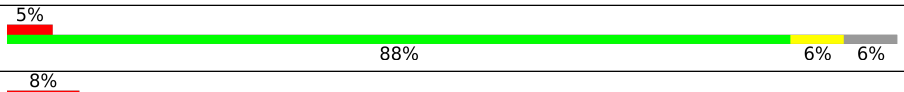
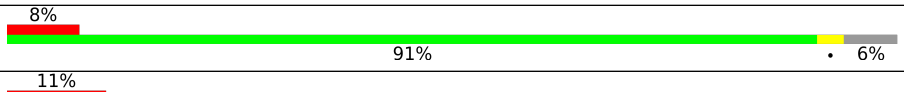
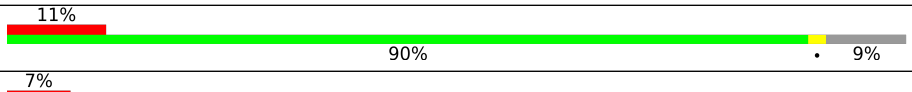
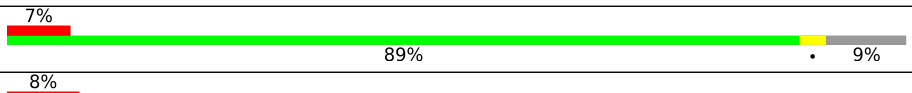
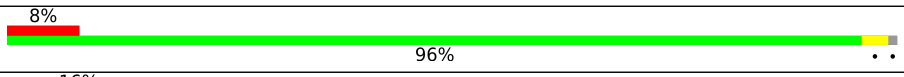
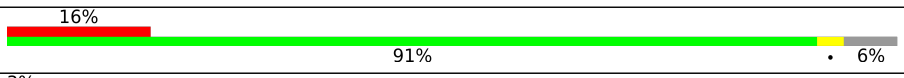
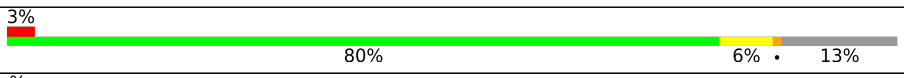
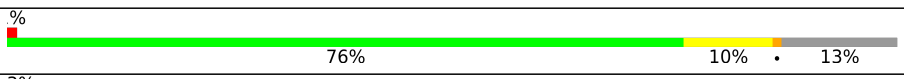
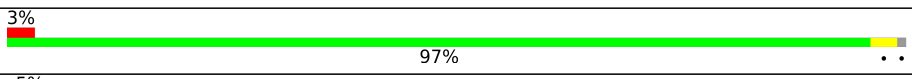
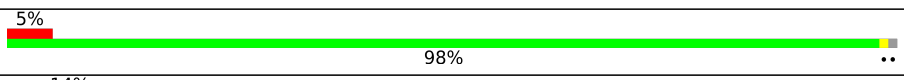
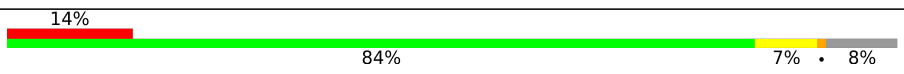
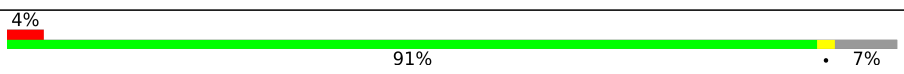
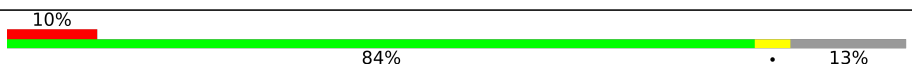
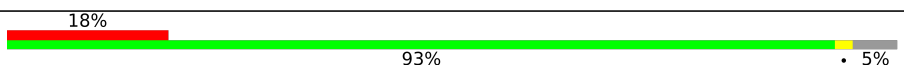
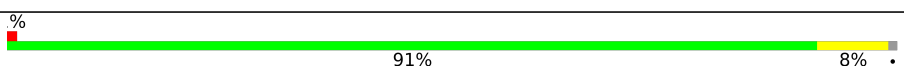
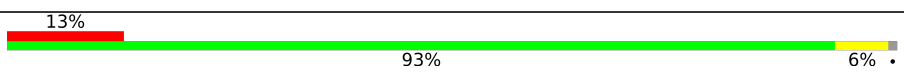
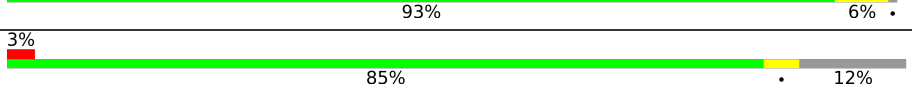
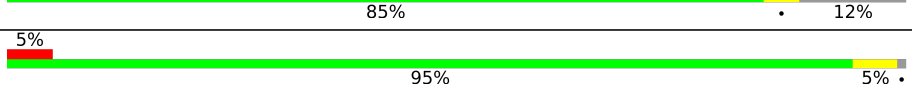
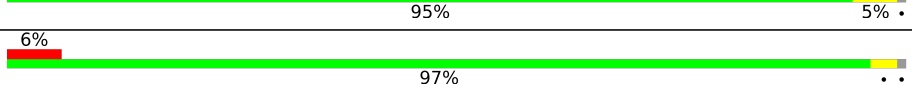
Mol	Chain	Length	Quality of chain
54	H	236	
54	s6	236	
55	I	190	
55	s7	190	
56	J	200	
56	s8	200	
57	K	197	
57	s9	197	
58	L	105	
58	c0	105	
59	M	156	
59	c1	156	
60	N	143	
60	c2	143	
61	O	151	
61	c3	151	
62	P	138	
62	c4	138	
63	Q	142	
63	c5	142	
64	R	143	
64	c6	143	
65	S	136	
66	T	146	
66	c8	146	

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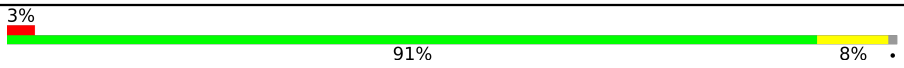
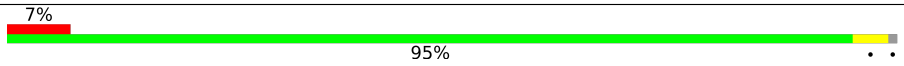
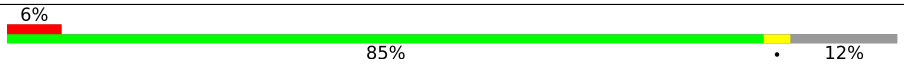
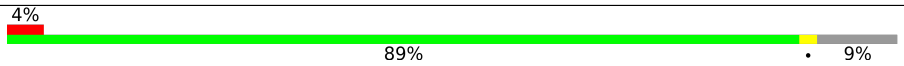
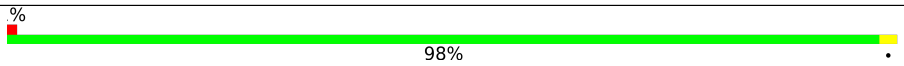
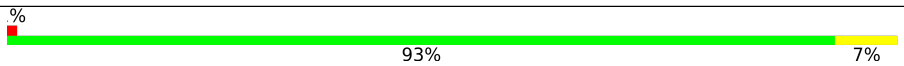
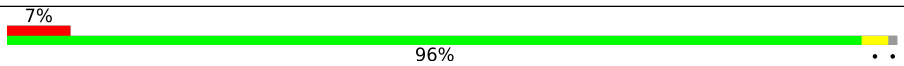
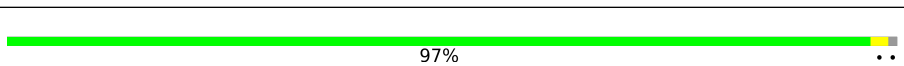
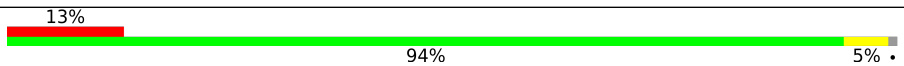
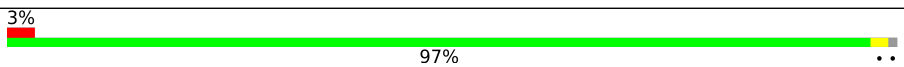
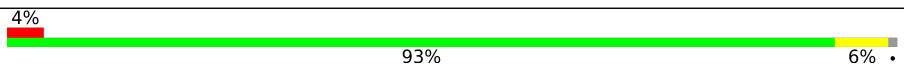
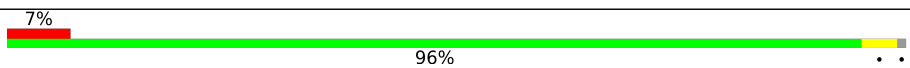
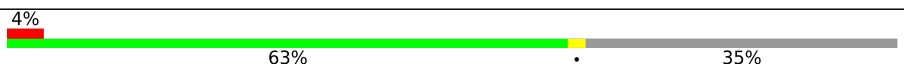
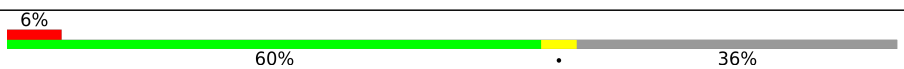
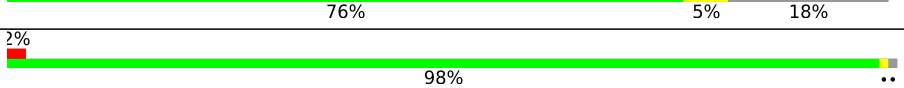
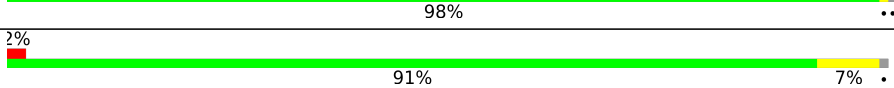
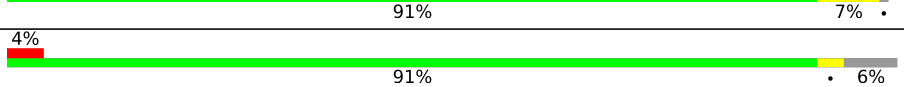
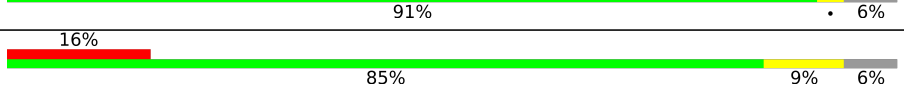
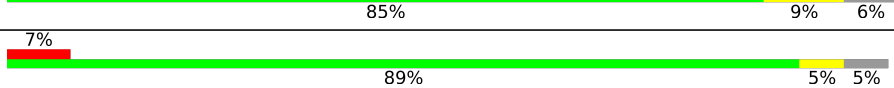
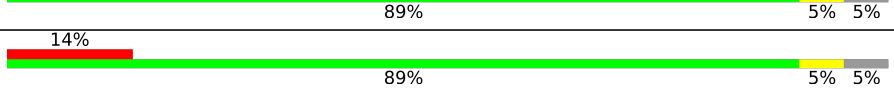
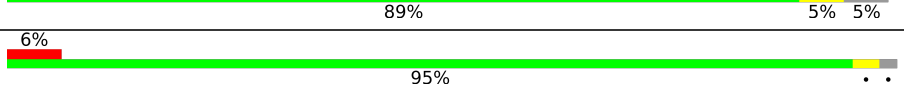
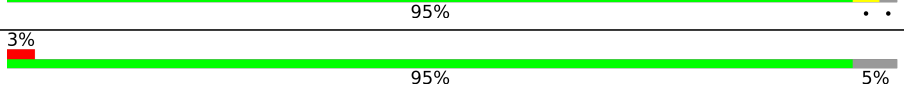
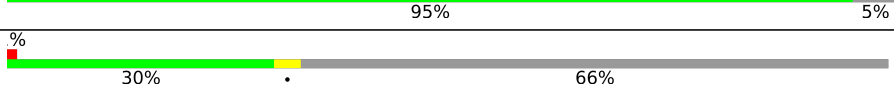
Mol	Chain	Length	Quality of chain
67	U	144	
67	c9	144	
68	V	121	
68	d0	121	
69	W	87	
69	d1	87	
70	X	130	
70	d2	130	
71	Y	145	
71	d3	145	
72	Z	135	
72	d4	135	
73	a	108	
73	d5	108	
74	b	119	
74	d6	119	
75	c	82	
75	d7	82	
76	d	67	
76	d8	67	
77	d9	56	
77	e	56	
78	e0	63	
78	f	63	
79	e1	152	

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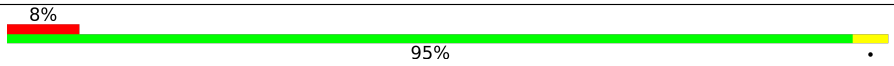
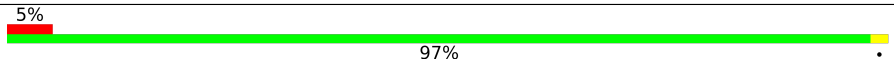
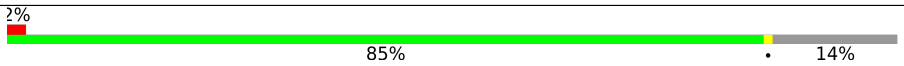
Mol	Chain	Length	Quality of chain
79	g	152	
80	Rb	319	
80	h	319	
81	c7	136	

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
83	MG	1	4009	-	-	-	X
83	MG	1	4031	-	-	-	X
83	MG	AR	3964	-	-	-	X
83	MG	AR	4007	-	-	-	X

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 409267 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	3147	Total	C	N	O	P	0	0	0
			67313	30067	12134	21965	3147			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called 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	S	0	0	0
			1053	675	199	177	2			
15	CO	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
25	CY	124	Total	C	N	O	S	0	0	0
			836	525	166	144	1			

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	9	126	Total	C	N	O	0	0	0
			993	625	192	176			
27	DA	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
			1087	706	201	180			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 45 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	i	159	Total	C	N	O	0	0	0
			1104	652	221	231			
45	sM	63	Total	C	N	O	0	0	0
			475	280	99	96			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	p0	143	Total	C	N	O	S	0	0	0
			1076	686	192	195	3			

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	A	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			
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
			1577	1014	278	283	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	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	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	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	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			
60	c2	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
			886	541	182	162	1			
62	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	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			
64	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	S	120	Total	C	N	O	S	0	0	0
			926	577	177	170	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	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
68	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	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	S	0	0	0
			397	249	73	71	4			

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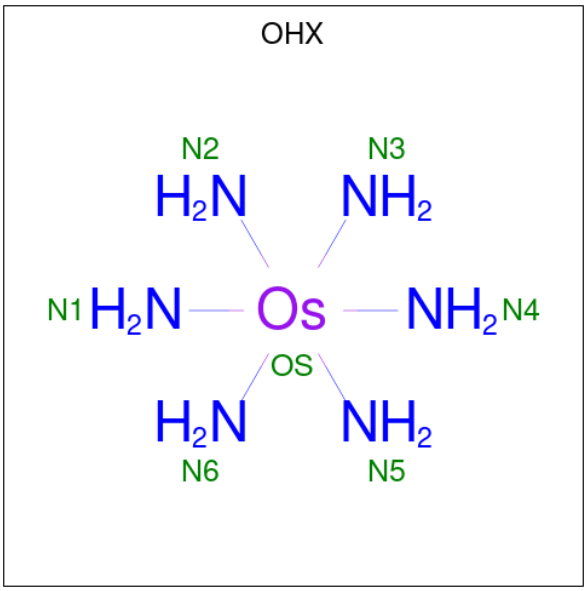
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	Rb	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 81 is a protein called 40S ribosomal protein S17-A.

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

- Molecule 82 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 14 12 2	0	1
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total Os 1 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 6 5 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 14 12 2	0	1
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 6 5 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	k	1	Total N Os 7 6 1	0	0
82	k	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	l	1	Total	N	Os	0	0
			7	6	1		
82	r	1	Total	N	Os	0	0
			7	6	1		
82	v	1	Total	N	Os	0	0
			7	6	1		
82	z	1	Total	N	Os	0	0
			7	6	1		
82	2	1	Total	N	Os	0	0
			7	6	1		
82	AC	1	Total	N	Os	0	0
			7	6	1		
82	AG	1	Total	N	Os	0	0
			7	6	1		
82	AK	1	Total	N	Os	0	0
			7	6	1		
82	AK	1	Total	N	Os	0	0
			7	6	1		
82	AP	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	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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82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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82	CE	1	Total 7	N 6	Os 1	0	0
82	CE	1	Total 7	N 6	Os 1	0	0
82	CG	1	Total 7	N 6	Os 1	0	0
82	CG	1	Total 7	N 6	Os 1	0	0
82	CG	1	Total 7	N 6	Os 1	0	0
82	CH	1	Total 7	N 6	Os 1	0	0
82	CK	1	Total 7	N 6	Os 1	0	0
82	CL	1	Total 7	N 6	Os 1	0	0
82	CL	1	Total 7	N 6	Os 1	0	0
82	CP	1	Total 7	N 6	Os 1	0	0
82	CS	1	Total 7	N 6	Os 1	0	0
82	CV	1	Total 7	N 6	Os 1	0	0
82	CX	1	Total 7	N 6	Os 1	0	0
82	DD	1	Total 7	N 6	Os 1	0	0
82	DH	1	Total 7	N 6	Os 1	0	0
82	DL	1	Total 7	N 6	Os 1	0	0
82	DQ	1	Total 7	N 6	Os 1	0	0
82	A	1	Total 7	N 6	Os 1	0	0
82	A	1	Total 7	N 6	Os 1	0	0
82	A	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	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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82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	J	1	Total N Os 7 6 1	0	0
82	O	1	Total N Os 7 6 1	0	0
82	Q	1	Total N Os 7 6 1	0	0
82	T	1	Total N Os 7 6 1	0	0
82	U	1	Total N Os 7 6 1	0	0
82	h	1	Total N Os 7 6 1	0	0

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	Rb	1	Total	N	Os	0	0
			7	6	1		
82	s1	1	Total	N	Os	0	0
			7	6	1		
82	s4	1	Total	N	Os	0	0
			7	6	1		
82	s8	1	Total	N	Os	0	0
			7	6	1		
82	c3	1	Total	N	Os	0	0
			7	6	1		
82	c5	1	Total	N	Os	0	0
			7	6	1		
82	c7	1	Total	N	Os	0	0
			7	6	1		
82	c8	1	Total	N	Os	0	0
			7	6	1		

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

- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	1	486	Total Mg 486 486	0	0
83	3	12	Total Mg 12 12	0	0
83	4	18	Total Mg 18 18	0	0
83	j	2	Total Mg 2 2	0	0
83	k	2	Total Mg 2 2	0	0
83	l	4	Total Mg 4 4	0	0
83	m	1	Total Mg 1 1	0	0
83	o	3	Total Mg 3 3	0	0
83	r	2	Total Mg 2 2	0	0
83	s	1	Total Mg 1 1	0	0
83	t	2	Total Mg 2 2	0	0
83	u	1	Total Mg 1 1	0	0
83	v	4	Total Mg 4 4	0	0
83	w	1	Total Mg 1 1	0	0
83	x	8	Total Mg 8 8	0	0
83	y	1	Total Mg 1 1	0	0
83	z	1	Total Mg 1 1	0	0
83	6	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	9	1	Total Mg 1 1	0	0
83	AB	5	Total Mg 5 5	0	0
83	AC	1	Total Mg 1 1	0	0
83	AF	2	Total Mg 2 2	0	0
83	AG	1	Total Mg 1 1	0	0
83	AH	2	Total Mg 2 2	0	0
83	AI	1	Total Mg 1 1	0	0
83	AP	1	Total Mg 1 1	0	0
83	i	1	Total Mg 1 1	0	0
83	AR	498	Total Mg 498 498	0	0
83	AS	19	Total Mg 19 19	0	0
83	AT	19	Total Mg 19 19	0	0
83	CD	1	Total Mg 1 1	0	0
83	CE	3	Total Mg 3 3	0	0
83	CF	5	Total Mg 5 5	0	0
83	CG	1	Total Mg 1 1	0	0
83	CI	2	Total Mg 2 2	0	0
83	CJ	1	Total Mg 1 1	0	0
83	CK	1	Total Mg 1 1	0	0
83	CL	2	Total Mg 2 2	0	0
83	CM	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	CO	1	Total Mg 1 1	0	0
83	CP	5	Total Mg 5 5	0	0
83	CQ	3	Total Mg 3 3	0	0
83	CR	8	Total Mg 8 8	0	0
83	CU	1	Total Mg 1 1	0	0
83	CX	1	Total Mg 1 1	0	0
83	DA	2	Total Mg 2 2	0	0
83	DC	2	Total Mg 2 2	0	0
83	DD	1	Total Mg 1 1	0	0
83	DH	2	Total Mg 2 2	0	0
83	DI	3	Total Mg 3 3	0	0
83	DL	2	Total Mg 2 2	0	0
83	DO	2	Total Mg 2 2	0	0
83	DP	1	Total Mg 1 1	0	0
83	DQ	2	Total Mg 2 2	0	0
83	sM	2	Total Mg 2 2	0	0
83	A	135	Total Mg 135 135	0	0
83	D	2	Total Mg 2 2	0	0
83	F	1	Total Mg 1 1	0	0
83	O	1	Total Mg 1 1	0	0
83	P	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	S	1	Total Mg 1 1	0	0
83	X	1	Total Mg 1 1	0	0
83	Y	1	Total Mg 1 1	0	0
83	b	1	Total Mg 1 1	0	0
83	sR	149	Total Mg 149 149	0	0
83	s1	1	Total Mg 1 1	0	0
83	s2	1	Total Mg 1 1	0	0
83	s4	1	Total Mg 1 1	0	0
83	s6	1	Total Mg 1 1	0	0
83	s8	2	Total Mg 2 2	0	0
83	s9	1	Total Mg 1 1	0	0
83	c1	1	Total Mg 1 1	0	0
83	c3	1	Total Mg 1 1	0	0
83	c4	2	Total Mg 2 2	0	0
83	c6	1	Total Mg 1 1	0	0
83	c8	1	Total Mg 1 1	0	0
83	c9	2	Total Mg 2 2	0	0
83	d3	3	Total Mg 3 3	0	0
83	d4	3	Total Mg 3 3	0	0
83	d5	1	Total Mg 1 1	0	0
83	d6	2	Total Mg 2 2	0	0

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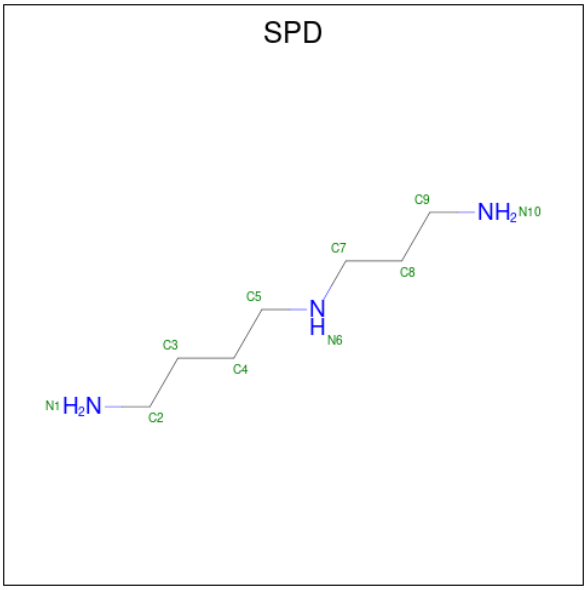
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	d9	1	Total Mg 1 1	0	0

- Molecule 84 is POTASSIUM ION (three-letter code: K) (formula: K).

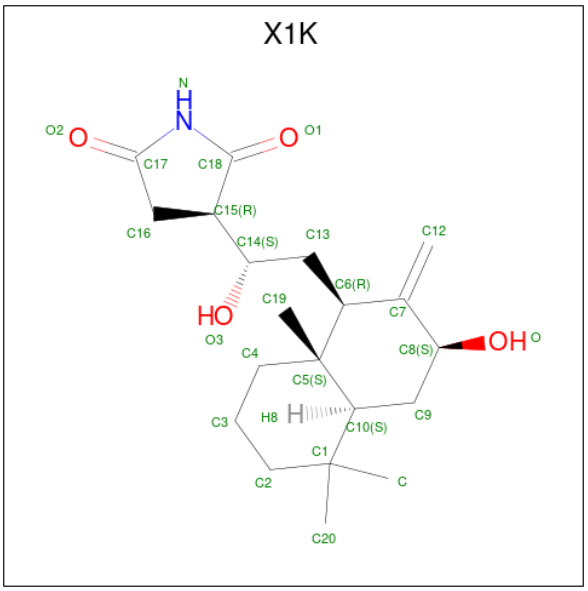
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	1	1	Total K 1 1	0	0
84	j	1	Total K 1 1	0	0
84	AR	4	Total K 4 4	0	0
84	sR	1	Total K 1 1	0	0

- Molecule 85 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	1	1	Total C N 10 7 3	0	0
85	AR	1	Total C N 10 7 3	0	0

- Molecule 86 is (3 {R})-3-[(1 {S})-2-[(1 {R},3 {S},4 {a} {S},8 {a} {S})-5,5,8 {a}-trimethyl-2-methylidene-3-oxidanyl-3,4,4 {a},6,7,8-hexahydro-1 {H}-naphthalen-1-yl]-1-oxidanyl-ethyl]pyrrolidine-2,5-dione (three-letter code: X1K) (formula: $C_{20}H_{31}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	1	1	Total C N O 25 20 1 4	0	0
86	AR	1	Total C N O 25 20 1 4	0	0

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

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

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

- Molecule 88 is OSMIUM ION (three-letter code: OS) (formula: Os).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	A	1	Total Os 1 1	0	0

- Molecule 89 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	1	148	Total O 148 148	0	0
89	4	14	Total O 14 14	0	0
89	j	1	Total O 1 1	0	0
89	x	4	Total O 4 4	0	0
89	AE	2	Total O 2 2	0	0
89	AO	1	Total O 1 1	0	0
89	AR	210	Total O 210 210	0	0
89	CD	1	Total O 1 1	0	0
89	CF	7	Total O 7 7	0	0
89	CI	1	Total O 1 1	0	0
89	CP	1	Total O 1 1	0	0

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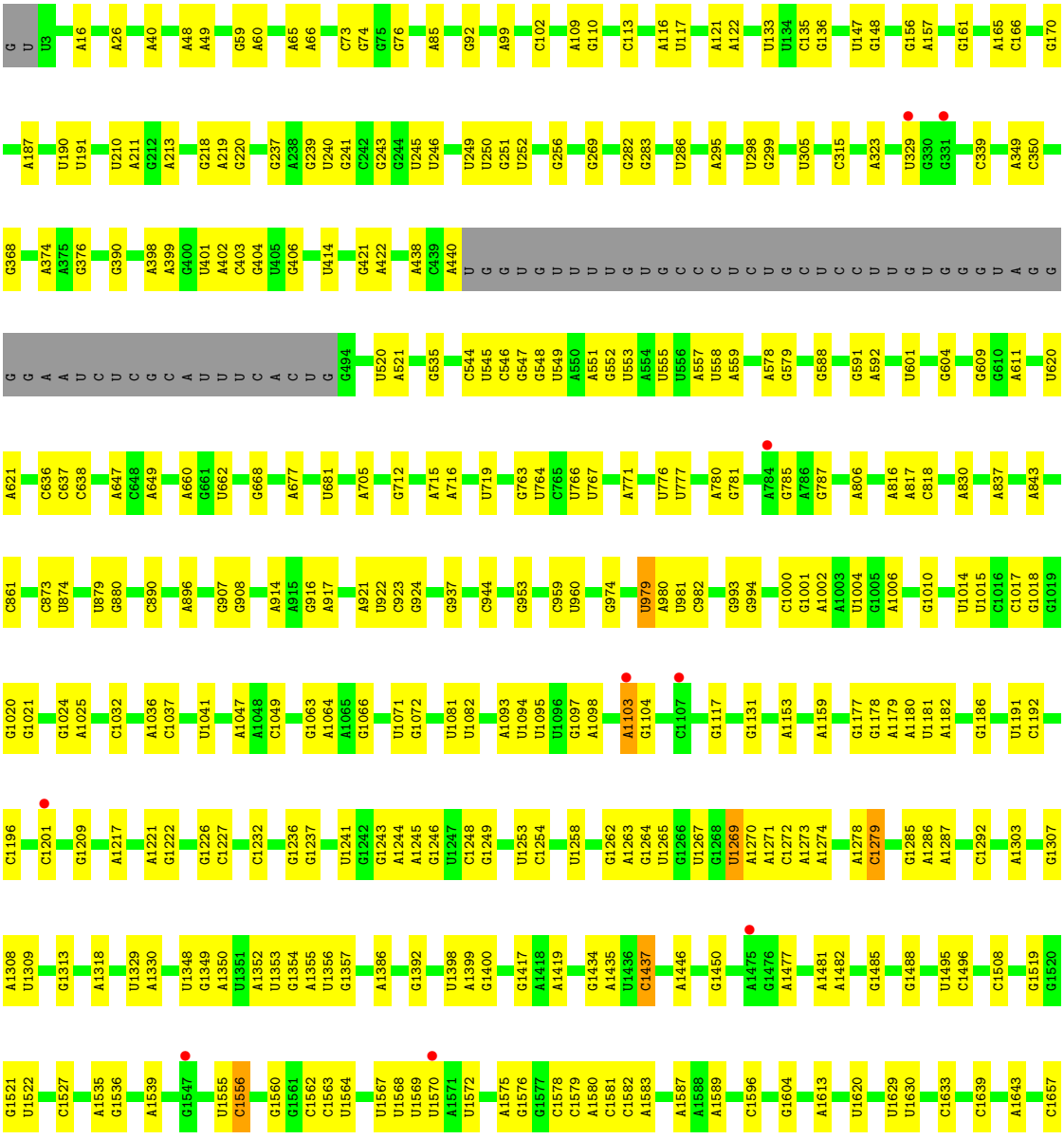
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	CR	1	Total O 1 1	0	0
89	CT	1	Total O 1 1	0	0
89	DG	1	Total O 1 1	0	0
89	A	57	Total O 57 57	0	0
89	R	1	Total O 1 1	0	0
89	S	6	Total O 6 6	0	0
89	Y	1	Total O 1 1	0	0
89	sR	41	Total O 41 41	0	0
89	s8	1	Total O 1 1	0	0
89	c1	1	Total O 1 1	0	0
89	c7	2	Total O 2 2	0	0

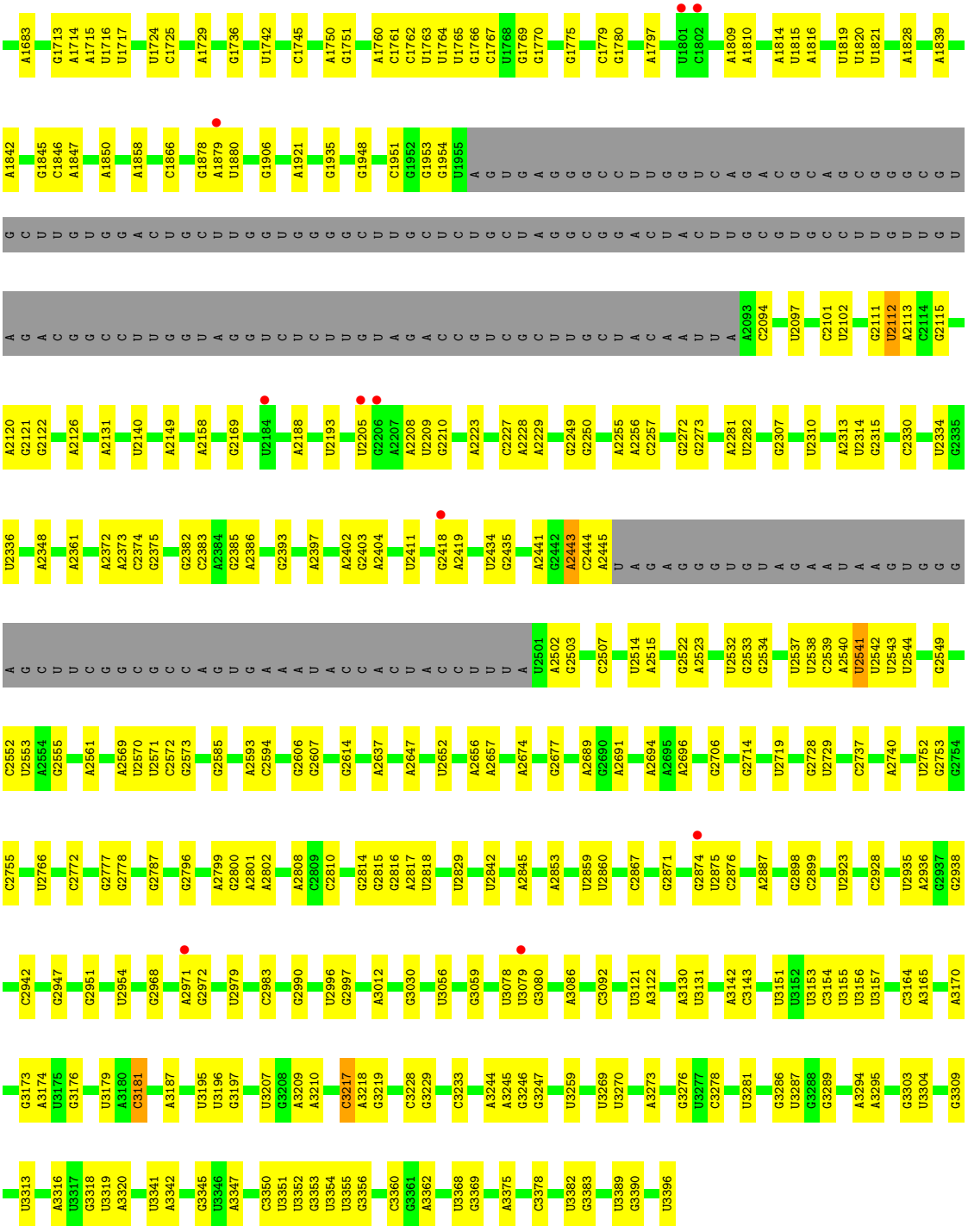
3 Residue-property plots (i)

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

• Molecule 1: 25S ribosomal RNA

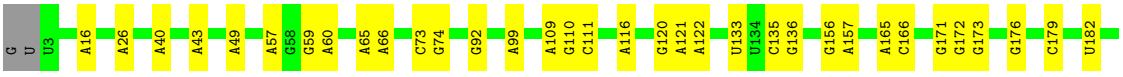
Chain 1:

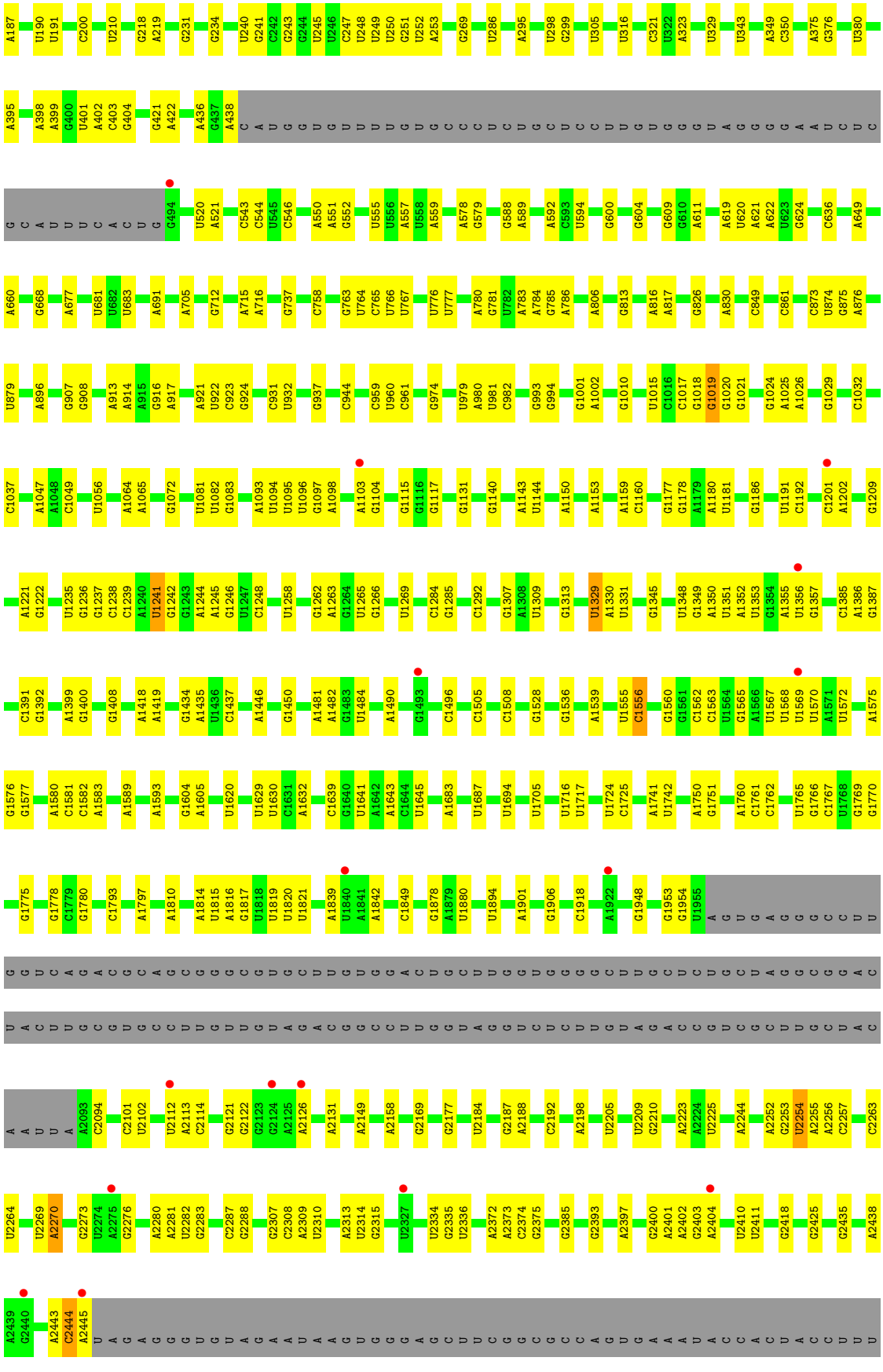


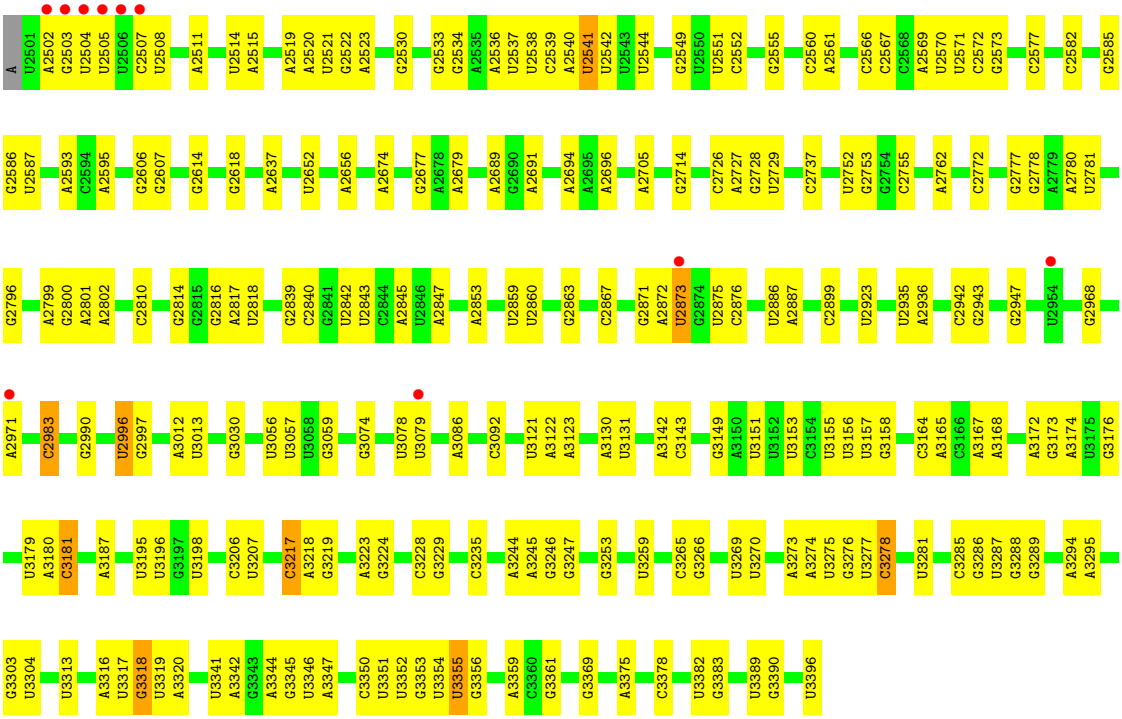


• Molecule 1: 25S ribosomal RNA

Chain AR:

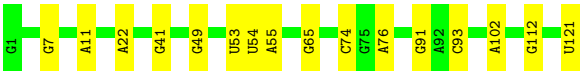



A187 U190 U191 C200 U210 G218 A219 G231 G234 U240 G241 C242 G243 G244 U245 U246 C247 U248 U249 U250 G251 U252 A253 G269 U286 A295 U298 G299 U305 U316 C321 U322 A323 U329 U343 A349 C350 A375 G376 U380
A395 A398 A399 G400 U401 A402 C403 G404 G421 A422 A436 G437 A438 C A U G G U G U U U U G U G C C C U C U G G C U C C U U G U G G G G U A G G G G A A U C U C
G C A U U U C A C U G G494 U520 A521 C543 C544 U545 C546 A550 A551 G552 U555 U556 A557 U558 A559 A578 G579 G588 A589 A592 C593 U594 G600 G604 G609 G610 A611 A619 U620 A621 A622 U623 G624 C636 A649
A660 G668 A677 U681 U682 U683 A691 A705 G712 A715 A716 G737 C758 G763 U764 C765 C766 U767 U776 U777 A780 G781 U782 A783 A784 G785 A786 A806 G813 A816 A817 G826 A830 C849 C861 C873 U874 G875 A876
U879 A896 G907 G908 A913 A914 A915 G916 A917 A921 U922 C923 G924 C931 U932 G937 C944 C959 U960 C961 G974 U979 A980 U981 C982 G993 G994 G1001 A1002 G1010 U1015 C1016 C1017 G1018 G1019 G1020 G1021 G1024 A1025 A1026 G1029 C1032
C1037 A1047 A1048 C1049 U1056 A1064 A1065 G1072 U1081 U1082 G1083 A1093 U1094 U1095 U1096 G1097 A1098 A1103 G1104 G1115 G1116 G1117 G1131 G1140 A1143 U1144 A1150 A1153 A1159 C1160 G1177 G1178 A1179 A1180 U1181 G1186 U1191 C1192 C1201 A1202 G1209
A1221 G1222 U1235 G1236 G1237 C1238 C1239 A1240 U1241 G1242 G1243 A1244 A1245 G1246 U1247 C1248 U1258 G1262 A1263 G1264 U1265 G1266 U1269 C1284 G1285 C1292 G1307 A1308 U1309 G1313 U1329 A1330 U1331 G1345 U1348 G1349 A1350 U1351 A1352 C1353 G1354 A1355 U1356 G1357 C1385 A1386 G1387
C1391 G1392 A1399 G1400 G1408 A1418 A1419 G1434 A1435 U1436 C1437 A1446 G1450 A1481 A1482 G1483 U1484 A1490 G1493 C1496 C1505 C1508 G1528 G1536 A1539 U1555 C1556 G1560 G1561 C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569 U1570 A1571 U1572 A1575
G1576 G1577 A1580 C1581 C1582 A1583 A1589 A1593 G1604 A1605 U1620 U1629 U1630 C1631 A1632 C1639 G1640 U1641 A1642 A1643 C1644 U1645 A1683 U1687 U1694 U1705 U1716 U1717 U1724 C1725 A1741 U1742 A1750 G1751 A1760 C1761 C1762 U1765 G1766 C1767 U1768 G1769 G1770
G1775 G1778 C1779 G1780 C1793 A1797 A1810 A1814 U1815 A1816 G1817 U1818 U1819 U1820 U1821 A1839 U1840 A1841 A1842 C1849 G1878 A1879 U1880 U1894 A1901 G1906 C1918 A1922 G1948 G1953 G1954 U1955 A G U G A G G G C C U U
G G U C A G A C G C A G C G G G C G U G C U U G U G G A C U G C U U G G U G G G G C U U G C U C U G C U A G G C G G A C
U A C U U G C G U G C C U U G U U G U A G A C G G C C U U G G U A G G U C U C U U G U A G A C C G U C G C U U G C U A C
A A U U A A2093 C2094 C2101 U2102 U2112 A2113 C2114 G2121 G2122 G2123 G2124 A2125 A2126 A2131 A2149 A2158 G2169 G2177 U2184 G2187 A2188 C2192 A2198 U2205 U2209 G2210 A2223 A2224 U2225 A2244 A2252 G2253 U2254 A2255 A2256 C2257 C2263
U2264 U2269 A2270 G2273 U2274 A2275 G2276 A2280 A2281 U2282 G2283 C2287 G2288 G2307 C2308 A2309 U2310 A2313 U2314 G2315 U2327 U2334 G2335 U2336 A2372 A2373 C2374 G2375 G2385 G2393 A2397 G2400 A2401 A2402 G2403 A2404 U2410 U2411 G2418 G2425 G2435 A2438
A2439 G2440 A2443 C2444 A2445 U A G A G G G U G U A G A A U A A G U G G G A G C U U C G G C G C C A G U G A A A U A C C A C U A C C U U U



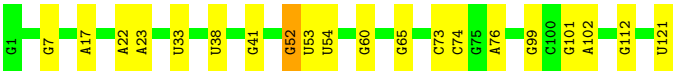
• Molecule 2: 5S ribosomal RNA

Chain 3:



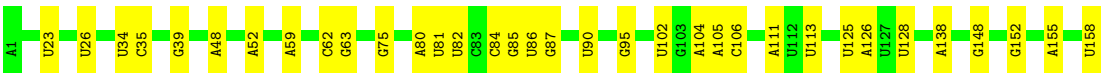
• Molecule 2: 5S ribosomal RNA

Chain AS:



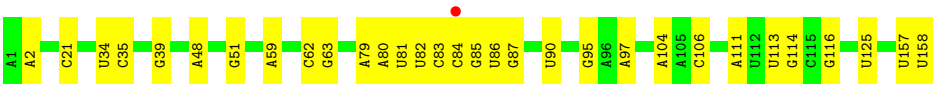
• Molecule 3: 5.8S ribosomal RNA

Chain 4:



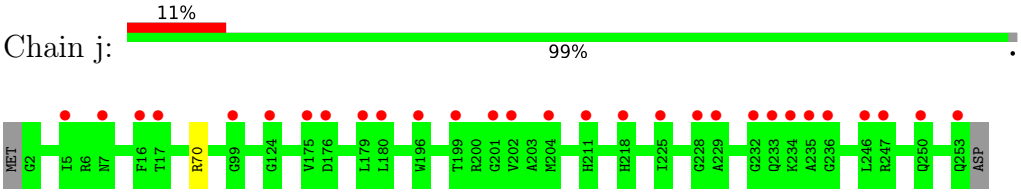
• Molecule 3: 5.8S ribosomal RNA

Chain AT:



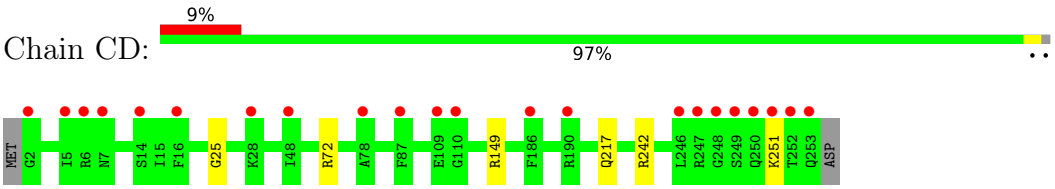
• Molecule 4: 60S ribosomal protein L2-A

Chain j:



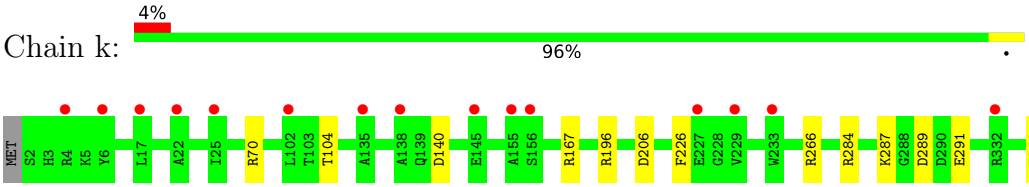
• Molecule 4: 60S ribosomal protein L2-A

Chain CD:



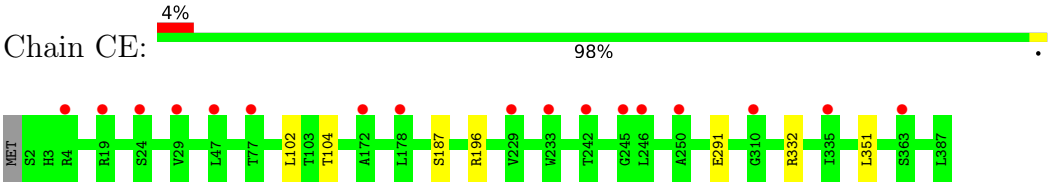
• Molecule 5: 60S ribosomal protein L3

Chain k:



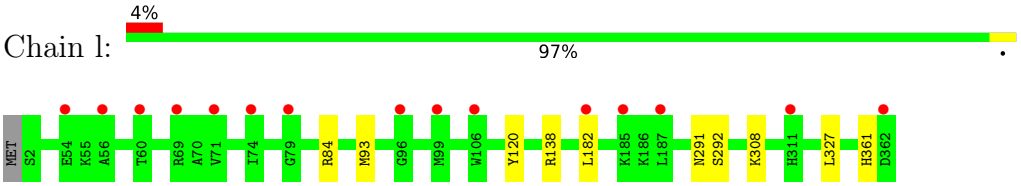
• Molecule 5: 60S ribosomal protein L3

Chain CE:



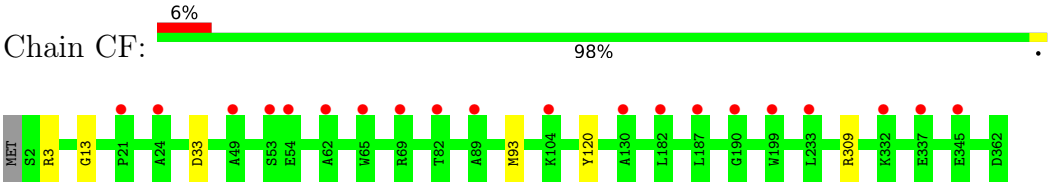
• Molecule 6: 60S ribosomal protein L4-A

Chain l:



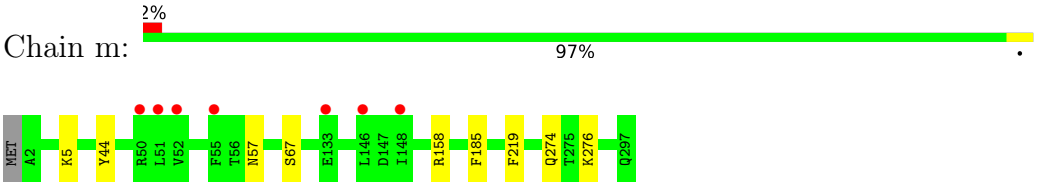
• Molecule 6: 60S ribosomal protein L4-A

Chain CF:



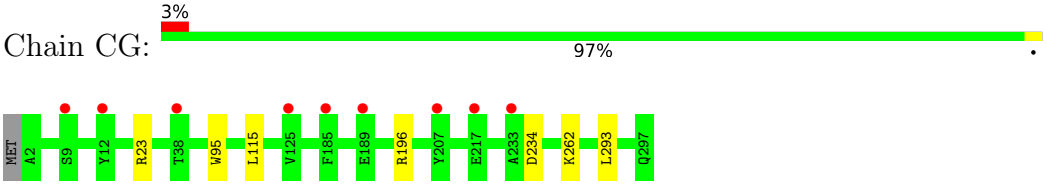
• Molecule 7: 60S ribosomal protein L5

Chain m:



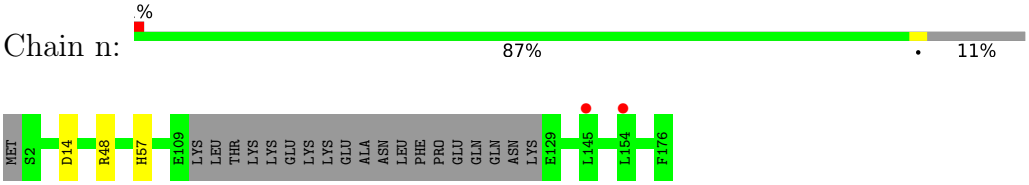
• Molecule 7: 60S ribosomal protein L5

Chain CG:



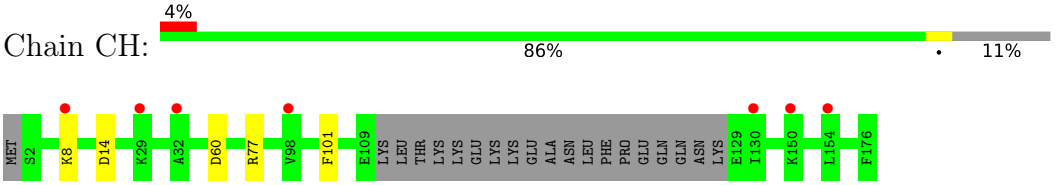
• Molecule 8: 60S ribosomal protein L6-A

Chain n:



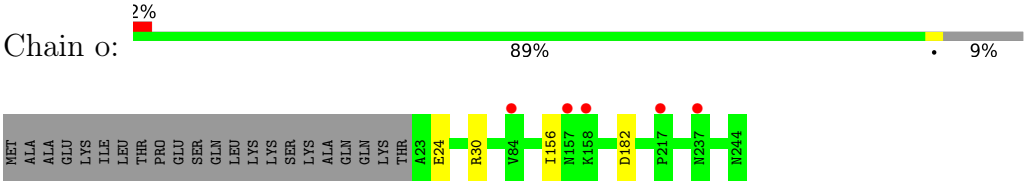
• Molecule 8: 60S ribosomal protein L6-A

Chain CH:



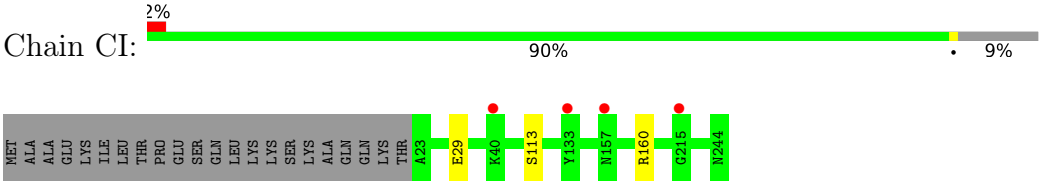
• Molecule 9: 60S ribosomal protein L7-A

Chain o:



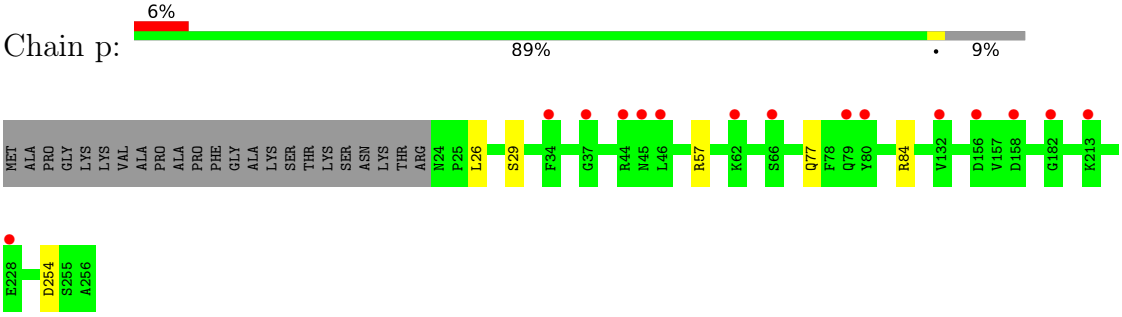
• Molecule 9: 60S ribosomal protein L7-A

Chain CI:



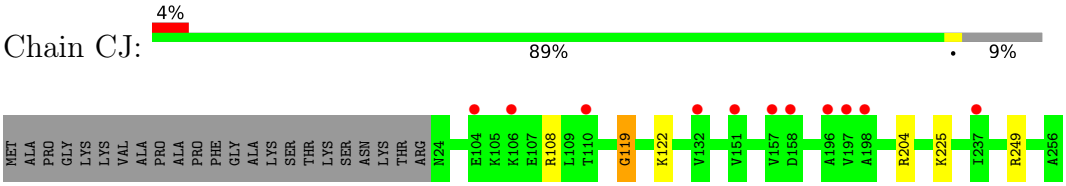
• Molecule 10: 60S ribosomal protein L8-A

Chain p:



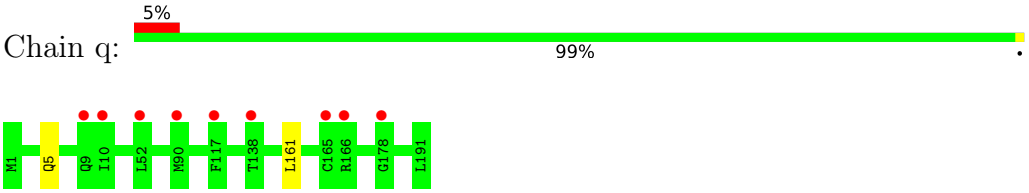
• Molecule 10: 60S ribosomal protein L8-A

Chain CJ:



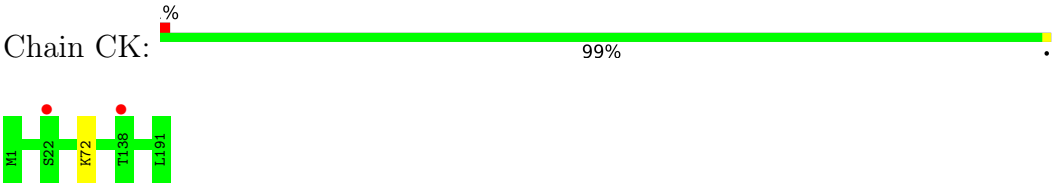
• Molecule 11: 60S ribosomal protein L9-A

Chain q:



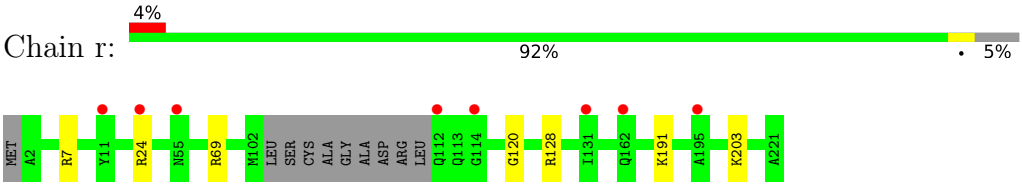
• Molecule 11: 60S ribosomal protein L9-A

Chain CK:



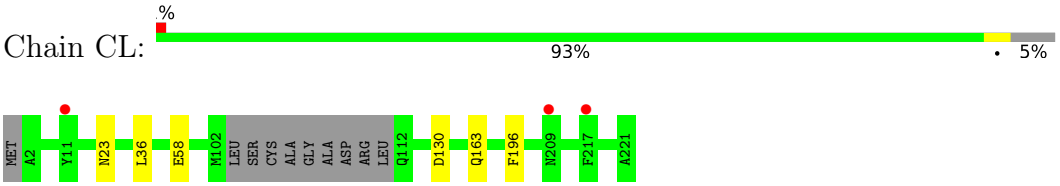
• Molecule 12: 60S ribosomal protein L10

Chain r:



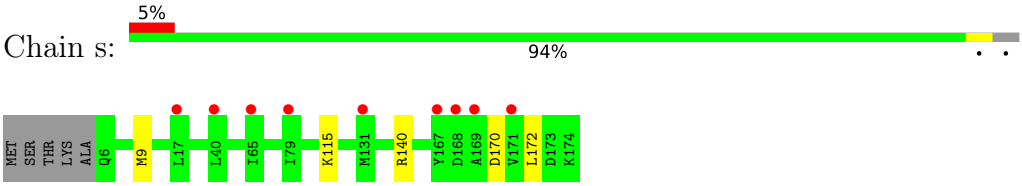
• Molecule 12: 60S ribosomal protein L10

Chain CL:



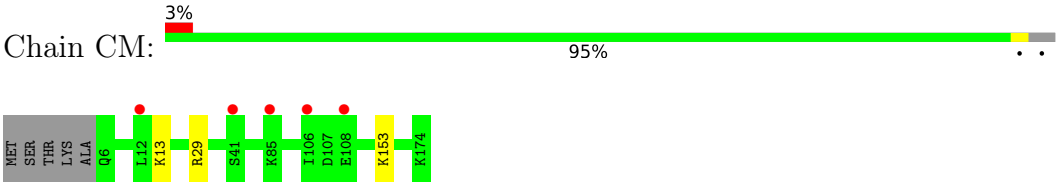
• Molecule 13: Large ribosomal subunit protein uL5B

Chain s:



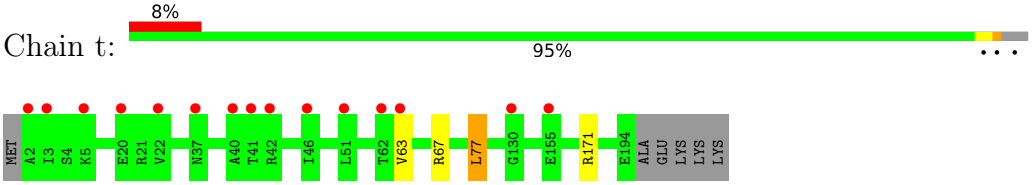
• Molecule 13: Large ribosomal subunit protein uL5B

Chain CM:



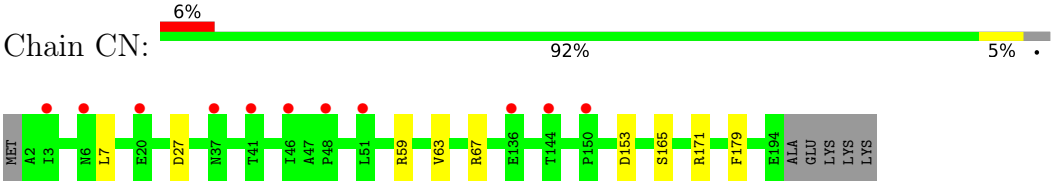
• Molecule 14: 60S ribosomal protein L13-A

Chain t:



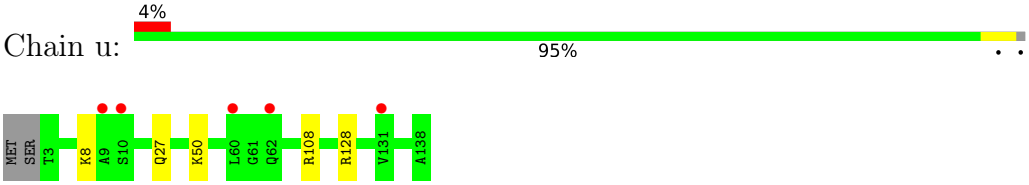
• Molecule 14: 60S ribosomal protein L13-A

Chain CN:



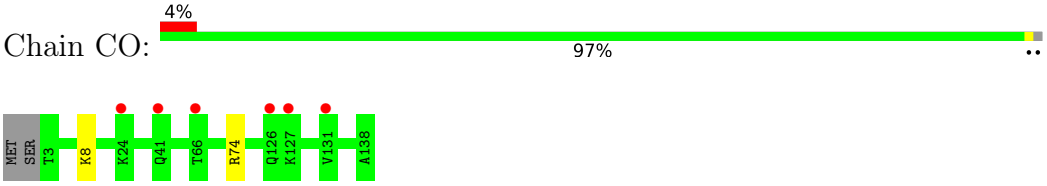
• Molecule 15: 60S ribosomal protein L14-A

Chain u:



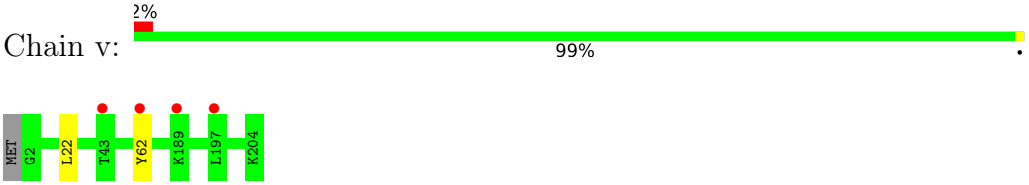
• Molecule 15: 60S ribosomal protein L14-A

Chain CO:



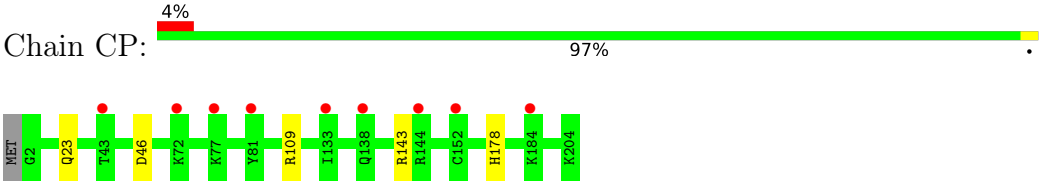
• Molecule 16: 60S ribosomal protein L15-A

Chain v:



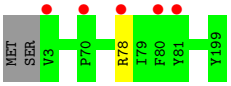
• Molecule 16: 60S ribosomal protein L15-A

Chain CP:



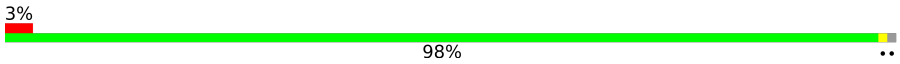
• Molecule 17: 60S ribosomal protein L16-A

Chain w:



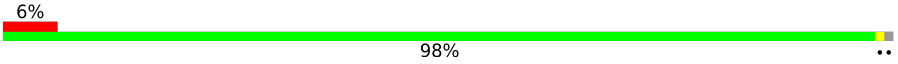
• Molecule 17: 60S ribosomal protein L16-A

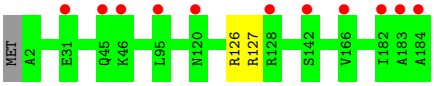
Chain CQ:



• Molecule 18: 60S ribosomal protein L17-A

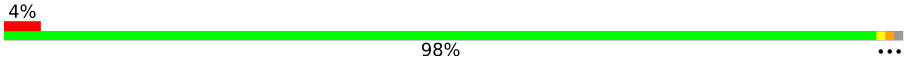
Chain x:

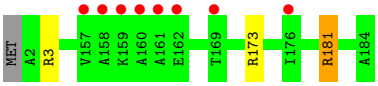




• Molecule 18: 60S ribosomal protein L17-A

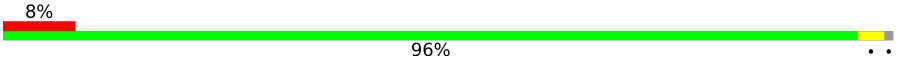
Chain CR:

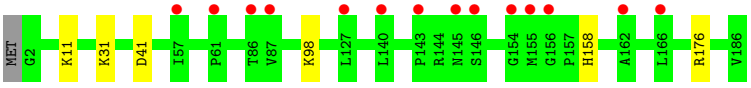




• Molecule 19: 60S ribosomal protein L18-A

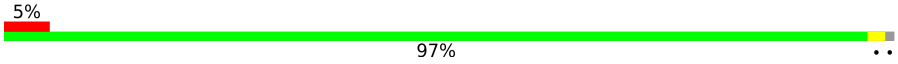
Chain y:

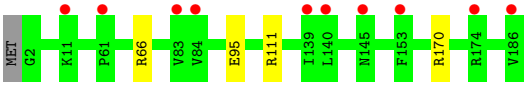




• Molecule 19: 60S ribosomal protein L18-A

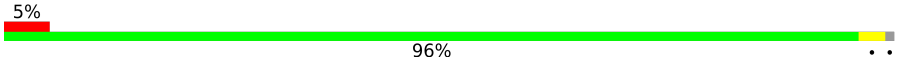
Chain CS:

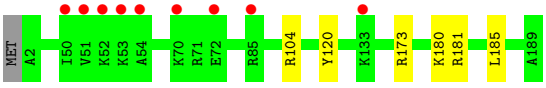




• Molecule 20: 60S ribosomal protein L19-A

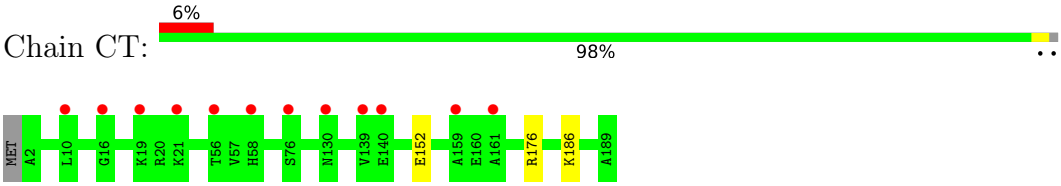
Chain z:





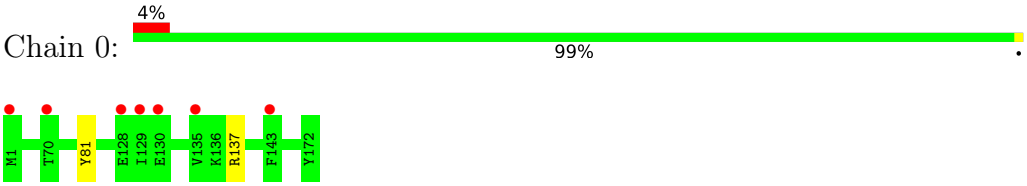
• Molecule 20: 60S ribosomal protein L19-A

Chain CT:



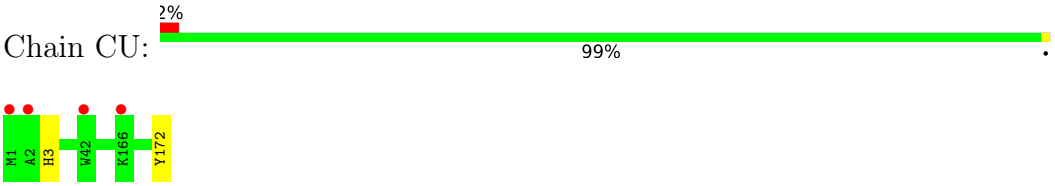
• Molecule 21: 60S ribosomal protein L20-A

Chain 0:



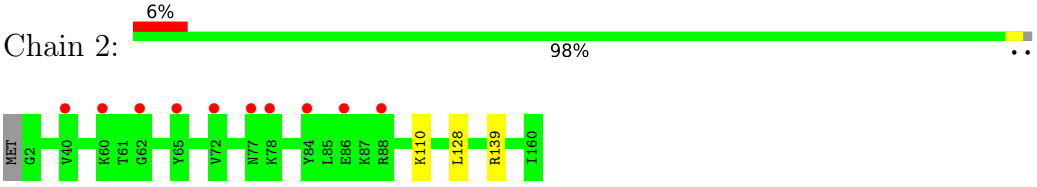
• Molecule 21: 60S ribosomal protein L20-A

Chain CU:



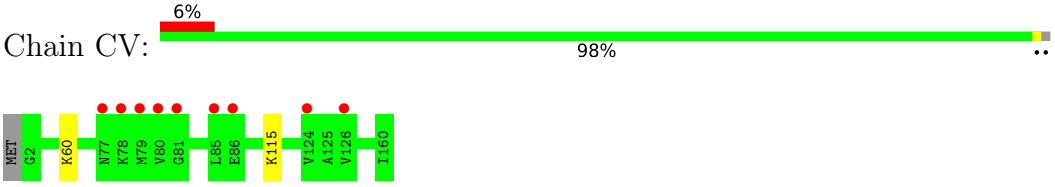
• Molecule 22: 60S ribosomal protein L21-A

Chain 2:



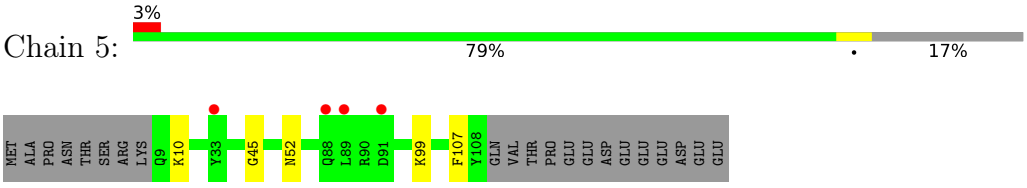
• Molecule 22: 60S ribosomal protein L21-A

Chain CV:



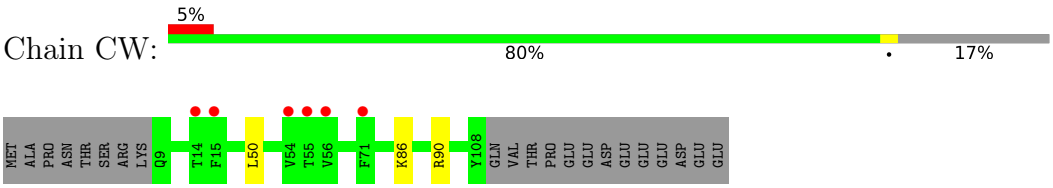
• Molecule 23: 60S ribosomal protein L22-A

Chain 5:



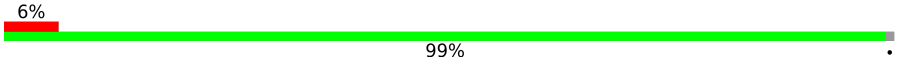
• Molecule 23: 60S ribosomal protein L22-A

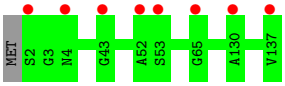
Chain CW:



• Molecule 24: 60S ribosomal protein L23-A

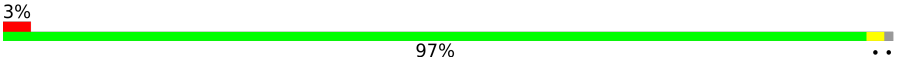
Chain 6:

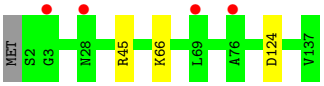




• Molecule 24: 60S ribosomal protein L23-A

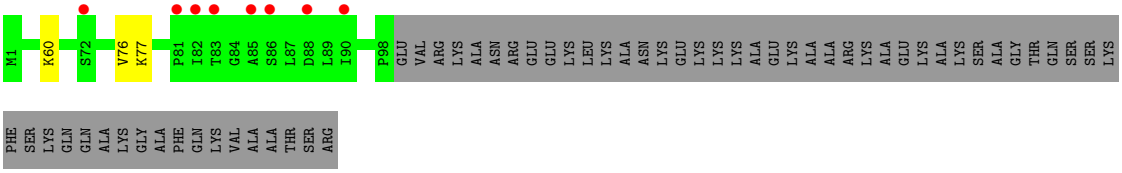
Chain CX:





