



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2020 – 12:57 pm BST

PDB ID : 6HHQ
Title : Crystal structure of compound C45 bound to the yeast 80S ribosome
Authors : Pellegrino, S.; Vanderwal, C.D.; Yusupov, M.
Deposited on : 2018-08-28
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

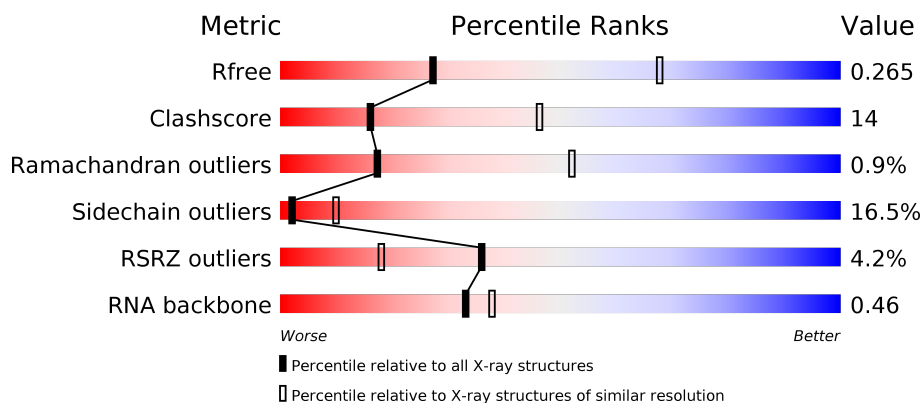
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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







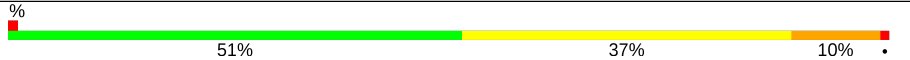
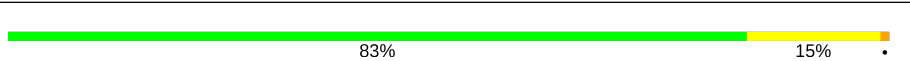
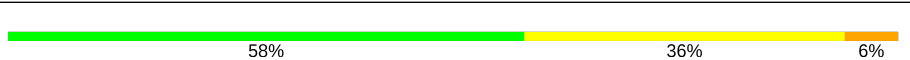
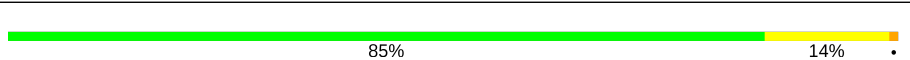
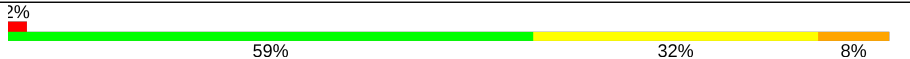
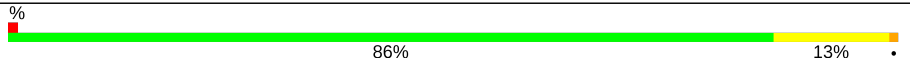
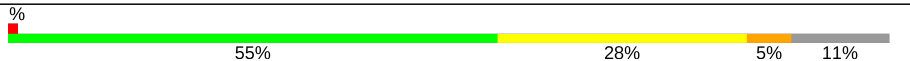
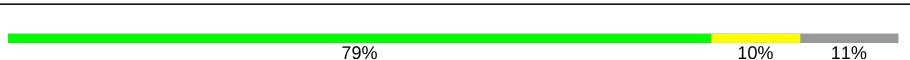
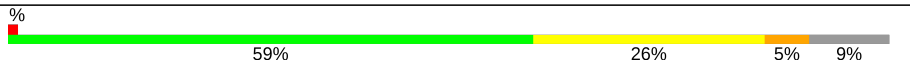
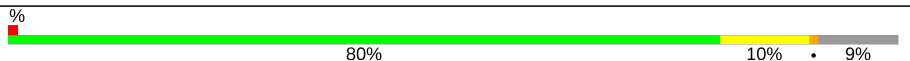


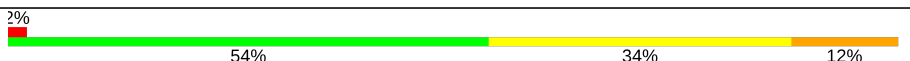
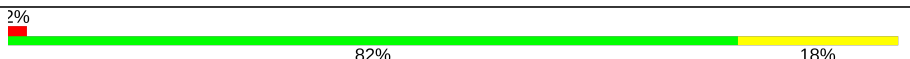


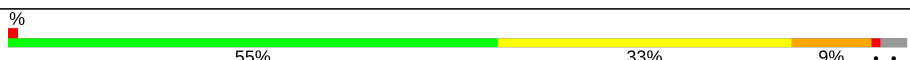
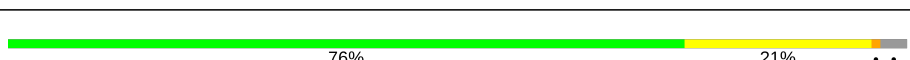
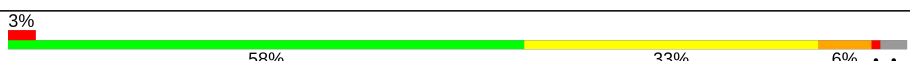
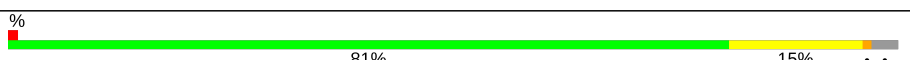
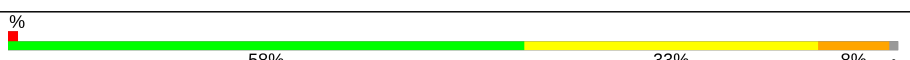
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	1	3396	
1	AR	3396	
2	3	121	
2	AS	121	

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


























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




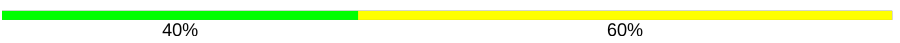








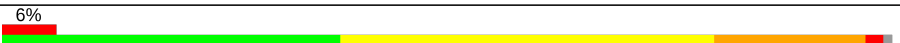
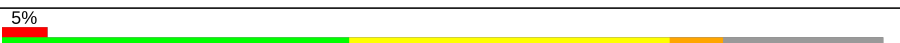


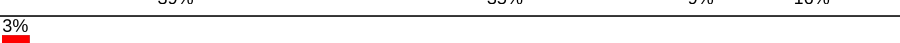
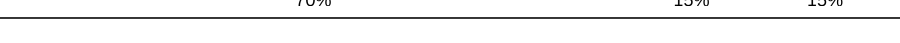
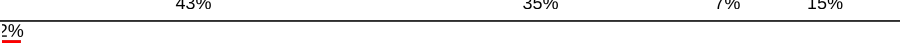

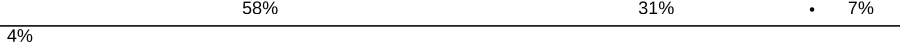
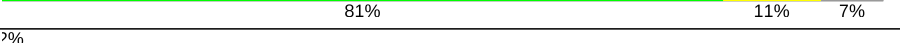



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Mol	Chain	Length	Quality of chain
28	AA	136	
28	DB	136	
29	AB	149	
29	DC	149	
30	AC	59	
30	DD	59	
31	AD	105	
31	DE	105	
32	AE	113	
32	DF	113	
33	AF	130	
33	DG	130	
34	AG	107	
34	DH	107	
35	AH	121	
35	DI	121	
36	AI	120	
36	DJ	120	
37	AJ	100	
37	DK	100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

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Mol	Chain	Length	Quality of chain
40	DN	51	
41	AN	128	
41	DO	128	
42	AO	25	
42	DP	25	
43	AP	106	
43	DQ	106	
44	AQ	92	
44	DR	92	
45	i	273	
45	sM	273	
46	p0	312	
47	A	1797	
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	
65	c7	136	
66	T	146	

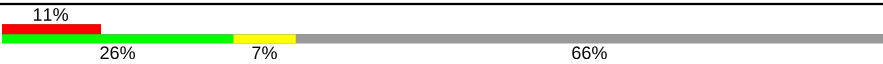

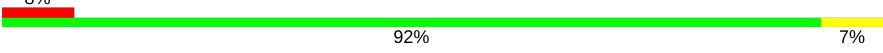


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Mol	Chain	Length	Quality of chain
66	c8	146	
67	U	144	
67	c9	144	
68	V	121	
68	d0	121	
69	W	87	
69	d1	87	
70	X	130	
70	d2	130	
71	Y	145	
71	d3	145	
72	Z	135	
72	d4	135	
73	a	108	
73	d5	108	
74	b	119	
74	d6	119	
75	c	82	
75	d7	82	
76	d	67	
76	d8	67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

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Mol	Chain	Length	Quality of chain
79	e1	152	
79	g	152	
80	Rb	319	
80	h	319	
81	sR	1800	

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
82	OHX	1	3405	-	-	X	-
82	OHX	1	3425	-	-	X	-
82	OHX	1	3467	-	-	X	-
82	OHX	1	3493	-	-	X	-
82	OHX	1	3505	-	-	X	-
82	OHX	1	3509	-	-	X	-
82	OHX	1	3537	-	-	X	-
82	OHX	1	3553	-	-	X	-
82	OHX	1	3562	-	-	X	-
82	OHX	1	3566	-	-	X	-
82	OHX	1	3577	-	-	X	-
82	OHX	1	3578	-	-	X	-
82	OHX	1	3588	-	-	X	-
82	OHX	1	3590	-	-	X	-
82	OHX	1	3617	-	-	X	-
82	OHX	1	3667	-	-	X	-
82	OHX	1	3673	-	-	X	-
82	OHX	1	3677	-	-	X	-
82	OHX	1	3681	-	-	X	-
82	OHX	1	3682	-	-	X	-
82	OHX	1	3683	-	-	X	-
82	OHX	1	3690	-	-	X	-
82	OHX	1	3697	-	-	X	-
82	OHX	1	3705	-	-	X	-
82	OHX	1	3719	-	-	X	-
82	OHX	1	3721	-	-	X	-
82	OHX	1	3722	-	-	X	-
82	OHX	1	3723	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
82	OHX	A	1809	-	-	X	-
82	OHX	A	1822	-	-	X	-
82	OHX	A	1853	-	-	X	-
82	OHX	A	1863	-	-	X	-
82	OHX	A	1867	-	-	X	-
82	OHX	A	1876	-	-	X	-
82	OHX	A	1886	-	-	X	-
82	OHX	A	1897	-	-	X	-
82	OHX	A	1920	-	-	X	-
82	OHX	A	1936	-	-	X	-
82	OHX	A	1941	-	-	X	-
82	OHX	AE	201	-	-	X	-
82	OHX	AK	102	-	-	X	-
82	OHX	AR	3443	-	-	X	-
82	OHX	AR	3458	-	-	X	-
82	OHX	AR	3463	-	-	X	-
82	OHX	AR	3479	-	-	X	-
82	OHX	AR	3486	-	-	X	-
82	OHX	AR	3503	-	-	X	-
82	OHX	AR	3504	-	-	X	-
82	OHX	AR	3513	-	-	X	-
82	OHX	AR	3523	-	-	X	-
82	OHX	AR	3526	-	-	X	-
82	OHX	AR	3530	-	-	X	-
82	OHX	AR	3536	-	-	X	-
82	OHX	AR	3538	-	-	X	-
82	OHX	AR	3558	-	-	X	-
82	OHX	AR	3569	-	-	X	-
82	OHX	AR	3584	-	-	X	-
82	OHX	AR	3593	-	-	X	-
82	OHX	AR	3597	-	-	X	-
82	OHX	AR	3598	-	-	X	-
82	OHX	AR	3683	-	-	X	-
82	OHX	AR	3691	-	-	X	-
82	OHX	AR	3692	-	-	X	-
82	OHX	AR	3693	-	-	X	-
82	OHX	AR	3696	-	-	X	-
82	OHX	AR	3709	-	-	X	-
82	OHX	AR	3723	-	-	X	-
82	OHX	AR	3725	-	-	X	-
82	OHX	AR	3728	-	-	X	-
82	OHX	AR	3736	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
82	OHX	AS	203	-	-	X	-
82	OHX	AS	209	-	-	X	-
82	OHX	AT	203	-	-	X	-
82	OHX	AT	212	-	-	X	-
82	OHX	AT	213	-	-	X	-
82	OHX	CF	401	-	-	X	-
82	OHX	CG	302	-	-	X	-
82	OHX	CL	301	-	-	X	-
82	OHX	DQ	502	-	-	X	-
83	MG	1	3728	-	-	-	X
83	MG	1	3731	-	-	-	X
83	MG	1	3780	-	-	-	X
83	MG	1	3803	-	-	-	X
83	MG	1	3828	-	-	-	X
83	MG	1	3931	-	-	-	X
83	MG	1	3958	-	-	-	X
83	MG	1	3962	-	-	-	X
83	MG	1	3992	-	-	-	X
83	MG	1	4008	-	-	-	X
83	MG	1	4029	-	-	-	X
83	MG	1	4136	-	-	-	X
83	MG	1	4143	-	-	-	X
83	MG	1	4158	-	-	-	X
83	MG	1	4205	-	-	-	X
83	MG	1	4210	-	-	-	X
83	MG	3	211	-	-	-	X
83	MG	3	217	-	-	-	X
83	MG	A	1946	-	-	-	X
83	MG	A	1954	-	-	-	X
83	MG	A	1961	-	-	-	X
83	MG	A	1962	-	-	-	X
83	MG	A	1969	-	-	-	X
83	MG	A	1988	-	-	-	X
83	MG	A	2001	-	-	-	X
83	MG	A	2005	-	-	-	X
83	MG	A	2010	-	-	-	X
83	MG	A	2012	-	-	-	X
83	MG	A	2018	-	-	-	X
83	MG	A	2021	-	-	-	X
83	MG	A	2025	-	-	-	X
83	MG	A	2058	-	-	-	X
83	MG	A	2061	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
83	MG	A	2062	-	-	-	X
83	MG	A	2068	-	-	-	X
83	MG	AR	3752	-	-	-	X
83	MG	AR	3794	-	-	-	X
83	MG	AR	3830	-	-	-	X
83	MG	AR	3895	-	-	-	X
83	MG	AR	3934	-	-	-	X
83	MG	AR	3953	-	-	-	X
83	MG	AR	3961	-	-	-	X
83	MG	AR	3969	-	-	-	X
83	MG	AR	3982	-	-	-	X
83	MG	AR	3994	-	-	-	X
83	MG	AR	4016	-	-	-	X
83	MG	AR	4062	-	-	-	X
83	MG	AR	4084	-	-	-	X
83	MG	AR	4089	-	-	-	X
83	MG	AR	4091	-	-	-	X
83	MG	AR	4105	-	-	-	X
83	MG	AR	4112	-	-	-	X
83	MG	AR	4113	-	-	-	X
83	MG	AR	4199	-	-	-	X
83	MG	AR	4222	-	-	-	X
83	MG	AR	4223	-	-	-	X
83	MG	AR	4235	-	-	-	X
83	MG	AR	4246	-	-	-	X
83	MG	AR	4260	-	-	-	X
83	MG	AT	225	-	-	-	X
83	MG	AT	228	-	-	-	X
83	MG	AT	230	-	-	-	X
83	MG	CD	301	-	-	-	X
83	MG	DA	201	-	-	-	X
83	MG	c6	201	-	-	-	X
83	MG	sR	2073	-	-	-	X
83	MG	sR	2079	-	-	-	X
83	MG	sR	2088	-	-	-	X
83	MG	sR	2107	-	-	-	X
83	MG	sR	2113	-	-	-	X
83	MG	sR	2128	-	-	-	X
83	MG	sR	2137	-	-	-	X
83	MG	sR	2154	-	-	-	X
83	MG	sR	2157	-	-	-	X
83	MG	sR	2159	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
83	MG	sR	2164	-	-	-	X
83	MG	sR	2180	-	-	-	X
83	MG	sR	2188	-	-	-	X
83	MG	sR	2189	-	-	-	X

2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 409486 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 60S ribosomal protein L11-B.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
25	CY	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
			1092	710	202	180				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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	S	0	0	0
			1104	652	221	231				
45	sM	63	Total	C	N	O	S	0	0	0
			475	280	99	96				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	p0	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			

- 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 40S ribosomal protein S3.

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	S	0	0	0
			1481	951	265	265				
55	s7	186	Total	C	N	O	S	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
			891	545	182	163	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-A.

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

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

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

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

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

- Molecule 68 is a protein called 40S ribosomal protein S20.

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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 40S ribosomal protein S26-B.

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 40S ribosomal protein S29-A.

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-40S ribosomal protein S31.

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			

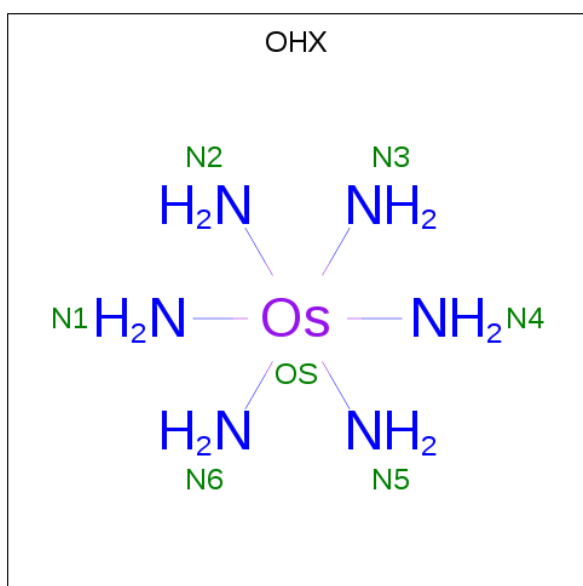
- Molecule 80 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

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

- Molecule 81 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	sR	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			

- Molecule 82 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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82	3	1	Total	N	Os	0	0
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82	3	1	Total	N	Os	0	0
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82	3	1	Total	N	Os	0	0
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82	4	1	Total	N	Os	0	0
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82	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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82	4	1	Total 7	N 6	Os 1	0	0
82	4	1	Total 7	N 6	Os 1	0	0
82	4	1	Total 7	N 6	Os 1	0	0
82	k	1	Total 7	N 6	Os 1	0	0
82	l	1	Total 7	N 6	Os 1	0	0
82	n	1	Total 7	N 6	Os 1	0	0
82	r	1	Total 7	N 6	Os 1	0	0
82	v	1	Total 7	N 6	Os 1	0	0
82	v	1	Total 7	N 6	Os 1	0	0
82	w	1	Total 7	N 6	Os 1	0	0
82	x	1	Total 7	N 6	Os 1	0	0
82	y	1	Total 7	N 6	Os 1	0	0
82	z	1	Total 7	N 6	Os 1	0	0
82	2	1	Total 7	N 6	Os 1	0	0
82	AC	1	Total 7	N 6	Os 1	0	0
82	AE	1	Total 7	N 6	Os 1	0	0
82	AG	1	Total 7	N 6	Os 1	0	0
82	AK	1	Total 7	N 6	Os 1	0	0
82	AK	1	Total 7	N 6	Os 1	0	0
82	AP	1	Total 7	N 6	Os 1	0	0

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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82	AR	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
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			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	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
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82	AT	1	Total	N	Os	0	0
			7	6	1		
82	CE	1	Total	N	Os	0	0
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82	CE	1	Total	N	Os	0	0
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82	CF	1	Total	N	Os	0	0
			7	6	1		
82	CG	1	Total	N	Os	0	0
			7	6	1		
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82	CH	1	Total	N	Os	0	0
			7	6	1		
82	CK	1	Total	N	Os	0	0
			7	6	1		
82	CL	1	Total	N	Os	0	0
			7	6	1		
82	CL	1	Total	N	Os	0	0
			7	6	1		
82	CM	1	Total	N	Os	0	0
			7	6	1		
82	CO	1	Total	N	Os	0	0
			7	6	1		
82	CP	1	Total	N	Os	0	0
			7	6	1		
82	CQ	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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82	CX	1	Total	N	Os	0	0
			7	6	1		
82	CX	1	Total	N	Os	0	0
			7	6	1		
82	DD	1	Total	N	Os	0	0
			7	6	1		
82	DG	1	Total	N	Os	0	0
			7	6	1		
82	DH	1	Total	N	Os	0	0
			7	6	1		
82	DQ	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
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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
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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
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	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
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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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	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	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
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	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
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	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
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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82	A	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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82	A	1	Total	N	Os	0	0
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82	O	1	Total	N	Os	0	0
			7	6	1		
82	Q	1	Total	N	Os	0	0
			7	6	1		
82	T	1	Total	N	Os	0	0
			7	6	1		
82	e	1	Total	N	Os	0	0
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82	h	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
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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		
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			7	6	1		
82	sR	1	Total	N	Os	0	0
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82	sR	1	Total	N	Os	0	0
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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		

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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		

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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		

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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		

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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	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	c1	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	c8	1	Total	N	Os	0	0
			7	6	1		
82	d4	1	Total	N	Os	0	0
			7	6	1		
82	d9	1	Total	N	Os	0	0
			7	6	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	AP	1	Total 1	Mg 1	0	0
83	AK	2	Total 2	Mg 2	0	0
83	DQ	3	Total 3	Mg 3	0	0
83	AB	8	Total 8	Mg 8	0	0
83	c6	1	Total 1	Mg 1	0	0
83	6	3	Total 3	Mg 3	0	0
83	DO	1	Total 1	Mg 1	0	0
83	sM	2	Total 2	Mg 2	0	0
83	d5	1	Total 1	Mg 1	0	0
83	t	3	Total 3	Mg 3	0	0
83	d9	1	Total 1	Mg 1	0	0
83	CD	3	Total 3	Mg 3	0	0
83	CR	8	Total 8	Mg 8	0	0
83	o	1	Total 1	Mg 1	0	0
83	DR	2	Total 2	Mg 2	0	0
83	DC	4	Total 4	Mg 4	0	0
83	AS	19	Total 19	Mg 19	0	0
83	DH	1	Total 1	Mg 1	0	0
83	J	1	Total 1	Mg 1	0	0
83	c9	1	Total 1	Mg 1	0	0
83	k	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	CO	1	Total 1	Mg 1	0	0
83	CU	2	Total 2	Mg 2	0	0
83	b	1	Total 1	Mg 1	0	0
83	e	1	Total 1	Mg 1	0	0
83	DL	1	Total 1	Mg 1	0	0
83	CY	1	Total 1	Mg 1	0	0
83	w	1	Total 1	Mg 1	0	0
83	c8	1	Total 1	Mg 1	0	0
83	CK	3	Total 3	Mg 3	0	0
83	CQ	2	Total 2	Mg 2	0	0
83	x	5	Total 5	Mg 5	0	0
83	sR	154	Total 154	Mg 154	0	0
83	AR	523	Total 523	Mg 523	0	0
83	d6	1	Total 1	Mg 1	0	0
83	F	1	Total 1	Mg 1	0	0
83	s	1	Total 1	Mg 1	0	0
83	DI	1	Total 1	Mg 1	0	0
83	AM	1	Total 1	Mg 1	0	0
83	j	2	Total 2	Mg 2	0	0
83	1	499	Total 499	Mg 499	0	0
83	D	1	Total 1	Mg 1	0	0

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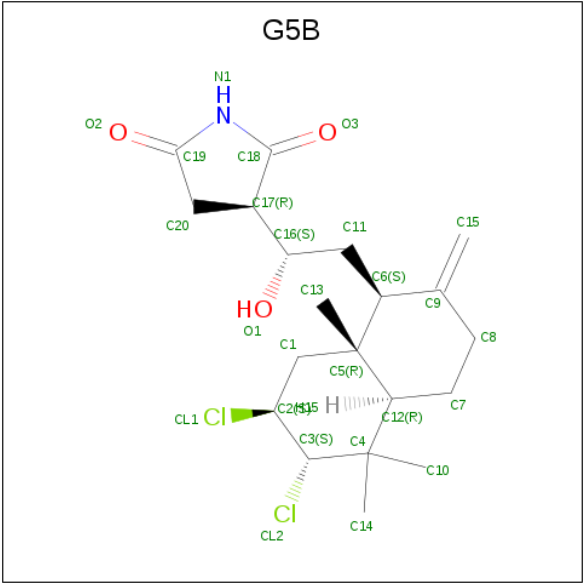
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	DD	1	Total 1	Mg 1	0	0
83	c4	1	Total 1	Mg 1	0	0
83	CM	1	Total 1	Mg 1	0	0
83	s2	1	Total 1	Mg 1	0	0
83	d3	3	Total 3	Mg 3	0	0
83	c1	2	Total 2	Mg 2	0	0
83	v	5	Total 5	Mg 5	0	0
83	CJ	1	Total 1	Mg 1	0	0
83	A	129	Total 129	Mg 129	0	0
83	CP	4	Total 4	Mg 4	0	0
83	4	23	Total 23	Mg 23	0	0
83	DA	2	Total 2	Mg 2	0	0
83	O	1	Total 1	Mg 1	0	0
83	r	2	Total 2	Mg 2	0	0
83	9	1	Total 1	Mg 1	0	0
83	CF	2	Total 2	Mg 2	0	0
83	CX	3	Total 3	Mg 3	0	0
83	AG	1	Total 1	Mg 1	0	0
83	DE	1	Total 1	Mg 1	0	0
83	Y	1	Total 1	Mg 1	0	0
83	s1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	AH	1	Total 1	Mg 1	0	0
83	DP	1	Total 1	Mg 1	0	0
83	s8	2	Total 2	Mg 2	0	0
83	CI	2	Total 2	Mg 2	0	0
83	d4	3	Total 3	Mg 3	0	0
83	H	1	Total 1	Mg 1	0	0
83	z	1	Total 1	Mg 1	0	0
83	DN	1	Total 1	Mg 1	0	0
83	AT	15	Total 15	Mg 15	0	0
83	CL	1	Total 1	Mg 1	0	0
83	s4	1	Total 1	Mg 1	0	0
83	CE	3	Total 3	Mg 3	0	0
83	CG	3	Total 3	Mg 3	0	0
83	1	3	Total 3	Mg 3	0	0
83	3	13	Total 13	Mg 13	0	0
83	AF	2	Total 2	Mg 2	0	0

- Molecule 84 is (3 {R})-3-[(1 {S})-2-[(1 {S},4 {a} {R},6 {S},7 {S},8 {a} {R})-6,7-bis(chloranyl)-5,5,8 {a}-trimethyl-2-methylidene-3,4,4 {a},6,7,8-hexahydro-1 {H}-naphthalen-1-yl]-1-oxidanyl-ethyl]pyrrolidine-2,5-dione (three-letter code: G5B) (formula: C₂₀H₂₉Cl₂NO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
84	1	1	Total 26	C 20	Cl 2	N 1	O 3	0	0
84	AR	1	Total 26	C 20	Cl 2	N 1	O 3	0	0

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

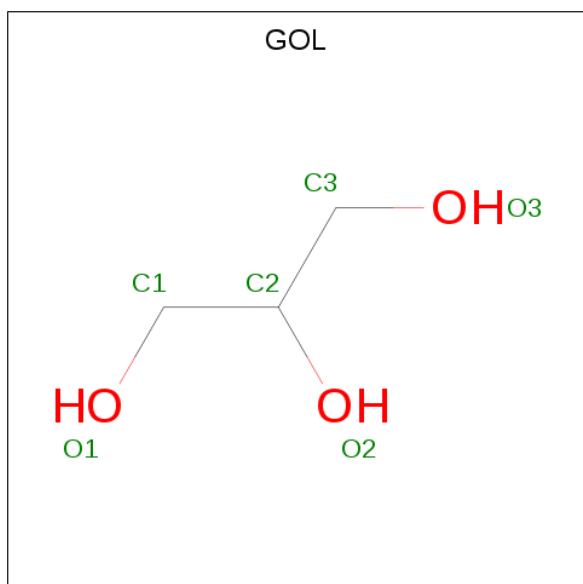
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AP	1	Total	Zn	0	0
			1	1		
85	g	1	Total	Zn	0	0
			1	1		
85	AQ	1	Total	Zn	0	0
			1	1		
85	AK	1	Total	Zn	0	0
			1	1		
85	DQ	1	Total	Zn	0	0
			1	1		
85	e	1	Total	Zn	0	0
			1	1		
85	b	1	Total	Zn	0	0
			1	1		
85	e1	1	Total	Zn	0	0
			1	1		
85	c	1	Total	Zn	0	0
			1	1		
85	DL	1	Total	Zn	0	0
			1	1		

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

- Molecule 86 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

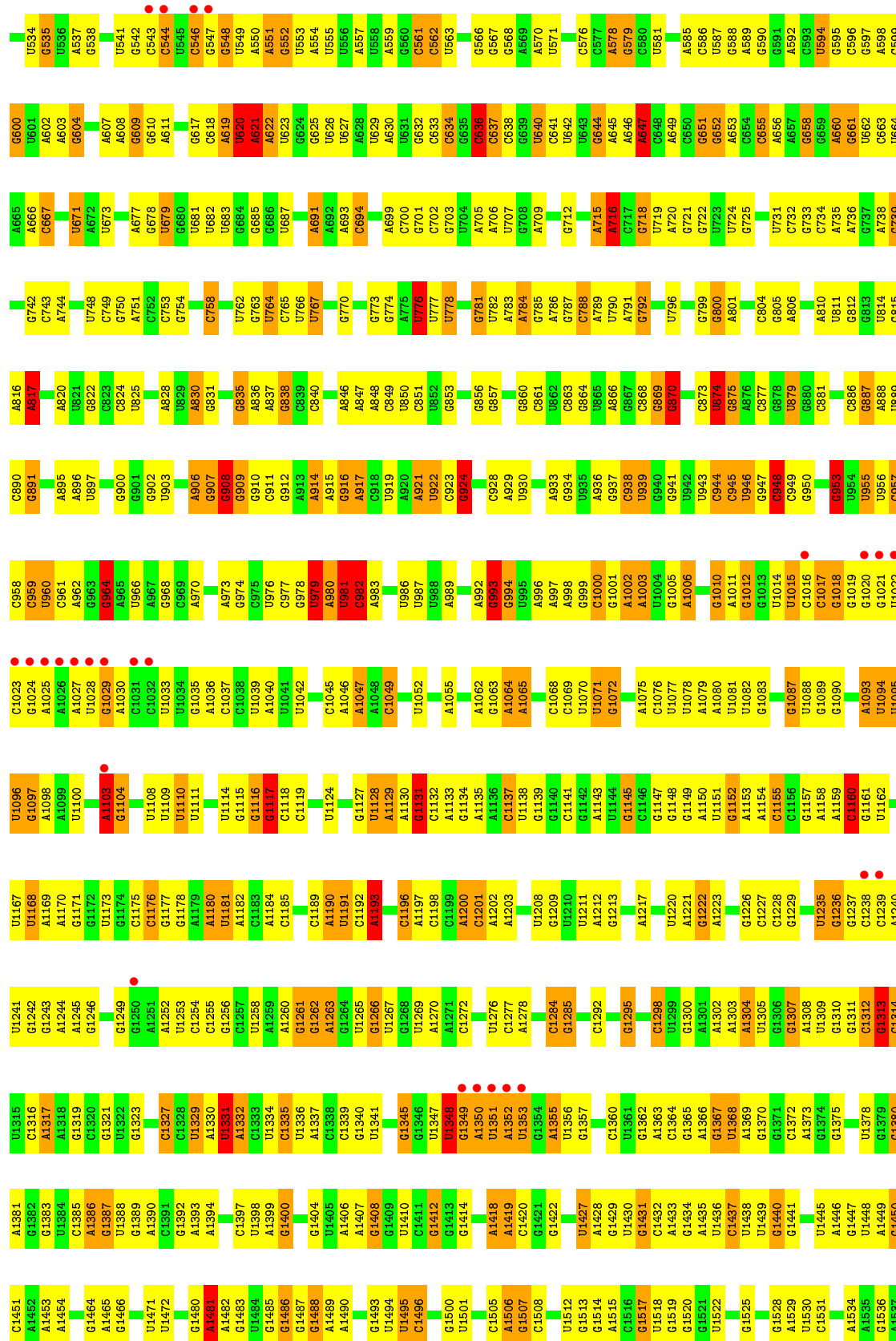


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	AR	1	Total	C	O	0	0
			6	3	3		
86	AR	1	Total	C	O	0	0
			6	3	3		

G1754	G1675	A1589	G1434	G1362	G1283	U1220	C1146	U1073	G999	A929	A847	A771
G1759	A1676	G1590	A1435	G1362	C1284	A1221	G1147	U1081	C1000	U930	A848	U772
A1760	G1680	G1591	U1436	A1363	G1285	G1222	G1148	U1082	A1001	C931	C849	G773
C1761	U1681	G1592	A1437	C1364	A1286	A1225	U1151	G1083	A1002	U932		U776
U1762	U1682	A1593	U1438	A1365	A1287	G1226	U1152	A1084	A1003	G934	A858	U777
U1763	A1683	U1595	U1439	A1366		C1227	A1153	G1087	U1004	G934	G859	
U1764	A1683	C1596	G1440	G1367	C1282	C1228			G1005	U935	G860	
U1765	U1688	C1597	G1443	A1368	U1283	G1229	G1157		A1006	G937	G861	A780
G1766	U1689	G1598	A1446	G1370	A1294	G1230	A1158	G1090	G1010	G938	U782	A781
C1767		G1599	A1446	G1371	C1296	A1231	A1159	A1091	G1014	C938	A783	
U1768	U1694		G1450	A1373	C1297	C1232	G1160	G1093	U1015	U942	A784	
G1769	U1695		A1453	G1374	U1298	G1233	G1161	U1094	U1016	U943	A785	
G1770	A1696		A1453	G1375	U1299	G1234	U1162	U1095	C944	U944	A786	
	C1697		A1454	G1376	A1301	U1235	G1166	U1096	G1017	U945	G867	
G1775	A1698		U1455	C1377	A1302	G1237		A1097	G1018	C946	G788	
U1776	G1537		G1538	U1378	A1303	C1238		A1098	G1019	U946	A789	
U1777	G1538				A1304	C1239	A1169	A1099	G1020	U947	U790	
	G1541		A1460	U1384	U1305	A1240	A1170	U1100	G1021	C948	A791	
G1780	G1542		A1461	C1385	U1306	A1241	A1171	U1101			U792	
U1785	G1543		A1462	C1386	G1307	G1242	G1172	U1102	G1024	G953	C802	
G1786	G1543		G1463	A1386	A1308	G1243	U1173	A1103	A1025	U954	C803	
A1787	G1547		G1464	G1387	A1309	A1244	G1174	A1104	A1026	U955	C804	
C1788			A1468	U1388	U1310	A1245	G1175	G1104	A1027	U956	G805	
G1789	G1552		A1475	A1390	G1310	G1246	G1177		U1028	C957	A806	
G1790	U1553		A1475	C1391	G1313	U1247		U1108	G1029	C958	A807	
C1791	U1554		C1478	G1392		U1247	G1178	U1109	A1030	C959	U808	
G1792	U1555		G1478	G1392	A1317	C1249	A1179	U1110	U1033	U960	G809	
C1793	C1556		G1480	A1393	A1318	G1250	U1180	U1111	U1034	C961	U810	
G1794			G1481	A1399	G1319	A1251	U1181	U1112	A982	A895	G806	
U1795	A1559		A1481	A1399	C1320	U1252	A1182	U1113	G963	U897	A807	
G1796	G1560		A1482	A1401	U1321	U1253		U1114	A1036	C964	A808	
A1797	G1561		G1483	A1401	G1323	C1254	G1186	U1115	U1039	U966	U898	
G1798	G1562		G1484	A1404		C1255	U1191	G1117	A1040	U967	G809	
A1799	C1563		G1485	G1405	G1327	G1257	A1192	G1118	U1041	A967	G900	
	U1564		G1486	A1406	C1328	U1258	A1193	G1119	U1042	G968	G901	
G1807	G1565		G1487	A1407	U1329	A1259	G1194	A1120	C1043	C969	G902	
G1808	U1566		G1488	A1407	U1330	A1260	A1195	U1121	U1044	A970	U903	
A1809	U1567		A1489	G1408	U1331	G1261	C1196	U1122	G1045	G974	A904	
A1810	U1568		A1490	G1409	U1332	G1262	A1197		A1046	C975	U905	
G1811	U1569		G1491	G1412	A1332	A1263	C1198	G1126	A1047	U976	A906	
G1812	U1570		G1492	G1413	G1333	G1264	C1199	U1127	U1048	G977	G908	
A1813	A1571		G1493	G1414	U1336	U1265	A1200	U1128	C1049	G978	U821	
U1814	U1572		U1494	G1415	U1337	G1266	G1201	A1129	U1052	U979		
U1815	G1573		U1495	U1416	U1337	U1267	A1202	A1130	A1053	A980	U829	
A1816	C1574		C1496	G1417		G1268	A1203	G1131	A1054	U981	A914	
U1740	U1575		C1497	A1418	G1340	U1269	A1204	G1132	A1055	C982	A915	
A1741	G1576		A1498	A1419	U1341	A1270	A1205	A1133	A1056	A983	G916	
U1818	U1577		C1499	G1500	U1342	A1271		G1134	U1056	G984	A917	
U1819	C1578		G1501	U1425	U1348	G1272	G1209	A1135		U985		
U1820	U1579		C1502	G1426	G1349	U1273	U1210		A1061	U986	A920	
C1822	A1580		A1503	U1427	A1350	A1274	U1211	U1138	A1062	U987	A921	
	C1581		U1506	U1428	U1351	A1275	G1213	G1139	G1063		U922	
G1833	C1582		A1506	A1429	U1352	G1276		G1140	A1064	G993	G923	
U1834	A1583		G1507	U1430	U1353	U1277	C1216	G1141	A1065	G994	G824	
A1835			G1508	U1431	G1354	C1277	U1217	G1142	G1066	U995	A925	
	G1586		U1509	G1432	U1355	C1278	A1218	A1143	U1067	A996	A926	
G1838	A1587		A1509	A1433	U1356	C1279	U1218	U1144		A997	C927	
A1839	A1588		G1510		G1357		C1219	G1145	G1072	A998	C928	







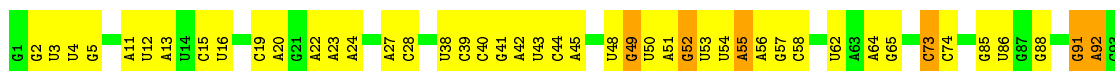






- Molecule 2: 5S ribosomal RNA

Chain AS: 50% 41% 7%



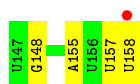
- Molecule 3: 5.8S ribosomal RNA

Chain 4: 44% 41% 14%



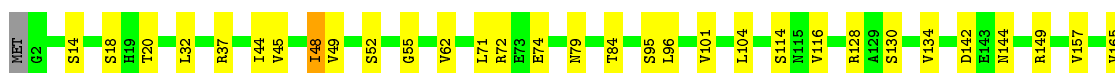
- Molecule 3: 5.8S ribosomal RNA

Chain AT: 41% 44% 13%



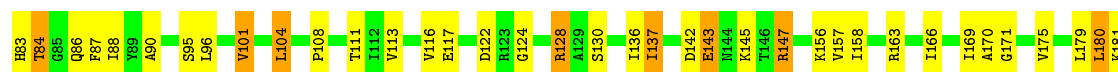
- Molecule 4: 60S ribosomal protein L2-A

Chain j: 81% 17%

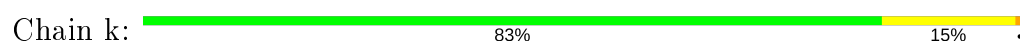




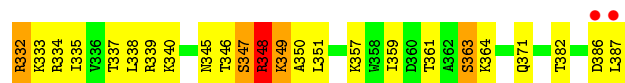
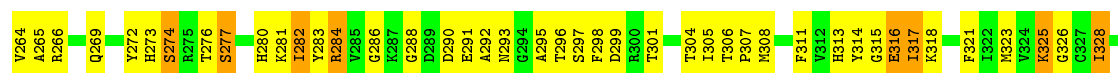
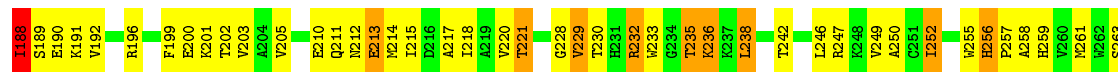
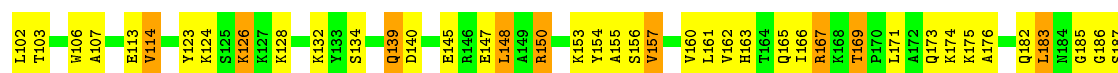
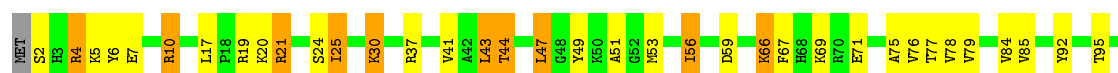
• Molecule 4: 60S ribosomal protein L2-A




• Molecule 5: 60S ribosomal protein L3

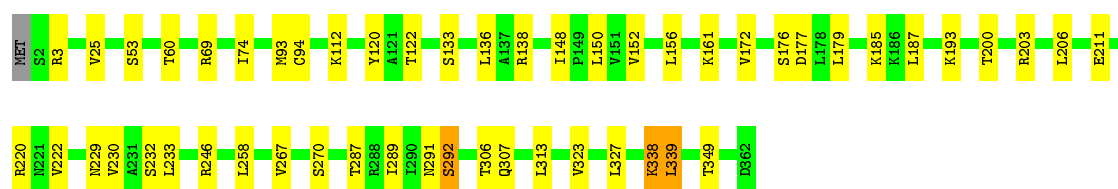


• Molecule 5: 60S ribosomal protein L3



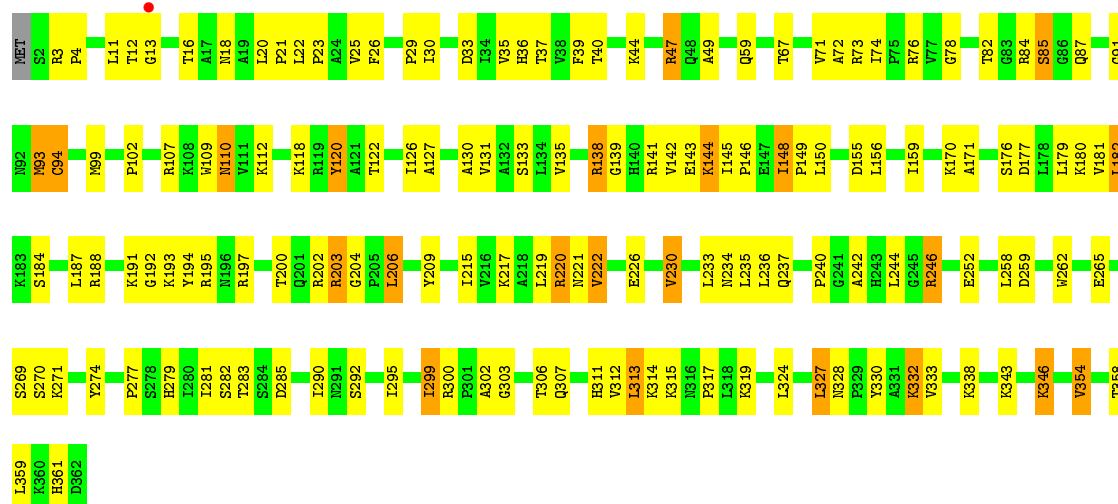
• Molecule 6: 60S ribosomal protein L4-A

Chain I: 




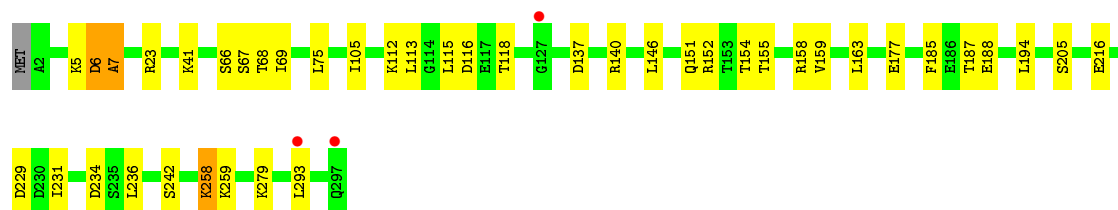
• Molecule 6: 60S ribosomal protein L4-A

Chain CF: 



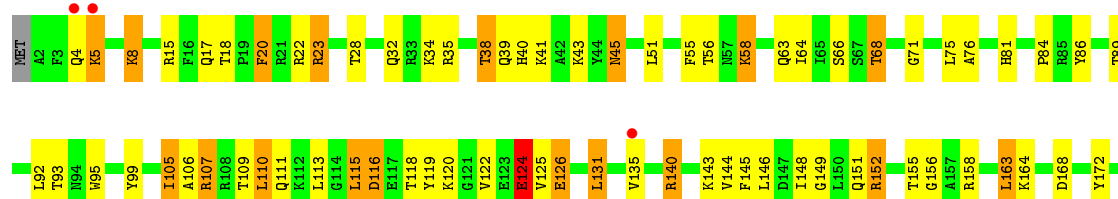
• Molecule 7: 60S ribosomal protein L5

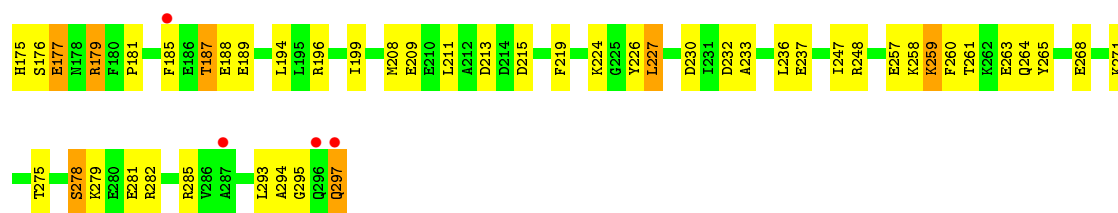
Chain m: 



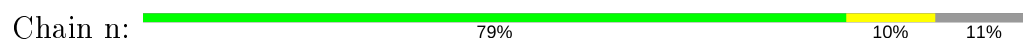
• Molecule 7: 60S ribosomal protein L5

Chain CG: 

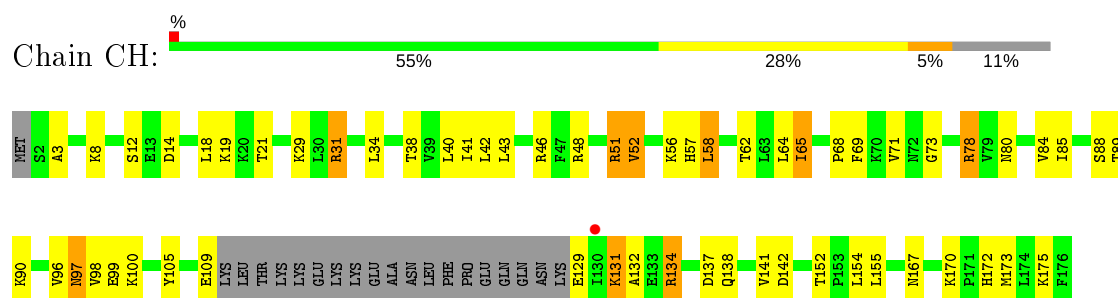




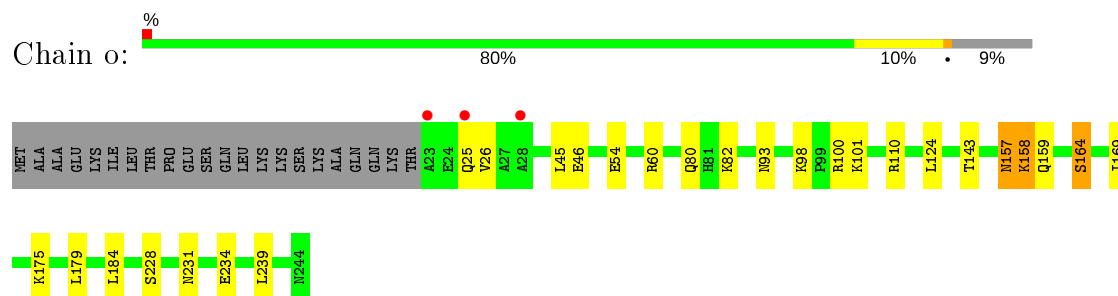
• Molecule 8: 60S ribosomal protein L6-A



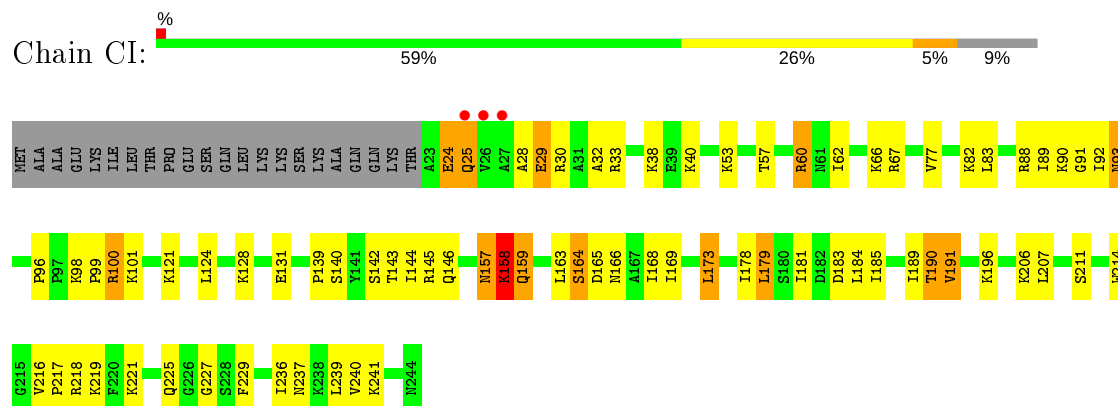
• Molecule 8: 60S ribosomal protein L6-A



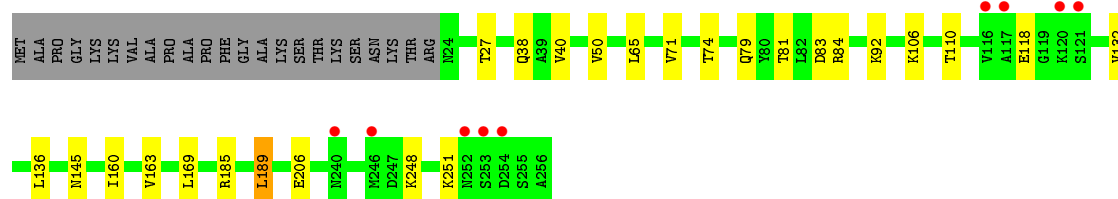
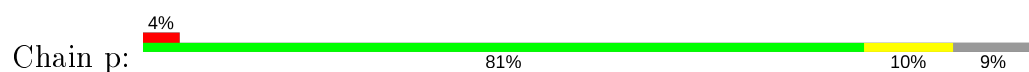
• Molecule 9: 60S ribosomal protein L7-A



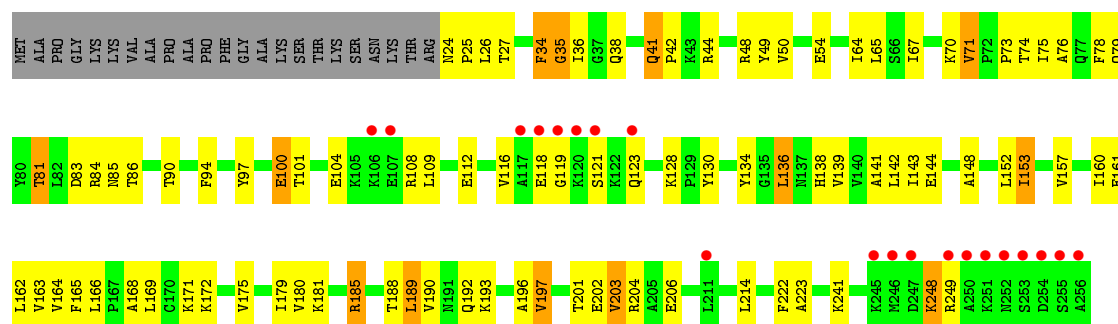
• Molecule 9: 60S ribosomal protein L7-A



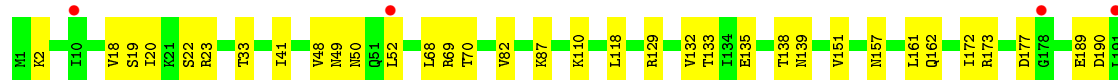
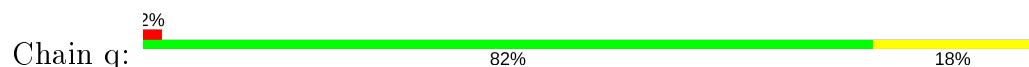
• Molecule 10: 60S ribosomal protein L8-A



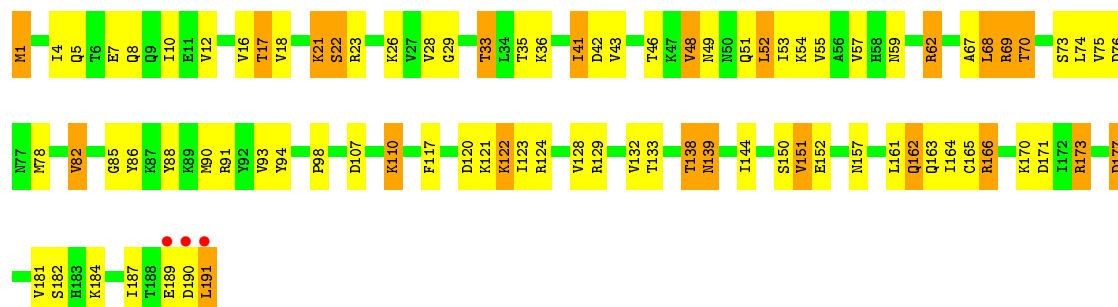
- Molecule 10: 60S ribosomal protein L8-A



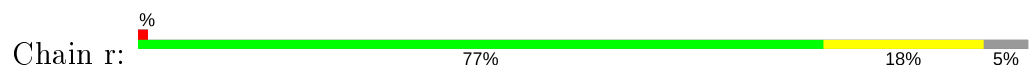
- Molecule 11: 60S ribosomal protein L9-A

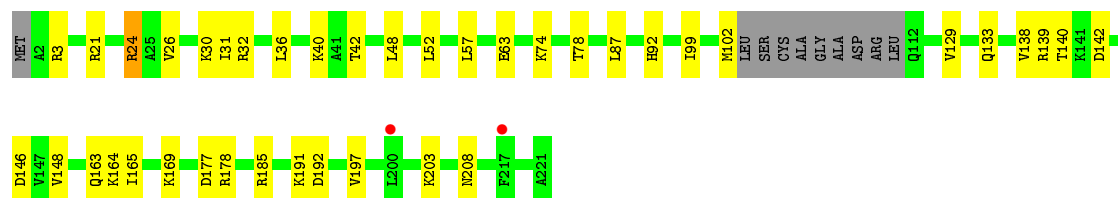


- Molecule 11: 60S ribosomal protein L9-A

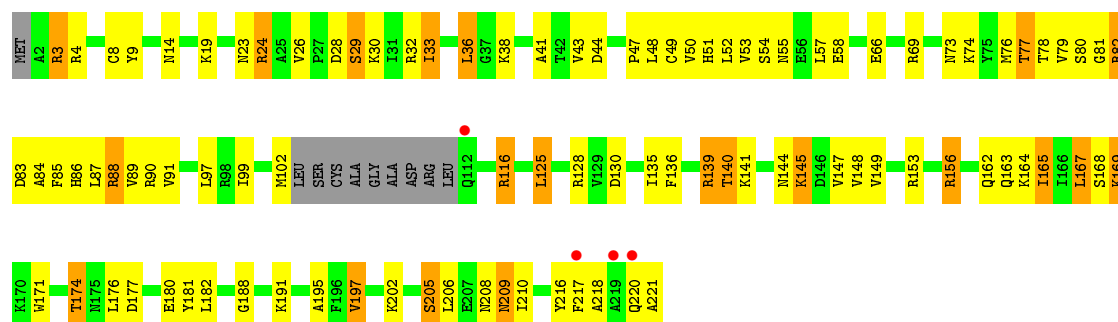


- Molecule 12: 60S ribosomal protein L10

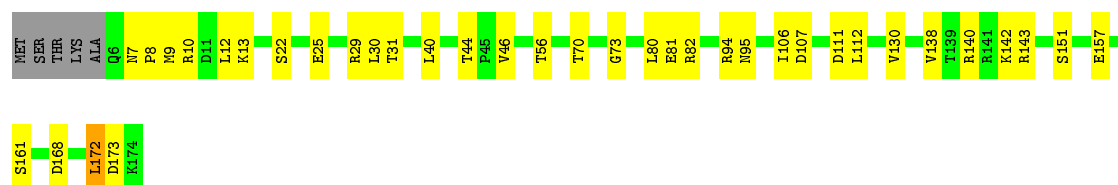




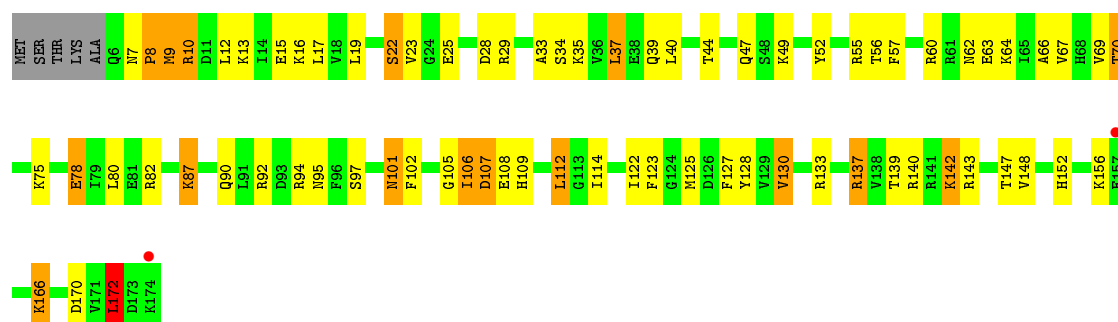
• Molecule 12: 60S ribosomal protein L10