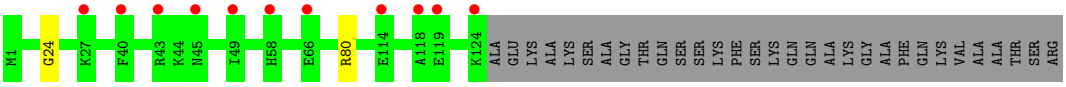
• Molecule 25: 60S ribosomal protein L24-A

Chain 7:



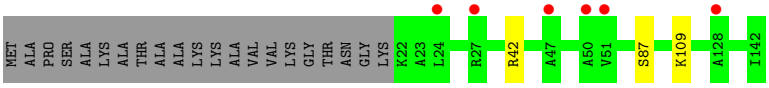
• Molecule 25: 60S ribosomal protein L24-A

Chain CY:



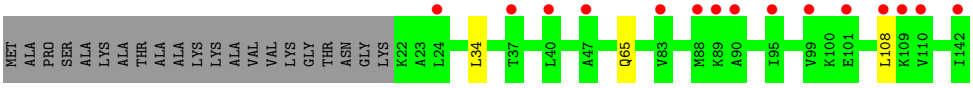
• Molecule 26: 60S ribosomal protein L25

Chain 8:



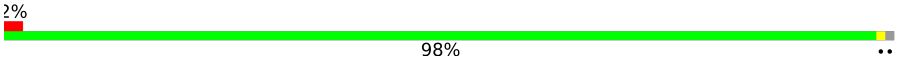
• Molecule 26: 60S ribosomal protein L25

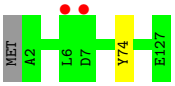
Chain CZ:



• Molecule 27: 60S ribosomal protein L26-A

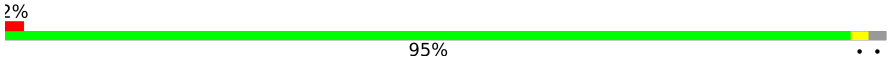
Chain 9:

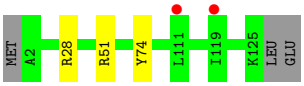




• Molecule 27: 60S ribosomal protein L26-A

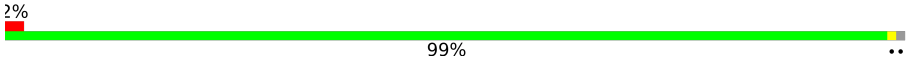
Chain DA:

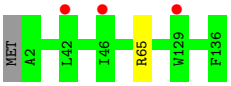




• Molecule 28: 60S ribosomal protein L27-A

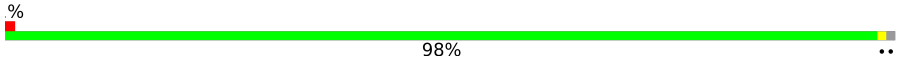
Chain AA:

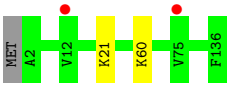




• Molecule 28: 60S ribosomal protein L27-A

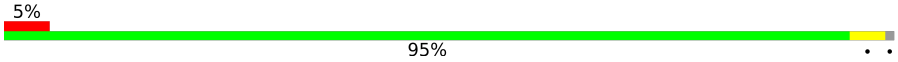
Chain DB:

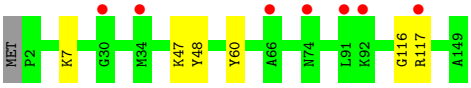




• Molecule 29: 60S ribosomal protein L28

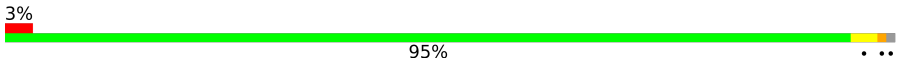
Chain AB:

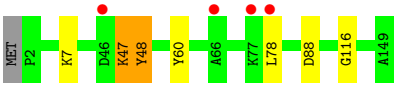




• Molecule 29: 60S ribosomal protein L28

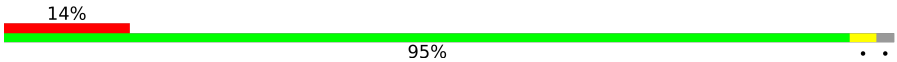
Chain DC:

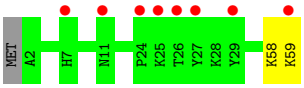




• Molecule 30: 60S ribosomal protein L29

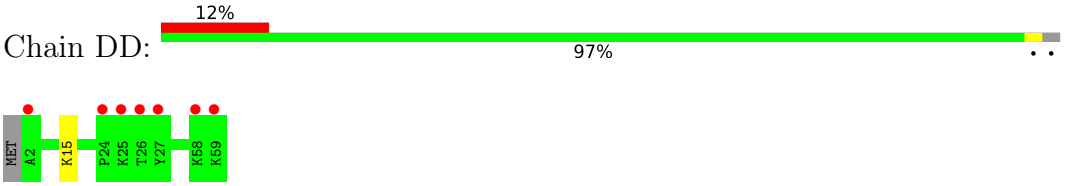
Chain AC:





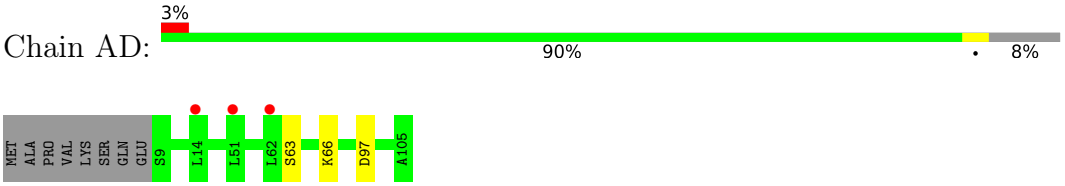
• Molecule 30: 60S ribosomal protein L29

Chain DD:



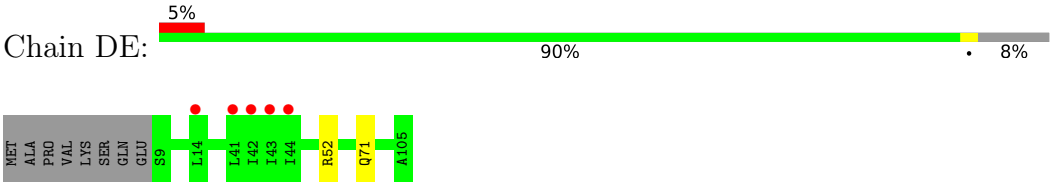
• Molecule 31: 60S ribosomal protein L30

Chain AD:



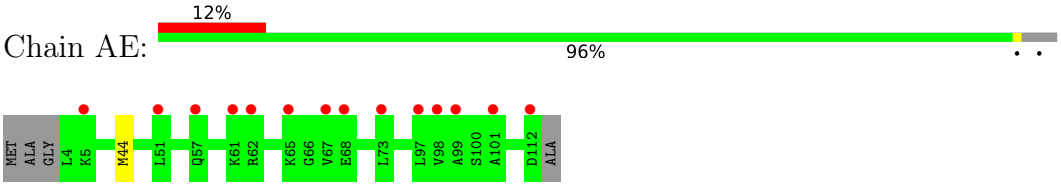
• Molecule 31: 60S ribosomal protein L30

Chain DE:



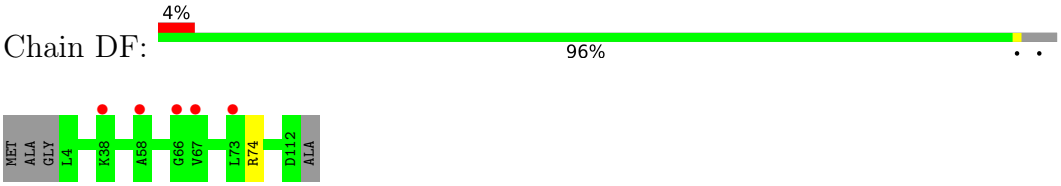
• Molecule 32: 60S ribosomal protein L31-A

Chain AE:



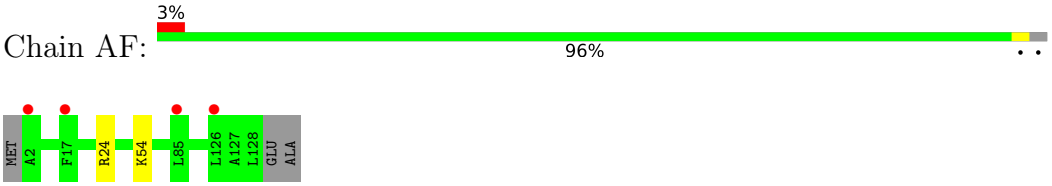
• Molecule 32: 60S ribosomal protein L31-A

Chain DF:



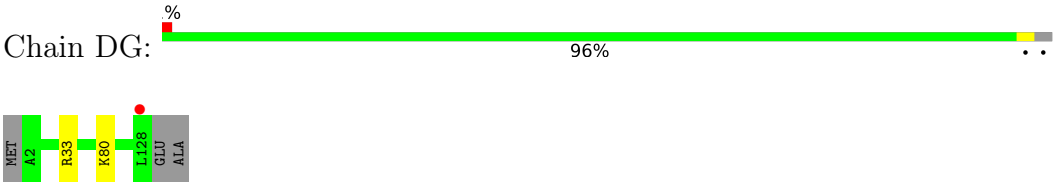
• Molecule 33: 60S ribosomal protein L32

Chain AF:



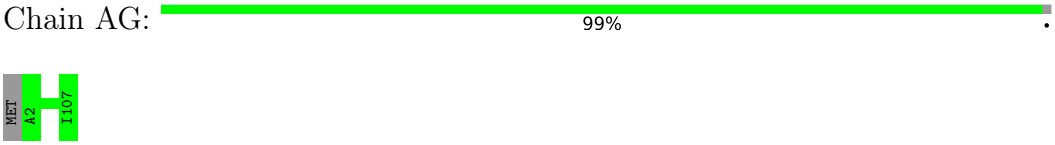
• Molecule 33: 60S ribosomal protein L32

Chain DG:



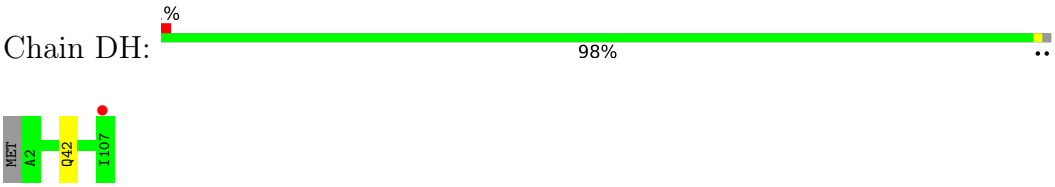
• Molecule 34: 60S ribosomal protein L33-A

Chain AG:



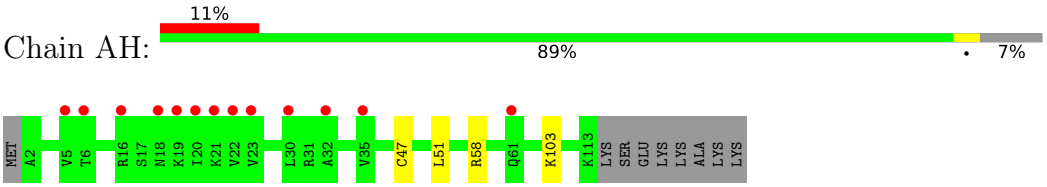
• Molecule 34: 60S ribosomal protein L33-A

Chain DH:



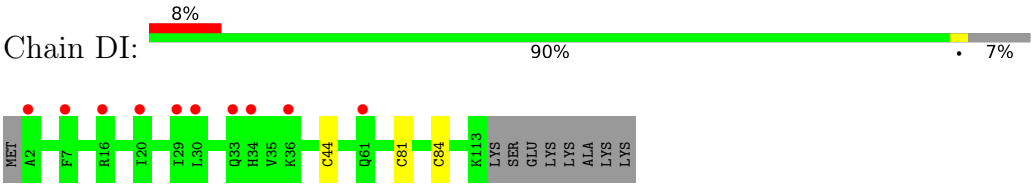
• Molecule 35: 60S ribosomal protein L34-A

Chain AH:



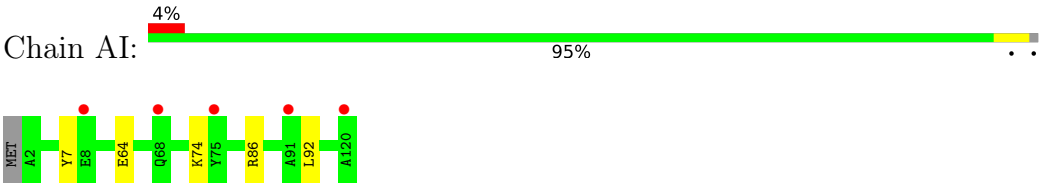
• Molecule 35: 60S ribosomal protein L34-A

Chain DI:



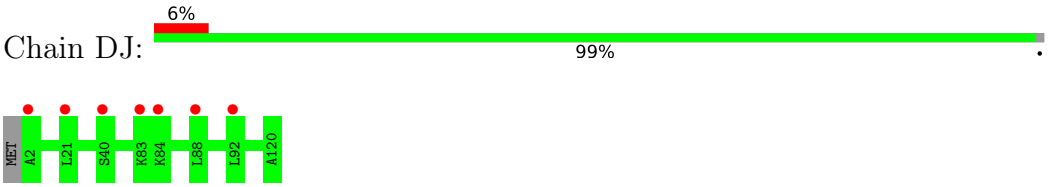
• Molecule 36: 60S ribosomal protein L35-A

Chain AI:



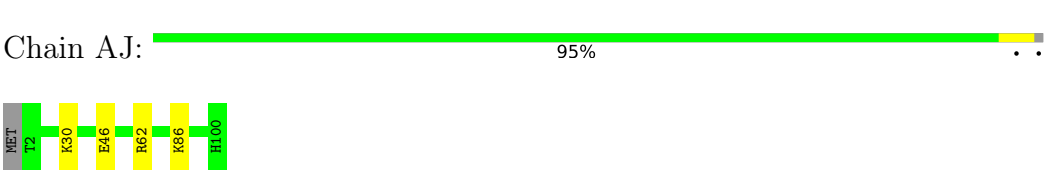
• Molecule 36: 60S ribosomal protein L35-A

Chain DJ:



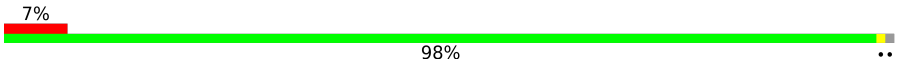
• Molecule 37: 60S ribosomal protein L36-A

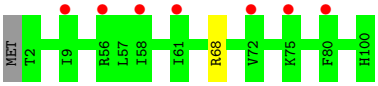
Chain AJ:



• Molecule 37: 60S ribosomal protein L36-A

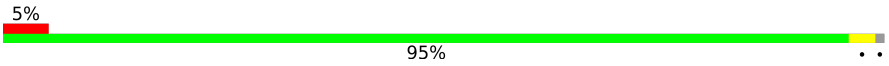
Chain DK:

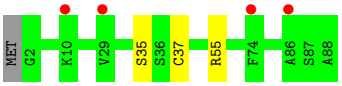




• Molecule 38: 60S ribosomal protein L37-A

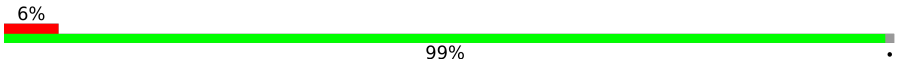
Chain AK:

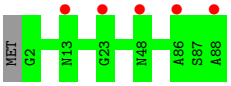




• Molecule 38: 60S ribosomal protein L37-A

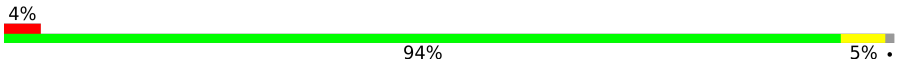
Chain DL:

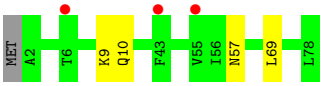




• Molecule 39: 60S ribosomal protein L38

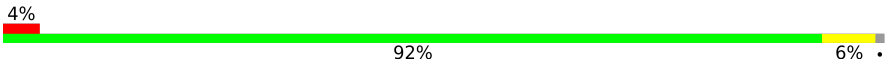
Chain AL:

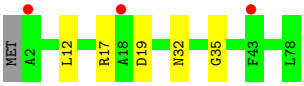




• Molecule 39: 60S ribosomal protein L38

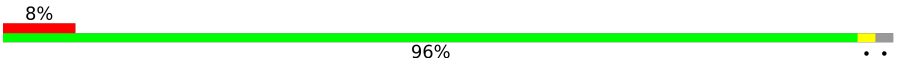
Chain DM:

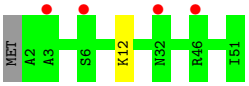




• Molecule 40: 60S ribosomal protein L39

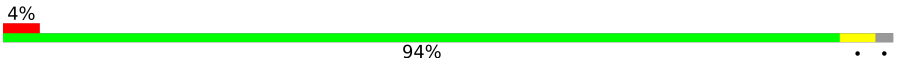
Chain AM:

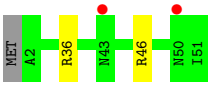




• Molecule 40: 60S ribosomal protein L39

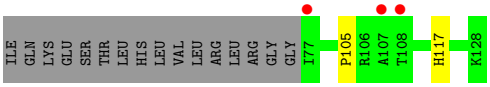
Chain DN:





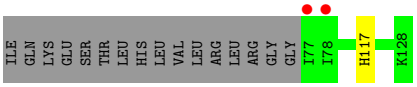
• Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain AN:



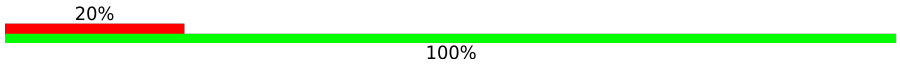
• Molecule 41: Ubiquitin-60S ribosomal protein L40

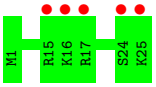
Chain DO:



• Molecule 42: 60S ribosomal protein L41-A

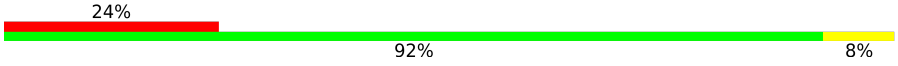
Chain AO:

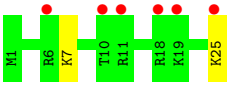




• Molecule 42: 60S ribosomal protein L41-A

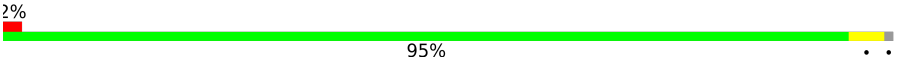
Chain DP:

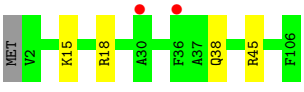




• Molecule 43: 60S ribosomal protein L42-A

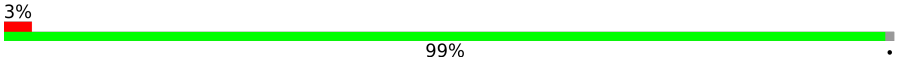
Chain AP:

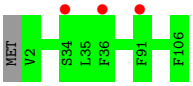




• Molecule 43: 60S ribosomal protein L42-A

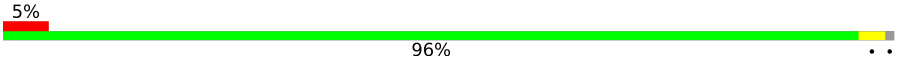
Chain DQ:

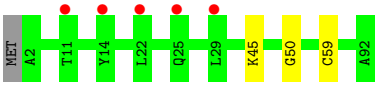




• Molecule 44: 60S ribosomal protein L43-A

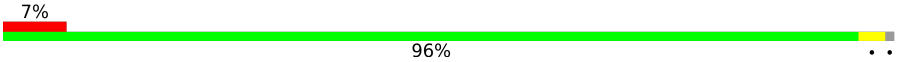
Chain AQ:

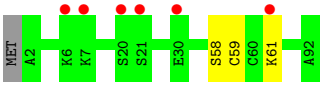




• Molecule 44: 60S ribosomal protein L43-A

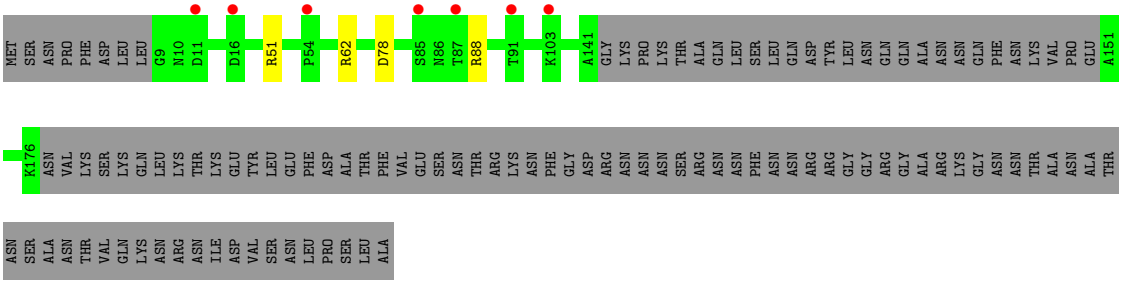
Chain DR:





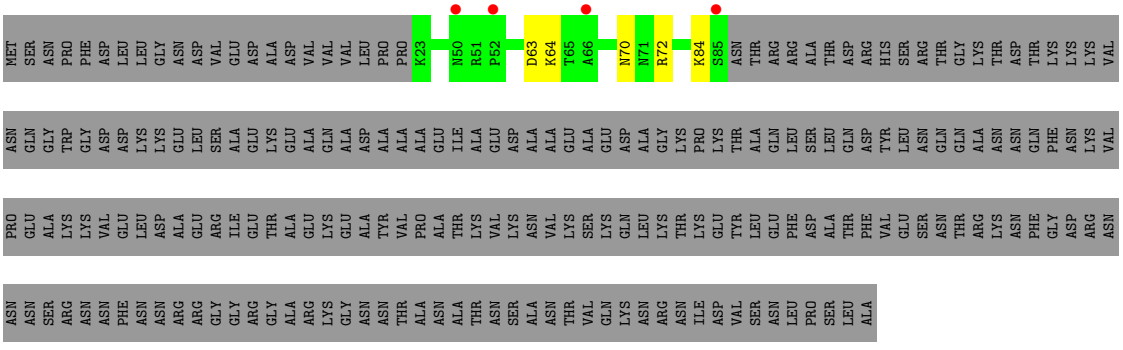
• Molecule 45: Suppressor protein STM1

Chain i:



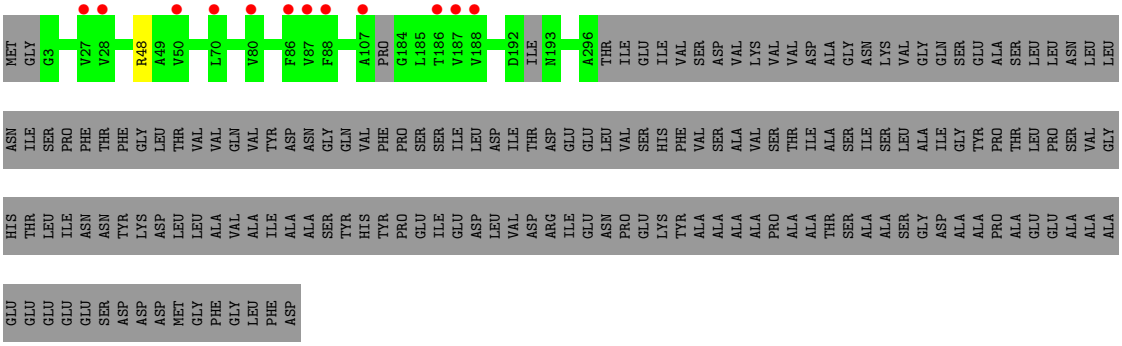
• Molecule 45: Suppressor protein STM1

Chain sM:



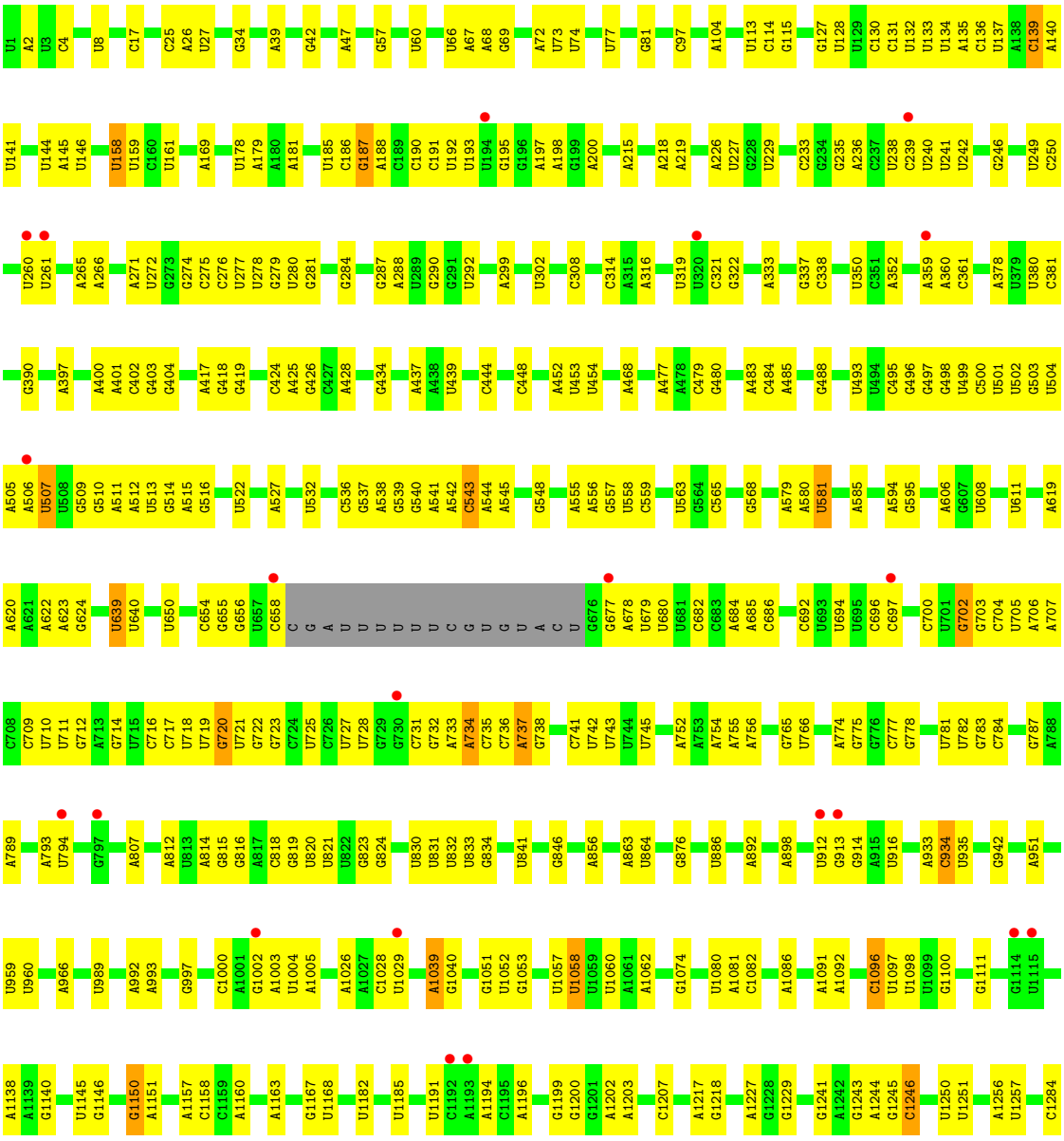
• Molecule 46: 60S acidic protein P0

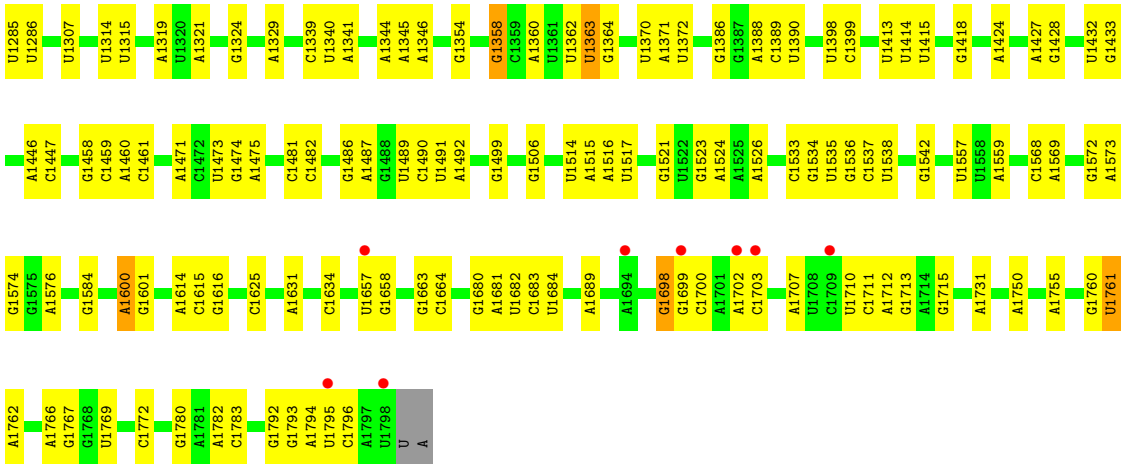
Chain p0:



• Molecule 47: 18S ribosomal RNA

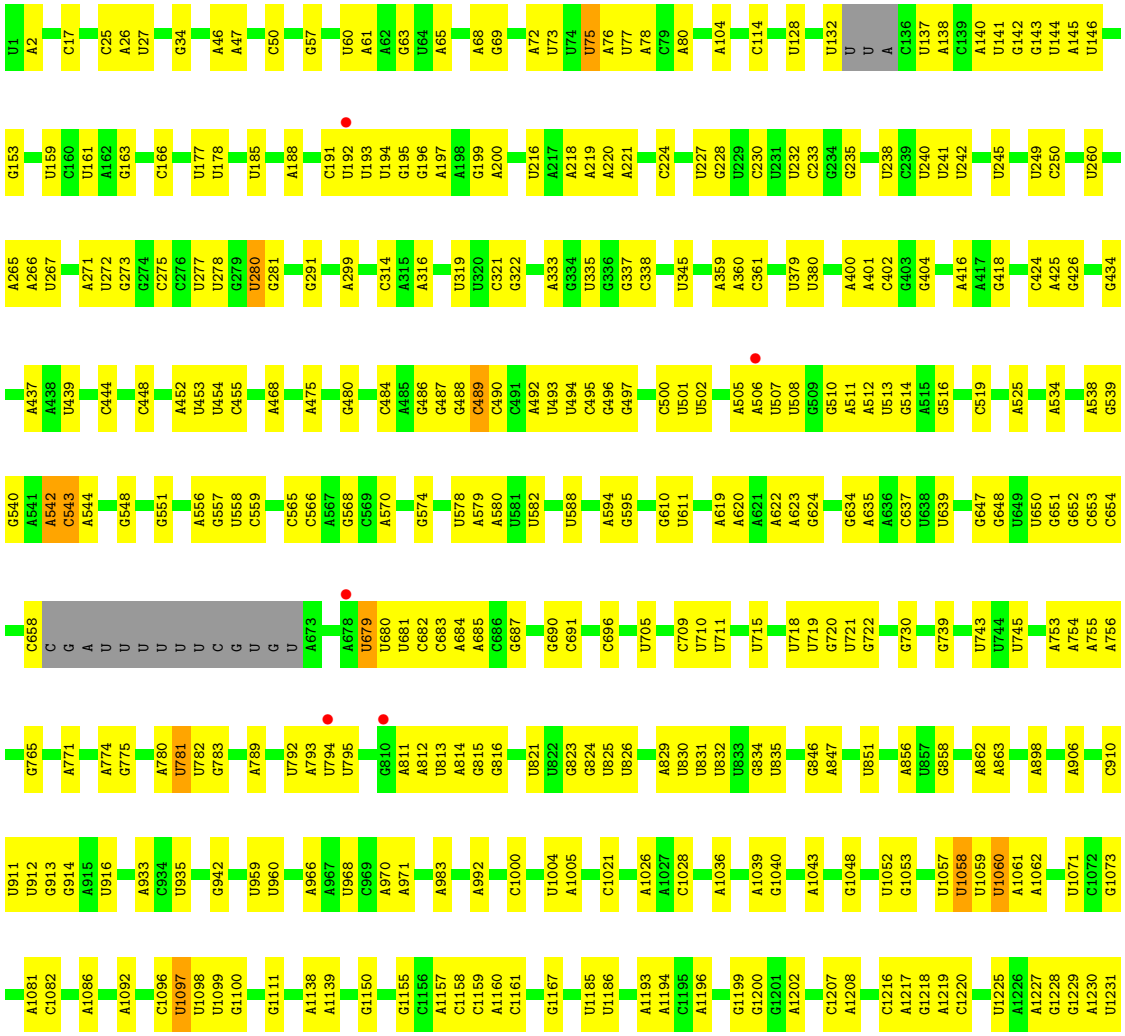
Chain A:

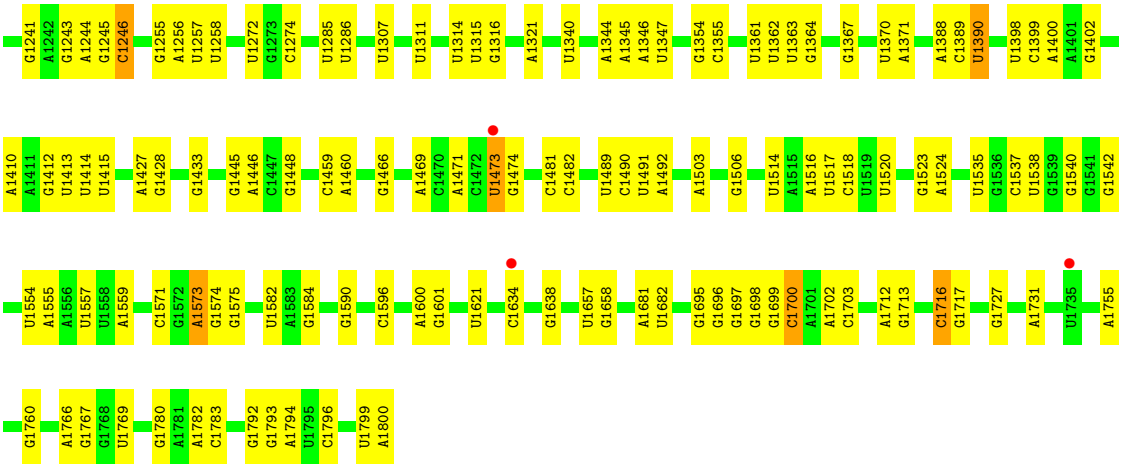




• Molecule 47: 18S ribosomal RNA

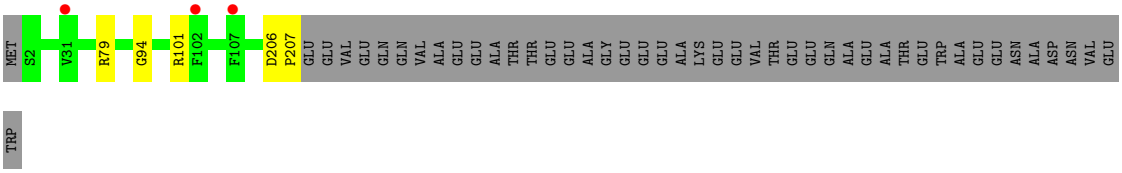
Chain sR:





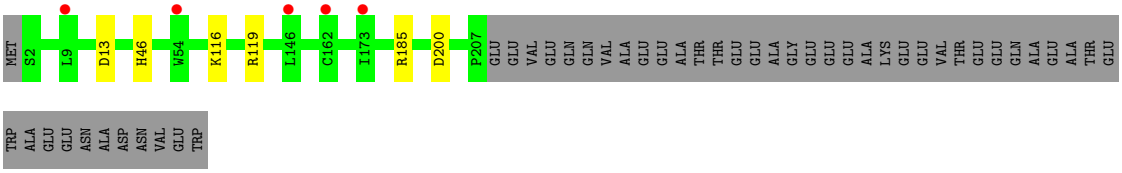
• Molecule 48: 40S ribosomal protein S0-A

Chain B:



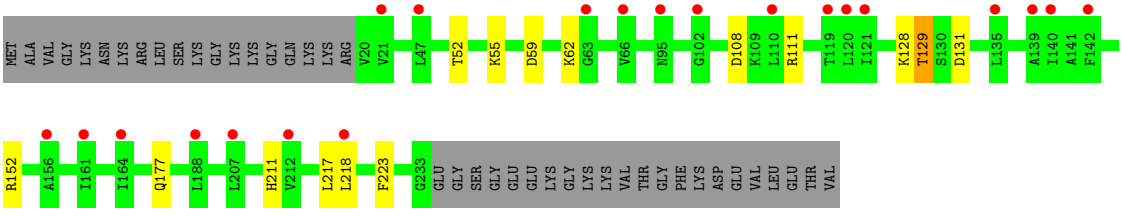
• Molecule 48: 40S ribosomal protein S0-A

Chain s0:



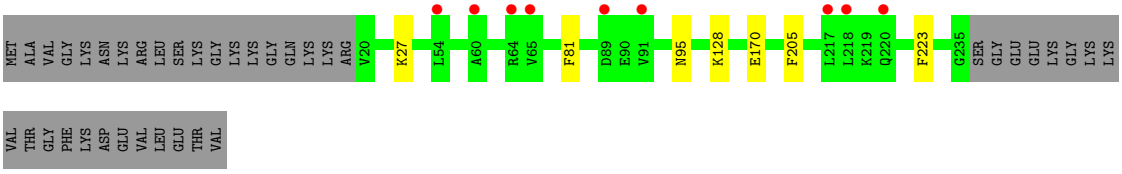
• Molecule 49: 40S ribosomal protein S1-A

Chain C:

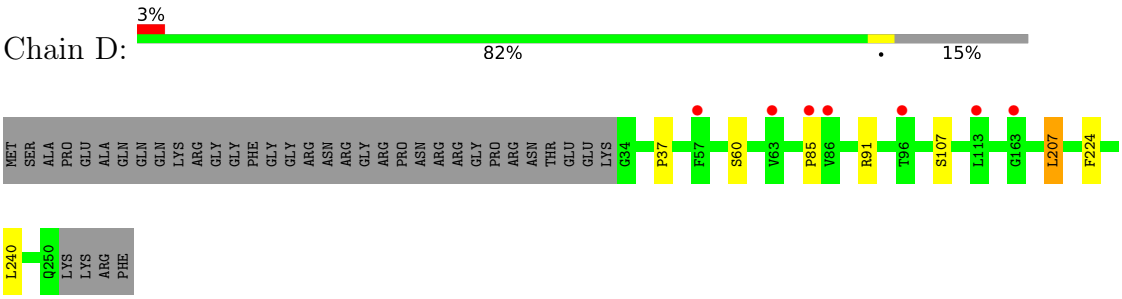


• Molecule 49: 40S ribosomal protein S1-A

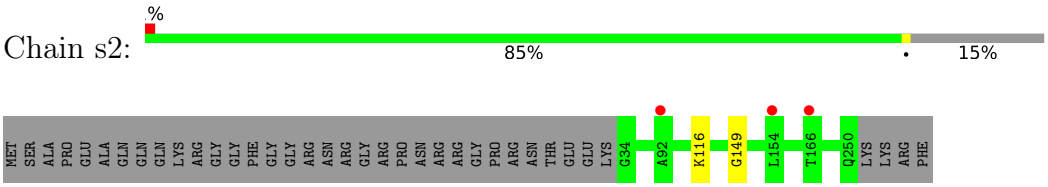
Chain s1:



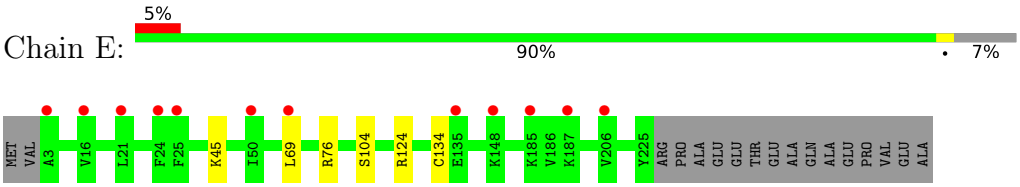
• Molecule 50: 40S ribosomal protein S2



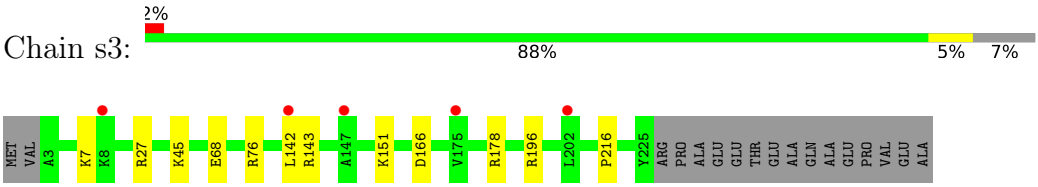
• Molecule 50: 40S ribosomal protein S2



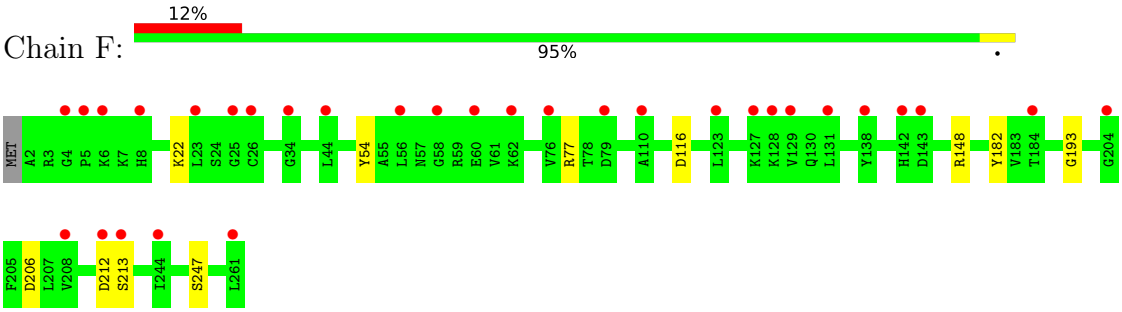
• Molecule 51: Small ribosomal subunit protein uS3



• Molecule 51: Small ribosomal subunit protein uS3

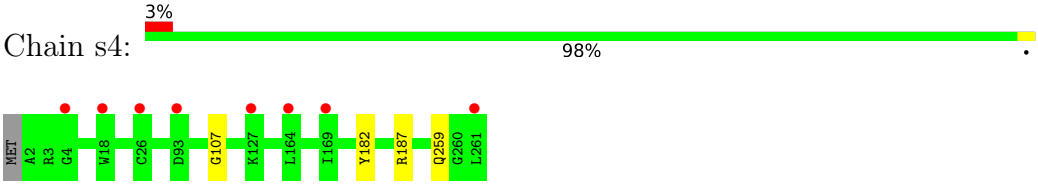


• Molecule 52: 40S ribosomal protein S4-A



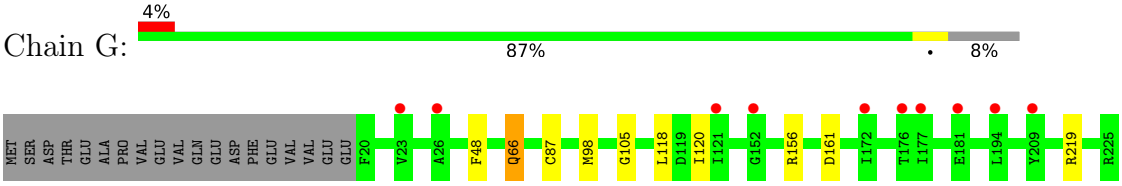
• Molecule 52: 40S ribosomal protein S4-A

Chain s4:



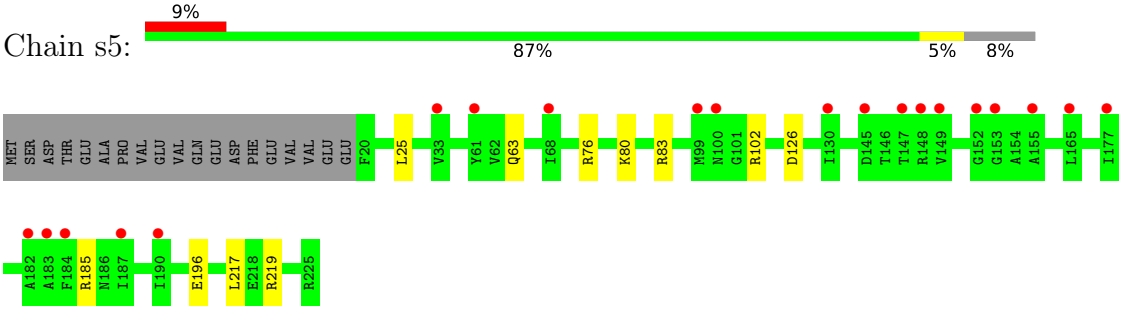
• Molecule 53: 40S ribosomal protein S5

Chain G:



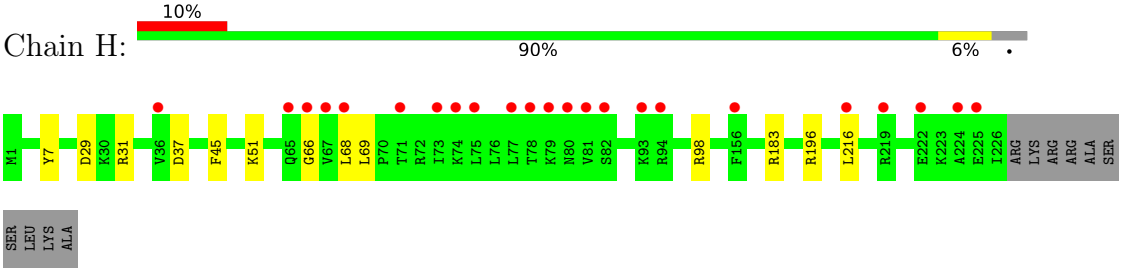
• Molecule 53: 40S ribosomal protein S5

Chain s5:



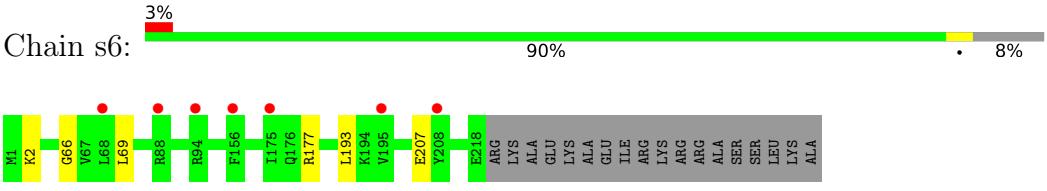
• Molecule 54: 40S ribosomal protein S6-A

Chain H:



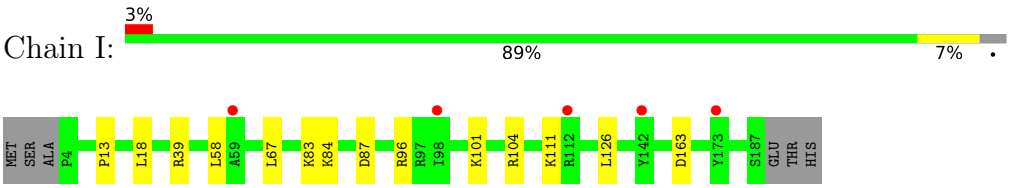
• Molecule 54: 40S ribosomal protein S6-A

Chain s6:



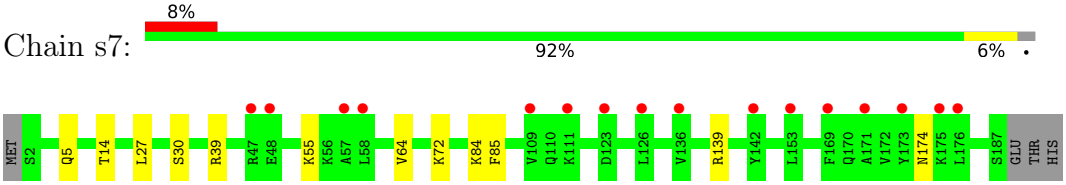
• Molecule 55: 40S ribosomal protein S7-A

Chain I:



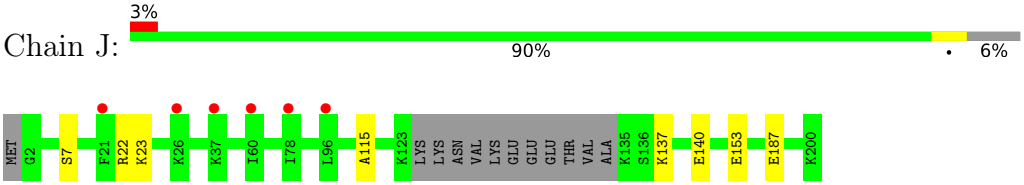
• Molecule 55: 40S ribosomal protein S7-A

Chain s7:



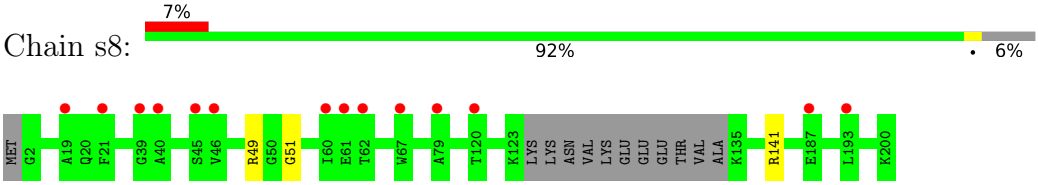
• Molecule 56: 40S ribosomal protein S8-A

Chain J:



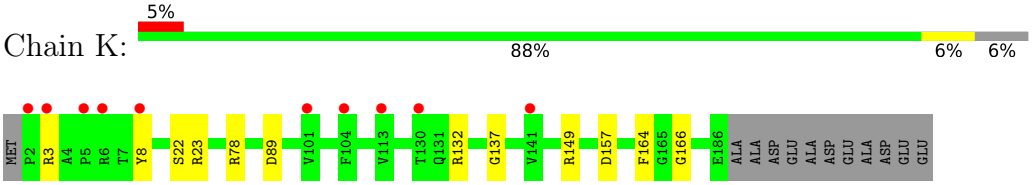
• Molecule 56: 40S ribosomal protein S8-A

Chain s8:



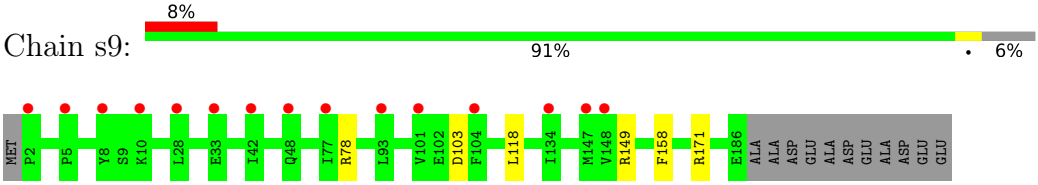
• Molecule 57: 40S ribosomal protein S9-A

Chain K:



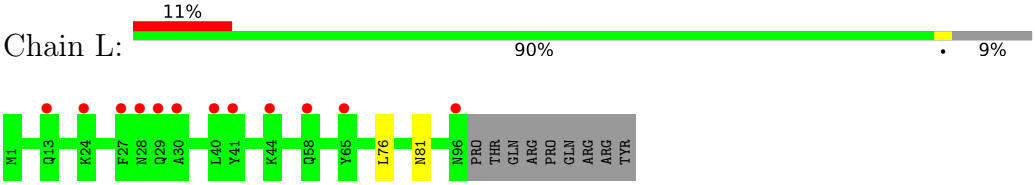
• Molecule 57: 40S ribosomal protein S9-A

Chain s9:



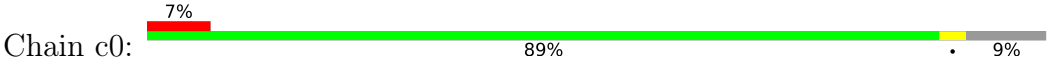
• Molecule 58: 40S ribosomal protein S10-A

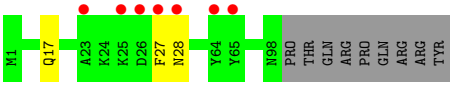
Chain L:



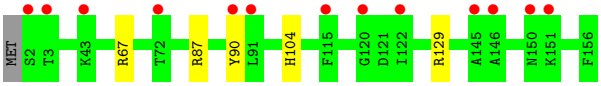
• Molecule 58: 40S ribosomal protein S10-A

Chain c0:

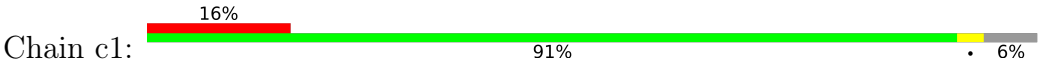


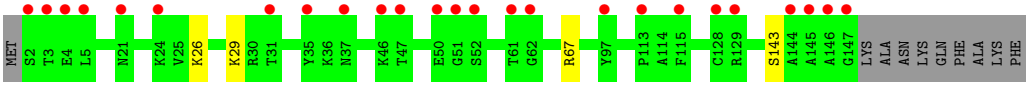


• Molecule 59: 40S ribosomal protein S11-A

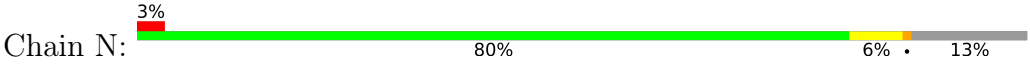


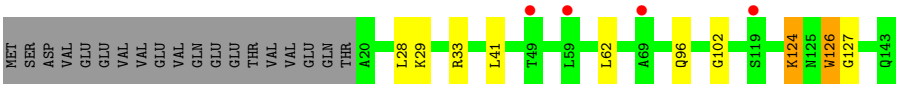
• Molecule 59: 40S ribosomal protein S11-A



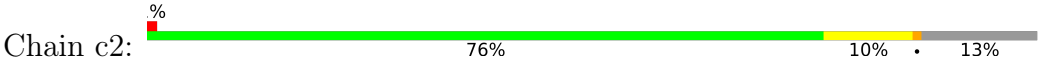


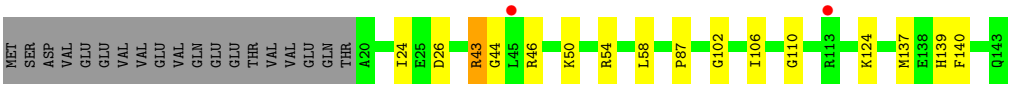
• Molecule 60: 40S ribosomal protein S12



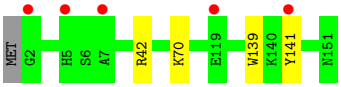


• Molecule 60: 40S ribosomal protein S12

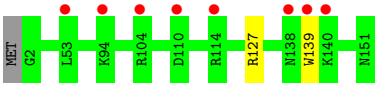




• Molecule 61: 40S ribosomal protein S13

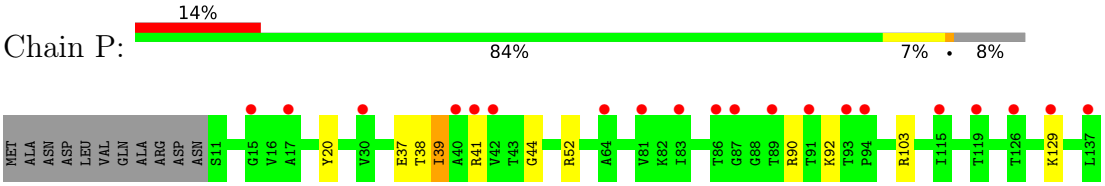


• Molecule 61: 40S ribosomal protein S13



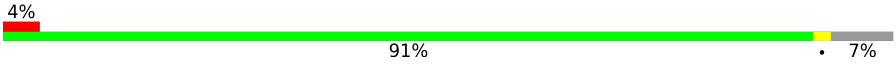
• Molecule 62: 40S ribosomal protein S14-B

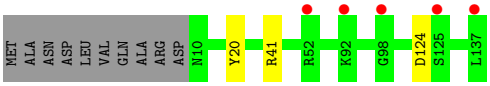
Chain P:



• Molecule 62: 40S ribosomal protein S14-B

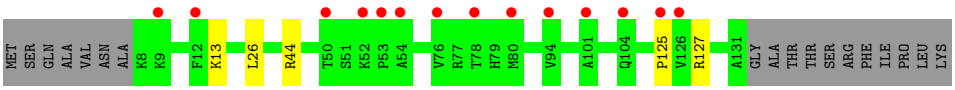
Chain c4:





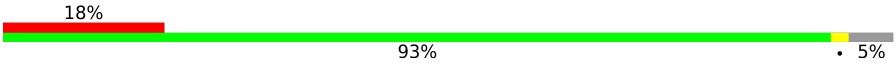
• Molecule 63: 40S ribosomal protein S15

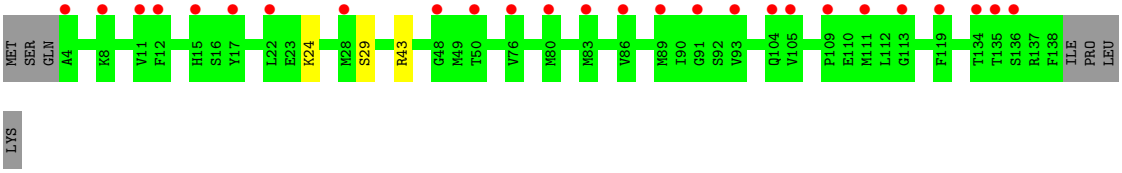
Chain Q:



• Molecule 63: 40S ribosomal protein S15

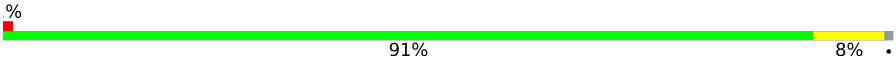
Chain c5:

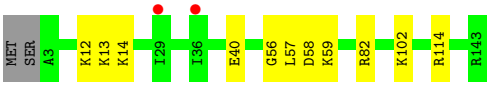




• Molecule 64: 40S ribosomal protein S16-A

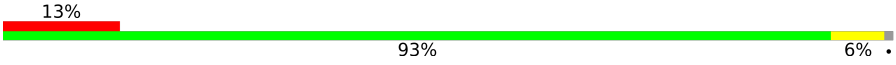
Chain R:

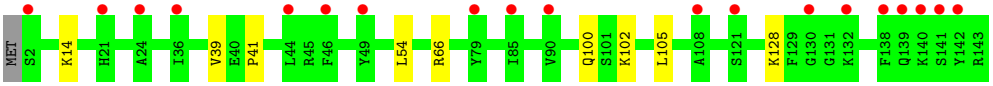




• Molecule 64: 40S ribosomal protein S16-A

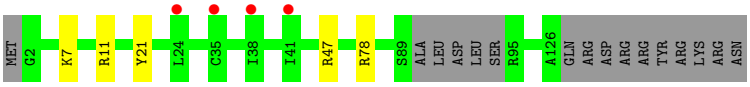
Chain c6:



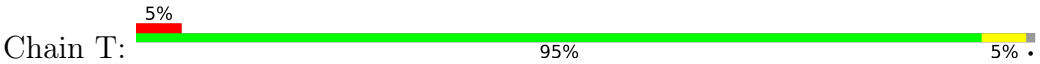


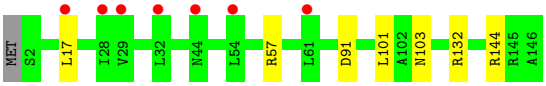
• Molecule 65: 40S ribosomal protein S17-B

Chain S:

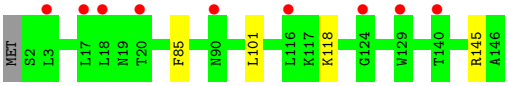


• Molecule 66: 40S ribosomal protein S18-A

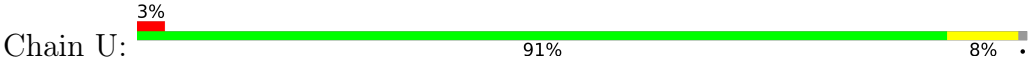




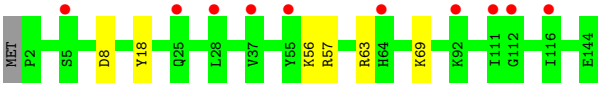
• Molecule 66: 40S ribosomal protein S18-A



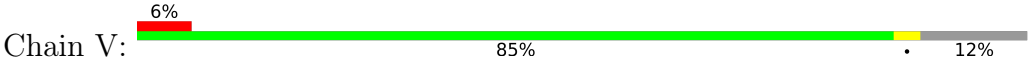
• Molecule 67: 40S ribosomal protein S19-A

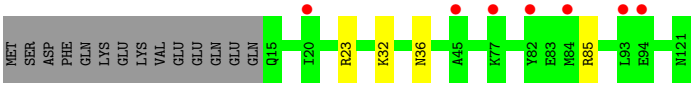


• Molecule 67: 40S ribosomal protein S19-A

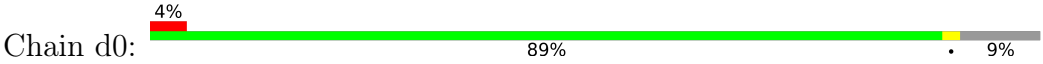


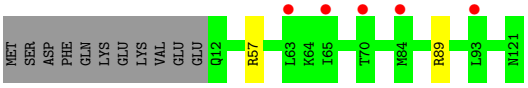
• Molecule 68: Small ribosomal subunit protein uS10





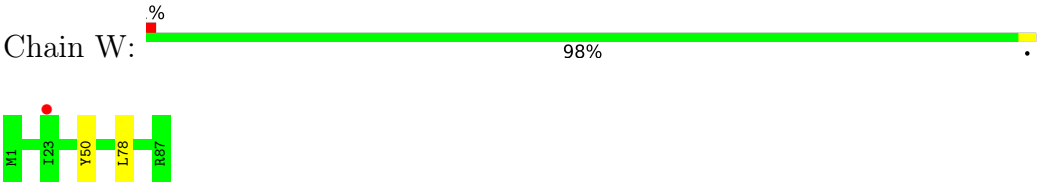
• Molecule 68: Small ribosomal subunit protein uS10





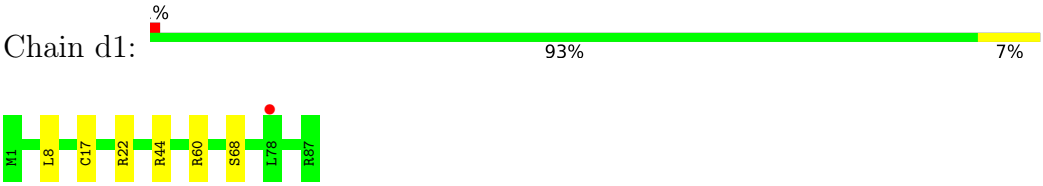
• Molecule 69: 40S ribosomal protein S21-A

Chain W:



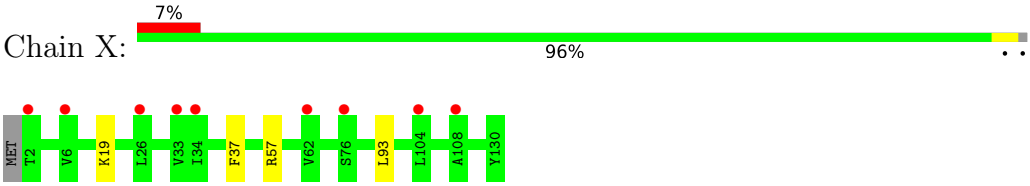
• Molecule 69: 40S ribosomal protein S21-A

Chain d1:



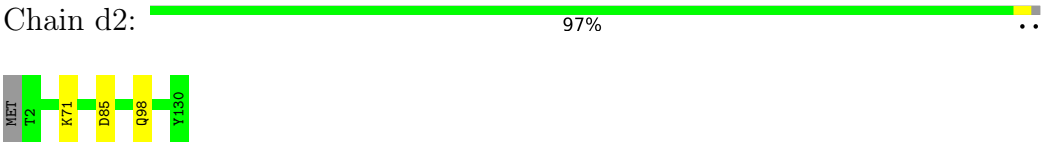
• Molecule 70: 40S ribosomal protein S22-A

Chain X:



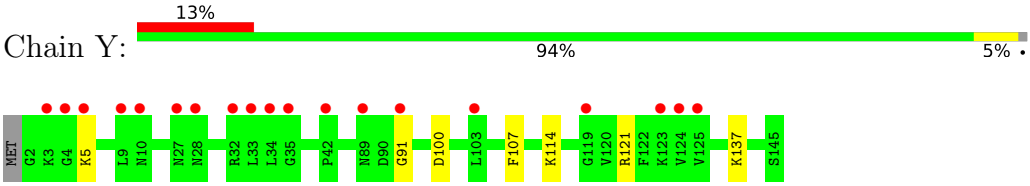
• Molecule 70: 40S ribosomal protein S22-A

Chain d2:



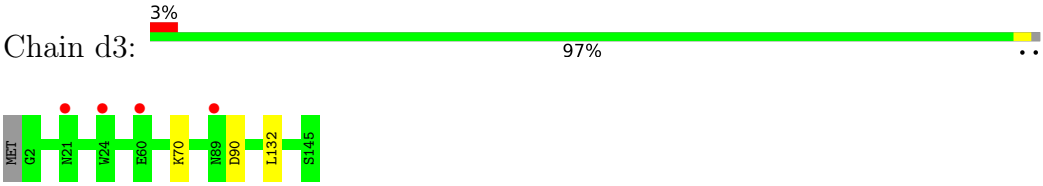
• Molecule 71: 40S ribosomal protein S23-A

Chain Y:



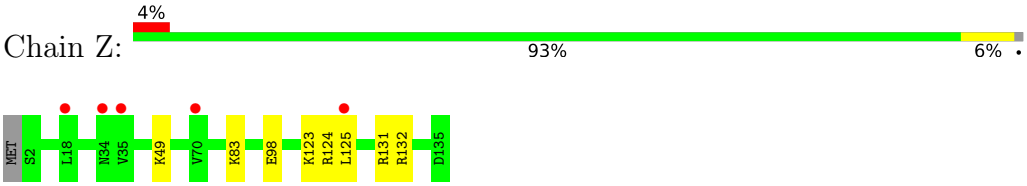
• Molecule 71: 40S ribosomal protein S23-A

Chain d3:



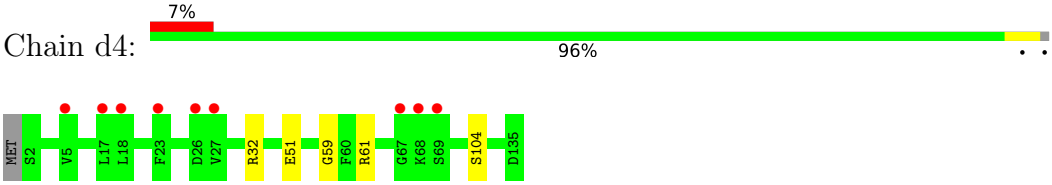
• Molecule 72: 40S ribosomal protein S24-A

Chain Z:



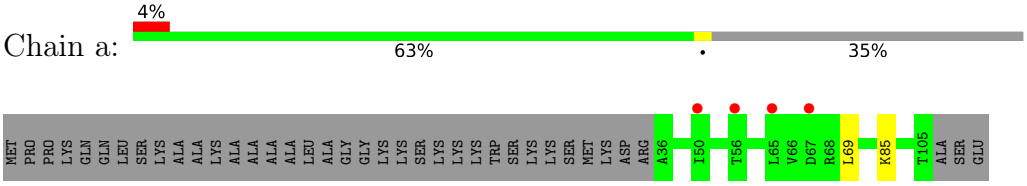
• Molecule 72: 40S ribosomal protein S24-A

Chain d4:



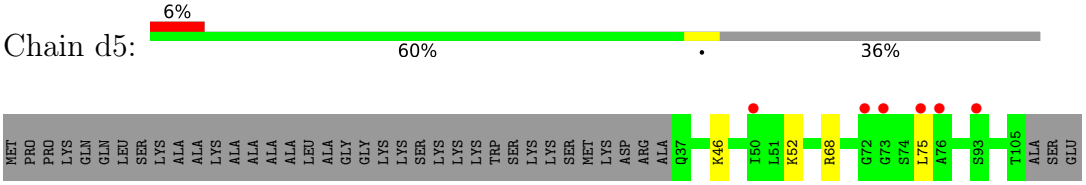
• Molecule 73: 40S ribosomal protein S25-A

Chain a:



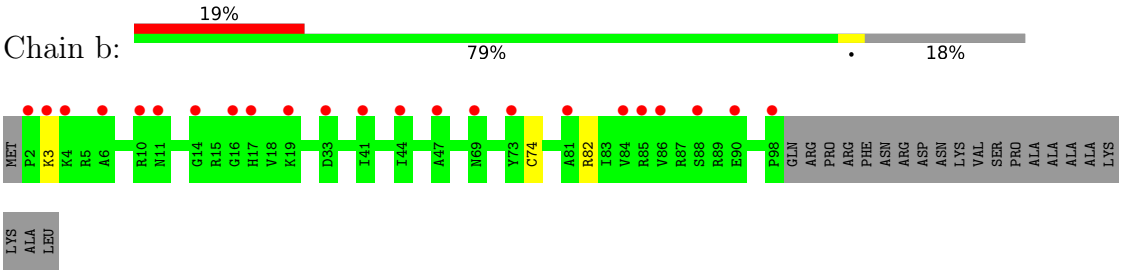
• Molecule 73: 40S ribosomal protein S25-A

Chain d5:



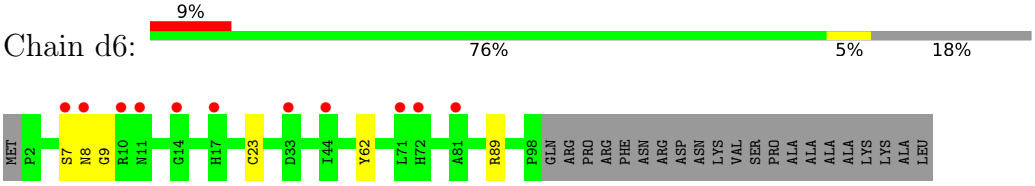
• Molecule 74: Small ribosomal subunit protein eS26B

Chain b:



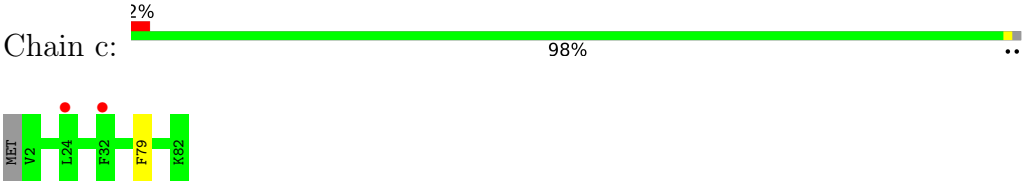
• Molecule 74: Small ribosomal subunit protein eS26B

Chain d6:



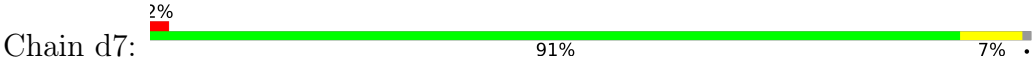
• Molecule 75: 40S ribosomal protein S27-A

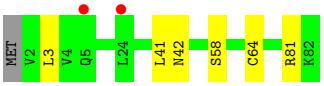
Chain c:



• Molecule 75: 40S ribosomal protein S27-A

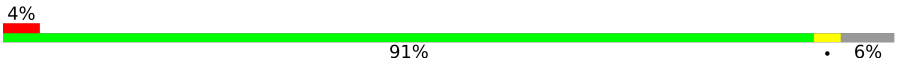
Chain d7:

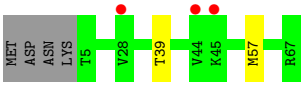




• Molecule 76: 40S ribosomal protein S28-A

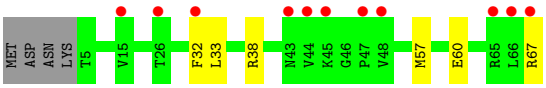
Chain d:





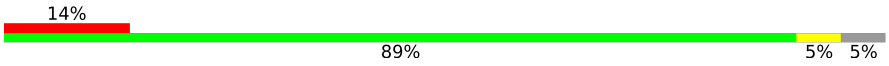
• Molecule 76: 40S ribosomal protein S28-A

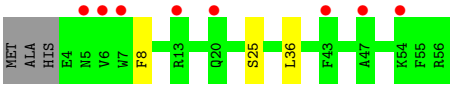
Chain d8:



• Molecule 77: Small ribosomal subunit protein uS14A

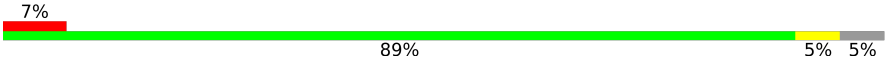
Chain e:

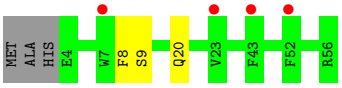




• Molecule 77: Small ribosomal subunit protein uS14A

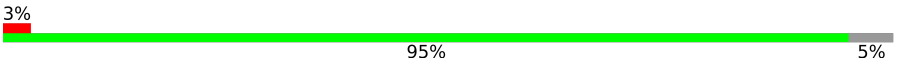
Chain d9:

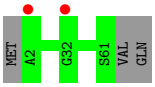




• Molecule 78: 40S ribosomal protein S30-A

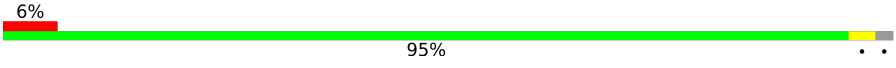
Chain f:

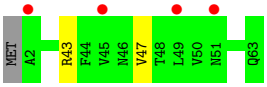




• Molecule 78: 40S ribosomal protein S30-A

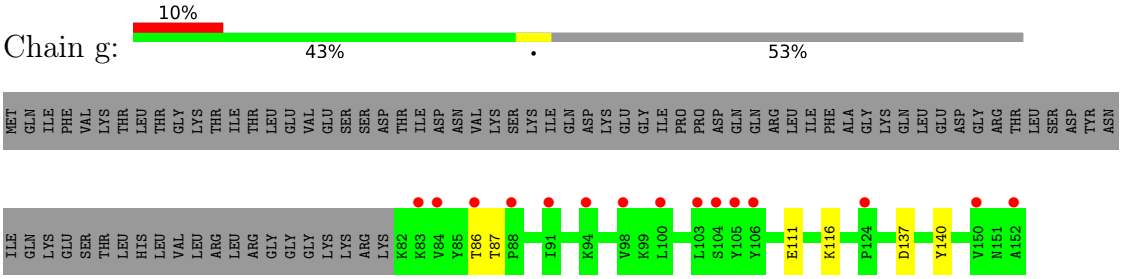
Chain e0:





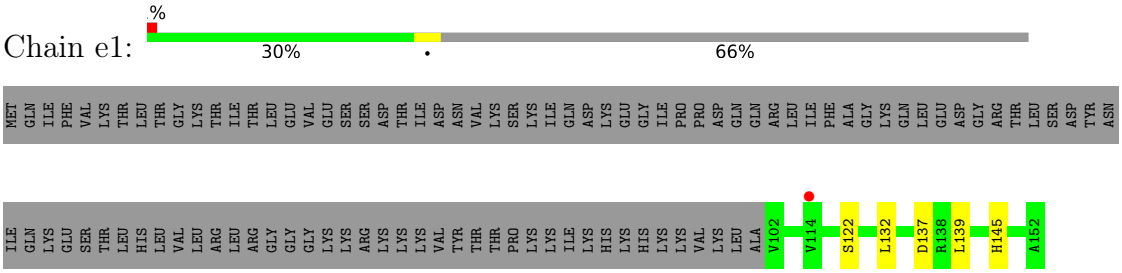
• Molecule 79: Ubiquitin

Chain g:



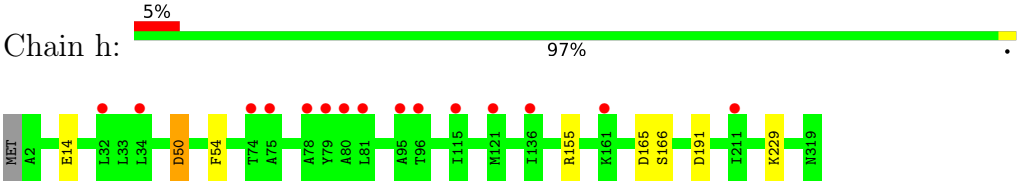
• Molecule 79: Ubiquitin

Chain e1:



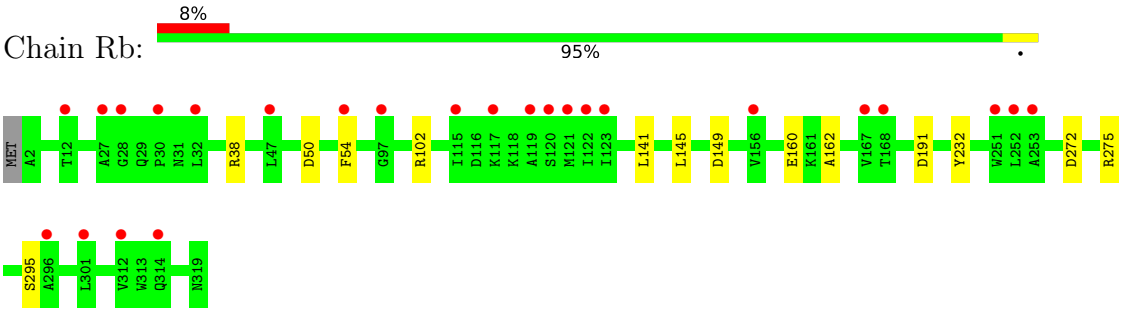
• Molecule 80: Guanine nucleotide-binding protein subunit beta-like protein

Chain h:



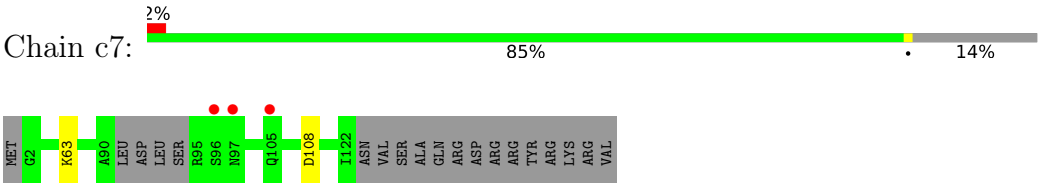
• Molecule 80: Guanine nucleotide-binding protein subunit beta-like protein

Chain Rb:



• Molecule 81: 40S ribosomal protein S17-A

Chain c7:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	302.58Å 285.05Å 433.72Å 90.00° 98.89° 90.00°	Depositor
Resolution (Å)	206.30 – 3.16 206.30 – 3.16	Depositor EDS
% Data completeness (in resolution range)	98.1 (206.30-3.16) 86.5 (206.30-3.16)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.52 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.223 , 0.251 0.225 , 0.251	Depositor DCC
R_{free} test set	1190791 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	72.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	409267	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OHX, X1K, K, OS, SPD, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.23	0/75394	0.83	35/117545 (0.0%)
1	AR	0.23	0/75347	0.83	39/117472 (0.0%)
2	3	0.21	0/2883	0.78	0/4491
2	AS	0.21	0/2883	0.79	0/4491
3	4	0.21	0/3746	0.79	0/5832
3	AT	0.20	0/3746	0.79	0/5832
4	CD	0.28	0/1948	0.71	1/2617 (0.0%)
4	j	0.28	0/1948	0.71	0/2617
5	CE	0.30	0/3146	0.70	2/4228 (0.0%)
5	k	0.29	0/3146	0.70	3/4228 (0.1%)
6	CF	0.28	0/2800	0.66	1/3790 (0.0%)
6	l	0.28	0/2800	0.70	4/3790 (0.1%)
7	CG	0.30	0/2425	0.70	1/3271 (0.0%)
7	m	0.28	0/2425	0.68	0/3271
8	CH	0.28	0/1260	0.64	0/1694
8	n	0.27	0/1260	0.63	0/1694
9	CI	0.28	0/1821	0.63	0/2451
9	o	0.28	0/1821	0.66	1/2451 (0.0%)
10	CJ	0.29	0/1836	0.70	2/2481 (0.1%)
10	p	0.29	0/1836	0.68	1/2481 (0.0%)
11	CK	0.29	0/1539	0.66	0/2073
11	q	0.29	0/1539	0.67	0/2073
12	CL	0.30	0/1741	0.69	0/2335
12	r	0.29	0/1741	0.67	1/2335 (0.0%)
13	CM	0.28	0/1374	0.70	0/1842
13	s	0.30	0/1374	0.76	2/1842 (0.1%)
14	CN	0.30	0/1568	0.79	2/2106 (0.1%)
14	t	0.29	0/1568	0.77	1/2106 (0.0%)
15	CO	0.30	0/1068	0.62	0/1438
15	u	0.31	0/1068	0.63	0/1438
16	CP	0.27	0/1757	0.67	0/2354
16	v	0.27	0/1757	0.70	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	CQ	0.27	0/1585	0.62	0/2128
17	w	0.27	0/1585	0.60	0/2128
18	CR	0.31	0/1443	0.68	0/1944
18	x	0.27	0/1443	0.67	0/1944
19	CS	0.29	0/1465	0.75	1/1965 (0.1%)
19	y	0.28	0/1465	0.70	1/1965 (0.1%)
20	CT	0.27	0/1538	0.70	0/2050
20	z	0.25	0/1538	0.66	1/2050 (0.0%)
21	0	0.30	0/1481	0.69	0/1990
21	CU	0.30	0/1481	0.66	0/1990
22	2	0.29	0/1300	0.65	0/1743
22	CV	0.28	0/1300	0.66	0/1743
23	5	0.30	0/812	0.67	1/1099 (0.1%)
23	CW	0.28	0/812	0.69	0/1099
24	6	0.29	0/1018	0.66	0/1369
24	CX	0.28	0/1018	0.64	0/1369
25	7	0.29	0/712	0.74	2/958 (0.2%)
25	CY	0.29	0/848	0.64	1/1146 (0.1%)
26	8	0.27	0/979	0.69	0/1321
26	CZ	0.27	0/979	0.67	0/1321
27	9	0.29	0/1004	0.68	0/1341
27	DA	0.28	0/987	0.64	0/1318
28	AA	0.32	0/1118	0.77	0/1497
28	DB	0.31	0/1113	0.67	1/1491 (0.1%)
29	AB	0.31	0/1204	0.87	3/1612 (0.2%)
29	DC	0.32	0/1204	0.80	4/1612 (0.2%)
30	AC	0.27	0/473	0.64	0/629
30	DD	0.28	0/473	0.67	0/629
31	AD	0.28	0/751	0.54	0/1008
31	DE	0.26	0/751	0.56	0/1008
32	AE	0.27	0/890	0.68	0/1196
32	DF	0.26	0/890	0.67	0/1196
33	AF	0.26	0/1041	0.65	0/1394
33	DG	0.25	0/1041	0.63	0/1394
34	AG	0.30	0/868	0.71	0/1168
34	DH	0.32	0/868	0.73	0/1168
35	AH	0.30	0/890	0.72	1/1189 (0.1%)
35	DI	0.47	2/890 (0.2%)	0.82	1/1189 (0.1%)
36	AI	0.28	0/978	0.76	1/1301 (0.1%)
36	DJ	0.27	0/978	0.63	0/1301
37	AJ	0.26	0/778	0.65	0/1034
37	DK	0.27	0/778	0.68	0/1034
38	AK	0.27	0/696	0.70	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DL	0.27	0/696	0.66	0/923
39	AL	0.31	0/618	0.73	0/826
39	DM	0.29	0/618	0.81	3/826 (0.4%)
40	AM	0.28	0/443	0.75	0/588
40	DN	0.26	0/443	0.78	0/588
41	AN	0.30	0/423	0.64	0/562
41	DO	0.30	0/423	0.68	0/562
42	AO	0.26	0/234	0.87	0/300
42	DP	0.27	0/234	0.80	0/300
43	AP	0.62	0/860	0.94	0/1136
43	DQ	0.62	0/860	0.93	0/1136
44	AQ	0.26	0/701	0.76	1/934 (0.1%)
44	DR	0.27	0/701	0.75	0/934
45	i	0.28	0/1113	0.68	0/1502
45	sM	0.31	0/480	0.85	0/642
46	p0	0.29	0/1091	0.74	0/1472
47	A	0.24	0/42443	0.87	53/66134 (0.1%)
47	sR	0.24	0/42490	0.85	49/66207 (0.1%)
48	B	0.33	0/1617	0.87	3/2215 (0.1%)
48	s0	0.30	0/1623	0.74	0/2222
49	C	0.33	0/1735	0.95	6/2335 (0.3%)
49	s1	0.27	0/1748	0.68	0/2352
50	D	0.30	0/1665	0.72	3/2263 (0.1%)
50	s2	0.29	0/1665	0.69	1/2263 (0.0%)
51	E	0.29	0/1759	0.70	0/2368
51	s3	0.32	0/1759	0.81	2/2368 (0.1%)
52	F	0.34	0/2109	0.80	2/2839 (0.1%)
52	s4	0.30	0/2109	0.73	1/2839 (0.0%)
53	G	0.30	0/1629	0.86	4/2202 (0.2%)
53	s5	0.28	0/1629	0.72	1/2202 (0.0%)
54	H	0.30	0/1823	0.81	5/2439 (0.2%)
54	s6	0.29	0/1779	0.76	2/2379 (0.1%)
55	I	0.33	0/1506	0.82	2/2028 (0.1%)
55	s7	0.32	0/1516	0.82	3/2043 (0.1%)
56	J	0.28	0/1514	0.81	2/2021 (0.1%)
56	s8	0.27	0/1514	0.70	1/2021 (0.0%)
57	K	0.29	0/1519	0.78	2/2035 (0.1%)
57	s9	0.28	0/1519	0.77	2/2035 (0.1%)
58	L	0.29	0/789	0.71	0/1067
58	c0	0.30	0/776	0.75	0/1047
59	M	0.29	0/1239	0.70	0/1673
59	c1	0.28	0/1194	0.72	1/1610 (0.1%)
60	N	0.34	0/898	1.03	7/1220 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	c2	0.33	0/898	1.16	11/1220 (0.9%)
61	O	0.27	0/1215	0.60	0/1638
61	c3	0.28	0/1215	0.63	0/1638
62	P	0.45	0/896	0.98	5/1210 (0.4%)
62	c4	0.28	0/960	0.80	0/1290
63	Q	0.32	0/998	0.85	2/1341 (0.1%)
63	c5	0.31	0/1060	0.80	0/1426
64	R	0.31	0/1125	0.75	2/1510 (0.1%)
64	c6	0.28	0/1131	0.81	3/1518 (0.2%)
65	S	0.30	0/935	0.80	0/1254
66	T	0.29	0/1211	0.80	1/1628 (0.1%)
66	c8	0.30	0/1211	0.83	1/1628 (0.1%)
67	U	0.31	0/1130	0.80	3/1517 (0.2%)
67	c9	0.27	0/1130	0.63	0/1517
68	V	0.30	0/865	0.82	0/1169
68	d0	0.29	0/892	0.81	0/1205
69	W	0.30	0/693	0.76	0/935
69	d1	0.28	0/693	0.78	1/935 (0.1%)
70	X	0.30	0/1038	0.76	0/1395
70	d2	0.30	0/1038	0.68	0/1395
71	Y	0.30	0/1139	0.82	2/1518 (0.1%)
71	d3	0.28	0/1139	0.70	1/1518 (0.1%)
72	Z	0.30	0/1087	0.72	2/1449 (0.1%)
72	d4	0.32	0/1087	0.82	3/1449 (0.2%)
73	a	0.30	0/571	0.80	1/768 (0.1%)
73	d5	0.28	0/566	0.79	1/761 (0.1%)
74	b	0.32	0/782	0.87	0/1047
74	d6	0.29	0/782	0.89	2/1047 (0.2%)
75	c	0.29	0/620	0.84	0/838
75	d7	0.27	0/620	0.82	2/838 (0.2%)
76	d	0.27	0/499	1.00	1/670 (0.1%)
76	d8	0.32	0/499	0.95	4/670 (0.6%)
77	d9	0.30	0/452	0.76	1/600 (0.2%)
77	e	0.28	0/452	0.74	1/600 (0.2%)
78	e0	0.29	0/499	0.77	0/665
78	f	0.26	0/483	0.78	0/643
79	e1	0.42	0/404	1.15	2/542 (0.4%)
79	g	0.37	0/577	1.00	3/770 (0.4%)
80	Rb	0.31	0/2495	0.83	4/3395 (0.1%)
80	h	0.30	0/2490	0.76	3/3389 (0.1%)
81	c7	0.27	0/914	0.74	0/1224
All	All	0.26	2/430026 (0.0%)	0.80	332/631405 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	u	0	1
49	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	DI	44	CYS	CB-SG	9.04	1.97	1.82
35	DI	84	CYS	CB-SG	5.94	1.92	1.82

All (332) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	G	120	ILE	C-N-CA	13.14	154.54	121.70
49	C	129	THR	C-N-CA	12.91	153.97	121.70
72	d4	32	ARG	C-N-CA	12.14	152.05	121.70
76	d	39	THR	C-N-CA	11.81	151.23	121.70
19	CS	95	GLU	C-N-CA	11.75	151.06	121.70
47	sR	1060	U	O5'-P-OP2	-11.21	95.61	105.70
35	DI	81	CYS	CA-CB-SG	-10.98	94.24	114.00
57	s9	118	LEU	CA-CB-CG	10.72	139.95	115.30
29	AB	116	GLY	N-CA-C	10.62	139.64	113.10
36	AI	92	LEU	CA-CB-CG	10.47	139.38	115.30
60	c2	44	GLY	C-N-CA	10.27	147.37	121.70
5	k	140	ASP	C-N-CA	10.04	143.39	122.30
48	B	206	ASP	C-N-CD	-10.03	98.53	120.60
53	G	118	LEU	CA-CB-CG	9.81	137.87	115.30
52	F	212	ASP	CB-CG-OD2	-9.37	109.86	118.30
62	P	38	THR	C-N-CA	9.28	144.91	121.70
47	sR	687	G	N3-C2-N2	-8.91	113.66	119.90
10	CJ	119	GLY	C-N-CA	8.86	143.84	121.70
71	Y	91	GLY	N-CA-C	-8.81	91.06	113.10
55	s7	27	LEU	CA-CB-CG	8.76	135.44	115.30
47	sR	453	U	C2-N1-C1'	8.71	128.15	117.70
9	o	156	ILE	C-N-CA	8.70	143.46	121.70
60	c2	24	ILE	C-N-CA	8.63	143.29	121.70
47	sR	453	U	N1-C2-O2	8.61	128.83	122.80
66	c8	101	LEU	C-N-CA	8.58	143.14	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	sR	453	U	N3-C2-O2	-8.48	116.26	122.20
1	1	3217	C	N1-C2-O2	8.46	123.98	118.90
1	AR	3217	C	N1-C2-O2	8.46	123.97	118.90
50	s2	149	GLY	N-CA-C	8.06	133.26	113.10
47	sR	163	G	N3-C4-N9	-8.03	121.18	126.00
1	1	3278	C	N1-C2-O2	7.91	123.64	118.90
47	A	543	C	N1-C2-O2	7.88	123.63	118.90
79	e1	139	LEU	CA-CB-CG	7.87	133.41	115.30
79	g	111	GLU	C-N-CA	7.81	138.71	122.30
73	d5	75	LEU	CA-CB-CG	7.81	133.26	115.30
1	1	3217	C	C2-N1-C1'	7.80	127.38	118.80
29	AB	47	LYS	C-N-CA	7.79	141.18	121.70
54	H	66	GLY	C-N-CA	-7.79	102.23	121.70
1	1	1269	U	C2-N1-C1'	7.66	126.89	117.70
74	d6	7	SER	C-N-CA	7.62	140.75	121.70
47	A	728	U	C2-N1-C1'	7.61	126.83	117.70
54	H	69	LEU	N-CA-C	7.56	131.41	111.00
60	c2	43	ARG	C-N-CA	7.51	138.07	122.30
76	d8	32	PHE	C-N-CA	7.45	140.33	121.70
75	d7	58	SER	C-N-CA	7.40	140.20	121.70
47	A	728	U	N1-C2-O2	7.32	127.93	122.80
75	d7	3	LEU	CA-CB-CG	7.31	132.12	115.30
47	A	1363	U	N1-C2-O2	7.29	127.91	122.80
29	DC	47	LYS	C-N-CA	7.28	139.91	121.70
14	CN	7	LEU	CA-CB-CG	7.26	132.00	115.30
54	s6	69	LEU	N-CA-C	7.26	130.60	111.00
1	AR	3217	C	C2-N1-C1'	7.25	126.78	118.80
69	d1	8	LEU	C-N-CA	7.23	139.77	121.70
47	A	702	G	C5-C6-O6	-7.19	124.28	128.60
13	s	170	ASP	C-N-CA	-7.17	103.77	121.70
1	AR	3278	C	C2-N1-C1'	7.14	126.65	118.80
1	1	1269	U	N1-C2-O2	7.13	127.79	122.80
60	N	62	LEU	CB-CG-CD1	-7.10	98.92	111.00
63	Q	125	PRO	N-CA-C	7.10	130.56	112.10
1	AR	2873	U	C2-N1-C1'	7.07	126.18	117.70
47	sR	1473	U	C2-N1-C1'	7.07	126.18	117.70
47	A	736	C	C2-N1-C1'	7.06	126.56	118.80
60	N	127	GLY	C-N-CA	7.02	139.24	121.70
60	N	126	TRP	C-N-CA	-7.01	107.57	122.30
55	s7	30	SER	C-N-CA	-6.99	104.24	121.70
1	1	3278	C	N3-C2-O2	-6.97	117.02	121.90
71	d3	132	LEU	CA-CB-CG	6.96	131.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	CF	13	GLY	N-CA-C	-6.94	95.76	113.10
60	c2	102	GLY	N-CA-C	6.94	130.44	113.10
47	A	728	U	N3-C2-O2	-6.93	117.35	122.20
47	A	1363	U	C2-N1-C1'	6.92	126.01	117.70
13	s	172	LEU	CA-CB-CG	-6.91	99.40	115.30
1	AR	2996	U	C2-N1-C1'	6.87	125.94	117.70
56	J	115	ALA	C-N-CA	6.86	138.86	121.70
47	sR	163	G	N3-C2-N2	-6.86	115.10	119.90
47	sR	280	U	C2-N1-C1'	6.86	125.94	117.70
1	1	3217	C	N3-C2-O2	-6.85	117.10	121.90
47	A	1363	U	N3-C2-O2	-6.85	117.41	122.20
54	H	37	ASP	C-N-CA	6.85	136.69	122.30
47	A	1000	C	N1-C2-O2	6.82	122.99	118.90
1	AR	3217	C	N3-C2-O2	-6.80	117.14	121.90
60	N	124	LYS	C-N-CA	6.75	138.58	121.70
49	C	52	THR	C-N-CA	-6.69	108.26	122.30
29	DC	116	GLY	N-CA-C	6.68	129.81	113.10
54	s6	66	GLY	C-N-CA	-6.67	105.03	121.70
47	A	1058	U	C2-N1-C1'	6.64	125.67	117.70
80	Rb	160	GLU	N-CA-C	-6.62	93.11	111.00
47	sR	687	G	N1-C2-N2	6.60	122.14	116.20
47	sR	687	G	N3-C4-N9	-6.60	122.04	126.00
5	CE	351	LEU	CA-CB-CG	6.58	130.44	115.30
39	DM	35	GLY	C-N-CA	6.55	138.08	121.70
1	1	1269	U	N3-C2-O2	-6.55	117.62	122.20
64	c6	41	PRO	C-N-CA	6.51	137.98	121.70
47	A	934	C	C2-N1-C1'	6.49	125.94	118.80
55	s7	72	LYS	C-N-CA	-6.47	105.53	121.70
1	1	1103	A	OP1-P-O3'	6.47	119.42	105.20
53	G	66	GLN	N-CA-C	6.47	128.46	111.00
47	A	1000	C	N3-C2-O2	-6.45	117.39	121.90
47	A	1000	C	C2-N1-C1'	6.41	125.85	118.80
76	d8	33	LEU	CB-CG-CD2	6.39	121.86	111.00
80	h	50	ASP	C-N-CA	6.38	137.66	121.70
1	1	2257	C	C2-N1-C1'	6.38	125.82	118.80
79	e1	122	SER	C-N-CA	6.36	137.60	121.70
64	R	57	LEU	C-N-CA	-6.34	105.86	121.70
47	A	507	U	C2-N1-C1'	6.33	125.29	117.70
50	D	60	SER	C-N-CA	-6.32	105.89	121.70
60	N	127	GLY	N-CA-C	6.30	128.84	113.10
4	CD	25	GLY	N-CA-C	6.29	128.81	113.10
1	AR	3278	C	N1-C2-O2	6.27	122.66	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AR	2996	U	N1-C2-O2	6.25	127.18	122.80
1	AR	2257	C	C2-N1-C1'	6.24	125.67	118.80
47	A	543	C	N3-C2-O2	-6.21	117.55	121.90
47	A	1389	C	C2-N1-C1'	6.20	125.62	118.80
47	A	702	G	N9-C4-C5	-6.19	102.92	105.40
47	sR	1389	C	C2-N1-C1'	6.19	125.61	118.80
53	G	105	GLY	N-CA-C	-6.18	97.65	113.10
67	U	51	GLU	N-CA-C	-6.15	94.39	111.00
1	1	979	U	P-O3'-C3'	6.14	127.07	119.70
77	d9	9	SER	C-N-CA	6.13	137.02	121.70
39	DM	12	LEU	CA-CB-CG	6.12	129.37	115.30
1	1	880	G	C4-N9-C1'	-6.10	118.57	126.50
10	CJ	122	LYS	C-N-CA	6.10	136.95	121.70
1	1	1103	A	P-O3'-C3'	6.09	127.01	119.70
1	1	880	G	C8-N9-C1'	6.07	134.89	127.00
47	sR	75	U	C2-N1-C1'	6.06	124.97	117.70
1	1	1279	C	C6-N1-C2	-6.05	117.88	120.30
62	P	44	GLY	N-CA-C	6.04	128.20	113.10
64	c6	39	VAL	C-N-CA	-6.04	106.61	121.70
50	D	37	PRO	C-N-CA	6.03	136.78	121.70
47	sR	163	G	N3-C4-C5	6.03	131.62	128.60
47	A	1150	G	P-O3'-C3'	6.01	126.92	119.70
1	1	2541	U	P-O3'-C3'	6.01	126.91	119.70
47	A	1096	C	C2-N1-C1'	6.00	125.40	118.80
14	t	77	LEU	CA-CB-CG	5.98	129.05	115.30
47	A	720	G	OP1-P-O3'	5.98	118.36	105.20
39	DM	32	ASN	C-N-CA	5.97	136.63	121.70
25	7	77	LYS	N-CA-C	5.96	127.09	111.00
1	AR	1115	G	C4-N9-C1'	5.96	134.25	126.50
62	P	39	ILE	CB-CA-C	-5.96	99.69	111.60
47	sR	1274	C	N1-C2-O2	5.95	122.47	118.90
60	c2	44	GLY	N-CA-C	5.95	127.97	113.10
47	A	543	C	C2-N1-C1'	5.94	125.33	118.80
66	T	101	LEU	C-N-CA	5.93	136.53	121.70
74	d6	9	GLY	CA-C-N	-5.93	104.15	117.20
47	sR	280	U	N1-C2-O2	5.93	126.95	122.80
64	R	56	GLY	N-CA-C	-5.92	98.29	113.10
60	c2	110	GLY	N-CA-C	-5.92	98.29	113.10
47	sR	795	U	C2-N1-C1'	5.91	124.79	117.70
47	sR	1097	U	P-O3'-C3'	5.88	126.76	119.70
77	e	36	LEU	CA-CB-CG	5.88	128.81	115.30
60	c2	46	ARG	CA-CB-CG	5.88	126.33	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	A	1150	G	OP2-P-O3'	5.87	118.12	105.20
47	sR	542	A	P-O3'-C3'	5.87	126.74	119.70
72	Z	125	LEU	CA-CB-CG	5.87	128.79	115.30
1	1	1556	C	N1-C2-O2	5.86	122.41	118.90
47	A	1000	C	C6-N1-C2	-5.84	117.96	120.30
47	A	639	U	N1-C2-O2	5.84	126.89	122.80
1	1	1279	C	C5-C6-N1	5.84	123.92	121.00
1	AR	1556	C	N1-C2-O2	5.83	122.40	118.90
79	g	87	THR	N-CA-C	5.82	126.72	111.00
1	1	545	U	C2-N1-C1'	5.82	124.68	117.70
1	AR	3181	C	N1-C2-O2	5.81	122.39	118.90
47	sR	75	U	O4'-C1'-N1	5.80	112.84	108.20
80	h	165	ASP	C-N-CA	5.79	136.18	121.70
7	CG	293	LEU	CA-CB-CG	5.79	128.62	115.30
1	AR	2873	U	N1-C2-O2	5.78	126.85	122.80
80	h	166	SER	N-CA-C	5.78	126.59	111.00
12	r	120	GLY	C-N-CA	5.77	136.13	121.70
80	Rb	145	LEU	CA-CB-CG	5.77	128.58	115.30
47	A	1039	A	O4'-C1'-N9	5.76	112.81	108.20
47	sR	1596	C	N1-C2-O2	5.75	122.35	118.90
1	AR	1019	G	N3-C2-N2	-5.75	115.88	119.90
1	1	406	G	O4'-C1'-N9	5.74	112.79	108.20
1	1	3181	C	N1-C2-O2	5.71	122.33	118.90
55	I	111	LYS	N-CA-C	5.70	126.39	111.00
60	c2	26	ASP	C-N-CA	-5.69	107.47	121.70
1	AR	2726	C	N3-C2-O2	-5.69	117.92	121.90
47	sR	1596	C	C2-N1-C1'	5.69	125.06	118.80
1	1	3217	C	C6-N1-C2	-5.67	118.03	120.30
1	1	3278	C	C2-N1-C1'	5.67	125.03	118.80
47	sR	679	U	C5-C6-N1	5.66	125.53	122.70
54	H	216	LEU	CA-CB-CG	5.66	128.32	115.30
10	p	26	LEU	CA-CB-CG	5.66	128.31	115.30
1	AR	2270	A	N7-C8-N9	5.64	116.62	113.80
20	z	185	LEU	CA-CB-CG	5.63	128.26	115.30
19	y	41	ASP	CB-CG-OD1	5.63	123.37	118.30
63	Q	26	LEU	CA-CB-CG	5.63	128.24	115.30
47	A	736	C	C6-N1-C1'	-5.62	114.05	120.80
47	A	737	A	O4'-C1'-N9	5.61	112.69	108.20
1	AR	2679	A	O4'-C1'-N9	5.61	112.69	108.20
47	sR	647	G	N3-C2-N2	-5.61	115.97	119.90
59	c1	29	LYS	N-CA-C	-5.61	95.86	111.00
47	sR	1390	U	C2-N1-C1'	5.60	124.42	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AR	2983	C	C2-N1-C1'	5.59	124.95	118.80
47	A	581	U	C2-N1-C1'	5.59	124.41	117.70
1	AR	2996	U	N3-C2-O2	-5.58	118.29	122.20
29	DC	48	TYR	CB-CA-C	-5.58	99.24	110.40
47	A	736	C	C5-C6-N1	5.57	123.79	121.00
1	1	922	U	C2-N1-C1'	5.57	124.38	117.70
67	U	132	LEU	CA-CB-CG	5.57	128.10	115.30
1	1	2443	A	O4'-C1'-N9	5.56	112.64	108.20
1	AR	922	U	C2-N1-C1'	5.56	124.37	117.70
54	H	68	LEU	CB-CG-CD2	5.55	120.43	111.00
47	A	1698	G	P-O3'-C3'	5.55	126.36	119.70
47	sR	1389	C	N1-C2-O2	5.54	122.22	118.90
47	A	639	U	N3-C2-O2	-5.51	118.34	122.20
50	D	207	LEU	CA-CB-CG	5.51	127.97	115.30
47	sR	1473	U	N1-C2-O2	5.50	126.65	122.80
47	sR	858	G	C4-N9-C1'	5.50	133.65	126.50
47	sR	280	U	N3-C2-O2	-5.50	118.35	122.20
1	1	3362	A	O4'-C1'-N9	5.50	112.60	108.20
5	k	346	THR	C-N-CA	5.49	135.43	121.70
47	sR	453	U	C6-N1-C1'	-5.49	113.51	121.20
47	sR	858	G	O4'-C1'-N9	5.49	112.59	108.20
23	5	45	GLY	N-CA-C	5.49	126.81	113.10
49	C	55	LYS	N-CA-C	-5.48	96.19	111.00
1	AR	3318	G	C4-N9-C1'	5.48	133.62	126.50
72	Z	98	GLU	C-N-CA	5.47	135.37	121.70
47	sR	1246	C	N1-C2-O2	5.47	122.18	118.90
47	A	1389	C	N1-C2-O2	5.46	122.18	118.90
1	AR	2726	C	C6-N1-C2	-5.45	118.12	120.30
47	A	702	G	C4-C5-N7	5.45	112.98	110.80
1	AR	2541	U	P-O3'-C3'	5.43	126.22	119.70
52	s4	107	GLY	N-CA-C	5.43	126.67	113.10
1	AR	3278	C	C6-N1-C1'	-5.43	114.29	120.80
76	d8	33	LEU	CB-CG-CD1	5.43	120.23	111.00
1	1	1556	C	C2-N1-C1'	5.41	124.75	118.80
57	s9	158	PHE	C-N-CA	-5.41	108.19	121.70
57	K	137	GLY	N-CA-C	-5.39	99.62	113.10
57	K	166	GLY	N-CA-C	5.39	126.58	113.10
47	A	734	A	OP1-P-O3'	5.38	117.05	105.20
1	AR	2263	C	C6-N1-C1'	-5.37	114.35	120.80
47	sR	687	G	N9-C4-C5	5.37	107.55	105.40
1	AR	1241	U	OP1-P-O3'	5.36	117.00	105.20
64	c6	105	LEU	CA-CB-CG	5.36	127.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	sR	1285	U	C2-N1-C1'	5.34	124.11	117.70
47	A	720	G	P-O3'-C3'	5.34	126.11	119.70
60	c2	58	LEU	CA-CB-CG	-5.33	103.03	115.30
6	l	292	SER	N-CA-C	5.33	125.39	111.00
47	sR	1097	U	OP2-P-O3'	5.33	116.92	105.20
76	d8	60	GLU	C-N-CA	5.33	135.02	121.70
1	AR	3318	G	C8-N9-C1'	-5.32	120.08	127.00
47	sR	1340	U	N1-C2-O2	5.32	126.53	122.80
47	A	934	C	N1-C2-O2	5.32	122.09	118.90
62	P	41	ARG	N-CA-C	5.32	125.35	111.00
1	AR	1329	U	P-O3'-C3'	5.31	126.08	119.70
67	U	103	LYS	CA-CB-CG	5.31	125.08	113.40
1	1	2553	U	C2-N1-C1'	5.30	124.06	117.70
14	CN	179	PHE	C-N-CA	-5.30	108.44	121.70
62	P	90	ARG	C-N-CA	5.30	134.96	121.70
1	AR	1604	G	N3-C4-C5	-5.30	125.95	128.60
72	d4	51	GLU	C-N-CA	5.29	134.93	121.70
47	sR	1573	A	OP2-P-O3'	5.29	116.84	105.20
25	CY	24	GLY	C-N-CA	-5.29	108.47	121.70
80	Rb	162	ALA	N-CA-C	-5.28	96.74	111.00
47	sR	1058	U	OP1-P-O3'	5.28	116.81	105.20
47	sR	543	C	N3-C2-O2	-5.27	118.21	121.90
1	1	3217	C	C6-N1-C1'	-5.26	114.48	120.80
25	7	76	VAL	C-N-CA	5.25	134.83	121.70
47	A	187	G	OP1-P-O3'	5.25	116.75	105.20
1	1	2996	U	C2-N1-C1'	5.25	124.00	117.70
47	sR	813	U	C2-N1-C1'	5.25	124.00	117.70
51	s3	142	LEU	CA-CB-CG	5.24	127.36	115.30
48	B	207	PRO	CA-N-CD	-5.24	104.17	111.50
1	AR	2873	U	N3-C2-O2	-5.24	118.54	122.20
1	AR	3217	C	C6-N1-C2	-5.23	118.21	120.30
47	A	453	U	C2-N1-C1'	5.23	123.98	117.70
48	B	94	GLY	N-CA-C	-5.23	100.03	113.10
1	1	2112	U	OP2-P-O3'	5.23	116.70	105.20
79	g	86	THR	C-N-CA	5.22	134.75	121.70
47	A	1182	U	N3-C2-O2	-5.21	118.55	122.20
47	A	1514	U	N1-C2-O2	5.21	126.45	122.80
47	sR	1000	C	C2-N1-C1'	5.21	124.53	118.80
47	A	287	G	O4'-C1'-N9	5.21	112.37	108.20
6	l	327	LEU	CA-CB-CG	5.20	127.27	115.30
60	c2	46	ARG	CB-CG-CD	-5.19	98.10	111.60
55	I	111	LYS	N-CA-CB	-5.18	101.27	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C	217	LEU	CB-CG-CD1	-5.18	102.19	111.00
44	AQ	50	GLY	N-CA-C	-5.18	100.15	113.10
47	A	1761	U	P-O3'-C3'	5.18	125.92	119.70
47	sR	1596	C	N3-C2-O2	-5.17	118.28	121.90
47	A	1458	G	C4-N9-C1'	5.17	133.22	126.50
56	s8	51	GLY	N-CA-C	-5.17	100.19	113.10
49	C	131	ASP	N-CA-C	-5.16	97.06	111.00
5	k	387	LEU	CA-CB-CG	5.16	127.17	115.30
56	J	153	GLU	C-N-CA	-5.16	108.81	121.70
29	AB	48	TYR	CB-CA-C	-5.15	100.10	110.40
6	l	291	ASN	C-N-CA	-5.14	108.84	121.70
49	C	211	HIS	C-N-CA	5.14	134.54	121.70
51	s3	216	PRO	N-CA-C	5.14	125.45	112.10
1	AR	2263	C	C2-N1-C1'	5.13	124.44	118.80
47	A	1600	A	OP1-P-O3'	5.13	116.48	105.20
47	A	959	U	N1-C2-O2	5.13	126.39	122.80
1	1	1604	G	C4-N9-C1'	5.12	133.16	126.50
52	F	193	GLY	N-CA-C	5.12	125.91	113.10
29	DC	78	LEU	CB-CG-CD2	5.12	119.71	111.00
47	A	1096	C	C6-N1-C1'	-5.12	114.65	120.80
47	A	1058	U	N1-C2-O2	5.12	126.38	122.80
1	AR	1019	G	N3-C4-N9	-5.11	122.93	126.00
1	AR	1115	G	C8-N9-C1'	-5.11	120.35	127.00
1	AR	3355	U	C2-N1-C1'	5.11	123.83	117.70
47	sR	781	U	N1-C2-O2	5.11	126.38	122.80
47	sR	1340	U	N3-C2-O2	-5.11	118.63	122.20
73	a	69	LEU	CA-CB-CG	5.10	127.03	115.30
60	N	41	LEU	CA-CB-CG	5.10	127.02	115.30
1	AR	1556	C	C2-N1-C1'	5.09	124.40	118.80
47	A	959	U	C2-N1-C1'	5.09	123.81	117.70
47	A	1246	C	C2-N1-C1'	5.09	124.40	118.80
80	Rb	141	LEU	C-N-CA	-5.09	108.98	121.70
53	s5	217	LEU	CA-CB-CG	5.08	127.00	115.30
1	1	1437	C	C2-N1-C1'	5.08	124.39	118.80
5	CE	102	LEU	CA-CB-CG	5.08	126.99	115.30
1	AR	2444	C	N1-C2-O2	5.07	121.94	118.90
47	A	158	U	P-O3'-C3'	5.07	125.79	119.70
1	1	545	U	N1-C2-O2	5.07	126.35	122.80
71	Y	114	LYS	C-N-CA	-5.06	111.68	122.30
60	c2	87	PRO	N-CA-C	5.05	125.24	112.10
60	N	102	GLY	N-CA-C	5.05	125.73	113.10
1	AR	2254	U	C2-N1-C1'	5.05	123.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2434	U	C2-N1-C1'	5.03	123.73	117.70
1	AR	1604	G	C4-N9-C1'	5.03	133.04	126.50
47	sR	489	C	C2-N1-C1'	5.03	124.33	118.80
47	sR	1503	A	O4'-C1'-N9	5.02	112.22	108.20
47	sR	1716	C	O4'-C1'-N1	5.02	112.22	108.20
47	A	1096	C	N1-C2-O2	5.02	121.91	118.90
6	l	182	LEU	CA-CB-CG	5.01	126.83	115.30
28	DB	60	LYS	C-N-CA	5.01	134.22	121.70
72	d4	59	GLY	N-CA-C	5.01	125.63	113.10
47	A	139	C	P-O3'-C3'	5.01	125.71	119.70
47	sR	1600	A	OP1-P-O3'	5.01	116.22	105.20
35	AH	51	LEU	CA-CB-CG	5.00	126.81	115.30
47	sR	1473	U	C6-N1-C1'	-5.00	114.20	121.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
49	C	129	THR	Peptide
15	u	128	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	250/254 (98%)	248 (99%)	2 (1%)	0	100	100
4	j	250/254 (98%)	250 (100%)	0	0	100	100
5	CE	384/387 (99%)	382 (100%)	2 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	k	384/387 (99%)	374 (97%)	10 (3%)	0	100	100
6	CF	359/362 (99%)	353 (98%)	6 (2%)	0	100	100
6	l	359/362 (99%)	350 (98%)	9 (2%)	0	100	100
7	CG	294/297 (99%)	289 (98%)	5 (2%)	0	100	100
7	m	294/297 (99%)	287 (98%)	7 (2%)	0	100	100
8	CH	152/176 (86%)	150 (99%)	2 (1%)	0	100	100
8	n	152/176 (86%)	152 (100%)	0	0	100	100
9	CI	220/244 (90%)	217 (99%)	3 (1%)	0	100	100
9	o	220/244 (90%)	210 (96%)	10 (4%)	0	100	100
10	CJ	231/256 (90%)	221 (96%)	10 (4%)	0	100	100
10	p	231/256 (90%)	226 (98%)	5 (2%)	0	100	100
11	CK	189/191 (99%)	185 (98%)	4 (2%)	0	100	100
11	q	189/191 (99%)	185 (98%)	4 (2%)	0	100	100
12	CL	207/221 (94%)	205 (99%)	2 (1%)	0	100	100
12	r	207/221 (94%)	205 (99%)	2 (1%)	0	100	100
13	CM	167/174 (96%)	162 (97%)	5 (3%)	0	100	100
13	s	167/174 (96%)	160 (96%)	7 (4%)	0	100	100
14	CN	191/199 (96%)	179 (94%)	11 (6%)	1 (0%)	25	57
14	t	191/199 (96%)	180 (94%)	9 (5%)	2 (1%)	13	43
15	CO	134/138 (97%)	134 (100%)	0	0	100	100
15	u	134/138 (97%)	131 (98%)	2 (2%)	1 (1%)	19	51
16	CP	201/204 (98%)	201 (100%)	0	0	100	100
16	v	201/204 (98%)	196 (98%)	5 (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	181/184 (98%)	181 (100%)	0	0	100	100
18	x	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
19	CS	183/186 (98%)	181 (99%)	2 (1%)	0	100	100
19	y	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
20	CT	186/189 (98%)	182 (98%)	4 (2%)	0	100	100
20	z	186/189 (98%)	183 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	0	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
21	CU	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
22	2	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
22	CV	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
23	5	98/121 (81%)	98 (100%)	0	0	100	100
23	CW	98/121 (81%)	96 (98%)	2 (2%)	0	100	100
24	6	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
24	CX	134/137 (98%)	134 (100%)	0	0	100	100
25	7	96/155 (62%)	94 (98%)	2 (2%)	0	100	100
25	CY	122/155 (79%)	118 (97%)	4 (3%)	0	100	100
26	8	119/142 (84%)	119 (100%)	0	0	100	100
26	CZ	119/142 (84%)	118 (99%)	1 (1%)	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%)	127 (96%)	6 (4%)	0	100	100
28	DB	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
29	AB	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
29	DC	146/149 (98%)	142 (97%)	4 (3%)	0	100	100
30	AC	56/59 (95%)	55 (98%)	1 (2%)	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%)	95 (100%)	0	0	100	100
32	AE	107/113 (95%)	101 (94%)	6 (6%)	0	100	100
32	DF	107/113 (95%)	104 (97%)	3 (3%)	0	100	100
33	AF	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
33	DG	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
34	AG	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
34	DH	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
35	AH	110/121 (91%)	110 (100%)	0	0	100	100
35	DI	110/121 (91%)	109 (99%)	1 (1%)	0	100	100
36	AI	117/120 (98%)	110 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	DJ	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
37	AJ	97/100 (97%)	95 (98%)	2 (2%)	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	85/88 (97%)	85 (100%)	0	0	100	100
39	AL	75/78 (96%)	75 (100%)	0	0	100	100
39	DM	75/78 (96%)	72 (96%)	3 (4%)	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%)	48 (96%)	2 (4%)	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%)	94 (91%)	8 (8%)	1 (1%)	13	43
43	DQ	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
44	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
44	DR	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	i	155/273 (57%)	147 (95%)	8 (5%)	0	100	100
45	sM	61/273 (22%)	57 (93%)	4 (7%)	0	100	100
46	p0	139/311 (45%)	139 (100%)	0	0	100	100
48	B	204/252 (81%)	185 (91%)	19 (9%)	0	100	100
48	s0	204/252 (81%)	194 (95%)	10 (5%)	0	100	100
49	C	212/255 (83%)	200 (94%)	12 (6%)	0	100	100
49	s1	214/255 (84%)	213 (100%)	1 (0%)	0	100	100
50	D	215/254 (85%)	207 (96%)	7 (3%)	1 (0%)	25	57
50	s2	215/254 (85%)	210 (98%)	5 (2%)	0	100	100
51	E	221/240 (92%)	215 (97%)	6 (3%)	0	100	100
51	s3	221/240 (92%)	208 (94%)	13 (6%)	0	100	100
52	F	258/261 (99%)	253 (98%)	5 (2%)	0	100	100
52	s4	258/261 (99%)	253 (98%)	5 (2%)	0	100	100
53	G	204/225 (91%)	198 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	s5	204/225 (91%)	195 (96%)	9 (4%)	0	100	100
54	H	224/236 (95%)	216 (96%)	8 (4%)	0	100	100
54	s6	216/236 (92%)	209 (97%)	7 (3%)	0	100	100
55	I	182/190 (96%)	175 (96%)	7 (4%)	0	100	100
55	s7	184/190 (97%)	173 (94%)	9 (5%)	2 (1%)	12	40
56	J	184/200 (92%)	170 (92%)	14 (8%)	0	100	100
56	s8	184/200 (92%)	184 (100%)	0	0	100	100
57	K	183/197 (93%)	174 (95%)	9 (5%)	0	100	100
57	s9	183/197 (93%)	178 (97%)	5 (3%)	0	100	100
58	L	94/105 (90%)	86 (92%)	8 (8%)	0	100	100
58	c0	92/105 (88%)	80 (87%)	12 (13%)	0	100	100
59	M	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
59	c1	144/156 (92%)	139 (96%)	5 (4%)	0	100	100
60	N	122/143 (85%)	111 (91%)	11 (9%)	0	100	100
60	c2	122/143 (85%)	109 (89%)	12 (10%)	1 (1%)	16	47
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%)	116 (93%)	7 (6%)	2 (2%)	8	33
62	c4	126/138 (91%)	119 (94%)	7 (6%)	0	100	100
63	Q	122/142 (86%)	111 (91%)	11 (9%)	0	100	100
63	c5	133/142 (94%)	123 (92%)	10 (8%)	0	100	100
64	R	139/143 (97%)	133 (96%)	4 (3%)	2 (1%)	9	36
64	c6	140/143 (98%)	136 (97%)	3 (2%)	1 (1%)	19	51
65	S	116/136 (85%)	110 (95%)	6 (5%)	0	100	100
66	T	143/146 (98%)	132 (92%)	10 (7%)	1 (1%)	19	51
66	c8	143/146 (98%)	126 (88%)	17 (12%)	0	100	100
67	U	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
67	c9	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
68	V	105/121 (87%)	96 (91%)	9 (9%)	0	100	100
68	d0	108/121 (89%)	102 (94%)	6 (6%)	0	100	100
69	W	85/87 (98%)	80 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	d1	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
70	X	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
70	d2	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
71	Y	142/145 (98%)	128 (90%)	14 (10%)	0	100	100
71	d3	142/145 (98%)	134 (94%)	8 (6%)	0	100	100
72	Z	132/135 (98%)	132 (100%)	0	0	100	100
72	d4	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
73	a	68/108 (63%)	62 (91%)	6 (9%)	0	100	100
73	d5	67/108 (62%)	67 (100%)	0	0	100	100
74	b	95/119 (80%)	86 (90%)	9 (10%)	0	100	100
74	d6	95/119 (80%)	89 (94%)	6 (6%)	0	100	100
75	c	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
75	d7	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
76	d	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
76	d8	61/67 (91%)	56 (92%)	5 (8%)	0	100	100
77	d9	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
77	e	51/56 (91%)	50 (98%)	0	1 (2%)	6	28
78	e0	60/63 (95%)	58 (97%)	1 (2%)	1 (2%)	7	32
78	f	58/63 (92%)	58 (100%)	0	0	100	100
79	e1	49/152 (32%)	42 (86%)	5 (10%)	2 (4%)	2	14
79	g	69/152 (45%)	57 (83%)	12 (17%)	0	100	100
80	Rb	316/319 (99%)	307 (97%)	9 (3%)	0	100	100
80	h	316/319 (99%)	304 (96%)	12 (4%)	0	100	100
81	c7	113/136 (83%)	110 (97%)	3 (3%)	0	100	100
All	All	22284/24619 (90%)	21584 (97%)	681 (3%)	19 (0%)	48	77

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	u	8	LYS
50	D	107	SER
62	P	37	GLU
64	R	40	GLU
64	R	59	LYS

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Mol	Chain	Res	Type
55	s7	64	VAL
79	e1	132	LEU
77	e	25	SER
60	c2	106	ILE
43	AP	15	LYS
64	c6	14	LYS
78	e0	47	VAL
79	e1	145	HIS
14	t	77	LEU
66	T	91	ASP
55	s7	14	THR
14	CN	63	VAL
14	t	63	VAL
62	P	39	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	CD	193/196 (98%)	188 (97%)	5 (3%)	41 66
4	j	193/196 (98%)	192 (100%)	1 (0%)	86 92
5	CE	319/323 (99%)	314 (98%)	5 (2%)	58 77
5	k	320/323 (99%)	309 (97%)	11 (3%)	32 60
6	CF	288/289 (100%)	283 (98%)	5 (2%)	56 75
6	l	288/289 (100%)	282 (98%)	6 (2%)	48 71
7	CG	244/245 (100%)	238 (98%)	6 (2%)	42 67
7	m	244/245 (100%)	235 (96%)	9 (4%)	29 57
8	CH	134/153 (88%)	129 (96%)	5 (4%)	29 57
8	n	134/153 (88%)	131 (98%)	3 (2%)	47 70
9	CI	186/205 (91%)	183 (98%)	3 (2%)	58 77
9	o	186/205 (91%)	183 (98%)	3 (2%)	58 77
10	CJ	187/208 (90%)	183 (98%)	4 (2%)	48 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	p	187/208 (90%)	182 (97%)	5 (3%)	40	65
11	CK	171/171 (100%)	170 (99%)	1 (1%)	84	91
11	q	171/171 (100%)	169 (99%)	2 (1%)	67	82
12	CL	177/187 (95%)	171 (97%)	6 (3%)	32	60
12	r	177/187 (95%)	171 (97%)	6 (3%)	32	60
13	CM	147/151 (97%)	144 (98%)	3 (2%)	50	72
13	s	147/151 (97%)	144 (98%)	3 (2%)	50	72
14	CN	154/159 (97%)	148 (96%)	6 (4%)	27	55
14	t	154/159 (97%)	152 (99%)	2 (1%)	65	81
15	CO	107/109 (98%)	105 (98%)	2 (2%)	52	73
15	u	107/109 (98%)	104 (97%)	3 (3%)	38	64
16	CP	175/176 (99%)	170 (97%)	5 (3%)	37	63
16	v	175/176 (99%)	173 (99%)	2 (1%)	70	84
17	CQ	160/162 (99%)	159 (99%)	1 (1%)	84	91
17	w	160/162 (99%)	159 (99%)	1 (1%)	84	91
18	CR	140/146 (96%)	137 (98%)	3 (2%)	48	71
18	x	140/146 (96%)	138 (99%)	2 (1%)	62	80
19	CS	150/151 (99%)	147 (98%)	3 (2%)	50	72
19	y	150/151 (99%)	145 (97%)	5 (3%)	33	60
20	CT	153/154 (99%)	150 (98%)	3 (2%)	50	72
20	z	153/154 (99%)	148 (97%)	5 (3%)	33	60
21	0	156/156 (100%)	154 (99%)	2 (1%)	65	81
21	CU	156/156 (100%)	154 (99%)	2 (1%)	65	81
22	2	136/137 (99%)	133 (98%)	3 (2%)	47	70
22	CV	136/137 (99%)	134 (98%)	2 (2%)	60	78
23	5	87/107 (81%)	83 (95%)	4 (5%)	23	52
23	CW	87/107 (81%)	84 (97%)	3 (3%)	32	60
24	6	104/105 (99%)	104 (100%)	0	100	100
24	CX	104/105 (99%)	101 (97%)	3 (3%)	37	63
25	7	57/129 (44%)	56 (98%)	1 (2%)	54	74
25	CY	58/129 (45%)	57 (98%)	1 (2%)	56	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	8	104/118 (88%)	101 (97%)	3 (3%)	37	63
26	CZ	104/118 (88%)	101 (97%)	3 (3%)	37	63
27	9	109/110 (99%)	108 (99%)	1 (1%)	75	87
27	DA	107/110 (97%)	104 (97%)	3 (3%)	38	64
28	AA	115/116 (99%)	114 (99%)	1 (1%)	75	87
28	DB	114/116 (98%)	113 (99%)	1 (1%)	75	87
29	AB	118/119 (99%)	115 (98%)	3 (2%)	42	67
29	DC	118/119 (99%)	113 (96%)	5 (4%)	25	53
30	AC	46/47 (98%)	44 (96%)	2 (4%)	25	53
30	DD	46/47 (98%)	45 (98%)	1 (2%)	47	70
31	AD	81/88 (92%)	78 (96%)	3 (4%)	29	57
31	DE	81/88 (92%)	79 (98%)	2 (2%)	42	67
32	AE	92/97 (95%)	91 (99%)	1 (1%)	70	84
32	DF	92/97 (95%)	91 (99%)	1 (1%)	70	84
33	AF	109/111 (98%)	107 (98%)	2 (2%)	54	74
33	DG	109/111 (98%)	107 (98%)	2 (2%)	54	74
34	AG	90/91 (99%)	90 (100%)	0	100	100
34	DH	90/91 (99%)	89 (99%)	1 (1%)	70	84
35	AH	95/103 (92%)	92 (97%)	3 (3%)	34	61
35	DI	95/103 (92%)	95 (100%)	0	100	100
36	AI	104/105 (99%)	100 (96%)	4 (4%)	28	56
36	DJ	104/105 (99%)	104 (100%)	0	100	100
37	AJ	81/82 (99%)	77 (95%)	4 (5%)	21	50
37	DK	81/82 (99%)	80 (99%)	1 (1%)	67	82
38	AK	70/71 (99%)	67 (96%)	3 (4%)	25	53
38	DL	70/71 (99%)	70 (100%)	0	100	100
39	AL	68/69 (99%)	64 (94%)	4 (6%)	16	43
39	DM	68/69 (99%)	66 (97%)	2 (3%)	37	63
40	AM	45/46 (98%)	44 (98%)	1 (2%)	47	70
40	DN	45/46 (98%)	43 (96%)	2 (4%)	24	52
41	AN	47/116 (40%)	45 (96%)	2 (4%)	25	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
41	DO	47/116 (40%)	46 (98%)	1 (2%)	48 71
42	AO	23/23 (100%)	23 (100%)	0	100 100
42	DP	23/23 (100%)	21 (91%)	2 (9%)	8 29
43	AP	90/91 (99%)	87 (97%)	3 (3%)	33 60
43	DQ	90/91 (99%)	90 (100%)	0	100 100
44	AQ	71/72 (99%)	69 (97%)	2 (3%)	38 64
44	DR	71/72 (99%)	68 (96%)	3 (4%)	25 53
45	i	97/228 (42%)	93 (96%)	4 (4%)	26 54
45	sM	54/228 (24%)	49 (91%)	5 (9%)	7 26
46	p0	105/248 (42%)	105 (100%)	0	100 100
48	B	164/210 (78%)	162 (99%)	2 (1%)	67 82
48	s0	165/210 (79%)	159 (96%)	6 (4%)	30 58
49	C	191/224 (85%)	182 (95%)	9 (5%)	22 51
49	s1	192/224 (86%)	185 (96%)	7 (4%)	30 58
50	D	176/205 (86%)	171 (97%)	5 (3%)	38 64
50	s2	176/205 (86%)	175 (99%)	1 (1%)	84 91
51	E	182/195 (93%)	176 (97%)	6 (3%)	33 60
51	s3	182/195 (93%)	172 (94%)	10 (6%)	18 46
52	F	221/222 (100%)	212 (96%)	9 (4%)	26 54
52	s4	221/222 (100%)	218 (99%)	3 (1%)	62 80
53	G	173/191 (91%)	166 (96%)	7 (4%)	27 55
53	s5	173/191 (91%)	163 (94%)	10 (6%)	17 44
54	H	188/201 (94%)	180 (96%)	8 (4%)	25 53
54	s6	187/201 (93%)	183 (98%)	4 (2%)	48 71
55	I	165/170 (97%)	152 (92%)	13 (8%)	10 33
55	s7	165/170 (97%)	158 (96%)	7 (4%)	25 53
56	J	150/161 (93%)	144 (96%)	6 (4%)	27 55
56	s8	150/161 (93%)	148 (99%)	2 (1%)	65 81
57	K	158/166 (95%)	148 (94%)	10 (6%)	15 42
57	s9	158/166 (95%)	154 (98%)	4 (2%)	42 67
58	L	77/98 (79%)	75 (97%)	2 (3%)	41 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	c0	73/98 (74%)	70 (96%)	3 (4%)	26	54
59	M	129/137 (94%)	124 (96%)	5 (4%)	27	55
59	c1	129/137 (94%)	126 (98%)	3 (2%)	45	69
60	N	88/119 (74%)	82 (93%)	6 (7%)	13	39
60	c2	88/119 (74%)	81 (92%)	7 (8%)	10	33
61	O	127/128 (99%)	123 (97%)	4 (3%)	35	62
61	c3	127/128 (99%)	125 (98%)	2 (2%)	58	77
62	P	79/105 (75%)	74 (94%)	5 (6%)	15	42
62	c4	97/105 (92%)	94 (97%)	3 (3%)	35	62
63	Q	101/118 (86%)	98 (97%)	3 (3%)	36	63
63	c5	103/118 (87%)	100 (97%)	3 (3%)	37	63
64	R	117/119 (98%)	110 (94%)	7 (6%)	16	43
64	c6	118/119 (99%)	113 (96%)	5 (4%)	25	53
65	S	94/124 (76%)	89 (95%)	5 (5%)	19	47
66	T	128/129 (99%)	123 (96%)	5 (4%)	27	55
66	c8	128/129 (99%)	125 (98%)	3 (2%)	45	69
67	U	115/116 (99%)	106 (92%)	9 (8%)	10	34
67	c9	115/116 (99%)	109 (95%)	6 (5%)	19	47
68	V	100/114 (88%)	96 (96%)	4 (4%)	27	55
68	d0	103/114 (90%)	101 (98%)	2 (2%)	52	73
69	W	74/74 (100%)	72 (97%)	2 (3%)	40	65
69	d1	74/74 (100%)	69 (93%)	5 (7%)	13	39
70	X	110/111 (99%)	106 (96%)	4 (4%)	30	58
70	d2	110/111 (99%)	107 (97%)	3 (3%)	40	65
71	Y	119/120 (99%)	114 (96%)	5 (4%)	25	53
71	d3	119/120 (99%)	117 (98%)	2 (2%)	56	75
72	Z	112/113 (99%)	106 (95%)	6 (5%)	18	46
72	d4	112/113 (99%)	110 (98%)	2 (2%)	54	74
73	a	61/89 (68%)	60 (98%)	1 (2%)	58	77
73	d5	61/89 (68%)	58 (95%)	3 (5%)	21	50
74	b	83/100 (83%)	80 (96%)	3 (4%)	30	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
74	d6	83/100 (83%)	79 (95%)	4 (5%)	21 50
75	c	70/71 (99%)	69 (99%)	1 (1%)	62 80
75	d7	70/71 (99%)	66 (94%)	4 (6%)	17 45
76	d	56/60 (93%)	55 (98%)	1 (2%)	54 74
76	d8	56/60 (93%)	53 (95%)	3 (5%)	18 46
77	d9	47/49 (96%)	45 (96%)	2 (4%)	25 53
77	e	47/49 (96%)	46 (98%)	1 (2%)	48 71
78	e0	53/54 (98%)	52 (98%)	1 (2%)	52 73
78	f	51/54 (94%)	51 (100%)	0	100 100
79	e1	43/135 (32%)	42 (98%)	1 (2%)	45 69
79	g	62/135 (46%)	59 (95%)	3 (5%)	21 50
80	Rb	260/262 (99%)	250 (96%)	10 (4%)	28 56
80	h	259/262 (99%)	253 (98%)	6 (2%)	45 69
81	c7	92/124 (74%)	90 (98%)	2 (2%)	47 70
All	All	18678/20672 (90%)	18145 (97%)	533 (3%)	37 63

All (533) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	j	70	ARG
5	k	70	ARG
5	k	104	THR
5	k	167	ARG
5	k	196	ARG
5	k	206	ASP
5	k	226	PHE
5	k	266	ARG
5	k	284	ARG
5	k	287	LYS
5	k	289	ASP
5	k	291	GLU
6	l	84	ARG
6	l	93	MET
6	l	120	TYR
6	l	138	ARG
6	l	308	LYS
6	l	361	HIS

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Mol	Chain	Res	Type
7	m	5	LYS
7	m	44	TYR
7	m	57	ASN
7	m	67	SER
7	m	158	ARG
7	m	185	PHE
7	m	219	PHE
7	m	274	GLN
7	m	276	LYS
8	n	14	ASP
8	n	48	ARG
8	n	57	HIS
9	o	24	GLU
9	o	30	ARG
9	o	182	ASP
10	p	29	SER
10	p	57	ARG
10	p	77	GLN
10	p	84	ARG
10	p	254	ASP
11	q	5	GLN
11	q	161	LEU
12	r	7	ARG
12	r	24	ARG
12	r	69	ARG
12	r	128	ARG
12	r	191	LYS
12	r	203	LYS
13	s	9	MET
13	s	115	LYS
13	s	140	ARG
14	t	67	ARG
14	t	171	ARG
15	u	27	GLN
15	u	50	LYS
15	u	108	ARG
16	v	22	LEU
16	v	62	TYR
17	w	78	ARG
18	x	126	ARG
18	x	127	ARG
19	y	11	LYS

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Mol	Chain	Res	Type
19	y	31	LYS
19	y	98	LYS
19	y	158	HIS
19	y	176	ARG
20	z	104	ARG
20	z	120	TYR
20	z	173	ARG
20	z	180	LYS
20	z	181	ARG
21	0	81	TYR
21	0	137	ARG
22	2	110	LYS
22	2	128	LEU
22	2	139	ARG
23	5	10	LYS
23	5	52	ASN
23	5	99	LYS
23	5	107	PHE
25	7	60	LYS
26	8	42	ARG
26	8	87	SER
26	8	109	LYS
27	9	74	TYR
28	AA	65	ARG
29	AB	7	LYS
29	AB	60	TYR
29	AB	117	ARG
30	AC	58	LYS
30	AC	59	LYS
31	AD	63	SER
31	AD	66	LYS
31	AD	97	ASP
32	AE	44	MET
33	AF	24	ARG
33	AF	54	LYS
35	AH	47	CYS
35	AH	58	ARG
35	AH	103	LYS
36	AI	7	TYR
36	AI	64	GLU
36	AI	74	LYS
36	AI	86	ARG

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Mol	Chain	Res	Type
37	AJ	30	LYS
37	AJ	46	GLU
37	AJ	62	ARG
37	AJ	86	LYS
38	AK	35	SER
38	AK	37	CYS
38	AK	55	ARG
39	AL	9	LYS
39	AL	10	GLN
39	AL	57	ASN
39	AL	69	LEU
40	AM	12	LYS
41	AN	105	PRO
41	AN	117	HIS
43	AP	18	ARG
43	AP	38	GLN
43	AP	45	ARG
44	AQ	45	LYS
44	AQ	59	CYS
45	i	51	ARG
45	i	62	ARG
45	i	78	ASP
45	i	88	ARG
4	CD	72	ARG
4	CD	149	ARG
4	CD	217	GLN
4	CD	242	ARG
4	CD	251	LYS
5	CE	104	THR
5	CE	187	SER
5	CE	196	ARG
5	CE	291	GLU
5	CE	332	ARG
6	CF	3	ARG
6	CF	33	ASP
6	CF	93	MET
6	CF	120	TYR
6	CF	309	ARG
7	CG	23	ARG
7	CG	95	TRP
7	CG	115	LEU
7	CG	196	ARG

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Mol	Chain	Res	Type
7	CG	234	ASP
7	CG	262	LYS
8	CH	8	LYS
8	CH	14	ASP
8	CH	60	ASP
8	CH	77	ARG
8	CH	101	PHE
9	CI	29	GLU
9	CI	113	SER
9	CI	160	ARG
10	CJ	108	ARG
10	CJ	204	ARG
10	CJ	225	LYS
10	CJ	249	ARG
11	CK	72	LYS
12	CL	23	ASN
12	CL	36	LEU
12	CL	58	GLU
12	CL	130	ASP
12	CL	163	GLN
12	CL	196	PHE
13	CM	13	LYS
13	CM	29	ARG
13	CM	153	LYS
14	CN	27	ASP
14	CN	59	ARG
14	CN	67	ARG
14	CN	153	ASP
14	CN	165	SER
14	CN	171	ARG
15	CO	8	LYS
15	CO	74	ARG
16	CP	23	GLN
16	CP	46	ASP
16	CP	109	ARG
16	CP	143	ARG
16	CP	178	HIS
17	CQ	66	LYS
18	CR	3	ARG
18	CR	173	ARG
18	CR	181	ARG
19	CS	66	ARG

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Mol	Chain	Res	Type
19	CS	111	ARG
19	CS	170	ARG
20	CT	152	GLU
20	CT	176	ARG
20	CT	186	LYS
21	CU	3	HIS
21	CU	172	TYR
22	CV	60	LYS
22	CV	115	LYS
23	CW	50	LEU
23	CW	86	LYS
23	CW	90	ARG
24	CX	45	ARG
24	CX	66	LYS
24	CX	124	ASP
25	CY	80	ARG
26	CZ	34	LEU
26	CZ	65	GLN
26	CZ	108	LEU
27	DA	28	ARG
27	DA	51	ARG
27	DA	74	TYR
28	DB	21	LYS
29	DC	7	LYS
29	DC	47	LYS
29	DC	48	TYR
29	DC	60	TYR
29	DC	88	ASP
30	DD	15	LYS
31	DE	52	ARG
31	DE	71	GLN
32	DF	74	ARG
33	DG	33	ARG
33	DG	80	LYS
34	DH	42	GLN
37	DK	68	ARG
39	DM	17	ARG
39	DM	19	ASP
40	DN	36	ARG
40	DN	46	ARG
41	DO	117	HIS
42	DP	7	LYS

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Mol	Chain	Res	Type
42	DP	25	LYS
44	DR	58	SER
44	DR	59	CYS
44	DR	61	LYS
45	sM	63	ASP
45	sM	64	LYS
45	sM	70	ASN
45	sM	72	ARG
45	sM	84	LYS
48	B	79	ARG
48	B	101	ARG
49	C	59	ASP
49	C	62	LYS
49	C	108	ASP
49	C	111	ARG
49	C	128	LYS
49	C	152	ARG
49	C	177	GLN
49	C	218	LEU
49	C	223	PHE
50	D	85	PRO
50	D	91	ARG
50	D	207	LEU
50	D	224	PHE
50	D	240	LEU
51	E	45	LYS
51	E	69	LEU
51	E	76	ARG
51	E	104	SER
51	E	124	ARG
51	E	134	CYS
52	F	22	LYS
52	F	54	TYR
52	F	77	ARG
52	F	116	ASP
52	F	148	ARG
52	F	182	TYR
52	F	206	ASP
52	F	213	SER
52	F	247	SER
53	G	48	PHE
53	G	66	GLN

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Mol	Chain	Res	Type
53	G	87	CYS
53	G	98	MET
53	G	156	ARG
53	G	161	ASP
53	G	219	ARG
54	H	7	TYR
54	H	29	ASP
54	H	31	ARG
54	H	45	PHE
54	H	51	LYS
54	H	98	ARG
54	H	183	ARG
54	H	196	ARG
55	I	13	PRO
55	I	18	LEU
55	I	39	ARG
55	I	58	LEU
55	I	67	LEU
55	I	83	LYS
55	I	84	LYS
55	I	87	ASP
55	I	96	ARG
55	I	101	LYS
55	I	104	ARG
55	I	126	LEU
55	I	163	ASP
56	J	7	SER
56	J	22	ARG
56	J	23	LYS
56	J	137	LYS
56	J	140	GLU
56	J	187	GLU
57	K	3	ARG
57	K	8	TYR
57	K	22	SER
57	K	23	ARG
57	K	78	ARG
57	K	89	ASP
57	K	132	ARG
57	K	149	ARG
57	K	157	ASP
57	K	164	PHE

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Mol	Chain	Res	Type
58	L	76	LEU
58	L	81	ASN
59	M	67	ARG
59	M	87	ARG
59	M	90	TYR
59	M	104	HIS
59	M	129	ARG
60	N	28	LEU
60	N	29	LYS
60	N	33	ARG
60	N	96	GLN
60	N	124	LYS
60	N	126	TRP
61	O	42	ARG
61	O	70	LYS
61	O	139	TRP
61	O	141	TYR
62	P	20	TYR
62	P	52	ARG
62	P	92	LYS
62	P	103	ARG
62	P	129	LYS
63	Q	13	LYS
63	Q	44	ARG
63	Q	127	ARG
64	R	12	LYS
64	R	13	LYS
64	R	14	LYS
64	R	58	ASP
64	R	82	ARG
64	R	102	LYS
64	R	114	ARG
65	S	7	LYS
65	S	11	ARG
65	S	21	TYR
65	S	47	ARG
65	S	78	ARG
66	T	17	LEU
66	T	57	ARG
66	T	103	ASN
66	T	132	ARG
66	T	144	ARG

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Mol	Chain	Res	Type
67	U	8	ASP
67	U	14	PHE
67	U	18	TYR
67	U	33	TYR
67	U	38	LYS
67	U	75	LYS
67	U	84	LYS
67	U	122	ARG
67	U	142	GLU
68	V	23	ARG
68	V	32	LYS
68	V	36	ASN
68	V	85	ARG
69	W	50	TYR
69	W	78	LEU
70	X	19	LYS
70	X	37	PHE
70	X	57	ARG
70	X	93	LEU
71	Y	5	LYS
71	Y	100	ASP
71	Y	107	PHE
71	Y	121	ARG
71	Y	137	LYS
72	Z	49	LYS
72	Z	83	LYS
72	Z	123	LYS
72	Z	124	ARG
72	Z	131	ARG
72	Z	132	ARG
73	a	85	LYS
74	b	3	LYS
74	b	74	CYS
74	b	82	ARG
75	c	79	PHE
76	d	57	MET
77	e	8	PHE
79	g	116	LYS
79	g	137	ASP
79	g	140	TYR
80	h	14	GLU
80	h	50	ASP

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Mol	Chain	Res	Type
80	h	54	PHE
80	h	155	ARG
80	h	191	ASP
80	h	229	LYS
80	Rb	38	ARG
80	Rb	50	ASP
80	Rb	54	PHE
80	Rb	102	ARG
80	Rb	149	ASP
80	Rb	191	ASP
80	Rb	232	TYR
80	Rb	272	ASP
80	Rb	275	ARG
80	Rb	295	SER
48	s0	13	ASP
48	s0	46	HIS
48	s0	116	LYS
48	s0	119	ARG
48	s0	185	ARG
48	s0	200	ASP
49	s1	27	LYS
49	s1	81	PHE
49	s1	95	ASN
49	s1	128	LYS
49	s1	170	GLU
49	s1	205	PHE
49	s1	223	PHE
50	s2	116	LYS
51	s3	7	LYS
51	s3	27	ARG
51	s3	45	LYS
51	s3	68	GLU
51	s3	76	ARG
51	s3	143	ARG
51	s3	151	LYS
51	s3	166	ASP
51	s3	178	ARG
51	s3	196	ARG
52	s4	182	TYR
52	s4	187	ARG
52	s4	259	GLN
53	s5	25	LEU

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Mol	Chain	Res	Type
53	s5	63	GLN
53	s5	76	ARG
53	s5	80	LYS
53	s5	83	ARG
53	s5	102	ARG
53	s5	126	ASP
53	s5	185	ARG
53	s5	196	GLU
53	s5	219	ARG
54	s6	2	LYS
54	s6	177	ARG
54	s6	193	LEU
54	s6	207	GLU
55	s7	5	GLN
55	s7	39	ARG
55	s7	55	LYS
55	s7	84	LYS
55	s7	85	PHE
55	s7	139	ARG
55	s7	174	ASN
56	s8	49	ARG
56	s8	141	ARG
57	s9	78	ARG
57	s9	103	ASP
57	s9	149	ARG
57	s9	171	ARG
58	c0	17	GLN
58	c0	27	PHE
58	c0	28	ASN
59	c1	26	LYS
59	c1	67	ARG
59	c1	143	SER
60	c2	43	ARG
60	c2	50	LYS
60	c2	54	ARG
60	c2	124	LYS
60	c2	137	MET
60	c2	139	HIS
60	c2	140	PHE
61	c3	127	ARG
61	c3	139	TRP
62	c4	20	TYR

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Mol	Chain	Res	Type
62	c4	41	ARG
62	c4	124	ASP
63	c5	24	LYS
63	c5	29	SER
63	c5	43	ARG
64	c6	54	LEU
64	c6	66	ARG
64	c6	100	GLN
64	c6	102	LYS
64	c6	128	LYS
81	c7	63	LYS
81	c7	108	ASP
66	c8	85	PHE
66	c8	118	LYS
66	c8	145	ARG
67	c9	8	ASP
67	c9	18	TYR
67	c9	56	LYS
67	c9	57	ARG
67	c9	63	ARG
67	c9	69	LYS
68	d0	57	ARG
68	d0	89	ARG
69	d1	17	CYS
69	d1	22	ARG
69	d1	44	ARG
69	d1	60	ARG
69	d1	68	SER
70	d2	71	LYS
70	d2	85	ASP
70	d2	98	GLN
71	d3	70	LYS
71	d3	90	ASP
72	d4	61	ARG
72	d4	104	SER
73	d5	46	LYS
73	d5	52	LYS
73	d5	68	ARG
74	d6	8	ASN
74	d6	23	CYS
74	d6	62	TYR
74	d6	89	ARG

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Mol	Chain	Res	Type
75	d7	41	LEU
75	d7	42	ASN
75	d7	64	CYS
75	d7	81	ARG
76	d8	38	ARG
76	d8	57	MET
76	d8	67	ARG
77	d9	8	PHE
77	d9	20	GLN
78	e0	43	ARG
79	e1	137	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
4	j	132	ASN
7	m	111	GLN
11	q	49	ASN
12	r	100	ASN
13	s	95	ASN
16	v	138	GLN
21	0	142	GLN
22	2	26	HIS
24	6	81	GLN
33	AF	71	HIS
12	CL	59	GLN
16	CP	23	GLN
16	CP	158	HIS
18	CR	137	ASN
30	DD	48	HIS
45	sM	71	ASN
48	B	140	ASN
49	C	211	HIS
52	F	67	GLN
53	G	44	ASN
53	G	66	GLN
53	G	104	ASN
55	I	150	GLN
56	J	94	ASN
56	J	159	GLN
64	R	8	GLN
68	V	17	GLN

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Mol	Chain	Res	Type
70	X	15	ASN
70	X	24	GLN
70	X	56	HIS
71	Y	79	ASN
72	Z	63	GLN
80	Rb	31	ASN
50	s2	152	HIS
53	s5	158	GLN
55	s7	71	HIS
58	c0	39	ASN
58	c0	62	GLN
59	c1	110	HIS
59	c1	138	ASN
66	c8	104	ASN
69	d1	29	HIS
69	d1	33	GLN
79	e1	123	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3396 (92%)	622 (19%)	49 (1%)
1	AR	3143/3396 (92%)	636 (20%)	46 (1%)
2	3	120/121 (99%)	15 (12%)	1 (0%)
2	AS	120/121 (99%)	20 (16%)	1 (0%)
3	4	157/158 (99%)	34 (21%)	2 (1%)
3	AT	157/158 (99%)	31 (19%)	1 (0%)
47	A	1778/1800 (98%)	489 (27%)	42 (2%)
47	sR	1780/1800 (98%)	452 (25%)	0
All	All	10400/10950 (94%)	2299 (22%)	142 (1%)

All (2299) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	16	A
1	1	26	A
1	1	40	A
1	1	48	A
1	1	49	A
1	1	59	G
1	1	60	A

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Mol	Chain	Res	Type
1	1	65	A
1	1	66	A
1	1	73	C
1	1	74	G
1	1	76	G
1	1	85	A
1	1	92	G
1	1	99	A
1	1	102	C
1	1	109	A
1	1	110	G
1	1	113	C
1	1	116	A
1	1	117	U
1	1	121	A
1	1	122	A
1	1	133	U
1	1	135	C
1	1	136	G
1	1	147	U
1	1	148	G
1	1	156	G
1	1	157	A
1	1	161	G
1	1	165	A
1	1	166	C
1	1	170	G
1	1	187	A
1	1	190	U
1	1	191	U
1	1	210	U
1	1	211	A
1	1	213	A
1	1	218	G
1	1	219	A
1	1	220	G
1	1	237	G
1	1	240	U
1	1	241	G
1	1	243	G
1	1	245	U
1	1	246	U