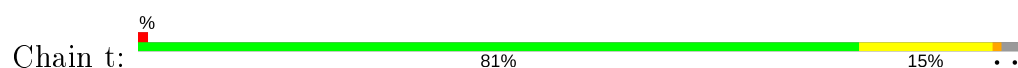
• Molecule 13: 60S ribosomal protein L11-B

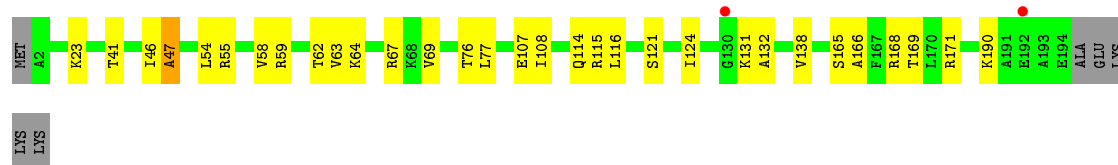


• Molecule 13: 60S ribosomal protein L11-B

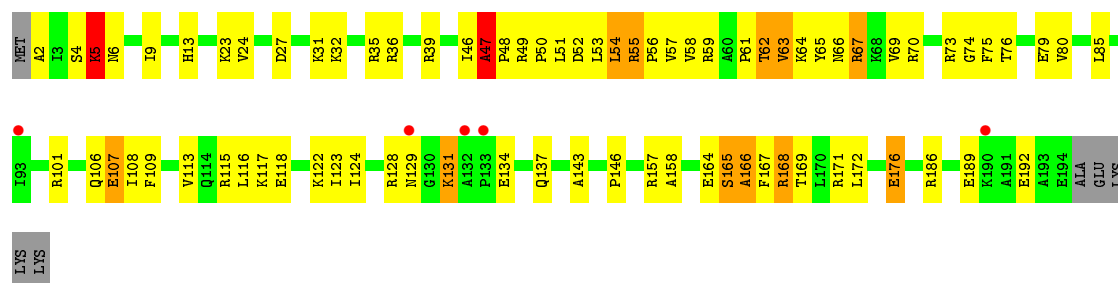


• Molecule 14: 60S ribosomal protein L13-A

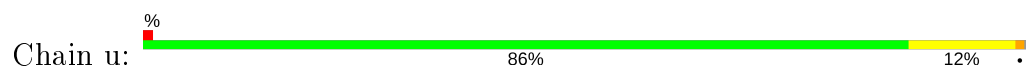




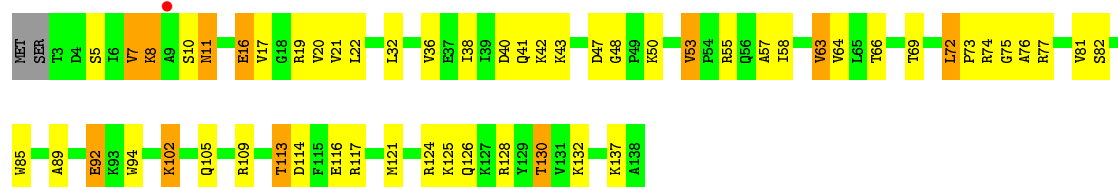
- Molecule 14: 60S ribosomal protein L13-A



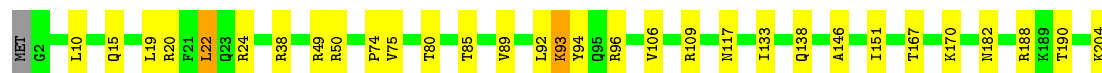
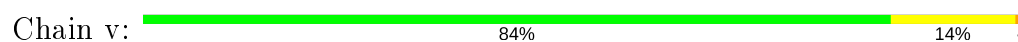
- Molecule 15: 60S ribosomal protein L14-A



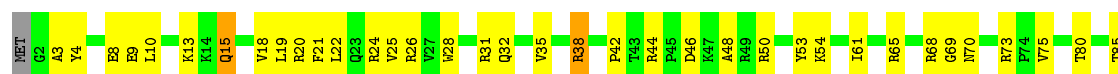
- Molecule 15: 60S ribosomal protein L14-A

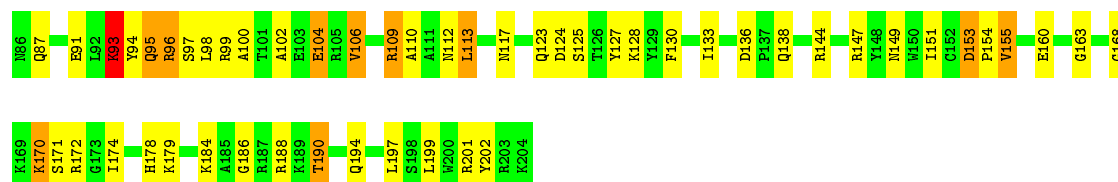


- Molecule 16: 60S ribosomal protein L15-A

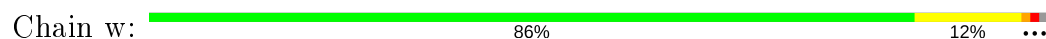


- Molecule 16: 60S ribosomal protein L15-A





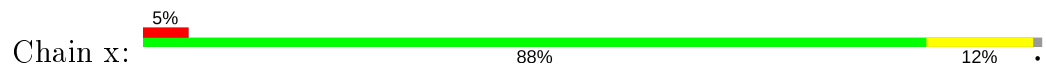
• Molecule 17: 60S ribosomal protein L16-A



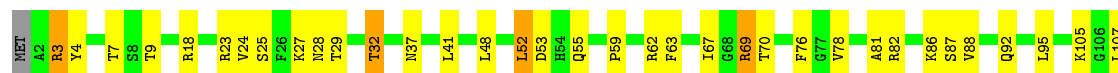
• Molecule 17: 60S ribosomal protein L16-A



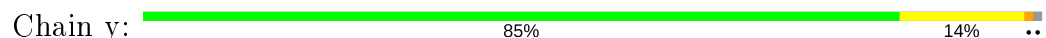
• Molecule 18: 60S ribosomal protein L17-A



• Molecule 18: 60S ribosomal protein L17-A



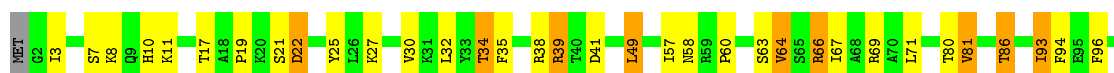
• Molecule 19: 60S ribosomal protein L18-A





- Molecule 19: 60S ribosomal protein L18-A

Chain CS: 62% 30% 8%



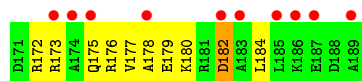
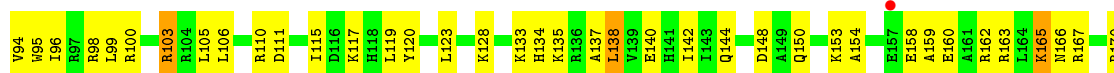
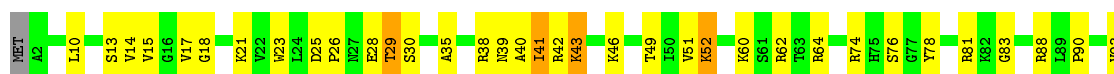
- Molecule 20: 60S ribosomal protein L19-A

Chain z: 4% 90% 10%



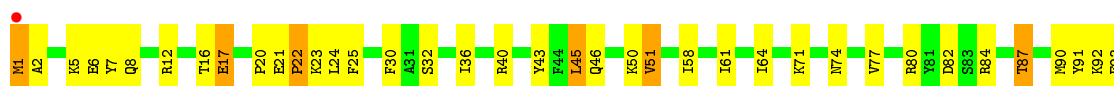
- Molecule 20: 60S ribosomal protein L19-A

Chain CT: 6% 56% 40%



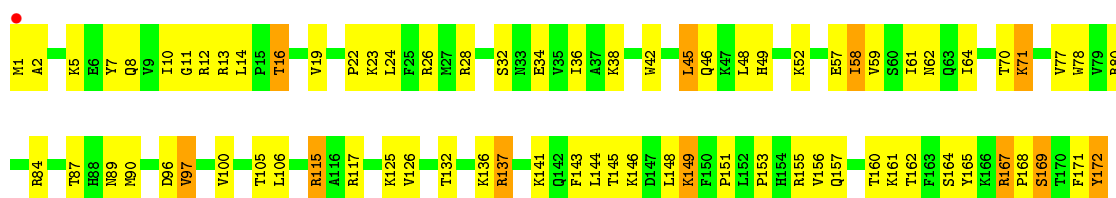
- Molecule 21: 60S ribosomal protein L20-A

Chain 0: % 58% 35% 7%



- Molecule 21: 60S ribosomal protein L20-A

Chain CU: % 56% 38% 6%



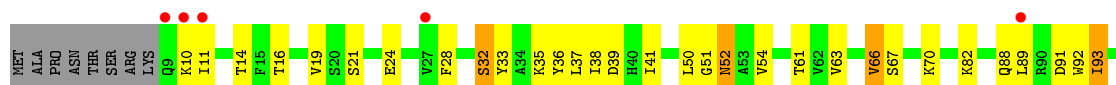
• Molecule 22: 60S ribosomal protein L21-A



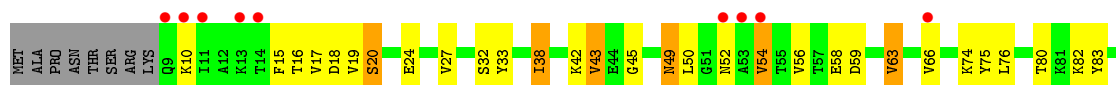
• Molecule 22: 60S ribosomal protein L21-A



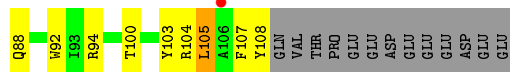
• Molecule 23: 60S ribosomal protein L22-A



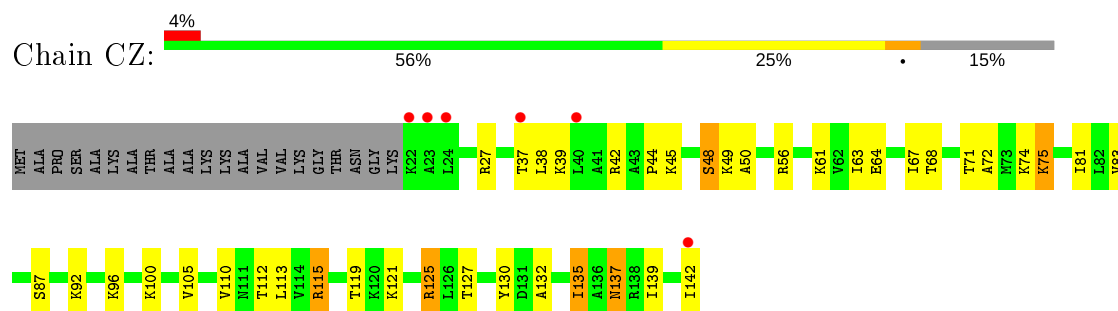
• Molecule 23: 60S ribosomal protein L22-A



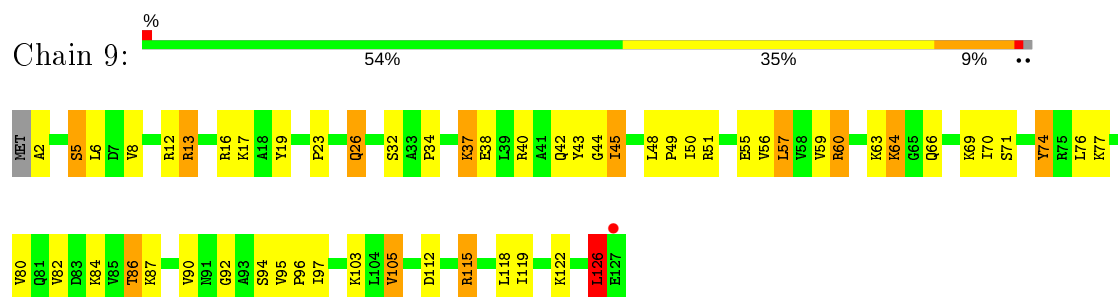
• Molecule 24: 60S ribosomal protein L23-A



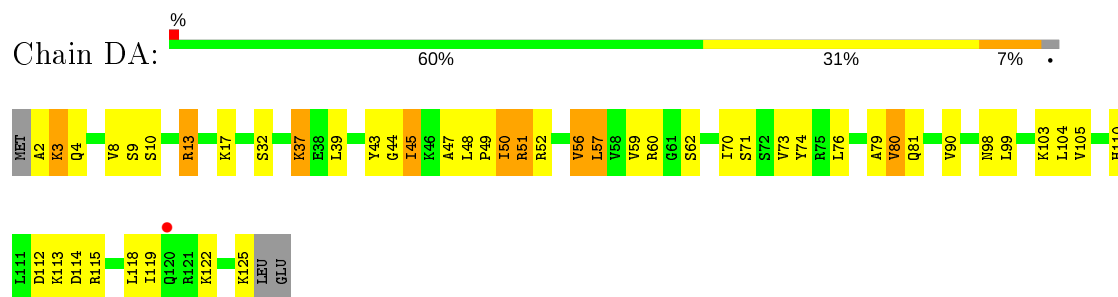
- Molecule 26: 60S ribosomal protein L25



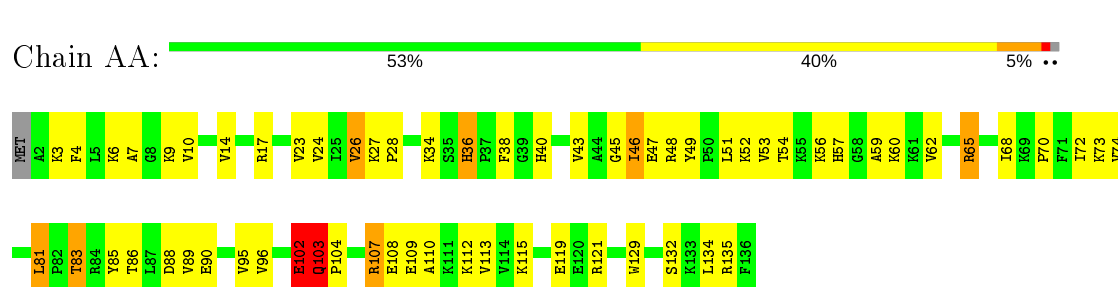
- Molecule 27: 60S ribosomal protein L26-A



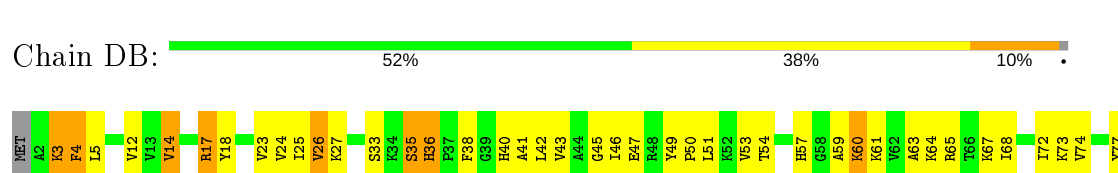
- Molecule 27: 60S ribosomal protein L26-A



- Molecule 28: 60S ribosomal protein L27-A



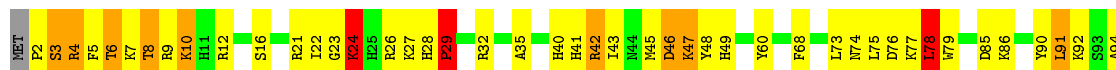
- Molecule 28: 60S ribosomal protein L27-A





- Molecule 29: 60S ribosomal protein L28

Chain AB: 58% 33% 7% ..



- Molecule 29: 60S ribosomal protein L28

Chain DC: 58% 32% 9% .



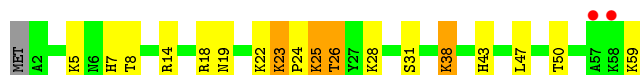
- Molecule 30: 60S ribosomal protein L29

Chain AC: 7% 49% 39% 10% .



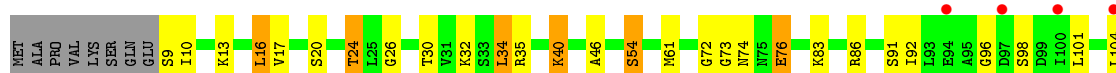
- Molecule 30: 60S ribosomal protein L29

Chain DD: 3% 68% 24% 7% .

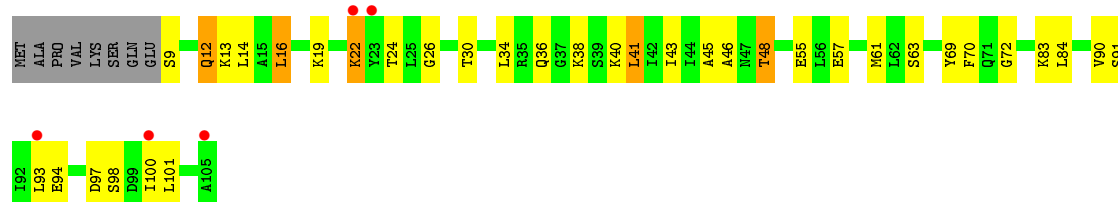


- Molecule 31: 60S ribosomal protein L30

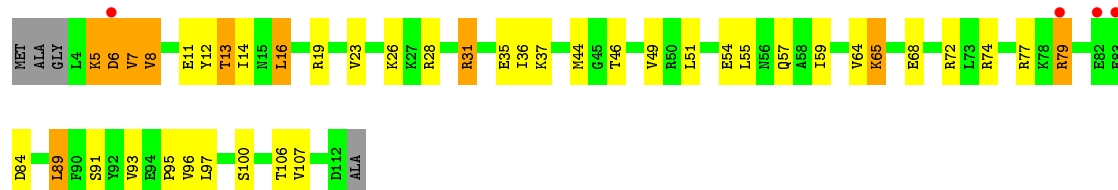
Chain AD: 5% 66% 21% 6% 8%



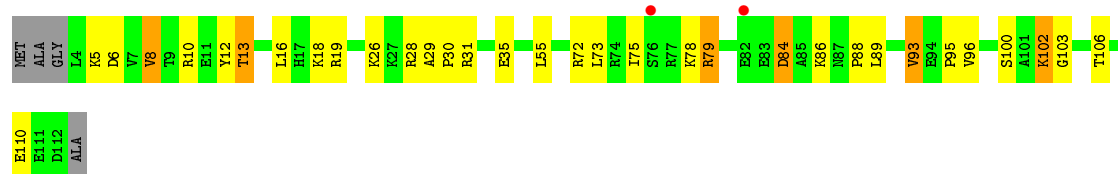
- Molecule 31: 60S ribosomal protein L30



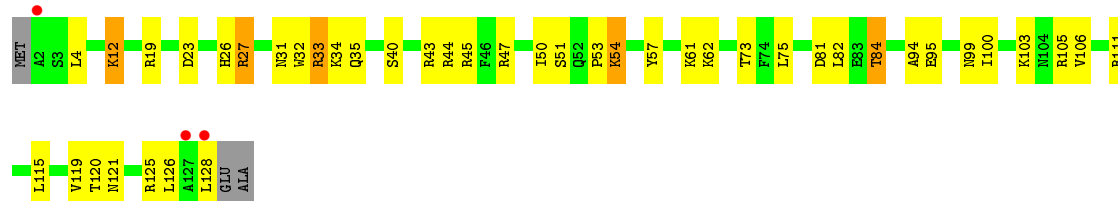
- Molecule 32: 60S ribosomal protein L31-A



- Molecule 32: 60S ribosomal protein L31-A



- Molecule 33: 60S ribosomal protein L32



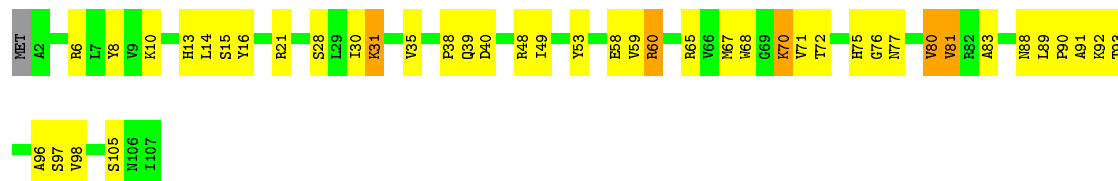
- Molecule 33: 60S ribosomal protein L32





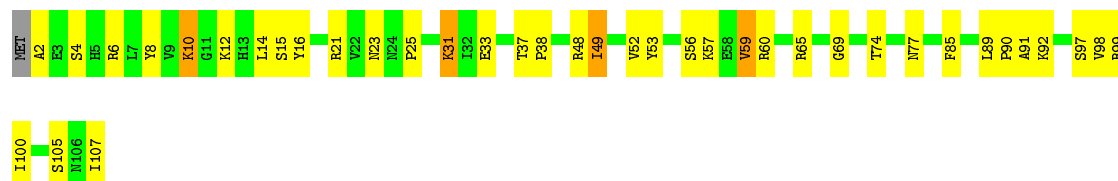
- Molecule 34: 60S ribosomal protein L33-A

Chain AG: 59% 36% 5% .



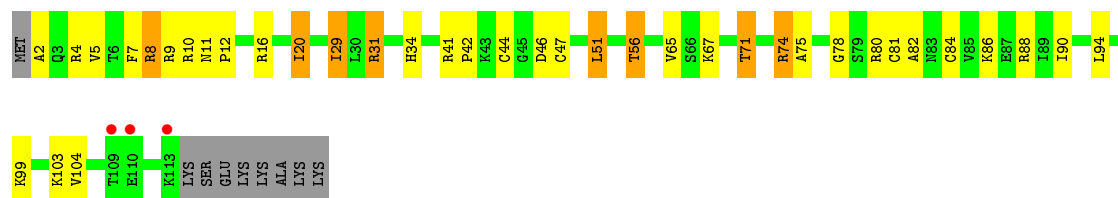
- Molecule 34: 60S ribosomal protein L33-A

Chain DH: 63% 33% . .



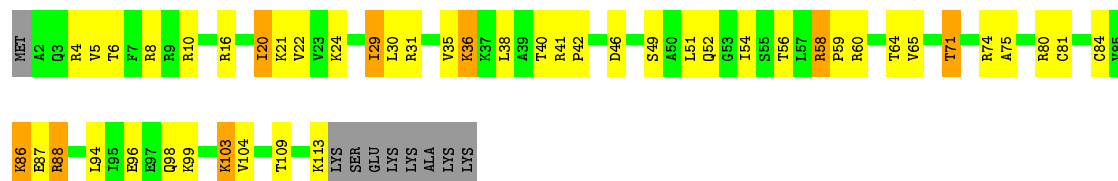
- Molecule 35: 60S ribosomal protein L34-A

Chain AH: 2% 61% 25% 7% 7%



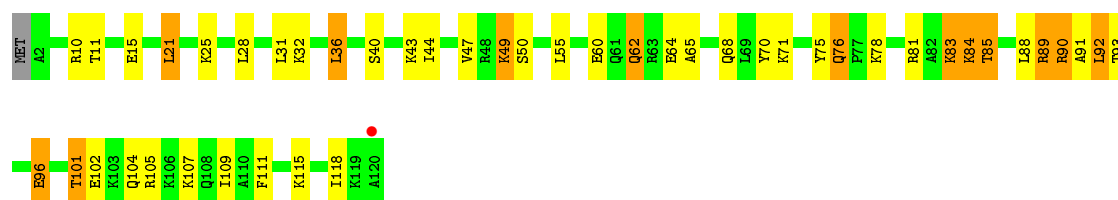
- Molecule 35: 60S ribosomal protein L34-A

Chain DI: 54% 32% 7% 7%

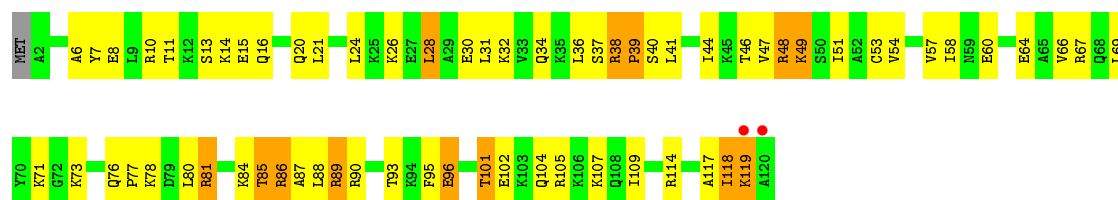
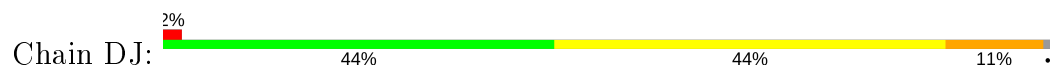


- Molecule 36: 60S ribosomal protein L35-A

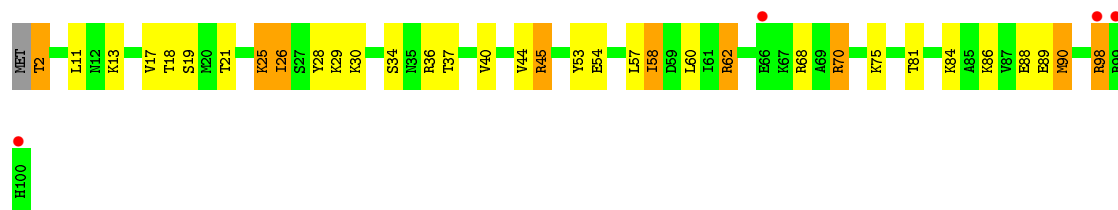
Chain AI: 61% 28% 11%



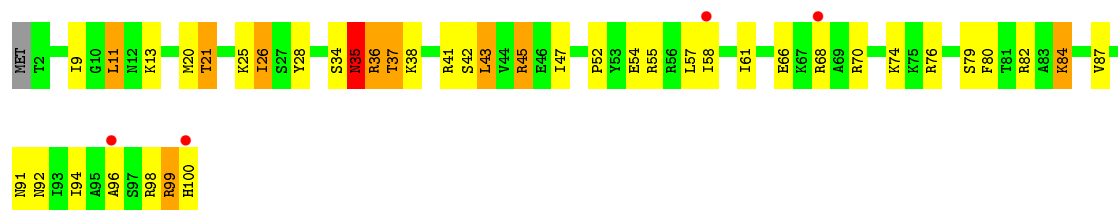
- Molecule 36: 60S ribosomal protein L35-A



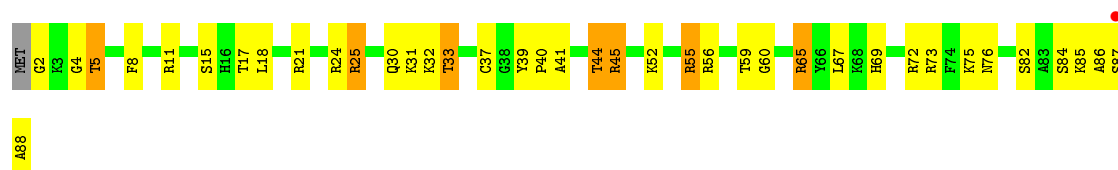
- Molecule 37: 60S ribosomal protein L36-A



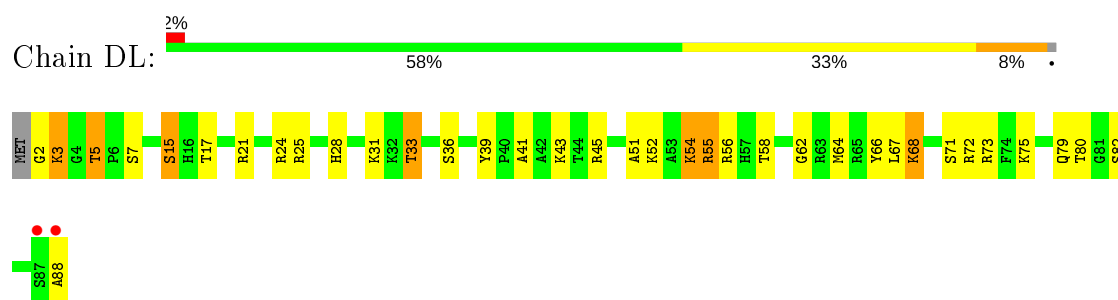
- Molecule 37: 60S ribosomal protein L36-A



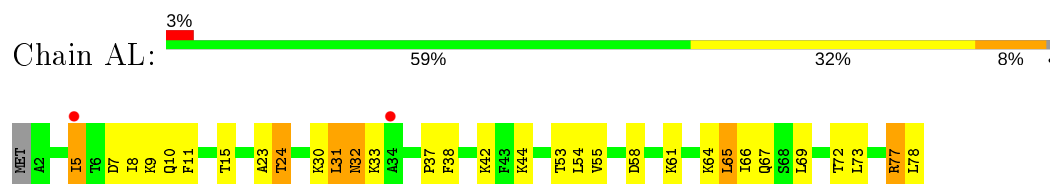
- Molecule 38: 60S ribosomal protein L37-A



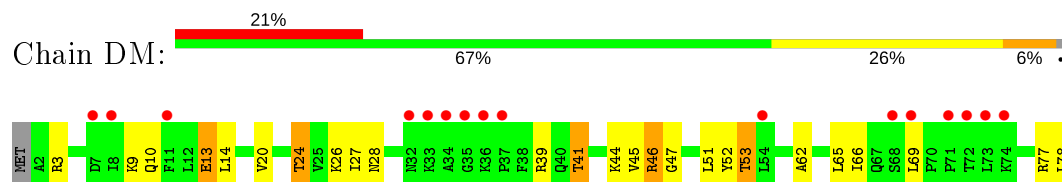
- Molecule 38: 60S ribosomal protein L37-A



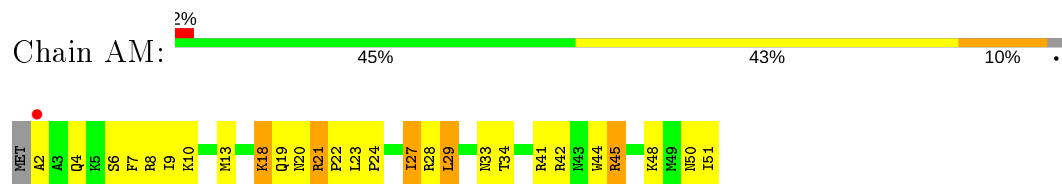
- Molecule 39: 60S ribosomal protein L38



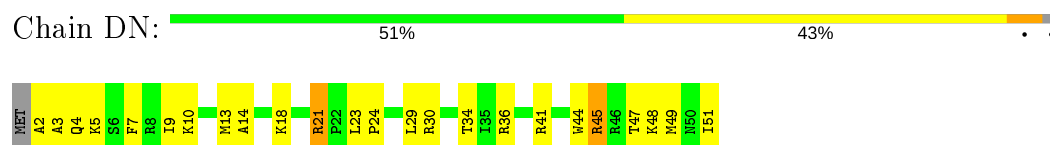
- Molecule 39: 60S ribosomal protein L38



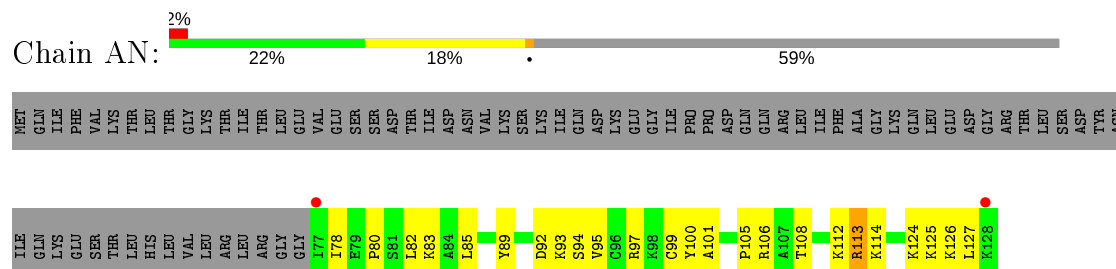
- Molecule 40: 60S ribosomal protein L39



- Molecule 40: 60S ribosomal protein L39



- Molecule 41: Ubiquitin-60S ribosomal protein L40



- Molecule 41: Ubiquitin-60S ribosomal protein L40



- Molecule 42: 60S ribosomal protein L41-B



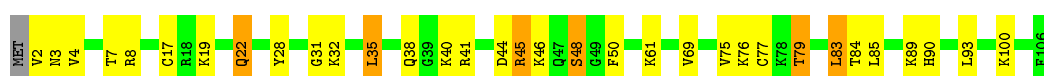
- Molecule 42: 60S ribosomal protein L41-B



- Molecule 43: 60S ribosomal protein L42-A



- Molecule 43: 60S ribosomal protein L42-A

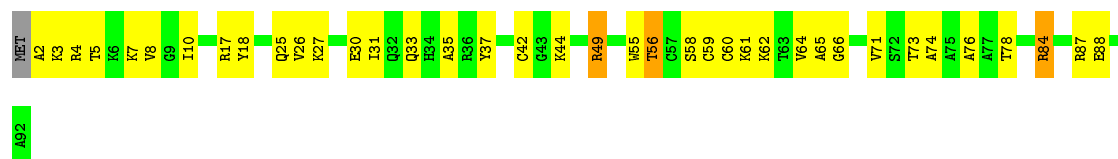


- Molecule 44: 60S ribosomal protein L43-A

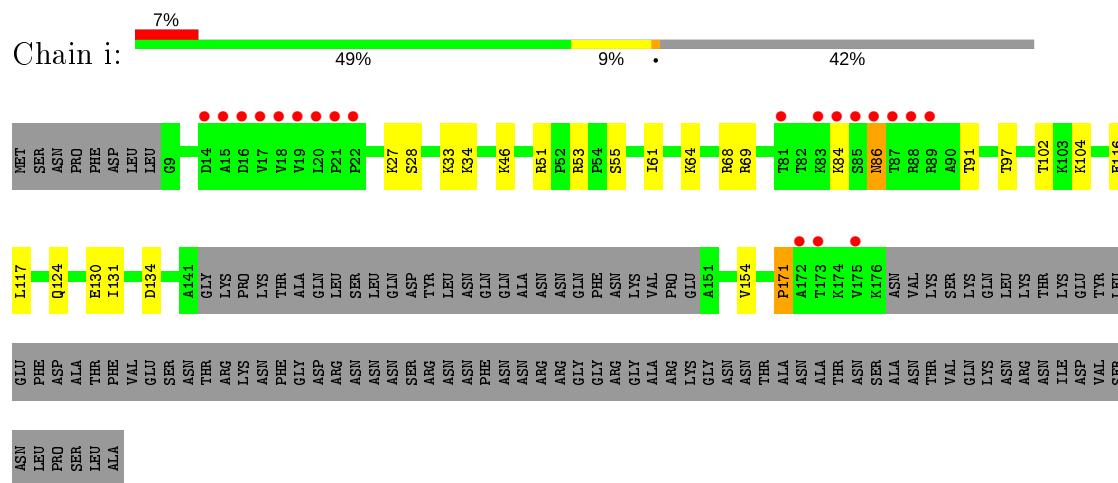


- Molecule 44: 60S ribosomal protein L43-A

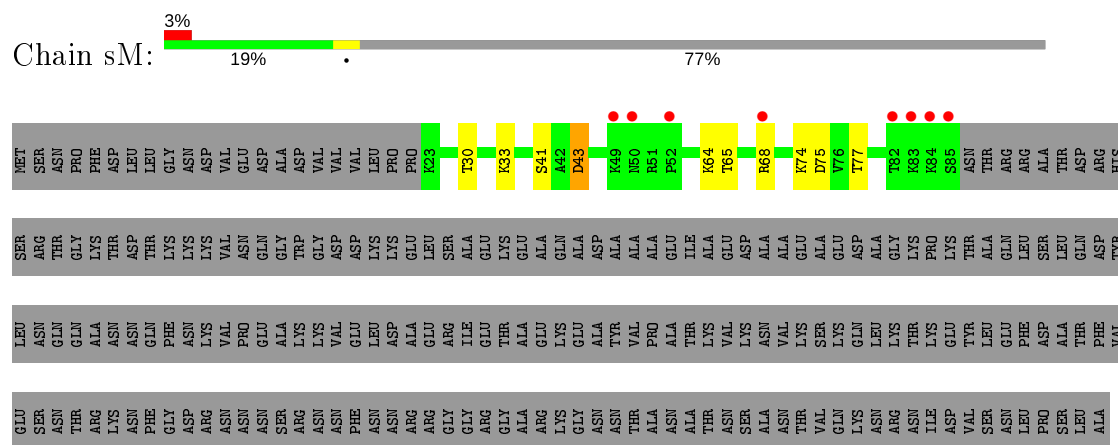




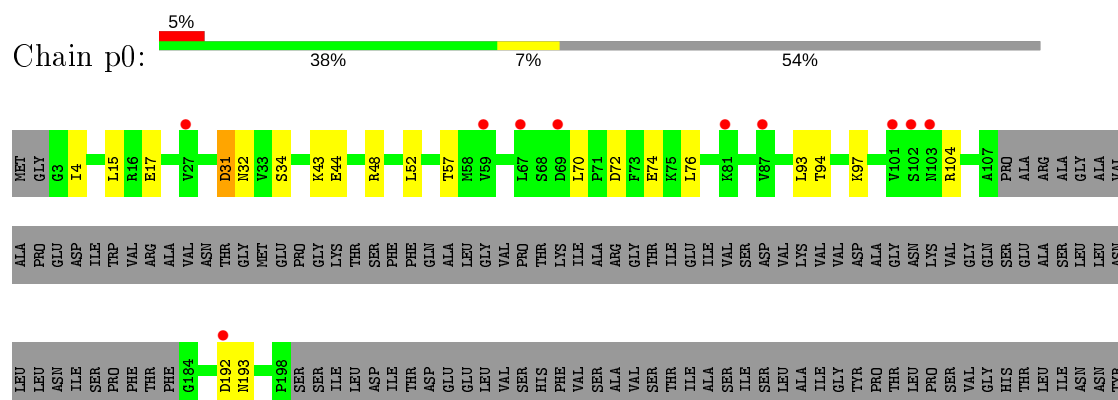
• Molecule 45: Suppressor protein STM1

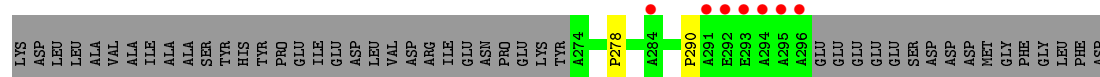


• Molecule 45: Suppressor protein STM1

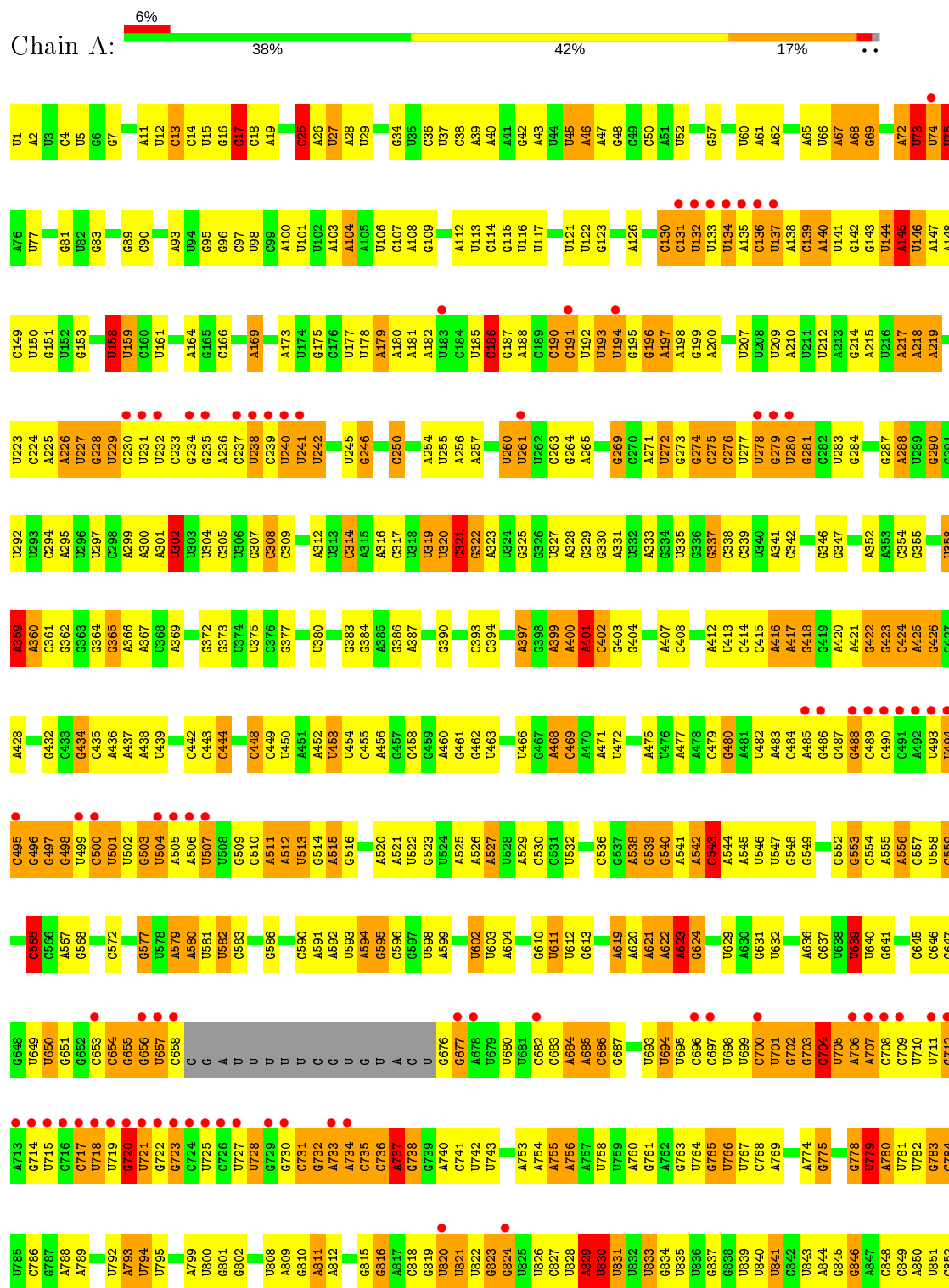


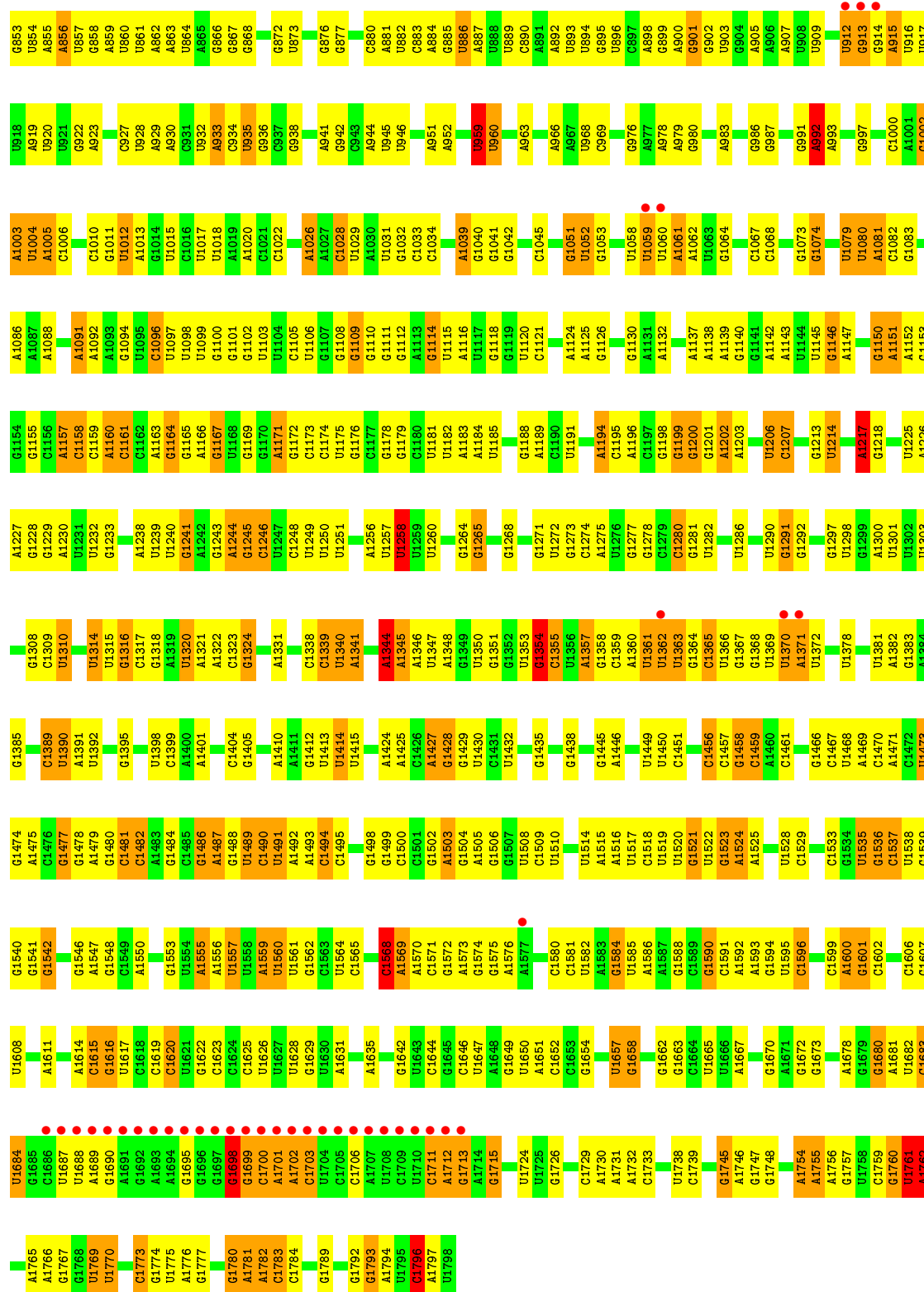
• Molecule 46: 60S acidic ribosomal protein P0

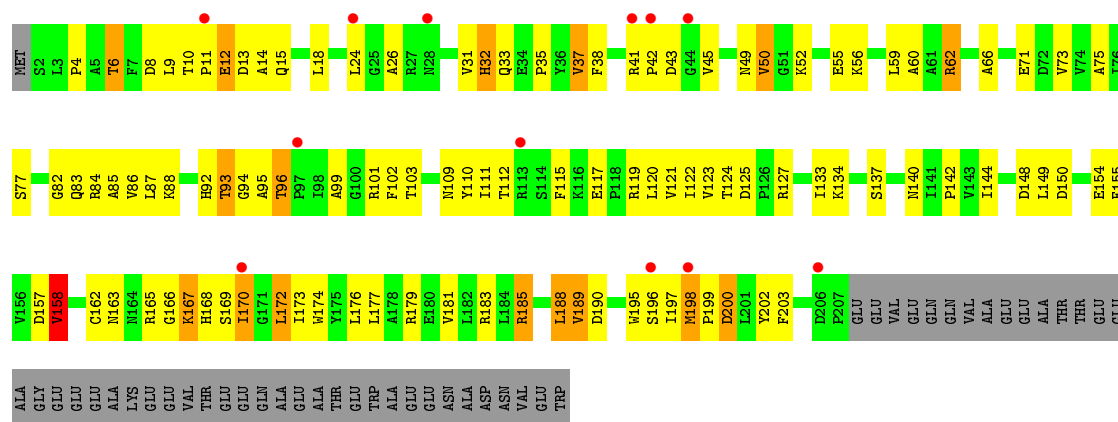




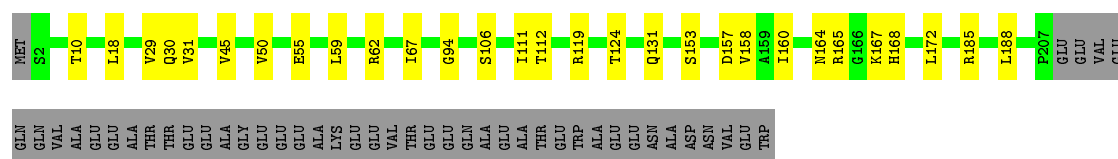
• Molecule 47: 18S ribosomal RNA



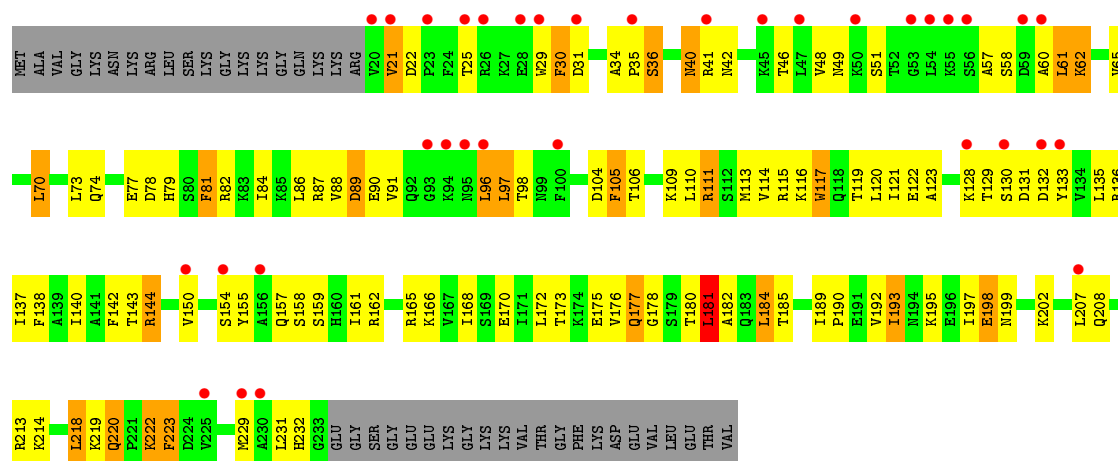




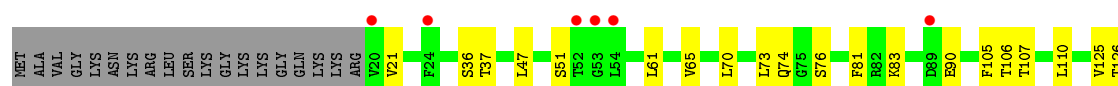
• Molecule 48: 40S ribosomal protein S0-A

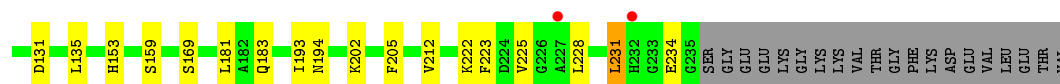


• Molecule 49: 40S ribosomal protein S1-A



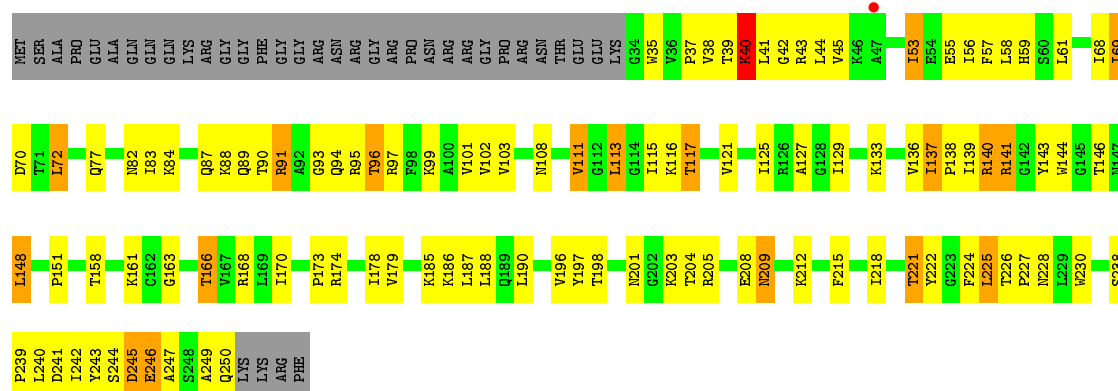
• Molecule 49: 40S ribosomal protein S1-A





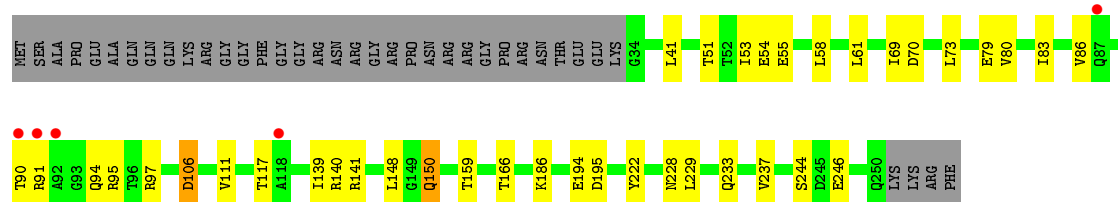
- Molecule 50: 40S ribosomal protein S2

Chain D: 43% 35% 7% 15%



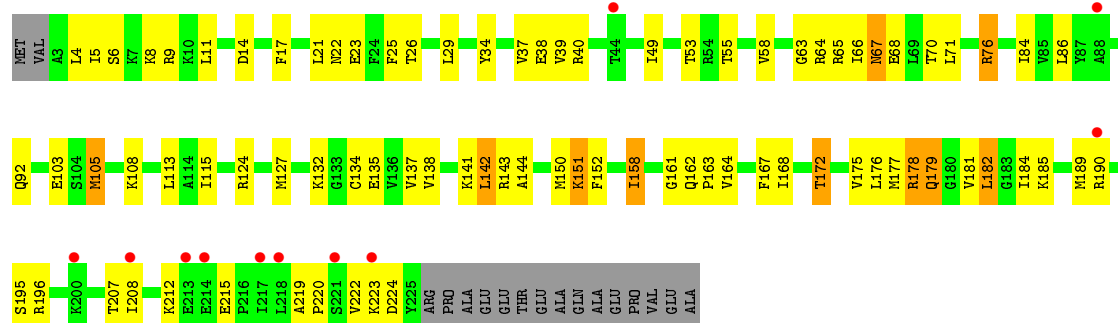
- Molecule 50: 40S ribosomal protein S2

Chain s2: 2% 70% 15% 15%



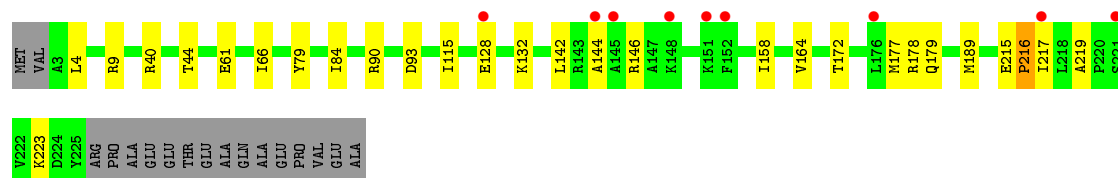
- Molecule 51: 40S ribosomal protein S3

Chain E: 5% 58% 31% 7%

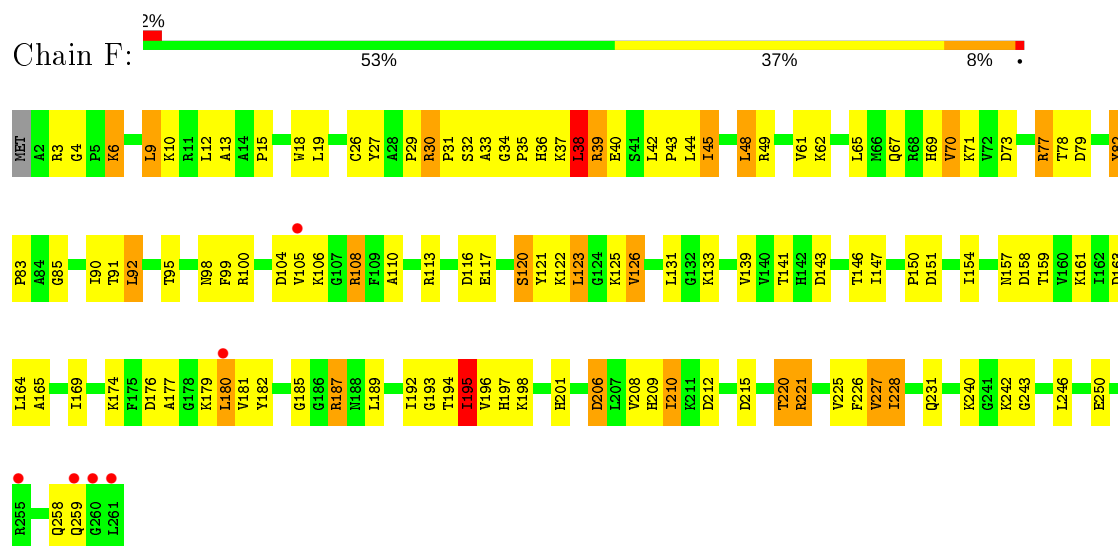


- Molecule 51: 40S ribosomal protein S3

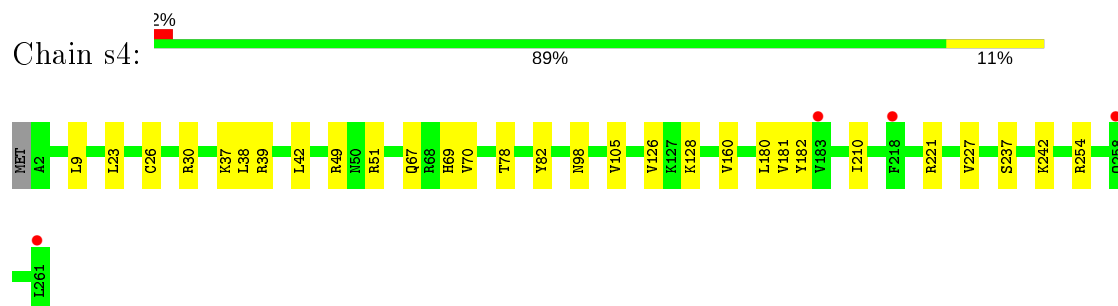
Chain s3: 4% 81% 11% 7%



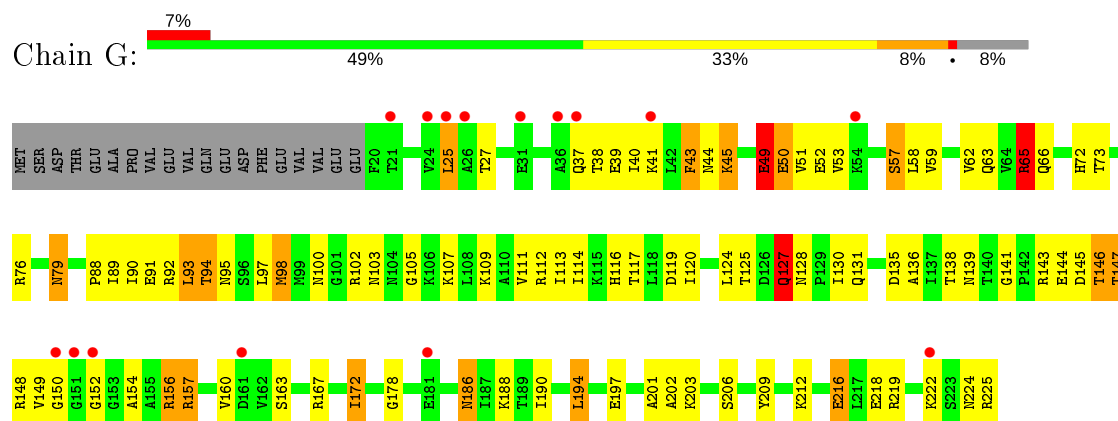
- Molecule 52: 40S ribosomal protein S4-A