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Mol	Chain	Res	Type
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	256	G
1	1	269	G
1	1	282	G
1	1	283	G
1	1	286	U
1	1	295	A
1	1	298	U
1	1	299	G
1	1	305	U
1	1	315	C
1	1	323	A
1	1	329	U
1	1	339	C
1	1	349	A
1	1	350	C
1	1	368	G
1	1	374	A
1	1	376	G
1	1	390	G
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	404	G
1	1	414	U
1	1	421	G
1	1	422	A
1	1	438	A
1	1	440	A
1	1	520	U
1	1	521	A
1	1	535	G
1	1	544	C
1	1	546	C
1	1	547	G
1	1	548	G
1	1	549	U

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Mol	Chain	Res	Type
1	1	551	A
1	1	552	G
1	1	553	U
1	1	555	U
1	1	557	A
1	1	558	U
1	1	559	A
1	1	578	A
1	1	579	G
1	1	591	G
1	1	592	A
1	1	601	U
1	1	604	G
1	1	609	G
1	1	611	A
1	1	620	U
1	1	621	A
1	1	636	C
1	1	637	C
1	1	638	C
1	1	647	A
1	1	649	A
1	1	660	A
1	1	662	U
1	1	668	G
1	1	677	A
1	1	681	U
1	1	705	A
1	1	712	G
1	1	715	A
1	1	716	A
1	1	719	U
1	1	763	G
1	1	764	U
1	1	766	U
1	1	767	U
1	1	771	A
1	1	776	U
1	1	777	U
1	1	780	A
1	1	781	G
1	1	785	G

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Mol	Chain	Res	Type
1	1	787	G
1	1	806	A
1	1	816	A
1	1	817	A
1	1	818	C
1	1	830	A
1	1	837	A
1	1	843	A
1	1	861	C
1	1	874	U
1	1	879	U
1	1	890	C
1	1	896	A
1	1	907	G
1	1	908	G
1	1	914	A
1	1	916	G
1	1	917	A
1	1	921	A
1	1	923	C
1	1	924	G
1	1	937	G
1	1	944	C
1	1	953	G
1	1	959	C
1	1	960	U
1	1	974	G
1	1	979	U
1	1	980	A
1	1	981	U
1	1	982	C
1	1	994	G
1	1	1000	C
1	1	1001	G
1	1	1002	A
1	1	1004	U
1	1	1006	A
1	1	1010	G
1	1	1014	U
1	1	1015	U
1	1	1017	C
1	1	1018	G

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Mol	Chain	Res	Type
1	1	1020	G
1	1	1021	G
1	1	1024	G
1	1	1025	A
1	1	1032	C
1	1	1036	A
1	1	1037	C
1	1	1041	U
1	1	1047	A
1	1	1049	C
1	1	1063	G
1	1	1064	A
1	1	1066	G
1	1	1071	U
1	1	1072	G
1	1	1081	U
1	1	1082	U
1	1	1093	A
1	1	1094	U
1	1	1095	U
1	1	1097	G
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1117	G
1	1	1131	G
1	1	1153	A
1	1	1159	A
1	1	1177	G
1	1	1178	G
1	1	1179	A
1	1	1180	A
1	1	1181	U
1	1	1182	A
1	1	1186	G
1	1	1191	U
1	1	1192	C
1	1	1201	C
1	1	1209	G
1	1	1217	A
1	1	1221	A
1	1	1222	G

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Mol	Chain	Res	Type
1	1	1226	G
1	1	1227	C
1	1	1232	C
1	1	1236	G
1	1	1237	G
1	1	1241	U
1	1	1243	G
1	1	1244	A
1	1	1245	A
1	1	1246	G
1	1	1248	C
1	1	1249	G
1	1	1253	U
1	1	1254	C
1	1	1258	U
1	1	1262	G
1	1	1263	A
1	1	1264	G
1	1	1265	U
1	1	1267	U
1	1	1269	U
1	1	1270	A
1	1	1271	A
1	1	1272	C
1	1	1273	A
1	1	1274	A
1	1	1278	A
1	1	1279	C
1	1	1285	G
1	1	1286	A
1	1	1287	A
1	1	1292	C
1	1	1303	A
1	1	1307	G
1	1	1308	A
1	1	1309	U
1	1	1313	G
1	1	1318	A
1	1	1330	A
1	1	1348	U
1	1	1349	G
1	1	1350	A

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Mol	Chain	Res	Type
1	1	1352	A
1	1	1353	U
1	1	1354	G
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1386	A
1	1	1392	G
1	1	1398	U
1	1	1399	A
1	1	1400	G
1	1	1417	G
1	1	1419	A
1	1	1434	G
1	1	1435	A
1	1	1437	C
1	1	1446	A
1	1	1450	G
1	1	1477	A
1	1	1481	A
1	1	1482	A
1	1	1485	G
1	1	1488	G
1	1	1495	U
1	1	1496	C
1	1	1508	C
1	1	1519	G
1	1	1521	G
1	1	1522	U
1	1	1527	C
1	1	1535	A
1	1	1536	G
1	1	1539	A
1	1	1555	U
1	1	1556	C
1	1	1560	G
1	1	1562	C
1	1	1563	C
1	1	1564	U
1	1	1567	U
1	1	1568	U
1	1	1569	U

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Mol	Chain	Res	Type
1	1	1570	U
1	1	1572	U
1	1	1575	A
1	1	1576	G
1	1	1578	C
1	1	1579	C
1	1	1580	A
1	1	1581	C
1	1	1582	C
1	1	1583	A
1	1	1587	A
1	1	1589	A
1	1	1596	C
1	1	1613	A
1	1	1620	U
1	1	1629	U
1	1	1630	U
1	1	1633	C
1	1	1639	C
1	1	1643	A
1	1	1657	C
1	1	1683	A
1	1	1713	G
1	1	1714	A
1	1	1715	A
1	1	1716	U
1	1	1717	U
1	1	1724	U
1	1	1725	C
1	1	1729	A
1	1	1736	G
1	1	1742	U
1	1	1745	C
1	1	1750	A
1	1	1751	G
1	1	1760	A
1	1	1761	C
1	1	1762	C
1	1	1763	U
1	1	1764	U
1	1	1765	U
1	1	1766	G

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Mol	Chain	Res	Type
1	1	1767	C
1	1	1769	G
1	1	1770	G
1	1	1775	G
1	1	1779	C
1	1	1780	G
1	1	1797	A
1	1	1809	A
1	1	1810	A
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1819	U
1	1	1820	U
1	1	1821	U
1	1	1828	A
1	1	1839	A
1	1	1842	A
1	1	1845	G
1	1	1846	C
1	1	1847	A
1	1	1850	A
1	1	1858	A
1	1	1866	C
1	1	1878	G
1	1	1879	A
1	1	1880	U
1	1	1906	G
1	1	1921	A
1	1	1935	G
1	1	1948	G
1	1	1951	C
1	1	1953	G
1	1	1954	G
1	1	2094	C
1	1	2097	U
1	1	2101	C
1	1	2102	U
1	1	2111	G
1	1	2113	A
1	1	2115	G
1	1	2120	A

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Mol	Chain	Res	Type
1	1	2121	G
1	1	2122	G
1	1	2126	A
1	1	2131	A
1	1	2140	U
1	1	2149	A
1	1	2158	A
1	1	2169	G
1	1	2188	A
1	1	2193	U
1	1	2205	U
1	1	2208	A
1	1	2210	G
1	1	2223	A
1	1	2228	A
1	1	2229	A
1	1	2249	G
1	1	2250	G
1	1	2255	A
1	1	2256	A
1	1	2272	G
1	1	2273	G
1	1	2281	A
1	1	2282	U
1	1	2307	G
1	1	2310	U
1	1	2313	A
1	1	2314	U
1	1	2315	G
1	1	2330	C
1	1	2334	U
1	1	2336	U
1	1	2348	A
1	1	2361	A
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2375	G
1	1	2382	G
1	1	2383	C
1	1	2385	G
1	1	2386	A

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Mol	Chain	Res	Type
1	1	2393	G
1	1	2397	A
1	1	2402	A
1	1	2403	G
1	1	2404	A
1	1	2411	U
1	1	2418	G
1	1	2419	A
1	1	2435	G
1	1	2441	A
1	1	2443	A
1	1	2444	C
1	1	2445	A
1	1	2502	A
1	1	2503	G
1	1	2507	C
1	1	2514	U
1	1	2515	A
1	1	2522	G
1	1	2523	A
1	1	2532	U
1	1	2533	G
1	1	2534	G
1	1	2537	U
1	1	2538	U
1	1	2539	C
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2544	U
1	1	2549	G
1	1	2552	C
1	1	2555	G
1	1	2561	A
1	1	2569	A
1	1	2570	U
1	1	2571	U
1	1	2572	C
1	1	2573	G
1	1	2585	G
1	1	2593	A

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Mol	Chain	Res	Type
1	1	2594	C
1	1	2606	G
1	1	2607	G
1	1	2614	G
1	1	2637	A
1	1	2647	A
1	1	2652	U
1	1	2656	A
1	1	2657	A
1	1	2674	A
1	1	2677	G
1	1	2689	A
1	1	2691	A
1	1	2694	A
1	1	2696	A
1	1	2706	G
1	1	2714	G
1	1	2719	U
1	1	2728	G
1	1	2729	U
1	1	2737	C
1	1	2740	A
1	1	2752	U
1	1	2753	G
1	1	2755	C
1	1	2766	U
1	1	2772	C
1	1	2777	G
1	1	2778	G
1	1	2787	G
1	1	2796	G
1	1	2799	A
1	1	2800	G
1	1	2801	A
1	1	2802	A
1	1	2808	A
1	1	2810	C
1	1	2814	G
1	1	2815	G
1	1	2816	G
1	1	2817	A
1	1	2818	U

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Mol	Chain	Res	Type
1	1	2829	U
1	1	2842	U
1	1	2845	A
1	1	2853	A
1	1	2860	U
1	1	2867	C
1	1	2871	G
1	1	2875	U
1	1	2876	C
1	1	2887	A
1	1	2898	G
1	1	2899	C
1	1	2923	U
1	1	2928	C
1	1	2935	U
1	1	2936	A
1	1	2938	G
1	1	2942	C
1	1	2947	G
1	1	2951	G
1	1	2954	U
1	1	2968	G
1	1	2971	A
1	1	2972	G
1	1	2979	U
1	1	2983	C
1	1	2990	G
1	1	2997	G
1	1	3012	A
1	1	3030	G
1	1	3056	U
1	1	3059	G
1	1	3078	U
1	1	3079	U
1	1	3080	G
1	1	3086	A
1	1	3092	C
1	1	3122	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C

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Mol	Chain	Res	Type
1	1	3151	U
1	1	3153	U
1	1	3154	C
1	1	3155	U
1	1	3156	U
1	1	3157	U
1	1	3164	C
1	1	3165	A
1	1	3170	A
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3181	C
1	1	3187	A
1	1	3195	U
1	1	3196	U
1	1	3197	G
1	1	3207	U
1	1	3209	A
1	1	3210	A
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3228	C
1	1	3229	G
1	1	3233	C
1	1	3244	A
1	1	3245	A
1	1	3246	G
1	1	3247	G
1	1	3259	U
1	1	3269	U
1	1	3270	U
1	1	3273	A
1	1	3276	G
1	1	3281	U
1	1	3286	G
1	1	3287	U
1	1	3289	G
1	1	3294	A
1	1	3295	A

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Mol	Chain	Res	Type
1	1	3303	G
1	1	3304	U
1	1	3309	G
1	1	3313	U
1	1	3316	A
1	1	3318	G
1	1	3319	U
1	1	3320	A
1	1	3341	U
1	1	3342	A
1	1	3345	G
1	1	3347	A
1	1	3351	U
1	1	3352	U
1	1	3354	U
1	1	3355	U
1	1	3356	G
1	1	3360	C
1	1	3368	U
1	1	3369	G
1	1	3375	A
1	1	3378	C
1	1	3382	U
1	1	3383	G
1	1	3389	U
1	1	3390	G
1	1	3396	U
2	3	7	G
2	3	11	A
2	3	22	A
2	3	41	G
2	3	53	U
2	3	54	U
2	3	55	A
2	3	65	G
2	3	74	C
2	3	76	A
2	3	91	G
2	3	93	C
2	3	102	A
2	3	112	G
2	3	121	U

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Mol	Chain	Res	Type
3	4	23	U
3	4	26	U
3	4	34	U
3	4	35	C
3	4	39	G
3	4	48	A
3	4	52	A
3	4	59	A
3	4	62	C
3	4	63	G
3	4	75	G
3	4	80	A
3	4	81	U
3	4	82	U
3	4	84	C
3	4	85	G
3	4	86	U
3	4	87	G
3	4	90	U
3	4	95	G
3	4	102	U
3	4	104	A
3	4	105	A
3	4	106	C
3	4	111	A
3	4	113	U
3	4	125	U
3	4	126	A
3	4	128	U
3	4	138	A
3	4	148	G
3	4	152	G
3	4	155	A
3	4	158	U
1	AR	16	A
1	AR	26	A
1	AR	40	A
1	AR	43	A
1	AR	49	A
1	AR	57	A
1	AR	59	G
1	AR	60	A

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Mol	Chain	Res	Type
1	AR	65	A
1	AR	66	A
1	AR	73	C
1	AR	74	G
1	AR	92	G
1	AR	99	A
1	AR	109	A
1	AR	110	G
1	AR	111	C
1	AR	116	A
1	AR	120	G
1	AR	121	A
1	AR	122	A
1	AR	133	U
1	AR	135	C
1	AR	136	G
1	AR	156	G
1	AR	157	A
1	AR	165	A
1	AR	166	C
1	AR	171	G
1	AR	172	G
1	AR	173	G
1	AR	176	G
1	AR	179	C
1	AR	182	U
1	AR	187	A
1	AR	190	U
1	AR	191	U
1	AR	200	C
1	AR	210	U
1	AR	218	G
1	AR	219	A
1	AR	231	G
1	AR	234	G
1	AR	240	U
1	AR	241	G
1	AR	243	G
1	AR	245	U
1	AR	247	C
1	AR	248	U
1	AR	249	U

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Mol	Chain	Res	Type
1	AR	250	U
1	AR	251	G
1	AR	252	U
1	AR	253	A
1	AR	269	G
1	AR	286	U
1	AR	295	A
1	AR	298	U
1	AR	299	G
1	AR	305	U
1	AR	316	U
1	AR	321	C
1	AR	323	A
1	AR	329	U
1	AR	343	U
1	AR	349	A
1	AR	350	C
1	AR	375	A
1	AR	376	G
1	AR	380	U
1	AR	395	A
1	AR	398	A
1	AR	399	A
1	AR	401	U
1	AR	402	A
1	AR	403	C
1	AR	404	G
1	AR	421	G
1	AR	422	A
1	AR	436	A
1	AR	438	A
1	AR	520	U
1	AR	521	A
1	AR	543	C
1	AR	544	C
1	AR	546	C
1	AR	550	A
1	AR	551	A
1	AR	552	G
1	AR	555	U
1	AR	557	A
1	AR	559	A

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Mol	Chain	Res	Type
1	AR	578	A
1	AR	579	G
1	AR	588	G
1	AR	589	A
1	AR	592	A
1	AR	600	G
1	AR	604	G
1	AR	609	G
1	AR	611	A
1	AR	619	A
1	AR	620	U
1	AR	621	A
1	AR	622	A
1	AR	624	G
1	AR	636	C
1	AR	649	A
1	AR	660	A
1	AR	668	G
1	AR	677	A
1	AR	681	U
1	AR	683	U
1	AR	691	A
1	AR	705	A
1	AR	712	G
1	AR	715	A
1	AR	716	A
1	AR	737	G
1	AR	758	C
1	AR	763	G
1	AR	764	U
1	AR	765	C
1	AR	766	U
1	AR	767	U
1	AR	776	U
1	AR	777	U
1	AR	780	A
1	AR	781	G
1	AR	783	A
1	AR	784	A
1	AR	785	G
1	AR	786	A
1	AR	806	A

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Mol	Chain	Res	Type
1	AR	813	G
1	AR	816	A
1	AR	817	A
1	AR	826	G
1	AR	830	A
1	AR	849	C
1	AR	861	C
1	AR	874	U
1	AR	875	G
1	AR	876	A
1	AR	879	U
1	AR	896	A
1	AR	907	G
1	AR	908	G
1	AR	913	A
1	AR	914	A
1	AR	916	G
1	AR	917	A
1	AR	921	A
1	AR	923	C
1	AR	924	G
1	AR	931	C
1	AR	932	U
1	AR	937	G
1	AR	944	C
1	AR	959	C
1	AR	960	U
1	AR	961	C
1	AR	974	G
1	AR	979	U
1	AR	980	A
1	AR	981	U
1	AR	982	C
1	AR	994	G
1	AR	1001	G
1	AR	1002	A
1	AR	1010	G
1	AR	1015	U
1	AR	1017	C
1	AR	1018	G
1	AR	1019	G
1	AR	1020	G

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Mol	Chain	Res	Type
1	AR	1021	G
1	AR	1024	G
1	AR	1025	A
1	AR	1026	A
1	AR	1029	G
1	AR	1032	C
1	AR	1037	C
1	AR	1047	A
1	AR	1049	C
1	AR	1056	U
1	AR	1064	A
1	AR	1065	A
1	AR	1072	G
1	AR	1081	U
1	AR	1082	U
1	AR	1083	G
1	AR	1093	A
1	AR	1094	U
1	AR	1095	U
1	AR	1096	U
1	AR	1097	G
1	AR	1098	A
1	AR	1103	A
1	AR	1104	G
1	AR	1117	G
1	AR	1131	G
1	AR	1140	G
1	AR	1143	A
1	AR	1144	U
1	AR	1150	A
1	AR	1153	A
1	AR	1159	A
1	AR	1160	C
1	AR	1177	G
1	AR	1178	G
1	AR	1180	A
1	AR	1181	U
1	AR	1186	G
1	AR	1191	U
1	AR	1192	C
1	AR	1201	C
1	AR	1202	A

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Mol	Chain	Res	Type
1	AR	1209	G
1	AR	1221	A
1	AR	1222	G
1	AR	1235	U
1	AR	1236	G
1	AR	1237	G
1	AR	1239	C
1	AR	1241	U
1	AR	1242	G
1	AR	1244	A
1	AR	1245	A
1	AR	1246	G
1	AR	1248	C
1	AR	1258	U
1	AR	1262	G
1	AR	1263	A
1	AR	1265	U
1	AR	1266	G
1	AR	1285	G
1	AR	1292	C
1	AR	1307	G
1	AR	1309	U
1	AR	1313	G
1	AR	1330	A
1	AR	1331	U
1	AR	1345	G
1	AR	1348	U
1	AR	1349	G
1	AR	1350	A
1	AR	1351	U
1	AR	1352	A
1	AR	1353	U
1	AR	1355	A
1	AR	1356	U
1	AR	1357	G
1	AR	1385	C
1	AR	1386	A
1	AR	1387	G
1	AR	1391	C
1	AR	1392	G
1	AR	1399	A
1	AR	1400	G

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Mol	Chain	Res	Type
1	AR	1408	G
1	AR	1418	A
1	AR	1419	A
1	AR	1434	G
1	AR	1435	A
1	AR	1437	C
1	AR	1446	A
1	AR	1450	G
1	AR	1481	A
1	AR	1482	A
1	AR	1484	U
1	AR	1490	A
1	AR	1496	C
1	AR	1505	C
1	AR	1508	C
1	AR	1528	G
1	AR	1536	G
1	AR	1539	A
1	AR	1555	U
1	AR	1556	C
1	AR	1560	G
1	AR	1562	C
1	AR	1563	C
1	AR	1565	G
1	AR	1567	U
1	AR	1568	U
1	AR	1569	U
1	AR	1570	U
1	AR	1572	U
1	AR	1575	A
1	AR	1576	G
1	AR	1577	G
1	AR	1580	A
1	AR	1581	C
1	AR	1582	C
1	AR	1583	A
1	AR	1589	A
1	AR	1593	A
1	AR	1605	A
1	AR	1620	U
1	AR	1629	U
1	AR	1630	U

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Mol	Chain	Res	Type
1	AR	1632	A
1	AR	1639	C
1	AR	1641	U
1	AR	1643	A
1	AR	1645	U
1	AR	1683	A
1	AR	1687	U
1	AR	1694	U
1	AR	1705	U
1	AR	1716	U
1	AR	1717	U
1	AR	1724	U
1	AR	1725	C
1	AR	1741	A
1	AR	1742	U
1	AR	1750	A
1	AR	1751	G
1	AR	1760	A
1	AR	1761	C
1	AR	1762	C
1	AR	1765	U
1	AR	1766	G
1	AR	1767	C
1	AR	1769	G
1	AR	1770	G
1	AR	1775	G
1	AR	1778	G
1	AR	1780	G
1	AR	1793	C
1	AR	1797	A
1	AR	1810	A
1	AR	1814	A
1	AR	1815	U
1	AR	1816	A
1	AR	1817	G
1	AR	1819	U
1	AR	1820	U
1	AR	1821	U
1	AR	1839	A
1	AR	1842	A
1	AR	1849	C
1	AR	1878	G

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Mol	Chain	Res	Type
1	AR	1880	U
1	AR	1894	U
1	AR	1901	A
1	AR	1906	G
1	AR	1918	C
1	AR	1948	G
1	AR	1953	G
1	AR	1954	G
1	AR	2094	C
1	AR	2101	C
1	AR	2102	U
1	AR	2112	U
1	AR	2113	A
1	AR	2114	C
1	AR	2121	G
1	AR	2122	G
1	AR	2126	A
1	AR	2131	A
1	AR	2149	A
1	AR	2158	A
1	AR	2169	G
1	AR	2177	G
1	AR	2184	U
1	AR	2187	G
1	AR	2188	A
1	AR	2192	C
1	AR	2198	A
1	AR	2205	U
1	AR	2209	U
1	AR	2210	G
1	AR	2223	A
1	AR	2225	U
1	AR	2244	A
1	AR	2252	A
1	AR	2253	G
1	AR	2254	U
1	AR	2255	A
1	AR	2256	A
1	AR	2264	U
1	AR	2269	U
1	AR	2270	A
1	AR	2273	G

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Mol	Chain	Res	Type
1	AR	2276	G
1	AR	2280	A
1	AR	2281	A
1	AR	2282	U
1	AR	2283	G
1	AR	2287	C
1	AR	2288	G
1	AR	2307	G
1	AR	2308	C
1	AR	2309	A
1	AR	2310	U
1	AR	2313	A
1	AR	2314	U
1	AR	2315	G
1	AR	2334	U
1	AR	2335	G
1	AR	2336	U
1	AR	2372	A
1	AR	2373	A
1	AR	2374	C
1	AR	2375	G
1	AR	2385	G
1	AR	2393	G
1	AR	2397	A
1	AR	2401	A
1	AR	2402	A
1	AR	2403	G
1	AR	2404	A
1	AR	2410	U
1	AR	2411	U
1	AR	2418	G
1	AR	2425	G
1	AR	2435	G
1	AR	2438	A
1	AR	2443	A
1	AR	2444	C
1	AR	2445	A
1	AR	2502	A
1	AR	2503	G
1	AR	2504	U
1	AR	2505	U
1	AR	2507	C

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Mol	Chain	Res	Type
1	AR	2508	U
1	AR	2511	A
1	AR	2514	U
1	AR	2515	A
1	AR	2519	A
1	AR	2520	A
1	AR	2521	U
1	AR	2522	G
1	AR	2523	A
1	AR	2530	G
1	AR	2533	G
1	AR	2534	G
1	AR	2536	A
1	AR	2538	U
1	AR	2539	C
1	AR	2540	A
1	AR	2541	U
1	AR	2542	U
1	AR	2544	U
1	AR	2549	G
1	AR	2551	U
1	AR	2552	C
1	AR	2555	G
1	AR	2560	C
1	AR	2561	A
1	AR	2566	C
1	AR	2567	C
1	AR	2569	A
1	AR	2570	U
1	AR	2571	U
1	AR	2572	C
1	AR	2573	G
1	AR	2577	C
1	AR	2582	C
1	AR	2585	G
1	AR	2587	U
1	AR	2593	A
1	AR	2595	A
1	AR	2606	G
1	AR	2607	G
1	AR	2614	G
1	AR	2618	G

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Mol	Chain	Res	Type
1	AR	2637	A
1	AR	2652	U
1	AR	2656	A
1	AR	2674	A
1	AR	2677	G
1	AR	2689	A
1	AR	2691	A
1	AR	2694	A
1	AR	2696	A
1	AR	2705	A
1	AR	2714	G
1	AR	2727	A
1	AR	2728	G
1	AR	2729	U
1	AR	2737	C
1	AR	2752	U
1	AR	2753	G
1	AR	2755	C
1	AR	2762	A
1	AR	2772	C
1	AR	2777	G
1	AR	2778	G
1	AR	2780	A
1	AR	2781	U
1	AR	2796	G
1	AR	2799	A
1	AR	2800	G
1	AR	2801	A
1	AR	2802	A
1	AR	2810	C
1	AR	2814	G
1	AR	2816	G
1	AR	2817	A
1	AR	2818	U
1	AR	2839	G
1	AR	2840	C
1	AR	2842	U
1	AR	2843	U
1	AR	2845	A
1	AR	2847	A
1	AR	2853	A
1	AR	2860	U

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Mol	Chain	Res	Type
1	AR	2863	G
1	AR	2867	C
1	AR	2871	G
1	AR	2872	A
1	AR	2873	U
1	AR	2875	U
1	AR	2876	C
1	AR	2886	U
1	AR	2887	A
1	AR	2899	C
1	AR	2923	U
1	AR	2935	U
1	AR	2936	A
1	AR	2942	C
1	AR	2943	G
1	AR	2947	G
1	AR	2968	G
1	AR	2971	A
1	AR	2983	C
1	AR	2990	G
1	AR	2996	U
1	AR	2997	G
1	AR	3012	A
1	AR	3013	U
1	AR	3030	G
1	AR	3056	U
1	AR	3057	U
1	AR	3059	G
1	AR	3074	G
1	AR	3078	U
1	AR	3079	U
1	AR	3086	A
1	AR	3092	C
1	AR	3122	A
1	AR	3123	A
1	AR	3130	A
1	AR	3131	U
1	AR	3142	A
1	AR	3143	C
1	AR	3149	G
1	AR	3151	U
1	AR	3153	U

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Mol	Chain	Res	Type
1	AR	3155	U
1	AR	3156	U
1	AR	3157	U
1	AR	3158	G
1	AR	3164	C
1	AR	3165	A
1	AR	3167	A
1	AR	3168	A
1	AR	3172	A
1	AR	3173	G
1	AR	3174	A
1	AR	3176	G
1	AR	3179	U
1	AR	3180	A
1	AR	3181	C
1	AR	3187	A
1	AR	3195	U
1	AR	3196	U
1	AR	3198	U
1	AR	3206	C
1	AR	3207	U
1	AR	3217	C
1	AR	3218	A
1	AR	3219	G
1	AR	3223	A
1	AR	3224	G
1	AR	3228	C
1	AR	3229	G
1	AR	3235	C
1	AR	3244	A
1	AR	3245	A
1	AR	3246	G
1	AR	3247	G
1	AR	3253	G
1	AR	3259	U
1	AR	3265	C
1	AR	3266	G
1	AR	3269	U
1	AR	3270	U
1	AR	3273	A
1	AR	3274	A
1	AR	3275	U

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Mol	Chain	Res	Type
1	AR	3276	G
1	AR	3277	U
1	AR	3278	C
1	AR	3281	U
1	AR	3285	C
1	AR	3286	G
1	AR	3287	U
1	AR	3288	G
1	AR	3289	G
1	AR	3294	A
1	AR	3295	A
1	AR	3304	U
1	AR	3313	U
1	AR	3316	A
1	AR	3317	U
1	AR	3318	G
1	AR	3319	U
1	AR	3320	A
1	AR	3341	U
1	AR	3342	A
1	AR	3344	A
1	AR	3345	G
1	AR	3346	U
1	AR	3347	A
1	AR	3351	U
1	AR	3352	U
1	AR	3353	G
1	AR	3354	U
1	AR	3355	U
1	AR	3356	G
1	AR	3359	A
1	AR	3361	G
1	AR	3369	G
1	AR	3375	A
1	AR	3378	C
1	AR	3382	U
1	AR	3383	G
1	AR	3389	U
1	AR	3390	G
1	AR	3396	U
2	AS	7	G
2	AS	17	A

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Mol	Chain	Res	Type
2	AS	22	A
2	AS	23	A
2	AS	33	U
2	AS	38	U
2	AS	41	G
2	AS	52	G
2	AS	53	U
2	AS	54	U
2	AS	60	G
2	AS	65	G
2	AS	73	C
2	AS	74	C
2	AS	76	A
2	AS	99	G
2	AS	101	G
2	AS	102	A
2	AS	112	G
2	AS	121	U
3	AT	2	A
3	AT	21	C
3	AT	34	U
3	AT	35	C
3	AT	39	G
3	AT	48	A
3	AT	51	G
3	AT	59	A
3	AT	62	C
3	AT	63	G
3	AT	79	A
3	AT	80	A
3	AT	81	U
3	AT	82	U
3	AT	83	C
3	AT	84	C
3	AT	85	G
3	AT	86	U
3	AT	87	G
3	AT	90	U
3	AT	95	G
3	AT	97	A
3	AT	104	A
3	AT	106	C

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Mol	Chain	Res	Type
3	AT	111	A
3	AT	113	U
3	AT	114	G
3	AT	116	G
3	AT	125	U
3	AT	157	U
3	AT	158	U
47	A	2	A
47	A	4	C
47	A	8	U
47	A	17	C
47	A	25	C
47	A	26	A
47	A	27	U
47	A	34	G
47	A	39	A
47	A	42	G
47	A	47	A
47	A	57	G
47	A	60	U
47	A	67	A
47	A	68	A
47	A	69	G
47	A	72	A
47	A	73	U
47	A	74	U
47	A	77	U
47	A	81	G
47	A	97	C
47	A	104	A
47	A	114	C
47	A	115	G
47	A	127	G
47	A	128	U
47	A	130	C
47	A	131	C
47	A	132	U
47	A	133	U
47	A	134	U
47	A	135	A
47	A	136	C
47	A	137	U

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Mol	Chain	Res	Type
47	A	140	A
47	A	141	U
47	A	144	U
47	A	145	A
47	A	146	U
47	A	158	U
47	A	159	U
47	A	161	U
47	A	169	A
47	A	178	U
47	A	179	A
47	A	181	A
47	A	185	U
47	A	186	C
47	A	188	A
47	A	190	C
47	A	191	C
47	A	192	U
47	A	193	U
47	A	195	G
47	A	197	A
47	A	198	A
47	A	200	A
47	A	215	A
47	A	218	A
47	A	219	A
47	A	226	A
47	A	227	U
47	A	229	U
47	A	233	C
47	A	235	G
47	A	236	A
47	A	238	U
47	A	239	C
47	A	240	U
47	A	241	U
47	A	242	U
47	A	246	G
47	A	249	U
47	A	250	C
47	A	260	U
47	A	261	U

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Mol	Chain	Res	Type
47	A	265	A
47	A	266	A
47	A	271	A
47	A	272	U
47	A	274	G
47	A	275	C
47	A	276	C
47	A	277	U
47	A	278	U
47	A	279	G
47	A	280	U
47	A	281	G
47	A	284	G
47	A	288	A
47	A	290	G
47	A	292	U
47	A	299	A
47	A	302	U
47	A	308	C
47	A	314	C
47	A	316	A
47	A	319	U
47	A	321	C
47	A	322	G
47	A	333	A
47	A	337	G
47	A	338	C
47	A	350	U
47	A	352	A
47	A	359	A
47	A	360	A
47	A	361	C
47	A	378	A
47	A	380	U
47	A	381	C
47	A	390	G
47	A	397	A
47	A	400	A
47	A	401	A
47	A	402	C
47	A	403	G
47	A	404	G

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Mol	Chain	Res	Type
47	A	418	G
47	A	419	G
47	A	424	C
47	A	425	A
47	A	426	G
47	A	428	A
47	A	434	G
47	A	437	A
47	A	439	U
47	A	444	C
47	A	448	C
47	A	452	A
47	A	454	U
47	A	468	A
47	A	477	A
47	A	479	C
47	A	480	G
47	A	483	A
47	A	484	C
47	A	485	A
47	A	488	G
47	A	493	U
47	A	495	C
47	A	496	G
47	A	497	G
47	A	498	G
47	A	499	U
47	A	500	C
47	A	502	U
47	A	503	G
47	A	504	U
47	A	505	A
47	A	506	A
47	A	507	U
47	A	509	G
47	A	510	G
47	A	511	A
47	A	512	A
47	A	513	U
47	A	514	G
47	A	515	A
47	A	516	G

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Mol	Chain	Res	Type
47	A	522	U
47	A	527	A
47	A	532	U
47	A	536	C
47	A	537	G
47	A	538	A
47	A	539	G
47	A	540	G
47	A	541	A
47	A	542	A
47	A	543	C
47	A	544	A
47	A	545	A
47	A	548	G
47	A	555	A
47	A	556	A
47	A	557	G
47	A	558	U
47	A	559	C
47	A	563	U
47	A	565	C
47	A	568	G
47	A	579	A
47	A	580	A
47	A	581	U
47	A	585	A
47	A	594	A
47	A	595	G
47	A	606	A
47	A	608	U
47	A	611	U
47	A	619	A
47	A	620	A
47	A	622	A
47	A	623	A
47	A	624	G
47	A	639	U
47	A	640	U
47	A	650	U
47	A	654	C
47	A	655	G
47	A	656	G

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Mol	Chain	Res	Type
47	A	658	C
47	A	677	G
47	A	678	A
47	A	679	U
47	A	680	U
47	A	682	C
47	A	684	A
47	A	686	C
47	A	692	C
47	A	694	U
47	A	696	C
47	A	697	C
47	A	700	C
47	A	702	G
47	A	703	G
47	A	704	C
47	A	705	U
47	A	706	A
47	A	707	A
47	A	709	C
47	A	710	U
47	A	711	U
47	A	712	G
47	A	714	G
47	A	716	C
47	A	717	C
47	A	718	U
47	A	719	U
47	A	720	G
47	A	721	U
47	A	722	G
47	A	723	G
47	A	725	U
47	A	727	U
47	A	731	C
47	A	732	G
47	A	733	A
47	A	734	A
47	A	735	C
47	A	737	A
47	A	738	G
47	A	741	C

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Mol	Chain	Res	Type
47	A	742	U
47	A	743	U
47	A	745	U
47	A	752	A
47	A	754	A
47	A	755	A
47	A	756	A
47	A	765	G
47	A	766	U
47	A	774	A
47	A	775	G
47	A	777	C
47	A	778	G
47	A	781	U
47	A	782	U
47	A	783	G
47	A	784	C
47	A	787	G
47	A	789	A
47	A	793	A
47	A	794	U
47	A	807	A
47	A	812	A
47	A	814	A
47	A	815	G
47	A	816	G
47	A	818	C
47	A	819	G
47	A	820	U
47	A	821	U
47	A	823	G
47	A	824	G
47	A	830	U
47	A	831	U
47	A	832	U
47	A	833	U
47	A	834	G
47	A	841	U
47	A	846	G
47	A	856	A
47	A	863	A
47	A	864	U

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Mol	Chain	Res	Type
47	A	876	G
47	A	886	U
47	A	892	A
47	A	898	A
47	A	912	U
47	A	913	G
47	A	914	G
47	A	916	U
47	A	933	A
47	A	934	C
47	A	935	U
47	A	942	G
47	A	951	A
47	A	960	U
47	A	966	A
47	A	989	U
47	A	992	A
47	A	993	A
47	A	997	G
47	A	1002	G
47	A	1003	A
47	A	1004	U
47	A	1005	A
47	A	1026	A
47	A	1028	C
47	A	1029	U
47	A	1039	A
47	A	1040	G
47	A	1052	U
47	A	1053	G
47	A	1057	U
47	A	1058	U
47	A	1060	U
47	A	1062	A
47	A	1074	G
47	A	1080	U
47	A	1082	C
47	A	1086	A
47	A	1091	A
47	A	1092	A
47	A	1096	C
47	A	1097	U

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Mol	Chain	Res	Type
47	A	1098	U
47	A	1100	G
47	A	1111	G
47	A	1138	A
47	A	1140	G
47	A	1145	U
47	A	1146	G
47	A	1150	G
47	A	1151	A
47	A	1157	A
47	A	1158	C
47	A	1160	A
47	A	1163	A
47	A	1167	G
47	A	1168	U
47	A	1185	U
47	A	1191	U
47	A	1194	A
47	A	1196	A
47	A	1199	G
47	A	1200	G
47	A	1202	A
47	A	1203	A
47	A	1207	C
47	A	1217	A
47	A	1218	G
47	A	1227	A
47	A	1229	G
47	A	1241	G
47	A	1243	G
47	A	1244	A
47	A	1245	G
47	A	1246	C
47	A	1251	U
47	A	1256	A
47	A	1257	U
47	A	1284	C
47	A	1285	U
47	A	1286	U
47	A	1307	U
47	A	1314	U
47	A	1315	U

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Mol	Chain	Res	Type
47	A	1319	A
47	A	1321	A
47	A	1324	G
47	A	1329	A
47	A	1339	C
47	A	1340	U
47	A	1341	A
47	A	1344	A
47	A	1345	A
47	A	1346	A
47	A	1354	G
47	A	1358	G
47	A	1360	A
47	A	1362	U
47	A	1363	U
47	A	1364	G
47	A	1370	U
47	A	1371	A
47	A	1372	U
47	A	1386	G
47	A	1388	A
47	A	1390	U
47	A	1398	U
47	A	1399	C
47	A	1413	U
47	A	1414	U
47	A	1415	U
47	A	1418	G
47	A	1424	A
47	A	1427	A
47	A	1428	G
47	A	1432	U
47	A	1433	G
47	A	1446	A
47	A	1447	C
47	A	1459	C
47	A	1460	A
47	A	1461	C
47	A	1471	A
47	A	1473	U
47	A	1474	G
47	A	1475	A

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Mol	Chain	Res	Type
47	A	1482	C
47	A	1486	G
47	A	1487	A
47	A	1489	U
47	A	1490	C
47	A	1491	U
47	A	1492	A
47	A	1499	G
47	A	1506	G
47	A	1515	A
47	A	1516	A
47	A	1517	U
47	A	1521	G
47	A	1523	G
47	A	1524	A
47	A	1526	A
47	A	1533	C
47	A	1534	G
47	A	1535	U
47	A	1536	G
47	A	1537	C
47	A	1538	U
47	A	1542	G
47	A	1557	U
47	A	1559	A
47	A	1569	A
47	A	1572	G
47	A	1574	G
47	A	1576	A
47	A	1584	G
47	A	1600	A
47	A	1601	G
47	A	1614	A
47	A	1615	C
47	A	1616	G
47	A	1625	C
47	A	1631	A
47	A	1634	C
47	A	1657	U
47	A	1658	G
47	A	1663	G
47	A	1664	C

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Mol	Chain	Res	Type
47	A	1680	G
47	A	1681	A
47	A	1682	U
47	A	1683	C
47	A	1684	U
47	A	1689	A
47	A	1698	G
47	A	1699	G
47	A	1700	C
47	A	1702	A
47	A	1703	C
47	A	1707	A
47	A	1710	U
47	A	1711	C
47	A	1712	A
47	A	1713	G
47	A	1715	G
47	A	1731	A
47	A	1750	A
47	A	1755	A
47	A	1760	G
47	A	1762	A
47	A	1766	A
47	A	1767	G
47	A	1769	U
47	A	1772	C
47	A	1780	G
47	A	1782	A
47	A	1783	C
47	A	1792	G
47	A	1793	G
47	A	1794	A
47	A	1795	U
47	A	1796	C
47	sR	2	A
47	sR	17	C
47	sR	25	C
47	sR	26	A
47	sR	27	U
47	sR	34	G
47	sR	46	A
47	sR	47	A

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Mol	Chain	Res	Type
47	sR	50	C
47	sR	57	G
47	sR	60	U
47	sR	61	A
47	sR	63	G
47	sR	65	A
47	sR	68	A
47	sR	69	G
47	sR	72	A
47	sR	73	U
47	sR	75	U
47	sR	76	A
47	sR	77	U
47	sR	78	A
47	sR	80	A
47	sR	104	A
47	sR	114	C
47	sR	128	U
47	sR	132	U
47	sR	137	U
47	sR	138	A
47	sR	140	A
47	sR	141	U
47	sR	142	G
47	sR	143	G
47	sR	144	U
47	sR	145	A
47	sR	146	U
47	sR	153	G
47	sR	159	U
47	sR	161	U
47	sR	166	C
47	sR	177	U
47	sR	178	U
47	sR	185	U
47	sR	188	A
47	sR	191	C
47	sR	192	U
47	sR	193	U
47	sR	194	U
47	sR	195	G
47	sR	196	G

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Mol	Chain	Res	Type
47	sR	197	A
47	sR	199	G
47	sR	200	A
47	sR	216	U
47	sR	218	A
47	sR	219	A
47	sR	220	A
47	sR	221	A
47	sR	224	C
47	sR	227	U
47	sR	228	G
47	sR	230	C
47	sR	232	U
47	sR	233	C
47	sR	235	G
47	sR	238	U
47	sR	240	U
47	sR	241	U
47	sR	242	U
47	sR	245	U
47	sR	249	U
47	sR	250	C
47	sR	260	U
47	sR	265	A
47	sR	266	A
47	sR	267	U
47	sR	271	A
47	sR	272	U
47	sR	273	G
47	sR	275	C
47	sR	277	U
47	sR	278	U
47	sR	280	U
47	sR	281	G
47	sR	291	G
47	sR	299	A
47	sR	314	C
47	sR	316	A
47	sR	319	U
47	sR	321	C
47	sR	322	G
47	sR	333	A

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Mol	Chain	Res	Type
47	sR	335	U
47	sR	337	G
47	sR	338	C
47	sR	345	U
47	sR	359	A
47	sR	360	A
47	sR	361	C
47	sR	379	U
47	sR	380	U
47	sR	400	A
47	sR	401	A
47	sR	402	C
47	sR	404	G
47	sR	416	A
47	sR	418	G
47	sR	424	C
47	sR	425	A
47	sR	426	G
47	sR	434	G
47	sR	437	A
47	sR	439	U
47	sR	444	C
47	sR	448	C
47	sR	452	A
47	sR	454	U
47	sR	455	C
47	sR	468	A
47	sR	475	A
47	sR	480	G
47	sR	484	C
47	sR	486	G
47	sR	487	G
47	sR	488	G
47	sR	489	C
47	sR	490	C
47	sR	492	A
47	sR	493	U
47	sR	494	U
47	sR	495	C
47	sR	496	G
47	sR	497	G
47	sR	500	C

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Mol	Chain	Res	Type
47	sR	501	U
47	sR	502	U
47	sR	505	A
47	sR	506	A
47	sR	507	U
47	sR	508	U
47	sR	510	G
47	sR	511	A
47	sR	512	A
47	sR	513	U
47	sR	514	G
47	sR	516	G
47	sR	519	C
47	sR	525	A
47	sR	534	A
47	sR	538	A
47	sR	539	G
47	sR	540	G
47	sR	542	A
47	sR	543	C
47	sR	544	A
47	sR	548	G
47	sR	551	G
47	sR	556	A
47	sR	557	G
47	sR	558	U
47	sR	559	C
47	sR	565	C
47	sR	566	C
47	sR	568	G
47	sR	570	A
47	sR	574	G
47	sR	578	U
47	sR	579	A
47	sR	580	A
47	sR	582	U
47	sR	588	U
47	sR	594	A
47	sR	595	G
47	sR	610	G
47	sR	611	U
47	sR	619	A

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Mol	Chain	Res	Type
47	sR	620	A
47	sR	622	A
47	sR	623	A
47	sR	624	G
47	sR	634	G
47	sR	635	A
47	sR	637	C
47	sR	639	U
47	sR	648	G
47	sR	650	U
47	sR	651	G
47	sR	652	G
47	sR	653	C
47	sR	654	C
47	sR	658	C
47	sR	679	U
47	sR	680	U
47	sR	681	U
47	sR	682	C
47	sR	683	C
47	sR	684	A
47	sR	685	A
47	sR	690	G
47	sR	691	C
47	sR	696	C
47	sR	705	U
47	sR	709	C
47	sR	710	U
47	sR	711	U
47	sR	715	U
47	sR	718	U
47	sR	719	U
47	sR	720	G
47	sR	721	U
47	sR	722	G
47	sR	730	G
47	sR	739	G
47	sR	743	U
47	sR	745	U
47	sR	753	A
47	sR	754	A
47	sR	755	A

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Mol	Chain	Res	Type
47	sR	756	A
47	sR	765	G
47	sR	771	A
47	sR	774	A
47	sR	775	G
47	sR	780	A
47	sR	781	U
47	sR	782	U
47	sR	783	G
47	sR	789	A
47	sR	792	U
47	sR	793	A
47	sR	794	U
47	sR	811	A
47	sR	812	A
47	sR	814	A
47	sR	815	G
47	sR	816	G
47	sR	821	U
47	sR	823	G
47	sR	824	G
47	sR	825	U
47	sR	826	U
47	sR	829	A
47	sR	830	U
47	sR	831	U
47	sR	832	U
47	sR	834	G
47	sR	835	U
47	sR	846	G
47	sR	847	A
47	sR	856	A
47	sR	862	A
47	sR	863	A
47	sR	898	A
47	sR	906	A
47	sR	910	C
47	sR	911	U
47	sR	912	U
47	sR	913	G
47	sR	914	G
47	sR	916	U

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Mol	Chain	Res	Type
47	sR	933	A
47	sR	935	U
47	sR	942	G
47	sR	959	U
47	sR	960	U
47	sR	966	A
47	sR	968	U
47	sR	970	A
47	sR	971	A
47	sR	983	A
47	sR	992	A
47	sR	1004	U
47	sR	1005	A
47	sR	1021	C
47	sR	1026	A
47	sR	1028	C
47	sR	1036	A
47	sR	1039	A
47	sR	1040	G
47	sR	1043	A
47	sR	1048	G
47	sR	1052	U
47	sR	1053	G
47	sR	1057	U
47	sR	1058	U
47	sR	1059	U
47	sR	1060	U
47	sR	1061	A
47	sR	1062	A
47	sR	1071	U
47	sR	1073	G
47	sR	1081	A
47	sR	1082	C
47	sR	1086	A
47	sR	1092	A
47	sR	1096	C
47	sR	1097	U
47	sR	1098	U
47	sR	1099	U
47	sR	1100	G
47	sR	1111	G
47	sR	1138	A

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Mol	Chain	Res	Type
47	sR	1139	A
47	sR	1150	G
47	sR	1155	G
47	sR	1157	A
47	sR	1158	C
47	sR	1159	C
47	sR	1160	A
47	sR	1161	C
47	sR	1167	G
47	sR	1185	U
47	sR	1186	U
47	sR	1193	A
47	sR	1194	A
47	sR	1196	A
47	sR	1199	G
47	sR	1200	G
47	sR	1202	A
47	sR	1207	C
47	sR	1208	A
47	sR	1216	C
47	sR	1217	A
47	sR	1218	G
47	sR	1219	A
47	sR	1220	C
47	sR	1225	U
47	sR	1227	A
47	sR	1228	G
47	sR	1229	G
47	sR	1230	A
47	sR	1231	U
47	sR	1241	G
47	sR	1243	G
47	sR	1244	A
47	sR	1245	G
47	sR	1246	C
47	sR	1255	G
47	sR	1256	A
47	sR	1257	U
47	sR	1258	U
47	sR	1272	U
47	sR	1286	U
47	sR	1307	U

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Mol	Chain	Res	Type
47	sR	1311	U
47	sR	1314	U
47	sR	1315	U
47	sR	1316	G
47	sR	1321	A
47	sR	1344	A
47	sR	1345	A
47	sR	1346	A
47	sR	1347	U
47	sR	1354	G
47	sR	1355	C
47	sR	1361	U
47	sR	1362	U
47	sR	1363	U
47	sR	1364	G
47	sR	1367	G
47	sR	1370	U
47	sR	1371	A
47	sR	1388	A
47	sR	1390	U
47	sR	1398	U
47	sR	1399	C
47	sR	1400	A
47	sR	1402	G
47	sR	1410	A
47	sR	1412	G
47	sR	1413	U
47	sR	1414	U
47	sR	1415	U
47	sR	1427	A
47	sR	1428	G
47	sR	1433	G
47	sR	1445	G
47	sR	1446	A
47	sR	1448	G
47	sR	1459	C
47	sR	1460	A
47	sR	1466	G
47	sR	1469	A
47	sR	1471	A
47	sR	1473	U
47	sR	1474	G

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Mol	Chain	Res	Type
47	sR	1481	C
47	sR	1482	C
47	sR	1489	U
47	sR	1490	C
47	sR	1491	U
47	sR	1492	A
47	sR	1506	G
47	sR	1514	U
47	sR	1516	A
47	sR	1517	U
47	sR	1518	C
47	sR	1520	U
47	sR	1523	G
47	sR	1524	A
47	sR	1535	U
47	sR	1537	C
47	sR	1538	U
47	sR	1540	G
47	sR	1542	G
47	sR	1554	U
47	sR	1555	A
47	sR	1557	U
47	sR	1559	A
47	sR	1571	C
47	sR	1573	A
47	sR	1574	G
47	sR	1575	G
47	sR	1582	U
47	sR	1584	G
47	sR	1590	G
47	sR	1601	G
47	sR	1621	U
47	sR	1634	C
47	sR	1638	G
47	sR	1657	U
47	sR	1658	G
47	sR	1681	A
47	sR	1682	U
47	sR	1695	G
47	sR	1696	G
47	sR	1697	G
47	sR	1698	G

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Mol	Chain	Res	Type
47	sR	1699	G
47	sR	1700	C
47	sR	1702	A
47	sR	1703	C
47	sR	1712	A
47	sR	1713	G
47	sR	1716	C
47	sR	1717	G
47	sR	1727	G
47	sR	1731	A
47	sR	1755	A
47	sR	1760	G
47	sR	1766	A
47	sR	1767	G
47	sR	1769	U
47	sR	1780	G
47	sR	1782	A
47	sR	1783	C
47	sR	1792	G
47	sR	1793	G
47	sR	1794	A
47	sR	1796	C
47	sR	1799	U
47	sR	1800	A

All (142) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	65	A
1	1	239	G
1	1	282	G
1	1	588	G
1	1	763	G
1	1	873	C
1	1	916	G
1	1	979	U
1	1	981	U
1	1	993	G
1	1	1094	U
1	1	1097	G
1	1	1103	A
1	1	1192	C

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Mol	Chain	Res	Type
1	1	1196	C
1	1	1264	G
1	1	1273	A
1	1	1329	U
1	1	1355	A
1	1	1562	C
1	1	1589	A
1	1	1716	U
1	1	1724	U
1	1	1820	U
1	1	2101	C
1	1	2112	U
1	1	2209	U
1	1	2227	C
1	1	2249	G
1	1	2418	G
1	1	2522	G
1	1	2537	U
1	1	2539	C
1	1	2541	U
1	1	2570	U
1	1	2593	A
1	1	2818	U
1	1	2859	U
1	1	2874	G
1	1	3078	U
1	1	3121	U
1	1	3196	U
1	1	3218	A
1	1	3228	C
1	1	3269	U
1	1	3303	G
1	1	3350	C
1	1	3351	U
1	1	3353	G
2	3	49	G
3	4	85	G
3	4	125	U
1	AR	65	A
1	AR	588	G
1	AR	594	U
1	AR	715	A

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Mol	Chain	Res	Type
1	AR	873	C
1	AR	896	A
1	AR	916	G
1	AR	979	U
1	AR	981	U
1	AR	993	G
1	AR	1064	A
1	AR	1094	U
1	AR	1097	G
1	AR	1238	C
1	AR	1241	U
1	AR	1284	C
1	AR	1329	U
1	AR	1352	A
1	AR	1355	A
1	AR	1562	C
1	AR	1716	U
1	AR	1815	U
1	AR	1820	U
1	AR	2101	C
1	AR	2112	U
1	AR	2252	A
1	AR	2255	A
1	AR	2269	U
1	AR	2400	G
1	AR	2537	U
1	AR	2541	U
1	AR	2586	G
1	AR	2728	G
1	AR	2801	A
1	AR	2818	U
1	AR	2859	U
1	AR	2871	G
1	AR	3121	U
1	AR	3157	U
1	AR	3218	A
1	AR	3228	C
1	AR	3269	U
1	AR	3276	G
1	AR	3303	G
1	AR	3350	C
1	AR	3375	A

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Mol	Chain	Res	Type
2	AS	52	G
3	AT	85	G
47	A	25	C
47	A	66	U
47	A	73	U
47	A	113	U
47	A	130	C
47	A	139	C
47	A	158	U
47	A	187	G
47	A	218	A
47	A	278	U
47	A	417	A
47	A	499	U
47	A	501	U
47	A	503	G
47	A	512	A
47	A	555	A
47	A	580	A
47	A	685	A
47	A	704	C
47	A	720	G
47	A	721	U
47	A	732	G
47	A	755	A
47	A	781	U
47	A	815	G
47	A	1051	G
47	A	1081	A
47	A	1150	G
47	A	1157	A
47	A	1244	A
47	A	1250	U
47	A	1370	U
47	A	1474	G
47	A	1481	C
47	A	1489	U
47	A	1537	C
47	A	1568	C
47	A	1573	A
47	A	1600	A
47	A	1657	U