- Molecule 52: 40S ribosomal protein S4-A

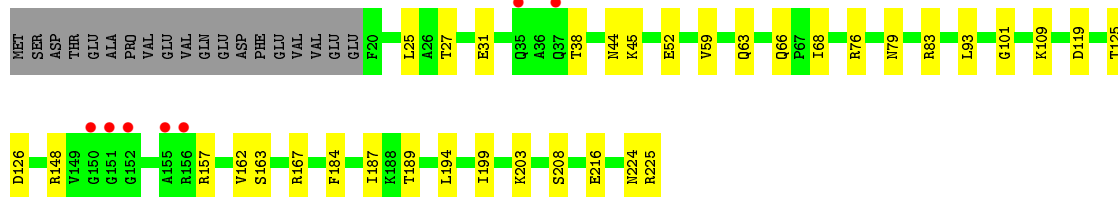


- Molecule 53: 40S ribosomal protein S5



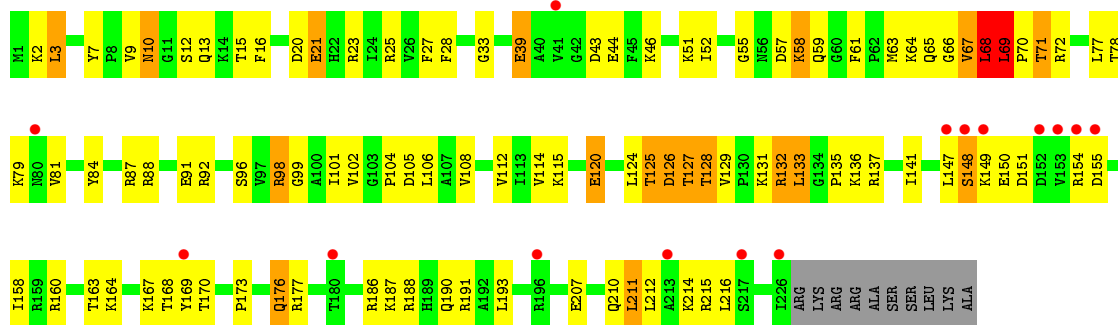
- Molecule 53: 40S ribosomal protein S5

Chain s5:



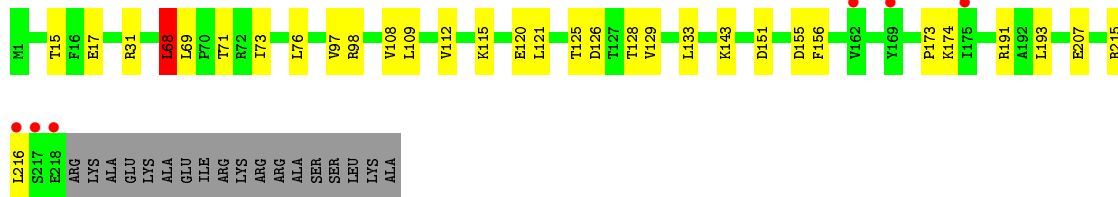
- Molecule 54: 40S ribosomal protein S6-A

Chain H:



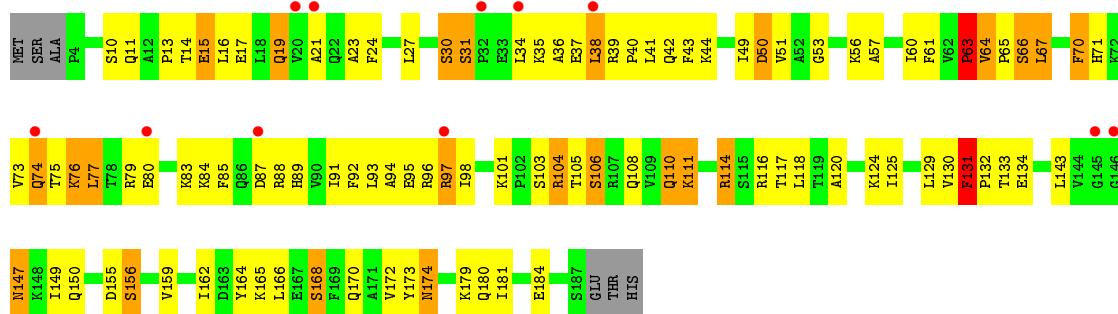
- Molecule 54: 40S ribosomal protein S6-A

Chain s6:

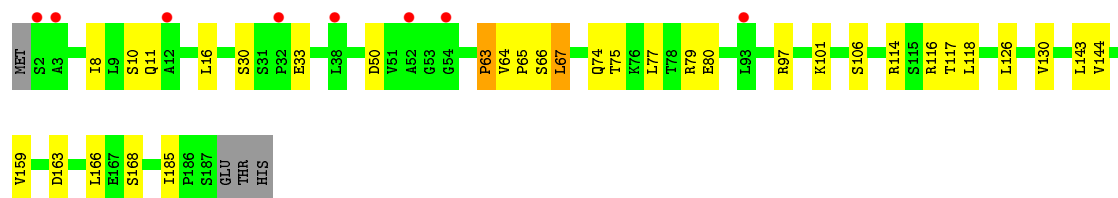
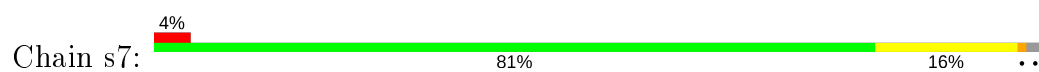


- Molecule 55: 40S ribosomal protein S7-A

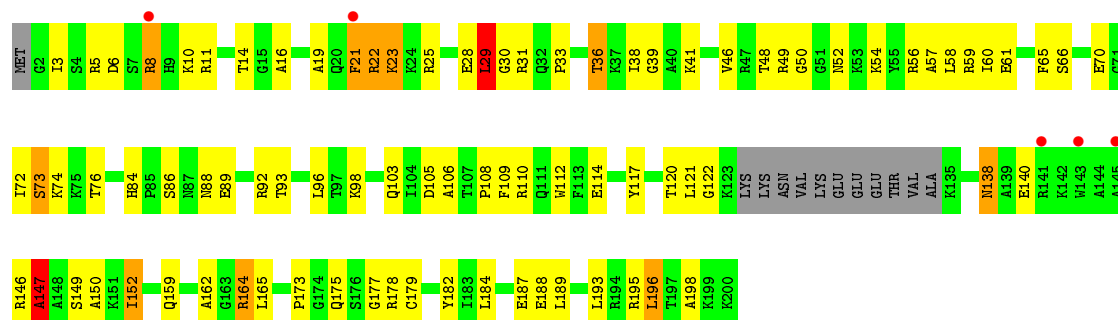
Chain I:



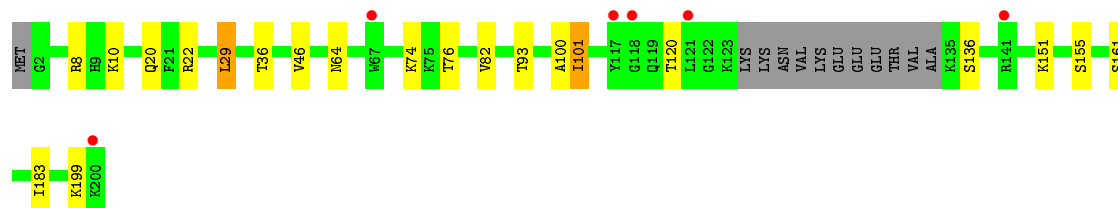
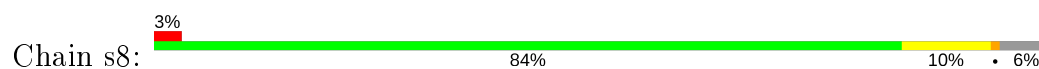
- Molecule 55: 40S ribosomal protein S7-A



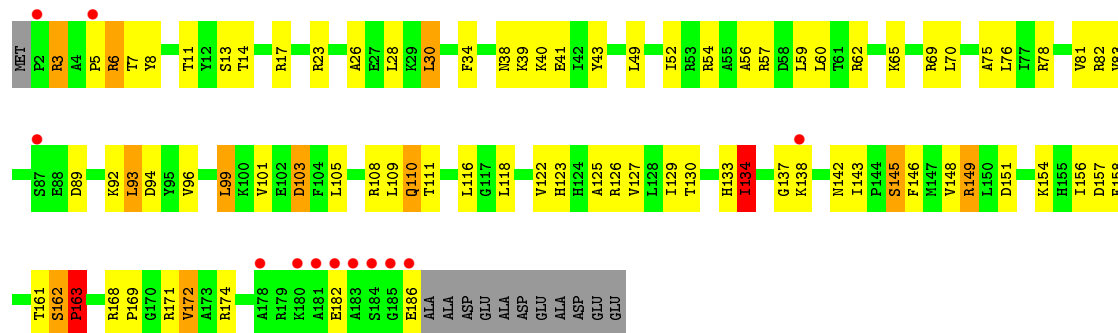
- Molecule 56: 40S ribosomal protein S8-A



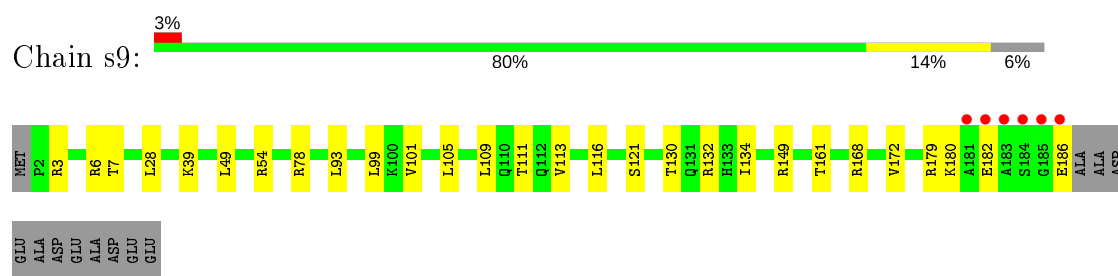
- Molecule 56: 40S ribosomal protein S8-A



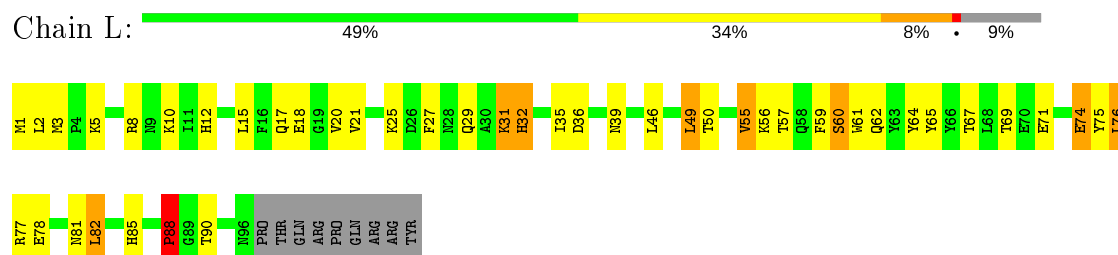
- Molecule 57: 40S ribosomal protein S9-A



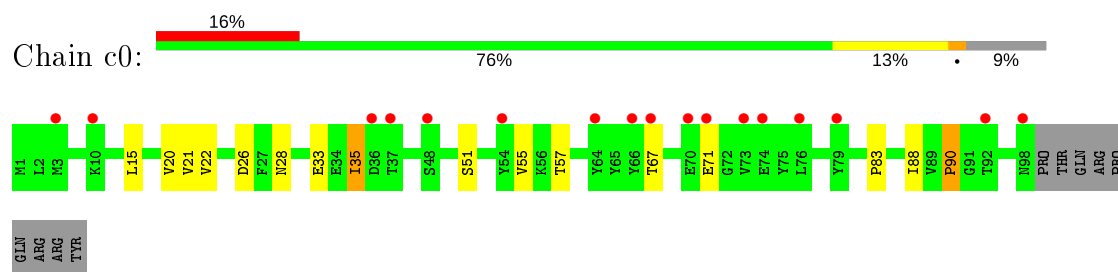
- Molecule 57: 40S ribosomal protein S9-A



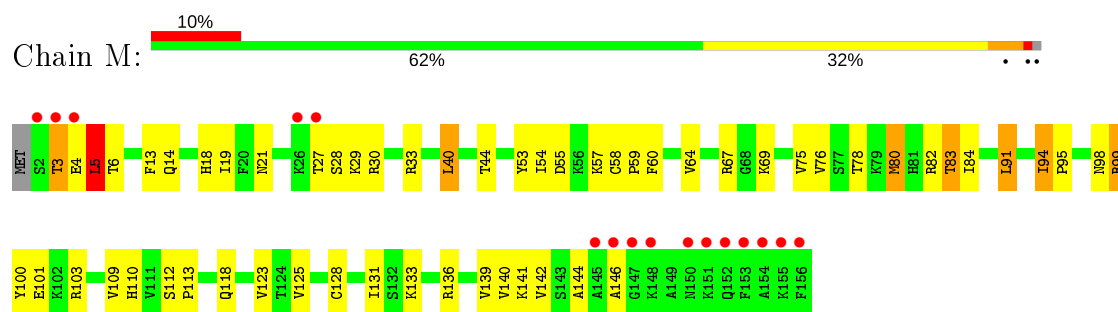
- Molecule 58: 40S ribosomal protein S10-A



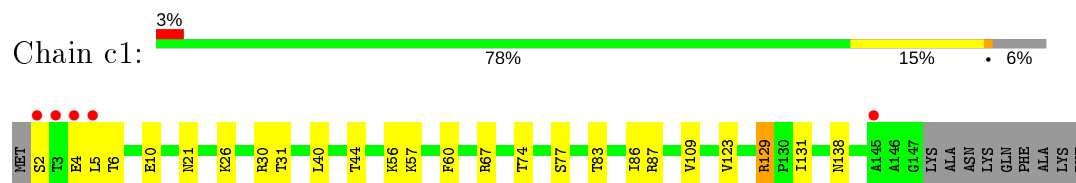
- Molecule 58: 40S ribosomal protein S10-A



- Molecule 59: 40S ribosomal protein S11-A

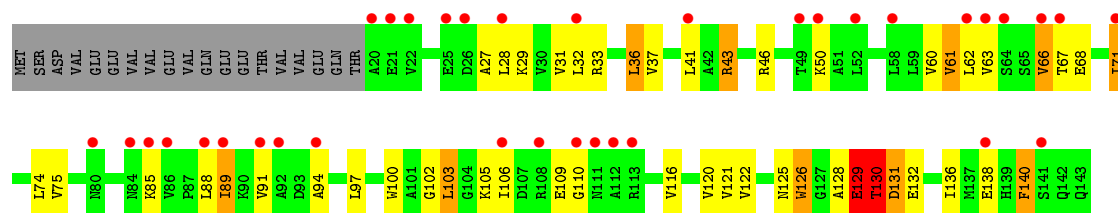


- Molecule 59: 40S ribosomal protein S11-A

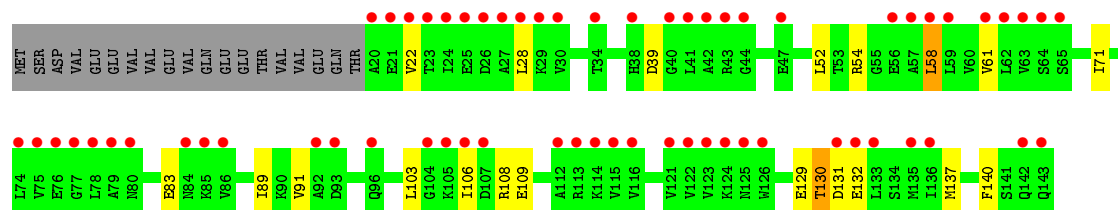
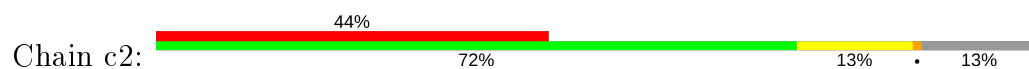


- Molecule 60: 40S ribosomal protein S12

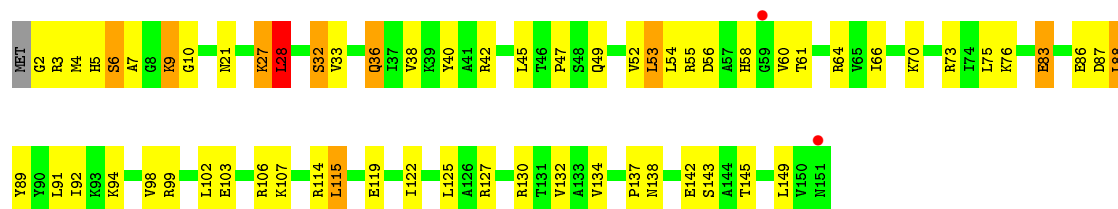




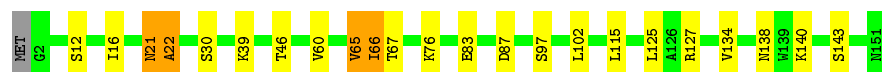
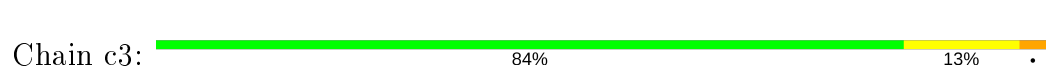
- Molecule 60: 40S ribosomal protein S12



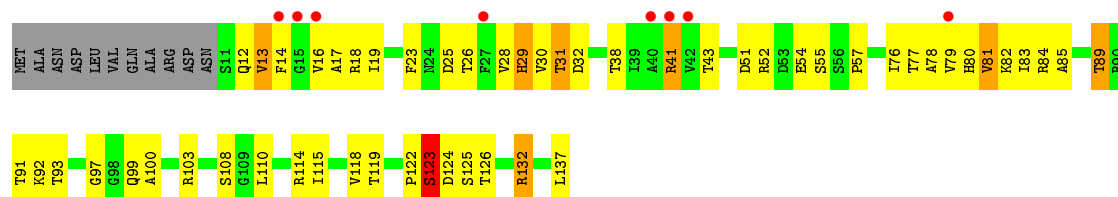
- Molecule 61: 40S ribosomal protein S13



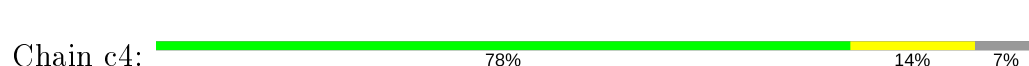
- Molecule 61: 40S ribosomal protein S13

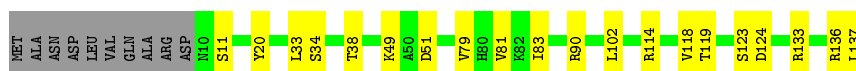


- Molecule 62: 40S ribosomal protein S14-B

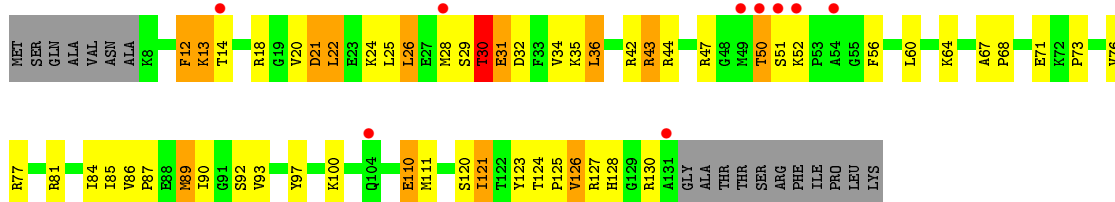


- Molecule 62: 40S ribosomal protein S14-B

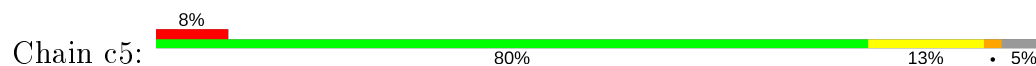




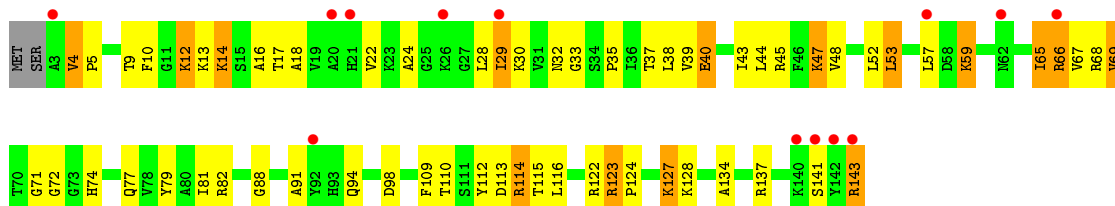
- Molecule 63: 40S ribosomal protein S15



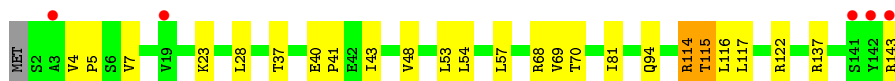
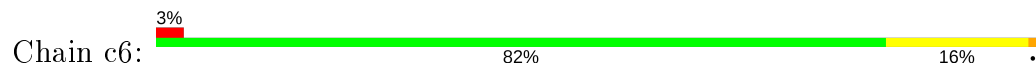
- Molecule 63: 40S ribosomal protein S15



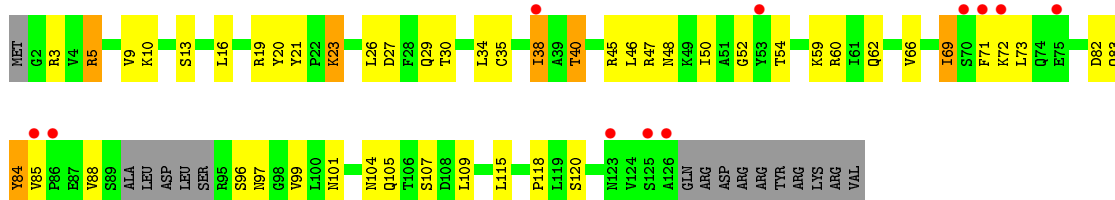
- Molecule 64: 40S ribosomal protein S16-A



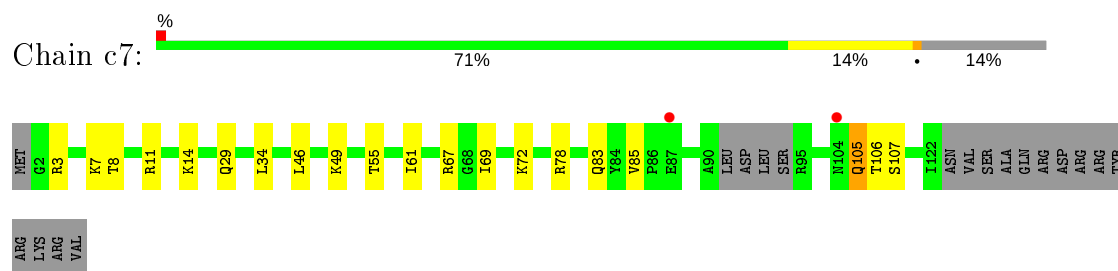
- Molecule 64: 40S ribosomal protein S16-A



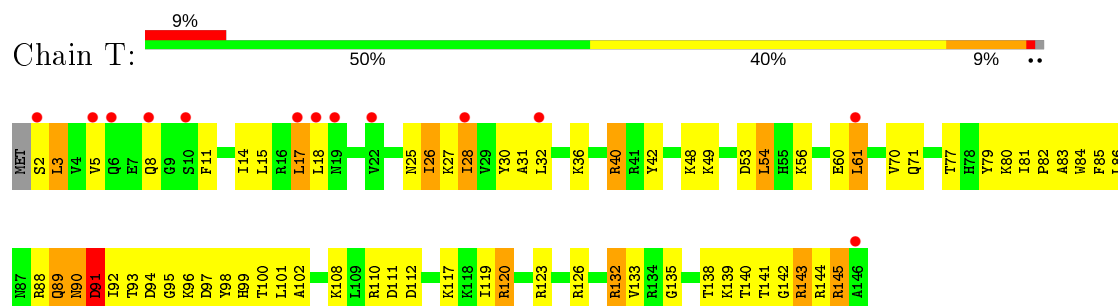
- Molecule 65: 40S ribosomal protein S17-A



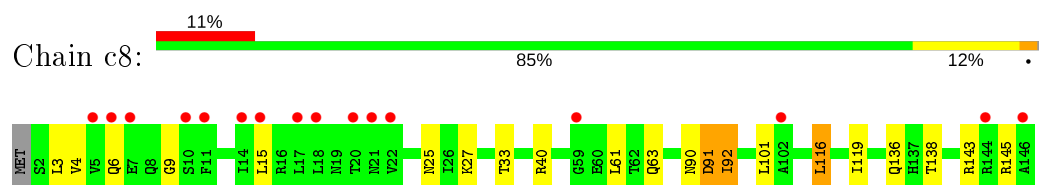
- Molecule 65: 40S ribosomal protein S17-A



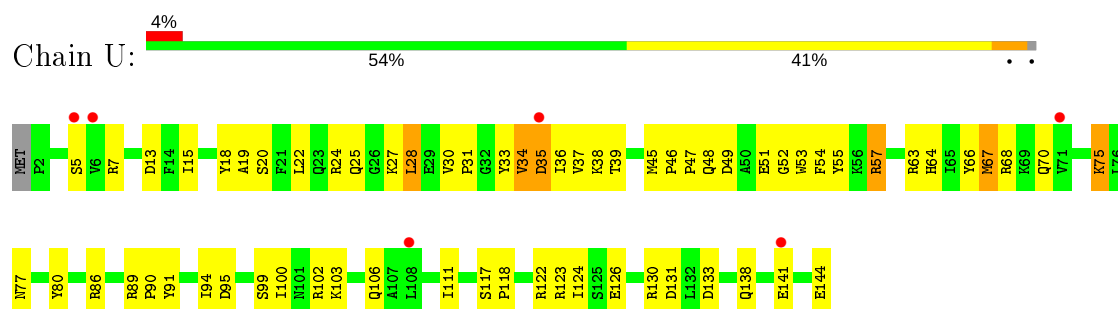
- Molecule 66: 40S ribosomal protein S18-A



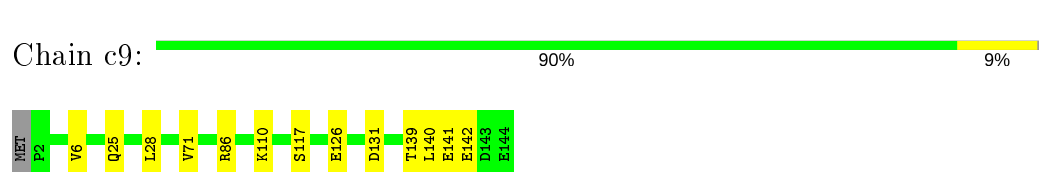
- Molecule 66: 40S ribosomal protein S18-A