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Mol	Chain	Res	Type
47	A	1698	G
47	A	1761	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 2462 ligands modelled in this entry, 1 is modelled with single atom and 1500 are monoatomic - leaving 961 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	$\#\|Z\| > 2$
82	OHX	3	206	-	0,6,6	-	-	-		
82	OHX	A	1969	-	0,6,6	-	-	-		
82	OHX	AR	3408	-	0,6,6	-	-	-		
82	OHX	A	2130	-	0,6,6	-	-	-		
82	OHX	sR	1972	-	0,6,6	-	-	-		
82	OHX	1	3599	-	0,6,6	-	-	-		
82	OHX	1	3553	-	0,6,6	-	-	-		
82	OHX	A	2104	-	0,6,6	-	-	-		
82	OHX	A	2142	-	0,6,6	-	-	-		
82	OHX	AR	4154	-	0,6,6	-	-	-		
82	OHX	sR	1925	-	0,6,6	-	-	-		
82	OHX	AR	3633	-	0,6,6	-	-	-		
82	OHX	AR	3492	-	0,6,6	-	-	-		
82	OHX	sR	1913	-	0,6,6	-	-	-		
82	OHX	AR	3645	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	OHX	AR	4159	-	0,6,6	-	-	-		
82	OHX	1	3412	-	0,6,6	-	-	-		
82	OHX	AR	3518	-	0,6,6	-	-	-		
82	OHX	AR	3572	-	0,6,6	-	-	-		
82	OHX	DQ	502	-	0,6,6	-	-	-		
82	OHX	sR	1909	-	0,6,6	-	-	-		
82	OHX	1	4132	-	0,6,6	-	-	-		
82	OHX	AR	3618	-	0,6,6	-	-	-		
82	OHX	sR	1983	-	0,6,6	-	-	-		
82	OHX	1	3487	-	0,6,6	-	-	-		
82	OHX	1	3506	-	0,6,6	-	-	-		
82	OHX	3	202	-	0,6,6	-	-	-		
82	OHX	r	303	-	0,6,6	-	-	-		
82	OHX	AR	3598	-	0,6,6	-	-	-		
82	OHX	sR	1912	-	0,6,6	-	-	-		
82	OHX	AR	3416	-	0,6,6	-	-	-		
82	OHX	AR	3407	-	0,6,6	-	-	-		
82	OHX	1	3576	-	0,6,6	-	-	-		
82	OHX	AR	3438	-	0,6,6	-	-	-		
82	OHX	AR	3651	-	0,6,6	-	-	-		
82	OHX	AR	3638	-	0,6,6	-	-	-		
82	OHX	A	1944	-	0,6,6	-	-	-		
82	OHX	AR	3513	-	0,6,6	-	-	-		
82	OHX	sR	1968	-	0,6,6	-	-	-		
82	OHX	1	3493	-	0,6,6	-	-	-		
82	OHX	sR	2022	-	0,6,6	-	-	-		
82	OHX	AR	3474	-	0,6,6	-	-	-		
82	OHX	AT	201	-	0,6,6	-	-	-		
82	OHX	AT	211	-	0,6,6	-	-	-		
82	OHX	1	3458	-	0,6,6	-	-	-		
82	OHX	A	1954	-	0,5,6	-	-	-		
82	OHX	sR	2019	-	0,6,6	-	-	-		
82	OHX	sR	1922	-	0,6,6	-	-	-		
82	OHX	4	202	-	0,6,6	-	-	-		
82	OHX	A	1928	-	0,6,6	-	-	-		
82	OHX	sR	2001	-	0,6,6	-	-	-		
82	OHX	AR	3586	-	0,6,6	-	-	-		
82	OHX	sR	1980	-	0,6,6	-	-	-		
82	OHX	AR	3445	-	0,6,6	-	-	-		
82	OHX	1	3591	-	0,6,6	-	-	-		
82	OHX	AR	3498	-	0,6,6	-	-	-		
82	OHX	A	1945	-	0,6,6	-	-	-		
82	OHX	1	3472	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	OHX	AR	3620	-	0,6,6	-	-	-		
82	OHX	sR	2017	-	0,6,6	-	-	-		
82	OHX	1	4072	-	0,6,6	-	-	-		
82	OHX	AR	3501	-	0,6,6	-	-	-		
82	OHX	AR	3462	-	0,6,6	-	-	-		
82	OHX	A	1946	-	0,6,6	-	-	-		
82	OHX	sR	1941	-	0,6,6	-	-	-		
82	OHX	A	2120	-	0,6,6	-	-	-		
82	OHX	sR	1953	-	0,6,6	-	-	-		
82	OHX	1	3501	-	0,6,6	-	-	-		
82	OHX	1	4075	-	0,6,6	-	-	-		
82	OHX	A	1925	-	0,6,6	-	-	-		
82	OHX	AR	3443	-	0,6,6	-	-	-		
82	OHX	A	2127	-	0,6,6	-	-	-		
82	OHX	A	1968	-	0,6,6	-	-	-		
82	OHX	AS	202	-	0,6,6	-	-	-		
82	OHX	sR	1964	-	0,6,6	-	-	-		
82	OHX	sR	1979	-	0,6,6	-	-	-		
82	OHX	1	3516	-	0,6,6	-	-	-		
82	OHX	AT	234	-	0,6,6	-	-	-		
82	OHX	O	201	-	0,6,6	-	-	-		
82	OHX	AT	213	-	0,6,6	-	-	-		
82	OHX	AK	103	-	0,6,6	-	-	-		
82	OHX	sR	1986	-	0,6,6	-	-	-		
82	OHX	AS	209	-	0,6,6	-	-	-		
82	OHX	sR	1926	-	0,6,6	-	-	-		
82	OHX	1	3419	-	0,6,6	-	-	-		
82	OHX	1	3499	-	0,6,6	-	-	-		
82	OHX	AR	3455	-	0,6,6	-	-	-		
82	OHX	AR	3601	-	0,6,6	-	-	-		
82	OHX	1	3402	-	0,6,6	-	-	-		
82	OHX	A	1912	-	0,6,6	-	-	-		
82	OHX	1	4147	-	0,6,6	-	-	-		
82	OHX	AR	3574	-	0,6,6	-	-	-		
82	OHX	1	3598	-	0,6,6	-	-	-		
82	OHX	AR	3670	-	0,6,6	-	-	-		
82	OHX	AS	207	-	0,6,6	-	-	-		
82	OHX	sR	1948	-	0,6,6	-	-	-		
82	OHX	1	3543	-	0,6,6	-	-	-		
82	OHX	1	4086	-	0,6,6	-	-	-		
82	OHX	AR	3525	-	0,6,6	-	-	-		
82	OHX	1	3551	-	0,6,6	-	-	-		
82	OHX	sR	1990	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3628	-	0,6,6	-	-	-		
82	OHX	1	4153	-	0,6,6	-	-	-		
82	OHX	AR	3466	-	0,6,6	-	-	-		
82	OHX	AR	3540	-	0,6,6	-	-	-		
82	OHX	AR	3425	-	0,6,6	-	-	-		
82	OHX	A	1964	-	0,6,6	-	-	-		
82	OHX	A	2141	-	0,6,6	-	-	-		
82	OHX	1	4150	-	0,6,6	-	-	-		
82	OHX	1	3463	-	0,6,6	-	-	-		
82	OHX	1	3495	-	0,6,6	-	-	-		
82	OHX	4	210	-	0,6,6	-	-	-		
82	OHX	AR	3617	-	0,6,6	-	-	-		
82	OHX	AR	3577	-	0,6,6	-	-	-		
82	OHX	A	2146	-	0,6,6	-	-	-		
86	X1K	1	4181	-	27,27,27	0.49	1 (3%)	35,43,43	2.30	8 (22%)
82	OHX	1	3594	-	0,6,6	-	-	-		
82	OHX	AR	3557	-	0,6,6	-	-	-		
82	OHX	1	4076	-	0,6,6	-	-	-		
82	OHX	AR	3548	-	0,6,6	-	-	-		
82	OHX	AR	3624	-	0,6,6	-	-	-		
82	OHX	A	1929	-	0,6,6	-	-	-		
82	OHX	AR	4142	-	0,6,6	-	-	-		
82	OHX	1	3504	-	0,6,6	-	-	-		
82	OHX	1	4094	-	0,6,6	-	-	-		
82	OHX	AR	3588	-	0,6,6	-	-	-		
82	OHX	AR	3668	-	0,6,6	-	-	-		
82	OHX	1	3558	-	0,6,6	-	-	-		
82	OHX	sR	1970	-	0,6,6	-	-	-		
82	OHX	1	3530	-	0,6,6	-	-	-		
82	OHX	1	3485	-	0,6,6	-	-	-		
82	OHX	3	205	-	0,6,6	-	-	-		
82	OHX	1	3483	-	0,6,6	-	-	-		
82	OHX	1	3600	-	0,6,6	-	-	-		
82	OHX	AR	3606	-	0,6,6	-	-	-		
82	OHX	A	1933	-	0,6,6	-	-	-		
82	OHX	1	3415	-	0,6,6	-	-	-		
82	OHX	1	4105	-	0,6,6	-	-	-		
86	X1K	AR	4205	-	27,27,27	0.68	2 (7%)	35,43,43	1.92	9 (25%)
85	SPD	1	4180	-	9,9,9	0.33	0	8,8,8	0.92	0
82	OHX	AR	3547	-	0,6,6	-	-	-		
82	OHX	AR	3484	-	0,6,6	-	-	-		
82	OHX	1	3414	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	3455	-	0,6,6	-	-	-		
82	OHX	A	1971	-	0,6,6	-	-	-		
82	OHX	1	4152	-	0,6,6	-	-	-		
82	OHX	AR	3419	-	0,6,6	-	-	-		
82	OHX	1	3524	-	0,6,6	-	-	-		
82	OHX	1	3605	-	0,6,6	-	-	-		
82	OHX	1	3479	-	0,6,6	-	-	-		
82	OHX	1	4096	-	0,6,6	-	-	-		
82	OHX	1	3523	-	0,6,6	-	-	-		
82	OHX	A	1914	-	0,6,6	-	-	-		
82	OHX	AR	3410	-	0,6,6	-	-	-		
82	OHX	AR	3531	-	0,6,6	-	-	-		
82	OHX	A	1922	-	0,6,6	-	-	-		
82	OHX	A	2126[B]	-	0,6,6	-	-	-		
82	OHX	AR	3502	-	0,6,6	-	-	-		
82	OHX	AR	3561	-	0,6,6	-	-	-		
82	OHX	A	2134	-	0,6,6	-	-	-		
82	OHX	sR	1911	-	0,6,6	-	-	-		
82	OHX	AR	3512	-	0,6,6	-	-	-		
82	OHX	A	1934	-	0,6,6	-	-	-		
82	OHX	A	1949	-	0,6,6	-	-	-		
82	OHX	1	3457	-	0,6,6	-	-	-		
82	OHX	A	1955	-	0,6,6	-	-	-		
82	OHX	AR	3573	-	0,6,6	-	-	-		
82	OHX	A	1903	-	0,6,6	-	-	-		
82	OHX	AR	3545	-	0,6,6	-	-	-		
82	OHX	1	3577	-	0,6,6	-	-	-		
82	OHX	AR	4143	-	0,6,6	-	-	-		
82	OHX	AR	3491	-	0,6,6	-	-	-		
82	OHX	1	3442	-	0,6,6	-	-	-		
82	OHX	1	3560	-	0,6,6	-	-	-		
82	OHX	AR	3439	-	0,6,6	-	-	-		
82	OHX	A	1973	-	0,6,6	-	-	-		
82	OHX	1	4114[B]	-	0,6,6	-	-	-		
82	OHX	1	4117	-	0,6,6	-	-	-		
82	OHX	1	3486	-	0,6,6	-	-	-		
82	OHX	1	4077	-	0,6,6	-	-	-		
82	OHX	AR	4157	-	0,6,6	-	-	-		
82	OHX	A	1977	-	0,6,6	-	-	-		
82	OHX	AR	3487	-	0,6,6	-	-	-		
82	OHX	1	3465	-	0,6,6	-	-	-		
82	OHX	AR	4153	-	0,6,6	-	-	-		
82	OHX	1	3427	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	sR	1906	-	0,6,6	-	-	-		
82	OHX	1	3451	-	0,6,6	-	-	-		
82	OHX	1	3454	-	0,6,6	-	-	-		
82	OHX	AR	3470	-	0,6,6	-	-	-		
82	OHX	AR	3527	-	0,6,6	-	-	-		
82	OHX	1	3441	-	0,6,6	-	-	-		
82	OHX	AR	3530	-	0,6,6	-	-	-		
82	OHX	AR	3648	-	0,6,6	-	-	-		
82	OHX	A	1967	-	0,6,6	-	-	-		
82	OHX	AR	3662	-	0,6,6	-	-	-		
82	OHX	A	2115	-	0,6,6	-	-	-		
82	OHX	A	1917	-	0,6,6	-	-	-		
82	OHX	s1	301	-	0,6,6	-	-	-		
82	OHX	AR	3627	-	0,6,6	-	-	-		
82	OHX	1	3535[B]	-	0,6,6	-	-	-		
82	OHX	1	3515	-	0,6,6	-	-	-		
82	OHX	A	1907	-	0,6,6	-	-	-		
82	OHX	1	3409	-	0,6,6	-	-	-		
82	OHX	1	4089	-	0,6,6	-	-	-		
82	OHX	sR	2167	-	0,6,6	-	-	-		
82	OHX	AR	4147	-	0,6,6	-	-	-		
82	OHX	AR	3597	-	0,6,6	-	-	-		
82	OHX	1	3556	-	0,6,6	-	-	-		
82	OHX	A	1927	-	0,6,6	-	-	-		
82	OHX	A	1906	-	0,6,6	-	-	-		
82	OHX	A	1918	-	0,6,6	-	-	-		
82	OHX	AR	3511	-	0,6,6	-	-	-		
82	OHX	1	3511	-	0,6,6	-	-	-		
82	OHX	AR	3667	-	0,6,6	-	-	-		
82	OHX	1	3480	-	0,6,6	-	-	-		
82	OHX	AR	3519	-	0,6,6	-	-	-		
82	OHX	AS	205	-	0,6,6	-	-	-		
82	OHX	A	1953	-	0,6,6	-	-	-		
82	OHX	sR	1949	-	0,6,6	-	-	-		
82	OHX	sR	1961	-	0,6,6	-	-	-		
82	OHX	A	2116	-	0,6,6	-	-	-		
82	OHX	AR	3640	-	0,6,6	-	-	-		
82	OHX	1	3490	-	0,6,6	-	-	-		
82	OHX	1	4138	-	0,6,6	-	-	-		
82	OHX	AR	3471	-	0,6,6	-	-	-		
82	OHX	1	3497	-	0,6,6	-	-	-		
82	OHX	A	1941	-	0,6,6	-	-	-		
82	OHX	AR	3488	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	sR	1998	-	0,6,6	-	-	-		
82	OHX	1	3447	-	0,6,6	-	-	-		
82	OHX	AR	3560	-	0,6,6	-	-	-		
82	OHX	sR	2004	-	0,6,6	-	-	-		
82	OHX	AR	3535	-	0,6,6	-	-	-		
82	OHX	1	4122	-	0,6,6	-	-	-		
82	OHX	CS	201	-	0,6,6	-	-	-		
82	OHX	1	4125	-	0,6,6	-	-	-		
82	OHX	1	3505	-	0,6,6	-	-	-		
82	OHX	A	1965	-	0,6,6	-	-	-		
82	OHX	sR	2000	-	0,6,6	-	-	-		
82	OHX	1	3581	-	0,6,6	-	-	-		
82	OHX	sR	1934	-	0,6,6	-	-	-		
82	OHX	sR	2014	-	0,6,6	-	-	-		
82	OHX	AT	207	-	0,6,6	-	-	-		
82	OHX	AR	3610	-	0,6,6	-	-	-		
82	OHX	AR	3441	-	0,6,6	-	-	-		
82	OHX	1	3568	-	0,6,6	-	-	-		
82	OHX	1	3464	-	0,6,6	-	-	-		
82	OHX	AR	3658	-	0,6,6	-	-	-		
82	OHX	1	3601	-	0,6,6	-	-	-		
82	OHX	1	4145	-	0,6,6	-	-	-		
82	OHX	CE	401	-	0,6,6	-	-	-		
82	OHX	A	1902	-	0,6,6	-	-	-		
82	OHX	1	4051	-	0,6,6	-	-	-		
82	OHX	1	3410	-	0,6,6	-	-	-		
82	OHX	AR	3422	-	0,6,6	-	-	-		
82	OHX	sR	1996	-	0,6,6	-	-	-		
82	OHX	AR	3622	-	0,6,6	-	-	-		
82	OHX	3	219	-	0,6,6	-	-	-		
82	OHX	J	301	-	0,6,6	-	-	-		
82	OHX	AR	3509	-	0,6,6	-	-	-		
82	OHX	AR	3516	-	0,6,6	-	-	-		
82	OHX	4	205	-	0,6,6	-	-	-		
82	OHX	1	3430	-	0,6,6	-	-	-		
82	OHX	AR	3478	-	0,6,6	-	-	-		
82	OHX	A	1916	-	0,6,6	-	-	-		
82	OHX	AR	3528	-	0,6,6	-	-	-		
82	OHX	1	3585	-	0,6,6	-	-	-		
82	OHX	CL	303	-	0,6,6	-	-	-		
82	OHX	sR	1991	-	0,6,6	-	-	-		
82	OHX	AR	3625	-	0,6,6	-	-	-		
82	OHX	1	4104	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	DH	202	-	0,6,6	-	-	-		
82	OHX	A	2103	-	0,6,6	-	-	-		
82	OHX	4	207	-	0,6,6	-	-	-		
82	OHX	A	1976	-	0,6,6	-	-	-		
82	OHX	1	3438	-	0,6,6	-	-	-		
82	OHX	A	1920	-	0,6,6	-	-	-		
82	OHX	AR	3482	-	0,6,6	-	-	-		
82	OHX	1	3513	-	0,6,6	-	-	-		
82	OHX	sR	1959	-	0,6,6	-	-	-		
82	OHX	1	4087	-	0,6,6	-	-	-		
82	OHX	AR	4156	-	0,6,6	-	-	-		
82	OHX	AR	3453	-	0,6,6	-	-	-		
82	OHX	A	1910	-	0,6,6	-	-	-		
82	OHX	AR	3580	-	0,6,6	-	-	-		
82	OHX	AR	3442	-	0,6,6	-	-	-		
82	OHX	sR	2179	-	0,6,6	-	-	-		
82	OHX	1	3586	-	0,6,6	-	-	-		
82	OHX	AC	102	-	0,6,6	-	-	-		
82	OHX	AR	3522	-	0,6,6	-	-	-		
82	OHX	A	2144	-	0,6,6	-	-	-		
82	OHX	sR	1907	-	0,6,6	-	-	-		
82	OHX	1	3481	-	0,6,6	-	-	-		
82	OHX	1	4144	1	0,5,6	-	-	-		
82	OHX	AR	3578	-	0,6,6	-	-	-		
82	OHX	A	2107	-	0,6,6	-	-	-		
82	OHX	1	4099	-	0,5,6	-	-	-		
82	OHX	sR	2024	-	0,6,6	-	-	-		
82	OHX	1	3470	-	0,6,6	-	-	-		
82	OHX	1	3462	-	0,6,6	-	-	-		
82	OHX	AR	3660	-	0,6,6	-	-	-		
82	OHX	1	4119	-	0,6,6	-	-	-		
82	OHX	1	3475	-	0,6,6	-	-	-		
82	OHX	1	3582	-	0,6,6	-	-	-		
82	OHX	4	213	-	0,6,6	-	-	-		
82	OHX	AR	3611	-	0,6,6	-	-	-		
82	OHX	AR	3526	-	0,6,6	-	-	-		
82	OHX	1	4123	-	0,6,6	-	-	-		
82	OHX	A	2118	-	0,6,6	-	-	-		
82	OHX	sR	1958	-	0,6,6	-	-	-		
82	OHX	1	4120	-	0,6,6	-	-	-		
82	OHX	1	3498	-	0,6,6	-	-	-		
82	OHX	1	3434	-	0,6,6	-	-	-		
82	OHX	AR	3555	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	Q	201	-	0,6,6	-	-	-		
82	OHX	1	4095	-	0,6,6	-	-	-		
82	OHX	AR	4148	-	0,6,6	-	-	-		
82	OHX	A	2105	-	0,6,6	-	-	-		
82	OHX	sR	1940	-	0,6,6	-	-	-		
82	OHX	AR	3562	-	0,6,6	-	-	-		
82	OHX	1	4093	-	0,6,6	-	-	-		
82	OHX	AR	3623	-	0,6,6	-	-	-		
82	OHX	1	3574	-	0,6,6	-	-	-		
82	OHX	sR	2174	-	0,6,6	-	-	-		
82	OHX	A	2132	-	0,6,6	-	-	-		
82	OHX	AR	3456	-	0,6,6	-	-	-		
82	OHX	AR	3591	-	0,6,6	-	-	-		
82	OHX	A	2131	-	0,6,6	-	-	-		
82	OHX	A	2102	-	0,6,6	-	-	-		
82	OHX	sR	1918	-	0,6,6	-	-	-		
82	OHX	1	3537	-	0,6,6	-	-	-		
82	OHX	A	2137	-	0,6,6	-	-	-		
82	OHX	1	3482	-	0,6,6	-	-	-		
82	OHX	1	3554	-	0,6,6	-	-	-		
82	OHX	sR	1997	-	0,6,6	-	-	-		
82	OHX	AR	3405	-	0,6,6	-	-	-		
82	OHX	1	3525	-	0,6,6	-	-	-		
82	OHX	CG	302	-	0,6,6	-	-	-		
82	OHX	A	1956	-	0,6,6	-	-	-		
82	OHX	1	3512	-	0,6,6	-	-	-		
82	OHX	1	4056	-	0,6,6	-	-	-		
82	OHX	A	1911	-	0,6,6	-	-	-		
82	OHX	sR	1916[A]	-	0,6,6	-	-	-		
82	OHX	AR	3556	-	0,6,6	-	-	-		
82	OHX	1	3597	-	0,6,6	-	-	-		
82	OHX	sR	1957	-	0,6,6	-	-	-		
82	OHX	sR	2177	-	0,6,6	-	-	-		
82	OHX	1	4128	-	0,6,6	-	-	-		
82	OHX	sR	1989	-	0,6,6	-	-	-		
82	OHX	1	4111	-	0,6,6	-	-	-		
82	OHX	AR	3564	-	0,6,6	-	-	-		
82	OHX	v	301	-	0,6,6	-	-	-		
82	OHX	AT	206	-	0,6,6	-	-	-		
82	OHX	AR	3650	-	0,6,6	-	-	-		
82	OHX	AR	3587	-	0,6,6	-	-	-		
82	OHX	1	3420	-	0,6,6	-	-	-		
82	OHX	1	3557	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3529	-	0,6,6	-	-	-		
82	OHX	1	3507	-	0,6,6	-	-	-		
82	OHX	sR	1956	-	0,6,6	-	-	-		
82	OHX	sR	2013	-	0,6,6	-	-	-		
82	OHX	1	3428	-	0,6,6	-	-	-		
82	OHX	1	4109	-	0,6,6	-	-	-		
82	OHX	AR	3655	-	0,6,6	-	-	-		
82	OHX	1	4106	-	0,6,6	-	-	-		
82	OHX	sR	1917	-	0,6,6	-	-	-		
82	OHX	A	2109	-	0,6,6	-	-	-		
82	OHX	Rb	401	-	0,6,6	-	-	-		
82	OHX	1	4050	-	0,6,6	-	-	-		
82	OHX	1	3508	-	0,6,6	-	-	-		
82	OHX	AR	3565	-	0,6,6	-	-	-		
82	OHX	AR	3581	-	0,6,6	-	-	-		
82	OHX	1	3571	-	0,6,6	-	-	-		
82	OHX	1	3547	-	0,6,6	-	-	-		
82	OHX	1	3484	-	0,6,6	-	-	-		
82	OHX	AR	4120	-	0,6,6	-	-	-		
82	OHX	sR	2026	-	0,6,6	-	-	-		
82	OHX	sR	1932	-	0,6,6	-	-	-		
82	OHX	sR	1939	-	0,6,6	-	-	-		
82	OHX	sR	1978	-	0,6,6	-	-	-		
82	OHX	sR	1973	-	0,6,6	-	-	-		
82	OHX	AR	3403	-	0,6,6	-	-	-		
82	OHX	1	4121	-	0,6,6	-	-	-		
82	OHX	AR	3644	-	0,6,6	-	-	-		
82	OHX	AR	4145	-	0,6,6	-	-	-		
82	OHX	1	3589	-	0,6,6	-	-	-		
82	OHX	1	3532	-	0,6,6	-	-	-		
82	OHX	AT	210	-	0,6,6	-	-	-		
82	OHX	AR	4162	-	0,6,6	-	-	-		
82	OHX	A	1975	-	0,6,6	-	-	-		
82	OHX	1	3531	-	0,6,6	-	-	-		
82	OHX	sR	1988	-	0,6,6	-	-	-		
82	OHX	sR	1904	-	0,6,6	-	-	-		
82	OHX	1	3453	-	0,6,6	-	-	-		
82	OHX	1	3502	-	0,6,6	-	-	-		
82	OHX	AR	3609	-	0,6,6	-	-	-		
82	OHX	A	1938	-	0,6,6	-	-	-		
82	OHX	A	1937	-	0,6,6	-	-	-		
82	OHX	1	3573	-	0,6,6	-	-	-		
82	OHX	A	1959	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	sR	2018	-	0,6,6	-	-	-		
82	OHX	AR	3536	-	0,6,6	-	-	-		
82	OHX	1	4084	-	0,6,6	-	-	-		
82	OHX	1	4143	-	0,6,6	-	-	-		
82	OHX	sR	1910	-	0,6,6	-	-	-		
82	OHX	1	4090	-	0,6,6	-	-	-		
82	OHX	1	3473	-	0,6,6	-	-	-		
82	OHX	AR	3614	-	0,6,6	-	-	-		
82	OHX	1	3449	-	0,6,6	-	-	-		
82	OHX	1	4110	-	0,6,6	-	-	-		
82	OHX	sR	2181	-	0,6,6	-	-	-		
82	OHX	1	3521	-	0,6,6	-	-	-		
82	OHX	1	4139	-	0,6,6	-	-	-		
82	OHX	c5	201	-	0,6,6	-	-	-		
82	OHX	1	3404	-	0,6,6	-	-	-		
82	OHX	A	2125	-	0,6,6	-	-	-		
82	OHX	AR	3426	-	0,6,6	-	-	-		
82	OHX	AR	3507	-	0,6,6	-	-	-		
82	OHX	1	3545	-	0,6,6	-	-	-		
82	OHX	4	201	-	0,6,6	-	-	-		
82	OHX	AR	3590	-	0,6,6	-	-	-		
82	OHX	AR	3533	-	0,6,6	-	-	-		
82	OHX	AR	3493	-	0,6,6	-	-	-		
82	OHX	AR	3448	-	0,6,6	-	-	-		
82	OHX	sR	1999	-	0,6,6	-	-	-		
82	OHX	1	3469	-	0,6,6	-	-	-		
82	OHX	CG	304	-	0,6,6	-	-	-		
82	OHX	1	3527	-	0,6,6	-	-	-		
82	OHX	AR	3480	-	0,6,6	-	-	-		
82	OHX	sR	1982	-	0,6,6	-	-	-		
82	OHX	AR	3579	-	0,6,6	-	-	-		
82	OHX	AS	204	-	0,6,6	-	-	-		
82	OHX	sR	1905	-	0,6,6	-	-	-		
82	OHX	1	4085	-	0,6,6	-	-	-		
82	OHX	AR	3570	-	0,6,6	-	-	-		
82	OHX	sR	2009	-	0,6,6	-	-	-		
82	OHX	AR	3664	-	0,6,6	-	-	-		
82	OHX	A	1957	-	0,6,6	-	-	-		
82	OHX	1	3408	-	0,6,6	-	-	-		
82	OHX	AR	3499	-	0,6,6	-	-	-		
82	OHX	1	3565	-	0,6,6	-	-	-		
82	OHX	AR	3505	-	0,6,6	-	-	-		
82	OHX	AR	3532	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3637	-	0,6,6	-	-	-		
82	OHX	1	3520	-	0,6,6	-	-	-		
82	OHX	AR	3634	-	0,6,6	-	-	-		
82	OHX	1	3583	-	0,6,6	-	-	-		
82	OHX	AR	3541	-	0,6,6	-	-	-		
82	OHX	AR	3566	-	0,6,6	-	-	-		
82	OHX	1	3592	-	0,6,6	-	-	-		
82	OHX	1	3514	-	0,6,6	-	-	-		
82	OHX	1	4097	-	0,6,6	-	-	-		
82	OHX	AR	3446	-	0,6,6	-	-	-		
82	OHX	AR	3465	-	0,6,6	-	-	-		
82	OHX	1	3440	-	0,6,6	-	-	-		
82	OHX	AR	3537	-	0,6,6	-	-	-		
82	OHX	1	4101	-	0,6,6	-	-	-		
82	OHX	AR	3661	-	0,6,6	-	-	-		
82	OHX	1	3572	-	0,6,6	-	-	-		
82	OHX	A	2108	-	0,6,6	-	-	-		
82	OHX	sR	1936	-	0,6,6	-	-	-		
82	OHX	1	3595	-	0,6,6	-	-	-		
82	OHX	AT	233	-	0,6,6	-	-	-		
82	OHX	DL	103	-	0,6,6	-	-	-		
82	OHX	AR	3552	-	0,6,6	-	-	-		
82	OHX	1	3596	-	0,6,6	-	-	-		
82	OHX	A	2136	-	0,6,6	-	-	-		
82	OHX	1	3503	-	0,6,6	-	-	-		
82	OHX	AR	3654	-	0,5,6	-	-	-		
82	OHX	AR	4139	-	0,6,6	-	-	-		
82	OHX	1	3429	-	0,6,6	-	-	-		
82	OHX	sR	1985	-	0,6,6	-	-	-		
82	OHX	1	4135	-	0,6,6	-	-	-		
82	OHX	AR	4116	-	0,6,6	-	-	-		
82	OHX	AR	3515	-	0,6,6	-	-	-		
82	OHX	sR	2016	-	0,6,6	-	-	-		
82	OHX	c8	201	-	0,6,6	-	-	-		
82	OHX	sR	1921	-	0,6,6	-	-	-		
82	OHX	AR	3454	-	0,6,6	-	-	-		
82	OHX	1	3433	-	0,6,6	-	-	-		
82	OHX	sR	1947	-	0,6,6	-	-	-		
82	OHX	1	3544	-	0,6,6	-	-	-		
82	OHX	1	3535[A]	-	0,6,6	-	-	-		
82	OHX	1	3550	-	0,6,6	-	-	-		
82	OHX	1	4060	-	0,6,6	-	-	-		
82	OHX	AR	3636	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	OHX	1	3488	-	0,6,6	-	-	-		
82	OHX	3	201	-	0,6,6	-	-	-		
82	OHX	1	3474	-	0,6,6	-	-	-		
82	OHX	AR	3415	-	0,6,6	-	-	-		
82	OHX	sR	2023	-	0,6,6	-	-	-		
82	OHX	AR	3659	-	0,6,6	-	-	-		
82	OHX	AR	4151	-	0,6,6	-	-	-		
82	OHX	AR	3414	-	0,6,6	-	-	-		
82	OHX	A	1923	-	0,6,6	-	-	-		
82	OHX	AT	215	-	0,6,6	-	-	-		
82	OHX	sR	1965	-	0,6,6	-	-	-		
82	OHX	A	2145	-	0,6,6	-	-	-		
82	OHX	AR	3605	-	0,6,6	-	-	-		
82	OHX	A	2114	-	0,6,6	-	-	-		
82	OHX	AR	3523	-	0,6,6	-	-	-		
82	OHX	AR	3451	-	0,6,6	-	-	-		
82	OHX	AR	3475	-	0,6,6	-	-	-		
82	OHX	AS	206	-	0,6,6	-	-	-		
82	OHX	1	3534	-	0,6,6	-	-	-		
82	OHX	1	3510	-	0,6,6	-	-	-		
82	OHX	AR	4160	-	0,6,6	-	-	-		
82	OHX	sR	1924	-	0,6,6	-	-	-		
82	OHX	3	222	-	0,6,6	-	-	-		
82	OHX	sR	1930	-	0,6,6	-	-	-		
82	OHX	1	3500	-	0,6,6	-	-	-		
82	OHX	DD	102	-	0,6,6	-	-	-		
82	OHX	CL	302	-	0,6,6	-	-	-		
82	OHX	sR	1994	-	0,6,6	-	-	-		
82	OHX	AR	3671	-	0,6,6	-	-	-		
82	OHX	sR	2178	-	0,6,6	-	-	-		
82	OHX	sR	1951	-	0,6,6	-	-	-		
82	OHX	AR	3449	-	0,6,6	-	-	-		
82	OHX	k	404	-	0,6,6	-	-	-		
82	OHX	1	3477	-	0,6,6	-	-	-		
82	OHX	AR	4138	-	0,6,6	-	-	-		
82	OHX	AR	3568	-	0,6,6	-	-	-		
82	OHX	AR	3643	-	0,6,6	-	-	-		
82	OHX	1	3529	-	0,6,6	-	-	-		
82	OHX	AR	3534	-	0,6,6	-	-	-		
82	OHX	sR	1966	-	0,6,6	-	-	-		
82	OHX	sR	2169	-	0,6,6	-	-	-		
82	OHX	sR	1929	-	0,6,6	-	-	-		
82	OHX	AS	208	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	c7	201	-	0,6,6	-	-	-		
82	OHX	1	3416	-	0,6,6	-	-	-		
82	OHX	1	4074	-	0,6,6	-	-	-		
82	OHX	sR	1967	-	0,6,6	-	-	-		
82	OHX	AT	202	-	0,6,6	-	-	-		
82	OHX	1	4126	-	0,6,6	-	-	-		
82	OHX	A	1974	-	0,6,6	-	-	-		
82	OHX	1	3540	-	0,6,6	-	-	-		
82	OHX	sR	2011	-	0,6,6	-	-	-		
82	OHX	AR	4158	-	0,6,6	-	-	-		
82	OHX	AR	4155	-	0,6,6	-	-	-		
82	OHX	sR	1962	-	0,6,6	-	-	-		
82	OHX	AR	3663	-	0,6,6	-	-	-		
82	OHX	1	4108	-	0,6,6	-	-	-		
82	OHX	sR	2015	-	0,6,6	-	-	-		
82	OHX	AR	3576	-	0,6,6	-	-	-		
82	OHX	AR	3517	-	0,6,6	-	-	-		
82	OHX	CH	201	-	0,6,6	-	-	-		
82	OHX	d4	201	-	0,6,6	-	-	-		
82	OHX	sR	1976	-	0,6,6	-	-	-		
82	OHX	AR	3559	-	0,6,6	-	-	-		
82	OHX	AR	3584	-	0,6,6	-	-	-		
82	OHX	AR	3649	-	0,6,6	-	-	-		
82	OHX	A	1943	-	0,6,6	-	-	-		
82	OHX	AT	235	-	0,6,6	-	-	-		
82	OHX	1	4137	-	0,6,6	-	-	-		
82	OHX	sR	2021	-	0,6,6	-	-	-		
82	OHX	sR	1977	-	0,6,6	-	-	-		
82	OHX	1	3509	-	0,6,6	-	-	-		
82	OHX	1	3444	-	0,6,6	-	-	-		
82	OHX	1	3578	-	0,6,6	-	-	-		
82	OHX	1	4083	-	0,6,6	-	-	-		
82	OHX	AR	3612	-	0,6,6	-	-	-		
82	OHX	1	3417	-	0,6,6	-	-	-		
82	OHX	1	4148	-	0,6,6	-	-	-		
82	OHX	AR	3567	-	0,6,6	-	-	-		
82	OHX	sR	1944	-	0,6,6	-	-	-		
82	OHX	1	3489	-	0,6,6	-	-	-		
82	OHX	1	3536	-	0,6,6	-	-	-		
82	OHX	1	3552	-	0,6,6	-	-	-		
82	OHX	sR	1987	-	0,6,6	-	-	-		
82	OHX	1	3604	-	0,6,6	-	-	-		
82	OHX	CX	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	OHX	1	4079	-	0,6,6	-	-	-		
82	OHX	AR	3569	-	0,6,6	-	-	-		
82	OHX	AR	3563	-	0,6,6	-	-	-		
82	OHX	AR	3583	-	0,6,6	-	-	-		
82	OHX	1	4112	-	0,6,6	-	-	-		
82	OHX	4	211	-	0,6,6	-	-	-		
82	OHX	AR	3626	-	0,6,6	-	-	-		
82	OHX	A	1940[B]	-	0,6,6	-	-	-		
82	OHX	sR	2012	-	0,6,6	-	-	-		
82	OHX	1	3456	-	0,6,6	-	-	-		
82	OHX	AR	3421	-	0,6,6	-	-	-		
82	OHX	AR	3477	-	0,6,6	-	-	-		
82	OHX	A	2122	-	0,6,6	-	-	-		
82	OHX	AR	3429	-	0,6,6	-	-	-		
82	OHX	A	1908	-	0,6,6	-	-	-		
82	OHX	A	1958	-	0,6,6	-	-	-		
82	OHX	sR	2180	-	0,6,6	-	-	-		
82	OHX	AR	4144	-	0,6,6	-	-	-		
82	OHX	sR	1955	-	0,6,6	-	-	-		
82	OHX	1	3575	-	0,6,6	-	-	-		
82	OHX	A	1960	-	0,6,6	-	-	-		
82	OHX	1	4073	-	0,6,6	-	-	-		
82	OHX	A	2128	-	0,6,6	-	-	-		
82	OHX	sR	1920	-	0,6,6	-	-	-		
82	OHX	AR	3496	-	0,6,6	-	-	-		
82	OHX	A	2110	-	0,6,6	-	-	-		
82	OHX	1	4134	-	0,6,6	-	-	-		
82	OHX	sR	2005	-	0,6,6	-	-	-		
82	OHX	AR	3593	-	0,6,6	-	-	-		
82	OHX	1	3538	-	0,6,6	-	-	-		
82	OHX	AR	3656	-	0,6,6	-	-	-		
82	OHX	sR	1938	-	0,6,6	-	-	-		
82	OHX	AR	3602	-	0,6,6	-	-	-		
82	OHX	1	3431	-	0,6,6	-	-	-		
82	OHX	1	3466	-	0,6,6	-	-	-		
82	OHX	1	3518	-	0,6,6	-	-	-		
82	OHX	1	4091	-	0,6,6	-	-	-		
82	OHX	1	3468	-	0,6,6	-	-	-		
82	OHX	sR	2170	-	0,6,6	-	-	-		
82	OHX	AS	201	-	0,6,6	-	-	-		
82	OHX	1	3445	-	0,6,6	-	-	-		
82	OHX	sR	1914	-	0,6,6	-	-	-		
82	OHX	1	3432	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	A	1932	-	0,6,6	-	-	-		
82	OHX	4	229	-	0,6,6	-	-	-		
82	OHX	AR	3464	-	0,6,6	-	-	-		
82	OHX	AR	3411	-	0,6,6	-	-	-		
82	OHX	AR	4150	-	0,6,6	-	-	-		
82	OHX	AR	3490	-	0,6,6	-	-	-		
82	OHX	A	1963	-	0,6,6	-	-	-		
82	OHX	sR	1992	-	0,6,6	-	-	-		
82	OHX	A	1905	-	0,6,6	-	-	-		
82	OHX	1	3459	-	0,6,6	-	-	-		
82	OHX	1	3424	-	0,6,6	-	-	-		
82	OHX	1	3562	-	0,6,6	-	-	-		
82	OHX	A	2135	-	0,6,6	-	-	-		
82	OHX	sR	1935	-	0,6,6	-	-	-		
82	OHX	AR	3635	-	0,6,6	-	-	-		
82	OHX	1	3443	-	0,6,6	-	-	-		
82	OHX	1	3450	-	0,6,6	-	-	-		
82	OHX	1	4082	-	0,6,6	-	-	-		
82	OHX	A	2117	-	0,6,6	-	-	-		
82	OHX	sR	1927	-	0,6,6	-	-	-		
82	OHX	A	1966	-	0,6,6	-	-	-		
82	OHX	AR	3436	-	0,6,6	-	-	-		
82	OHX	1	3448	-	0,6,6	-	-	-		
82	OHX	AR	3585	-	0,6,6	-	-	-		
82	OHX	AR	3447	-	0,6,6	-	-	-		
82	OHX	1	3559	-	0,6,6	-	-	-		
82	OHX	3	203	-	0,6,6	-	-	-		
82	OHX	sR	1952	-	0,6,6	-	-	-		
82	OHX	1	3422	-	0,6,6	-	-	-		
82	OHX	1	3549	-	0,6,6	-	-	-		
82	OHX	4	228	-	0,6,6	-	-	-		
82	OHX	1	3403	-	0,6,6	-	-	-		
82	OHX	AR	3483	-	0,6,6	-	-	-		
82	OHX	AR	3435	-	0,6,6	-	-	-		
82	OHX	sR	2175	-	0,6,6	-	-	-		
82	OHX	AR	3546	-	0,6,6	-	-	-		
82	OHX	AT	214	-	0,6,6	-	-	-		
82	OHX	1	4102	-	0,6,6	-	-	-		
82	OHX	1	4062	-	0,6,6	-	-	-		
82	OHX	1	3478	-	0,6,6	-	-	-		
82	OHX	AR	3514	-	0,6,6	-	-	-		
82	OHX	1	3461	-	0,6,6	-	-	-		
82	OHX	sR	1919	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	OHX	1	3437	-	0,6,6	-	-	-		
82	OHX	A	2113	-	0,6,6	-	-	-		
82	OHX	1	3603	-	0,6,6	-	-	-		
82	OHX	AR	3468	-	0,6,6	-	-	-		
82	OHX	sR	1933	-	0,6,6	-	-	-		
82	OHX	1	3425	-	0,6,6	-	-	-		
82	OHX	AR	3430	-	0,6,6	-	-	-		
82	OHX	sR	1995	-	0,6,6	-	-	-		
82	OHX	1	3566	-	0,6,6	-	-	-		
82	OHX	1	4129	-	0,6,6	-	-	-		
82	OHX	sR	1923	-	0,6,6	-	-	-		
82	OHX	AR	3431	-	0,6,6	-	-	-		
82	OHX	AR	3457	-	0,6,6	-	-	-		
82	OHX	A	1915	-	0,6,6	-	-	-		
82	OHX	AR	3647	-	0,6,6	-	-	-		
82	OHX	1	3426	-	0,6,6	-	-	-		
82	OHX	1	3579	-	0,6,6	-	-	-		
82	OHX	1	4133	-	0,6,6	-	-	-		
82	OHX	1	3569	-	0,6,6	-	-	-		
82	OHX	AR	3476	-	0,6,6	-	-	-		
82	OHX	AR	3665	-	0,6,6	-	-	-		
82	OHX	AR	3619	-	0,6,6	-	-	-		
82	OHX	1	4118	-	0,6,6	-	-	-		
82	OHX	AR	3642	-	0,6,6	-	-	-		
82	OHX	AT	216	-	0,6,6	-	-	-		
82	OHX	A	2133	-	0,6,6	-	-	-		
82	OHX	sR	1943	-	0,6,6	-	-	-		
82	OHX	A	2139	-	0,6,6	-	-	-		
82	OHX	CE	402	-	0,6,6	-	-	-		
82	OHX	AR	3503	-	0,6,6	-	-	-		
82	OHX	1	4142	-	0,6,6	-	-	-		
82	OHX	AR	3495	-	0,6,6	-	-	-		
82	OHX	AR	3542	-	0,6,6	-	-	-		
82	OHX	AR	3460	-	0,6,6	-	-	-		
82	OHX	AR	3424	-	0,6,6	-	-	-		
82	OHX	AR	3481	-	0,6,6	-	-	-		
82	OHX	AP	502	-	0,6,6	-	-	-		
82	OHX	1	3533	-	0,6,6	-	-	-		
82	OHX	AR	3631	-	0,6,6	-	-	-		
82	OHX	1	3588	-	0,6,6	-	-	-		
82	OHX	AR	3550	-	0,6,6	-	-	-		
82	OHX	1	3541	-	0,6,6	-	-	-		
82	OHX	1	4136	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	3570	-	0,6,6	-	-	-		
82	OHX	AR	3434	-	0,6,6	-	-	-		
82	OHX	1	3446	-	0,6,6	-	-	-		
82	OHX	AT	209	-	0,6,6	-	-	-		
82	OHX	AR	3469	-	0,6,6	-	-	-		
82	OHX	A	1930	-	0,6,6	-	-	-		
82	OHX	1	3496	-	0,6,6	-	-	-		
82	OHX	AR	3489	-	0,6,6	-	-	-		
82	OHX	1	4140	-	0,6,6	-	-	-		
82	OHX	AR	3401	-	0,6,6	-	-	-		
82	OHX	sR	1916[B]	-	0,6,6	-	-	-		
82	OHX	1	3405	-	0,6,6	-	-	-		
82	OHX	sR	2007	-	0,6,6	-	-	-		
82	OHX	sR	2008	-	0,6,6	-	-	-		
82	OHX	CV	201	-	0,6,6	-	-	-		
82	OHX	1	3580	-	0,6,6	-	-	-		
82	OHX	1	4155	-	0,6,6	-	-	-		
82	OHX	AR	3553	-	0,6,6	-	-	-		
82	OHX	sR	2176	-	0,6,6	-	-	-		
82	OHX	A	1942	-	0,6,6	-	-	-		
82	OHX	A	1921	-	0,6,6	-	-	-		
82	OHX	AR	3575	-	0,5,6	-	-	-		
82	OHX	AT	212	-	0,6,6	-	-	-		
82	OHX	A	1901	-	0,6,6	-	-	-		
82	OHX	A	1947	-	0,6,6	-	-	-		
82	OHX	AR	3428	-	0,6,6	-	-	-		
82	OHX	AR	3669	-	0,5,6	-	-	-		
82	OHX	1	4080	-	0,6,6	-	-	-		
82	OHX	AR	3452	-	0,6,6	-	-	-		
82	OHX	sR	1946	-	0,6,6	-	-	-		
82	OHX	AR	3418	-	0,6,6	-	-	-		
82	OHX	A	2147	-	0,6,6	-	-	-		
82	OHX	1	3452	-	0,6,6	-	-	-		
82	OHX	1	4100	-	0,6,6	-	-	-		
82	OHX	1	4149	-	0,6,6	-	-	-		
82	OHX	AR	3440	-	0,6,6	-	-	-		
82	OHX	1	3418	-	0,6,6	-	-	-		
82	OHX	1	4058	-	0,6,6	-	-	-		
82	OHX	A	2126[A]	-	0,6,6	-	-	-		
82	OHX	c3	202	-	0,6,6	-	-	-		
82	OHX	AR	3621	-	0,6,6	-	-	-		
82	OHX	CG	303	-	0,6,6	-	-	-		
82	OHX	1	3561	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3450	-	0,6,6	-	-	-		
82	OHX	1	3593	-	0,6,6	-	-	-		
82	OHX	AR	3432	-	0,6,6	-	-	-		
82	OHX	4	212	-	0,6,6	-	-	-		
82	OHX	AR	3594	-	0,6,6	-	-	-		
82	OHX	A	1936	-	0,6,6	-	-	-		
82	OHX	1	4115	-	0,6,6	-	-	-		
82	OHX	sR	2003	-	0,6,6	-	-	-		
82	OHX	AR	3596	-	0,6,6	-	-	-		
82	OHX	AR	3420	-	0,6,6	-	-	-		
82	OHX	k	403	-	0,6,6	-	-	-		
82	OHX	1	4116	-	0,6,6	-	-	-		
82	OHX	AR	3459	-	0,6,6	-	-	-		
82	OHX	1	4092	-	0,6,6	-	-	-		
82	OHX	1	4114[A]	-	0,6,6	-	-	-		
82	OHX	AR	3592	-	0,6,6	-	-	-		
82	OHX	1	3491	-	0,6,6	-	-	-		
82	OHX	AR	3629	-	0,6,6	-	-	-		
82	OHX	AR	3641	-	0,6,6	-	-	-		
82	OHX	1	3517	-	0,6,6	-	-	-		
82	OHX	1	3555	-	0,6,6	-	-	-		
82	OHX	1	4078	-	0,6,6	-	-	-		
82	OHX	AR	4136	-	0,6,6	-	-	-		
82	OHX	sR	1984	-	0,6,6	-	-	-		
82	OHX	1	3542	-	0,6,6	-	-	-		
82	OHX	1	4131	-	0,6,6	-	-	-		
82	OHX	AR	3544	-	0,6,6	-	-	-		
82	OHX	A	1951	-	0,6,6	-	-	-		
82	OHX	1	3563	-	0,6,6	-	-	-		
82	OHX	1	3546	-	0,6,6	-	-	-		
82	OHX	sR	1903	-	0,6,6	-	-	-		
82	OHX	A	1948	-	0,6,6	-	-	-		
82	OHX	A	2112	-	0,6,6	-	-	-		
82	OHX	AR	3549	-	0,6,6	-	-	-		
82	OHX	A	1909	-	0,6,6	-	-	-		
82	OHX	AR	3607	-	0,6,6	-	-	-		
82	OHX	sR	1928	-	0,6,6	-	-	-		
82	OHX	AR	3472	-	0,6,6	-	-	-		
82	OHX	sR	1981	-	0,6,6	-	-	-		
82	OHX	sR	1945	-	0,6,6	-	-	-		
82	OHX	sR	1915	-	0,6,6	-	-	-		
82	OHX	AR	4140	-	0,6,6	-	-	-		
82	OHX	AR	3444	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3402	-	0,6,6	-	-	-		
82	OHX	A	2138	-	0,6,6	-	-	-		
82	OHX	A	1950	-	0,6,6	-	-	-		
82	OHX	AR	3437	-	0,6,6	-	-	-		
82	OHX	AR	3554	-	0,6,6	-	-	-		
82	OHX	1	3602	-	0,6,6	-	-	-		
82	OHX	AR	3603	-	0,6,6	-	-	-		
82	OHX	AR	3666	-	0,6,6	-	-	-		
82	OHX	AR	3615	-	0,6,6	-	-	-		
82	OHX	sR	2006	-	0,6,6	-	-	-		
82	OHX	AR	3613	-	0,6,6	-	-	-		
82	OHX	1	3423	-	0,6,6	-	-	-		
82	OHX	AR	3467	-	0,6,6	-	-	-		
82	OHX	AR	3510	-	0,6,6	-	-	-		
82	OHX	sR	2002	-	0,6,6	-	-	-		
82	OHX	1	3548	-	0,6,6	-	-	-		
82	OHX	1	3439	-	0,6,6	-	-	-		
82	OHX	1	3584	-	0,6,6	-	-	-		
82	OHX	1	3471	-	0,6,6	-	-	-		
82	OHX	AR	4149	-	0,6,6	-	-	-		
82	OHX	A	1970	-	0,6,6	-	-	-		
82	OHX	AR	3589	-	0,6,6	-	-	-		
85	SPD	AR	4204	-	9,9,9	0.33	0	8,8,8	0.88	0
82	OHX	AR	4141	-	0,6,6	-	-	-		
82	OHX	AR	3463	-	0,6,6	-	-	-		
82	OHX	1	3401	-	0,6,6	-	-	-		
82	OHX	1	4130	-	0,6,6	-	-	-		
82	OHX	1	4141	-	0,6,6	-	-	-		
82	OHX	s8	301	-	0,6,6	-	-	-		
82	OHX	AR	3521	-	0,6,6	-	-	-		
82	OHX	CK	201	-	0,6,6	-	-	-		
82	OHX	AR	3608	-	0,6,6	-	-	-		
82	OHX	1	3567	-	0,6,6	-	-	-		
82	OHX	A	1919	-	0,6,6	-	-	-		
82	OHX	1	3519	-	0,6,6	-	-	-		
82	OHX	1	3587	-	0,6,6	-	-	-		
82	OHX	A	2111	-	0,6,6	-	-	-		
82	OHX	sR	2020	-	0,6,6	-	-	-		
82	OHX	1	3526	-	0,6,6	-	-	-		
82	OHX	AR	3539	-	0,6,6	-	-	-		
82	OHX	AR	3520	-	0,6,6	-	-	-		
82	OHX	AR	3595	-	0,6,6	-	-	-		
82	OHX	AR	3582	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	sR	2171	-	0,6,6	-	-	-		
82	OHX	AR	3558	-	0,6,6	-	-	-		
82	OHX	sR	1942	-	0,6,6	-	-	-		
82	OHX	AR	3485	-	0,6,6	-	-	-		
82	OHX	AR	4161	-	0,6,6	-	-	-		
82	OHX	AR	3524	-	0,6,6	-	-	-		
82	OHX	3	221	-	0,6,6	-	-	-		
82	OHX	AR	3494	-	0,6,6	-	-	-		
82	OHX	AR	3504	-	0,6,6	-	-	-		
82	OHX	AR	3427	-	0,6,6	-	-	-		
82	OHX	sR	1969	-	0,6,6	-	-	-		
82	OHX	AR	3479	-	0,6,6	-	-	-		
82	OHX	AR	4137	-	0,6,6	-	-	-		
82	OHX	1	3528	-	0,6,6	-	-	-		
82	OHX	1	4154	-	0,6,6	-	-	-		
82	OHX	1	3494	-	0,6,6	-	-	-		
82	OHX	A	2124	-	0,6,6	-	-	-		
82	OHX	AR	3600	-	0,6,6	-	-	-		
82	OHX	4	209	-	0,6,6	-	-	-		
82	OHX	A	2123	-	0,6,6	-	-	-		
82	OHX	sR	2010	-	0,6,6	-	-	-		
82	OHX	AR	3412	-	0,6,6	-	-	-		
82	OHX	s4	301	-	0,6,6	-	-	-		
82	OHX	sR	1931	-	0,6,6	-	-	-		
82	OHX	1	4103	-	0,6,6	-	-	-		
82	OHX	AR	3473	-	0,6,6	-	-	-		
82	OHX	AT	208	-	0,6,6	-	-	-		
82	OHX	AR	4146	-	0,6,6	-	-	-		
82	OHX	sR	1971	-	0,6,6	-	-	-		
82	OHX	1	4081	-	0,6,6	-	-	-		
82	OHX	1	3406	-	0,6,6	-	-	-		
82	OHX	1	4098	-	0,6,6	-	-	-		
82	OHX	AR	3616	-	0,6,6	-	-	-		
82	OHX	4	206	-	0,6,6	-	-	-		
82	OHX	1	4146	-	0,6,6	-	-	-		
82	OHX	AG	202	-	0,6,6	-	-	-		
82	OHX	1	3411	-	0,6,6	-	-	-		
82	OHX	3	220	-	0,6,6	-	-	-		
82	OHX	A	1924	-	0,6,6	-	-	-		
82	OHX	A	1935	-	0,6,6	-	-	-		
82	OHX	1	3590	-	0,6,6	-	-	-		
82	OHX	1	4088	-	0,6,6	-	-	-		
82	OHX	AK	102	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	OHX	A	1939	-	0,6,6	-	-	-		
82	OHX	A	1940[A]	-	0,6,6	-	-	-		
82	OHX	1	3467	-	0,6,6	-	-	-		
82	OHX	1	3539	-	0,6,6	-	-	-		
82	OHX	sR	1908	-	0,6,6	-	-	-		
82	OHX	T	201	-	0,6,6	-	-	-		
82	OHX	AR	3543	-	0,6,6	-	-	-		
82	OHX	sR	1960	-	0,6,6	-	-	-		
82	OHX	1	3407	-	0,6,6	-	-	-		
82	OHX	A	1952	-	0,6,6	-	-	-		
82	OHX	AR	3551	-	0,6,6	-	-	-		
82	OHX	sR	1993	-	0,6,6	-	-	-		
82	OHX	sR	1937	-	0,6,6	-	-	-		
82	OHX	AR	3538	-	0,6,6	-	-	-		
82	OHX	4	208	-	0,6,6	-	-	-		
82	OHX	1	3435	-	0,6,6	-	-	-		
82	OHX	1	3522	-	0,6,6	-	-	-		
82	OHX	AR	3508	-	0,6,6	-	-	-		
82	OHX	A	1931	-	0,6,6	-	-	-		
82	OHX	A	2119	-	0,6,6	-	-	-		
82	OHX	l	405	-	0,6,6	-	-	-		
82	OHX	AR	3486	-	0,6,6	-	-	-		
82	OHX	AR	3571	-	0,6,6	-	-	-		
82	OHX	1	3413	-	0,6,6	-	-	-		
82	OHX	AR	3458	-	0,6,6	-	-	-		
82	OHX	1	3421	-	0,6,6	-	-	-		
82	OHX	1	3436	-	0,6,6	-	-	-		
82	OHX	A	1962	-	0,6,6	-	-	-		
82	OHX	sR	1950	-	0,6,6	-	-	-		
82	OHX	z	202	-	0,6,6	-	-	-		
82	OHX	A	1961	-	0,6,6	-	-	-		
82	OHX	sR	1963	-	0,6,6	-	-	-		
82	OHX	sR	2025	-	0,6,6	-	-	-		
82	OHX	AR	3500	-	0,6,6	-	-	-		
82	OHX	AR	4163	-	0,6,6	-	-	-		
82	OHX	CP	302	-	0,6,6	-	-	-		
82	OHX	AR	3652	-	0,6,6	-	-	-		
82	OHX	sR	1954	-	0,6,6	-	-	-		
82	OHX	1	4127	-	0,6,6	-	-	-		
82	OHX	AR	3409	-	0,6,6	-	-	-		
82	OHX	AR	3599	-	0,6,6	-	-	-		
82	OHX	1	4124	-	0,6,6	-	-	-		
82	OHX	AR	4126	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3433	-	0,6,6	-	-	-		
82	OHX	A	1972	-	0,6,6	-	-	-		
82	OHX	1	4113	-	0,6,6	-	-	-		
82	OHX	A	2140	-	0,6,6	-	-	-		
82	OHX	sR	2173	-	0,6,6	-	-	-		
82	OHX	4	204	-	0,6,6	-	-	-		
82	OHX	AR	3423	-	0,6,6	-	-	-		
82	OHX	1	3564	-	0,6,6	-	-	-		
82	OHX	A	2129	-	0,6,6	-	-	-		
82	OHX	AR	3406	-	0,6,6	-	-	-		
82	OHX	AR	4152	-	0,6,6	-	-	-		
82	OHX	A	1913	-	0,6,6	-	-	-		
82	OHX	1	3492	-	0,6,6	-	-	-		
82	OHX	1	3476	-	0,6,6	-	-	-		
82	OHX	1	3460	-	0,6,6	-	-	-		
82	OHX	AR	3461	-	0,6,6	-	-	-		
82	OHX	sR	2172	-	0,6,6	-	-	-		
82	OHX	AR	3657	-	0,6,6	-	-	-		
82	OHX	AR	3404	-	0,6,6	-	-	-		
82	OHX	A	1904	-	0,6,6	-	-	-		
82	OHX	sR	1974	-	0,6,6	-	-	-		
82	OHX	A	2121	-	0,6,6	-	-	-		
82	OHX	A	2143	-	0,6,6	-	-	-		
82	OHX	AR	3417	-	0,6,6	-	-	-		
82	OHX	sR	1901	-	0,6,6	-	-	-		
82	OHX	AR	3630	-	0,6,6	-	-	-		
82	OHX	AR	3653	-	0,6,6	-	-	-		
82	OHX	h	401	-	0,6,6	-	-	-		
82	OHX	AS	203	-	0,6,6	-	-	-		
82	OHX	AR	3639	-	0,6,6	-	-	-		
82	OHX	U	201	-	0,6,6	-	-	-		
82	OHX	AR	3632	-	0,6,6	-	-	-		
82	OHX	1	4151	-	0,6,6	-	-	-		
82	OHX	AR	3506	-	0,6,6	-	-	-		
82	OHX	sR	1975	-	0,6,6	-	-	-		
82	OHX	AR	3497	-	0,6,6	-	-	-		
82	OHX	AR	3604	-	0,6,6	-	-	-		
82	OHX	AR	3646	-	0,6,6	-	-	-		
82	OHX	A	2106	-	0,6,6	-	-	-		
82	OHX	A	1926	-	0,6,6	-	-	-		
82	OHX	3	204	-	0,6,6	-	-	-		
82	OHX	AR	3413	-	0,6,6	-	-	-		
82	OHX	2	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	4107	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	X1K	AR	4205	-	-	0/8/58/58	0/3/3/3
85	SPD	AR	4204	-	-	2/7/7/7	-
86	X1K	1	4181	-	-	2/8/58/58	0/3/3/3
85	SPD	1	4180	-	-	2/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	AR	4205	X1K	C1-C10	-2.44	1.52	1.56
86	AR	4205	X1K	C5-C10	2.09	1.59	1.56
86	1	4181	X1K	C5-C10	2.03	1.59	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	1	4181	X1K	C1-C10-C5	-7.82	107.86	116.78
86	1	4181	X1K	C20-C1-C2	-5.82	97.05	109.03
86	AR	4205	X1K	C1-C10-C5	-5.21	110.83	116.78
86	1	4181	X1K	C20-C1-C	-4.51	101.24	107.89
86	AR	4205	X1K	C20-C1-C	-4.22	101.68	107.89
86	AR	4205	X1K	C20-C1-C2	-3.98	100.83	109.03
86	AR	4205	X1K	C20-C1-C10	-3.84	99.95	111.53
86	1	4181	X1K	C2-C1-C10	3.67	113.89	108.42
86	1	4181	X1K	C20-C1-C10	-3.57	100.77	111.53
86	1	4181	X1K	C-C1-C10	3.37	121.69	111.53
86	1	4181	X1K	C-C1-C2	3.36	115.94	109.03
86	AR	4205	X1K	C-C1-C10	3.34	121.63	111.53
86	AR	4205	X1K	C-C1-C2	3.17	115.56	109.03
86	AR	4205	X1K	C2-C1-C10	2.69	112.43	108.42
86	1	4181	X1K	C9-C8-C7	2.27	113.95	110.84
86	AR	4205	X1K	O-C8-C7	2.17	115.72	110.25
86	AR	4205	X1K	C9-C8-C7	2.10	113.71	110.84

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	1	4181	X1K	C13-C14-C15-C16
85	AR	4204	SPD	C3-C4-C5-N6
85	1	4180	SPD	C3-C4-C5-N6
86	1	4181	X1K	C6-C13-C14-C15
85	AR	4204	SPD	N1-C2-C3-C4
85	1	4180	SPD	C2-C3-C4-C5

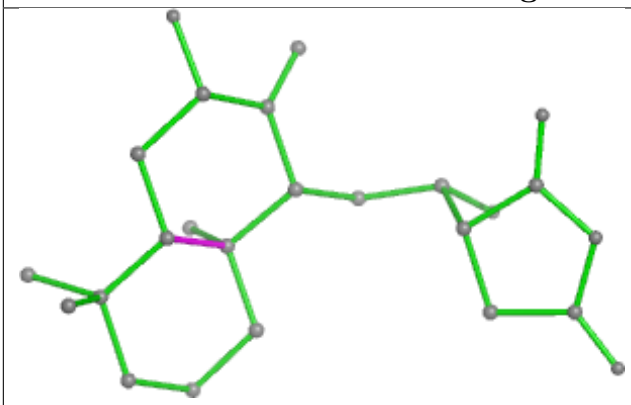
There are no ring outliers.

2 monomers are involved in 2 short contacts:

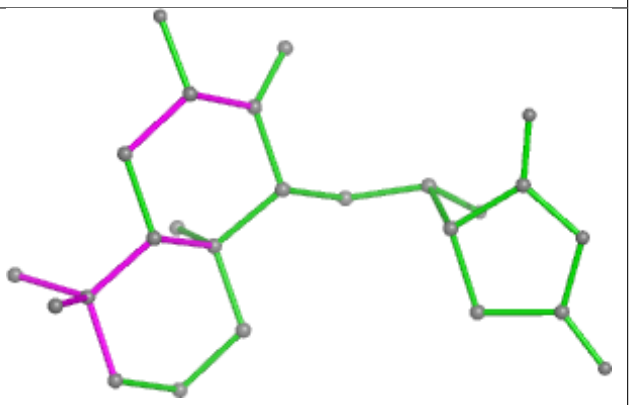
Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	CG	304	OHX	0	1
82	AR	3440	OHX	0	1

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

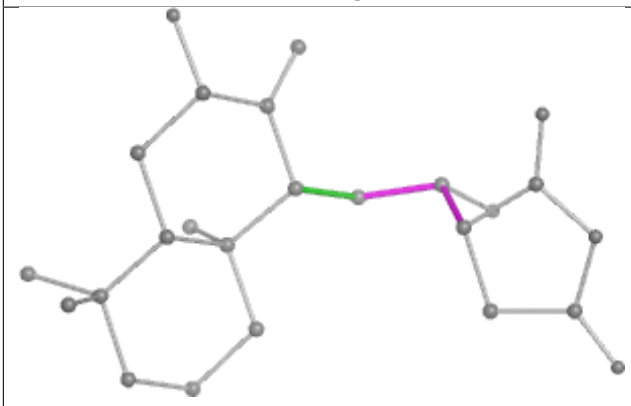
Ligand X1K 1 4181



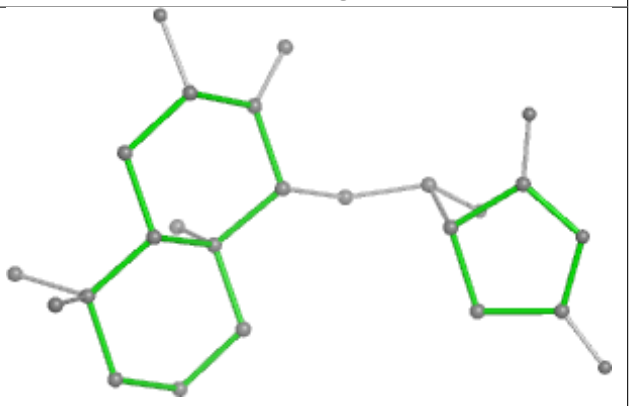
Bond lengths



Bond angles

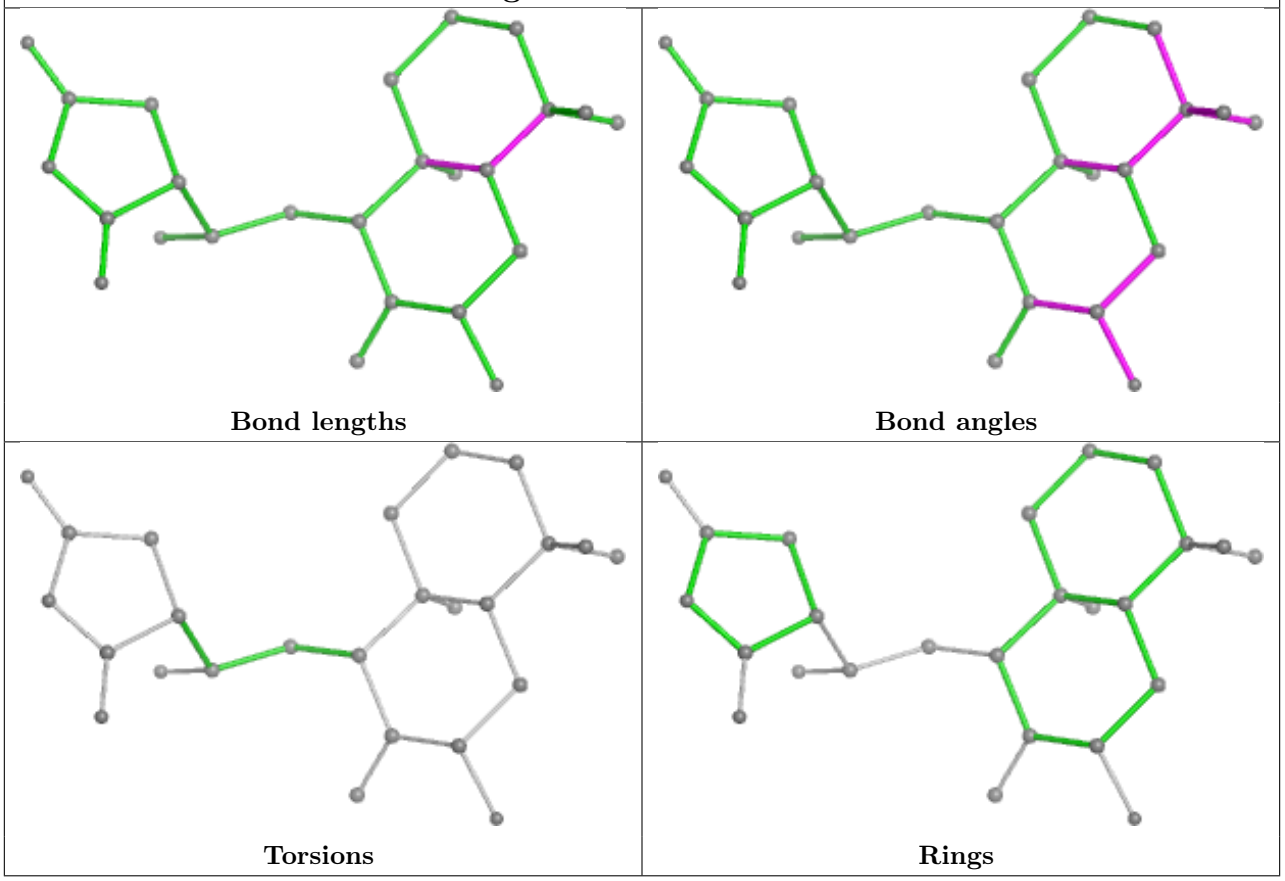


Torsions



Rings

Ligand X1K AR 4205



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
58	c0	1
47	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c0	84:GLU	C	87:HIS	N	9.31
1	A	1716:C	O3'	1717:G	P	4.49

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	3149/3396 (92%)	-0.15	19 (0%) 85 75	48, 78, 189, 306	0
1	AR	3147/3396 (92%)	-0.13	26 (0%) 82 69	50, 76, 175, 286	0
2	3	121/121 (100%)	-0.40	0 100 100	61, 92, 117, 150	0
2	AS	121/121 (100%)	-0.43	0 100 100	60, 80, 95, 157	0
3	4	158/158 (100%)	-0.38	0 100 100	59, 79, 145, 230	0
3	AT	158/158 (100%)	-0.22	1 (0%) 85 75	62, 85, 163, 234	0
4	CD	252/254 (99%)	0.63	22 (8%) 17 12	52, 79, 112, 181	0
4	j	252/254 (99%)	0.72	29 (11%) 11 7	49, 77, 104, 155	0
5	CE	386/387 (99%)	0.39	17 (4%) 39 26	48, 69, 98, 157	0
5	k	386/387 (99%)	0.47	15 (3%) 44 29	50, 79, 111, 168	0
6	CF	361/362 (99%)	0.46	20 (5%) 32 20	49, 78, 111, 149	0
6	l	361/362 (99%)	0.35	15 (4%) 41 27	47, 74, 113, 161	0
7	CG	296/297 (99%)	0.31	9 (3%) 52 37	58, 83, 135, 238	0
7	m	296/297 (99%)	0.27	7 (2%) 59 44	65, 102, 154, 184	0
8	CH	156/176 (88%)	0.30	7 (4%) 39 25	54, 80, 121, 166	0
8	n	156/176 (88%)	0.34	2 (1%) 74 59	55, 76, 113, 156	0
9	CI	222/244 (90%)	0.36	4 (1%) 67 52	52, 68, 111, 187	0
9	o	222/244 (90%)	0.19	5 (2%) 61 45	51, 70, 122, 188	0
10	CJ	233/256 (91%)	0.55	11 (4%) 37 24	76, 114, 158, 185	0
10	p	233/256 (91%)	0.68	15 (6%) 27 17	67, 103, 162, 211	0
11	CK	191/191 (100%)	0.18	2 (1%) 79 65	54, 77, 116, 203	0
11	q	191/191 (100%)	0.48	9 (4%) 37 24	63, 89, 122, 192	0
12	CL	211/221 (95%)	0.12	3 (1%) 73 58	50, 79, 119, 152	0
12	r	211/221 (95%)	0.20	8 (3%) 44 30	53, 81, 132, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	CM	169/174 (97%)	0.40	5 (2%) 52 37	58, 84, 117, 181	0
13	s	169/174 (97%)	0.60	9 (5%) 33 21	76, 104, 139, 197	0
14	CN	193/199 (96%)	0.42	11 (5%) 30 19	56, 89, 149, 196	0
14	t	193/199 (96%)	0.41	15 (7%) 20 14	51, 83, 132, 176	0
15	CO	136/138 (98%)	0.28	6 (4%) 39 26	58, 75, 105, 139	0
15	u	136/138 (98%)	0.21	5 (3%) 45 30	60, 77, 112, 184	0
16	CP	203/204 (99%)	0.47	9 (4%) 39 26	61, 83, 102, 115	0
16	v	203/204 (99%)	0.56	4 (1%) 64 49	51, 77, 94, 111	0
17	CQ	197/199 (98%)	0.25	6 (3%) 52 37	50, 64, 112, 171	0
17	w	197/199 (98%)	0.07	5 (2%) 58 42	50, 69, 102, 139	0
18	CR	183/184 (99%)	0.34	8 (4%) 39 26	53, 73, 210, 245	0
18	x	183/184 (99%)	0.42	11 (6%) 29 18	51, 74, 157, 193	0
19	CS	185/186 (99%)	0.59	10 (5%) 32 21	56, 78, 96, 125	0
19	y	185/186 (99%)	0.59	14 (7%) 21 14	55, 73, 93, 112	0
20	CT	188/189 (99%)	0.43	12 (6%) 27 17	62, 91, 170, 224	0
20	z	188/189 (99%)	0.30	9 (4%) 36 24	63, 95, 173, 222	0
21	0	172/172 (100%)	0.12	7 (4%) 42 28	55, 75, 109, 161	0
21	CU	172/172 (100%)	0.07	4 (2%) 61 45	53, 71, 101, 133	0
22	2	159/160 (99%)	0.42	10 (6%) 27 17	51, 79, 124, 175	0
22	CV	159/160 (99%)	0.41	9 (5%) 30 19	54, 72, 135, 215	0
23	5	100/121 (82%)	0.42	4 (4%) 43 28	87, 130, 170, 182	0
23	CW	100/121 (82%)	0.58	6 (6%) 29 18	82, 121, 165, 174	0
24	6	136/137 (99%)	0.59	8 (5%) 29 19	57, 79, 116, 164	0
24	CX	136/137 (99%)	0.41	4 (2%) 54 38	49, 69, 99, 160	0
25	7	98/155 (63%)	0.67	8 (8%) 19 13	62, 94, 197, 210	0
25	CY	124/155 (80%)	0.62	11 (8%) 17 11	56, 100, 182, 220	0
26	8	121/142 (85%)	0.36	6 (4%) 35 23	63, 88, 123, 174	0
26	CZ	121/142 (85%)	0.87	15 (12%) 9 6	64, 93, 132, 194	0
27	9	126/127 (99%)	0.11	2 (1%) 70 55	61, 83, 115, 144	0
27	DA	124/127 (97%)	0.47	2 (1%) 70 55	58, 86, 110, 149	0
28	AA	135/136 (99%)	0.37	3 (2%) 62 46	83, 117, 153, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DB	135/136 (99%)	0.30	2 (1%) 71 57	94, 125, 164, 185	0
29	AB	148/149 (99%)	0.44	7 (4%) 37 24	48, 73, 109, 147	0
29	DC	148/149 (99%)	0.36	4 (2%) 56 40	47, 74, 115, 159	0
30	AC	58/59 (98%)	0.84	8 (13%) 8 5	52, 87, 140, 194	0
30	DD	58/59 (98%)	0.81	7 (12%) 10 7	52, 82, 114, 138	0
31	AD	97/105 (92%)	0.12	3 (3%) 51 36	80, 110, 148, 176	0
31	DE	97/105 (92%)	0.38	5 (5%) 34 22	80, 110, 153, 183	0
32	AE	109/113 (96%)	0.96	14 (12%) 9 6	61, 91, 150, 200	0
32	DF	109/113 (96%)	0.54	5 (4%) 38 25	57, 84, 148, 190	0
33	AF	127/130 (97%)	0.44	4 (3%) 51 36	51, 69, 100, 146	0
33	DG	127/130 (97%)	0.24	1 (0%) 82 69	52, 71, 99, 150	0
34	AG	106/107 (99%)	0.08	0 100 100	51, 68, 96, 128	0
34	DH	106/107 (99%)	0.32	1 (0%) 81 67	50, 68, 108, 140	0
35	AH	112/121 (92%)	0.90	13 (11%) 11 7	60, 96, 140, 188	0
35	DI	112/121 (92%)	0.53	10 (8%) 17 11	63, 96, 150, 185	0
36	AI	119/120 (99%)	0.37	5 (4%) 41 27	57, 88, 122, 144	0
36	DJ	119/120 (99%)	0.46	7 (5%) 29 19	69, 97, 127, 151	0
37	AJ	99/100 (99%)	0.20	0 100 100	66, 93, 142, 176	0
37	DK	99/100 (99%)	0.49	7 (7%) 23 16	69, 103, 146, 194	0
38	AK	87/88 (98%)	0.41	4 (4%) 38 25	57, 71, 91, 191	0
38	DL	87/88 (98%)	0.53	5 (5%) 30 19	54, 74, 114, 156	0
39	AL	77/78 (98%)	0.52	3 (3%) 44 29	81, 118, 162, 170	0
39	DM	77/78 (98%)	0.53	3 (3%) 44 29	86, 122, 165, 198	0
40	AM	50/51 (98%)	0.50	4 (8%) 20 13	57, 80, 99, 119	0
40	DN	50/51 (98%)	0.50	2 (4%) 43 28	64, 82, 102, 127	0
41	AN	52/128 (40%)	0.27	3 (5%) 30 19	58, 79, 113, 144	0
41	DO	52/128 (40%)	0.19	2 (3%) 44 30	51, 67, 95, 173	0
42	AO	25/25 (100%)	1.39	5 (20%) 3 2	68, 81, 103, 108	0
42	DP	25/25 (100%)	1.25	6 (24%) 2 2	56, 77, 99, 108	0
43	AP	105/106 (99%)	0.20	2 (1%) 66 50	53, 82, 122, 163	0
43	DQ	105/106 (99%)	0.21	3 (2%) 54 38	55, 78, 124, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	AQ	91/92 (98%)	0.51	5 (5%) 32 20	54, 84, 113, 158	0
44	DR	91/92 (98%)	0.62	6 (6%) 26 17	60, 83, 119, 125	0
45	i	159/273 (58%)	0.45	7 (4%) 39 26	72, 125, 187, 206	0
45	sM	63/273 (23%)	0.70	4 (6%) 27 17	61, 137, 179, 196	0
46	p0	143/311 (45%)	0.60	12 (8%) 18 12	89, 145, 187, 210	0
47	A	1781/1800 (98%)	0.02	29 (1%) 70 55	74, 110, 232, 314	0
47	sR	1783/1800 (99%)	-0.08	8 (0%) 89 80	60, 104, 221, 293	0
48	B	206/252 (81%)	0.35	3 (1%) 71 57	89, 134, 178, 198	0
48	s0	206/252 (81%)	0.35	5 (2%) 59 44	82, 122, 159, 205	0
49	C	214/255 (83%)	0.80	21 (9%) 14 10	93, 151, 197, 234	0
49	s1	216/255 (84%)	0.35	9 (4%) 41 27	65, 110, 149, 197	0
50	D	217/254 (85%)	0.18	7 (3%) 50 35	81, 113, 148, 190	0
50	s2	217/254 (85%)	0.06	3 (1%) 73 58	67, 103, 144, 163	0
51	E	223/240 (92%)	0.34	12 (5%) 32 21	82, 120, 159, 208	0
51	s3	223/240 (92%)	0.14	5 (2%) 62 46	97, 138, 185, 230	0
52	F	260/261 (99%)	0.82	31 (11%) 10 7	73, 114, 150, 177	0
52	s4	260/261 (99%)	0.41	8 (3%) 51 36	73, 102, 135, 191	0
53	G	206/225 (91%)	0.52	10 (4%) 36 23	94, 140, 177, 200	0
53	s5	206/225 (91%)	0.91	20 (9%) 15 10	92, 146, 183, 211	0
54	H	226/236 (95%)	0.58	23 (10%) 13 9	73, 122, 160, 191	0
54	s6	218/236 (92%)	0.18	7 (3%) 50 35	61, 103, 153, 192	0
55	I	184/190 (96%)	0.51	5 (2%) 56 40	85, 144, 192, 220	0
55	s7	186/190 (97%)	0.68	16 (8%) 18 12	74, 132, 187, 212	0
56	J	188/200 (94%)	0.48	6 (3%) 50 35	57, 99, 150, 171	0
56	s8	188/200 (94%)	0.60	14 (7%) 22 15	71, 97, 153, 174	0
57	K	185/197 (93%)	0.59	10 (5%) 32 21	84, 123, 164, 226	0
57	s9	185/197 (93%)	0.65	15 (8%) 19 13	72, 105, 158, 200	0
58	L	96/105 (91%)	0.75	12 (12%) 9 6	89, 133, 185, 197	0
58	c0	96/105 (91%)	0.46	7 (7%) 22 15	118, 154, 202, 225	0
59	M	155/156 (99%)	0.66	13 (8%) 18 12	68, 98, 189, 220	0
59	c1	146/156 (93%)	1.14	25 (17%) 5 3	62, 94, 159, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
60	N	124/143 (86%)	0.43	4 (3%) 50 35	119, 182, 209, 234	0
60	c2	124/143 (86%)	0.48	2 (1%) 70 55	152, 192, 221, 243	0
61	O	150/151 (99%)	0.32	5 (3%) 49 34	70, 111, 148, 172	0
61	c3	150/151 (99%)	0.47	8 (5%) 33 21	67, 103, 136, 165	0
62	P	127/138 (92%)	1.18	20 (15%) 6 4	82, 145, 187, 212	0
62	c4	128/138 (92%)	0.44	5 (3%) 44 29	64, 112, 151, 166	0
63	Q	124/142 (87%)	0.81	14 (11%) 11 8	80, 117, 189, 204	0
63	c5	135/142 (95%)	1.06	26 (19%) 4 3	91, 142, 183, 203	0
64	R	141/143 (98%)	0.38	2 (1%) 73 58	83, 127, 156, 170	0
64	c6	142/143 (99%)	0.81	19 (13%) 8 5	81, 133, 179, 206	0
65	S	120/136 (88%)	0.23	4 (3%) 49 34	79, 134, 183, 202	0
66	T	145/146 (99%)	0.32	7 (4%) 36 24	71, 127, 175, 198	0
66	c8	145/146 (99%)	0.57	9 (6%) 28 18	99, 135, 181, 210	0
67	U	143/144 (99%)	0.37	5 (3%) 47 32	88, 126, 163, 175	0
67	c9	143/144 (99%)	0.70	10 (6%) 24 16	88, 132, 164, 185	0
68	V	107/121 (88%)	0.64	7 (6%) 26 17	77, 133, 191, 200	0
68	d0	110/121 (90%)	0.55	5 (4%) 39 25	88, 156, 200, 221	0
69	W	87/87 (100%)	0.21	1 (1%) 77 62	96, 129, 162, 189	0
69	d1	87/87 (100%)	0.07	1 (1%) 77 62	71, 110, 156, 176	0
70	X	129/130 (99%)	0.72	9 (6%) 24 16	80, 110, 134, 162	0
70	d2	129/130 (99%)	0.23	0 100 100	66, 91, 118, 141	0
71	Y	144/145 (99%)	0.98	19 (13%) 8 5	62, 93, 121, 149	0
71	d3	144/145 (99%)	0.44	4 (2%) 55 39	59, 82, 109, 155	0
72	Z	134/135 (99%)	0.52	5 (3%) 45 30	79, 122, 171, 211	0
72	d4	134/135 (99%)	0.51	9 (6%) 25 17	69, 106, 148, 173	0
73	a	70/108 (64%)	0.46	4 (5%) 30 19	99, 160, 196, 215	0
73	d5	69/108 (63%)	0.58	6 (8%) 17 12	117, 158, 192, 203	0
74	b	97/119 (81%)	1.31	23 (23%) 2 2	83, 123, 187, 223	0
74	d6	97/119 (81%)	0.74	11 (11%) 11 8	66, 96, 144, 177	0
75	c	81/82 (98%)	0.24	2 (2%) 58 42	80, 127, 180, 205	0
75	d7	81/82 (98%)	0.11	2 (2%) 58 42	70, 116, 178, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
76	d	63/67 (94%)	0.38	3 (4%) 36 24	84, 146, 178, 207	0
76	d8	63/67 (94%)	1.04	11 (17%) 5 3	106, 155, 194, 231	0
77	d9	53/56 (94%)	0.97	4 (7%) 22 15	89, 115, 175, 196	0
77	e	53/56 (94%)	1.20	8 (15%) 6 4	79, 107, 137, 194	0
78	e0	62/63 (98%)	0.41	4 (6%) 26 17	83, 118, 170, 210	0
78	f	60/63 (95%)	0.38	2 (3%) 49 34	83, 119, 183, 202	0
79	e1	51/152 (33%)	0.88	1 (1%) 64 49	150, 184, 233, 248	0
79	g	71/152 (46%)	1.11	15 (21%) 3 2	115, 164, 199, 215	0
80	Rb	318/319 (99%)	0.63	25 (7%) 20 14	113, 162, 197, 217	0
80	h	318/319 (99%)	0.35	15 (4%) 37 24	89, 139, 181, 205	0
81	c7	117/136 (86%)	0.23	3 (2%) 57 41	88, 128, 171, 206	0
All	All	33026/35569 (92%)	0.28	1326 (4%) 43 28	47, 95, 178, 314	0

All (1326) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
59	c1	4	GLU	10.2
53	s5	153	GLY	7.7
59	c1	3	THR	7.3
25	CY	43	ARG	7.3
22	CV	86	GLU	6.7
4	j	250	GLN	5.9
35	AH	20	ILE	5.7
1	1	2205	U	5.7
59	c1	2	SER	5.6
35	DI	34	HIS	5.5
73	a	65	LEU	5.4
4	CD	253	GLN	5.4
25	7	82	ILE	5.3
56	J	21	PHE	5.3
18	x	184	ALA	5.2
64	c6	138	PHE	5.1
4	CD	190	ARG	5.1
60	N	119	SER	4.9
1	AR	2971	A	4.9
54	H	80	ASN	4.9
71	Y	3	LYS	4.9
52	F	142	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
78	f	2	ALA	4.9
52	F	25	GLY	4.9
38	DL	48	ASN	4.8
80	h	79	TYR	4.8
5	k	17	LEU	4.8
54	H	68	LEU	4.8
57	K	3	ARG	4.8
63	Q	101	ALA	4.8
22	CV	77	ASN	4.8
20	z	72	GLU	4.7
5	CE	245	GLY	4.7
43	AP	36	PHE	4.7
39	AL	6	THR	4.7
6	l	54	GLU	4.7
77	e	5	ASN	4.7
1	AR	2505	U	4.7
74	b	2	PRO	4.6
76	d8	26	THR	4.6
46	p0	27	VAL	4.6
62	P	89	THR	4.6
80	h	78	ALA	4.6
23	5	89	LEU	4.6
38	DL	88	ALA	4.5
66	c8	17	LEU	4.5
74	b	85	ARG	4.5
19	y	145	ASN	4.5
20	z	51	VAL	4.5
73	d5	50	ILE	4.5
62	P	40	ALA	4.4
59	c1	50	GLU	4.4
61	O	2	GLY	4.4
80	Rb	27	ALA	4.4
24	6	137	VAL	4.4
59	M	150	ASN	4.4
10	CJ	106	LYS	4.4
54	H	74	LYS	4.4
1	1	3079	U	4.4
4	j	235	ALA	4.4
46	p0	86	PHE	4.4
49	s1	218	LEU	4.4
59	c1	21	ASN	4.4
5	k	4	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
14	CN	46	ILE	4.3
47	A	1193	A	4.3
14	t	46	ILE	4.3
54	H	65	GLN	4.3
80	h	81	LEU	4.3
30	AC	26	THR	4.2
4	CD	246	LEU	4.2
4	CD	252	THR	4.2
47	A	913	G	4.2
59	M	120	GLY	4.2
4	j	176	ASP	4.2
66	T	28	ILE	4.2
53	G	26	ALA	4.2
17	CQ	182	ASN	4.1
53	s5	182	ALA	4.1
64	c6	44	LEU	4.1
17	CQ	3	VAL	4.1
9	o	157	ASN	4.1
58	L	24	LYS	4.1
58	L	30	ALA	4.1
71	d3	21	ASN	4.0
46	p0	28	VAL	4.0
52	F	58	GLY	4.0
55	I	98	ILE	4.0
71	Y	91	GLY	4.0
80	h	136	ILE	4.0
66	T	17	LEU	4.0
72	d4	18	LEU	4.0
22	CV	79	MET	4.0
36	DJ	84	LYS	4.0
56	s8	61	GLU	4.0
58	c0	25	LYS	3.9
63	c5	105	VAL	3.9
6	l	96	GLY	3.9
56	s8	60	ILE	3.9
18	CR	160	ALA	3.9
66	T	44	ASN	3.9
1	AR	2504	U	3.9
35	AH	19	LYS	3.9
70	X	2	THR	3.9
57	s9	101	VAL	3.9
70	X	26	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
62	P	83	ILE	3.9
47	A	658	C	3.9
47	A	1657	U	3.9
26	CZ	37	THR	3.8
15	u	60	LEU	3.8
6	CF	332	LYS	3.8
17	w	80	PHE	3.8
76	d	44	VAL	3.8
23	CW	56	VAL	3.8
30	AC	29	TYR	3.8
18	CR	161	ALA	3.8
77	e	20	GLN	3.8
71	Y	103	LEU	3.8
18	CR	159	LYS	3.8
53	s5	147	THR	3.8
19	y	154	GLY	3.8
72	d4	69	SER	3.8
74	d6	7	SER	3.8
54	H	156	PHE	3.8
74	b	86	VAL	3.8
29	DC	78	LEU	3.8
1	AR	2506	U	3.8
51	E	50	ILE	3.8
61	O	141	TYR	3.8
46	p0	87	VAL	3.7
31	AD	14	LEU	3.7
23	CW	14	THR	3.7
53	s5	152	GLY	3.7
26	CZ	99	VAL	3.7
20	CT	19	LYS	3.7
19	y	61	PRO	3.7
57	K	2	PRO	3.7
74	b	19	LYS	3.7
10	p	182	GLY	3.7
35	DI	33	GLN	3.7
19	CS	145	ASN	3.7
57	s9	104	PHE	3.6
52	F	56	LEU	3.6
64	c6	90	VAL	3.6
4	CD	250	GLN	3.6
71	Y	89	ASN	3.6
21	CU	2	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
53	G	181	GLU	3.6
12	r	112	GLN	3.6
63	c5	119	PHE	3.6
49	C	164	ILE	3.6
17	CQ	183	ALA	3.6
71	Y	28	ASN	3.6
57	s9	5	PRO	3.6
24	6	2	SER	3.5
24	6	4	ASN	3.5
79	g	124	PRO	3.5
4	CD	249	SER	3.5
22	2	86	GLU	3.5
74	b	3	LYS	3.5
63	Q	53	PRO	3.5
4	j	180	LEU	3.5
4	j	232	GLY	3.5
52	F	4	GLY	3.5
71	Y	119	GLY	3.5
22	CV	80	VAL	3.5
47	A	1699	G	3.5
57	s9	42	ILE	3.5
64	c6	140	LYS	3.5
17	CQ	187	GLU	3.5
55	s7	58	LEU	3.5
80	h	95	ALA	3.5
1	AR	1201	C	3.5
6	CF	182	LEU	3.5
10	p	80	TYR	3.5
44	AQ	22	LEU	3.5
49	s1	217	LEU	3.5
23	CW	54	VAL	3.5
50	D	86	VAL	3.5
51	E	25	PHE	3.5
63	c5	91	GLY	3.5
42	AO	25	LYS	3.5
45	i	87	THR	3.4
46	p0	186	THR	3.4
62	c4	92	LYS	3.4
35	AH	61	GLN	3.4
56	J	96	LEU	3.4
63	c5	109	PRO	3.4
59	c1	146	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
12	r	114	GLY	3.4
64	c6	132	LYS	3.4
58	L	29	GLN	3.4
21	0	1	MET	3.4
21	CU	1	MET	3.4
62	P	42	VAL	3.4
67	c9	55	TYR	3.4
64	c6	139	GLN	3.4
71	Y	27	ASN	3.4
35	AH	21	LYS	3.4
18	CR	158	ALA	3.4
36	AI	91	ALA	3.4
6	CF	199	TRP	3.4
59	M	2	SER	3.4
26	8	50	ALA	3.3
48	s0	173	ILE	3.3
56	s8	62	THR	3.3
6	l	106	TRP	3.3
6	l	99	MET	3.3
46	p0	80	VAL	3.3
63	c5	86	VAL	3.3
62	P	41	ARG	3.3
32	AE	101	ALA	3.3
64	R	29	ILE	3.3
57	s9	33	GLU	3.3
15	CO	127	LYS	3.3
62	P	81	VAL	3.3
54	s6	68	LEU	3.3
55	s7	173	TYR	3.3
76	d8	67	ARG	3.3
18	x	166	VAL	3.3
20	CT	16	GLY	3.3
26	CZ	40	LEU	3.3
51	E	148	LYS	3.2
79	g	106	TYR	3.2
47	A	506	A	3.2
5	k	135	ALA	3.2
32	AE	99	ALA	3.2
77	d9	43	PHE	3.2
30	DD	24	PRO	3.2
67	c9	111	ILE	3.2
79	g	88	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
6	l	182	LEU	3.2
54	H	77	LEU	3.2
26	CZ	83	VAL	3.2
50	s2	166	THR	3.2
36	DJ	83	LYS	3.2
69	W	23	ILE	3.2
4	CD	14	SER	3.2
12	r	55	ASN	3.2
59	c1	129	ARG	3.2
24	CX	76	ALA	3.2
41	AN	107	ALA	3.2
18	x	182	ILE	3.2
20	z	52	LYS	3.2
35	DI	36	LYS	3.2
49	C	140	ILE	3.2
52	F	127	LYS	3.2
76	d8	45	LYS	3.2
51	s3	142	LEU	3.2
72	Z	18	LEU	3.2
53	s5	145	ASP	3.2
59	c1	52	SER	3.2
76	d8	43	ASN	3.2
57	s9	8	TYR	3.2
64	c6	142	TYR	3.2
14	t	63	VAL	3.2
56	s8	19	ALA	3.2
35	AH	6	THR	3.2
24	CX	3	GLY	3.2
7	m	51	LEU	3.2
66	c8	18	LEU	3.2
4	j	236	GLY	3.1
12	CL	209	ASN	3.1
55	I	142	TYR	3.1
57	s9	148	VAL	3.1
58	c0	64	TYR	3.1
63	Q	76	VAL	3.1
6	l	56	ALA	3.1
80	h	80	ALA	3.1
62	P	137	LEU	3.1
18	x	128	ARG	3.1
74	b	16	GLY	3.1
63	Q	126	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
71	d3	60	GLU	3.1
54	H	75	LEU	3.1
73	d5	75	LEU	3.1
41	AN	77	ILE	3.1
49	C	161	ILE	3.1
59	M	122	ILE	3.1
74	d6	10	ARG	3.1
30	DD	26	THR	3.1
59	M	3	THR	3.1
6	l	79	GLY	3.1
1	AR	1103	A	3.1
39	DM	2	ALA	3.1
41	DO	77	ILE	3.1
59	c1	61	THR	3.1
22	CV	78	LYS	3.1
35	AH	22	VAL	3.1
10	p	46	LEU	3.1
16	v	62	TYR	3.1
54	H	73	ILE	3.1
19	y	146	SER	3.1
26	CZ	101	GLU	3.1
5	CE	242	THR	3.1
14	CN	41	THR	3.1
62	P	87	GLY	3.1
4	CD	247	ARG	3.1
52	F	60	GLU	3.0
77	d9	7	TRP	3.0
5	CE	77	THR	3.0
4	j	202	VAL	3.0
22	CV	126	VAL	3.0
4	j	179	LEU	3.0
53	G	194	LEU	3.0
56	s8	21	PHE	3.0
4	j	229	ALA	3.0
20	z	54	ALA	3.0
21	0	130	GLU	3.0
79	g	94	LYS	3.0
42	AO	24	SER	3.0
44	DR	20	SER	3.0
59	c1	51	GLY	3.0
5	CE	229	VAL	3.0
10	p	44	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
42	DP	11	ARG	3.0
14	CN	3	ILE	3.0
64	c6	85	ILE	3.0
7	CG	9	SER	3.0
18	x	95	LEU	3.0
55	s7	153	LEU	3.0
57	K	6	ARG	3.0
79	g	103	LEU	3.0
1	AR	1922	A	3.0
24	6	52	ALA	3.0
55	I	59	ALA	3.0
16	CP	72	LYS	3.0
47	A	1115	U	3.0
61	c3	140	LYS	3.0
66	c8	124	GLY	3.0
50	D	63	VAL	3.0
5	CE	363	SER	3.0
7	CG	38	THR	3.0
49	s1	54	LEU	3.0
40	AM	32	ASN	3.0
58	L	28	ASN	3.0
41	DO	78	ILE	3.0
80	Rb	30	PRO	3.0
22	CV	85	LEU	3.0
48	s0	146	LEU	3.0
49	C	66	VAL	3.0
59	c1	5	LEU	3.0
58	c0	26	ASP	3.0
53	s5	184	PHE	3.0
55	s7	169	PHE	3.0
56	s8	45	SER	3.0
28	AA	46	ILE	3.0
44	DR	6	LYS	2.9
1	AR	2503	G	2.9
20	z	85	ARG	2.9
13	s	40	LEU	2.9
32	AE	67	VAL	2.9
33	AF	85	LEU	2.9
53	s5	149	VAL	2.9
60	c2	45	LEU	2.9
49	C	142	PHE	2.9
6	l	60	THR	2.9