- Molecule 67: 40S ribosomal protein S19-A

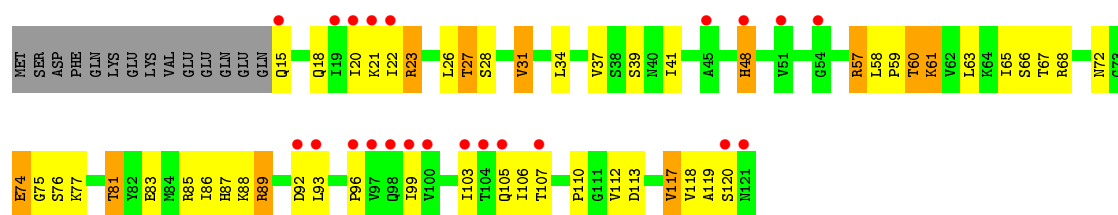


- Molecule 67: 40S ribosomal protein S19-A

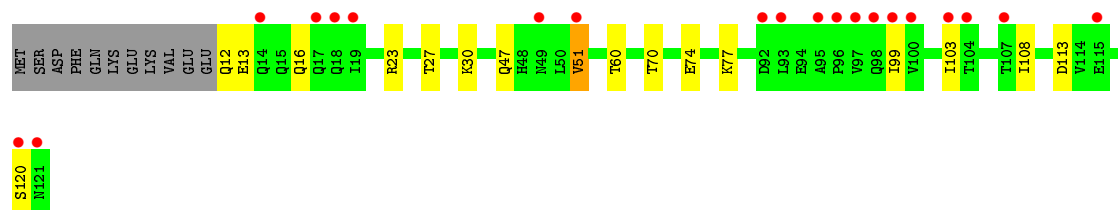
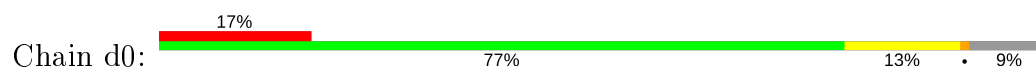


- Molecule 68: 40S ribosomal protein S20

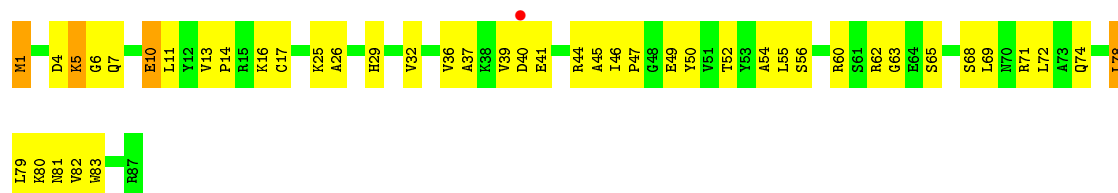




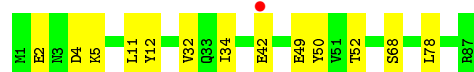
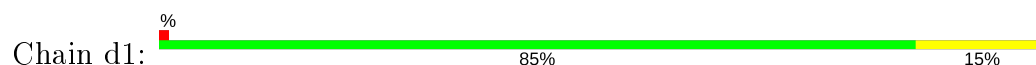
- Molecule 68: 40S ribosomal protein S20



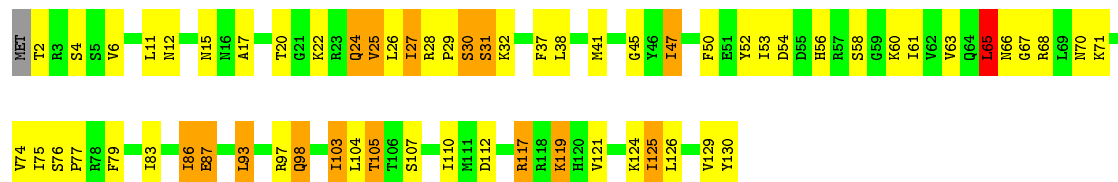
- Molecule 69: 40S ribosomal protein S21-A



- Molecule 69: 40S ribosomal protein S21-A



- Molecule 70: 40S ribosomal protein S22-A



- Molecule 70: 40S ribosomal protein S22-A

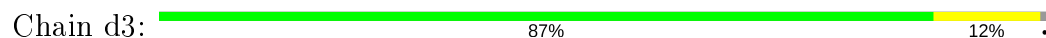




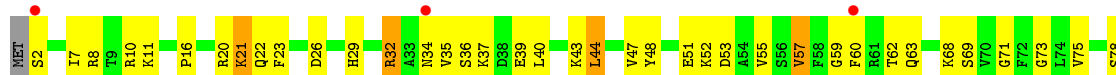
- Molecule 71: 40S ribosomal protein S23-A



- Molecule 71: 40S ribosomal protein S23-A



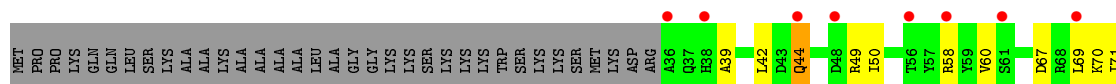
- Molecule 72: 40S ribosomal protein S24-A



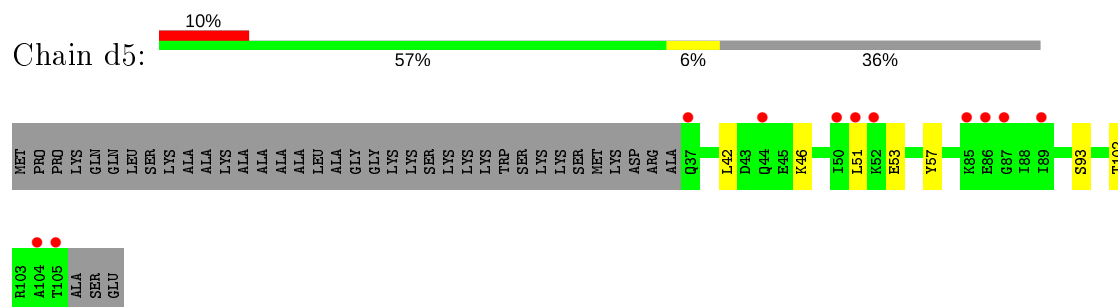
- Molecule 72: 40S ribosomal protein S24-A



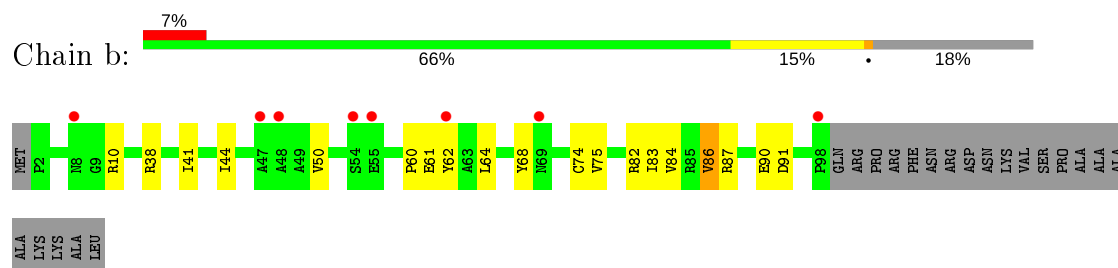
- Molecule 73: 40S ribosomal protein S25-A



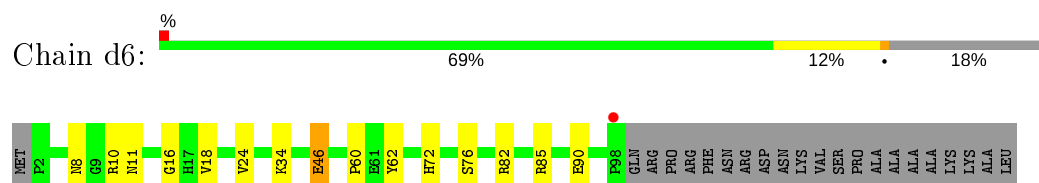
- Molecule 73: 40S ribosomal protein S25-A



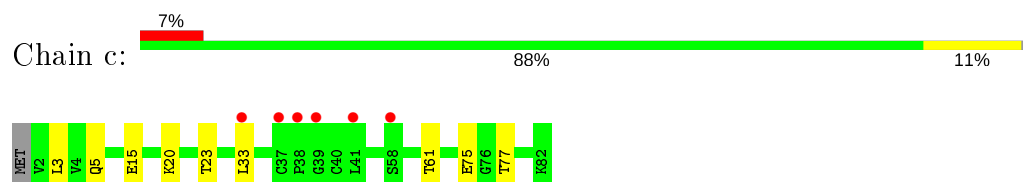
- Molecule 74: 40S ribosomal protein S26-B



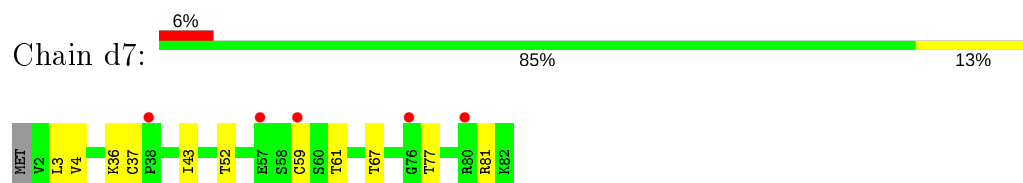
- Molecule 74: 40S ribosomal protein S26-B



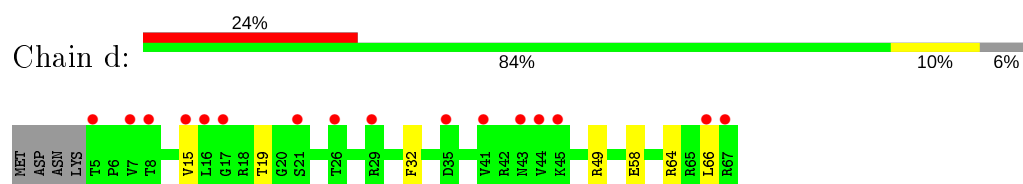
- Molecule 75: 40S ribosomal protein S27-A



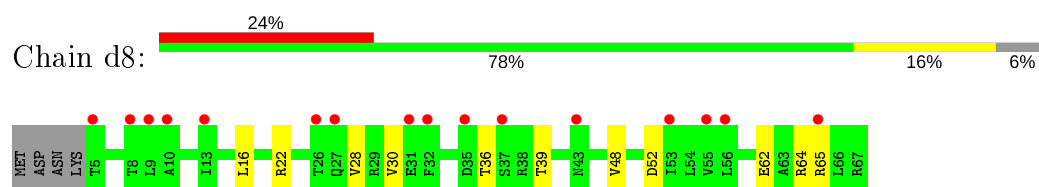
- Molecule 75: 40S ribosomal protein S27-A



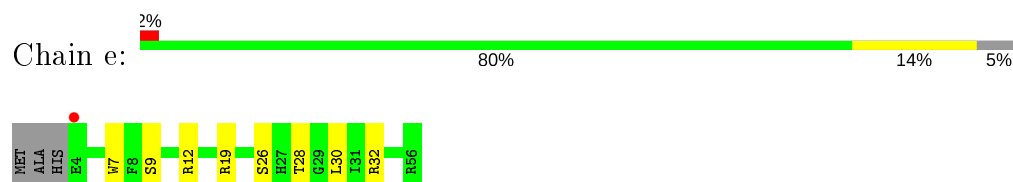
- Molecule 76: 40S ribosomal protein S28-A



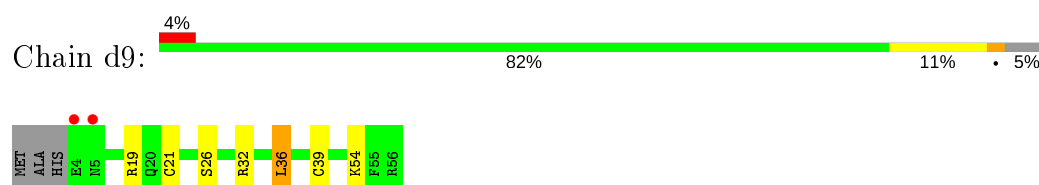
- Molecule 76: 40S ribosomal protein S28-A



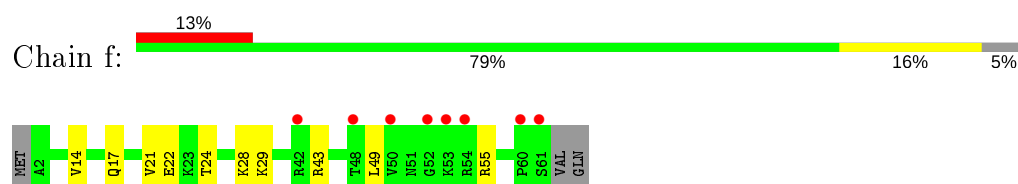
- Molecule 77: 40S ribosomal protein S29-A



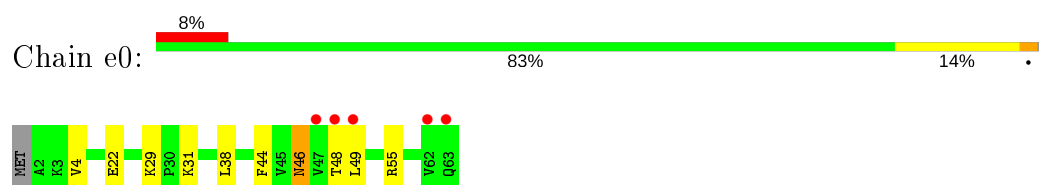
- Molecule 77: 40S ribosomal protein S29-A



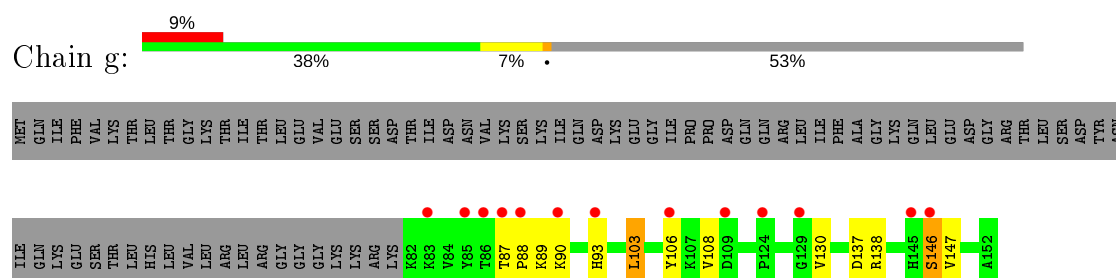
- Molecule 78: 40S ribosomal protein S30-A



- Molecule 78: 40S ribosomal protein S30-A

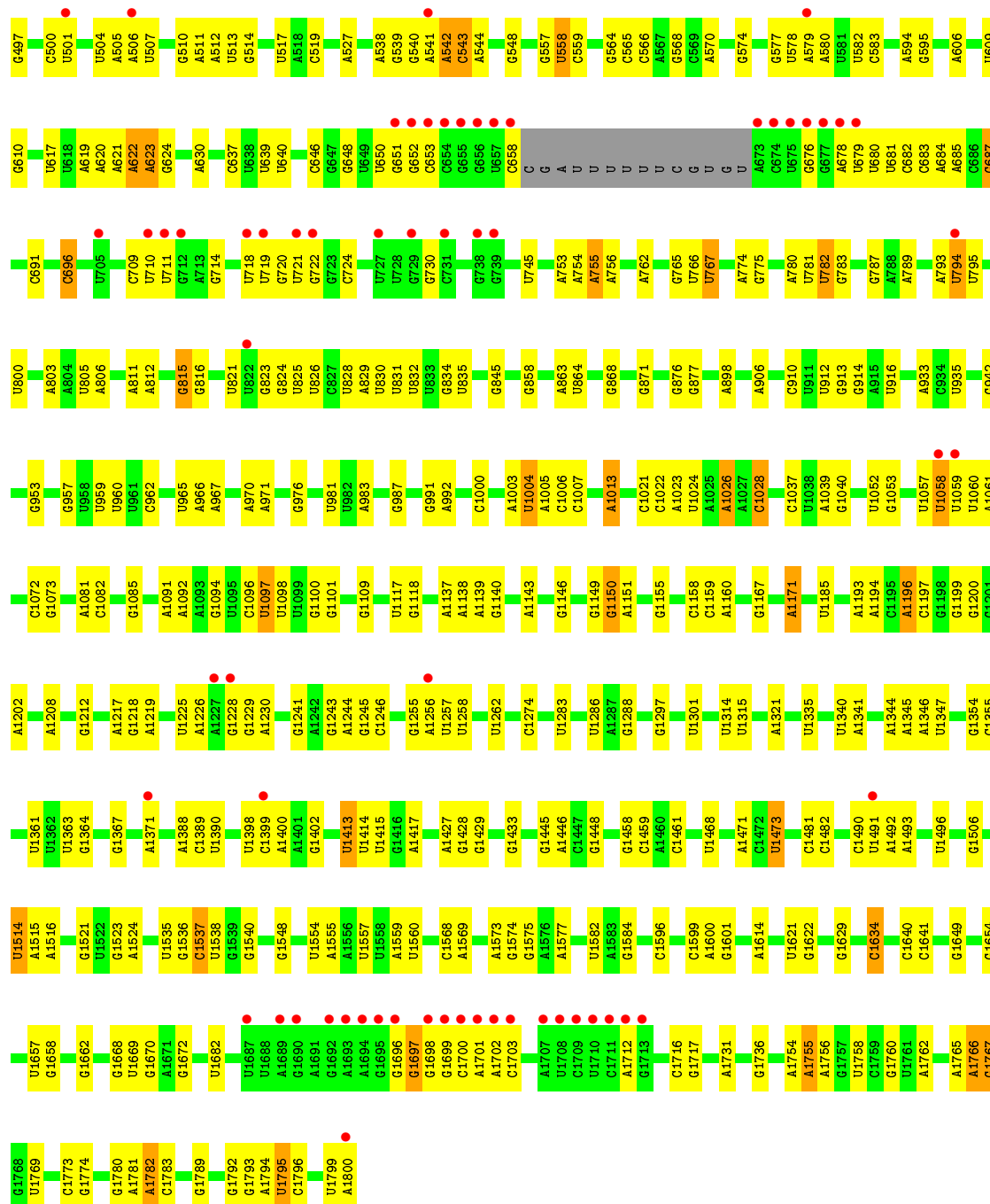


- Molecule 79: Ubiquitin-40S ribosomal protein S31



- Molecule 79: Ubiquitin-40S ribosomal protein S31





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	303.77Å 287.95Å 435.45Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	54.71 – 3.10 54.71 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.71-3.10) 100.0 (54.71-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.13Å)	Xtriage
Refinement program	PHENIX dev_2450, PHENIX dev_2450	Depositor
R, R_{free}	0.217 , 0.264 0.217 , 0.265	Depositor DCC
R_{free} test set	26494 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	409486	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, OHX, MG, G5B

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	1.00	49/75394 (0.1%)	1.43	925/117545 (0.8%)
1	AR	1.04	61/75347 (0.1%)	1.44	947/117472 (0.8%)
2	3	0.82	0/2883	1.25	7/4491 (0.2%)
2	AS	0.97	2/2883 (0.1%)	1.37	16/4491 (0.4%)
3	4	0.96	0/3746	1.35	28/5832 (0.5%)
3	AT	0.88	2/3746 (0.1%)	1.28	17/5832 (0.3%)
4	CD	0.54	0/1948	0.72	0/2617
4	j	0.54	0/1948	0.74	1/2617 (0.0%)
5	CE	0.63	0/3146	0.74	1/4228 (0.0%)
5	k	0.55	0/3146	0.70	1/4228 (0.0%)
6	CF	0.59	1/2800 (0.0%)	0.74	2/3790 (0.1%)
6	l	0.62	1/2800 (0.0%)	0.79	2/3790 (0.1%)
7	CG	0.61	1/2425 (0.0%)	0.69	0/3271
7	m	0.46	0/2425	0.64	0/3271
8	CH	0.60	0/1260	0.71	1/1694 (0.1%)
8	n	0.59	0/1260	0.69	1/1694 (0.1%)
9	CI	0.63	0/1821	0.73	2/2451 (0.1%)
9	o	0.59	0/1821	0.74	0/2451
10	CJ	0.44	0/1836	0.59	0/2481
10	p	0.47	0/1836	0.59	1/2481 (0.0%)
11	CK	0.56	0/1539	0.68	0/2073
11	q	0.53	0/1539	0.66	0/2073
12	CL	0.58	1/1741 (0.1%)	0.75	2/2335 (0.1%)
12	r	0.63	1/1741 (0.1%)	0.72	3/2335 (0.1%)
13	CM	0.53	1/1374 (0.1%)	0.72	2/1842 (0.1%)
13	s	0.43	0/1374	0.65	0/1842
14	CN	0.51	0/1568	0.63	0/2106
14	t	0.79	1/1568 (0.1%)	0.68	0/2106
15	CO	0.58	0/1068	0.68	0/1438
15	u	0.55	0/1068	0.65	0/1438
16	CP	0.52	0/1757	0.67	0/2354
16	v	0.59	0/1757	0.74	1/2354 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CQ	0.73	0/1585	0.80	3/2128 (0.1%)
17	w	0.64	0/1585	0.72	1/2128 (0.0%)
18	CR	0.62	0/1443	0.71	0/1944
18	x	0.58	0/1443	0.70	0/1944
19	CS	0.59	0/1465	0.80	2/1965 (0.1%)
19	y	0.60	0/1465	0.77	1/1965 (0.1%)
20	CT	0.49	0/1538	0.61	0/2050
20	z	0.44	0/1538	0.60	0/2050
21	0	0.59	0/1481	0.70	0/1990
21	CU	0.65	0/1481	0.69	0/1990
22	2	0.58	0/1300	0.69	0/1743
22	CV	0.62	0/1300	0.70	0/1743
23	5	0.37	0/812	0.55	0/1099
23	CW	0.44	0/812	0.59	0/1099
24	6	0.59	0/1018	0.73	0/1369
24	CX	0.62	0/1018	0.73	0/1369
25	7	0.42	0/712	0.55	0/958
25	CY	0.49	0/848	0.57	0/1146
26	8	0.50	0/979	0.65	0/1321
26	CZ	0.49	0/979	0.68	0/1321
27	9	0.56	0/1004	0.79	1/1341 (0.1%)
27	DA	0.52	0/987	0.70	0/1318
28	AA	0.51	1/1118 (0.1%)	0.62	1/1497 (0.1%)
28	DB	0.49	1/1118 (0.1%)	0.56	0/1497
29	AB	0.63	0/1204	0.81	1/1612 (0.1%)
29	DC	0.58	0/1204	0.74	1/1612 (0.1%)
30	AC	0.54	0/473	0.67	0/629
30	DD	0.53	0/473	0.69	0/629
31	AD	0.41	0/751	0.59	0/1008
31	DE	0.41	0/751	0.61	1/1008 (0.1%)
32	AE	0.50	0/890	0.60	0/1196
32	DF	0.57	0/890	0.65	0/1196
33	AF	0.62	0/1041	0.73	0/1394
33	DG	0.63	0/1041	0.75	0/1394
34	AG	0.70	0/868	0.73	0/1168
34	DH	0.68	0/868	0.71	0/1168
35	AH	0.48	0/890	0.70	0/1189
35	DI	0.52	0/890	0.64	0/1189
36	AI	0.57	1/978 (0.1%)	0.72	2/1301 (0.2%)
36	DJ	0.50	0/978	0.66	1/1301 (0.1%)
37	AJ	0.50	0/778	0.65	0/1034
37	DK	0.45	0/778	0.60	0/1034
38	AK	0.59	0/696	0.78	1/923 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DL	0.58	0/696	0.71	0/923
39	AL	0.44	0/618	0.56	0/826
39	DM	0.40	0/618	0.60	0/826
40	AM	0.64	0/443	0.76	0/588
40	DN	0.58	0/443	0.75	0/588
41	AN	0.59	0/423	0.77	0/562
41	DO	0.71	0/423	0.79	0/562
42	AO	0.48	0/234	0.70	0/300
42	DP	0.68	0/234	0.81	0/300
43	AP	0.60	0/860	0.76	1/1136 (0.1%)
43	DQ	0.62	0/860	0.78	0/1136
44	AQ	0.58	0/701	0.70	0/934
44	DR	0.58	0/701	0.78	0/934
45	i	0.40	0/1113	0.64	1/1502 (0.1%)
45	sM	0.42	0/480	0.69	0/642
46	p0	0.41	0/1091	0.60	2/1472 (0.1%)
47	A	0.64	9/42443 (0.0%)	1.16	193/66134 (0.3%)
48	B	0.38	0/1617	0.59	0/2215
48	s0	0.47	1/1623 (0.1%)	0.60	0/2222
49	C	0.30	0/1735	0.58	1/2335 (0.0%)
49	s1	0.42	0/1748	0.61	1/2352 (0.0%)
50	D	0.39	0/1665	0.60	0/2263
50	s2	0.45	0/1665	0.67	0/2263
51	E	0.39	0/1759	0.55	0/2368
51	s3	0.38	0/1759	0.55	0/2368
52	F	0.44	1/2109 (0.0%)	0.63	1/2839 (0.0%)
52	s4	0.53	1/2109 (0.0%)	0.64	0/2839
53	G	0.32	0/1629	0.54	0/2202
53	s5	0.35	0/1629	0.53	0/2202
54	H	0.38	0/1823	0.60	1/2439 (0.0%)
54	s6	0.47	0/1779	0.63	0/2379
55	I	0.37	0/1506	0.58	0/2028
55	s7	0.40	0/1516	0.58	0/2043
56	J	0.42	0/1514	0.67	1/2021 (0.0%)
56	s8	0.47	0/1514	0.63	1/2021 (0.0%)
57	K	0.39	0/1519	0.60	1/2035 (0.0%)
57	s9	0.43	0/1519	0.60	0/2035
58	L	0.34	0/789	0.60	1/1067 (0.1%)
58	c0	0.33	0/776	0.58	2/1047 (0.2%)
59	M	0.46	0/1239	0.62	0/1673
59	c1	0.52	1/1194 (0.1%)	0.65	0/1610
60	N	0.34	0/898	0.62	0/1220
60	c2	0.27	0/898	0.61	1/1220 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	O	0.42	0/1215	0.56	0/1638
61	c3	0.45	0/1215	0.69	3/1638 (0.2%)
62	P	0.31	0/901	0.59	0/1217
62	c4	0.45	0/960	0.66	0/1290
63	Q	0.40	0/998	0.57	0/1341
63	c5	0.41	0/1060	0.62	0/1426
64	R	0.35	0/1125	0.59	0/1510
64	c6	0.37	0/1131	0.65	1/1518 (0.1%)
65	S	0.35	0/935	0.55	0/1254
65	c7	0.40	0/914	0.61	0/1224
66	T	0.36	0/1211	0.57	0/1628
66	c8	0.39	0/1211	0.60	2/1628 (0.1%)
67	U	0.36	0/1130	0.54	0/1517
67	c9	0.38	0/1130	0.54	0/1517
68	V	0.37	0/865	0.55	0/1169
68	d0	0.39	0/892	0.57	0/1205
69	W	0.36	0/693	0.58	0/935
69	d1	0.41	0/693	0.65	0/935
70	X	0.41	0/1038	0.64	2/1395 (0.1%)
70	d2	0.48	0/1038	0.66	0/1395
71	Y	0.47	0/1139	0.70	1/1518 (0.1%)
71	d3	0.54	0/1139	0.68	0/1518
72	Z	0.39	0/1087	0.54	0/1449
72	d4	0.43	0/1087	0.64	0/1449
73	a	0.32	0/571	0.55	0/768
73	d5	0.35	0/566	0.51	0/761
74	b	0.35	0/782	0.66	0/1047
74	d6	0.48	0/782	0.69	0/1047
75	c	0.36	0/620	0.62	0/838
75	d7	0.47	1/620 (0.2%)	0.63	0/838
76	d	0.32	0/499	0.55	0/670
76	d8	0.35	0/499	0.66	0/670
77	d9	0.42	0/452	0.62	1/600 (0.2%)
77	e	0.42	0/452	0.61	0/600
78	e0	0.44	0/499	0.61	0/665
78	f	0.38	0/483	0.52	0/643
79	e1	0.31	0/404	0.56	0/542
79	g	0.37	0/577	0.61	0/770
80	Rb	0.33	0/2495	0.55	0/3395
80	h	0.32	0/2490	0.54	0/3389
81	sR	0.78	17/42490 (0.0%)	1.24	270/66207 (0.4%)
All	All	0.77	155/430036 (0.0%)	1.14	2464/631418 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	j	0	1
5	CE	0	2
5	k	0	2
6	CF	0	1
6	l	0	3
7	CG	0	4
7	m	0	3
8	CH	0	1
9	CI	0	2
9	o	0	2
10	CJ	0	3
11	CK	0	1
11	q	0	1
13	CM	0	1
13	s	0	1
14	CN	0	1
14	t	0	1
15	CO	0	1
15	u	0	2
16	CP	0	1
16	v	0	2
17	CQ	0	2
17	w	0	1
19	CS	0	1
21	0	0	1
22	2	0	1
28	AA	0	1
28	DB	0	1
29	AB	0	1
29	DC	0	1
30	AC	0	1
30	DD	0	1
32	AE	0	2
36	AI	0	1
36	DJ	0	1
43	DQ	0	1
46	p0	0	1
48	B	0	2
48	s0	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
50	s2	0	1
51	E	0	1
51	s3	0	3
52	F	0	1
53	G	0	2
53	s5	0	1
54	H	0	2
54	s6	0	1
55	I	0	4
55	s7	0	2
56	J	0	2
56	s8	0	1
57	K	0	2
59	M	0	2
60	N	0	4
60	c2	0	2
61	O	0	1
61	c3	0	2
62	P	0	1
62	c4	0	3
63	c5	0	2
64	R	0	1
64	c6	0	3
65	c7	0	1
66	T	0	3
66	c8	0	3
69	d1	0	1
71	Y	0	2
71	d3	0	1
72	d4	0	1
73	a	0	1
74	b	0	3
78	e0	0	1
79	e1	0	1
79	g	0	3
80	Rb	0	2
All	All	0	124

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	132	ALA	C-N	21.63	1.75	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AR	870	G	C8-N7	13.78	1.39	1.30
52	s4	82	TYR	C-N	-13.10	1.09	1.34
81	sR	1662	G	C8-N7	11.30	1.37	1.30
12	r	92	HIS	C-N	10.69	1.54	1.34

The worst 5 of 2464 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	870	G	C5-N7-C8	-19.96	94.32	104.30
81	sR	1672	G	C5-N7-C8	-16.95	95.82	104.30
1	1	86	G	O5'-P-OP2	-16.12	91.19	105.70
1	AR	870	G	N7-C8-N9	15.53	120.86	113.10
1	AR	2700	G	C5-N7-C8	-14.21	97.19	104.30

There are no chirality outliers.