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Mol	Chain	Res	Type	RSRZ
13	s	168	ASP	2.9
10	CJ	196	ALA	2.9
53	s5	155	ALA	2.9
59	c1	46	LYS	2.9
62	P	119	THR	2.9
10	p	79	GLN	2.9
5	k	332	ARG	2.9
32	AE	62	ARG	2.9
32	DF	67	VAL	2.9
5	k	227	GLU	2.9
4	CD	28	LYS	2.9
4	CD	251	LYS	2.9
10	CJ	237	ILE	2.9
16	CP	184	LYS	2.9
77	e	43	PHE	2.9
1	1	1107	C	2.9
25	7	85	ALA	2.9
61	O	7	ALA	2.9
63	c5	135	THR	2.9
80	Rb	12	THR	2.9
6	CF	65	TRP	2.9
9	o	217	PRO	2.9
14	t	22	VAL	2.9
58	L	65	TYR	2.9
76	d8	48	VAL	2.9
71	Y	5	LYS	2.9
80	Rb	115	ILE	2.9
6	CF	69	ARG	2.9
35	AH	16	ARG	2.9
3	AT	84	C	2.9
47	A	239	C	2.9
6	CF	233	LEU	2.9
6	CF	345	GLU	2.9
11	q	10	ILE	2.9
31	DE	43	ILE	2.9
35	DI	7	PHE	2.9
11	q	165	CYS	2.9
49	s1	89	ASP	2.9
46	p0	70	LEU	2.9
52	F	8	HIS	2.9
53	s5	165	LEU	2.9
4	CD	2	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
15	CO	131	VAL	2.9
72	d4	27	VAL	2.9
76	d	28	VAL	2.9
79	g	98	VAL	2.9
25	CY	27	LYS	2.9
32	AE	61	LYS	2.9
44	DR	7	LYS	2.9
55	s7	111	LYS	2.9
56	J	37	LYS	2.9
1	1	1802	C	2.9
1	1	2971	A	2.9
27	DA	119	ILE	2.9
6	CF	54	GLU	2.8
6	CF	62	ALA	2.8
59	c1	47	THR	2.8
44	AQ	25	GLN	2.8
6	CF	104	LYS	2.8
63	Q	52	LYS	2.8
59	c1	62	GLY	2.8
76	d8	47	PRO	2.8
26	CZ	95	ILE	2.8
30	DD	27	TYR	2.8
37	DK	9	ILE	2.8
53	s5	130	ILE	2.8
62	P	115	ILE	2.8
14	CN	136	GLU	2.8
59	c1	144	ALA	2.8
5	CE	47	LEU	2.8
80	h	32	LEU	2.8
57	K	101	VAL	2.8
71	Y	123	LYS	2.8
10	p	66	SER	2.8
45	sM	85	SER	2.8
67	U	94	ILE	2.8
77	d9	52	PHE	2.8
4	CD	6	ARG	2.8
36	AI	8	GLU	2.8
61	c3	53	LEU	2.8
54	H	79	LYS	2.8
10	CJ	151	VAL	2.8
42	DP	10	THR	2.8
55	s7	109	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
56	s8	46	VAL	2.8
57	K	130	THR	2.8
57	K	5	PRO	2.8
24	6	53	SER	2.8
43	DQ	34	SER	2.8
4	j	7	ASN	2.8
4	j	196	TRP	2.8
71	Y	10	ASN	2.8
74	b	11	ASN	2.8
4	CD	109	GLU	2.8
5	CE	246	LEU	2.8
71	Y	33	LEU	2.8
76	d	45	LYS	2.8
15	u	131	VAL	2.8
49	s1	65	VAL	2.8
67	U	71	VAL	2.8
64	c6	130	GLY	2.8
72	d4	23	PHE	2.8
80	Rb	122	ILE	2.8
29	DC	46	ASP	2.8
64	c6	141	SER	2.8
67	U	50	ALA	2.8
74	d6	8	ASN	2.8
18	x	46	LYS	2.8
32	AE	73	LEU	2.8
58	L	44	LYS	2.8
68	d0	84	MET	2.8
17	w	3	VAL	2.8
46	p0	187	VAL	2.8
52	F	129	VAL	2.8
24	6	65	GLY	2.8
4	j	253	GLN	2.7
21	0	143	PHE	2.8
39	DM	43	PHE	2.8
53	s5	68	ILE	2.8
4	CD	78	ALA	2.7
52	s4	18	TRP	2.7
53	G	209	TYR	2.7
55	s7	123	ASP	2.7
56	J	26	LYS	2.7
8	n	145	LEU	2.7
50	s2	154	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
29	AB	34	MET	2.7
28	DB	75	VAL	2.7
6	CF	190	GLY	2.7
17	w	78	ARG	2.7
44	AQ	11	THR	2.7
59	M	72	THR	2.7
63	c5	48	GLY	2.7
4	j	233	GLN	2.7
25	CY	58	HIS	2.7
74	b	17	HIS	2.7
55	s7	57	ALA	2.7
52	F	128	LYS	2.7
26	CZ	24	LEU	2.7
27	9	6	LEU	2.7
10	p	158	ASP	2.7
22	2	77	ASN	2.7
74	d6	11	ASN	2.7
12	r	131	ILE	2.7
18	CR	176	ILE	2.7
54	H	71	THR	2.7
59	c1	31	THR	2.7
59	c1	115	PHE	2.7
63	Q	50	THR	2.7
45	sM	66	ALA	2.7
57	s9	10	LYS	2.7
57	s9	48	GLN	2.7
67	c9	25	GLN	2.7
13	CM	12	LEU	2.7
14	t	51	LEU	2.7
66	c8	3	LEU	2.7
75	c	24	LEU	2.7
48	s0	54	TRP	2.7
68	V	84	MET	2.7
66	T	29	VAL	2.7
47	sR	1473	U	2.7
42	AO	17	ARG	2.7
6	l	74	ILE	2.7
26	CZ	142	ILE	2.7
74	b	44	ILE	2.7
48	B	107	PHE	2.7
25	CY	124	LYS	2.7
59	c1	24	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
5	CE	172	ALA	2.7
13	s	169	ALA	2.7
36	DJ	2	ALA	2.7
51	s3	147	ALA	2.7
47	A	1192	C	2.7
49	C	188	LEU	2.7
68	V	93	LEU	2.7
58	c0	65	TYR	2.7
11	CK	22	SER	2.7
27	9	7	ASP	2.7
4	CD	48	ILE	2.7
30	AC	11	ASN	2.7
1	AR	3079	U	2.7
9	CI	215	GLY	2.7
58	L	27	PHE	2.7
59	c1	147	GLY	2.7
25	7	81	PRO	2.7
80	h	96	THR	2.7
4	j	218	HIS	2.7
5	k	22	ALA	2.7
77	e	47	ALA	2.7
18	x	45	GLN	2.7
1	AR	2126	A	2.7
19	CS	84	VAL	2.7
20	CT	139	VAL	2.7
53	s5	177	ILE	2.6
4	j	234	LYS	2.6
9	o	158	LYS	2.6
55	s7	175	LYS	2.6
64	c6	2	SER	2.6
67	U	92	LYS	2.6
80	h	161	LYS	2.6
8	CH	32	ALA	2.6
15	CO	66	THR	2.6
30	DD	2	ALA	2.6
75	d7	24	LEU	2.6
47	A	194	U	2.6
47	A	261	U	2.6
47	sR	1735	U	2.6
12	r	162	GLN	2.6
52	F	208	VAL	2.6
70	X	6	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
22	2	84	TYR	2.6
47	A	677	G	2.6
1	1	784	A	2.6
16	v	189	LYS	2.6
29	AB	92	LYS	2.6
47	A	1694	A	2.6
47	sR	506	A	2.6
65	S	41	ILE	2.6
80	h	211	ILE	2.6
4	j	124	GLY	2.6
21	0	128	GLU	2.6
54	H	66	GLY	2.6
19	CS	140	LEU	2.6
24	CX	28	ASN	2.6
74	d6	71	LEU	2.6
59	M	146	ALA	2.6
63	Q	125	PRO	2.6
64	c6	21	HIS	2.6
42	DP	18	ARG	2.6
48	B	31	VAL	2.6
77	d9	23	VAL	2.6
20	z	53	LYS	2.6
30	DD	25	LYS	2.6
45	i	103	LYS	2.6
8	CH	130	ILE	2.6
14	t	3	ILE	2.6
4	j	228	GLY	2.6
31	DE	41	LEU	2.6
52	s4	26	CYS	2.6
66	T	54	LEU	2.6
1	AR	2502	A	2.6
29	DC	66	ALA	2.6
46	p0	107	ALA	2.6
61	c3	138	ASN	2.6
47	sR	1634	C	2.6
66	c8	20	THR	2.6
74	b	10	ARG	2.6
80	Rb	168	THR	2.6
26	8	51	VAL	2.6
63	Q	94	VAL	2.6
70	X	33	VAL	2.6
63	c5	104	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
6	l	185	LYS	2.6
44	DR	61	LYS	2.6
59	M	151	LYS	2.6
1	1	1570	U	2.6
19	y	57	ILE	2.6
53	G	172	ILE	2.6
4	CD	110	GLY	2.6
62	P	15	GLY	2.6
24	CX	69	LEU	2.6
70	X	104	LEU	2.6
74	b	81	ALA	2.6
25	7	88	ASP	2.6
74	b	33	ASP	2.6
79	g	104	SER	2.6
35	AH	23	VAL	2.6
53	s5	100	ASN	2.6
63	c5	134	THR	2.6
76	d8	44	VAL	2.6
1	AR	2124	G	2.6
28	AA	129	TRP	2.6
79	g	91	ILE	2.6
44	AQ	14	TYR	2.6
31	AD	62	LEU	2.6
52	F	23	LEU	2.6
80	Rb	97	GLY	2.6
1	1	329	U	2.6
1	AR	2873	U	2.6
47	A	794	U	2.6
6	CF	337	GLU	2.6
5	CE	19	ARG	2.6
74	b	6	ALA	2.6
53	s5	99	MET	2.6
42	DP	19	LYS	2.6
20	CT	56	THR	2.6
45	i	16	ASP	2.6
4	CD	7	ASN	2.6
10	p	34	PHE	2.5
47	sR	678	A	2.5
49	C	218	LEU	2.5
57	K	8	TYR	2.5
72	Z	125	LEU	2.5
63	c5	113	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
35	AH	32	ALA	2.5
50	s2	92	ALA	2.5
56	s8	40	ALA	2.5
59	c1	145	ALA	2.5
1	AR	494	G	2.5
25	CY	119	GLU	2.5
63	Q	80	MET	2.5
10	p	62	LYS	2.5
42	AO	16	LYS	2.5
57	K	141	VAL	2.5
6	l	362	ASP	2.5
63	c5	15	HIS	2.5
80	Rb	120	SER	2.5
5	k	25	ILE	2.5
9	CI	157	ASN	2.5
10	p	45	ASN	2.5
5	k	102	LEU	2.5
60	N	59	LEU	2.5
58	L	41	TYR	2.5
64	c6	49	TYR	2.5
4	CD	248	GLY	2.5
14	t	130	GLY	2.5
62	c4	52	ARG	2.5
71	Y	32	ARG	2.5
5	k	138	ALA	2.5
15	u	9	ALA	2.5
33	AF	2	ALA	2.5
45	sM	52	PRO	2.5
57	s9	2	PRO	2.5
59	c1	113	PRO	2.5
9	o	84	VAL	2.5
77	e	6	VAL	2.5
5	k	156	SER	2.5
53	s5	190	ILE	2.5
48	B	102	PHE	2.5
56	s8	193	LEU	2.5
69	d1	78	LEU	2.5
12	r	11	TYR	2.5
49	C	102	GLY	2.5
53	s5	61	TYR	2.5
74	b	73	TYR	2.5
77	e	13	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
79	g	105	TYR	2.5
35	DI	2	ALA	2.5
67	c9	92	LYS	2.5
57	s9	147	MET	2.5
14	CN	150	PRO	2.5
38	AK	29	VAL	2.5
20	z	50	ILE	2.5
52	s4	169	ILE	2.5
27	DA	111	LEU	2.5
33	AF	17	PHE	2.5
36	DJ	92	LEU	2.5
44	DR	21	SER	2.5
54	H	219	ARG	2.5
64	c6	121	SER	2.5
45	i	11	ASP	2.5
71	d3	24	TRP	2.5
9	o	237	ASN	2.5
59	c1	37	ASN	2.5
56	s8	39	GLY	2.5
67	c9	112	GLY	2.5
74	b	14	GLY	2.5
5	CE	250	ALA	2.5
1	1	2874	G	2.5
51	s3	175	VAL	2.5
52	F	76	VAL	2.5
71	Y	42	PRO	2.5
78	e0	45	VAL	2.5
37	DK	58	ILE	2.5
49	C	121	ILE	2.5
80	Rb	123	ILE	2.5
8	n	154	LEU	2.5
26	CZ	108	LEU	2.5
51	s3	202	LEU	2.5
57	s9	93	LEU	2.5
80	Rb	252	LEU	2.5
4	CD	16	PHE	2.5
6	CF	82	THR	2.5
14	t	42	ARG	2.5
23	CW	15	PHE	2.5
49	C	119	THR	2.5
60	N	49	THR	2.5
4	j	99	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
23	5	88	GLN	2.5
52	F	34	GLY	2.5
52	F	213	SER	2.5
59	c1	128	CYS	2.5
73	a	67	ASP	2.5
9	CI	133	TYR	2.5
63	c5	17	TYR	2.5
1	1	1201	C	2.5
5	k	229	VAL	2.5
49	s1	91	VAL	2.5
19	CS	61	PRO	2.5
25	CY	66	GLU	2.5
5	CE	178	LEU	2.4
80	Rb	301	LEU	2.4
1	1	331	G	2.4
1	AR	1493	G	2.4
6	l	69	ARG	2.4
39	AL	43	PHE	2.4
51	E	24	PHE	2.4
14	t	41	THR	2.4
15	CO	24	LYS	2.4
19	CS	11	LYS	2.4
30	AC	25	LYS	2.4
66	c8	140	THR	2.4
38	DL	86	ALA	2.4
59	M	145	ALA	2.4
63	c5	89	MET	2.4
64	c6	108	ALA	2.4
52	F	212	ASP	2.4
5	CE	29	VAL	2.4
22	2	72	VAL	2.4
57	K	113	VAL	2.4
5	CE	335	ILE	2.4
64	c6	36	ILE	2.4
55	s7	47	ARG	2.4
80	Rb	32	LEU	2.4
13	CM	85	LYS	2.4
22	CV	81	GLY	2.4
7	CG	233	ALA	2.4
63	Q	104	GLN	2.4
80	Rb	121	MET	2.4
13	s	171	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
19	y	87	VAL	2.4
19	CS	186	VAL	2.4
32	AE	98	VAL	2.4
46	p0	50	VAL	2.4
62	c4	125	SER	2.4
72	Z	35	VAL	2.4
30	AC	24	PRO	2.4
72	Z	34	ASN	2.4
21	0	129	ILE	2.4
68	V	20	ILE	2.4
54	H	222	GLU	2.4
17	CQ	192	LYS	2.4
19	CS	153	PHE	2.4
30	DD	59	LYS	2.4
32	AE	5	LYS	2.4
51	E	185	LYS	2.4
63	c5	8	LYS	2.4
26	8	47	ALA	2.4
36	AI	68	GLN	2.4
46	p0	188	VAL	2.4
13	s	167	TYR	2.4
40	AM	6	SER	2.4
45	i	54	PRO	2.4
18	x	120	ASN	2.4
26	8	27	ARG	2.4
34	DH	107	ILE	2.4
52	s4	261	LEU	2.4
65	S	24	LEU	2.4
72	d4	26	ASP	2.4
42	DP	25	LYS	2.4
74	b	4	LYS	2.4
20	CT	140	GLU	2.4
43	DQ	36	PHE	2.4
1	AR	2404	A	2.4
30	AC	7	HIS	2.4
4	j	201	GLY	2.4
5	k	155	ALA	2.4
17	CQ	184	THR	2.4
29	AB	66	ALA	2.4
47	A	1795	U	2.4
54	H	78	THR	2.4
7	CG	125	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
12	CL	11	TYR	2.4
19	y	143	PRO	2.4
42	AO	15	ARG	2.4
19	CS	139	ILE	2.4
33	AF	126	LEU	2.4
52	F	244	ILE	2.4
67	c9	5	SER	2.4
80	h	34	LEU	2.4
16	CP	77	LYS	2.4
52	F	6	LYS	2.4
14	CN	37	ASN	2.4
10	CJ	198	ALA	2.4
19	y	155	MET	2.4
25	CY	118	ALA	2.4
38	AK	86	ALA	2.4
62	P	17	ALA	2.4
63	Q	54	ALA	2.4
80	Rb	296	ALA	2.4
10	p	132	VAL	2.4
11	q	138	THR	2.4
25	7	83	THR	2.4
51	E	206	VAL	2.4
63	c5	50	THR	2.4
68	d0	70	THR	2.4
76	d8	15	VAL	2.4
1	AR	2954	U	2.4
37	DK	56	ARG	2.4
54	H	94	ARG	2.4
58	L	13	GLN	2.4
11	q	52	LEU	2.3
17	w	81	TYR	2.3
22	2	65	TYR	2.3
35	DI	20	ILE	2.3
35	DI	29	ILE	2.3
50	D	85	PRO	2.3
53	s5	187	ILE	2.3
59	M	91	LEU	2.3
80	h	115	ILE	2.3
4	j	16	PHE	2.3
49	C	95	ASN	2.3
7	m	133	GLU	2.3
53	G	152	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
63	c5	111	MET	2.3
73	d5	73	GLY	2.3
35	AH	35	VAL	2.3
37	DK	72	VAL	2.3
14	t	62	THR	2.3
77	e	7	TRP	2.3
80	Rb	251	TRP	2.3
4	j	225	ILE	2.3
21	CU	166	LYS	2.3
52	F	44	LEU	2.3
62	c4	137	LEU	2.3
63	Q	9	LYS	2.3
66	T	61	LEU	2.3
67	c9	116	ILE	2.3
74	d6	44	ILE	2.3
68	V	82	TYR	2.3
47	sR	794	U	2.3
1	1	1547	G	2.3
14	t	37	ASN	2.3
14	t	20	GLU	2.3
22	2	40	VAL	2.3
24	6	130	ALA	2.3
26	CZ	47	ALA	2.3
35	AH	5	VAL	2.3
60	c2	113	ARG	2.3
79	g	84	VAL	2.3
7	m	146	LEU	2.3
20	CT	21	LYS	2.3
36	DJ	21	LEU	2.3
49	C	47	LEU	2.3
56	s8	67	TRP	2.3
68	d0	93	LEU	2.3
71	Y	34	LEU	2.3
15	u	62	GLN	2.3
15	u	10	SER	2.3
1	1	1879	A	2.3
10	CJ	104	GLU	2.3
13	CM	108	GLU	2.3
25	CY	114	GLU	2.3
4	j	175	VAL	2.3
6	CF	130	ALA	2.3
54	H	67	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
55	s7	171	ALA	2.3
47	A	1114	G	2.3
51	E	187	LYS	2.3
67	c9	64	HIS	2.3
79	g	83	LYS	2.3
6	CF	187	LEU	2.3
36	DJ	88	LEU	2.3
58	L	40	LEU	2.3
37	DK	61	ILE	2.3
65	S	38	ILE	2.3
1	AR	2507	C	2.3
41	AN	108	THR	2.3
14	CN	48	PRO	2.3
52	F	138	TYR	2.3
54	s6	208	TYR	2.3
59	M	115	PHE	2.3
64	c6	79	TYR	2.3
49	s1	64	ARG	2.3
25	7	86	SER	2.3
10	p	213	LYS	2.3
14	t	155	GLU	2.3
26	CZ	110	VAL	2.3
50	D	163	GLY	2.3
51	E	135	GLU	2.3
60	N	69	ALA	2.3
63	c5	76	VAL	2.3
63	c5	136	SER	2.3
26	CZ	109	LYS	2.3
38	DL	23	GLY	2.3
81	c7	97	ASN	2.3
55	s7	176	LEU	2.3
66	c8	116	LEU	2.3
67	c9	28	LEU	2.3
74	d6	72	HIS	2.3
76	d8	66	LEU	2.3
1	AR	2445	A	2.3
10	CJ	110	THR	2.3
11	CK	138	THR	2.3
56	s8	120	THR	2.3
12	CL	217	PHE	2.3
63	c5	12	PHE	2.3
47	A	1709	C	2.3

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Mol	Chain	Res	Type	RSRZ
40	AM	46	ARG	2.3
61	c3	104	ARG	2.3
80	h	121	MET	2.3
19	CS	83	VAL	2.3
20	z	133	LYS	2.3
22	CV	124	VAL	2.3
72	Z	70	VAL	2.3
74	b	84	VAL	2.3
79	g	150	VAL	2.3
80	Rb	28	GLY	2.3
4	j	246	LEU	2.3
18	CR	162	GLU	2.3
44	DR	30	GLU	2.3
52	F	261	LEU	2.3
66	T	32	LEU	2.3
72	d4	17	LEU	2.3
74	b	88	SER	2.3
52	F	26	CYS	2.2
54	s6	156	PHE	2.2
65	S	35	CYS	2.2
74	b	98	PRO	2.2
4	j	204	MET	2.2
80	Rb	117	LYS	2.2
28	DB	12	VAL	2.2
71	Y	124	VAL	2.2
72	d4	5	VAL	2.2
6	l	187	LEU	2.2
31	AD	51	LEU	2.2
49	C	110	LEU	2.2
62	c4	98	GLY	2.2
74	b	47	ALA	2.2
78	f	32	GLY	2.2
80	Rb	47	LEU	2.2
47	A	1002	G	2.2
4	j	211	HIS	2.2
6	l	311	HIS	2.2
13	s	79	ILE	2.2
70	X	76	SER	2.2
10	p	156	ASP	2.2
61	c3	110	ASP	2.2
43	DQ	91	PHE	2.2
63	Q	12	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
73	a	56	THR	2.2
80	h	74	THR	2.2
32	AE	57	GLN	2.2
47	A	260	U	2.2
54	s6	94	ARG	2.2
80	Rb	314	GLN	2.2
55	s7	136	VAL	2.2
62	P	30	VAL	2.2
8	CH	154	LEU	2.2
16	v	197	LEU	2.2
19	y	140	LEU	2.2
78	e0	2	ALA	2.2
19	y	156	GLY	2.2
10	p	228	GLU	2.2
32	AE	68	GLU	2.2
61	O	119	GLU	2.2
74	d6	17	HIS	2.2
5	CE	24	SER	2.2
4	CD	186	PHE	2.2
21	CU	42	TRP	2.2
10	CJ	158	ASP	2.2
40	DN	43	ASN	2.2
52	F	143	ASP	2.2
42	DP	6	ARG	2.2
1	1	2206	G	2.2
1	1	2418	G	2.2
47	A	797	G	2.2
11	q	90	MET	2.2
10	CJ	197	VAL	2.2
63	c5	93	VAL	2.2
32	AE	51	LEU	2.2
52	F	123	LEU	2.2
63	c5	22	LEU	2.2
68	d0	63	LEU	2.2
26	8	128	ALA	2.2
43	AP	30	ALA	2.2
70	X	108	ALA	2.2
73	d5	76	ALA	2.2
79	g	152	ALA	2.2
5	CE	310	GLY	2.2
10	p	37	GLY	2.2
71	Y	4	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
13	CM	106	ILE	2.2
31	DE	42	ILE	2.2
54	s6	175	ILE	2.2
68	V	94	GLU	2.2
7	CG	185	PHE	2.2
16	CP	144	ARG	2.2
22	2	88	ARG	2.2
58	c0	27	PHE	2.2
64	c6	46	PHE	2.2
81	c7	96	SER	2.2
61	c3	94	LYS	2.2
52	F	79	ASP	2.2
4	j	199	THR	2.2
52	F	184	THR	2.2
49	C	207	LEU	2.2
54	H	216	LEU	2.2
58	L	58	GLN	2.2
14	t	2	ALA	2.2
49	s1	60	ALA	2.2
68	V	45	ALA	2.2
74	d6	81	ALA	2.2
80	Rb	253	ALA	2.2
1	AR	2440	G	2.2
25	7	90	ILE	2.2
47	A	730	G	2.2
56	J	60	ILE	2.2
56	J	78	ILE	2.2
1	1	2184	U	2.2
1	AR	1840	U	2.2
1	AR	2327	U	2.2
5	CE	4	ARG	2.2
35	DI	16	ARG	2.2
61	O	5	HIS	2.2
38	AK	10	LYS	2.2
1	1	1103	A	2.2
1	1	1475	A	2.2
1	AR	2275	A	2.2
36	DJ	40	SER	2.2
20	CT	130	ASN	2.2
63	c5	28	MET	2.2
71	d3	89	ASN	2.2
32	DF	73	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
51	E	16	VAL	2.2
51	E	21	LEU	2.2
52	s4	164	LEU	2.2
71	Y	125	VAL	2.2
80	Rb	312	VAL	2.2
18	x	183	ALA	2.1
32	DF	58	ALA	2.1
36	AI	120	ALA	2.1
49	C	156	ALA	2.1
53	s5	183	ALA	2.1
54	H	224	ALA	2.1
75	d7	5	GLN	2.2
80	h	75	ALA	2.1
11	q	178	GLY	2.1
4	j	5	ILE	2.1
53	G	121	ILE	2.1
68	d0	65	ILE	2.1
47	A	1703	C	2.1
4	j	247	ARG	2.1
19	CS	174	ARG	2.1
61	c3	114	ARG	2.1
38	AK	74	PHE	2.1
46	p0	88	PHE	2.1
50	D	57	PHE	2.1
47	sR	192	U	2.1
19	y	166	LEU	2.1
49	C	212	VAL	2.1
53	s5	33	VAL	2.1
54	H	36	VAL	2.1
23	CW	55	THR	2.1
45	i	91	THR	2.1
45	sM	50	ASN	2.1
62	P	86	THR	2.1
62	P	126	THR	2.1
79	g	86	THR	2.1
15	CO	41	GLN	2.1
15	CO	126	GLN	2.1
52	F	110	ALA	2.1
67	U	96	ALA	2.1
47	A	359	A	2.1
47	A	1702	A	2.1
4	CD	5	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
16	CP	152	CYS	2.1
13	s	17	LEU	2.1
26	8	24	LEU	2.1
26	CZ	88	MET	2.1
31	DE	14	LEU	2.1
52	F	131	LEU	2.1
6	l	71	VAL	2.1
1	AR	1569	U	2.1
73	d5	93	SER	2.1
6	CF	24	ALA	2.1
12	r	195	ALA	2.1
20	CT	159	ALA	2.1
20	CT	161	ALA	2.1
63	Q	78	THR	2.1
35	AH	18	ASN	2.1
36	AI	75	TYR	2.1
38	DL	13	ASN	2.1
59	M	90	TYR	2.1
11	q	9	GLN	2.1
71	Y	35	GLY	2.1
8	CH	150	LYS	2.1
26	CZ	89	LYS	2.1
29	DC	77	LYS	2.1
54	H	93	LYS	2.1
7	m	55	PHE	2.1
74	b	90	GLU	2.1
14	CN	51	LEU	2.1
29	AB	91	LEU	2.1
32	AE	97	LEU	2.1
44	AQ	29	LEU	2.1
57	s9	28	LEU	2.1
71	Y	9	LEU	2.1
10	CJ	157	VAL	2.1
39	AL	55	VAL	2.1
63	c5	11	VAL	2.1
67	c9	37	VAL	2.1
80	Rb	156	VAL	2.1
14	t	40	ALA	2.1
47	A	697	C	2.1
51	E	3	ALA	2.1
63	c5	4	ALA	2.1
18	CR	169	THR	2.1

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Mol	Chain	Res	Type	RSRZ
19	y	86	THR	2.1
50	D	96	THR	2.1
1	AR	2112	U	2.1
8	CH	29	LYS	2.1
12	r	24	ARG	2.1
16	CP	81	TYR	2.1
22	2	60	LYS	2.1
29	AB	117	ARG	2.1
30	AC	27	TYR	2.1
14	CN	6	ASN	2.1
16	CP	138	GLN	2.1
29	AB	74	ASN	2.1
32	DF	38	LYS	2.1
40	DN	50	ASN	2.1
47	A	1798	U	2.1
58	c0	28	ASN	2.1
74	b	69	ASN	2.1
11	q	117	PHE	2.1
25	CY	40	PHE	2.1
19	y	127	LEU	2.1
20	CT	10	LEU	2.1
33	DG	128	LEU	2.1
47	sR	810	G	2.1
49	C	120	LEU	2.1
50	D	113	LEU	2.1
62	P	94	PRO	2.1
63	c5	83	MET	2.1
78	e0	49	LEU	2.1
79	g	100	LEU	2.1
5	k	145	GLU	2.1
14	CN	20	GLU	2.1
5	k	233	TRP	2.1
7	m	52	VAL	2.1
54	H	81	VAL	2.1
54	s6	195	VAL	2.1
79	e1	114	VAL	2.1
6	CF	49	ALA	2.1
6	CF	89	ALA	2.1
49	C	139	ALA	2.1
7	m	50	ARG	2.1
7	m	148	ILE	2.1
8	CH	8	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
11	q	166	ARG	2.1
16	CP	133	ILE	2.1
20	z	70	LYS	2.1
30	DD	58	LYS	2.1
52	s4	127	LYS	2.1
53	s5	148	ARG	2.1
57	s9	134	ILE	2.1
68	V	77	LYS	2.1
73	a	50	ILE	2.1
6	CF	53	SER	2.1
7	CG	12	TYR	2.1
14	CN	144	THR	2.1
52	F	204	GLY	2.1
53	G	176	THR	2.1
55	s7	142	TYR	2.1
59	c1	35	TYR	2.1
62	P	93	THR	2.1
13	CM	41	SER	2.1
25	7	72	SER	2.1
45	i	85	SER	2.1
25	CY	45	ASN	2.1
58	L	96	ASN	2.1
66	c8	90	ASN	2.1
78	e0	51	ASN	2.1
23	CW	71	PHE	2.1
74	d6	33	ASP	2.1
75	c	32	PHE	2.1
80	Rb	54	PHE	2.1
13	s	131	MET	2.1
28	AA	42	LEU	2.1
35	DI	30	LEU	2.1
63	c5	80	MET	2.1
18	CR	157	VAL	2.1
20	CT	58	HIS	2.1
49	C	21	VAL	2.1
52	F	5	PRO	2.1
53	G	23	VAL	2.1
54	H	225	GLU	2.1
55	s7	48	GLU	2.1
5	CE	233	TRP	2.0
61	c3	139	TRP	2.0
19	y	162	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
22	2	78	LYS	2.0
26	CZ	90	ALA	2.0
31	DE	44	ILE	2.0
39	DM	18	ALA	2.0
51	s3	8	LYS	2.0
53	G	177	ILE	2.0
56	s8	79	ALA	2.0
57	s9	77	ILE	2.0
62	P	64	ALA	2.0
64	R	36	ILE	2.0
64	c6	24	ALA	2.0
22	2	62	GLY	2.0
24	6	43	GLY	2.0
29	AB	30	GLY	2.0
73	d5	72	GLY	2.0
74	d6	14	GLY	2.0
5	k	6	TYR	2.0
16	v	43	THR	2.0
16	CP	43	THR	2.0
62	P	91	THR	2.0
20	CT	76	SER	2.0
35	DI	61	GLN	2.0
81	c7	105	GLN	2.0
4	CD	87	PHE	2.0
57	K	104	PHE	2.0
32	AE	112	ASP	2.0
55	s7	126	LEU	2.0
1	1	1801	U	2.0
10	CJ	132	VAL	2.0
17	w	70	PRO	2.0
21	0	135	VAL	2.0
80	Rb	167	VAL	2.0
7	CG	189	GLU	2.0
7	CG	217	GLU	2.0
9	CI	40	LYS	2.0
14	t	5	LYS	2.0
37	DK	75	LYS	2.0
55	I	112	ARG	2.0
56	s8	187	GLU	2.0
62	P	129	LYS	2.0
72	d4	68	LYS	2.0
76	d8	65	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
77	e	54	LYS	2.0
13	s	65	ILE	2.0
40	AM	3	ALA	2.0
48	s0	162	CYS	2.0
70	X	34	ILE	2.0
74	b	41	ILE	2.0
52	s4	4	GLY	2.0
72	d4	67	GLY	2.0
4	j	17	THR	2.0
7	CG	207	TYR	2.0
21	0	70	THR	2.0
23	5	33	TYR	2.0
55	I	173	TYR	2.0
59	c1	97	TYR	2.0
37	DK	80	PHE	2.0
49	s1	220	GLN	2.0
76	d8	32	PHE	2.0
18	x	142	SER	2.0
35	AH	30	LEU	2.0
48	s0	9	LEU	2.0
49	C	135	LEU	2.0
51	E	69	LEU	2.0
54	H	82	SER	2.0
8	CH	98	VAL	2.0
23	5	91	ASP	2.0
52	s4	93	ASP	2.0
70	X	62	VAL	2.0
6	CF	21	PRO	2.0
30	AC	59	LYS	2.0
32	AE	65	LYS	2.0
52	F	62	LYS	2.0
54	s6	88	ARG	2.0
59	M	43	LYS	2.0
18	x	31	GLU	2.0
1	AR	1356	U	2.0
25	CY	49	ILE	2.0
47	A	912	U	2.0
47	A	1029	U	2.0
58	c0	23	ALA	2.0
66	c8	129	TRP	2.0
47	A	320	U	2.0
80	Rb	119	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
32	DF	66	GLY	2.0
49	C	63	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	A	2084	1/1	0.32	0.18	122,122,122,122	0
83	MG	AS	222	1/1	0.41	0.14	77,77,77,77	0
83	MG	sR	2139	1/1	0.43	0.16	100,100,100,100	0
83	MG	AR	3942	1/1	0.45	0.22	99,99,99,99	0
83	MG	AR	3718	1/1	0.45	0.21	73,73,73,73	0
83	MG	sR	2189	1/1	0.47	0.25	103,103,103,103	0
83	MG	1	4024	1/1	0.50	0.31	69,69,69,69	0
83	MG	CR	204	1/1	0.51	0.30	140,140,140,140	0
83	MG	1	4009	1/1	0.51	0.43	102,102,102,102	0
83	MG	AR	3859	1/1	0.52	0.25	73,73,73,73	0
83	MG	s	300	1/1	0.56	0.16	94,94,94,94	0
83	MG	sR	2037	1/1	0.56	0.26	89,89,89,89	0
83	MG	A	2085	1/1	0.57	0.24	97,97,97,97	0
83	MG	A	2037	1/1	0.57	0.24	90,90,90,90	0
83	MG	A	2039	1/1	0.57	0.12	113,113,113,113	0
83	MG	AR	3878	1/1	0.57	0.25	61,61,61,61	0
83	MG	AR	3961	1/1	0.58	0.14	86,86,86,86	0
82	OHX	1	4118	7/7	0.58	0.27	141,144,153,265	0
83	MG	A	2012	1/1	0.59	0.25	71,71,71,71	0
83	MG	1	3903	1/1	0.59	0.24	72,72,72,72	0
83	MG	CF	401	1/1	0.60	0.25	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	3928	1/1	0.60	0.26	97,97,97,97	0
83	MG	A	2049	1/1	0.60	0.22	90,90,90,90	0
83	MG	AR	3850	1/1	0.60	0.14	75,75,75,75	0
83	MG	1	3797	1/1	0.61	0.21	84,84,84,84	0
83	MG	1	4000	1/1	0.61	0.24	95,95,95,95	0
83	MG	AR	4013	1/1	0.61	0.34	90,90,90,90	0
83	MG	AR	4079	1/1	0.61	0.36	82,82,82,82	0
83	MG	AR	3893	1/1	0.62	0.30	99,99,99,99	0
83	MG	sR	2141	1/1	0.62	0.10	81,81,81,81	0
83	MG	1	3876	1/1	0.62	0.28	71,71,71,71	0
83	MG	1	3710	1/1	0.63	0.20	52,52,52,52	0
83	MG	CR	205	1/1	0.63	0.19	90,90,90,90	0
83	MG	AR	3940	1/1	0.64	0.11	76,76,76,76	0
83	MG	A	1985	1/1	0.64	0.18	79,79,79,79	0
83	MG	sR	2041	1/1	0.65	0.19	71,71,71,71	0
83	MG	sR	2056	1/1	0.65	0.21	84,84,84,84	0
83	MG	AR	3788	1/1	0.65	0.26	73,73,73,73	0
83	MG	AR	4070	1/1	0.65	0.27	100,100,100,100	0
83	MG	AR	4007	1/1	0.65	0.45	90,90,90,90	0
82	OHX	1	4145	7/7	0.66	0.14	216,230,238,336	0
83	MG	AR	3916	1/1	0.66	0.15	77,77,77,77	0
83	MG	A	2045	1/1	0.66	0.11	79,79,79,79	0
83	MG	sR	2120	1/1	0.66	0.15	60,60,60,60	0
82	OHX	AR	4154	7/7	0.66	0.14	188,198,207,310	0
83	MG	A	2002	1/1	0.66	0.19	94,94,94,94	0
83	MG	1	3965	1/1	0.66	0.32	90,90,90,90	0
83	MG	1	4038	1/1	0.67	0.17	72,72,72,72	0
83	MG	AR	3987	1/1	0.67	0.21	89,89,89,89	0
83	MG	sR	2116	1/1	0.67	0.18	88,88,88,88	0
83	MG	A	2060	1/1	0.67	0.20	94,94,94,94	0
83	MG	AR	3776	1/1	0.67	0.19	48,48,48,48	0
83	MG	1	3920	1/1	0.67	0.30	84,84,84,84	0
83	MG	AR	3817	1/1	0.67	0.24	48,48,48,48	0
83	MG	AR	4017	1/1	0.68	0.17	84,84,84,84	0
83	MG	A	2030	1/1	0.68	0.12	108,108,108,108	0
83	MG	CO	201	1/1	0.68	0.20	91,91,91,91	0
82	OHX	1	4146	7/7	0.68	0.13	259,262,267,335	0
83	MG	sR	2091	1/1	0.68	0.21	92,92,92,92	0
83	MG	AR	3684	1/1	0.68	0.32	46,46,46,46	0
83	MG	AR	4127	1/1	0.68	0.25	87,87,87,87	0
83	MG	A	1992	1/1	0.68	0.35	90,90,90,90	0
83	MG	A	2062	1/1	0.68	0.24	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	sR	2144	1/1	0.68	0.15	88,88,88,88	0
82	OHX	A	2141	7/7	0.68	0.15	203,208,221,316	0
83	MG	1	3808	1/1	0.69	0.20	59,59,59,59	0
83	MG	AR	4077	1/1	0.69	0.23	76,76,76,76	0
82	OHX	1	4141	7/7	0.69	0.12	222,234,247,330	0
83	MG	AR	4103	1/1	0.69	0.26	70,70,70,70	0
83	MG	A	2038	1/1	0.69	0.29	85,85,85,85	0
83	MG	b	202	1/1	0.69	0.25	92,92,92,92	0
83	MG	AR	3699	1/1	0.69	0.24	67,67,67,67	0
83	MG	sR	2188	1/1	0.69	0.13	98,98,98,98	0
82	OHX	AR	3663	7/7	0.69	0.11	193,198,213,299	0
82	OHX	1	4153	7/7	0.70	0.16	167,171,174,238	7
83	MG	1	3704	1/1	0.70	0.23	81,81,81,81	0
83	MG	AR	4005	1/1	0.70	0.24	86,86,86,86	0
83	MG	x	206	1/1	0.70	0.22	95,95,95,95	0
83	MG	sR	2112	1/1	0.70	0.14	89,89,89,89	0
83	MG	1	3856	1/1	0.70	0.21	88,88,88,88	0
83	MG	1	4001	1/1	0.70	0.24	79,79,79,79	0
82	OHX	AR	3635	7/7	0.70	0.20	143,160,193,285	0
83	MG	AR	3719	1/1	0.70	0.25	62,62,62,62	0
83	MG	sR	2143	1/1	0.70	0.16	72,72,72,72	0
83	MG	1	3746	1/1	0.70	0.26	57,57,57,57	0
83	MG	1	4037	1/1	0.70	0.28	85,85,85,85	0
83	MG	A	2021	1/1	0.70	0.18	82,82,82,82	0
83	MG	sR	2070	1/1	0.71	0.23	79,79,79,79	0
83	MG	AR	4088	1/1	0.71	0.29	73,73,73,73	0
83	MG	1	3625	1/1	0.71	0.22	72,72,72,72	0
83	MG	1	3761	1/1	0.71	0.17	70,70,70,70	0
83	MG	AR	4009	1/1	0.71	0.23	73,73,73,73	0
83	MG	1	3671	1/1	0.71	0.20	82,82,82,82	0
83	MG	D	302	1/1	0.71	0.20	64,64,64,64	0
83	MG	AR	3825	1/1	0.71	0.24	49,49,49,49	0
82	OHX	A	1973	7/7	0.71	0.12	199,215,230,299	0
83	MG	sR	2161	1/1	0.71	0.27	92,92,92,92	0
82	OHX	1	3601	7/7	0.71	0.13	177,183,217,304	0
83	MG	1	4046	1/1	0.71	0.22	78,78,78,78	0
83	MG	s2	301	1/1	0.71	0.14	61,61,61,61	0
83	MG	1	3769	1/1	0.72	0.30	55,55,55,55	0
83	MG	1	3970	1/1	0.72	0.22	101,101,101,101	0
83	MG	sR	2151	1/1	0.72	0.25	128,128,128,128	0
83	MG	1	3883	1/1	0.72	0.14	88,88,88,88	0
83	MG	1	3855	1/1	0.72	0.29	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3678	1/1	0.72	0.16	59,59,59,59	0
83	MG	1	3942	1/1	0.72	0.31	83,83,83,83	0
83	MG	A	2068	1/1	0.73	0.21	94,94,94,94	0
83	MG	1	3736	1/1	0.73	0.21	62,62,62,62	0
83	MG	AR	4059	1/1	0.73	0.21	75,75,75,75	0
83	MG	A	2159	1/1	0.73	0.24	87,87,87,87	0
83	MG	A	1986	1/1	0.73	0.15	70,70,70,70	0
83	MG	F	301	1/1	0.73	0.18	73,73,73,73	0
83	MG	AR	4061	1/1	0.73	0.18	87,87,87,87	0
83	MG	A	1994	1/1	0.73	0.16	52,52,52,52	0
83	MG	1	4035	1/1	0.73	0.17	70,70,70,70	0
83	MG	A	2004	1/1	0.73	0.24	69,69,69,69	0
83	MG	1	3962	1/1	0.73	0.23	67,67,67,67	0
82	OHX	sR	2181	7/7	0.73	0.11	204,210,219,318	0
83	MG	sR	2104	1/1	0.73	0.13	75,75,75,75	0
83	MG	A	2023	1/1	0.73	0.18	89,89,89,89	0
83	MG	A	2029	1/1	0.73	0.14	91,91,91,91	0
82	OHX	AR	3662	7/7	0.73	0.14	191,195,217,316	0
83	MG	A	2034	1/1	0.73	0.21	74,74,74,74	0
83	MG	AR	4101	1/1	0.73	0.34	87,87,87,87	0
83	MG	AR	3979	1/1	0.73	0.34	69,69,69,69	0
83	MG	3	212	1/1	0.73	0.16	61,61,61,61	0
83	MG	1	3996	1/1	0.73	0.27	77,77,77,77	0
83	MG	1	3907	1/1	0.73	0.13	71,71,71,71	0
83	MG	A	2053	1/1	0.73	0.22	80,80,80,80	0
83	MG	1	3910	1/1	0.73	0.19	54,54,54,54	0
82	OHX	sR	2025	7/7	0.73	0.12	235,236,247,328	0
83	MG	sR	2101	1/1	0.74	0.15	77,77,77,77	0
83	MG	1	3825	1/1	0.74	0.19	68,68,68,68	0
83	MG	AR	3862	1/1	0.74	0.20	115,115,115,115	0
83	MG	1	3971	1/1	0.74	0.20	80,80,80,80	0
83	MG	AG	201	1/1	0.74	0.12	78,78,78,78	0
83	MG	AR	3894	1/1	0.74	0.30	78,78,78,78	0
82	OHX	AR	3664	7/7	0.74	0.14	219,223,230,341	0
83	MG	AR	3919	1/1	0.74	0.16	47,47,47,47	0
83	MG	3	216	1/1	0.74	0.13	90,90,90,90	0
83	MG	AR	4032	1/1	0.74	0.35	84,84,84,84	0
83	MG	sR	2160	1/1	0.74	0.32	80,80,80,80	0
83	MG	sR	2065	1/1	0.74	0.19	61,61,61,61	0
83	MG	AR	3702	1/1	0.74	0.27	61,61,61,61	0
83	MG	sR	2089	1/1	0.74	0.24	88,88,88,88	0
83	MG	AR	3709	1/1	0.74	0.24	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3888	1/1	0.75	0.32	100,100,100,100	0
83	MG	AR	4102	1/1	0.75	0.21	70,70,70,70	0
82	OHX	AR	3632	7/7	0.75	0.14	180,203,230,310	0
83	MG	1	3904	1/1	0.75	0.29	70,70,70,70	0
83	MG	AR	3990	1/1	0.75	0.33	74,74,74,74	0
83	MG	AS	223	1/1	0.75	0.10	73,73,73,73	0
82	OHX	A	2125	7/7	0.75	0.15	190,194,208,296	0
83	MG	1	3723	1/1	0.75	0.26	45,45,45,45	0
83	MG	CP	305	1/1	0.75	0.14	73,73,73,73	0
83	MG	1	3656	1/1	0.75	0.20	64,64,64,64	0
83	MG	1	4022	1/1	0.75	0.30	70,70,70,70	0
83	MG	sR	2125	1/1	0.75	0.24	72,72,72,72	0
83	MG	A	2061	1/1	0.75	0.12	75,75,75,75	0
83	MG	AR	3685	1/1	0.75	0.17	55,55,55,55	0
83	MG	1	3926	1/1	0.75	0.15	71,71,71,71	0
83	MG	1	4031	1/1	0.75	0.42	86,86,86,86	0
82	OHX	1	4154	7/7	0.75	0.11	218,222,231,326	0
83	MG	AR	3712	1/1	0.75	0.26	90,90,90,90	0
83	MG	1	3677	1/1	0.75	0.22	83,83,83,83	0
82	OHX	AR	4163	7/7	0.75	0.18	143,147,151,216	7
83	MG	A	2014	1/1	0.75	0.27	66,66,66,66	0
83	MG	AR	3741	1/1	0.75	0.23	63,63,63,63	0
83	MG	sR	2048	1/1	0.76	0.20	58,58,58,58	0
82	OHX	AR	3661	7/7	0.76	0.16	179,187,199,306	0
83	MG	AR	4078	1/1	0.76	0.24	60,60,60,60	0
82	OHX	sR	2175	7/7	0.76	0.12	202,212,219,315	0
83	MG	sR	2084	1/1	0.76	0.18	97,97,97,97	0
83	MG	AR	3866	1/1	0.76	0.19	65,65,65,65	0
83	MG	1	4028	1/1	0.76	0.20	49,49,49,49	0
83	MG	sR	2100	1/1	0.76	0.16	100,100,100,100	0
83	MG	A	2000	1/1	0.76	0.20	73,73,73,73	0
82	OHX	1	4142	7/7	0.76	0.15	183,190,207,327	0
83	MG	AR	3753	1/1	0.76	0.26	65,65,65,65	0
83	MG	A	2006	1/1	0.76	0.24	86,86,86,86	0
83	MG	A	2070	1/1	0.76	0.17	66,66,66,66	0
83	MG	sR	2123	1/1	0.76	0.18	66,66,66,66	0
83	MG	A	2083	1/1	0.76	0.18	112,112,112,112	0
83	MG	AR	4011	1/1	0.76	0.29	68,68,68,68	0
83	MG	AS	219	1/1	0.76	0.29	62,62,62,62	0
83	MG	1	3613	1/1	0.76	0.27	67,67,67,67	0
83	MG	1	3691	1/1	0.76	0.26	87,87,87,87	0
83	MG	sR	2149	1/1	0.76	0.29	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	3792	1/1	0.76	0.25	48,48,48,48	0
83	MG	sR	2156	1/1	0.76	0.27	85,85,85,85	0
83	MG	1	3622	1/1	0.76	0.19	52,52,52,52	0
83	MG	sR	1902	1/1	0.76	0.19	83,83,83,83	0
83	MG	sR	2035	1/1	0.76	0.22	95,95,95,95	0
82	OHX	AR	3657	7/7	0.76	0.15	246,255,276,392	0
83	MG	1	4012	1/1	0.76	0.15	63,63,63,63	0
83	MG	AR	3860	1/1	0.77	0.15	63,63,63,63	0
83	MG	1	3755	1/1	0.77	0.28	94,94,94,94	0
82	OHX	A	2140	7/7	0.77	0.23	195,209,215,324	0
83	MG	DO	201	1/1	0.77	0.14	71,71,71,71	0
83	MG	AR	3705	1/1	0.77	0.23	47,47,47,47	0
83	MG	1	3969	1/1	0.77	0.14	76,76,76,76	0
83	MG	A	1990	1/1	0.77	0.23	80,80,80,80	0
82	OHX	z	202	7/7	0.77	0.10	162,166,170,226	7
83	MG	1	3901	1/1	0.77	0.13	86,86,86,86	0
83	MG	1	3977	1/1	0.77	0.14	96,96,96,96	0
83	MG	sR	2124	1/1	0.77	0.14	54,54,54,54	0
83	MG	1	4052	1/1	0.77	0.25	62,62,62,62	0
83	MG	AR	3752	1/1	0.77	0.18	69,69,69,69	0
83	MG	1	3787	1/1	0.77	0.30	46,46,46,46	0
82	OHX	sR	1999	7/7	0.77	0.15	181,192,213,301	0
83	MG	AR	3964	1/1	0.77	0.49	75,75,75,75	0
82	OHX	sR	2021	7/7	0.77	0.14	212,242,247,335	0
83	MG	AR	4105	1/1	0.77	0.29	80,80,80,80	0
83	MG	1	3822	1/1	0.77	0.21	87,87,87,87	0
82	OHX	1	4143	7/7	0.77	0.14	184,210,220,309	0
83	MG	AR	4002	1/1	0.77	0.24	73,73,73,73	0
83	MG	AI	201	1/1	0.77	0.18	74,74,74,74	0
82	OHX	1	4149	7/7	0.77	0.19	134,145,156,203	7
82	OHX	sR	2178	7/7	0.77	0.11	198,210,226,310	0
83	MG	d4	203	1/1	0.77	0.10	83,83,83,83	0
84	K	j	303	1/1	0.77	0.39	111,111,111,111	0
83	MG	AR	3848	1/1	0.78	0.15	59,59,59,59	0
83	MG	AR	3937	1/1	0.78	0.16	68,68,68,68	0
83	MG	AR	3734	1/1	0.78	0.15	62,62,62,62	0
83	MG	AS	218	1/1	0.78	0.24	88,88,88,88	0
83	MG	AR	3941	1/1	0.78	0.28	59,59,59,59	0
83	MG	A	2094	1/1	0.78	0.33	79,79,79,79	0
83	MG	A	2097	1/1	0.78	0.28	80,80,80,80	0
83	MG	AR	3737	1/1	0.78	0.15	77,77,77,77	0
83	MG	AR	4053	1/1	0.78	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	sR	2126	1/1	0.78	0.23	68,68,68,68	0
83	MG	AS	228	1/1	0.78	0.30	76,76,76,76	0
83	MG	1	3727	1/1	0.78	0.32	71,71,71,71	0
82	OHX	sR	2024	7/7	0.78	0.14	212,212,237,322	0
83	MG	AR	4068	1/1	0.78	0.27	86,86,86,86	0
83	MG	sR	2145	1/1	0.78	0.21	84,84,84,84	0
82	OHX	AR	3669	6/7	0.78	0.12	157,176,185,285	0
83	MG	sR	2040	1/1	0.78	0.29	80,80,80,80	0
83	MG	1	3749	1/1	0.78	0.26	47,47,47,47	0
83	MG	sR	2158	1/1	0.78	0.20	64,64,64,64	0
83	MG	DD	101	1/1	0.78	0.17	51,51,51,51	0
82	OHX	AR	3552	7/7	0.78	0.17	122,141,148,243	0
83	MG	AR	3999	1/1	0.78	0.22	85,85,85,85	0
82	OHX	3	206	7/7	0.78	0.11	194,196,207,290	0
83	MG	AR	4094	1/1	0.78	0.17	72,72,72,72	0
83	MG	i	301	1/1	0.78	0.20	60,60,60,60	0
83	MG	1	3931	1/1	0.78	0.12	64,64,64,64	0
83	MG	1	4033	1/1	0.79	0.24	65,65,65,65	0
83	MG	AR	3761	1/1	0.79	0.20	57,57,57,57	0
83	MG	AT	226	1/1	0.79	0.23	60,60,60,60	0
82	OHX	AR	4157	7/7	0.79	0.14	194,204,218,308	0
83	MG	A	2042	1/1	0.79	0.15	87,87,87,87	0
83	MG	CI	301	1/1	0.79	0.17	61,61,61,61	0
83	MG	AR	4056	1/1	0.79	0.21	86,86,86,86	0
83	MG	A	2051	1/1	0.79	0.18	59,59,59,59	0
82	OHX	3	222	7/7	0.79	0.10	189,197,214,301	0
82	OHX	sR	1996	7/7	0.79	0.13	176,192,211,292	0
82	OHX	A	1963	7/7	0.79	0.16	211,216,222,304	0
83	MG	1	3949	1/1	0.79	0.20	63,63,63,63	0
83	MG	A	2064	1/1	0.79	0.15	81,81,81,81	0
83	MG	AR	3963	1/1	0.79	0.14	74,74,74,74	0
83	MG	AR	3829	1/1	0.79	0.33	46,46,46,46	0
83	MG	A	2071	1/1	0.79	0.14	76,76,76,76	0
83	MG	sR	2132	1/1	0.79	0.33	80,80,80,80	0
83	MG	sR	2138	1/1	0.79	0.21	86,86,86,86	0
83	MG	AR	3965	1/1	0.79	0.23	65,65,65,65	0
83	MG	1	4159	1/1	0.79	0.17	73,73,73,73	0
83	MG	AR	4089	1/1	0.79	0.27	75,75,75,75	0
82	OHX	AR	4153	7/7	0.79	0.14	187,197,211,324	0
83	MG	AR	3714	1/1	0.79	0.20	60,60,60,60	0
83	MG	1	4020	1/1	0.79	0.40	52,52,52,52	0
83	MG	sR	2150	1/1	0.79	0.28	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	sR	2022	7/7	0.79	0.11	225,230,246,348	0
83	MG	AR	3731	1/1	0.79	0.16	63,63,63,63	0
83	MG	Y	201	1/1	0.79	0.13	60,60,60,60	0
83	MG	v	305	1/1	0.79	0.20	76,76,76,76	0
83	MG	AR	4188	1/1	0.79	0.11	102,102,102,102	0
83	MG	AS	212	1/1	0.79	0.16	73,73,73,73	0
83	MG	1	3836	1/1	0.79	0.27	80,80,80,80	0
83	MG	1	3837	1/1	0.79	0.19	88,88,88,88	0
83	MG	c8	202	1/1	0.79	0.24	90,90,90,90	0
82	OHX	AR	3659	7/7	0.79	0.11	227,244,262,365	0
83	MG	A	2033	1/1	0.79	0.17	81,81,81,81	0
84	K	sR	2182	1/1	0.79	0.36	146,146,146,146	0
83	MG	sR	2073	1/1	0.80	0.24	58,58,58,58	0
83	MG	AR	3722	1/1	0.80	0.18	50,50,50,50	0
83	MG	AR	3727	1/1	0.80	0.23	69,69,69,69	0
83	MG	AR	3877	1/1	0.80	0.17	72,72,72,72	0
83	MG	1	3815	1/1	0.80	0.23	57,57,57,57	0
83	MG	AR	4012	1/1	0.80	0.24	87,87,87,87	0
83	MG	sR	2102	1/1	0.80	0.16	75,75,75,75	0
83	MG	1	4023	1/1	0.80	0.25	50,50,50,50	0
83	MG	1	3963	1/1	0.80	0.13	61,61,61,61	0
83	MG	AR	4026	1/1	0.80	0.20	74,74,74,74	0
83	MG	6	202	1/1	0.80	0.11	86,86,86,86	0
83	MG	AR	4042	1/1	0.80	0.12	48,48,48,48	0
82	OHX	sR	2011	7/7	0.80	0.11	232,247,262,320	0
82	OHX	sR	2013	7/7	0.80	0.11	225,235,242,338	0
83	MG	CR	208	1/1	0.80	0.17	73,73,73,73	0
83	MG	1	3752	1/1	0.80	0.26	56,56,56,56	0
83	MG	1	3610	1/1	0.80	0.17	60,60,60,60	0
83	MG	AR	4063	1/1	0.80	0.23	80,80,80,80	0
82	OHX	AR	4156	7/7	0.80	0.12	172,178,193,301	0
82	OHX	1	4134	7/7	0.80	0.12	186,187,195,310	0
83	MG	AR	3948	1/1	0.80	0.17	74,74,74,74	0
83	MG	AR	3959	1/1	0.80	0.14	69,69,69,69	0
82	OHX	1	4106	7/7	0.80	0.20	154,167,185,301	0
83	MG	AR	3824	1/1	0.80	0.18	47,47,47,47	0
83	MG	1	3938	1/1	0.80	0.19	78,78,78,78	0
83	MG	1	4068	1/1	0.80	0.27	72,72,72,72	0
82	OHX	1	4108	7/7	0.80	0.11	220,224,236,318	0
83	MG	1	3947	1/1	0.80	0.14	68,68,68,68	0
83	MG	AR	3988	1/1	0.80	0.17	61,61,61,61	0
82	OHX	1	3574	7/7	0.80	0.12	190,198,221,292	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	4122	1/1	0.80	0.22	78,78,78,78	0
83	MG	4	220	1/1	0.80	0.11	77,77,77,77	0
83	MG	s9	201	1/1	0.80	0.29	76,76,76,76	0
83	MG	sR	2053	1/1	0.80	0.12	62,62,62,62	0
83	MG	AR	4185	1/1	0.80	0.09	123,123,123,123	0
83	MG	AR	3861	1/1	0.80	0.25	66,66,66,66	0
83	MG	AR	4004	1/1	0.80	0.16	70,70,70,70	0
82	OHX	1	4140	7/7	0.81	0.10	238,246,255,348	0
83	MG	1	3657	1/1	0.81	0.19	54,54,54,54	0
83	MG	sR	2058	1/1	0.81	0.44	83,83,83,83	0
83	MG	A	2026	1/1	0.81	0.24	85,85,85,85	0
83	MG	1	3936	1/1	0.81	0.20	48,48,48,48	0
83	MG	1	3881	1/1	0.81	0.20	89,89,89,89	0
83	MG	AS	211	1/1	0.81	0.14	49,49,49,49	0
83	MG	AR	3762	1/1	0.81	0.21	60,60,60,60	0
83	MG	AR	3930	1/1	0.81	0.10	96,96,96,96	0
83	MG	AR	4022	1/1	0.81	0.24	84,84,84,84	0
83	MG	1	3667	1/1	0.81	0.24	60,60,60,60	0
83	MG	1	4054	1/1	0.81	0.22	77,77,77,77	0
83	MG	1	3886	1/1	0.81	0.20	106,106,106,106	0
83	MG	sR	2110	1/1	0.81	0.25	69,69,69,69	0
83	MG	AR	4051	1/1	0.81	0.19	62,62,62,62	0
83	MG	A	2050	1/1	0.81	0.15	77,77,77,77	0
83	MG	AR	3804	1/1	0.81	0.30	51,51,51,51	0
83	MG	1	4013	1/1	0.81	0.19	47,47,47,47	0
83	MG	1	3734	1/1	0.81	0.29	71,71,71,71	0
83	MG	AR	3960	1/1	0.81	0.19	64,64,64,64	0
83	MG	CR	201	1/1	0.81	0.15	109,109,109,109	0
82	OHX	A	2130	7/7	0.81	0.12	238,242,260,344	0
83	MG	AR	4065	1/1	0.81	0.19	63,63,63,63	0
82	OHX	AR	3578	7/7	0.81	0.13	140,142,171,259	0
83	MG	AR	3839	1/1	0.81	0.26	64,64,64,64	0
82	OHX	1	3554	7/7	0.81	0.16	154,175,182,280	0
83	MG	t	201	1/1	0.81	0.26	79,79,79,79	0
83	MG	AR	3980	1/1	0.81	0.21	79,79,79,79	0
82	OHX	sR	1995	7/7	0.81	0.10	233,246,257,341	0
83	MG	A	2096	1/1	0.81	0.20	94,94,94,94	0
83	MG	x	202	1/1	0.81	0.26	105,105,105,105	0
83	MG	sR	2153	1/1	0.81	0.20	76,76,76,76	0
83	MG	sR	2154	1/1	0.81	0.25	66,66,66,66	0
83	MG	AR	4090	1/1	0.81	0.25	51,51,51,51	0
83	MG	AR	4091	1/1	0.81	0.24	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	3728	1/1	0.81	0.18	69,69,69,69	0
83	MG	A	2003	1/1	0.81	0.35	60,60,60,60	0
83	MG	sR	2163	1/1	0.81	0.18	69,69,69,69	0
83	MG	1	3694	1/1	0.81	0.15	86,86,86,86	0
83	MG	A	2005	1/1	0.81	0.18	59,59,59,59	0
83	MG	sR	2033	1/1	0.81	0.16	76,76,76,76	0
83	MG	s8	302	1/1	0.81	0.22	69,69,69,69	0
83	MG	6	201	1/1	0.81	0.23	55,55,55,55	0
83	MG	A	2007	1/1	0.81	0.25	78,78,78,78	0
83	MG	1	3652	1/1	0.81	0.15	54,54,54,54	0
83	MG	AR	3740	1/1	0.81	0.09	68,68,68,68	0
83	MG	A	2017	1/1	0.81	0.25	69,69,69,69	0
82	OHX	AR	3666	7/7	0.82	0.11	213,224,234,323	0
83	MG	1	4055	1/1	0.82	0.25	70,70,70,70	0
83	MG	1	3849	1/1	0.82	0.22	69,69,69,69	0
82	OHX	AS	208	7/7	0.82	0.12	189,201,221,304	0
83	MG	1	3631	1/1	0.82	0.21	89,89,89,89	0
83	MG	sR	2059	1/1	0.82	0.20	81,81,81,81	0
83	MG	AR	3944	1/1	0.82	0.12	72,72,72,72	0
83	MG	sR	2068	1/1	0.82	0.17	75,75,75,75	0
83	MG	AR	3750	1/1	0.82	0.12	66,66,66,66	0
83	MG	1	3738	1/1	0.82	0.27	75,75,75,75	0
83	MG	sR	2074	1/1	0.82	0.36	73,73,73,73	0
83	MG	sR	2080	1/1	0.82	0.26	64,64,64,64	0
82	OHX	AT	234	7/7	0.82	0.11	183,190,217,317	0
83	MG	4	223	1/1	0.82	0.17	69,69,69,69	0
82	OHX	AR	3667	7/7	0.82	0.14	186,206,226,342	0
83	MG	1	3979	1/1	0.82	0.26	59,59,59,59	0
83	MG	1	3750	1/1	0.82	0.28	46,46,46,46	0
83	MG	AR	3972	1/1	0.82	0.08	66,66,66,66	0
83	MG	A	2035	1/1	0.82	0.23	84,84,84,84	0
82	OHX	AR	3588	7/7	0.82	0.18	191,199,209,345	0
83	MG	AR	3798	1/1	0.82	0.23	45,45,45,45	0
82	OHX	A	1976	7/7	0.82	0.11	198,201,219,281	0
83	MG	1	4003	1/1	0.82	0.19	46,46,46,46	0
83	MG	A	2044	1/1	0.82	0.27	89,89,89,89	0
82	OHX	AR	4145	7/7	0.82	0.12	176,178,193,295	0
83	MG	1	4011	1/1	0.82	0.11	57,57,57,57	0
82	OHX	sR	2172	7/7	0.82	0.16	155,164,178,268	0
83	MG	1	3771	1/1	0.82	0.23	47,47,47,47	0
83	MG	AR	3845	1/1	0.82	0.07	63,63,63,63	0
82	OHX	AR	4151	7/7	0.82	0.15	214,221,230,313	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AT	225	1/1	0.82	0.36	55,55,55,55	0
83	MG	AR	3849	1/1	0.82	0.10	54,54,54,54	0
83	MG	1	3791	1/1	0.82	0.15	57,57,57,57	0
83	MG	CG	301	1/1	0.82	0.29	52,52,52,52	0
83	MG	AR	3686	1/1	0.82	0.10	78,78,78,78	0
82	OHX	sR	2177	7/7	0.82	0.10	224,228,236,317	0
82	OHX	AR	3601	7/7	0.82	0.16	115,138,154,256	0
83	MG	1	3702	1/1	0.82	0.25	48,48,48,48	0
83	MG	AR	4025	1/1	0.82	0.13	78,78,78,78	0
82	OHX	1	4120	7/7	0.82	0.12	162,171,200,283	0
83	MG	AR	3872	1/1	0.82	0.17	65,65,65,65	0
82	OHX	1	4122	7/7	0.82	0.13	161,168,195,292	0
83	MG	1	4034	1/1	0.82	0.29	78,78,78,78	0
83	MG	D	301	1/1	0.82	0.20	65,65,65,65	0
83	MG	AR	4052	1/1	0.82	0.13	78,78,78,78	0
83	MG	AR	3880	1/1	0.82	0.08	51,51,51,51	0
83	MG	1	3943	1/1	0.82	0.15	84,84,84,84	0
83	MG	1	3831	1/1	0.82	0.25	56,56,56,56	0
83	MG	1	3948	1/1	0.82	0.16	71,71,71,71	0
83	MG	A	1995	1/1	0.82	0.28	64,64,64,64	0
83	MG	AR	3918	1/1	0.82	0.09	66,66,66,66	0
83	MG	d5	201	1/1	0.82	0.17	94,94,94,94	0
83	MG	d9	102	1/1	0.82	0.09	100,100,100,100	0
82	OHX	1	4124	7/7	0.82	0.15	132,136,141,244	0
83	MG	1	3953	1/1	0.82	0.26	76,76,76,76	0
82	OHX	sR	2019	7/7	0.83	0.12	199,200,229,308	0
83	MG	AR	3832	1/1	0.83	0.39	56,56,56,56	0
83	MG	A	2019	1/1	0.83	0.20	84,84,84,84	0
83	MG	sR	2062	1/1	0.83	0.26	60,60,60,60	0
83	MG	AR	3975	1/1	0.83	0.11	73,73,73,73	0
82	OHX	AR	4162	7/7	0.83	0.14	171,181,192,299	0
83	MG	AR	3842	1/1	0.83	0.38	49,49,49,49	0
83	MG	1	3633	1/1	0.83	0.18	87,87,87,87	0
83	MG	1	3635	1/1	0.83	0.33	61,61,61,61	0
83	MG	sR	2077	1/1	0.83	0.27	67,67,67,67	0
82	OHX	A	2137	7/7	0.83	0.11	203,207,212,298	0
83	MG	sR	2081	1/1	0.83	0.32	53,53,53,53	0
83	MG	AR	4187	1/1	0.83	0.10	94,94,94,94	0
83	MG	AR	3997	1/1	0.83	0.13	72,72,72,72	0
82	OHX	1	3585	7/7	0.83	0.16	143,161,168,288	0
82	OHX	AR	3643	7/7	0.83	0.13	169,181,207,299	0
83	MG	1	3662	1/1	0.83	0.26	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	A	2144	7/7	0.83	0.20	133,137,142,175	7
83	MG	sR	2103	1/1	0.83	0.08	84,84,84,84	0
83	MG	1	3754	1/1	0.83	0.33	58,58,58,58	0
83	MG	1	4063	1/1	0.83	0.12	84,84,84,84	0
83	MG	AR	3723	1/1	0.83	0.19	50,50,50,50	0
82	OHX	sR	1976	7/7	0.83	0.16	136,144,165,249	0
82	OHX	sR	1980	7/7	0.83	0.11	210,219,239,333	0
83	MG	CE	403	1/1	0.83	0.37	48,48,48,48	0
83	MG	1	3892	1/1	0.83	0.21	88,88,88,88	0
83	MG	CF	402	1/1	0.83	0.24	85,85,85,85	0
83	MG	AR	3890	1/1	0.83	0.31	75,75,75,75	0
83	MG	sR	2130	1/1	0.83	0.17	56,56,56,56	0
83	MG	A	2063	1/1	0.83	0.12	81,81,81,81	0
82	OHX	AR	3652	7/7	0.83	0.10	158,171,190,292	0
83	MG	3	217	1/1	0.83	0.16	95,95,95,95	0
83	MG	AR	4031	1/1	0.83	0.12	62,62,62,62	0
83	MG	1	3680	1/1	0.83	0.35	91,91,91,91	0
83	MG	A	2076	1/1	0.83	0.19	78,78,78,78	0
82	OHX	1	4105	7/7	0.83	0.09	190,194,218,314	0
83	MG	AR	4044	1/1	0.83	0.10	78,78,78,78	0
83	MG	1	3906	1/1	0.83	0.17	73,73,73,73	0
83	MG	A	2087	1/1	0.83	0.13	67,67,67,67	0
83	MG	AR	3925	1/1	0.83	0.27	79,79,79,79	0
83	MG	1	3789	1/1	0.83	0.37	47,47,47,47	0
83	MG	t	202	1/1	0.83	0.15	57,57,57,57	0
83	MG	AR	3934	1/1	0.83	0.13	94,94,94,94	0
83	MG	A	1987	1/1	0.83	0.32	56,56,56,56	0
82	OHX	s8	301	7/7	0.83	0.13	167,179,185,281	0
83	MG	1	3697	1/1	0.83	0.17	79,79,79,79	0
83	MG	AR	3772	1/1	0.83	0.12	62,62,62,62	0
83	MG	1	3925	1/1	0.83	0.29	70,70,70,70	0
82	OHX	AR	3665	7/7	0.83	0.11	189,203,222,316	0
83	MG	sR	2030	1/1	0.83	0.18	90,90,90,90	0
83	MG	1	3929	1/1	0.83	0.13	60,60,60,60	0
83	MG	AR	3953	1/1	0.83	0.22	66,66,66,66	0
82	OHX	4	229	7/7	0.83	0.13	185,200,206,312	0
82	OHX	AR	3660	7/7	0.83	0.10	199,210,226,315	0
83	MG	1	3824	1/1	0.83	0.14	62,62,62,62	0
83	MG	AR	3682	1/1	0.83	0.27	62,62,62,62	0
84	K	AR	4164	1/1	0.83	0.18	126,126,126,126	0
83	MG	1	3940	1/1	0.83	0.14	92,92,92,92	0
83	MG	1	3724	1/1	0.84	0.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	3957	1/1	0.84	0.07	68,68,68,68	0
83	MG	1	3826	1/1	0.84	0.20	67,67,67,67	0
83	MG	AR	3743	1/1	0.84	0.30	63,63,63,63	0
83	MG	AT	205	1/1	0.84	0.16	60,60,60,60	0
83	MG	AT	221	1/1	0.84	0.13	70,70,70,70	0
83	MG	1	3725	1/1	0.84	0.20	48,48,48,48	0
82	OHX	AR	4149	7/7	0.84	0.12	159,166,179,299	0
83	MG	1	3636	1/1	0.84	0.24	59,59,59,59	0
83	MG	1	3961	1/1	0.84	0.12	57,57,57,57	0
82	OHX	AS	209	7/7	0.84	0.11	163,183,198,276	0
83	MG	AR	3763	1/1	0.84	0.20	70,70,70,70	0
82	OHX	1	4133	7/7	0.84	0.11	194,197,206,307	0
83	MG	CK	202	1/1	0.84	0.27	70,70,70,70	0
83	MG	1	3739	1/1	0.84	0.17	54,54,54,54	0
83	MG	AR	3778	1/1	0.84	0.32	46,46,46,46	0
83	MG	AR	3781	1/1	0.84	0.35	60,60,60,60	0
83	MG	AR	3989	1/1	0.84	0.12	65,65,65,65	0
83	MG	1	3743	1/1	0.84	0.14	59,59,59,59	0
83	MG	sR	2057	1/1	0.84	0.23	78,78,78,78	0
83	MG	o	301	1/1	0.84	0.32	90,90,90,90	0
83	MG	1	3877	1/1	0.84	0.13	72,72,72,72	0
83	MG	AR	3801	1/1	0.84	0.16	58,58,58,58	0
83	MG	sM	302	1/1	0.84	0.16	64,64,64,64	0
83	MG	1	3880	1/1	0.84	0.15	62,62,62,62	0
83	MG	1	3973	1/1	0.84	0.17	71,71,71,71	0
83	MG	AR	3822	1/1	0.84	0.24	45,45,45,45	0
83	MG	AR	3823	1/1	0.84	0.28	67,67,67,67	0
82	OHX	A	2146	7/7	0.84	0.17	161,174,185,278	0
82	OHX	AT	235	7/7	0.84	0.13	140,148,153,220	7
83	MG	x	203	1/1	0.84	0.21	53,53,53,53	0
83	MG	1	3989	1/1	0.84	0.21	65,65,65,65	0
83	MG	AR	4020	1/1	0.84	0.10	117,117,117,117	0
83	MG	z	201	1/1	0.84	0.17	113,113,113,113	0
83	MG	sR	2099	1/1	0.84	0.15	74,74,74,74	0
82	OHX	CE	402	7/7	0.84	0.09	197,214,224,306	0
83	MG	1	3997	1/1	0.84	0.14	80,80,80,80	0
83	MG	AB	205	1/1	0.84	0.21	76,76,76,76	0
83	MG	1	3998	1/1	0.84	0.12	66,66,66,66	0
82	OHX	1	3549	7/7	0.84	0.12	167,173,184,276	0
83	MG	1	3673	1/1	0.84	0.26	81,81,81,81	0
83	MG	AR	3681	1/1	0.84	0.24	56,56,56,56	0
83	MG	A	2018	1/1	0.84	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3893	1/1	0.84	0.36	59,59,59,59	0
82	OHX	sR	2180	7/7	0.84	0.12	201,209,219,271	7
83	MG	A	2022	1/1	0.84	0.09	70,70,70,70	0
83	MG	1	3756	1/1	0.84	0.17	50,50,50,50	0
82	OHX	1	4139	7/7	0.84	0.12	179,184,201,306	0
83	MG	AR	3875	1/1	0.84	0.24	71,71,71,71	0
83	MG	AR	3687	1/1	0.84	0.33	66,66,66,66	0
83	MG	sR	2136	1/1	0.84	0.19	115,115,115,115	0
83	MG	AR	3698	1/1	0.84	0.12	88,88,88,88	0
82	OHX	s4	301	7/7	0.84	0.11	175,178,202,279	0
83	MG	AR	3701	1/1	0.84	0.16	72,72,72,72	0
83	MG	AR	3892	1/1	0.84	0.17	52,52,52,52	0
83	MG	1	4018	1/1	0.84	0.25	47,47,47,47	0
83	MG	1	3683	1/1	0.84	0.15	63,63,63,63	0
83	MG	AR	3899	1/1	0.84	0.17	70,70,70,70	0
83	MG	AR	3905	1/1	0.84	0.11	50,50,50,50	0
83	MG	AR	3707	1/1	0.84	0.27	47,47,47,47	0
83	MG	1	3908	1/1	0.84	0.17	83,83,83,83	0
83	MG	AR	4092	1/1	0.84	0.24	67,67,67,67	0
83	MG	1	3776	1/1	0.84	0.16	59,59,59,59	0
83	MG	AR	4096	1/1	0.84	0.30	47,47,47,47	0
83	MG	AR	3920	1/1	0.84	0.14	87,87,87,87	0
83	MG	AR	3921	1/1	0.84	0.18	59,59,59,59	0
83	MG	1	3686	1/1	0.84	0.23	84,84,84,84	0
82	OHX	1	3521	7/7	0.84	0.13	157,163,177,260	0
83	MG	AR	4110	1/1	0.84	0.28	46,46,46,46	0
83	MG	A	2065	1/1	0.84	0.23	56,56,56,56	0
82	OHX	1	4126	7/7	0.84	0.11	181,192,206,292	0
82	OHX	sR	2012	7/7	0.84	0.09	182,186,201,287	0
83	MG	c4	2202	1/1	0.84	0.11	64,64,64,64	0
83	MG	1	3806	1/1	0.84	0.17	51,51,51,51	0
83	MG	A	2072	1/1	0.84	0.11	75,75,75,75	0
82	OHX	1	4131	7/7	0.84	0.12	144,147,155,258	0
82	OHX	sR	2018	7/7	0.84	0.13	175,195,204,289	0
82	OHX	A	2135	7/7	0.84	0.10	222,226,236,296	0
83	MG	1	3941	1/1	0.84	0.24	56,56,56,56	0
82	OHX	AR	4146	7/7	0.84	0.11	160,172,195,285	0
87	ZN	d7	101	1/1	0.84	0.08	252,252,252,252	0
83	MG	sR	2027	1/1	0.85	0.24	55,55,55,55	0
83	MG	sR	2028	1/1	0.85	0.23	65,65,65,65	0
83	MG	r	301	1/1	0.85	0.08	51,51,51,51	0
83	MG	sR	2031	1/1	0.85	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	3915	1/1	0.85	0.09	55,55,55,55	0
83	MG	1	3882	1/1	0.85	0.12	74,74,74,74	0
82	OHX	AT	233	7/7	0.85	0.11	162,166,168,271	0
82	OHX	sR	2179	7/7	0.85	0.08	233,239,247,320	0
83	MG	AR	3755	1/1	0.85	0.22	47,47,47,47	0
83	MG	sR	2046	1/1	0.85	0.38	84,84,84,84	0
83	MG	AR	3758	1/1	0.85	0.10	51,51,51,51	0
83	MG	1	3679	1/1	0.85	0.20	72,72,72,72	0
82	OHX	1	3556	7/7	0.85	0.14	172,176,195,283	0
82	OHX	AR	4139	7/7	0.85	0.10	158,177,186,273	0
83	MG	AR	4067	1/1	0.85	0.23	72,72,72,72	0
82	OHX	AR	3653	7/7	0.85	0.12	175,186,209,315	0
82	OHX	CL	303	7/7	0.85	0.14	132,136,165,235	0
83	MG	1	3609	1/1	0.85	0.32	65,65,65,65	0
83	MG	sR	2067	1/1	0.85	0.30	52,52,52,52	0
83	MG	1	3696	1/1	0.85	0.17	67,67,67,67	0
82	OHX	sR	2001	7/7	0.85	0.12	192,195,213,288	0
83	MG	1	3698	1/1	0.85	0.12	64,64,64,64	0
83	MG	1	3804	1/1	0.85	0.14	46,46,46,46	0
82	OHX	1	3550	7/7	0.85	0.11	171,196,204,303	0
83	MG	sR	2079	1/1	0.85	0.21	53,53,53,53	0
83	MG	1	3703	1/1	0.85	0.18	60,60,60,60	0
83	MG	AR	3958	1/1	0.85	0.15	51,51,51,51	0
82	OHX	1	3504	7/7	0.85	0.18	125,127,141,250	0
83	MG	A	2020	1/1	0.85	0.11	66,66,66,66	0
83	MG	1	3623	1/1	0.85	0.27	59,59,59,59	0
83	MG	sR	2092	1/1	0.85	0.18	76,76,76,76	0
82	OHX	1	4151	7/7	0.85	0.13	175,176,189,295	0
83	MG	1	3629	1/1	0.85	0.22	59,59,59,59	0
82	OHX	1	3586	7/7	0.85	0.14	162,167,180,283	0
83	MG	A	2028	1/1	0.85	0.16	90,90,90,90	0
83	MG	AR	3826	1/1	0.85	0.14	49,49,49,49	0
83	MG	AR	4109	1/1	0.85	0.21	65,65,65,65	0
83	MG	1	3939	1/1	0.85	0.10	55,55,55,55	0
83	MG	1	3830	1/1	0.85	0.21	61,61,61,61	0
83	MG	AR	3976	1/1	0.85	0.28	57,57,57,57	0
83	MG	sR	2117	1/1	0.85	0.11	67,67,67,67	0
83	MG	AR	4134	1/1	0.85	0.13	70,70,70,70	0
83	MG	AR	4178	1/1	0.85	0.09	134,134,134,134	0
82	OHX	1	4127	7/7	0.85	0.11	152,165,169,278	0
83	MG	1	3832	1/1	0.85	0.16	65,65,65,65	0
83	MG	AR	3984	1/1	0.85	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3630	7/7	0.85	0.12	166,179,194,274	0
83	MG	A	2047	1/1	0.85	0.16	81,81,81,81	0
83	MG	sR	2133	1/1	0.85	0.33	90,90,90,90	0
83	MG	AR	3706	1/1	0.85	0.18	67,67,67,67	0
83	MG	AS	214	1/1	0.85	0.28	48,48,48,48	0
83	MG	1	4043	1/1	0.85	0.24	60,60,60,60	0
82	OHX	A	2136	7/7	0.85	0.12	177,185,201,271	0
83	MG	AR	3996	1/1	0.85	0.12	101,101,101,101	0
83	MG	1	3839	1/1	0.85	0.19	51,51,51,51	0
83	MG	AS	227	1/1	0.85	0.21	61,61,61,61	0
83	MG	AR	3998	1/1	0.85	0.12	51,51,51,51	0
83	MG	1	3843	1/1	0.85	0.31	74,74,74,74	0
83	MG	AT	219	1/1	0.85	0.13	65,65,65,65	0
83	MG	AR	3717	1/1	0.85	0.21	60,60,60,60	0
82	OHX	1	4155	7/7	0.85	0.16	139,143,149,205	7
82	OHX	1	3600	7/7	0.85	0.14	168,173,196,280	0
83	MG	AT	227	1/1	0.85	0.13	57,57,57,57	0
83	MG	A	2075	1/1	0.85	0.17	100,100,100,100	0
82	OHX	sR	2169	7/7	0.85	0.11	183,196,209,283	0
83	MG	CE	404	1/1	0.85	0.25	55,55,55,55	0
83	MG	sR	2168	1/1	0.85	0.16	66,66,66,66	0
83	MG	1	3866	1/1	0.85	0.14	56,56,56,56	0
83	MG	AR	3876	1/1	0.85	0.09	57,57,57,57	0
83	MG	1	4183	1/1	0.85	0.23	59,59,59,59	0
83	MG	A	2091	1/1	0.85	0.32	58,58,58,58	0
83	MG	1	3871	1/1	0.85	0.10	68,68,68,68	0
82	OHX	sR	2170	7/7	0.85	0.10	213,216,228,298	0
83	MG	c6	201	1/1	0.85	0.15	102,102,102,102	0
83	MG	CM	201	1/1	0.85	0.20	65,65,65,65	0
82	OHX	AR	3640	7/7	0.85	0.16	139,153,157,277	0
83	MG	CP	303	1/1	0.85	0.14	63,63,63,63	0
83	MG	AR	3735	1/1	0.85	0.25	69,69,69,69	0
82	OHX	1	4132	7/7	0.85	0.11	177,187,201,284	0
82	OHX	AR	3668	7/7	0.85	0.11	207,215,224,293	0
83	MG	1	3974	1/1	0.85	0.10	63,63,63,63	0
83	MG	AR	3902	1/1	0.85	0.16	66,66,66,66	0
83	MG	1	3786	1/1	0.86	0.12	66,66,66,66	0
82	OHX	A	2132	7/7	0.86	0.11	166,167,184,266	0
82	OHX	1	3602	7/7	0.86	0.12	159,165,193,278	0
83	MG	DC	201	1/1	0.86	0.17	48,48,48,48	0
83	MG	AR	3901	1/1	0.86	0.26	69,69,69,69	0
82	OHX	AR	3656	7/7	0.86	0.10	176,195,208,297	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3981	1/1	0.86	0.09	69,69,69,69	0
83	MG	A	1984	1/1	0.86	0.27	52,52,52,52	0
83	MG	1	3792	1/1	0.86	0.21	48,48,48,48	0
83	MG	AR	4060	1/1	0.86	0.11	55,55,55,55	0
83	MG	1	3990	1/1	0.86	0.06	56,56,56,56	0
83	MG	AR	4062	1/1	0.86	0.12	59,59,59,59	0
83	MG	v	304	1/1	0.86	0.21	63,63,63,63	0
82	OHX	sR	2023	7/7	0.86	0.12	196,200,220,312	0
83	MG	AR	3757	1/1	0.86	0.15	69,69,69,69	0
83	MG	A	1997	1/1	0.86	0.23	62,62,62,62	0
83	MG	A	1999	1/1	0.86	0.14	54,54,54,54	0
83	MG	x	201	1/1	0.86	0.22	48,48,48,48	0
83	MG	AR	4069	1/1	0.86	0.19	51,51,51,51	0
83	MG	AR	3760	1/1	0.86	0.28	48,48,48,48	0
83	MG	AR	4072	1/1	0.86	0.29	56,56,56,56	0
82	OHX	AR	3615	7/7	0.86	0.10	201,208,222,316	0
83	MG	1	3805	1/1	0.86	0.11	56,56,56,56	0
82	OHX	A	2139	7/7	0.86	0.10	208,213,228,304	0
83	MG	AR	4084	1/1	0.86	0.12	88,88,88,88	0
83	MG	AR	4085	1/1	0.86	0.25	51,51,51,51	0
83	MG	AR	3765	1/1	0.86	0.20	52,52,52,52	0
82	OHX	AR	3671	7/7	0.86	0.12	159,163,184,297	0
83	MG	sR	2087	1/1	0.86	0.13	85,85,85,85	0
83	MG	1	3812	1/1	0.86	0.09	56,56,56,56	0
82	OHX	AR	3526	7/7	0.86	0.15	124,141,160,251	0
83	MG	AR	3780	1/1	0.86	0.29	50,50,50,50	0
83	MG	6	203	1/1	0.86	0.23	73,73,73,73	0
83	MG	AR	3950	1/1	0.86	0.21	76,76,76,76	0
83	MG	AR	3782	1/1	0.86	0.32	50,50,50,50	0
82	OHX	AR	4141	7/7	0.86	0.10	152,157,177,265	0
83	MG	1	3823	1/1	0.86	0.38	86,86,86,86	0
83	MG	1	3917	1/1	0.86	0.10	67,67,67,67	0
83	MG	sR	2107	1/1	0.86	0.32	88,88,88,88	0
83	MG	sR	2108	1/1	0.86	0.16	85,85,85,85	0
83	MG	1	3658	1/1	0.86	0.24	69,69,69,69	0
83	MG	AR	3803	1/1	0.86	0.27	58,58,58,58	0
83	MG	1	3660	1/1	0.86	0.14	60,60,60,60	0
83	MG	AR	3809	1/1	0.86	0.24	51,51,51,51	0
83	MG	AR	4128	1/1	0.86	0.15	66,66,66,66	0
83	MG	sR	2122	1/1	0.86	0.21	69,69,69,69	0
83	MG	AR	4129	1/1	0.86	0.23	76,76,76,76	0
83	MG	AR	4130	1/1	0.86	0.14	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	4021	1/1	0.86	0.18	52,52,52,52	0
83	MG	AR	3820	1/1	0.86	0.26	48,48,48,48	0
83	MG	1	3737	1/1	0.86	0.29	46,46,46,46	0
83	MG	1	3827	1/1	0.86	0.20	67,67,67,67	0
82	OHX	sR	2173	7/7	0.86	0.11	182,199,211,290	0
82	OHX	AR	4143	7/7	0.86	0.13	148,150,164,272	0
82	OHX	AR	3631	7/7	0.86	0.12	152,158,168,258	0
83	MG	1	3835	1/1	0.86	0.20	63,63,63,63	0
83	MG	AR	3700	1/1	0.86	0.10	51,51,51,51	0
83	MG	sR	2142	1/1	0.86	0.16	62,62,62,62	0
82	OHX	1	4144	6/7	0.86	0.18	128,139,143,217	6
82	OHX	1	3565	7/7	0.86	0.11	183,193,199,284	0
82	OHX	A	1960	7/7	0.86	0.10	174,190,199,275	0
82	OHX	sR	1997	7/7	0.86	0.13	177,183,200,280	0
83	MG	A	2066	1/1	0.86	0.17	83,83,83,83	0
83	MG	A	2067	1/1	0.86	0.13	84,84,84,84	0
83	MG	1	4039	1/1	0.86	0.14	46,46,46,46	0
83	MG	AR	3708	1/1	0.86	0.23	50,50,50,50	0
82	OHX	AR	4150	7/7	0.86	0.15	152,172,187,311	0
82	OHX	A	1967	7/7	0.86	0.11	180,188,198,287	0
83	MG	A	2073	1/1	0.86	0.10	91,91,91,91	0
82	OHX	sR	2002	7/7	0.86	0.11	178,186,192,275	0
83	MG	1	3857	1/1	0.86	0.28	53,53,53,53	0
83	MG	AR	3863	1/1	0.86	0.16	68,68,68,68	0
83	MG	AT	230	1/1	0.86	0.19	51,51,51,51	0
83	MG	1	3956	1/1	0.86	0.16	78,78,78,78	0
82	OHX	AR	3637	7/7	0.86	0.11	158,171,194,295	0
83	MG	CE	405	1/1	0.86	0.30	72,72,72,72	0
83	MG	1	3867	1/1	0.86	0.07	60,60,60,60	0
83	MG	AR	4015	1/1	0.86	0.15	60,60,60,60	0
83	MG	1	3765	1/1	0.86	0.32	47,47,47,47	0
83	MG	A	2151	1/1	0.86	0.27	106,106,106,106	0
83	MG	d4	202	1/1	0.86	0.09	79,79,79,79	0
83	MG	AR	4019	1/1	0.86	0.14	70,70,70,70	0
83	MG	AR	3725	1/1	0.86	0.22	46,46,46,46	0
83	MG	1	3873	1/1	0.86	0.24	72,72,72,72	0
82	OHX	1	3584	7/7	0.86	0.10	159,167,177,273	0
83	MG	AR	3889	1/1	0.86	0.07	68,68,68,68	0
82	OHX	AR	3589	7/7	0.86	0.17	75,99,121,217	0
82	OHX	AR	3592	7/7	0.86	0.13	118,129,142,224	0
88	OS	A	2158	1/1	0.86	0.07	290,290,290,290	0
83	MG	AR	3720	1/1	0.87	0.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	A	2013	1/1	0.87	0.26	54,54,54,54	0
82	OHX	A	2147	7/7	0.87	0.12	152,153,158,179	7
83	MG	1	3890	1/1	0.87	0.18	62,62,62,62	0
83	MG	sR	2063	1/1	0.87	0.25	70,70,70,70	0
83	MG	4	218	1/1	0.87	0.09	57,57,57,57	0
83	MG	AR	3853	1/1	0.87	0.19	47,47,47,47	0
83	MG	AR	3857	1/1	0.87	0.13	48,48,48,48	0
83	MG	AR	3858	1/1	0.87	0.13	65,65,65,65	0
82	OHX	J	301	7/7	0.87	0.08	209,213,226,304	0
83	MG	1	3654	1/1	0.87	0.19	54,54,54,54	0
83	MG	4	226	1/1	0.87	0.14	55,55,55,55	0
83	MG	1	3655	1/1	0.87	0.17	60,60,60,60	0
83	MG	AR	4181	1/1	0.87	0.11	119,119,119,119	0
83	MG	1	3817	1/1	0.87	0.14	69,69,69,69	0
83	MG	AR	4001	1/1	0.87	0.22	63,63,63,63	0
83	MG	AR	3736	1/1	0.87	0.16	86,86,86,86	0
83	MG	AR	3870	1/1	0.87	0.07	61,61,61,61	0
83	MG	1	3818	1/1	0.87	0.07	84,84,84,84	0
83	MG	AS	213	1/1	0.87	0.30	71,71,71,71	0
83	MG	sR	2098	1/1	0.87	0.20	51,51,51,51	0
82	OHX	O	201	7/7	0.87	0.08	199,205,223,293	0
83	MG	AR	4008	1/1	0.87	0.08	58,58,58,58	0
83	MG	1	3732	1/1	0.87	0.14	65,65,65,65	0
82	OHX	sR	1963	7/7	0.87	0.13	151,157,169,247	0
83	MG	AR	3748	1/1	0.87	0.23	65,65,65,65	0
82	OHX	sR	2174	7/7	0.87	0.10	156,165,173,254	0
83	MG	sR	2106	1/1	0.87	0.10	74,74,74,74	0
83	MG	AR	4014	1/1	0.87	0.12	67,67,67,67	0
82	OHX	1	3508	7/7	0.87	0.13	140,155,170,257	0
82	OHX	1	3579	7/7	0.87	0.11	168,177,200,294	0
83	MG	A	2054	1/1	0.87	0.16	60,60,60,60	0
83	MG	A	2057	1/1	0.87	0.14	77,77,77,77	0
83	MG	A	2059	1/1	0.87	0.26	73,73,73,73	0
83	MG	sR	2119	1/1	0.87	0.27	70,70,70,70	0
83	MG	AR	3891	1/1	0.87	0.14	46,46,46,46	0
83	MG	1	3666	1/1	0.87	0.13	48,48,48,48	0
82	OHX	1	3502	7/7	0.87	0.11	121,157,174,276	0
82	OHX	1	3603	7/7	0.87	0.11	150,161,171,272	0
82	OHX	1	4123	7/7	0.87	0.14	150,151,172,268	0
83	MG	1	3935	1/1	0.87	0.34	55,55,55,55	0
83	MG	sR	2128	1/1	0.87	0.17	71,71,71,71	0
82	OHX	AR	3595	7/7	0.87	0.10	172,179,192,255	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	4033	1/1	0.87	0.15	56,56,56,56	0
83	MG	AB	201	1/1	0.87	0.16	64,64,64,64	0
82	OHX	A	2128	7/7	0.87	0.12	177,179,193,258	0
82	OHX	AR	3598	7/7	0.87	0.13	141,150,190,272	0
82	OHX	AR	4120	7/7	0.87	0.10	184,199,209,297	0
82	OHX	AR	3600	7/7	0.87	0.12	178,182,201,258	0
83	MG	1	4029	1/1	0.87	0.12	63,63,63,63	0
83	MG	1	3612	1/1	0.87	0.21	57,57,57,57	0
83	MG	AR	3923	1/1	0.87	0.15	79,79,79,79	0
82	OHX	1	3561	7/7	0.87	0.14	128,152,174,242	0
83	MG	sR	2146	1/1	0.87	0.36	68,68,68,68	0
83	MG	1	3692	1/1	0.87	0.21	61,61,61,61	0
83	MG	1	3693	1/1	0.87	0.21	47,47,47,47	0
82	OHX	AT	202	7/7	0.87	0.12	163,173,186,286	0
83	MG	1	3780	1/1	0.87	0.41	69,69,69,69	0
82	OHX	4	228	7/7	0.87	0.10	179,192,220,313	0
83	MG	1	3958	1/1	0.87	0.24	75,75,75,75	0
83	MG	AR	3808	1/1	0.87	0.12	101,101,101,101	0
83	MG	1	4045	1/1	0.87	0.31	47,47,47,47	0
83	MG	A	1981	1/1	0.87	0.17	65,65,65,65	0
83	MG	AR	3810	1/1	0.87	0.24	65,65,65,65	0
82	OHX	1	4147	7/7	0.87	0.21	122,124,129,152	7
82	OHX	1	3551	7/7	0.87	0.16	123,132,144,236	0
83	MG	1	3699	1/1	0.87	0.24	80,80,80,80	0
83	MG	1	3964	1/1	0.87	0.20	69,69,69,69	0
83	MG	AR	4087	1/1	0.87	0.24	65,65,65,65	0
82	OHX	AR	4147	7/7	0.87	0.10	168,179,190,289	0
82	OHX	A	2145	7/7	0.87	0.14	144,150,154,206	7
82	OHX	1	4150	7/7	0.87	0.10	172,177,179,285	0
83	MG	1	3707	1/1	0.87	0.40	62,62,62,62	0
83	MG	d3	202	1/1	0.87	0.20	92,92,92,92	0
83	MG	1	4184	1/1	0.87	0.19	52,52,52,52	0
83	MG	AR	4093	1/1	0.87	0.17	62,62,62,62	0
83	MG	1	3887	1/1	0.87	0.28	61,61,61,61	0
83	MG	AR	4095	1/1	0.87	0.11	53,53,53,53	0
83	MG	3	214	1/1	0.87	0.13	62,62,62,62	0
83	MG	AR	3974	1/1	0.87	0.12	55,55,55,55	0
83	MG	sR	2050	1/1	0.87	0.15	72,72,72,72	0
83	MG	AR	3844	1/1	0.87	0.12	51,51,51,51	0
83	MG	A	2010	1/1	0.87	0.23	68,68,68,68	0
83	MG	1	3653	1/1	0.88	0.14	49,49,49,49	0
83	MG	AR	3945	1/1	0.88	0.13	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	3946	1/1	0.88	0.23	90,90,90,90	0
83	MG	AR	4206	1/1	0.88	0.18	64,64,64,64	0
83	MG	A	2090	1/1	0.88	0.23	69,69,69,69	0
83	MG	AS	210	1/1	0.88	0.28	54,54,54,54	0
83	MG	1	3912	1/1	0.88	0.13	66,66,66,66	0
82	OHX	sR	2006	7/7	0.88	0.12	155,165,184,265	0
83	MG	1	3919	1/1	0.88	0.15	63,63,63,63	0
83	MG	A	2099	1/1	0.88	0.12	79,79,79,79	0
83	MG	1	3775	1/1	0.88	0.28	46,46,46,46	0
83	MG	A	2154	1/1	0.88	0.08	120,120,120,120	0
83	MG	A	2155	1/1	0.88	0.14	118,118,118,118	0
83	MG	1	4064	1/1	0.88	0.20	47,47,47,47	0
82	OHX	sR	2007	7/7	0.88	0.10	170,185,210,286	0
83	MG	1	4071	1/1	0.88	0.07	67,67,67,67	0
82	OHX	AR	3670	7/7	0.88	0.11	161,170,194,261	0
83	MG	1	4182	1/1	0.88	0.26	54,54,54,54	0
82	OHX	A	1962	7/7	0.88	0.09	184,203,216,286	0
82	OHX	1	3507	7/7	0.88	0.13	121,130,142,226	0
83	MG	AT	217	1/1	0.88	0.15	70,70,70,70	0
83	MG	AR	3971	1/1	0.88	0.10	68,68,68,68	0
82	OHX	sR	2015	7/7	0.88	0.12	147,155,185,270	0
82	OHX	AR	3634	7/7	0.88	0.11	161,171,198,284	0
83	MG	AR	3773	1/1	0.88	0.15	55,55,55,55	0
82	OHX	AR	3525	7/7	0.88	0.14	117,124,139,197	0
83	MG	sR	2036	1/1	0.88	0.28	59,59,59,59	0
83	MG	AT	229	1/1	0.88	0.29	60,60,60,60	0
83	MG	1	3793	1/1	0.88	0.20	47,47,47,47	0
82	OHX	1	3553	7/7	0.88	0.11	139,143,180,259	0
83	MG	sR	2045	1/1	0.88	0.19	70,70,70,70	0
82	OHX	A	1977	7/7	0.88	0.10	179,185,208,272	0
83	MG	4	222	1/1	0.88	0.18	58,58,58,58	0
82	OHX	A	2114	7/7	0.88	0.10	165,176,190,266	0
83	MG	AR	3791	1/1	0.88	0.14	49,49,49,49	0
82	OHX	AR	3639	7/7	0.88	0.09	165,179,197,275	0
83	MG	AR	3993	1/1	0.88	0.13	67,67,67,67	0
83	MG	AR	3995	1/1	0.88	0.11	66,66,66,66	0
83	MG	AR	3796	1/1	0.88	0.15	49,49,49,49	0
83	MG	k	401	1/1	0.88	0.13	57,57,57,57	0
83	MG	1	3807	1/1	0.88	0.11	59,59,59,59	0
83	MG	o	302	1/1	0.88	0.20	59,59,59,59	0
82	OHX	A	2127	7/7	0.88	0.09	252,258,261,330	0
82	OHX	sR	2026	7/7	0.88	0.11	171,177,200,271	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	sR	2167	7/7	0.88	0.12	158,165,177,257	0
82	OHX	AR	3535	7/7	0.88	0.13	116,130,152,218	0
82	OHX	AR	3642	7/7	0.88	0.11	161,164,177,289	0
82	OHX	1	3582	7/7	0.88	0.11	135,150,162,246	0
83	MG	sR	2078	1/1	0.88	0.30	53,53,53,53	0
82	OHX	AR	4148	7/7	0.88	0.09	157,165,176,276	0
82	OHX	AR	3645	7/7	0.88	0.11	139,154,176,262	0
82	OHX	1	3605	7/7	0.88	0.10	162,182,206,284	0
83	MG	sR	2083	1/1	0.88	0.16	68,68,68,68	0
82	OHX	sR	2176	7/7	0.88	0.13	175,179,199,288	0
83	MG	1	3966	1/1	0.88	0.12	69,69,69,69	0
83	MG	sR	2088	1/1	0.88	0.10	73,73,73,73	0
83	MG	1	3967	1/1	0.88	0.25	68,68,68,68	0
82	OHX	AR	3586	7/7	0.88	0.11	151,158,165,250	0
83	MG	AR	3833	1/1	0.88	0.22	48,48,48,48	0
83	MG	A	1991	1/1	0.88	0.25	74,74,74,74	0
82	OHX	AR	3587	7/7	0.88	0.14	145,150,157,261	0
82	OHX	1	3564	7/7	0.88	0.11	166,179,211,279	0
83	MG	AR	3843	1/1	0.88	0.10	58,58,58,58	0
83	MG	AB	202	1/1	0.88	0.14	67,67,67,67	0
83	MG	1	3701	1/1	0.88	0.23	52,52,52,52	0
82	OHX	AR	3658	7/7	0.88	0.11	144,162,177,262	0
83	MG	1	3976	1/1	0.88	0.11	69,69,69,69	0
82	OHX	1	3523	7/7	0.88	0.10	170,193,212,283	0
83	MG	AR	3677	1/1	0.88	0.18	74,74,74,74	0
83	MG	sR	2109	1/1	0.88	0.11	117,117,117,117	0
83	MG	AR	4048	1/1	0.88	0.16	60,60,60,60	0
83	MG	AR	4049	1/1	0.88	0.12	62,62,62,62	0
82	OHX	1	3568	7/7	0.88	0.10	162,172,187,267	0
83	MG	1	3705	1/1	0.88	0.13	55,55,55,55	0
83	MG	1	3982	1/1	0.88	0.21	55,55,55,55	0
83	MG	1	3988	1/1	0.88	0.16	81,81,81,81	0
83	MG	AR	4057	1/1	0.88	0.25	68,68,68,68	0
83	MG	A	2015	1/1	0.88	0.26	73,73,73,73	0
82	OHX	1	4112	7/7	0.88	0.12	179,184,189,237	0
82	OHX	c3	202	7/7	0.88	0.10	188,197,219,281	0
83	MG	AR	3689	1/1	0.88	0.20	49,49,49,49	0
83	MG	AR	3691	1/1	0.88	0.22	51,51,51,51	0
83	MG	1	3993	1/1	0.88	0.13	58,58,58,58	0
83	MG	1	3712	1/1	0.88	0.10	54,54,54,54	0
82	OHX	c7	201	7/7	0.88	0.07	235,249,260,342	0
82	OHX	1	4113	7/7	0.88	0.10	169,172,197,290	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	1	3591	7/7	0.88	0.12	188,197,216,325	0
83	MG	AR	3704	1/1	0.88	0.27	54,54,54,54	0
82	OHX	1	3594	7/7	0.88	0.10	193,200,211,300	0
83	MG	A	2032	1/1	0.88	0.26	89,89,89,89	0
82	OHX	sR	1973	7/7	0.88	0.09	217,230,239,321	0
83	MG	1	3618	1/1	0.88	0.20	61,61,61,61	0
83	MG	1	3620	1/1	0.88	0.12	92,92,92,92	0
83	MG	1	3621	1/1	0.88	0.19	53,53,53,53	0
82	OHX	4	202	7/7	0.88	0.12	154,167,182,277	0
82	OHX	AR	3628	7/7	0.88	0.12	189,195,207,308	0
83	MG	AR	3895	1/1	0.88	0.10	71,71,71,71	0
83	MG	AR	3716	1/1	0.88	0.10	47,47,47,47	0
83	MG	1	3741	1/1	0.88	0.24	58,58,58,58	0
83	MG	1	3624	1/1	0.88	0.15	76,76,76,76	0
82	OHX	sR	1985	7/7	0.88	0.09	174,187,199,267	0
83	MG	AR	3911	1/1	0.88	0.12	68,68,68,68	0
82	OHX	AR	3629	7/7	0.88	0.09	141,157,166,258	0
83	MG	sR	2162	1/1	0.88	0.16	62,62,62,62	0
83	MG	A	2052	1/1	0.88	0.14	72,72,72,72	0
82	OHX	1	3596	7/7	0.88	0.09	143,158,175,280	0
82	OHX	CG	302	7/7	0.88	0.09	190,197,203,279	0
83	MG	1	3634	1/1	0.88	0.20	67,67,67,67	0
83	MG	AR	3726	1/1	0.88	0.14	52,52,52,52	0
82	OHX	1	3572	7/7	0.88	0.10	147,153,175,244	0
83	MG	AR	3922	1/1	0.88	0.20	60,60,60,60	0
83	MG	c3	201	1/1	0.88	0.26	55,55,55,55	0
83	MG	AR	4106	1/1	0.88	0.17	46,46,46,46	0
83	MG	1	3895	1/1	0.88	0.15	69,69,69,69	0
82	OHX	A	1955	7/7	0.88	0.10	145,152,172,248	0
83	MG	c9	201	1/1	0.88	0.26	82,82,82,82	0
83	MG	AR	4118	1/1	0.88	0.27	56,56,56,56	0
83	MG	AR	3926	1/1	0.88	0.08	57,57,57,57	0
83	MG	1	3760	1/1	0.88	0.29	47,47,47,47	0
83	MG	1	3648	1/1	0.88	0.17	47,47,47,47	0
83	MG	1	3905	1/1	0.88	0.13	59,59,59,59	0
83	MG	1	3762	1/1	0.88	0.12	51,51,51,51	0
82	OHX	A	1959	7/7	0.88	0.11	165,169,189,263	0
83	MG	AR	4175	1/1	0.88	0.17	64,64,64,64	0
85	SPD	1	4180	10/10	0.88	0.17	54,59,62,64	0
83	MG	1	3767	1/1	0.88	0.27	52,52,52,52	0
83	MG	AR	3742	1/1	0.88	0.14	61,61,61,61	0
83	MG	1	4161	1/1	0.89	0.09	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	4024	1/1	0.89	0.11	73,73,73,73	0
83	MG	1	4174	1/1	0.89	0.10	102,102,102,102	0
82	OHX	CG	304	7/7	0.89	0.10	229,230,235,324	0
82	OHX	AR	3570	7/7	0.89	0.11	151,155,173,265	0
83	MG	1	3850	1/1	0.89	0.16	53,53,53,53	0
83	MG	AR	3884	1/1	0.89	0.12	61,61,61,61	0
83	MG	CR	203	1/1	0.89	0.24	45,45,45,45	0
83	MG	sR	2032	1/1	0.89	0.19	53,53,53,53	0
83	MG	AR	4034	1/1	0.89	0.10	68,68,68,68	0
83	MG	AR	4040	1/1	0.89	0.27	71,71,71,71	0
83	MG	AR	3888	1/1	0.89	0.23	50,50,50,50	0
83	MG	AR	3733	1/1	0.89	0.30	64,64,64,64	0
82	OHX	sR	1972	7/7	0.89	0.10	175,182,191,255	0
82	OHX	A	1942	7/7	0.89	0.12	159,168,178,251	0
83	MG	sR	2042	1/1	0.89	0.23	90,90,90,90	0
83	MG	DO	203	1/1	0.89	0.20	74,74,74,74	0
83	MG	DP	101	1/1	0.89	0.25	72,72,72,72	0
82	OHX	AR	3574	7/7	0.89	0.15	131,139,151,254	0
82	OHX	sR	1977	7/7	0.89	0.08	203,206,232,292	0
83	MG	4	215	1/1	0.89	0.18	57,57,57,57	0
83	MG	1	3676	1/1	0.89	0.21	47,47,47,47	0
82	OHX	AR	4140	7/7	0.89	0.10	184,190,199,289	0
83	MG	AR	3900	1/1	0.89	0.18	48,48,48,48	0
82	OHX	sR	1981	7/7	0.89	0.10	139,148,162,267	0
83	MG	sR	2060	1/1	0.89	0.21	86,86,86,86	0
83	MG	AR	3747	1/1	0.89	0.28	74,74,74,74	0
83	MG	AR	3904	1/1	0.89	0.11	57,57,57,57	0
82	OHX	AR	3575	6/7	0.89	0.10	146,168,180,264	0
83	MG	4	225	1/1	0.89	0.14	61,61,61,61	0
82	OHX	sR	1993	7/7	0.89	0.10	212,214,216,294	0
83	MG	A	1998	1/1	0.89	0.11	64,64,64,64	0
83	MG	sR	2071	1/1	0.89	0.17	57,57,57,57	0
82	OHX	AR	4142	7/7	0.89	0.10	178,189,199,277	0
83	MG	1	402	1/1	0.89	0.20	76,76,76,76	0
83	MG	sR	2076	1/1	0.89	0.30	66,66,66,66	0
83	MG	A	2001	1/1	0.89	0.26	70,70,70,70	0
83	MG	1	3975	1/1	0.89	0.15	69,69,69,69	0
83	MG	AR	4071	1/1	0.89	0.28	70,70,70,70	0
83	MG	1	3684	1/1	0.89	0.20	51,51,51,51	0
83	MG	AR	4076	1/1	0.89	0.23	62,62,62,62	0
83	MG	sR	2082	1/1	0.89	0.20	71,71,71,71	0
82	OHX	1	3519	7/7	0.89	0.11	121,130,146,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	c8	201	7/7	0.89	0.09	181,187,202,258	0
83	MG	sR	2086	1/1	0.89	0.12	77,77,77,77	0
83	MG	1	3884	1/1	0.89	0.19	50,50,50,50	0
83	MG	AR	4080	1/1	0.89	0.17	49,49,49,49	0
83	MG	AR	4081	1/1	0.89	0.21	55,55,55,55	0
82	OHX	1	3583	7/7	0.89	0.12	151,161,177,257	0
83	MG	1	3985	1/1	0.89	0.17	47,47,47,47	0
83	MG	AR	3769	1/1	0.89	0.18	50,50,50,50	0
83	MG	1	3781	1/1	0.89	0.23	49,49,49,49	0
83	MG	1	3785	1/1	0.89	0.21	52,52,52,52	0
82	OHX	1	3573	7/7	0.89	0.09	169,177,198,288	0
82	OHX	AR	3649	7/7	0.89	0.09	176,190,210,301	0
83	MG	x	205	1/1	0.89	0.17	54,54,54,54	0
82	OHX	1	4130	7/7	0.89	0.08	151,163,186,280	0
83	MG	AR	3943	1/1	0.89	0.09	50,50,50,50	0
82	OHX	sR	2004	7/7	0.89	0.12	218,228,242,340	0
83	MG	1	3619	1/1	0.89	0.26	47,47,47,47	0
83	MG	1	3999	1/1	0.89	0.23	92,92,92,92	0
82	OHX	1	3524	7/7	0.89	0.11	172,180,198,268	0
83	MG	AR	3949	1/1	0.89	0.16	69,69,69,69	0
83	MG	sR	2114	1/1	0.89	0.15	103,103,103,103	0
83	MG	1	3796	1/1	0.89	0.14	59,59,59,59	0
82	OHX	4	212	7/7	0.89	0.09	155,162,175,277	0
83	MG	AR	3800	1/1	0.89	0.12	45,45,45,45	0
83	MG	1	3800	1/1	0.89	0.14	60,60,60,60	0
83	MG	AR	3802	1/1	0.89	0.23	69,69,69,69	0
83	MG	1	4010	1/1	0.89	0.23	48,48,48,48	0
82	OHX	sR	2009	7/7	0.89	0.09	213,216,223,267	0
83	MG	AR	3806	1/1	0.89	0.30	46,46,46,46	0
83	MG	AR	3807	1/1	0.89	0.23	66,66,66,66	0
82	OHX	4	213	7/7	0.89	0.11	162,168,187,275	0
82	OHX	1	3575	7/7	0.89	0.10	204,208,228,309	0
83	MG	1	4015	1/1	0.89	0.22	52,52,52,52	0
82	OHX	A	2129	7/7	0.89	0.09	220,231,238,318	0
83	MG	sR	2134	1/1	0.89	0.20	70,70,70,70	0
83	MG	1	3916	1/1	0.89	0.11	49,49,49,49	0
82	OHX	1	4119	7/7	0.89	0.10	134,137,153,248	0
83	MG	A	2055	1/1	0.89	0.12	73,73,73,73	0
82	OHX	k	404	7/7	0.89	0.13	110,122,138,206	0
83	MG	A	2058	1/1	0.89	0.26	53,53,53,53	0
82	OHX	A	2134	7/7	0.89	0.11	153,158,163,246	0
83	MG	AR	4189	1/1	0.89	0.10	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	4195	1/1	0.89	0.07	98,98,98,98	0
83	MG	1	3921	1/1	0.89	0.28	73,73,73,73	0
83	MG	sR	2147	1/1	0.89	0.26	54,54,54,54	0
83	MG	AR	3690	1/1	0.89	0.10	53,53,53,53	0
83	MG	1	3922	1/1	0.89	0.24	57,57,57,57	0
82	OHX	AR	3602	7/7	0.89	0.10	163,176,201,261	0
82	OHX	1	4148	7/7	0.89	0.16	125,135,142,210	7
83	MG	AR	3837	1/1	0.89	0.22	46,46,46,46	0
82	OHX	AR	3616	7/7	0.89	0.12	150,151,176,247	0
83	MG	A	2069	1/1	0.89	0.14	68,68,68,68	0
83	MG	1	3637	1/1	0.89	0.15	64,64,64,64	0
82	OHX	AR	3618	7/7	0.89	0.09	196,213,217,285	0
83	MG	1	3650	1/1	0.89	0.23	50,50,50,50	0
83	MG	AS	224	1/1	0.89	0.23	64,64,64,64	0
82	OHX	1	3590	7/7	0.89	0.11	161,174,195,291	0
82	OHX	1	4136	7/7	0.89	0.09	173,185,206,296	0
83	MG	A	2081	1/1	0.89	0.33	55,55,55,55	0
83	MG	1	3828	1/1	0.89	0.23	60,60,60,60	0
83	MG	s4	302	1/1	0.89	0.13	69,69,69,69	0
83	MG	1	4044	1/1	0.89	0.28	48,48,48,48	0
83	MG	AR	3851	1/1	0.89	0.23	47,47,47,47	0
83	MG	A	2086	1/1	0.89	0.21	53,53,53,53	0
82	OHX	1	3483	7/7	0.89	0.14	74,109,118,210	0
83	MG	A	2088	1/1	0.89	0.09	63,63,63,63	0
82	OHX	AR	3542	7/7	0.89	0.12	134,142,156,226	0
83	MG	1	3740	1/1	0.89	0.23	69,69,69,69	0
83	MG	A	2092	1/1	0.89	0.28	65,65,65,65	0
82	OHX	AR	3551	7/7	0.89	0.09	151,158,173,280	0
82	OHX	1	3593	7/7	0.89	0.09	176,195,209,291	0
83	MG	d4	204	1/1	0.89	0.28	58,58,58,58	0
83	MG	1	3744	1/1	0.89	0.18	62,62,62,62	0
83	MG	AT	232	1/1	0.89	0.09	63,63,63,63	0
83	MG	1	3950	1/1	0.89	0.15	73,73,73,73	0
82	OHX	AR	3566	7/7	0.89	0.14	111,121,140,204	0
83	MG	AR	3721	1/1	0.89	0.26	46,46,46,46	0
83	MG	1	3954	1/1	0.89	0.18	80,80,80,80	0
85	SPD	AR	4204	10/10	0.89	0.18	51,56,61,62	0
83	MG	1	3840	1/1	0.89	0.16	49,49,49,49	0
83	MG	AR	4021	1/1	0.89	0.17	61,61,61,61	0
82	OHX	CK	201	7/7	0.90	0.10	146,154,166,256	0
82	OHX	1	4098	7/7	0.90	0.10	134,143,164,231	0
83	MG	1	3626	1/1	0.90	0.19	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	A	1939	7/7	0.90	0.11	126,147,152,213	0
83	MG	1	3742	1/1	0.90	0.06	45,45,45,45	0
83	MG	AR	3910	1/1	0.90	0.07	61,61,61,61	0
83	MG	A	2074	1/1	0.90	0.14	63,63,63,63	0
83	MG	AR	4111	1/1	0.90	0.26	64,64,64,64	0
83	MG	AR	4117	1/1	0.90	0.13	60,60,60,60	0
83	MG	A	2078	1/1	0.90	0.27	84,84,84,84	0
83	MG	A	2080	1/1	0.90	0.25	52,52,52,52	0
83	MG	1	4014	1/1	0.90	0.26	47,47,47,47	0
83	MG	1	3630	1/1	0.90	0.09	47,47,47,47	0
83	MG	AR	4124	1/1	0.90	0.12	58,58,58,58	0
83	MG	AR	4125	1/1	0.90	0.20	61,61,61,61	0
83	MG	1	4017	1/1	0.90	0.10	70,70,70,70	0
83	MG	AR	3917	1/1	0.90	0.18	72,72,72,72	0
82	OHX	1	4099	6/7	0.90	0.11	168,180,202,291	0
83	MG	1	3885	1/1	0.90	0.19	66,66,66,66	0
83	MG	AR	4133	1/1	0.90	0.23	56,56,56,56	0
82	OHX	sR	2000	7/7	0.90	0.11	164,172,176,291	0
83	MG	A	2093	1/1	0.90	0.33	80,80,80,80	0
83	MG	AR	4171	1/1	0.90	0.11	109,109,109,109	0
82	OHX	A	1946	7/7	0.90	0.11	155,162,172,238	0
82	OHX	A	1951	7/7	0.90	0.10	180,183,193,269	0
82	OHX	1	405	7/7	0.90	0.07	194,201,215,302	0
83	MG	A	2101	1/1	0.90	0.09	68,68,68,68	0
83	MG	1	4026	1/1	0.90	0.18	55,55,55,55	0
82	OHX	AR	3606	7/7	0.90	0.09	166,170,186,269	0
83	MG	AR	3927	1/1	0.90	0.08	67,67,67,67	0
83	MG	1	3641	1/1	0.90	0.21	63,63,63,63	0
83	MG	1	3644	1/1	0.90	0.24	62,62,62,62	0
83	MG	AR	4199	1/1	0.90	0.11	69,69,69,69	0
83	MG	AR	4202	1/1	0.90	0.09	101,101,101,101	0
83	MG	1	3898	1/1	0.90	0.13	63,63,63,63	0
83	MG	1	3899	1/1	0.90	0.09	66,66,66,66	0
83	MG	1	3758	1/1	0.90	0.28	53,53,53,53	0
83	MG	1	3646	1/1	0.90	0.20	83,83,83,83	0
82	OHX	AR	3611	7/7	0.90	0.09	152,172,184,254	0
83	MG	sR	2029	1/1	0.90	0.21	65,65,65,65	0
82	OHX	sR	2008	7/7	0.90	0.10	144,162,182,257	0
83	MG	AS	215	1/1	0.90	0.13	55,55,55,55	0
82	OHX	1	4104	7/7	0.90	0.13	144,159,164,259	0
82	OHX	AR	3478	7/7	0.90	0.17	102,118,120,170	0
82	OHX	A	1966	7/7	0.90	0.10	170,176,188,255	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3493	7/7	0.90	0.10	130,135,158,219	0
83	MG	1	3773	1/1	0.90	0.26	46,46,46,46	0
83	MG	1	3913	1/1	0.90	0.11	66,66,66,66	0
82	OHX	sR	2014	7/7	0.90	0.09	193,202,212,284	0
83	MG	1	4061	1/1	0.90	0.11	54,54,54,54	0
83	MG	sR	2043	1/1	0.90	0.18	60,60,60,60	0
83	MG	sR	2044	1/1	0.90	0.10	57,57,57,57	0
82	OHX	A	1970	7/7	0.90	0.10	135,146,164,221	0
83	MG	AT	218	1/1	0.90	0.14	48,48,48,48	0
83	MG	1	3779	1/1	0.90	0.26	61,61,61,61	0
83	MG	AR	3756	1/1	0.90	0.20	56,56,56,56	0
83	MG	sR	2051	1/1	0.90	0.22	65,65,65,65	0
83	MG	1	4067	1/1	0.90	0.20	60,60,60,60	0
82	OHX	sR	2017	7/7	0.90	0.08	222,233,237,319	0
83	MG	1	4069	1/1	0.90	0.12	85,85,85,85	0
83	MG	1	3659	1/1	0.90	0.23	55,55,55,55	0
83	MG	AR	3966	1/1	0.90	0.15	78,78,78,78	0
82	OHX	AR	3624	7/7	0.90	0.10	197,201,202,278	0
82	OHX	AR	3501	7/7	0.90	0.15	102,108,121,204	0
82	OHX	AR	3510	7/7	0.90	0.13	90,114,132,192	0
83	MG	AR	3768	1/1	0.90	0.23	45,45,45,45	0
82	OHX	1	4125	7/7	0.90	0.11	129,130,143,233	0
83	MG	AR	3770	1/1	0.90	0.40	47,47,47,47	0
83	MG	CF	403	1/1	0.90	0.14	59,59,59,59	0
83	MG	1	3670	1/1	0.90	0.12	71,71,71,71	0
83	MG	AR	3982	1/1	0.90	0.29	60,60,60,60	0
83	MG	1	3932	1/1	0.90	0.15	78,78,78,78	0
83	MG	AR	3774	1/1	0.90	0.30	46,46,46,46	0
83	MG	CM	202	1/1	0.90	0.20	74,74,74,74	0
83	MG	3	208	1/1	0.90	0.12	61,61,61,61	0
83	MG	AR	3777	1/1	0.90	0.14	58,58,58,58	0
83	MG	1	3933	1/1	0.90	0.13	79,79,79,79	0
83	MG	AR	3992	1/1	0.90	0.15	64,64,64,64	0
82	OHX	1	3597	7/7	0.90	0.10	153,159,175,266	0
82	OHX	1	3599	7/7	0.90	0.10	149,154,167,236	0
82	OHX	1	4129	7/7	0.90	0.11	131,138,156,241	0
82	OHX	1	3559	7/7	0.90	0.09	144,150,170,242	0
83	MG	DA	202	1/1	0.90	0.19	55,55,55,55	0
82	OHX	AR	3636	7/7	0.90	0.11	129,142,157,264	0
83	MG	4	219	1/1	0.90	0.14	72,72,72,72	0
83	MG	DL	101	1/1	0.90	0.19	64,64,64,64	0
83	MG	AR	3795	1/1	0.90	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	sR	2096	1/1	0.90	0.10	73,73,73,73	0
82	OHX	1	4109	7/7	0.90	0.10	143,147,173,256	0
83	MG	4	221	1/1	0.90	0.15	60,60,60,60	0
83	MG	AR	3799	1/1	0.90	0.23	49,49,49,49	0
82	OHX	AR	3638	7/7	0.90	0.10	134,141,150,250	0
83	MG	A	1982	1/1	0.90	0.24	61,61,61,61	0
83	MG	1	3681	1/1	0.90	0.24	61,61,61,61	0
83	MG	1	3945	1/1	0.90	0.12	71,71,71,71	0
83	MG	sR	2105	1/1	0.90	0.10	67,67,67,67	0
83	MG	AR	4010	1/1	0.90	0.17	56,56,56,56	0
83	MG	1	3682	1/1	0.90	0.13	84,84,84,84	0
83	MG	4	230	1/1	0.90	0.07	108,108,108,108	0
82	OHX	AR	3564	7/7	0.90	0.10	163,166,174,233	0
82	OHX	1	4111	7/7	0.90	0.07	209,218,228,314	0
83	MG	sR	2111	1/1	0.90	0.20	56,56,56,56	0
83	MG	l	403	1/1	0.90	0.12	103,103,103,103	0
83	MG	sR	2113	1/1	0.90	0.12	60,60,60,60	0
83	MG	1	3813	1/1	0.90	0.44	73,73,73,73	0
82	OHX	AR	3569	7/7	0.90	0.09	155,164,184,258	0
83	MG	AR	3814	1/1	0.90	0.28	57,57,57,57	0
83	MG	sR	2118	1/1	0.90	0.10	86,86,86,86	0
83	MG	o	303	1/1	0.90	0.13	67,67,67,67	0
82	OHX	A	2138	7/7	0.90	0.10	145,155,158,246	0
83	MG	r	302	1/1	0.90	0.11	49,49,49,49	0
82	OHX	1	4152	7/7	0.90	0.07	176,182,195,293	0
83	MG	1	3819	1/1	0.90	0.10	60,60,60,60	0
83	MG	1	3960	1/1	0.90	0.13	58,58,58,58	0
82	OHX	1	3527	7/7	0.90	0.10	133,139,158,238	0
83	MG	AR	3828	1/1	0.90	0.25	49,49,49,49	0
82	OHX	AR	3646	7/7	0.90	0.08	179,191,211,275	0
83	MG	AR	4038	1/1	0.90	0.08	84,84,84,84	0
82	OHX	AR	4158	7/7	0.90	0.08	161,163,180,262	0
82	OHX	AR	4159	7/7	0.90	0.14	112,117,127,188	7
82	OHX	1	3563	7/7	0.90	0.10	153,157,176,251	0
83	MG	sR	2137	1/1	0.90	0.21	59,59,59,59	0
82	OHX	1	4135	7/7	0.90	0.09	153,162,174,273	0
83	MG	AR	3841	1/1	0.90	0.17	60,60,60,60	0
82	OHX	1	3541	7/7	0.90	0.14	143,151,156,250	0
83	MG	y	201	1/1	0.90	0.14	65,65,65,65	0
83	MG	1	3968	1/1	0.90	0.20	70,70,70,70	0
82	OHX	3	219	7/7	0.90	0.13	136,148,158,230	0
82	OHX	c5	201	7/7	0.90	0.09	182,189,197,257	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	4058	1/1	0.90	0.15	62,62,62,62	0
83	MG	A	2025	1/1	0.90	0.15	70,70,70,70	0
82	OHX	Q	201	7/7	0.90	0.09	201,205,215,281	0
83	MG	1	3833	1/1	0.90	0.14	62,62,62,62	0
82	OHX	U	201	7/7	0.90	0.10	228,241,243,327	0
82	OHX	d4	201	7/7	0.90	0.09	182,184,197,276	0
83	MG	1	3708	1/1	0.90	0.19	48,48,48,48	0
83	MG	AH	202	1/1	0.90	0.21	71,71,71,71	0
82	OHX	sR	1953	7/7	0.90	0.12	169,170,181,231	0
83	MG	1	3711	1/1	0.90	0.31	46,46,46,46	0
83	MG	AR	3673	1/1	0.90	0.07	53,53,53,53	0
83	MG	AR	3676	1/1	0.90	0.07	55,55,55,55	0
83	MG	1	3980	1/1	0.90	0.12	58,58,58,58	0
83	MG	sR	2164	1/1	0.90	0.14	76,76,76,76	0