5 of 124 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	j	48	ILE	Peptide
5	k	139	GLN	Peptide
5	k	315	GLY	Peptide
6	l	291	ASN	Peptide
6	l	292	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	67355	0	33845	1134	0
1	AR	67313	0	33820	1287	0
2	3	2579	0	1304	32	0
2	AS	2579	0	1304	39	1
3	4	3353	0	1695	66	1
3	AT	3353	0	1695	70	0
4	CD	1914	0	1981	83	0
4	j	1914	0	1981	0	0
5	CE	3075	0	3142	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	k	3075	0	3142	0	0
6	CF	2748	0	2859	115	0
6	l	2748	0	2859	0	0
7	CG	2375	0	2324	85	0
7	m	2375	0	2325	0	0
8	CH	1239	0	1326	38	0
8	n	1239	0	1326	0	0
9	CI	1784	0	1862	55	0
9	o	1784	0	1862	0	0
10	CJ	1804	0	1877	60	0
10	p	1804	0	1877	0	0
11	CK	1518	0	1587	60	0
11	q	1518	0	1587	0	0
12	CL	1705	0	1736	64	0
12	r	1705	0	1736	0	0
13	CM	1353	0	1383	51	0
13	s	1353	0	1383	0	0
14	CN	1543	0	1608	73	0
14	t	1543	0	1608	0	0
15	CO	1053	0	1149	43	0
15	u	1053	0	1149	0	0
16	CP	1720	0	1779	66	0
16	v	1720	0	1779	0	0
17	CQ	1555	0	1659	49	0
17	w	1555	0	1659	0	0
18	CR	1420	0	1437	56	0
18	x	1420	0	1437	0	0
19	CS	1441	0	1543	51	0
19	y	1441	0	1543	0	0
20	CT	1521	0	1617	55	0
20	z	1521	0	1617	0	0
21	0	1445	0	1487	47	0
21	CU	1445	0	1487	51	0
22	2	1276	0	1323	43	0
22	CV	1276	0	1323	46	0
23	5	796	0	812	15	0
23	CW	796	0	812	24	0
24	6	1003	0	1048	49	0
24	CX	1003	0	1048	34	0
25	7	699	0	640	10	0
25	CY	836	0	721	9	0
26	8	964	0	1025	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	CZ	964	0	1025	20	0
27	9	993	0	1081	37	0
27	DA	976	0	1064	29	0
28	AA	1092	0	1155	49	0
28	DB	1092	0	1155	45	0
29	AB	1173	0	1215	56	0
29	DC	1173	0	1215	53	0
30	AC	462	0	491	20	0
30	DD	462	0	491	15	0
31	AD	743	0	797	18	0
31	DE	743	0	797	19	0
32	AE	876	0	912	28	0
32	DF	876	0	912	20	0
33	AF	1020	0	1090	32	0
33	DG	1020	0	1090	43	0
34	AG	850	0	880	33	0
34	DH	850	0	880	24	0
35	AH	880	0	945	34	0
35	DI	880	0	945	32	0
36	AI	969	0	1078	27	0
36	DJ	969	0	1078	47	0
37	AJ	771	0	849	20	0
37	DK	771	0	849	37	0
38	AK	681	0	683	30	0
38	DL	681	0	683	28	0
39	AL	612	0	682	17	0
39	DM	612	0	682	15	0
40	AM	436	0	475	29	0
40	DN	436	0	475	19	0
41	AN	417	0	455	18	0
41	DO	417	0	455	9	0
42	AO	233	0	284	12	0
42	DP	233	0	284	12	0
43	AP	847	0	914	19	0
43	DQ	847	0	914	20	0
44	AQ	694	0	734	31	0
44	DR	694	0	734	29	0
45	i	1104	0	1002	0	0
45	sM	475	0	492	0	0
46	p0	1076	0	1076	0	0
47	A	37948	0	19089	879	1
48	B	1577	0	1567	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	s0	1583	0	1578	0	0
49	C	1709	0	1784	87	0
49	s1	1722	0	1793	0	0
50	D	1635	0	1723	71	0
50	s2	1635	0	1723	0	0
51	E	1734	0	1817	47	0
51	s3	1734	0	1817	0	0
52	F	2068	0	2154	89	0
52	s4	2068	0	2154	0	0
53	G	1609	0	1675	76	0
53	s5	1609	0	1675	0	0
54	H	1799	0	1879	74	0
54	s6	1755	0	1846	0	0
55	I	1481	0	1572	80	0
55	s7	1491	0	1578	0	0
56	J	1489	0	1525	70	0
56	s8	1489	0	1525	0	0
57	K	1494	0	1573	52	0
57	s9	1494	0	1573	0	0
58	L	772	0	727	39	0
58	c0	761	0	698	0	0
59	M	1213	0	1257	33	0
59	c1	1168	0	1233	0	0
60	N	890	0	887	27	0
60	c2	890	0	887	0	0
61	O	1192	0	1255	39	0
61	c3	1192	0	1255	0	0
62	P	891	0	883	46	0
62	c4	949	0	985	0	0
63	Q	977	0	1002	44	0
63	c5	1039	0	1050	0	0
64	R	1105	0	1166	48	0
64	c6	1111	0	1171	0	0
65	S	926	0	930	31	0
65	c7	906	0	909	0	0
66	T	1192	0	1222	46	0
66	c8	1192	0	1222	0	0
67	U	1112	0	1124	43	0
67	c9	1112	0	1124	0	0
68	V	855	0	917	39	0
68	d0	882	0	939	0	0
69	W	684	0	672	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	d1	684	0	672	0	0
70	X	1021	0	1060	49	0
70	d2	1021	0	1060	0	0
71	Y	1121	0	1196	40	0
71	d3	1121	0	1196	0	0
72	Z	1073	0	1132	52	0
72	d4	1073	0	1132	0	0
73	a	563	0	603	0	0
73	d5	558	0	598	0	0
74	b	769	0	814	0	0
74	d6	769	0	814	0	0
75	c	610	0	633	0	0
75	d7	610	0	633	0	0
76	d	497	0	535	0	0
76	d8	497	0	535	0	0
77	d9	442	0	428	0	0
77	e	442	0	428	0	0
78	e0	491	0	542	0	0
78	f	475	0	525	0	0
79	e1	397	0	396	0	0
79	g	566	0	601	0	0
80	Rb	2442	0	2392	0	0
80	h	2437	0	2386	0	0
81	sR	37990	0	19111	0	0
82	1	2262	0	0	316	0
82	2	7	0	0	0	0
82	3	63	0	0	4	0
82	4	98	0	0	7	0
82	A	994	0	0	148	0
82	AC	7	0	0	2	0
82	AE	7	0	0	9	0
82	AG	7	0	0	1	0
82	AK	14	0	0	6	0
82	AP	7	0	0	3	0
82	AR	2366	0	0	354	1
82	AS	70	0	0	12	0
82	AT	112	0	0	34	0
82	CE	14	0	0	4	0
82	CF	7	0	0	4	0
82	CG	21	0	0	8	0
82	CH	7	0	0	2	0
82	CK	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	CL	14	0	0	6	0
82	CM	7	0	0	0	0
82	CO	7	0	0	0	0
82	CP	7	0	0	1	0
82	CQ	7	0	0	1	0
82	CS	1	0	0	0	0
82	CX	14	0	0	1	0
82	DD	7	0	0	1	0
82	DG	7	0	0	1	0
82	DH	7	0	0	0	0
82	DQ	7	0	0	4	0
82	J	14	0	0	2	0
82	O	7	0	0	0	0
82	Q	7	0	0	1	0
82	Rb	7	0	0	0	0
82	T	7	0	0	2	0
82	c1	7	0	0	0	0
82	c3	7	0	0	0	0
82	c5	7	0	0	0	0
82	c8	7	0	0	0	0
82	d4	7	0	0	0	0
82	d9	7	0	0	0	0
82	e	7	0	0	0	0
82	h	7	0	0	0	0
82	k	7	0	0	0	0
82	l	7	0	0	0	0
82	n	7	0	0	0	0
82	r	7	0	0	0	0
82	s1	7	0	0	0	0
82	s4	7	0	0	0	0
82	s8	7	0	0	0	0
82	sR	1043	0	0	0	0
82	v	14	0	0	0	0
82	w	7	0	0	0	0
82	x	7	0	0	0	0
82	y	7	0	0	0	0
82	z	7	0	0	0	0
83	1	499	0	0	0	0
83	3	13	0	0	0	0
83	4	23	0	0	0	0
83	6	3	0	0	0	0
83	9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	A	129	0	0	0	0
83	AB	8	0	0	0	0
83	AF	2	0	0	0	0
83	AG	1	0	0	0	0
83	AH	1	0	0	0	0
83	AK	2	0	0	0	0
83	AM	1	0	0	0	0
83	AP	1	0	0	0	0
83	AR	523	0	0	0	0
83	AS	19	0	0	0	0
83	AT	15	0	0	0	0
83	CD	3	0	0	0	0
83	CE	3	0	0	0	0
83	CF	2	0	0	0	0
83	CG	3	0	0	0	0
83	CI	2	0	0	0	0
83	CJ	1	0	0	0	0
83	CK	3	0	0	0	0
83	CL	1	0	0	0	0
83	CM	1	0	0	0	0
83	CO	1	0	0	0	0
83	CP	4	0	0	0	0
83	CQ	2	0	0	0	0
83	CR	8	0	0	0	0
83	CU	2	0	0	0	0
83	CX	3	0	0	0	0
83	CY	1	0	0	0	0
83	D	1	0	0	0	0
83	DA	2	0	0	0	0
83	DC	4	0	0	0	0
83	DD	1	0	0	0	0
83	DE	1	0	0	0	0
83	DH	1	0	0	0	0
83	DI	1	0	0	0	0
83	DL	1	0	0	0	0
83	DN	1	0	0	0	0
83	DO	1	0	0	0	0
83	DP	1	0	0	0	0
83	DQ	3	0	0	0	0
83	DR	2	0	0	0	0
83	F	1	0	0	0	0
83	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	J	1	0	0	0	0
83	O	1	0	0	0	0
83	Y	1	0	0	0	0
83	b	1	0	0	0	0
83	c1	2	0	0	0	0
83	c4	1	0	0	0	0
83	c6	1	0	0	0	0
83	c8	1	0	0	0	0
83	c9	1	0	0	0	0
83	d3	3	0	0	0	0
83	d4	3	0	0	0	0
83	d5	1	0	0	0	0
83	d6	1	0	0	0	0
83	d9	1	0	0	0	0
83	e	1	0	0	0	0
83	j	2	0	0	0	0
83	k	1	0	0	0	0
83	l	3	0	0	0	0
83	o	1	0	0	0	0
83	r	2	0	0	0	0
83	s	1	0	0	0	0
83	s1	1	0	0	0	0
83	s2	1	0	0	0	0
83	s4	1	0	0	0	0
83	s8	2	0	0	0	0
83	sM	2	0	0	0	0
83	sR	154	0	0	0	0
83	t	3	0	0	0	0
83	v	5	0	0	0	0
83	w	1	0	0	0	0
83	x	5	0	0	0	0
83	z	1	0	0	0	0
84	1	26	0	0	1	0
84	AR	26	0	0	0	0
85	AK	1	0	0	0	0
85	AN	1	0	0	0	0
85	AP	1	0	0	0	0
85	AQ	1	0	0	0	0
85	DL	1	0	0	0	0
85	DO	1	0	0	0	0
85	DQ	1	0	0	0	0
85	DR	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	b	1	0	0	0	0
85	c	1	0	0	0	0
85	d6	1	0	0	0	0
85	d7	1	0	0	0	0
85	d9	1	0	0	0	0
85	e	1	0	0	0	0
85	e1	1	0	0	0	0
85	g	1	0	0	0	0
86	AR	12	0	16	0	0
All	All	409486	0	296719	6599	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 6599 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2395:G:N7	82:1:3722:OHX:N1	2.04	1.05
47:A:320:U:H3'	47:A:321:C:H5''	1.41	1.02
1:1:1481:A:O2'	1:1:1858:A:N3	1.91	1.01
12:CL:174:THR:HG23	12:CL:176:LEU:H	1.24	1.01
5:CE:41:VAL:HA	5:CE:185:GLY:HA3	1.42	1.00

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AS:52:G:OP1	82:AR:3441:OHX:N2[2_756]	1.31	0.89
3:4:158:U:O2'	47:A:236:A:O2'[2_655]	2.01	0.19

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%)	225 (90%)	25 (10%)	0	100	100
4	j	250/254 (98%)	223 (89%)	26 (10%)	1 (0%)	34	69
5	CE	384/387 (99%)	347 (90%)	34 (9%)	3 (1%)	19	54
5	k	384/387 (99%)	343 (89%)	37 (10%)	4 (1%)	15	49
6	CF	359/362 (99%)	315 (88%)	44 (12%)	0	100	100
6	l	359/362 (99%)	322 (90%)	35 (10%)	2 (1%)	25	59
7	CG	294/297 (99%)	240 (82%)	49 (17%)	5 (2%)	9	36
7	m	294/297 (99%)	252 (86%)	39 (13%)	3 (1%)	15	49
8	CH	152/176 (86%)	135 (89%)	16 (10%)	1 (1%)	22	57
8	n	152/176 (86%)	143 (94%)	9 (6%)	0	100	100
9	CI	220/244 (90%)	201 (91%)	15 (7%)	4 (2%)	8	34
9	o	220/244 (90%)	198 (90%)	18 (8%)	4 (2%)	8	34
10	CJ	231/256 (90%)	204 (88%)	26 (11%)	1 (0%)	34	69
10	p	231/256 (90%)	205 (89%)	25 (11%)	1 (0%)	34	69
11	CK	189/191 (99%)	173 (92%)	16 (8%)	0	100	100
11	q	189/191 (99%)	164 (87%)	23 (12%)	2 (1%)	14	46
12	CL	207/221 (94%)	184 (89%)	23 (11%)	0	100	100
12	r	207/221 (94%)	185 (89%)	22 (11%)	0	100	100
13	CM	167/174 (96%)	136 (81%)	30 (18%)	1 (1%)	25	59
13	s	167/174 (96%)	133 (80%)	31 (19%)	3 (2%)	8	34
14	CN	191/199 (96%)	165 (86%)	20 (10%)	6 (3%)	4	23
14	t	191/199 (96%)	168 (88%)	17 (9%)	6 (3%)	4	23
15	CO	134/138 (97%)	120 (90%)	13 (10%)	1 (1%)	22	57
15	u	134/138 (97%)	117 (87%)	16 (12%)	1 (1%)	22	57
16	CP	201/204 (98%)	182 (90%)	18 (9%)	1 (0%)	29	64
16	v	201/204 (98%)	181 (90%)	16 (8%)	4 (2%)	7	31
17	CQ	195/199 (98%)	185 (95%)	9 (5%)	1 (0%)	29	64
17	w	195/199 (98%)	186 (95%)	7 (4%)	2 (1%)	15	49
18	CR	181/184 (98%)	154 (85%)	27 (15%)	0	100	100
18	x	181/184 (98%)	159 (88%)	22 (12%)	0	100	100
19	CS	183/186 (98%)	156 (85%)	26 (14%)	1 (0%)	29	64
19	y	183/186 (98%)	170 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	CT	186/189 (98%)	165 (89%)	21 (11%)	0	100	100
20	z	186/189 (98%)	174 (94%)	12 (6%)	0	100	100
21	0	170/172 (99%)	154 (91%)	16 (9%)	0	100	100
21	CU	170/172 (99%)	157 (92%)	12 (7%)	1 (1%)	25	59
22	2	157/160 (98%)	140 (89%)	16 (10%)	1 (1%)	25	59
22	CV	157/160 (98%)	143 (91%)	14 (9%)	0	100	100
23	5	98/121 (81%)	85 (87%)	13 (13%)	0	100	100
23	CW	98/121 (81%)	81 (83%)	17 (17%)	0	100	100
24	6	134/137 (98%)	127 (95%)	7 (5%)	0	100	100
24	CX	134/137 (98%)	124 (92%)	10 (8%)	0	100	100
25	7	96/155 (62%)	81 (84%)	15 (16%)	0	100	100
25	CY	122/155 (79%)	107 (88%)	12 (10%)	3 (2%)	5	27
26	8	119/142 (84%)	113 (95%)	6 (5%)	0	100	100
26	CZ	119/142 (84%)	108 (91%)	11 (9%)	0	100	100
27	9	124/127 (98%)	109 (88%)	15 (12%)	0	100	100
27	DA	122/127 (96%)	117 (96%)	5 (4%)	0	100	100
28	AA	133/136 (98%)	112 (84%)	17 (13%)	4 (3%)	4	23
28	DB	133/136 (98%)	114 (86%)	15 (11%)	4 (3%)	4	23
29	AB	146/149 (98%)	119 (82%)	25 (17%)	2 (1%)	11	40
29	DC	146/149 (98%)	120 (82%)	23 (16%)	3 (2%)	7	30
30	AC	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	8	34
30	DD	56/59 (95%)	47 (84%)	9 (16%)	0	100	100
31	AD	95/105 (90%)	89 (94%)	6 (6%)	0	100	100
31	DE	95/105 (90%)	88 (93%)	7 (7%)	0	100	100
32	AE	107/113 (95%)	98 (92%)	8 (8%)	1 (1%)	17	52
32	DF	107/113 (95%)	97 (91%)	10 (9%)	0	100	100
33	AF	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
33	DG	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
34	AG	104/107 (97%)	97 (93%)	7 (7%)	0	100	100
34	DH	104/107 (97%)	95 (91%)	9 (9%)	0	100	100
35	AH	110/121 (91%)	101 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	DI	110/121 (91%)	103 (94%)	7 (6%)	0	100	100
36	AI	117/120 (98%)	104 (89%)	12 (10%)	1 (1%)	17	52
36	DJ	117/120 (98%)	102 (87%)	13 (11%)	2 (2%)	9	36
37	AJ	97/100 (97%)	81 (84%)	16 (16%)	0	100	100
37	DK	97/100 (97%)	84 (87%)	12 (12%)	1 (1%)	15	49
38	AK	85/88 (97%)	74 (87%)	11 (13%)	0	100	100
38	DL	85/88 (97%)	79 (93%)	6 (7%)	0	100	100
39	AL	75/78 (96%)	64 (85%)	11 (15%)	0	100	100
39	DM	75/78 (96%)	61 (81%)	14 (19%)	0	100	100
40	AM	48/51 (94%)	42 (88%)	6 (12%)	0	100	100
40	DN	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
41	AN	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
41	DO	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
42	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
42	DP	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
43	AP	103/106 (97%)	87 (84%)	16 (16%)	0	100	100
43	DQ	103/106 (97%)	90 (87%)	13 (13%)	0	100	100
44	AQ	89/92 (97%)	79 (89%)	10 (11%)	0	100	100
44	DR	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
45	i	155/273 (57%)	115 (74%)	37 (24%)	3 (2%)	8	33
45	sM	61/273 (22%)	44 (72%)	16 (26%)	1 (2%)	9	37
46	p0	139/312 (45%)	125 (90%)	12 (9%)	2 (1%)	11	40
48	B	204/252 (81%)	157 (77%)	44 (22%)	3 (2%)	10	39
48	s0	204/252 (81%)	162 (79%)	39 (19%)	3 (2%)	10	39
49	C	212/255 (83%)	161 (76%)	50 (24%)	1 (0%)	29	64
49	s1	214/255 (84%)	179 (84%)	33 (15%)	2 (1%)	17	52
50	D	215/254 (85%)	192 (89%)	22 (10%)	1 (0%)	29	64
50	s2	215/254 (85%)	193 (90%)	20 (9%)	2 (1%)	17	52
51	E	221/240 (92%)	198 (90%)	22 (10%)	1 (0%)	29	64
51	s3	221/240 (92%)	194 (88%)	26 (12%)	1 (0%)	29	64
52	F	258/261 (99%)	225 (87%)	32 (12%)	1 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	s4	258/261 (99%)	230 (89%)	28 (11%)	0	100	100
53	G	204/225 (91%)	160 (78%)	40 (20%)	4 (2%)	7	31
53	s5	204/225 (91%)	169 (83%)	33 (16%)	2 (1%)	15	49
54	H	224/236 (95%)	199 (89%)	21 (9%)	4 (2%)	8	34
54	s6	216/236 (92%)	197 (91%)	16 (7%)	3 (1%)	11	40
55	I	182/190 (96%)	156 (86%)	20 (11%)	6 (3%)	4	21
55	s7	184/190 (97%)	152 (83%)	26 (14%)	6 (3%)	4	21
56	J	184/200 (92%)	157 (85%)	24 (13%)	3 (2%)	9	37
56	s8	184/200 (92%)	158 (86%)	25 (14%)	1 (0%)	29	64
57	K	183/197 (93%)	157 (86%)	24 (13%)	2 (1%)	14	46
57	s9	183/197 (93%)	162 (88%)	21 (12%)	0	100	100
58	L	94/105 (90%)	69 (73%)	23 (24%)	2 (2%)	7	30
58	c0	92/105 (88%)	63 (68%)	26 (28%)	3 (3%)	4	21
59	M	153/156 (98%)	130 (85%)	20 (13%)	3 (2%)	7	31
59	c1	144/156 (92%)	128 (89%)	15 (10%)	1 (1%)	22	57
60	N	122/143 (85%)	85 (70%)	32 (26%)	5 (4%)	3	16
60	c2	122/143 (85%)	86 (70%)	31 (25%)	5 (4%)	3	16
61	O	148/151 (98%)	132 (89%)	14 (10%)	2 (1%)	11	40
61	c3	148/151 (98%)	127 (86%)	18 (12%)	3 (2%)	7	31
62	P	125/138 (91%)	96 (77%)	29 (23%)	0	100	100
62	c4	126/138 (91%)	104 (82%)	22 (18%)	0	100	100
63	Q	122/142 (86%)	93 (76%)	25 (20%)	4 (3%)	4	21
63	c5	133/142 (94%)	99 (74%)	30 (23%)	4 (3%)	4	23
64	R	139/143 (97%)	120 (86%)	18 (13%)	1 (1%)	22	57
64	c6	140/143 (98%)	123 (88%)	14 (10%)	3 (2%)	7	30
65	S	116/136 (85%)	97 (84%)	19 (16%)	0	100	100
65	c7	113/136 (83%)	96 (85%)	17 (15%)	0	100	100
66	T	143/146 (98%)	120 (84%)	21 (15%)	2 (1%)	11	40
66	c8	143/146 (98%)	117 (82%)	23 (16%)	3 (2%)	7	30
67	U	141/144 (98%)	124 (88%)	17 (12%)	0	100	100
67	c9	141/144 (98%)	130 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	V	105/121 (87%)	92 (88%)	12 (11%)	1 (1%)	15	49
68	d0	108/121 (89%)	92 (85%)	15 (14%)	1 (1%)	17	52
69	W	85/87 (98%)	63 (74%)	19 (22%)	3 (4%)	3	20
69	d1	85/87 (98%)	72 (85%)	13 (15%)	0	100	100
70	X	127/130 (98%)	113 (89%)	14 (11%)	0	100	100
70	d2	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
71	Y	142/145 (98%)	112 (79%)	28 (20%)	2 (1%)	11	40
71	d3	142/145 (98%)	122 (86%)	20 (14%)	0	100	100
72	Z	132/135 (98%)	113 (86%)	18 (14%)	1 (1%)	19	54
72	d4	132/135 (98%)	113 (86%)	17 (13%)	2 (2%)	10	39
73	a	68/108 (63%)	53 (78%)	13 (19%)	2 (3%)	4	24
73	d5	67/108 (62%)	58 (87%)	9 (13%)	0	100	100
74	b	95/119 (80%)	68 (72%)	23 (24%)	4 (4%)	3	16
74	d6	95/119 (80%)	69 (73%)	21 (22%)	5 (5%)	2	12
75	c	79/82 (96%)	63 (80%)	16 (20%)	0	100	100
75	d7	79/82 (96%)	64 (81%)	15 (19%)	0	100	100
76	d	61/67 (91%)	52 (85%)	9 (15%)	0	100	100
76	d8	61/67 (91%)	45 (74%)	16 (26%)	0	100	100
77	d9	51/56 (91%)	45 (88%)	6 (12%)	0	100	100
77	e	51/56 (91%)	47 (92%)	4 (8%)	0	100	100
78	e0	60/63 (95%)	52 (87%)	8 (13%)	0	100	100
78	f	58/63 (92%)	44 (76%)	14 (24%)	0	100	100
79	e1	49/152 (32%)	32 (65%)	17 (35%)	0	100	100
79	g	69/152 (45%)	37 (54%)	32 (46%)	0	100	100
80	Rb	316/319 (99%)	276 (87%)	39 (12%)	1 (0%)	41	73
80	h	316/319 (99%)	281 (89%)	35 (11%)	0	100	100
All	All	22284/24620 (90%)	19305 (87%)	2782 (12%)	197 (1%)	17	52

5 of 197 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	l	339	LEU
7	m	7	ALA