83	MG	sR	2166	1/1	0.90	0.11	63,63,63,63	0
83	MG	A	2041	1/1	0.90	0.11	62,62,62,62	0
82	OHX	AT	201	7/7	0.90	0.10	129,138,156,253	0
83	MG	1	3844	1/1	0.90	0.20	53,53,53,53	0
83	MG	1	3845	1/1	0.90	0.11	68,68,68,68	0
83	MG	A	2046	1/1	0.90	0.12	74,74,74,74	0
83	MG	1	3716	1/1	0.90	0.22	50,50,50,50	0
82	OHX	1	4137	7/7	0.90	0.10	123,138,154,264	0
83	MG	1	3854	1/1	0.90	0.07	64,64,64,64	0
83	MG	c4	2201	1/1	0.90	0.10	75,75,75,75	0
83	MG	1	3991	1/1	0.90	0.16	61,61,61,61	0
83	MG	AR	4083	1/1	0.90	0.23	65,65,65,65	0
82	OHX	AT	216	7/7	0.90	0.10	156,166,190,294	0
83	MG	1	3994	1/1	0.90	0.08	69,69,69,69	0
83	MG	c9	202	1/1	0.90	0.16	99,99,99,99	0
83	MG	AR	3886	1/1	0.90	0.21	50,50,50,50	0
83	MG	A	2056	1/1	0.90	0.12	57,57,57,57	0
83	MG	AR	3695	1/1	0.90	0.23	69,69,69,69	0
83	MG	AR	3696	1/1	0.90	0.22	61,61,61,61	0
82	OHX	1	4138	7/7	0.90	0.10	123,132,150,223	0
83	MG	d6	203	1/1	0.90	0.19	68,68,68,68	0
82	OHX	1	3588	7/7	0.90	0.11	151,155,172,244	0
82	OHX	1	3606	1/7	0.90	0.14	221,221,221,221	0
82	OHX	AR	3596	7/7	0.90	0.11	167,171,173,271	0
83	MG	1	3869	1/1	0.90	0.26	62,62,62,62	0
82	OHX	1	4121	7/7	0.90	0.09	167,180,193,281	0
83	MG	AR	3898	1/1	0.90	0.18	46,46,46,46	0
83	MG	AR	4099	1/1	0.90	0.19	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3599	7/7	0.90	0.09	171,174,205,287	0
83	MG	AR	4047	1/1	0.91	0.16	52,52,52,52	0
82	OHX	sR	1987	7/7	0.91	0.09	147,157,161,256	0
82	OHX	1	3562	7/7	0.91	0.09	174,177,188,299	0
82	OHX	1	3517	7/7	0.91	0.10	158,167,193,252	0
83	MG	1	3909	1/1	0.91	0.10	62,62,62,62	0
83	MG	sR	2034	1/1	0.91	0.20	69,69,69,69	0
83	MG	AR	3897	1/1	0.91	0.24	68,68,68,68	0
82	OHX	AR	3594	7/7	0.91	0.10	120,133,139,225	0
83	MG	1	3733	1/1	0.91	0.20	46,46,46,46	0
83	MG	1	4005	1/1	0.91	0.21	69,69,69,69	0
83	MG	1	4006	1/1	0.91	0.23	60,60,60,60	0
83	MG	u	201	1/1	0.91	0.08	76,76,76,76	0
82	OHX	Rb	401	7/7	0.91	0.08	231,232,242,307	0
83	MG	A	1979	1/1	0.91	0.24	53,53,53,53	0
83	MG	1	3915	1/1	0.91	0.13	61,61,61,61	0
83	MG	AR	3908	1/1	0.91	0.09	62,62,62,62	0
83	MG	A	1983	1/1	0.91	0.11	70,70,70,70	0
83	MG	AR	3764	1/1	0.91	0.34	49,49,49,49	0
83	MG	w	201	1/1	0.91	0.11	57,57,57,57	0
83	MG	AR	3914	1/1	0.91	0.17	74,74,74,74	0
83	MG	sR	2054	1/1	0.91	0.14	64,64,64,64	0
83	MG	1	3820	1/1	0.91	0.10	46,46,46,46	0
83	MG	1	3821	1/1	0.91	0.12	66,66,66,66	0
83	MG	1	3735	1/1	0.91	0.23	49,49,49,49	0
82	OHX	AR	3561	7/7	0.91	0.14	104,114,136,217	0
83	MG	AR	4075	1/1	0.91	0.26	46,46,46,46	0
82	OHX	AR	3563	7/7	0.91	0.11	126,134,162,222	0
83	MG	A	1996	1/1	0.91	0.14	55,55,55,55	0
83	MG	1	4016	1/1	0.91	0.16	63,63,63,63	0
82	OHX	AG	202	7/7	0.91	0.10	136,148,161,253	0
82	OHX	1	3598	7/7	0.91	0.12	132,136,146,238	0
82	OHX	1	4128	7/7	0.91	0.09	133,138,159,244	0
83	MG	AR	3779	1/1	0.91	0.22	47,47,47,47	0
83	MG	sR	2072	1/1	0.91	0.21	63,63,63,63	0
82	OHX	AT	213	7/7	0.91	0.10	150,165,177,267	0
83	MG	1	3930	1/1	0.91	0.28	64,64,64,64	0
82	OHX	1	3480	7/7	0.91	0.12	116,132,139,198	0
83	MG	AR	3786	1/1	0.91	0.20	72,72,72,72	0
83	MG	AR	3933	1/1	0.91	0.10	72,72,72,72	0
82	OHX	AR	3571	7/7	0.91	0.11	132,138,148,237	0
83	MG	A	2009	1/1	0.91	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	3790	1/1	0.91	0.33	46,46,46,46	0
83	MG	1	3675	1/1	0.91	0.16	47,47,47,47	0
82	OHX	AR	3605	7/7	0.91	0.11	144,151,164,256	0
83	MG	AR	3794	1/1	0.91	0.18	46,46,46,46	0
83	MG	1	3747	1/1	0.91	0.19	57,57,57,57	0
83	MG	A	2016	1/1	0.91	0.15	95,95,95,95	0
83	MG	AP	503	1/1	0.91	0.16	77,77,77,77	0
82	OHX	AR	3641	7/7	0.91	0.09	134,140,171,244	0
83	MG	AR	4097	1/1	0.91	0.27	63,63,63,63	0
82	OHX	1	3560	7/7	0.91	0.10	132,139,157,248	0
83	MG	1	3838	1/1	0.91	0.08	75,75,75,75	0
83	MG	sR	2097	1/1	0.91	0.30	52,52,52,52	0
82	OHX	AR	3610	7/7	0.91	0.12	103,125,151,228	0
83	MG	AR	3680	1/1	0.91	0.17	53,53,53,53	0
83	MG	AR	3951	1/1	0.91	0.21	60,60,60,60	0
83	MG	AR	3952	1/1	0.91	0.13	64,64,64,64	0
83	MG	AR	4108	1/1	0.91	0.23	49,49,49,49	0
82	OHX	AR	3644	7/7	0.91	0.11	130,136,155,250	0
83	MG	AR	3955	1/1	0.91	0.15	63,63,63,63	0
82	OHX	1	3576	7/7	0.91	0.11	134,154,174,241	0
82	OHX	1	3511	7/7	0.91	0.10	138,140,157,233	0
83	MG	1	4042	1/1	0.91	0.10	48,48,48,48	0
83	MG	AR	4119	1/1	0.91	0.19	60,60,60,60	0
83	MG	1	3757	1/1	0.91	0.24	47,47,47,47	0
82	OHX	sR	2016	7/7	0.91	0.09	157,173,190,287	0
83	MG	AR	3962	1/1	0.91	0.11	61,61,61,61	0
83	MG	A	2040	1/1	0.91	0.13	73,73,73,73	0
82	OHX	CS	201	7/7	0.91	0.10	117,122,125,220	0
83	MG	AR	3813	1/1	0.91	0.17	71,71,71,71	0
83	MG	1	3853	1/1	0.91	0.28	67,67,67,67	0
82	OHX	A	1936	7/7	0.91	0.08	186,190,197,263	0
83	MG	AR	4131	1/1	0.91	0.13	67,67,67,67	0
83	MG	1	3687	1/1	0.91	0.16	60,60,60,60	0
83	MG	1	3688	1/1	0.91	0.34	66,66,66,66	0
83	MG	AR	4135	1/1	0.91	0.12	77,77,77,77	0
83	MG	AR	3697	1/1	0.91	0.28	60,60,60,60	0
83	MG	1	3689	1/1	0.91	0.18	57,57,57,57	0
83	MG	1	3858	1/1	0.91	0.06	46,46,46,46	0
83	MG	AR	3978	1/1	0.91	0.09	76,76,76,76	0
83	MG	1	3860	1/1	0.91	0.26	70,70,70,70	0
83	MG	sR	2129	1/1	0.91	0.12	91,91,91,91	0
83	MG	AR	3827	1/1	0.91	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	sR	2131	1/1	0.91	0.27	65,65,65,65	0
83	MG	1	4065	1/1	0.91	0.21	56,56,56,56	0
82	OHX	A	1938	7/7	0.91	0.09	195,201,219,265	0
83	MG	AR	3986	1/1	0.91	0.17	73,73,73,73	0
82	OHX	sR	2020	7/7	0.91	0.12	184,200,228,322	0
83	MG	1	3772	1/1	0.91	0.16	53,53,53,53	0
83	MG	1	3628	1/1	0.91	0.28	63,63,63,63	0
82	OHX	AR	3648	7/7	0.91	0.10	152,158,170,255	0
83	MG	AR	3840	1/1	0.91	0.33	58,58,58,58	0
83	MG	1	3695	1/1	0.91	0.17	54,54,54,54	0
82	OHX	A	1941	7/7	0.91	0.10	142,143,159,240	0
82	OHX	AR	3581	7/7	0.91	0.09	142,147,167,247	0
82	OHX	AR	3651	7/7	0.91	0.08	192,197,208,295	0
82	OHX	AR	3617	7/7	0.91	0.09	151,157,172,249	0
82	OHX	A	1954	6/7	0.91	0.09	221,229,232,268	0
83	MG	AS	221	1/1	0.91	0.22	84,84,84,84	0
83	MG	3	209	1/1	0.91	0.26	56,56,56,56	0
82	OHX	AR	3529	7/7	0.91	0.14	75,97,108,191	0
83	MG	sR	2152	1/1	0.91	0.21	64,64,64,64	0
82	OHX	A	1956	7/7	0.91	0.11	148,158,171,218	0
83	MG	AS	226	1/1	0.91	0.35	56,56,56,56	0
83	MG	sR	2155	1/1	0.91	0.21	52,52,52,52	0
83	MG	1	3640	1/1	0.91	0.20	57,57,57,57	0
82	OHX	AR	3654	6/7	0.91	0.10	192,208,228,313	0
83	MG	A	2079	1/1	0.91	0.16	65,65,65,65	0
82	OHX	AR	3620	7/7	0.91	0.10	139,152,171,242	0
83	MG	AR	3724	1/1	0.91	0.12	63,63,63,63	0
83	MG	4	217	1/1	0.91	0.28	50,50,50,50	0
82	OHX	AR	3621	7/7	0.91	0.08	167,179,196,260	0
83	MG	1	3647	1/1	0.91	0.08	91,91,91,91	0
83	MG	AT	223	1/1	0.91	0.22	77,77,77,77	0
82	OHX	AR	3622	7/7	0.91	0.09	184,195,202,271	0
83	MG	AR	3865	1/1	0.91	0.10	64,64,64,64	0
83	MG	AR	3729	1/1	0.91	0.15	75,75,75,75	0
83	MG	AR	3869	1/1	0.91	0.07	47,47,47,47	0
83	MG	s6	301	1/1	0.91	0.09	115,115,115,115	0
83	MG	1	3984	1/1	0.91	0.10	81,81,81,81	0
83	MG	AT	231	1/1	0.91	0.10	45,45,45,45	0
83	MG	1	3801	1/1	0.91	0.10	63,63,63,63	0
83	MG	A	2095	1/1	0.91	0.20	71,71,71,71	0
83	MG	AR	3874	1/1	0.91	0.28	65,65,65,65	0
82	OHX	1	3569	7/7	0.91	0.08	202,203,219,273	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	4	224	1/1	0.91	0.07	57,57,57,57	0
82	OHX	1	3571	7/7	0.91	0.09	150,172,185,253	0
83	MG	1	3718	1/1	0.91	0.24	46,46,46,46	0
83	MG	d3	201	1/1	0.91	0.17	69,69,69,69	0
83	MG	A	2153	1/1	0.91	0.08	134,134,134,134	0
83	MG	d3	203	1/1	0.91	0.22	58,58,58,58	0
83	MG	AR	4027	1/1	0.91	0.07	55,55,55,55	0
83	MG	AR	3738	1/1	0.91	0.21	62,62,62,62	0
83	MG	1	3902	1/1	0.91	0.11	51,51,51,51	0
83	MG	j	302	1/1	0.91	0.16	71,71,71,71	0
83	MG	AR	3887	1/1	0.91	0.25	54,54,54,54	0
83	MG	1	3722	1/1	0.91	0.40	46,46,46,46	0
83	MG	P	201	1/1	0.91	0.07	72,72,72,72	0
83	MG	X	201	1/1	0.91	0.10	54,54,54,54	0
84	K	AR	4167	1/1	0.91	0.13	139,139,139,139	0
83	MG	l	401	1/1	0.91	0.34	45,45,45,45	0
82	OHX	A	1969	7/7	0.91	0.09	219,231,237,294	0
83	MG	CP	304	1/1	0.91	0.11	73,73,73,73	0
83	MG	1	3809	1/1	0.91	0.32	48,48,48,48	0
83	MG	AR	4045	1/1	0.91	0.10	63,63,63,63	0
83	MG	1	4177	1/1	0.92	0.09	82,82,82,82	0
83	MG	1	3875	1/1	0.92	0.22	68,68,68,68	0
82	OHX	1	4110	7/7	0.92	0.08	212,217,233,310	0
82	OHX	AR	3604	7/7	0.92	0.11	125,143,155,248	0
83	MG	AR	3831	1/1	0.92	0.28	50,50,50,50	0
83	MG	AR	4100	1/1	0.92	0.21	66,66,66,66	0
83	MG	1	3627	1/1	0.92	0.14	60,60,60,60	0
82	OHX	1	3570	7/7	0.92	0.09	134,146,179,262	0
83	MG	AR	3834	1/1	0.92	0.29	44,44,44,44	0
82	OHX	A	2133	7/7	0.92	0.10	169,172,175,253	0
83	MG	AR	3968	1/1	0.92	0.14	53,53,53,53	0
83	MG	A	2008	1/1	0.92	0.30	53,53,53,53	0
83	MG	AR	4107	1/1	0.92	0.09	54,54,54,54	0
83	MG	AR	3969	1/1	0.92	0.15	59,59,59,59	0
83	MG	AR	3838	1/1	0.92	0.23	48,48,48,48	0
83	MG	sR	2069	1/1	0.92	0.23	54,54,54,54	0
83	MG	3	213	1/1	0.92	0.07	49,49,49,49	0
82	OHX	k	403	7/7	0.92	0.11	119,122,130,204	0
83	MG	AR	4112	1/1	0.92	0.14	50,50,50,50	0
83	MG	1	3790	1/1	0.92	0.26	58,58,58,58	0
82	OHX	AR	3609	7/7	0.92	0.12	121,125,139,250	0
83	MG	1	3632	1/1	0.92	0.06	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	1	3547	7/7	0.92	0.09	130,145,163,238	0
83	MG	AR	4123	1/1	0.92	0.13	70,70,70,70	0
82	OHX	A	1928	7/7	0.92	0.10	178,187,198,257	0
83	MG	1	3706	1/1	0.92	0.16	48,48,48,48	0
82	OHX	1	3528	7/7	0.92	0.10	158,166,172,253	0
82	OHX	AR	3613	7/7	0.92	0.10	135,148,154,248	0
82	OHX	1	3587	7/7	0.92	0.09	152,156,172,256	0
83	MG	A	2027	1/1	0.92	0.19	69,69,69,69	0
83	MG	1	3897	1/1	0.92	0.11	61,61,61,61	0
83	MG	AR	3730	1/1	0.92	0.25	48,48,48,48	0
82	OHX	1	3530	7/7	0.92	0.08	136,141,157,234	0
82	OHX	1	3531	7/7	0.92	0.09	127,134,136,225	0
83	MG	1	3900	1/1	0.92	0.09	53,53,53,53	0
83	MG	AR	3994	1/1	0.92	0.14	62,62,62,62	0
83	MG	sR	2093	1/1	0.92	0.18	65,65,65,65	0
83	MG	sR	2094	1/1	0.92	0.18	56,56,56,56	0
82	OHX	A	1945	7/7	0.92	0.09	177,187,204,276	0
82	OHX	1	4051	7/7	0.92	0.09	121,128,139,236	0
82	OHX	1	3537	7/7	0.92	0.12	104,107,122,211	0
83	MG	1	3810	1/1	0.92	0.13	66,66,66,66	0
82	OHX	A	1953	7/7	0.92	0.10	156,161,174,235	0
83	MG	AR	3868	1/1	0.92	0.16	54,54,54,54	0
82	OHX	AR	3579	7/7	0.92	0.10	115,125,136,208	0
82	OHX	1	3506	7/7	0.92	0.10	97,110,124,198	0
83	MG	AR	3871	1/1	0.92	0.08	64,64,64,64	0
83	MG	1	4002	1/1	0.92	0.09	52,52,52,52	0
83	MG	AR	3873	1/1	0.92	0.13	49,49,49,49	0
83	MG	A	2048	1/1	0.92	0.10	76,76,76,76	0
82	OHX	AR	3584	7/7	0.92	0.10	115,125,150,223	0
83	MG	1	4004	1/1	0.92	0.17	62,62,62,62	0
83	MG	AR	3749	1/1	0.92	0.17	46,46,46,46	0
82	OHX	AR	3626	7/7	0.92	0.09	121,129,138,226	0
82	OHX	3	204	7/7	0.92	0.09	150,156,162,243	0
82	OHX	sR	1967	7/7	0.92	0.11	152,152,164,224	0
83	MG	AS	216	1/1	0.92	0.14	57,57,57,57	0
82	OHX	1	4103	7/7	0.92	0.10	105,125,142,219	0
83	MG	AR	4016	1/1	0.92	0.27	66,66,66,66	0
82	OHX	1	3546	7/7	0.92	0.08	209,216,228,290	0
83	MG	AR	4018	1/1	0.92	0.18	65,65,65,65	0
83	MG	v	302	1/1	0.92	0.10	56,56,56,56	0
82	OHX	A	1964	7/7	0.92	0.08	163,174,182,244	0
83	MG	AS	225	1/1	0.92	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3532	7/7	0.92	0.10	122,123,146,221	0
82	OHX	AR	3533	7/7	0.92	0.14	143,147,156,250	0
83	MG	1	3664	1/1	0.92	0.19	46,46,46,46	0
83	MG	1	3665	1/1	0.92	0.18	46,46,46,46	0
82	OHX	A	1968	7/7	0.92	0.09	160,178,181,256	0
83	MG	1	3924	1/1	0.92	0.10	68,68,68,68	0
83	MG	AR	4028	1/1	0.92	0.14	47,47,47,47	0
83	MG	1	4019	1/1	0.92	0.23	49,49,49,49	0
83	MG	x	207	1/1	0.92	0.21	49,49,49,49	0
83	MG	AT	224	1/1	0.92	0.08	71,71,71,71	0
82	OHX	1	3580	7/7	0.92	0.07	209,216,225,297	0
83	MG	1	3668	1/1	0.92	0.19	68,68,68,68	0
83	MG	AR	4035	1/1	0.92	0.07	57,57,57,57	0
82	OHX	AR	3537	7/7	0.92	0.12	125,140,155,208	0
83	MG	sR	2140	1/1	0.92	0.09	67,67,67,67	0
82	OHX	sR	1988	7/7	0.92	0.08	157,172,192,271	0
82	OHX	sR	1989	7/7	0.92	0.09	157,167,188,264	0
83	MG	9	201	1/1	0.92	0.09	45,45,45,45	0
82	OHX	A	1972	7/7	0.92	0.08	176,188,203,268	0
83	MG	A	2082	1/1	0.92	0.28	52,52,52,52	0
83	MG	1	4027	1/1	0.92	0.20	73,73,73,73	0
83	MG	AB	204	1/1	0.92	0.10	55,55,55,55	0
82	OHX	AT	211	7/7	0.92	0.09	132,150,164,255	0
83	MG	AR	4050	1/1	0.92	0.14	52,52,52,52	0
83	MG	AR	3913	1/1	0.92	0.20	50,50,50,50	0
83	MG	1	3753	1/1	0.92	0.25	47,47,47,47	0
83	MG	AR	3785	1/1	0.92	0.31	46,46,46,46	0
82	OHX	A	1975	7/7	0.92	0.07	238,244,257,327	0
83	MG	CL	301	1/1	0.92	0.11	51,51,51,51	0
83	MG	1	4032	1/1	0.92	0.25	57,57,57,57	0
83	MG	AR	3789	1/1	0.92	0.19	52,52,52,52	0
82	OHX	1	3581	7/7	0.92	0.08	171,189,205,286	0
83	MG	1	3607	1/1	0.92	0.28	56,56,56,56	0
82	OHX	AT	215	7/7	0.92	0.08	172,178,199,270	0
82	OHX	A	2113	7/7	0.92	0.11	115,120,129,203	0
83	MG	A	2100	1/1	0.92	0.09	79,79,79,79	0
83	MG	CQ	202	1/1	0.92	0.35	97,97,97,97	0
83	MG	CQ	203	1/1	0.92	0.10	50,50,50,50	0
83	MG	sR	2184	1/1	0.92	0.07	95,95,95,95	0
83	MG	1	3611	1/1	0.92	0.15	55,55,55,55	0
83	MG	CR	202	1/1	0.92	0.20	48,48,48,48	0
83	MG	s1	302	1/1	0.92	0.11	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3548	7/7	0.92	0.09	112,120,142,205	0
83	MG	1	4041	1/1	0.92	0.11	58,58,58,58	0
83	MG	1	3944	1/1	0.92	0.13	59,59,59,59	0
82	OHX	A	2122	7/7	0.92	0.10	138,149,160,233	0
83	MG	CU	201	1/1	0.92	0.25	74,74,74,74	0
83	MG	CX	202	1/1	0.92	0.22	47,47,47,47	0
83	MG	1	3763	1/1	0.92	0.32	49,49,49,49	0
83	MG	1	3617	1/1	0.92	0.19	50,50,50,50	0
82	OHX	sR	2003	7/7	0.92	0.09	156,160,171,255	0
83	MG	AR	4074	1/1	0.92	0.07	66,66,66,66	0
82	OHX	1	3557	7/7	0.92	0.10	127,131,162,213	0
83	MG	AR	3805	1/1	0.92	0.24	53,53,53,53	0
83	MG	1	3952	1/1	0.92	0.10	77,77,77,77	0
82	OHX	A	2126[A]	7/7	0.92	0.14	114,116,119,153	7
83	MG	1	3690	1/1	0.92	0.22	51,51,51,51	0
83	MG	1	3861	1/1	0.92	0.33	70,70,70,70	0
83	MG	1	3864	1/1	0.92	0.09	50,50,50,50	0
83	MG	AR	4082	1/1	0.92	0.19	50,50,50,50	0
83	MG	1	3865	1/1	0.92	0.11	75,75,75,75	0
83	MG	AR	3947	1/1	0.92	0.16	66,66,66,66	0
82	OHX	A	2126[B]	7/7	0.92	0.14	116,116,121,149	7
83	MG	sR	2038	1/1	0.92	0.34	61,61,61,61	0
83	MG	1	3774	1/1	0.92	0.30	51,51,51,51	0
83	MG	AR	3819	1/1	0.92	0.21	46,46,46,46	0
83	MG	1	3868	1/1	0.92	0.15	72,72,72,72	0
82	OHX	1	3558	7/7	0.92	0.09	147,154,173,249	0
82	OHX	AR	3554	7/7	0.92	0.11	138,145,160,238	0
87	ZN	c	101	1/1	0.92	0.06	226,226,226,226	0
83	MG	1	3872	1/1	0.92	0.09	47,47,47,47	0
82	OHX	sR	2010	7/7	0.92	0.08	169,173,184,257	0
83	MG	1	3911	1/1	0.93	0.11	68,68,68,68	0
83	MG	AR	3854	1/1	0.93	0.14	59,59,59,59	0
82	OHX	A	1943	7/7	0.93	0.10	161,163,179,243	0
82	OHX	AR	4144	7/7	0.93	0.08	148,152,173,255	0
83	MG	1	3794	1/1	0.93	0.10	50,50,50,50	0
82	OHX	sR	1916[A]	7/7	0.93	0.20	94,95,100,109	7
83	MG	CF	405	1/1	0.93	0.18	67,67,67,67	0
82	OHX	sR	1916[B]	7/7	0.93	0.20	86,90,100,103	7
82	OHX	sR	1927	7/7	0.93	0.13	113,116,131,164	0
83	MG	AR	3710	1/1	0.93	0.12	54,54,54,54	0
83	MG	AR	3864	1/1	0.93	0.19	63,63,63,63	0
82	OHX	sR	1941	7/7	0.93	0.09	169,171,183,227	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	4029	1/1	0.93	0.06	68,68,68,68	0
83	MG	AR	4030	1/1	0.93	0.18	84,84,84,84	0
83	MG	1	3803	1/1	0.93	0.11	50,50,50,50	0
83	MG	AR	3715	1/1	0.93	0.34	61,61,61,61	0
82	OHX	sR	1944	7/7	0.93	0.13	110,121,140,175	0
83	MG	CQ	201	1/1	0.93	0.14	59,59,59,59	0
82	OHX	sR	1951	7/7	0.93	0.11	130,139,147,194	0
82	OHX	1	4062	7/7	0.93	0.09	121,128,149,221	0
82	OHX	sR	1961	7/7	0.93	0.11	117,125,143,215	0
83	MG	AR	4039	1/1	0.93	0.12	60,60,60,60	0
82	OHX	sR	1962	7/7	0.93	0.12	120,125,145,220	0
83	MG	AR	4041	1/1	0.93	0.15	60,60,60,60	0
83	MG	1	4059	1/1	0.93	0.20	51,51,51,51	0
83	MG	CR	206	1/1	0.93	0.12	51,51,51,51	0
83	MG	CR	207	1/1	0.93	0.18	49,49,49,49	0
83	MG	AR	4043	1/1	0.93	0.16	57,57,57,57	0
82	OHX	A	1949	7/7	0.93	0.09	164,170,174,229	0
82	OHX	AR	3557	7/7	0.93	0.09	137,146,156,225	0
83	MG	1	3700	1/1	0.93	0.17	58,58,58,58	0
82	OHX	sR	1970	7/7	0.93	0.11	122,136,153,218	0
83	MG	sR	2055	1/1	0.93	0.23	62,62,62,62	0
83	MG	1	3934	1/1	0.93	0.10	64,64,64,64	0
83	MG	DH	201	1/1	0.93	0.17	54,54,54,54	0
83	MG	DI	203	1/1	0.93	0.13	73,73,73,73	0
83	MG	1	3814	1/1	0.93	0.25	75,75,75,75	0
82	OHX	A	1952	7/7	0.93	0.08	165,171,181,249	0
82	OHX	AR	3558	7/7	0.93	0.08	140,144,157,224	0
83	MG	1	3614	1/1	0.93	0.14	48,48,48,48	0
83	MG	DQ	503	1/1	0.93	0.06	69,69,69,69	0
83	MG	sM	301	1/1	0.93	0.07	53,53,53,53	0
83	MG	AR	4054	1/1	0.93	0.18	101,101,101,101	0
83	MG	AR	4055	1/1	0.93	0.17	89,89,89,89	0
82	OHX	sR	1974	7/7	0.93	0.09	135,136,145,210	0
83	MG	1	4163	1/1	0.93	0.08	63,63,63,63	0
82	OHX	1	4087	7/7	0.93	0.11	113,128,135,188	0
83	MG	1	4176	1/1	0.93	0.10	106,106,106,106	0
82	OHX	AR	3562	7/7	0.93	0.10	124,136,153,225	0
83	MG	sR	2075	1/1	0.93	0.14	68,68,68,68	0
82	OHX	sR	1978	7/7	0.93	0.10	151,158,174,234	0
82	OHX	1	4091	7/7	0.93	0.10	109,111,119,208	0
83	MG	AR	3896	1/1	0.93	0.17	61,61,61,61	0
83	MG	AR	4064	1/1	0.93	0.13	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	3739	1/1	0.93	0.18	66,66,66,66	0
82	OHX	A	1957	7/7	0.93	0.08	176,185,198,257	0
82	OHX	sR	1982	7/7	0.93	0.10	150,156,161,226	0
82	OHX	AR	3647	7/7	0.93	0.12	119,130,141,232	0
83	MG	1	3717	1/1	0.93	0.28	47,47,47,47	0
82	OHX	AR	4152	7/7	0.93	0.08	197,209,222,285	0
83	MG	1	3720	1/1	0.93	0.12	49,49,49,49	0
83	MG	1	3721	1/1	0.93	0.06	48,48,48,48	0
82	OHX	A	1961	7/7	0.93	0.07	195,201,211,281	0
83	MG	sR	2090	1/1	0.93	0.31	61,61,61,61	0
83	MG	AR	3909	1/1	0.93	0.38	72,72,72,72	0
83	MG	3	218	1/1	0.93	0.18	61,61,61,61	0
82	OHX	1	4092	7/7	0.93	0.09	118,130,155,215	0
83	MG	AR	3754	1/1	0.93	0.05	48,48,48,48	0
83	MG	1	3957	1/1	0.93	0.17	55,55,55,55	0
82	OHX	sR	1990	7/7	0.93	0.09	161,169,182,257	0
83	MG	1	3959	1/1	0.93	0.13	75,75,75,75	0
82	OHX	sR	1991	7/7	0.93	0.09	143,153,162,230	0
83	MG	AR	3759	1/1	0.93	0.19	54,54,54,54	0
83	MG	1	3726	1/1	0.93	0.23	49,49,49,49	0
82	OHX	1	3552	7/7	0.93	0.08	169,176,185,249	0
83	MG	1	3728	1/1	0.93	0.28	48,48,48,48	0
83	MG	1	3730	1/1	0.93	0.19	45,45,45,45	0
82	OHX	AR	3650	7/7	0.93	0.08	193,197,207,263	0
82	OHX	AR	3567	7/7	0.93	0.09	134,145,161,234	0
83	MG	AR	3767	1/1	0.93	0.31	48,48,48,48	0
82	OHX	AR	3612	7/7	0.93	0.11	122,137,152,239	0
82	OHX	sR	1998	7/7	0.93	0.08	141,142,147,236	0
83	MG	AR	3929	1/1	0.93	0.08	63,63,63,63	0
82	OHX	AR	3568	7/7	0.93	0.09	108,118,141,214	0
83	MG	k	402	1/1	0.93	0.20	48,48,48,48	0
83	MG	A	2024	1/1	0.93	0.14	64,64,64,64	0
83	MG	1	3851	1/1	0.93	0.23	78,78,78,78	0
83	MG	sR	2115	1/1	0.93	0.17	73,73,73,73	0
82	OHX	AR	4160	7/7	0.93	0.18	88,90,98,118	7
83	MG	AR	3939	1/1	0.93	0.23	50,50,50,50	0
83	MG	1	3972	1/1	0.93	0.21	47,47,47,47	0
83	MG	l	404	1/1	0.93	0.36	49,49,49,49	0
82	OHX	AR	3614	7/7	0.93	0.08	152,164,172,251	0
83	MG	sR	2121	1/1	0.93	0.19	70,70,70,70	0
83	MG	A	2031	1/1	0.93	0.17	53,53,53,53	0
82	OHX	AR	3655	7/7	0.93	0.09	173,177,184,268	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AS	204	7/7	0.93	0.12	109,116,130,204	0
83	MG	1	3642	1/1	0.93	0.20	46,46,46,46	0
82	OHX	A	1974	7/7	0.93	0.09	134,142,163,220	0
83	MG	A	2036	1/1	0.93	0.19	70,70,70,70	0
83	MG	1	3859	1/1	0.93	0.09	73,73,73,73	0
83	MG	1	3645	1/1	0.93	0.15	72,72,72,72	0
83	MG	AR	3787	1/1	0.93	0.23	45,45,45,45	0
82	OHX	sR	2005	7/7	0.93	0.09	166,170,183,261	0
83	MG	1	3863	1/1	0.93	0.13	57,57,57,57	0
82	OHX	1	3543	7/7	0.93	0.07	141,154,166,228	0
82	OHX	AR	3492	7/7	0.93	0.12	106,115,126,206	0
83	MG	1	3987	1/1	0.93	0.20	77,77,77,77	0
83	MG	AR	3956	1/1	0.93	0.13	56,56,56,56	0
83	MG	AR	3793	1/1	0.93	0.14	58,58,58,58	0
83	MG	1	3748	1/1	0.93	0.14	54,54,54,54	0
82	OHX	1	4101	7/7	0.93	0.10	143,147,156,219	0
82	OHX	3	203	7/7	0.93	0.09	131,142,163,218	0
82	OHX	1	3544	7/7	0.93	0.10	127,143,156,226	0
82	OHX	AR	3513	7/7	0.93	0.14	103,107,118,188	0
82	OHX	A	2123	7/7	0.93	0.11	128,131,137,198	0
82	OHX	AR	3514	7/7	0.93	0.10	121,136,142,208	0
83	MG	1	3874	1/1	0.93	0.09	63,63,63,63	0
83	MG	sR	2148	1/1	0.93	0.21	52,52,52,52	0
82	OHX	3	205	7/7	0.93	0.10	157,160,166,226	0
83	MG	AR	4172	1/1	0.93	0.06	97,97,97,97	0
82	OHX	AR	3625	7/7	0.93	0.08	142,155,162,242	0
82	OHX	1	3516	7/7	0.93	0.09	126,138,162,233	0
83	MG	1	3878	1/1	0.93	0.11	59,59,59,59	0
83	MG	AR	4183	1/1	0.93	0.07	101,101,101,101	0
82	OHX	1	3491	7/7	0.93	0.11	93,114,116,205	0
82	OHX	3	220	7/7	0.93	0.08	171,177,179,289	0
82	OHX	1	3548	7/7	0.93	0.08	155,160,173,237	0
83	MG	sR	2159	1/1	0.93	0.21	72,72,72,72	0
82	OHX	A	2131	7/7	0.93	0.08	221,221,229,323	0
83	MG	1	3764	1/1	0.93	0.15	49,49,49,49	0
83	MG	1	4008	1/1	0.93	0.10	93,93,93,93	0
83	MG	AR	3815	1/1	0.93	0.25	50,50,50,50	0
83	MG	AR	4203	1/1	0.93	0.12	123,123,123,123	0
83	MG	AR	3981	1/1	0.93	0.27	69,69,69,69	0
82	OHX	4	201	7/7	0.93	0.12	102,105,121,182	0
82	OHX	AR	3590	7/7	0.93	0.12	137,141,145,228	0
83	MG	AR	3985	1/1	0.93	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3591	7/7	0.93	0.08	166,175,187,285	0
83	MG	1	3669	1/1	0.93	0.15	54,54,54,54	0
83	MG	1	3889	1/1	0.93	0.16	97,97,97,97	0
83	MG	A	2077	1/1	0.93	0.16	70,70,70,70	0
83	MG	AR	3675	1/1	0.93	0.14	55,55,55,55	0
83	MG	AS	217	1/1	0.93	0.07	68,68,68,68	0
82	OHX	1	3492	7/7	0.93	0.10	117,130,140,216	0
83	MG	c1	201	1/1	0.93	0.20	75,75,75,75	0
82	OHX	A	1915	7/7	0.93	0.11	103,119,132,183	0
83	MG	AS	220	1/1	0.93	0.29	54,54,54,54	0
83	MG	AR	3678	1/1	0.93	0.18	48,48,48,48	0
82	OHX	A	1918	7/7	0.93	0.12	114,128,138,194	0
82	OHX	A	1920	7/7	0.93	0.10	144,154,164,220	0
82	OHX	AR	4138	7/7	0.93	0.12	131,134,143,233	0
83	MG	1	3777	1/1	0.93	0.17	46,46,46,46	0
83	MG	1	3778	1/1	0.93	0.16	45,45,45,45	0
82	OHX	A	1934	7/7	0.93	0.10	137,145,157,212	0
82	OHX	A	1935	7/7	0.93	0.11	140,151,157,236	0
83	MG	AR	3688	1/1	0.93	0.08	54,54,54,54	0
83	MG	AR	4003	1/1	0.93	0.22	46,46,46,46	0
82	OHX	A	2142	7/7	0.93	0.23	100,102,110,115	7
83	MG	1	3782	1/1	0.93	0.31	46,46,46,46	0
82	OHX	1	3592	7/7	0.93	0.09	133,147,157,255	0
83	MG	AR	3694	1/1	0.93	0.07	48,48,48,48	0
82	OHX	A	1937	7/7	0.93	0.08	146,153,171,241	0
82	OHX	AR	3546	7/7	0.93	0.09	109,120,131,224	0
84	K	AR	4166	1/1	0.93	0.08	94,94,94,94	0
83	MG	1	3788	1/1	0.93	0.30	46,46,46,46	0
83	MG	AR	3847	1/1	0.93	0.15	59,59,59,59	0
83	MG	1	4030	1/1	0.93	0.19	60,60,60,60	0
82	OHX	1	3539	7/7	0.93	0.08	135,142,153,228	0
82	OHX	1	3512	7/7	0.93	0.10	153,155,177,251	0
83	MG	A	2156	1/1	0.93	0.06	91,91,91,91	0
82	OHX	1	3595	7/7	0.93	0.12	125,127,146,225	0
83	MG	DL	102	1/1	0.94	0.12	46,46,46,46	0
83	MG	AR	3932	1/1	0.94	0.18	64,64,64,64	0
83	MG	AF	202	1/1	0.94	0.07	62,62,62,62	0
82	OHX	A	1924	7/7	0.94	0.09	143,144,150,216	0
82	OHX	A	1926	7/7	0.94	0.10	128,137,150,196	0
83	MG	1	3923	1/1	0.94	0.12	56,56,56,56	0
82	OHX	A	1927	7/7	0.94	0.09	152,157,166,214	0
83	MG	sR	2047	1/1	0.94	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	A	1978	1/1	0.94	0.15	64,64,64,64	0
82	OHX	1	3578	7/7	0.94	0.07	157,160,167,220	0
82	OHX	A	1929	7/7	0.94	0.11	116,118,135,205	0
83	MG	sR	2052	1/1	0.94	0.10	53,53,53,53	0
83	MG	AR	3674	1/1	0.94	0.07	56,56,56,56	0
83	MG	1	3829	1/1	0.94	0.14	61,61,61,61	0
82	OHX	A	1932	7/7	0.94	0.10	132,142,150,233	0
82	OHX	AR	4137	7/7	0.94	0.10	156,165,180,275	0
82	OHX	AR	3505	7/7	0.94	0.10	95,111,129,188	0
83	MG	AR	3679	1/1	0.94	0.22	49,49,49,49	0
82	OHX	1	3534	7/7	0.94	0.09	133,145,147,222	0
83	MG	1	3834	1/1	0.94	0.29	56,56,56,56	0
82	OHX	AR	3512	7/7	0.94	0.09	164,168,179,219	0
83	MG	A	1993	1/1	0.94	0.15	54,54,54,54	0
83	MG	1	4040	1/1	0.94	0.13	48,48,48,48	0
83	MG	sR	2066	1/1	0.94	0.18	49,49,49,49	0
82	OHX	AR	3576	7/7	0.94	0.10	145,151,156,203	0
83	MG	1	3937	1/1	0.94	0.13	57,57,57,57	0
82	OHX	1	3536	7/7	0.94	0.07	124,137,157,232	0
82	OHX	1	3500	7/7	0.94	0.09	148,162,166,209	0
83	MG	1	3661	1/1	0.94	0.23	70,70,70,70	0
83	MG	AR	3818	1/1	0.94	0.24	46,46,46,46	0
82	OHX	AR	3633	7/7	0.94	0.07	137,148,160,231	0
83	MG	1	3841	1/1	0.94	0.09	47,47,47,47	0
83	MG	AR	3821	1/1	0.94	0.18	46,46,46,46	0
83	MG	AR	4104	1/1	0.94	0.08	49,49,49,49	0
83	MG	1	3663	1/1	0.94	0.29	47,47,47,47	0
82	OHX	AR	3580	7/7	0.94	0.14	121,128,141,210	0
83	MG	1	4057	1/1	0.94	0.06	49,49,49,49	0
82	OHX	h	401	7/7	0.94	0.07	205,207,214,275	0
83	MG	AR	3967	1/1	0.94	0.25	65,65,65,65	0
82	OHX	sR	1901	7/7	0.94	0.08	142,143,147,241	0
82	OHX	AR	3517	7/7	0.94	0.10	122,132,137,196	0
83	MG	AR	3970	1/1	0.94	0.12	46,46,46,46	0
83	MG	sR	2085	1/1	0.94	0.13	75,75,75,75	0
82	OHX	AR	3518	7/7	0.94	0.10	92,107,112,177	0
83	MG	1	3852	1/1	0.94	0.20	66,66,66,66	0
83	MG	AR	3973	1/1	0.94	0.11	56,56,56,56	0
83	MG	1	4066	1/1	0.94	0.23	63,63,63,63	0
83	MG	AR	3703	1/1	0.94	0.32	49,49,49,49	0
82	OHX	sR	1920	7/7	0.94	0.12	90,109,123,159	0
82	OHX	sR	2171	7/7	0.94	0.10	99,114,123,207	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3519	7/7	0.94	0.10	118,136,146,215	0
83	MG	1	3955	1/1	0.94	0.16	69,69,69,69	0
83	MG	sR	2095	1/1	0.94	0.18	63,63,63,63	0
83	MG	1	4158	1/1	0.94	0.09	97,97,97,97	0
82	OHX	AR	3520	7/7	0.94	0.09	89,105,145,192	0
83	MG	AR	3983	1/1	0.94	0.09	73,73,73,73	0
82	OHX	AR	3523	7/7	0.94	0.09	131,137,161,231	0
82	OHX	sR	1945	7/7	0.94	0.09	144,154,158,200	0
83	MG	1	4167	1/1	0.94	0.08	98,98,98,98	0
82	OHX	1	3469	7/7	0.94	0.11	103,109,124,167	0
82	OHX	1	3540	7/7	0.94	0.07	150,152,174,244	0
83	MG	AR	3846	1/1	0.94	0.21	61,61,61,61	0
82	OHX	sR	1955	7/7	0.94	0.09	184,185,189,237	0
83	MG	AR	3991	1/1	0.94	0.04	73,73,73,73	0
83	MG	1	4178	1/1	0.94	0.07	120,120,120,120	0
83	MG	AR	4184	1/1	0.94	0.07	111,111,111,111	0
83	MG	1	4179	1/1	0.94	0.08	78,78,78,78	0
83	MG	AR	4186	1/1	0.94	0.09	69,69,69,69	0
82	OHX	sR	1956	7/7	0.94	0.09	165,169,177,208	0
83	MG	1	3768	1/1	0.94	0.25	50,50,50,50	0
83	MG	AR	3852	1/1	0.94	0.13	46,46,46,46	0
83	MG	AR	4192	1/1	0.94	0.12	53,53,53,53	0
82	OHX	sR	1960	7/7	0.94	0.09	133,138,152,205	0
82	OHX	1	3474	7/7	0.94	0.10	104,110,130,180	0
83	MG	AR	4201	1/1	0.94	0.12	97,97,97,97	0
82	OHX	AR	3530	7/7	0.94	0.10	123,129,140,206	0
83	MG	3	211	1/1	0.94	0.23	49,49,49,49	0
82	OHX	AR	3593	7/7	0.94	0.08	119,130,158,213	0
82	OHX	1	3525	7/7	0.94	0.07	137,145,163,218	0
83	MG	1	3870	1/1	0.94	0.08	62,62,62,62	0
82	OHX	sR	1968	7/7	0.94	0.11	130,134,150,205	0
82	OHX	sR	1969	7/7	0.94	0.10	127,136,147,225	0
82	OHX	4	208	7/7	0.94	0.07	117,134,149,251	0
83	MG	4	214	1/1	0.94	0.16	45,45,45,45	0
82	OHX	sR	1971	7/7	0.94	0.08	139,150,161,235	0
82	OHX	1	3514	7/7	0.94	0.09	143,149,162,227	0
82	OHX	AR	3536	7/7	0.94	0.10	119,126,150,200	0
82	OHX	1	3505	7/7	0.94	0.08	135,137,154,226	0
82	OHX	1	4107	7/7	0.94	0.07	174,179,190,287	0
83	MG	1	3783	1/1	0.94	0.15	49,49,49,49	0
83	MG	1	3784	1/1	0.94	0.20	55,55,55,55	0
82	OHX	AR	3544	7/7	0.94	0.09	106,119,132,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AS	207	7/7	0.94	0.09	121,129,136,198	0
82	OHX	1	3468	7/7	0.94	0.12	104,119,126,181	0
83	MG	AR	3745	1/1	0.94	0.22	47,47,47,47	0
82	OHX	AR	3547	7/7	0.94	0.09	127,138,153,224	0
83	MG	AR	3879	1/1	0.94	0.16	67,67,67,67	0
83	MG	AT	204	1/1	0.94	0.24	54,54,54,54	0
83	MG	AR	4023	1/1	0.94	0.06	57,57,57,57	0
83	MG	1	3986	1/1	0.94	0.13	54,54,54,54	0
82	OHX	1	3604	7/7	0.94	0.12	93,111,130,155	0
83	MG	AR	3885	1/1	0.94	0.13	48,48,48,48	0
82	OHX	1	3589	7/7	0.94	0.11	100,103,119,178	0
83	MG	AT	222	1/1	0.94	0.07	85,85,85,85	0
82	OHX	sR	1986	7/7	0.94	0.09	142,147,168,228	0
82	OHX	AT	209	7/7	0.94	0.10	144,152,178,226	0
82	OHX	AR	3607	7/7	0.94	0.09	105,112,120,211	0
83	MG	1	3891	1/1	0.94	0.07	72,72,72,72	0
82	OHX	1	3495	7/7	0.94	0.12	105,113,120,172	0
83	MG	AT	228	1/1	0.94	0.32	77,77,77,77	0
83	MG	m	301	1/1	0.94	0.27	54,54,54,54	0
83	MG	1	3795	1/1	0.94	0.22	60,60,60,60	0
83	MG	1	3894	1/1	0.94	0.30	51,51,51,51	0
83	MG	AR	4036	1/1	0.94	0.15	67,67,67,67	0
82	OHX	1	3532	7/7	0.94	0.10	122,128,143,216	0
83	MG	1	3896	1/1	0.94	0.29	82,82,82,82	0
82	OHX	1	3577	7/7	0.94	0.08	135,145,158,235	0
82	OHX	sR	1992	7/7	0.94	0.08	152,158,182,238	0
82	OHX	AP	502	7/7	0.94	0.11	106,116,122,224	0
83	MG	1	3709	1/1	0.94	0.21	52,52,52,52	0
83	MG	AR	3766	1/1	0.94	0.27	47,47,47,47	0
82	OHX	sR	1994	7/7	0.94	0.08	157,172,185,238	0
83	MG	AR	3903	1/1	0.94	0.22	56,56,56,56	0
83	MG	CI	302	1/1	0.94	0.10	61,61,61,61	0
82	OHX	AR	3559	7/7	0.94	0.09	116,120,148,210	0
82	OHX	AR	3451	7/7	0.94	0.10	109,123,130,145	0
83	MG	CL	304	1/1	0.94	0.23	48,48,48,48	0
83	MG	AR	3906	1/1	0.94	0.17	49,49,49,49	0
83	MG	1	3713	1/1	0.94	0.15	46,46,46,46	0
83	MG	s8	303	1/1	0.94	0.12	62,62,62,62	0
83	MG	AR	3771	1/1	0.94	0.30	46,46,46,46	0
82	OHX	CE	401	7/7	0.94	0.10	104,111,129,178	0
82	OHX	AR	3472	7/7	0.94	0.14	99,104,117,187	0
83	MG	AR	3912	1/1	0.94	0.09	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	1	4117	7/7	0.94	0.12	90,104,117,204	0
83	MG	AR	3775	1/1	0.94	0.14	52,52,52,52	0
82	OHX	CG	303	7/7	0.94	0.07	193,206,216,288	0
82	OHX	AR	3481	7/7	0.94	0.11	84,103,125,154	0
82	OHX	AR	3565	7/7	0.94	0.08	132,137,154,239	0
83	MG	O	202	1/1	0.94	0.16	67,67,67,67	0
82	OHX	CL	302	7/7	0.94	0.09	124,131,143,198	0
82	OHX	AR	3619	7/7	0.94	0.08	150,159,179,243	0
83	MG	1	3638	1/1	0.94	0.13	66,66,66,66	0
83	MG	1	3914	1/1	0.94	0.05	105,105,105,105	0
83	MG	AR	3783	1/1	0.94	0.30	45,45,45,45	0
83	MG	AR	4066	1/1	0.94	0.25	83,83,83,83	0
82	OHX	AR	3487	7/7	0.94	0.10	110,120,129,179	0
82	OHX	DH	202	7/7	0.94	0.10	122,127,143,208	0
82	OHX	3	202	7/7	0.94	0.09	117,130,133,198	0
83	MG	1	3918	1/1	0.94	0.09	48,48,48,48	0
83	MG	DC	202	1/1	0.94	0.17	61,61,61,61	0
82	OHX	1	4074	7/7	0.94	0.19	95,106,117,119	0
82	OHX	AR	3498	7/7	0.94	0.10	80,114,124,171	0
83	MG	DI	201	1/1	0.94	0.19	50,50,50,50	0
83	MG	DI	202	1/1	0.94	0.24	70,70,70,70	0
86	X1K	1	4181	25/25	0.94	0.12	66,74,78,78	0
86	X1K	AR	4205	25/25	0.94	0.12	64,73,79,80	0
83	MG	AR	4073	1/1	0.94	0.19	69,69,69,69	0
83	MG	1	4025	1/1	0.94	0.16	49,49,49,49	0
83	MG	sR	2039	1/1	0.94	0.32	51,51,51,51	0
83	MG	3	207	1/1	0.95	0.16	60,60,60,60	0
82	OHX	1	3498	7/7	0.95	0.10	102,111,124,184	0
82	OHX	A	2143	7/7	0.95	0.14	117,118,125,136	7
83	MG	AR	3744	1/1	0.95	0.13	55,55,55,55	0
83	MG	3	210	1/1	0.95	0.14	49,49,49,49	0
83	MG	DA	201	1/1	0.95	0.08	65,65,65,65	0
83	MG	1	3951	1/1	0.95	0.14	110,110,110,110	0
82	OHX	AR	3560	7/7	0.95	0.08	144,145,157,232	0
82	OHX	1	3470	7/7	0.95	0.11	93,106,111,174	0
82	OHX	AR	3441	7/7	0.95	0.12	72,96,100,135	0
83	MG	3	215	1/1	0.95	0.26	69,69,69,69	0
83	MG	DH	203	1/1	0.95	0.09	75,75,75,75	0
82	OHX	1	3501	7/7	0.95	0.09	149,160,170,224	0
82	OHX	AR	3466	7/7	0.95	0.12	97,111,125,166	0
82	OHX	AR	3471	7/7	0.95	0.11	97,105,119,183	0
82	OHX	1	3529	7/7	0.95	0.08	122,128,140,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3473	7/7	0.95	0.14	76,86,106,130	0
83	MG	4	216	1/1	0.95	0.11	44,44,44,44	0
83	MG	1	3715	1/1	0.95	0.27	50,50,50,50	0
82	OHX	AR	3474	7/7	0.95	0.10	90,107,128,157	0
82	OHX	CP	302	7/7	0.95	0.09	132,143,156,205	0
82	OHX	AR	3477	7/7	0.95	0.12	93,104,119,164	0
83	MG	1	3719	1/1	0.95	0.13	51,51,51,51	0
82	OHX	1	3473	7/7	0.95	0.10	120,128,135,182	0
83	MG	1	3842	1/1	0.95	0.27	57,57,57,57	0
83	MG	A	1980	1/1	0.95	0.15	64,64,64,64	0
82	OHX	A	1908	7/7	0.95	0.12	96,116,125,154	0
82	OHX	sR	1922	7/7	0.95	0.12	126,132,140,155	0
83	MG	sR	2064	1/1	0.95	0.07	66,66,66,66	0
82	OHX	sR	1925	7/7	0.95	0.11	100,110,125,154	0
83	MG	1	3846	1/1	0.95	0.08	47,47,47,47	0
83	MG	j	301	1/1	0.95	0.08	47,47,47,47	0
83	MG	1	3847	1/1	0.95	0.16	57,57,57,57	0
82	OHX	A	1914	7/7	0.95	0.10	132,135,146,194	0
82	OHX	sR	1929	7/7	0.95	0.12	126,137,141,170	0
83	MG	AR	4086	1/1	0.95	0.25	48,48,48,48	0
82	OHX	sR	1940	7/7	0.95	0.09	114,118,130,185	0
82	OHX	1	3457	7/7	0.95	0.12	106,108,118,158	0
83	MG	AR	3931	1/1	0.95	0.14	50,50,50,50	0
83	MG	1	3615	1/1	0.95	0.07	48,48,48,48	0
83	MG	1	3729	1/1	0.95	0.10	58,58,58,58	0
83	MG	1	3616	1/1	0.95	0.18	47,47,47,47	0
83	MG	AR	3936	1/1	0.95	0.07	60,60,60,60	0
82	OHX	sR	1942	7/7	0.95	0.10	87,110,117,157	0
82	OHX	A	1916	7/7	0.95	0.10	128,136,151,190	0
82	OHX	A	1917	7/7	0.95	0.09	148,159,174,219	0
83	MG	1	3983	1/1	0.95	0.14	126,126,126,126	0
82	OHX	sR	1946	7/7	0.95	0.09	124,124,136,191	0
83	MG	AR	3784	1/1	0.95	0.15	48,48,48,48	0
82	OHX	sR	1947	7/7	0.95	0.10	131,135,147,219	0
82	OHX	AR	3572	7/7	0.95	0.10	113,127,145,206	0
82	OHX	AR	3573	7/7	0.95	0.08	126,133,140,211	0
82	OHX	A	1923	7/7	0.95	0.10	111,120,133,179	0
82	OHX	AR	3483	7/7	0.95	0.08	104,122,134,204	0
82	OHX	sR	1958	7/7	0.95	0.10	119,129,136,193	0
82	OHX	1	3477	7/7	0.95	0.11	100,106,117,157	0
83	MG	1	3992	1/1	0.95	0.07	55,55,55,55	0
82	OHX	AR	3491	7/7	0.95	0.10	101,109,131,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	1	3533	7/7	0.95	0.08	151,152,164,218	0
83	MG	AR	3954	1/1	0.95	0.18	50,50,50,50	0
83	MG	1	3995	1/1	0.95	0.05	57,57,57,57	0
82	OHX	1	3478	7/7	0.95	0.11	92,100,129,169	0
83	MG	AR	3797	1/1	0.95	0.17	46,46,46,46	0
82	OHX	sR	1965	7/7	0.95	0.09	120,128,144,205	0
83	MG	AR	4121	1/1	0.95	0.13	52,52,52,52	0
82	OHX	sR	1966	7/7	0.95	0.08	115,131,152,216	0
82	OHX	A	1930	7/7	0.95	0.07	134,143,158,205	0
82	OHX	AR	3494	7/7	0.95	0.11	112,117,124,200	0
82	OHX	A	1933	7/7	0.95	0.10	125,127,148,192	0
82	OHX	1	3460	7/7	0.95	0.11	100,108,115,158	0
82	OHX	AR	3582	7/7	0.95	0.10	115,122,145,201	0
82	OHX	AR	3500	7/7	0.95	0.11	105,106,117,172	0
83	MG	1	3639	1/1	0.95	0.17	46,46,46,46	0
82	OHX	AR	3585	7/7	0.95	0.07	139,150,171,246	0
83	MG	1	4007	1/1	0.95	0.21	48,48,48,48	0
82	OHX	1	3482	7/7	0.95	0.10	114,121,132,214	0
83	MG	AC	101	1/1	0.95	0.15	48,48,48,48	0
83	MG	AR	3812	1/1	0.95	0.24	47,47,47,47	0
82	OHX	AR	3502	7/7	0.95	0.10	101,106,118,173	0
82	OHX	AR	3503	7/7	0.95	0.10	101,111,119,176	0
83	MG	AH	201	1/1	0.95	0.27	59,59,59,59	0
83	MG	AR	4179	1/1	0.95	0.08	94,94,94,94	0
83	MG	AR	3816	1/1	0.95	0.37	48,48,48,48	0
82	OHX	1	4116	7/7	0.95	0.11	98,108,119,179	0
82	OHX	AR	3506	7/7	0.95	0.08	126,134,140,194	0
82	OHX	A	1944	7/7	0.95	0.09	135,142,144,235	0
83	MG	A	2043	1/1	0.95	0.19	65,65,65,65	0
82	OHX	AR	3508	7/7	0.95	0.09	77,95,114,197	0
83	MG	AR	3672	1/1	0.95	0.09	48,48,48,48	0
83	MG	1	3766	1/1	0.95	0.23	53,53,53,53	0
82	OHX	1	3538	7/7	0.95	0.08	109,117,120,195	0
83	MG	sR	2127	1/1	0.95	0.09	85,85,85,85	0
83	MG	1	3651	1/1	0.95	0.09	55,55,55,55	0
82	OHX	A	1947	7/7	0.95	0.09	149,153,156,204	0
82	OHX	AR	3511	7/7	0.95	0.10	110,114,134,202	0
82	OHX	1	3510	7/7	0.95	0.10	126,130,138,220	0
82	OHX	1	3463	7/7	0.95	0.10	93,100,113,150	0
82	OHX	1	3485	7/7	0.95	0.10	96,110,127,173	0
83	MG	AR	3830	1/1	0.95	0.20	46,46,46,46	0
83	MG	sR	2135	1/1	0.95	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3597	7/7	0.95	0.08	132,150,162,238	0
82	OHX	AR	3516	7/7	0.95	0.09	108,140,151,206	0
82	OHX	1	3542	7/7	0.95	0.09	129,131,137,216	0
82	OHX	1	3486	7/7	0.95	0.12	112,121,131,190	0
83	MG	AR	3835	1/1	0.95	0.19	54,54,54,54	0
82	OHX	1	3515	7/7	0.95	0.09	128,142,151,216	0
82	OHX	1	3545	7/7	0.95	0.08	162,169,180,241	0
82	OHX	AR	3603	7/7	0.95	0.10	135,137,142,234	0
82	OHX	AR	3521	7/7	0.95	0.10	104,109,136,182	0
83	MG	AR	4000	1/1	0.95	0.27	99,99,99,99	0
82	OHX	AR	3522	7/7	0.95	0.09	110,116,127,199	0
82	OHX	1	3488	7/7	0.95	0.12	87,100,115,183	0
82	OHX	AR	3524	7/7	0.95	0.11	118,124,136,187	0
82	OHX	AR	3608	7/7	0.95	0.11	128,139,153,241	0
82	OHX	1	3489	7/7	0.95	0.11	80,105,113,161	0
83	MG	AR	4006	1/1	0.95	0.07	59,59,59,59	0
83	MG	1	4036	1/1	0.95	0.16	47,47,47,47	0
82	OHX	1	3518	7/7	0.95	0.08	144,151,172,239	0
82	OHX	AR	3527	7/7	0.95	0.09	89,100,109,179	0
83	MG	AT	203	1/1	0.95	0.05	69,69,69,69	0
83	MG	1	3672	1/1	0.95	0.10	58,58,58,58	0
83	MG	sR	2157	1/1	0.95	0.14	65,65,65,65	0
82	OHX	1	3464	7/7	0.95	0.11	101,109,122,174	0
83	MG	1	3674	1/1	0.95	0.14	57,57,57,57	0
82	OHX	1	3520	7/7	0.95	0.08	137,146,154,224	0
82	OHX	1	4090	7/7	0.95	0.09	85,118,129,182	0
83	MG	AT	220	1/1	0.95	0.10	53,53,53,53	0
82	OHX	4	206	7/7	0.95	0.09	109,117,138,191	0
82	OHX	AR	4155	7/7	0.95	0.10	91,104,116,201	0
82	OHX	4	207	7/7	0.95	0.08	131,139,150,217	0
83	MG	1	3798	1/1	0.95	0.32	65,65,65,65	0
83	MG	1	4053	1/1	0.95	0.10	46,46,46,46	0
83	MG	sR	2185	1/1	0.95	0.07	109,109,109,109	0
83	MG	sR	2187	1/1	0.95	0.06	96,96,96,96	0
83	MG	1	3799	1/1	0.95	0.24	57,57,57,57	0
83	MG	AR	3711	1/1	0.95	0.09	66,66,66,66	0
82	OHX	1	3436	7/7	0.95	0.12	92,102,118,142	0
83	MG	A	2089	1/1	0.95	0.20	59,59,59,59	0
83	MG	AR	3713	1/1	0.95	0.10	54,54,54,54	0
82	OHX	4	210	7/7	0.95	0.06	146,153,168,235	0
82	OHX	A	2117	7/7	0.95	0.09	120,121,133,214	0
82	OHX	AR	3538	7/7	0.95	0.08	131,135,143,195	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3540	7/7	0.95	0.10	106,110,132,187	0
83	MG	1	3927	1/1	0.95	0.13	47,47,47,47	0
82	OHX	4	211	7/7	0.95	0.07	154,159,166,242	0
82	OHX	1	3522	7/7	0.95	0.08	118,125,136,197	0
82	OHX	AS	203	7/7	0.95	0.09	81,103,111,166	0
82	OHX	1	4096	7/7	0.95	0.09	120,125,151,213	0
82	OHX	1	4097	7/7	0.95	0.08	119,124,138,200	0
83	MG	1	3811	1/1	0.95	0.06	56,56,56,56	0
82	OHX	1	3444	7/7	0.95	0.10	108,116,129,166	0
82	OHX	AR	3627	7/7	0.95	0.07	141,147,154,242	0
83	MG	CJ	301	1/1	0.95	0.12	70,70,70,70	0
83	MG	AR	4037	1/1	0.95	0.07	65,65,65,65	0
82	OHX	AR	3549	7/7	0.95	0.10	106,111,119,199	0
82	OHX	1	3497	7/7	0.95	0.09	132,139,148,198	0
83	MG	AR	3881	1/1	0.95	0.21	54,54,54,54	0
83	MG	AR	3883	1/1	0.95	0.07	53,53,53,53	0
83	MG	d6	201	1/1	0.95	0.31	55,55,55,55	0
82	OHX	AT	207	7/7	0.95	0.10	96,115,127,180	0
82	OHX	1	4100	7/7	0.95	0.10	93,105,120,170	0
83	MG	S	201	1/1	0.95	0.05	135,135,135,135	0
83	MG	1	4175	1/1	0.95	0.07	89,89,89,89	0
83	MG	AR	3732	1/1	0.95	0.20	47,47,47,47	0
83	MG	CP	306	1/1	0.95	0.11	78,78,78,78	0
82	OHX	AT	210	7/7	0.95	0.08	112,120,135,201	0
82	OHX	AR	3553	7/7	0.95	0.12	118,126,134,222	0
82	OHX	AT	212	7/7	0.95	0.09	128,137,158,222	0
82	OHX	1	3555	7/7	0.95	0.09	136,142,152,229	0
82	OHX	AR	3555	7/7	0.95	0.10	116,123,128,204	0
82	OHX	v	301	7/7	0.95	0.10	114,128,142,207	0
87	ZN	g	501	1/1	0.95	0.05	162,162,162,162	0
82	OHX	1	4102	7/7	0.95	0.11	113,128,140,191	0
83	MG	1	4185	1/1	0.95	0.21	48,48,48,48	0
82	OHX	1	3459	7/7	0.96	0.10	93,104,123,150	0
82	OHX	1	3442	7/7	0.96	0.09	98,105,122,163	0
82	OHX	1	3513	7/7	0.96	0.09	119,126,147,204	0
82	OHX	1	4114[A]	7/7	0.96	0.16	90,96,106,125	7
82	OHX	1	4114[B]	7/7	0.96	0.16	97,97,103,109	7
82	OHX	sR	1911	7/7	0.96	0.11	110,124,138,152	0
82	OHX	r	303	7/7	0.96	0.10	91,98,109,148	0
82	OHX	AR	3515	7/7	0.96	0.09	103,107,114,175	0
82	OHX	1	3535[A]	7/7	0.96	0.16	104,105,111,146	7
82	OHX	sR	1921	7/7	0.96	0.08	110,111,129,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	1	3535[B]	7/7	0.96	0.16	101,102,106,128	7
82	OHX	sR	1923	7/7	0.96	0.11	105,108,111,167	0
83	MG	1	3685	1/1	0.96	0.06	59,59,59,59	0
83	MG	4	231	1/1	0.96	0.05	100,100,100,100	0
82	OHX	1	3475	7/7	0.96	0.08	85,96,116,167	0
82	OHX	sR	1926	7/7	0.96	0.11	97,101,121,152	0
82	OHX	AK	102	7/7	0.96	0.10	100,100,119,159	0
82	OHX	1	4079	7/7	0.96	0.12	81,86,109,119	0
82	OHX	sR	1932	7/7	0.96	0.11	100,106,129,171	0
82	OHX	sR	1933	7/7	0.96	0.09	91,114,128,159	0
82	OHX	sR	1935	7/7	0.96	0.09	135,143,153,189	0
83	MG	AR	3977	1/1	0.96	0.21	74,74,74,74	0
82	OHX	sR	1936	7/7	0.96	0.09	107,115,126,184	0
82	OHX	sR	1937	7/7	0.96	0.11	98,103,119,147	0
82	OHX	AR	4161	7/7	0.96	0.16	112,114,119,137	7
82	OHX	AR	3438	7/7	0.96	0.13	97,105,118,118	0
82	OHX	AR	3440	7/7	0.96	0.11	88,95,114,134	0
82	OHX	sR	1943	7/7	0.96	0.08	138,142,158,205	0
83	MG	AR	3751	1/1	0.96	0.14	73,73,73,73	0
83	MG	AR	3867	1/1	0.96	0.10	48,48,48,48	0
82	OHX	A	1950	7/7	0.96	0.10	113,117,134,174	0
82	OHX	AR	3583	7/7	0.96	0.06	136,149,163,220	0
83	MG	1	3802	1/1	0.96	0.06	68,68,68,68	0
82	OHX	1	4080	7/7	0.96	0.12	107,110,115,140	0
82	OHX	AS	205	7/7	0.96	0.09	114,117,127,175	0
82	OHX	sR	1950	7/7	0.96	0.07	138,146,154,210	0
82	OHX	AS	206	7/7	0.96	0.08	117,124,132,183	0
82	OHX	AR	3442	7/7	0.96	0.14	65,86,99,132	0
82	OHX	sR	1954	7/7	0.96	0.09	115,127,141,173	0
82	OHX	AR	3449	7/7	0.96	0.09	103,120,131,154	0
82	OHX	1	4085	7/7	0.96	0.11	77,86,100,138	0
82	OHX	A	1958	7/7	0.96	0.07	130,148,161,216	0
82	OHX	sR	1959	7/7	0.96	0.09	109,113,125,184	0
82	OHX	AR	3452	7/7	0.96	0.10	101,111,121,152	0
82	OHX	AR	3528	7/7	0.96	0.10	91,99,114,190	0
82	OHX	AR	3455	7/7	0.96	0.12	86,104,112,144	0
83	MG	1	3816	1/1	0.96	0.08	56,56,56,56	0
83	MG	1	3714	1/1	0.96	0.28	66,66,66,66	0
83	MG	DQ	504	1/1	0.96	0.06	49,49,49,49	0
82	OHX	AT	208	7/7	0.96	0.09	99,102,117,183	0
83	MG	A	2150	1/1	0.96	0.05	95,95,95,95	0
82	OHX	sR	1964	7/7	0.96	0.09	111,118,120,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3460	7/7	0.96	0.11	80,96,103,146	0
82	OHX	AR	3464	7/7	0.96	0.09	96,99,111,144	0
82	OHX	A	1965	7/7	0.96	0.09	134,136,150,221	0
83	MG	AR	4132	1/1	0.96	0.11	81,81,81,81	0
83	MG	AB	203	1/1	0.96	0.10	47,47,47,47	0
82	OHX	1	3493	7/7	0.96	0.08	118,120,144,197	0
82	OHX	AR	3467	7/7	0.96	0.10	87,100,114,155	0
82	OHX	1	3494	7/7	0.96	0.09	112,122,130,205	0
82	OHX	1	3476	7/7	0.96	0.07	124,127,143,186	0
82	OHX	1	3496	7/7	0.96	0.08	104,118,140,184	0
83	MG	AR	4177	1/1	0.96	0.05	103,103,103,103	0
82	OHX	A	1971	7/7	0.96	0.11	85,115,126,139	0
82	OHX	1	4093	7/7	0.96	0.10	112,120,132,176	0
82	OHX	sR	1975	7/7	0.96	0.08	125,139,147,206	0
82	OHX	AR	3541	7/7	0.96	0.08	154,156,169,193	0
82	OHX	AR	3475	7/7	0.96	0.12	77,108,119,162	0
82	OHX	AR	3543	7/7	0.96	0.10	82,96,115,170	0
83	MG	1	3731	1/1	0.96	0.25	54,54,54,54	0
82	OHX	sR	1979	7/7	0.96	0.09	114,123,133,197	0
82	OHX	1	3461	7/7	0.96	0.09	96,98,105,189	0
82	OHX	AR	3545	7/7	0.96	0.08	115,119,140,211	0
83	MG	AR	4191	1/1	0.96	0.06	52,52,52,52	0
82	OHX	A	2102	7/7	0.96	0.11	104,105,126,167	0
82	OHX	sR	1983	7/7	0.96	0.07	141,144,158,211	0
83	MG	AR	4197	1/1	0.96	0.06	99,99,99,99	0
83	MG	1	3946	1/1	0.96	0.27	64,64,64,64	0
82	OHX	1	3435	7/7	0.96	0.14	69,86,105,144	0
82	OHX	1	3566	7/7	0.96	0.07	183,187,198,236	0
82	OHX	1	3567	7/7	0.96	0.08	103,110,120,195	0
82	OHX	A	2118	7/7	0.96	0.09	135,143,147,201	0
82	OHX	A	2120	7/7	0.96	0.08	106,118,124,185	0
83	MG	A	2011	1/1	0.96	0.25	54,54,54,54	0
83	MG	sR	2186	1/1	0.96	0.06	71,71,71,71	0
82	OHX	A	2121	7/7	0.96	0.09	123,133,142,199	0
82	OHX	1	3479	7/7	0.96	0.08	87,99,117,199	0
82	OHX	AR	3550	7/7	0.96	0.08	139,145,148,199	0
83	MG	1	3745	1/1	0.96	0.18	47,47,47,47	0
82	OHX	AR	3489	7/7	0.96	0.10	97,101,115,179	0
83	MG	sR	2049	1/1	0.96	0.08	73,73,73,73	0
82	OHX	1	3451	7/7	0.96	0.13	75,94,104,142	0
83	MG	AR	3693	1/1	0.96	0.10	47,47,47,47	0
83	MG	AR	3924	1/1	0.96	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	1	3466	7/7	0.96	0.09	88,111,128,167	0
82	OHX	DL	103	7/7	0.96	0.10	104,114,127,169	0
82	OHX	DQ	502	7/7	0.96	0.09	113,119,125,226	0
83	MG	1	4166	1/1	0.96	0.07	57,57,57,57	0
82	OHX	A	1907	7/7	0.96	0.10	138,148,152,185	0
83	MG	AR	4046	1/1	0.96	0.13	72,72,72,72	0
83	MG	1	4173	1/1	0.96	0.09	48,48,48,48	0
82	OHX	1	3456	7/7	0.96	0.11	91,103,117,151	0
83	MG	sR	2061	1/1	0.96	0.26	52,52,52,52	0
82	OHX	4	205	7/7	0.96	0.08	84,94,108,164	0
82	OHX	AR	3556	7/7	0.96	0.09	106,115,138,201	0
82	OHX	AR	3495	7/7	0.96	0.10	90,104,115,180	0
82	OHX	AR	3496	7/7	0.96	0.08	126,139,145,190	0
82	OHX	AR	3497	7/7	0.96	0.08	113,119,133,179	0
83	MG	AR	3938	1/1	0.96	0.16	64,64,64,64	0
83	MG	1	3862	1/1	0.96	0.20	57,57,57,57	0
83	MG	1	3759	1/1	0.96	0.26	46,46,46,46	0
82	OHX	A	1919	7/7	0.96	0.08	124,131,141,181	0
82	OHX	1	3484	7/7	0.96	0.08	115,116,127,184	0
82	OHX	A	1921	7/7	0.96	0.08	132,139,163,191	0
82	OHX	1	3526	7/7	0.96	0.07	126,134,148,209	0
84	K	AR	4165	1/1	0.96	0.09	94,94,94,94	0
82	OHX	1	3431	7/7	0.96	0.10	79,97,115,133	0
82	OHX	A	1925	7/7	0.96	0.09	122,126,137,203	0
82	OHX	1	3458	7/7	0.96	0.10	100,106,110,160	0
82	OHX	1	3487	7/7	0.96	0.09	102,103,114,196	0
83	MG	1	3978	1/1	0.96	0.12	107,107,107,107	0
82	OHX	AR	3623	7/7	0.96	0.07	135,140,147,219	0
82	OHX	AR	3504	7/7	0.96	0.09	107,110,124,194	0
83	MG	1	3770	1/1	0.96	0.29	46,46,46,46	0
82	OHX	1	3509	7/7	0.96	0.07	121,122,126,216	0
82	OHX	A	1931	7/7	0.96	0.08	125,134,136,197	0
82	OHX	1	3471	7/7	0.96	0.09	93,106,117,161	0
83	MG	AR	4198	1/1	0.97	0.07	97,97,97,97	0
82	OHX	AR	3490	7/7	0.97	0.07	96,99,105,167	0
83	MG	AR	4200	1/1	0.97	0.05	101,101,101,101	0
82	OHX	1	3438	7/7	0.97	0.10	94,101,111,140	0
82	OHX	1	3462	7/7	0.97	0.07	115,118,130,167	0
82	OHX	1	3440	7/7	0.97	0.11	68,93,109,150	0
82	OHX	1	3441	7/7	0.97	0.10	90,106,118,145	0
82	OHX	AT	214	7/7	0.97	0.05	146,155,163,223	0
83	MG	1	3879	1/1	0.97	0.28	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	1	3465	7/7	0.97	0.11	85,95,101,153	0
83	MG	1	3649	1/1	0.97	0.04	56,56,56,56	0
82	OHX	1	3426	7/7	0.97	0.10	105,115,120,121	0
82	OHX	1	4050	7/7	0.97	0.11	91,97,109,134	0
82	OHX	A	2105	7/7	0.97	0.11	113,118,128,133	0
82	OHX	A	2106	7/7	0.97	0.13	113,124,126,131	0
82	OHX	A	2107	7/7	0.97	0.09	97,100,109,148	0
82	OHX	A	2111	7/7	0.97	0.11	101,106,109,152	0
82	OHX	1	3467	7/7	0.97	0.10	83,95,101,141	0
83	MG	v	303	1/1	0.97	0.05	68,68,68,68	0
82	OHX	sR	1984	7/7	0.97	0.09	126,138,144,199	0
82	OHX	AR	3499	7/7	0.97	0.09	105,114,127,168	0
82	OHX	A	2115	7/7	0.97	0.08	98,113,121,181	0
82	OHX	A	2116	7/7	0.97	0.09	124,127,141,200	0
82	OHX	1	4060	7/7	0.97	0.08	95,104,119,174	0
82	OHX	1	3429	7/7	0.97	0.11	97,102,120,124	0
83	MG	AR	3907	1/1	0.97	0.07	49,49,49,49	0
83	MG	x	204	1/1	0.97	0.21	46,46,46,46	0
82	OHX	A	2119	7/7	0.97	0.07	137,148,160,185	0
82	OHX	1	3490	7/7	0.97	0.09	90,105,114,182	0
82	OHX	1	3445	7/7	0.97	0.09	93,98,104,153	0
83	MG	x	208	1/1	0.97	0.06	92,92,92,92	0
82	OHX	AR	3577	7/7	0.97	0.09	94,103,110,167	0
82	OHX	1	3447	7/7	0.97	0.13	85,97,110,114	0
82	OHX	AK	103	7/7	0.97	0.09	95,105,121,166	0
82	OHX	1	4081	7/7	0.97	0.10	94,100,109,138	0
82	OHX	AR	3507	7/7	0.97	0.09	87,88,103,135	0
82	OHX	AR	3401	7/7	0.97	0.14	68,76,82,85	0
82	OHX	AR	3509	7/7	0.97	0.09	115,118,132,168	0
82	OHX	AR	3411	7/7	0.97	0.14	90,98,110,116	0
82	OHX	AR	3412	7/7	0.97	0.13	87,98,106,110	0
82	OHX	A	1901	7/7	0.97	0.13	93,108,118,126	0
82	OHX	A	1903	7/7	0.97	0.10	92,106,123,134	0
82	OHX	A	1906	7/7	0.97	0.09	107,120,128,145	0
82	OHX	AR	3427	7/7	0.97	0.12	61,83,107,109	0
82	OHX	AR	3429	7/7	0.97	0.10	89,103,112,118	0
83	MG	CD	301	1/1	0.97	0.14	47,47,47,47	0
82	OHX	A	1911	7/7	0.97	0.09	101,114,125,151	0
82	OHX	A	1912	7/7	0.97	0.07	125,133,139,182	0
82	OHX	A	1913	7/7	0.97	0.06	125,143,145,198	0
82	OHX	AR	3432	7/7	0.97	0.11	80,98,108,109	0
82	OHX	AR	3433	7/7	0.97	0.10	97,109,124,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3435	7/7	0.97	0.11	96,99,121,124	0
82	OHX	AR	3436	7/7	0.97	0.09	82,92,113,131	0
82	OHX	1	4082	7/7	0.97	0.09	97,101,114,176	0
82	OHX	1	4083	7/7	0.97	0.10	94,100,112,147	0
82	OHX	1	3448	7/7	0.97	0.11	83,92,106,132	0
82	OHX	1	4086	7/7	0.97	0.09	92,101,109,156	0
82	OHX	A	1922	7/7	0.97	0.07	126,128,136,190	0
82	OHX	AR	3443	7/7	0.97	0.12	78,82,105,123	0
82	OHX	AR	3444	7/7	0.97	0.10	76,91,121,121	0
82	OHX	AR	4116	7/7	0.97	0.11	77,92,103,129	0
82	OHX	T	201	7/7	0.97	0.10	103,120,137,143	0
83	MG	AR	3811	1/1	0.97	0.18	47,47,47,47	0
83	MG	CP	301	1/1	0.97	0.07	66,66,66,66	0
83	MG	1	3928	1/1	0.97	0.10	51,51,51,51	0
83	MG	1	4048	1/1	0.97	0.05	100,100,100,100	0
82	OHX	AR	3446	7/7	0.97	0.10	65,85,110,116	0
82	OHX	AR	4126	7/7	0.97	0.10	95,102,116,155	0
82	OHX	AR	4136	7/7	0.97	0.07	91,104,110,143	0
82	OHX	sR	1904	7/7	0.97	0.13	89,106,116,125	0
82	OHX	sR	1910	7/7	0.97	0.14	97,99,112,120	0
82	OHX	AR	3447	7/7	0.97	0.09	99,102,113,131	0
82	OHX	sR	1912	7/7	0.97	0.12	89,94,101,107	0
82	OHX	sR	1913	7/7	0.97	0.09	90,102,108,116	0
82	OHX	sR	1915	7/7	0.97	0.11	95,107,117,132	0
82	OHX	1	3472	7/7	0.97	0.09	97,106,115,163	0
82	OHX	AR	3450	7/7	0.97	0.11	88,98,110,125	0
82	OHX	sR	1918	7/7	0.97	0.10	97,106,113,133	0
82	OHX	3	201	7/7	0.97	0.08	88,96,115,134	0
82	OHX	1	4088	7/7	0.97	0.08	112,121,135,175	0
83	MG	1	4070	1/1	0.97	0.09	103,103,103,103	0
82	OHX	1	4089	7/7	0.97	0.11	79,92,104,130	0
82	OHX	AR	3531	7/7	0.97	0.07	147,150,158,206	0
83	MG	A	2152	1/1	0.97	0.15	67,67,67,67	0
82	OHX	AR	3456	7/7	0.97	0.11	96,103,126,140	0
82	OHX	1	3430	7/7	0.97	0.10	87,92,100,119	0
82	OHX	AR	3534	7/7	0.97	0.11	86,99,112,156	0
83	MG	AR	4098	1/1	0.97	0.15	47,47,47,47	0
83	MG	1	4164	1/1	0.97	0.07	83,83,83,83	0
82	OHX	AR	3461	7/7	0.97	0.09	97,102,109,152	0
83	MG	AR	3836	1/1	0.97	0.10	73,73,73,73	0
82	OHX	sR	1931	7/7	0.97	0.09	94,104,113,150	0
82	OHX	A	1940[A]	7/7	0.97	0.18	103,109,114,138	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	A	1940[B]	7/7	0.97	0.18	109,112,112,143	7
82	OHX	sR	1934	7/7	0.97	0.09	92,102,109,152	0
82	OHX	AR	3462	7/7	0.97	0.10	99,102,113,136	0
82	OHX	AR	3463	7/7	0.97	0.11	96,97,109,136	0
82	OHX	1	3452	7/7	0.97	0.09	101,107,127,155	0
83	MG	1	3608	1/1	0.97	0.08	48,48,48,48	0
82	OHX	sR	1938	7/7	0.97	0.07	112,113,123,166	0
82	OHX	sR	1939	7/7	0.97	0.09	103,113,122,164	0
82	OHX	AR	3539	7/7	0.97	0.08	94,99,105,185	0
82	OHX	1	3453	7/7	0.97	0.08	96,104,121,137	0
82	OHX	1	3407	7/7	0.97	0.13	90,92,104,105	0
82	OHX	AR	3468	7/7	0.97	0.08	94,108,117,136	0
82	OHX	A	1948	7/7	0.97	0.07	160,167,174,209	0
82	OHX	AR	3469	7/7	0.97	0.07	100,103,121,152	0
82	OHX	AR	3470	7/7	0.97	0.08	112,115,130,156	0
83	MG	1	3848	1/1	0.97	0.07	61,61,61,61	0
83	MG	AR	3855	1/1	0.97	0.31	60,60,60,60	0
82	OHX	1	4094	7/7	0.97	0.07	105,112,124,177	0
83	MG	A	1988	1/1	0.97	0.19	52,52,52,52	0
82	OHX	sR	1948	7/7	0.97	0.08	117,119,129,182	0
82	OHX	sR	1949	7/7	0.97	0.08	106,117,123,179	0
82	OHX	3	221	7/7	0.97	0.08	98,99,121,162	0
82	OHX	1	4095	7/7	0.97	0.08	107,112,120,196	0
82	OHX	sR	1952	7/7	0.97	0.07	112,127,136,165	0
83	MG	4	203	1/1	0.97	0.06	64,64,64,64	0
82	OHX	1	3499	7/7	0.97	0.08	127,137,146,190	0
82	OHX	1	3432	7/7	0.97	0.11	93,101,108,130	0
82	OHX	AR	3476	7/7	0.97	0.09	102,105,113,156	0
82	OHX	1	3434	7/7	0.97	0.11	101,107,116,135	0
83	MG	AR	4174	1/1	0.97	0.10	105,105,105,105	0
82	OHX	sR	1957	7/7	0.97	0.07	161,165,175,201	0
83	MG	AR	4176	1/1	0.97	0.05	65,65,65,65	0
82	OHX	AS	202	7/7	0.97	0.09	105,111,120,138	0
82	OHX	1	3423	7/7	0.97	0.13	67,90,101,116	0
82	OHX	AR	3479	7/7	0.97	0.09	94,104,112,158	0
82	OHX	1	3503	7/7	0.97	0.10	97,109,118,168	0
82	OHX	AR	3482	7/7	0.97	0.09	97,98,102,155	0
82	OHX	1	3425	7/7	0.97	0.11	92,99,111,112	0
82	OHX	AR	3484	7/7	0.97	0.10	106,113,119,154	0
83	MG	AR	3746	1/1	0.97	0.17	66,66,66,66	0
83	MG	1	3751	1/1	0.97	0.06	52,52,52,52	0
82	OHX	AR	3485	7/7	0.97	0.09	93,99,103,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	AR	3486	7/7	0.97	0.08	93,102,113,168	0
83	MG	AR	4190	1/1	0.97	0.06	87,87,87,87	0
82	OHX	4	209	7/7	0.97	0.07	121,123,141,202	0
87	ZN	DQ	501	1/1	0.97	0.04	105,105,105,105	0
82	OHX	AR	3488	7/7	0.97	0.10	99,103,110,163	0
83	MG	AR	4194	1/1	0.97	0.09	48,48,48,48	0
83	MG	AR	3882	1/1	0.97	0.13	47,47,47,47	0
82	OHX	1	3481	7/7	0.97	0.06	109,119,132,164	0
82	OHX	AR	3421	7/7	0.98	0.11	96,100,116,120	0
82	OHX	AR	3423	7/7	0.98	0.11	101,102,113,113	0
82	OHX	AR	3424	7/7	0.98	0.12	85,90,105,108	0
83	MG	AR	3692	1/1	0.98	0.09	49,49,49,49	0
82	OHX	AR	3425	7/7	0.98	0.10	89,93,106,112	0
82	OHX	1	3450	7/7	0.98	0.08	100,102,108,135	0
82	OHX	AR	3428	7/7	0.98	0.10	85,90,108,121	0
82	OHX	1	3405	7/7	0.98	0.12	75,87,99,104	0
82	OHX	AR	3430	7/7	0.98	0.10	90,95,112,115	0
82	OHX	1	3406	7/7	0.98	0.11	91,96,100,103	0
82	OHX	A	2124	7/7	0.98	0.14	92,96,103,107	0
82	OHX	1	3427	7/7	0.98	0.11	93,97,121,132	0
83	MG	AR	4168	1/1	0.98	0.04	63,63,63,63	0
83	MG	AR	4170	1/1	0.98	0.05	72,72,72,72	0
82	OHX	AR	3434	7/7	0.98	0.10	98,103,112,114	0
82	OHX	1	3454	7/7	0.98	0.07	90,107,118,151	0
83	MG	AR	4173	1/1	0.98	0.06	88,88,88,88	0
82	OHX	1	3455	7/7	0.98	0.09	102,114,118,141	0
82	OHX	AR	3437	7/7	0.98	0.09	94,101,109,114	0
82	OHX	1	3428	7/7	0.98	0.09	88,98,111,113	0
82	OHX	AR	3439	7/7	0.98	0.08	109,112,124,144	0
82	OHX	1	3402	7/7	0.98	0.10	71,72,80,80	0
82	OHX	1	3408	7/7	0.98	0.11	89,94,99,101	0
82	OHX	1	3410	7/7	0.98	0.10	88,95,101,107	0
83	MG	AR	4182	1/1	0.98	0.09	99,99,99,99	0
82	OHX	1	3411	7/7	0.98	0.12	83,86,96,116	0
82	OHX	1	3433	7/7	0.98	0.11	90,102,106,120	0
82	OHX	AR	3445	7/7	0.98	0.09	85,89,104,126	0
82	OHX	4	204	7/7	0.98	0.11	74,81,88,92	0
83	MG	A	2098	1/1	0.98	0.05	105,105,105,105	0
82	OHX	AS	201	7/7	0.98	0.09	91,104,111,114	0
82	OHX	1	3412	7/7	0.98	0.10	87,93,108,110	0
82	OHX	AR	3448	7/7	0.98	0.07	98,103,113,131	0
83	MG	A	2148	1/1	0.98	0.06	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	A	2149	1/1	0.98	0.04	97,97,97,97	0
82	OHX	1	3415	7/7	0.98	0.14	84,95,103,106	0
82	OHX	1	3416	7/7	0.98	0.09	98,105,107,114	0
82	OHX	1	3437	7/7	0.98	0.10	90,97,115,129	0
82	OHX	1	3417	7/7	0.98	0.13	90,95,108,120	0
83	MG	A	1989	1/1	0.98	0.06	58,58,58,58	0
82	OHX	AR	3453	7/7	0.98	0.10	89,100,102,134	0
83	MG	AR	4196	1/1	0.98	0.05	86,86,86,86	0
83	MG	A	2157	1/1	0.98	0.03	94,94,94,94	0
83	MG	AR	3935	1/1	0.98	0.04	47,47,47,47	0
82	OHX	AR	3454	7/7	0.98	0.08	108,109,120,138	0
83	MG	4	227	1/1	0.98	0.27	47,47,47,47	0
82	OHX	1	3439	7/7	0.98	0.07	112,113,122,158	0
82	OHX	1	3418	7/7	0.98	0.11	95,110,115,116	0
83	MG	4	232	1/1	0.98	0.04	94,94,94,94	0
82	OHX	AT	206	7/7	0.98	0.12	83,84,95,108	0
82	OHX	AR	3457	7/7	0.98	0.07	93,100,102,126	0
82	OHX	AR	3458	7/7	0.98	0.10	83,90,105,142	0
83	MG	1	3643	1/1	0.98	0.19	47,47,47,47	0
82	OHX	AR	3459	7/7	0.98	0.09	83,94,106,117	0
82	OHX	1	3419	7/7	0.98	0.11	90,102,109,113	0
82	OHX	1	4058	7/7	0.98	0.10	87,97,110,124	0
82	OHX	sR	1903	7/7	0.98	0.12	76,82,87,90	0
82	OHX	1	3420	7/7	0.98	0.10	90,102,107,108	0
82	OHX	sR	1905	7/7	0.98	0.13	94,96,102,111	0
82	OHX	sR	1907	7/7	0.98	0.09	85,104,113,120	0
82	OHX	sR	1909	7/7	0.98	0.09	75,104,110,110	0
82	OHX	1	3443	7/7	0.98	0.09	88,93,101,144	0
82	OHX	1	4072	7/7	0.98	0.17	80,84,93,97	0
82	OHX	AR	3465	7/7	0.98	0.10	100,107,116,136	0
82	OHX	1	4073	7/7	0.98	0.10	74,76,83,87	0
82	OHX	sR	1914	7/7	0.98	0.09	100,112,118,120	0
82	OHX	1	3421	7/7	0.98	0.07	87,98,107,138	0
82	OHX	1	4075	7/7	0.98	0.12	95,100,106,107	0
82	OHX	1	4076	7/7	0.98	0.10	87,92,101,103	0
82	OHX	sR	1917	7/7	0.98	0.08	101,104,111,129	0
82	OHX	1	4077	7/7	0.98	0.15	88,95,98,105	0
82	OHX	sR	1919	7/7	0.98	0.07	98,101,108,131	0
83	MG	AR	3856	1/1	0.98	0.04	48,48,48,48	0
82	OHX	AC	102	7/7	0.98	0.10	70,91,100,101	0
82	OHX	1	3422	7/7	0.98	0.11	79,97,110,115	0
82	OHX	1	3446	7/7	0.98	0.07	98,104,105,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	OHX	1	4115	7/7	0.98	0.11	94,97,103,105	0
82	OHX	sR	1924	7/7	0.98	0.07	100,104,111,135	0
82	OHX	CH	201	7/7	0.98	0.12	71,75,82,88	0
82	OHX	1	3404	7/7	0.98	0.11	86,90,97,99	0
82	OHX	1	3424	7/7	0.98	0.10	84,92,118,122	0
83	MG	1	4047	1/1	0.98	0.05	63,63,63,63	0
82	OHX	sR	1928	7/7	0.98	0.07	99,106,119,172	0
83	MG	1	4049	1/1	0.98	0.03	70,70,70,70	0
82	OHX	AR	3402	7/7	0.98	0.13	60,62,67,79	0
82	OHX	sR	1930	7/7	0.98	0.07	154,156,164,192	0
82	OHX	AR	3405	7/7	0.98	0.13	81,82,88,90	0
82	OHX	AR	3406	7/7	0.98	0.11	81,92,98,99	0
82	OHX	CV	201	7/7	0.98	0.10	76,79,84,85	0
82	OHX	CX	201	7/7	0.98	0.08	95,99,119,142	0
82	OHX	DD	102	7/7	0.98	0.10	69,95,100,108	0
82	OHX	AR	3480	7/7	0.98	0.07	95,106,127,168	0
82	OHX	AR	3409	7/7	0.98	0.12	70,75,83,85	0
83	MG	AF	201	1/1	0.98	0.12	55,55,55,55	0
82	OHX	1	3449	7/7	0.98	0.08	107,114,122,160	0
82	OHX	1	4084	7/7	0.98	0.09	94,97,104,151	0
83	MG	CF	404	1/1	0.98	0.05	81,81,81,81	0
82	OHX	A	1902	7/7	0.98	0.10	98,100,114,116	0
82	OHX	AR	3413	7/7	0.98	0.14	92,95,106,108	0
82	OHX	A	1904	7/7	0.98	0.07	112,117,130,134	0
82	OHX	A	2103	7/7	0.98	0.13	95,105,106,112	0
82	OHX	A	2104	7/7	0.98	0.10	100,103,116,122	0
82	OHX	A	1905	7/7	0.98	0.10	107,113,116,139	0
82	OHX	AR	3415	7/7	0.98	0.13	78,83,99,110	0
83	MG	1	4160	1/1	0.98	0.04	77,77,77,77	0
84	K	1	4156	1/1	0.98	0.15	65,65,65,65	0
82	OHX	AR	3416	7/7	0.98	0.11	94,97,105,110	0
83	MG	1	4162	1/1	0.98	0.05	86,86,86,86	0
82	OHX	A	2108	7/7	0.98	0.09	101,108,113,145	0
82	OHX	A	2109	7/7	0.98	0.11	107,114,118,134	0
83	MG	1	4165	1/1	0.98	0.04	93,93,93,93	0
82	OHX	s1	301	7/7	0.98	0.09	101,107,119,119	0
82	OHX	A	2110	7/7	0.98	0.09	104,106,122,137	0
83	MG	1	4169	1/1	0.98	0.15	70,70,70,70	0
83	MG	AR	3683	1/1	0.98	0.11	55,55,55,55	0
83	MG	AR	4113	1/1	0.98	0.09	71,71,71,71	0
87	ZN	AP	501	1/1	0.98	0.05	109,109,109,109	0
83	MG	1	4171	1/1	0.98	0.08	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	ZN	b	201	1/1	0.98	0.05	96,96,96,96	0
82	OHX	AR	3417	7/7	0.98	0.11	81,98,109,116	0
82	OHX	A	2112	7/7	0.98	0.07	128,132,139,174	0
87	ZN	d6	202	1/1	0.98	0.04	77,77,77,77	0
82	OHX	A	1909	7/7	0.98	0.10	111,113,124,141	0
82	OHX	A	1910	7/7	0.98	0.08	114,117,122,148	0
82	OHX	1	4078	7/7	0.99	0.10	93,102,104,110	0
82	OHX	1	3413	7/7	0.99	0.09	85,95,107,108	0
82	OHX	AR	3414	7/7	0.99	0.11	89,94,105,116	0
82	OHX	1	3414	7/7	0.99	0.11	97,104,108,122	0
82	OHX	1	4056	7/7	0.99	0.08	61,72,77,81	0
82	OHX	AR	3403	7/7	0.99	0.11	50,55,58,72	0
83	MG	1	4168	1/1	0.99	0.03	60,60,60,60	0
82	OHX	AR	3418	7/7	0.99	0.09	91,94,99,113	0
83	MG	1	4170	1/1	0.99	0.11	88,88,88,88	0
82	OHX	AR	3419	7/7	0.99	0.08	97,100,103,112	0
83	MG	sR	2165	1/1	0.99	0.12	64,64,64,64	0
83	MG	1	4172	1/1	0.99	0.06	61,61,61,61	0
83	MG	AR	4193	1/1	0.99	0.03	65,65,65,65	0
83	MG	sR	2183	1/1	0.99	0.03	74,74,74,74	0
82	OHX	sR	1906	7/7	0.99	0.09	86,103,113,116	0
82	OHX	AR	3420	7/7	0.99	0.09	92,98,103,107	0
82	OHX	sR	1908	7/7	0.99	0.10	100,103,107,108	0
82	OHX	AR	3404	7/7	0.99	0.11	78,84,90,99	0
82	OHX	AR	3422	7/7	0.99	0.09	92,98,102,102	0
82	OHX	2	201	7/7	0.99	0.10	85,90,101,110	0
83	MG	AR	4169	1/1	0.99	0.03	49,49,49,49	0
82	OHX	1	3403	7/7	0.99	0.12	57,59,70,73	0
82	OHX	AR	3407	7/7	0.99	0.11	80,84,90,91	0
82	OHX	AR	3426	7/7	0.99	0.08	78,87,98,103	0
87	ZN	AN	500	1/1	0.99	0.03	70,70,70,70	0
82	OHX	AR	3408	7/7	0.99	0.10	89,94,100,102	0
87	ZN	AQ	501	1/1	0.99	0.05	85,85,85,85	0
87	ZN	DL	104	1/1	0.99	0.03	70,70,70,70	0
87	ZN	DO	202	1/1	0.99	0.03	62,62,62,62	0
83	MG	1	4157	1/1	0.99	0.06	55,55,55,55	0
87	ZN	DR	501	1/1	0.99	0.05	83,83,83,83	0
82	OHX	1	3401	7/7	0.99	0.12	59,63,69,74	0
82	OHX	AR	3410	7/7	0.99	0.11	83,90,93,98	0
87	ZN	e	101	1/1	0.99	0.04	103,103,103,103	0
82	OHX	1	3409	7/7	0.99	0.11	94,95,106,109	0
83	MG	AR	4114	1/1	0.99	0.04	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AR	4115	1/1	0.99	0.07	46,46,46,46	0
87	ZN	d9	101	1/1	0.99	0.05	108,108,108,108	0
82	OHX	AR	3431	7/7	0.99	0.10	97,104,113,116	0
87	ZN	AK	101	1/1	1.00	0.02	62,62,62,62	0
83	MG	AR	4180	1/1	1.00	0.03	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.