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Mol	Chain	Res	Type
9	o	159	GLN
9	o	234	GLU
11	q	50	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	193/196 (98%)	152 (79%)	41 (21%)	1	5
4	j	193/196 (98%)	150 (78%)	43 (22%)	1	3
5	CE	320/323 (99%)	254 (79%)	66 (21%)	1	5
5	k	320/323 (99%)	259 (81%)	61 (19%)	1	6
6	CF	288/289 (100%)	249 (86%)	39 (14%)	4	16
6	l	288/289 (100%)	241 (84%)	47 (16%)	2	10
7	CG	244/245 (100%)	198 (81%)	46 (19%)	1	6
7	m	244/245 (100%)	205 (84%)	39 (16%)	2	11
8	CH	134/153 (88%)	114 (85%)	20 (15%)	3	13
8	n	134/153 (88%)	118 (88%)	16 (12%)	5	20
9	CI	186/205 (91%)	162 (87%)	24 (13%)	4	18
9	o	186/205 (91%)	162 (87%)	24 (13%)	4	18
10	CJ	187/208 (90%)	163 (87%)	24 (13%)	4	18
10	p	187/208 (90%)	162 (87%)	25 (13%)	4	16
11	CK	171/171 (100%)	138 (81%)	33 (19%)	1	6
11	q	171/171 (100%)	140 (82%)	31 (18%)	1	7
12	CL	177/187 (95%)	140 (79%)	37 (21%)	1	5
12	r	177/187 (95%)	140 (79%)	37 (21%)	1	5
13	CM	147/151 (97%)	123 (84%)	24 (16%)	2	10
13	s	147/151 (97%)	113 (77%)	34 (23%)	1	3
14	CN	154/159 (97%)	134 (87%)	20 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	t	154/159 (97%)	130 (84%)	24 (16%)	2	11
15	CO	107/109 (98%)	90 (84%)	17 (16%)	2	11
15	u	107/109 (98%)	91 (85%)	16 (15%)	3	12
16	CP	175/176 (99%)	146 (83%)	29 (17%)	2	9
16	v	175/176 (99%)	149 (85%)	26 (15%)	3	13
17	CQ	160/162 (99%)	141 (88%)	19 (12%)	5	20
17	w	160/162 (99%)	136 (85%)	24 (15%)	3	12
18	CR	140/146 (96%)	117 (84%)	23 (16%)	2	10
18	x	140/146 (96%)	118 (84%)	22 (16%)	2	11
19	CS	150/151 (99%)	128 (85%)	22 (15%)	3	13
19	y	150/151 (99%)	123 (82%)	27 (18%)	1	7
20	CT	153/154 (99%)	131 (86%)	22 (14%)	3	14
20	z	153/154 (99%)	135 (88%)	18 (12%)	5	21
21	0	156/156 (100%)	129 (83%)	27 (17%)	2	9
21	CU	156/156 (100%)	128 (82%)	28 (18%)	2	8
22	2	136/137 (99%)	111 (82%)	25 (18%)	1	7
22	CV	136/137 (99%)	108 (79%)	28 (21%)	1	5
23	5	87/107 (81%)	73 (84%)	14 (16%)	2	10
23	CW	87/107 (81%)	71 (82%)	16 (18%)	1	7
24	6	104/105 (99%)	82 (79%)	22 (21%)	1	5
24	CX	104/105 (99%)	88 (85%)	16 (15%)	2	11
25	7	57/129 (44%)	50 (88%)	7 (12%)	4	19
25	CY	58/129 (45%)	50 (86%)	8 (14%)	3	16
26	8	104/118 (88%)	85 (82%)	19 (18%)	1	7
26	CZ	104/118 (88%)	87 (84%)	17 (16%)	2	10
27	9	109/110 (99%)	84 (77%)	25 (23%)	1	3
27	DA	107/110 (97%)	88 (82%)	19 (18%)	2	8
28	AA	115/116 (99%)	100 (87%)	15 (13%)	4	18
28	DB	115/116 (99%)	99 (86%)	16 (14%)	3	15
29	AB	118/119 (99%)	97 (82%)	21 (18%)	2	8
29	DC	118/119 (99%)	99 (84%)	19 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	AC	46/47 (98%)	35 (76%)	11 (24%)	0	2
30	DD	46/47 (98%)	38 (83%)	8 (17%)	2	9
31	AD	81/88 (92%)	71 (88%)	10 (12%)	4	19
31	DE	81/88 (92%)	70 (86%)	11 (14%)	3	16
32	AE	92/97 (95%)	74 (80%)	18 (20%)	1	6
32	DF	92/97 (95%)	77 (84%)	15 (16%)	2	10
33	AF	109/111 (98%)	96 (88%)	13 (12%)	5	20
33	DG	109/111 (98%)	89 (82%)	20 (18%)	1	7
34	AG	90/91 (99%)	78 (87%)	12 (13%)	4	16
34	DH	90/91 (99%)	79 (88%)	11 (12%)	5	19
35	AH	95/103 (92%)	83 (87%)	12 (13%)	4	18
35	DI	95/103 (92%)	76 (80%)	19 (20%)	1	5
36	AI	104/105 (99%)	83 (80%)	21 (20%)	1	5
36	DJ	104/105 (99%)	82 (79%)	22 (21%)	1	5
37	AJ	81/82 (99%)	63 (78%)	18 (22%)	1	4
37	DK	81/82 (99%)	68 (84%)	13 (16%)	2	11
38	AK	70/71 (99%)	58 (83%)	12 (17%)	2	9
38	DL	70/71 (99%)	55 (79%)	15 (21%)	1	4
39	AL	68/69 (99%)	56 (82%)	12 (18%)	2	8
39	DM	68/69 (99%)	56 (82%)	12 (18%)	2	8
40	AM	45/46 (98%)	37 (82%)	8 (18%)	2	8
40	DN	45/46 (98%)	37 (82%)	8 (18%)	2	8
41	AN	47/116 (40%)	40 (85%)	7 (15%)	3	13
41	DO	47/116 (40%)	40 (85%)	7 (15%)	3	13
42	AO	23/23 (100%)	18 (78%)	5 (22%)	1	4
42	DP	23/23 (100%)	17 (74%)	6 (26%)	0	1
43	AP	90/91 (99%)	74 (82%)	16 (18%)	2	8
43	DQ	90/91 (99%)	75 (83%)	15 (17%)	2	9
44	AQ	71/72 (99%)	55 (78%)	16 (22%)	1	3
44	DR	71/72 (99%)	63 (89%)	8 (11%)	6	23
45	i	97/228 (42%)	73 (75%)	24 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	sM	54/228 (24%)	44 (82%)	10 (18%)	1	7
46	p0	105/254 (41%)	86 (82%)	19 (18%)	1	7
48	B	164/210 (78%)	137 (84%)	27 (16%)	2	10
48	s0	165/210 (79%)	141 (86%)	24 (14%)	3	13
49	C	191/224 (85%)	160 (84%)	31 (16%)	2	10
49	s1	192/224 (86%)	156 (81%)	36 (19%)	1	6
50	D	176/205 (86%)	143 (81%)	33 (19%)	1	6
50	s2	176/205 (86%)	138 (78%)	38 (22%)	1	4
51	E	182/195 (93%)	150 (82%)	32 (18%)	2	8
51	s3	182/195 (93%)	157 (86%)	25 (14%)	3	16
52	F	221/222 (100%)	180 (81%)	41 (19%)	1	7
52	s4	221/222 (100%)	193 (87%)	28 (13%)	4	18
53	G	173/191 (91%)	146 (84%)	27 (16%)	2	11
53	s5	173/191 (91%)	141 (82%)	32 (18%)	1	7
54	H	188/201 (94%)	155 (82%)	33 (18%)	2	8
54	s6	187/201 (93%)	157 (84%)	30 (16%)	2	11
55	I	165/170 (97%)	134 (81%)	31 (19%)	1	6
55	s7	165/170 (97%)	138 (84%)	27 (16%)	2	10
56	J	150/161 (93%)	131 (87%)	19 (13%)	4	18
56	s8	150/161 (93%)	130 (87%)	20 (13%)	4	16
57	K	158/166 (95%)	126 (80%)	32 (20%)	1	5
57	s9	158/166 (95%)	130 (82%)	28 (18%)	2	8
58	L	77/98 (79%)	67 (87%)	10 (13%)	4	18
58	c0	73/98 (74%)	60 (82%)	13 (18%)	2	8
59	M	129/137 (94%)	109 (84%)	20 (16%)	2	11
59	c1	129/137 (94%)	105 (81%)	24 (19%)	1	7
60	N	88/119 (74%)	71 (81%)	17 (19%)	1	6
60	c2	88/119 (74%)	73 (83%)	15 (17%)	2	9
61	O	127/128 (99%)	108 (85%)	19 (15%)	3	12
61	c3	127/128 (99%)	107 (84%)	20 (16%)	2	11
62	P	81/105 (77%)	66 (82%)	15 (18%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	c4	97/105 (92%)	80 (82%)	17 (18%)	2	8
63	Q	101/118 (86%)	82 (81%)	19 (19%)	1	6
63	c5	103/118 (87%)	85 (82%)	18 (18%)	2	8
64	R	117/119 (98%)	95 (81%)	22 (19%)	1	6
64	c6	118/119 (99%)	98 (83%)	20 (17%)	2	9
65	S	94/124 (76%)	80 (85%)	14 (15%)	3	13
65	c7	92/124 (74%)	72 (78%)	20 (22%)	1	4
66	T	128/129 (99%)	103 (80%)	25 (20%)	1	6
66	c8	128/129 (99%)	112 (88%)	16 (12%)	4	18
67	U	115/116 (99%)	97 (84%)	18 (16%)	2	11
67	c9	115/116 (99%)	102 (89%)	13 (11%)	6	23
68	V	100/114 (88%)	81 (81%)	19 (19%)	1	6
68	d0	103/114 (90%)	86 (84%)	17 (16%)	2	10
69	W	74/74 (100%)	64 (86%)	10 (14%)	4	16
69	d1	74/74 (100%)	62 (84%)	12 (16%)	2	10
70	X	110/111 (99%)	87 (79%)	23 (21%)	1	5
70	d2	110/111 (99%)	98 (89%)	12 (11%)	6	25
71	Y	119/120 (99%)	105 (88%)	14 (12%)	5	21
71	d3	119/120 (99%)	102 (86%)	17 (14%)	3	14
72	Z	112/113 (99%)	101 (90%)	11 (10%)	8	29
72	d4	112/113 (99%)	103 (92%)	9 (8%)	12	40
73	a	61/89 (68%)	43 (70%)	18 (30%)	0	1
73	d5	61/89 (68%)	54 (88%)	7 (12%)	5	22
74	b	83/100 (83%)	70 (84%)	13 (16%)	2	11
74	d6	83/100 (83%)	72 (87%)	11 (13%)	4	16
75	c	70/71 (99%)	61 (87%)	9 (13%)	4	18
75	d7	70/71 (99%)	60 (86%)	10 (14%)	3	14
76	d	56/60 (93%)	49 (88%)	7 (12%)	4	18
76	d8	56/60 (93%)	45 (80%)	11 (20%)	1	6
77	d9	47/49 (96%)	40 (85%)	7 (15%)	3	13
77	e	47/49 (96%)	39 (83%)	8 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	e0	53/54 (98%)	43 (81%)	10 (19%)	1	6
78	f	51/54 (94%)	41 (80%)	10 (20%)	1	6
79	e1	43/135 (32%)	33 (77%)	10 (23%)	1	3
79	g	62/135 (46%)	50 (81%)	12 (19%)	1	6
80	Rb	260/262 (99%)	238 (92%)	22 (8%)	10	37
80	h	259/262 (99%)	232 (90%)	27 (10%)	7	27
All	All	18682/20678 (90%)	15601 (84%)	3081 (16%)	2	10

5 of 3081 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	CT	43	LYS
40	DN	21	ARG
62	c4	49	LYS
21	CU	164	SER
29	DC	42	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
49	C	177	GLN
53	G	95	ASN
55	s7	71	HIS
50	D	94	GLN
53	G	131	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3396 (92%)	643 (20%)	74 (2%)
1	AR	3143/3396 (92%)	642 (20%)	75 (2%)
2	3	120/121 (99%)	15 (12%)	2 (1%)
2	AS	120/121 (99%)	16 (13%)	1 (0%)
3	4	157/158 (99%)	35 (22%)	2 (1%)
3	AT	157/158 (99%)	32 (20%)	3 (1%)
47	A	1778/1797 (98%)	453 (25%)	53 (2%)
81	sR	1780/1800 (98%)	433 (24%)	0
All	All	10400/10947 (95%)	2269 (21%)	210 (2%)

5 of 2269 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	16	A
1	1	18	G
1	1	26	A
1	1	40	A
1	1	43	A

5 of 210 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AR	1103	A
1	AR	2101	C
47	A	1150	G
1	AR	1238	C
1	AR	1507	G

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2586 ligands modelled in this entry, 2 are modelled with single atom and 1525 are monoatomic - leaving 1059 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	1	3720	-	0,6,6	0.00	-	-		
82	OHX	A	1913	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3620	-	0,6,6	0.00	-	-		
82	OHX	1	3584	-	0,6,6	0.00	-	-		
82	OHX	AR	3487	-	0,6,6	0.00	-	-		
82	OHX	1	3557	-	0,6,6	0.00	-	-		
82	OHX	AR	3663	-	0,6,6	0.00	-	-		
82	OHX	AR	3575	-	0,6,6	0.00	-	-		
82	OHX	A	1911	-	0,6,6	0.00	-	-		
82	OHX	A	1889	-	0,6,6	0.00	-	-		
82	OHX	1	3601	-	0,6,6	0.00	-	-		
82	OHX	DD	101	-	0,6,6	0.00	-	-		
82	OHX	AR	3706	-	0,6,6	0.00	-	-		
82	OHX	sR	1990	-	0,6,6	0.00	-	-		
82	OHX	sR	1931	-	0,6,6	0.00	-	-		
82	OHX	AR	3415	-	0,6,6	0.00	-	-		
82	OHX	AR	3677	-	0,6,6	0.00	-	-		
82	OHX	sR	2039	-	0,6,6	0.00	-	-		
82	OHX	1	3566	-	0,6,6	0.00	-	-		
82	OHX	A	1899	-	0,6,6	0.00	-	-		
82	OHX	sR	2017	-	0,6,6	0.00	-	-		
82	OHX	AR	3448	-	0,6,6	0.00	-	-		
82	OHX	A	1890	-	0,6,6	0.00	-	-		
82	OHX	sR	1960	-	0,6,6	0.00	-	-		
82	OHX	1	3613	-	0,6,6	0.00	-	-		
82	OHX	AR	3494	-	0,6,6	0.00	-	-		
82	OHX	sR	1911	-	0,6,6	0.00	-	-		
82	OHX	AR	3576	-	0,6,6	0.00	-	-		
82	OHX	sR	1951	-	0,6,6	0.00	-	-		
82	OHX	AR	3691	-	0,6,6	0.00	-	-		
82	OHX	AR	3467	-	0,6,6	0.00	-	-		
82	OHX	1	3526	-	0,6,6	0.00	-	-		
82	OHX	1	3440	-	0,6,6	0.00	-	-		
82	OHX	1	3696	-	0,6,6	0.00	-	-		
82	OHX	AR	3406	-	0,6,6	0.00	-	-		
82	OHX	A	1819	-	0,6,6	0.00	-	-		
82	OHX	AR	3545	-	0,6,6	0.00	-	-		
82	OHX	sR	2026	-	0,6,6	0.00	-	-		
82	OHX	AR	3658	-	0,6,6	0.00	-	-		
82	OHX	sR	1956	-	0,6,6	0.00	-	-		
82	OHX	sR	1913	-	0,6,6	0.00	-	-		
82	OHX	sR	1933	-	0,6,6	0.00	-	-		
82	OHX	AR	3413	-	0,6,6	0.00	-	-		
82	OHX	AR	3427	-	0,6,6	0.00	-	-		
82	OHX	sR	1905	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3513	-	0,6,6	0.00	-	-		
82	OHX	1	3456	-	0,6,6	0.00	-	-		
82	OHX	AR	3686	-	0,6,6	0.00	-	-		
82	OHX	sR	2006	-	0,6,6	0.00	-	-		
82	OHX	1	3581	-	0,6,6	0.00	-	-		
82	OHX	1	3654	-	0,6,6	0.00	-	-		
82	OHX	n	201	-	0,6,6	0.00	-	-		
82	OHX	sR	2010	-	0,6,6	0.00	-	-		
82	OHX	c1	201	-	0,6,6	0.00	-	-		
82	OHX	AR	3465	-	0,6,6	0.00	-	-		
82	OHX	A	1834	-	0,6,6	0.00	-	-		
82	OHX	AR	3684	-	0,6,6	0.00	-	-		
82	OHX	sR	2047	-	0,6,6	0.00	-	-		
82	OHX	sR	2024	-	0,6,6	0.00	-	-		
82	OHX	AR	3565	-	0,6,6	0.00	-	-		
82	OHX	AR	3719	-	0,6,6	0.00	-	-		
82	OHX	AR	3473	-	0,6,6	0.00	-	-		
82	OHX	A	1914	-	0,6,6	0.00	-	-		
82	OHX	AR	3613	-	0,6,6	0.00	-	-		
82	OHX	1	3538	-	0,6,6	0.00	-	-		
82	OHX	1	3586	-	0,6,6	0.00	-	-		
82	OHX	AR	3528	-	0,6,6	0.00	-	-		
82	OHX	c5	201	-	0,6,6	0.00	-	-		
82	OHX	A	1938	-	0,6,6	0.00	-	-		
82	OHX	AR	3644	-	0,6,6	0.00	-	-		
82	OHX	AR	3432	-	0,6,6	0.00	-	-		
82	OHX	1	3642	-	0,6,6	0.00	-	-		
82	OHX	4	204	-	0,6,6	0.00	-	-		
82	OHX	1	3615	-	0,6,6	0.00	-	-		
82	OHX	AR	3570	-	0,6,6	0.00	-	-		
82	OHX	A	1839	-	0,6,6	0.00	-	-		
82	OHX	1	3417	-	0,6,6	0.00	-	-		
82	OHX	A	1856	-	0,6,6	0.00	-	-		
82	OHX	A	1934	-	0,6,6	0.00	-	-		
82	OHX	J	301	-	0,6,6	0.00	-	-		
82	OHX	AR	3690	-	0,6,6	0.00	-	-		
82	OHX	AR	3516	-	0,6,6	0.00	-	-		
82	OHX	1	3701	-	0,6,6	0.00	-	-		
82	OHX	AK	102	-	0,6,6	0.00	-	-		
82	OHX	AR	3665	-	0,6,6	0.00	-	-		
82	OHX	AR	3581	-	0,6,6	0.00	-	-		
82	OHX	sR	1957	-	0,6,6	0.00	-	-		
82	OHX	1	3540	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	A	1808	-	0,6,6	0.00	-	-		
82	OHX	DG	201	-	0,6,6	0.00	-	-		
82	OHX	AT	205	-	0,6,6	0.00	-	-		
82	OHX	AR	3419	-	0,6,6	0.00	-	-		
82	OHX	A	1931	-	0,6,6	0.00	-	-		
82	OHX	1	3576	-	0,6,6	0.00	-	-		
82	OHX	1	3573	-	0,6,6	0.00	-	-		
82	OHX	AR	3435	-	0,6,6	0.00	-	-		
82	OHX	sR	1908	-	0,6,6	0.00	-	-		
82	OHX	AR	3416	-	0,6,6	0.00	-	-		
82	OHX	AR	3493	-	0,6,6	0.00	-	-		
82	OHX	A	1806	-	0,6,6	0.00	-	-		
82	OHX	1	3494	-	0,6,6	0.00	-	-		
82	OHX	A	1909	-	0,6,6	0.00	-	-		
82	OHX	sR	1965	-	0,6,6	0.00	-	-		
82	OHX	AR	3549	-	0,6,6	0.00	-	-		
82	OHX	CF	401	-	0,6,6	0.00	-	-		
82	OHX	AR	3634	-	0,6,6	0.00	-	-		
82	OHX	AT	204	-	0,6,6	0.00	-	-		
82	OHX	3	204	-	0,6,6	0.00	-	-		
82	OHX	1	3483	-	0,6,6	0.00	-	-		
82	OHX	AR	3724	-	0,6,6	0.00	-	-		
82	OHX	AR	3525	-	0,6,6	0.00	-	-		
82	OHX	1	3574	-	0,6,6	0.00	-	-		
82	OHX	AR	3707	-	0,6,6	0.00	-	-		
82	OHX	CG	303	-	0,6,6	0.00	-	-		
82	OHX	AR	3424	-	0,6,6	0.00	-	-		
82	OHX	1	3462	-	0,6,6	0.00	-	-		
82	OHX	1	3433	-	0,6,6	0.00	-	-		
82	OHX	AR	3498	-	0,6,6	0.00	-	-		
82	OHX	A	1832	-	0,6,6	0.00	-	-		
82	OHX	AR	3455	-	0,6,6	0.00	-	-		
82	OHX	AR	3472	-	0,6,6	0.00	-	-		
82	OHX	4	206	-	0,6,6	0.00	-	-		
82	OHX	AK	103	-	0,6,6	0.00	-	-		
82	OHX	sR	1994	-	0,6,6	0.00	-	-		
82	OHX	sR	1962	-	0,6,6	0.00	-	-		
82	OHX	AR	3705	-	0,6,6	0.00	-	-		
82	OHX	AR	3682	-	0,6,6	0.00	-	-		
82	OHX	A	1912	-	0,6,6	0.00	-	-		
82	OHX	AR	3469	-	0,6,6	0.00	-	-		
82	OHX	A	1860	-	0,6,6	0.00	-	-		
82	OHX	sR	1914	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3699	-	0,6,6	0.00	-	-		
82	OHX	AR	3522	-	0,6,6	0.00	-	-		
82	OHX	CG	302	-	0,6,6	0.00	-	-		
82	OHX	sR	1904	-	0,6,6	0.00	-	-		
82	OHX	AR	3482	-	0,6,6	0.00	-	-		
82	OHX	1	3530	-	0,6,6	0.00	-	-		
82	OHX	sR	2040	-	0,6,6	0.00	-	-		
82	OHX	1	3718	-	0,6,6	0.00	-	-		
82	OHX	A	1827	-	0,6,6	0.00	-	-		
82	OHX	1	3564	-	0,6,6	0.00	-	-		
82	OHX	AR	3597	-	0,6,6	0.00	-	-		
82	OHX	sR	2033	-	0,6,6	0.00	-	-		
82	OHX	AR	3637	-	0,6,6	0.00	-	-		
82	OHX	1	3630	-	0,6,6	0.00	-	-		
82	OHX	1	3569	-	0,6,6	0.00	-	-		
82	OHX	AR	3620	-	0,6,6	0.00	-	-		
82	OHX	AR	3535	-	0,6,6	0.00	-	-		
82	OHX	1	3711	-	0,6,6	0.00	-	-		
82	OHX	1	3517	-	0,6,6	0.00	-	-		
82	OHX	sR	1982	-	0,6,6	0.00	-	-		
82	OHX	A	1876	82	0,6,6	0.00	-	-		
82	OHX	A	1903	-	0,6,6	0.00	-	-		
82	OHX	1	3636	-	0,6,6	0.00	-	-		
82	OHX	AR	3678	-	0,6,6	0.00	-	-		
82	OHX	1	3638	-	0,6,6	0.00	-	-		
82	OHX	AR	3479	-	0,6,6	0.00	-	-		
82	OHX	sR	1950	-	0,6,6	0.00	-	-		
82	OHX	AR	3731	-	0,6,6	0.00	-	-		
82	OHX	sR	2045	-	0,6,6	0.00	-	-		
82	OHX	1	3710	-	0,6,6	0.00	-	-		
82	OHX	sR	1986	-	0,6,6	0.00	-	-		
82	OHX	sR	1993	-	0,6,6	0.00	-	-		
82	OHX	sR	1987	-	0,6,6	0.00	-	-		
82	OHX	sR	1902	-	0,6,6	0.00	-	-		
82	OHX	A	1896	-	0,6,6	0.00	-	-		
82	OHX	1	3506	-	0,6,6	0.00	-	-		
82	OHX	1	3614	-	0,6,6	0.00	-	-		
82	OHX	1	3585	-	0,6,6	0.00	-	-		
82	OHX	1	3403	-	0,6,6	0.00	-	-		
82	OHX	1	3580	-	0,6,6	0.00	-	-		
82	OHX	A	1881	-	0,6,6	0.00	-	-		
82	OHX	A	1870	-	0,6,6	0.00	-	-		
82	OHX	1	3679	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3715	-	0,6,6	0.00	-	-		
82	OHX	1	3648	-	0,6,6	0.00	-	-		
82	OHX	AR	3571	-	0,6,6	0.00	-	-		
82	OHX	A	1850	-	0,6,6	0.00	-	-		
82	OHX	AR	3429	-	0,6,6	0.00	-	-		
82	OHX	4	214	-	0,6,6	0.00	-	-		
82	OHX	1	3459	-	0,6,6	0.00	-	-		
82	OHX	A	1936	-	0,6,6	0.00	-	-		
82	OHX	A	1883	-	0,6,6	0.00	-	-		
82	OHX	AR	3502	-	0,6,6	0.00	-	-		
82	OHX	1	3673	-	0,6,6	0.00	-	-		
82	OHX	1	3535	-	0,6,6	0.00	-	-		
82	OHX	sR	1945	-	0,6,6	0.00	-	-		
82	OHX	1	3706	-	0,6,6	0.00	-	-		
82	OHX	sR	1959	-	0,6,6	0.00	-	-		
82	OHX	AS	201	-	0,6,6	0.00	-	-		
82	OHX	1	3480	-	0,6,6	0.00	-	-		
82	OHX	1	3419	-	0,6,6	0.00	-	-		
82	OHX	AR	3676	-	0,6,6	0.00	-	-		
82	OHX	AR	3627	-	0,6,6	0.00	-	-		
82	OHX	sR	1923	-	0,6,6	0.00	-	-		
82	OHX	AR	3401	-	0,6,6	0.00	-	-		
82	OHX	AR	3508	-	0,6,6	0.00	-	-		
82	OHX	1	3430	-	0,6,6	0.00	-	-		
82	OHX	sR	1912	-	0,6,6	0.00	-	-		
82	OHX	A	1862	-	0,6,6	0.00	-	-		
82	OHX	sR	1998	-	0,6,6	0.00	-	-		
82	OHX	4	205	-	0,6,6	0.00	-	-		
82	OHX	sR	1973	-	0,6,6	0.00	-	-		
82	OHX	1	3611	-	0,6,6	0.00	-	-		
82	OHX	AR	3579	-	0,6,6	0.00	-	-		
82	OHX	AR	3737	1	0,6,6	0.00	-	-		
82	OHX	1	3409	-	0,6,6	0.00	-	-		
82	OHX	1	3522	-	0,6,6	0.00	-	-		
82	OHX	1	3495	-	0,6,6	0.00	-	-		
82	OHX	A	1873	-	0,6,6	0.00	-	-		
82	OHX	AR	3503	-	0,6,6	0.00	-	-		
82	OHX	AR	3461	-	0,6,6	0.00	-	-		
82	OHX	1	3516	-	0,6,6	0.00	-	-		
82	OHX	AR	3666	-	0,6,6	0.00	-	-		
82	OHX	A	1880	-	0,6,6	0.00	-	-		
82	OHX	3	207	-	0,6,6	0.00	-	-		
82	OHX	1	3481	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	1903	-	0,6,6	0.00	-	-		
82	OHX	AR	3649	-	0,6,6	0.00	-	-		
82	OHX	1	3577	-	0,6,6	0.00	-	-		
82	OHX	sR	1992	-	0,6,6	0.00	-	-		
82	OHX	1	3640	-	0,6,6	0.00	-	-		
82	OHX	AR	3630	-	0,6,6	0.00	-	-		
82	OHX	sR	1930	-	0,6,6	0.00	-	-		
82	OHX	AR	3735	-	0,6,6	0.00	-	-		
82	OHX	AR	3588	-	0,6,6	0.00	-	-		
82	OHX	AR	3687	-	0,6,6	0.00	-	-		
82	OHX	AR	3595	-	0,6,6	0.00	-	-		
82	OHX	A	1838	-	0,6,6	0.00	-	-		
82	OHX	AR	3500	-	0,6,6	0.00	-	-		
82	OHX	A	1906	47	0,6,6	0.00	-	-		
82	OHX	AR	3505	-	0,6,6	0.00	-	-		
82	OHX	1	3631	-	0,6,6	0.00	-	-		
82	OHX	1	3612	-	0,6,6	0.00	-	-		
82	OHX	1	3447	-	0,6,6	0.00	-	-		
82	OHX	1	3452	-	0,6,6	0.00	-	-		
82	OHX	1	3550	-	0,6,6	0.00	-	-		
82	OHX	sR	2011	-	0,6,6	0.00	-	-		
82	OHX	1	3476	-	0,6,6	0.00	-	-		
82	OHX	1	3532	-	0,6,6	0.00	-	-		
82	OHX	AR	3402	-	0,6,6	0.00	-	-		
82	OHX	AR	3667	-	0,6,6	0.00	-	-		
82	OHX	AR	3646	-	0,6,6	0.00	-	-		
82	OHX	1	3420	-	0,6,6	0.00	-	-		
82	OHX	1	3541	-	0,6,6	0.00	-	-		
82	OHX	1	3484	-	0,6,6	0.00	-	-		
82	OHX	1	3548	-	0,6,6	0.00	-	-		
82	OHX	A	1885	-	0,6,6	0.00	-	-		
82	OHX	1	3477	-	0,6,6	0.00	-	-		
82	OHX	A	1811	-	0,6,6	0.00	-	-		
82	OHX	1	3425	-	0,6,6	0.00	-	-		
82	OHX	AR	3458	-	0,6,6	0.00	-	-		
82	OHX	AR	3464	-	0,6,6	0.00	-	-		
82	OHX	A	1820	-	0,6,6	0.00	-	-		
82	OHX	1	3421	-	0,6,6	0.00	-	-		
82	OHX	AR	3536	-	0,6,6	0.00	-	-		
82	OHX	AR	3405	-	0,6,6	0.00	-	-		
82	OHX	v	302	-	0,6,6	0.00	-	-		
82	OHX	A	1816	-	0,6,6	0.00	-	-		
82	OHX	AT	201	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	s4	301	-	0,6,6	0.00	-	-		
82	OHX	AR	3517	-	0,6,6	0.00	-	-		
82	OHX	AR	3587	-	0,6,6	0.00	-	-		
82	OHX	sR	1938	-	0,6,6	0.00	-	-		
82	OHX	1	3423	-	0,6,6	0.00	-	-		
82	OHX	AG	201	-	0,6,6	0.00	-	-		
82	OHX	1	3635	-	0,6,6	0.00	-	-		
82	OHX	AS	206	-	0,6,6	0.00	-	-		
82	OHX	AR	3606	-	0,6,6	0.00	-	-		
82	OHX	1	3594	-	0,6,6	0.00	-	-		
82	OHX	1	3634	-	0,6,6	0.00	-	-		
82	OHX	AR	3654	-	0,6,6	0.00	-	-		
82	OHX	A	1801	-	0,6,6	0.00	-	-		
82	OHX	4	207	-	0,6,6	0.00	-	-		
82	OHX	1	3474	-	0,6,6	0.00	-	-		
82	OHX	O	201	-	0,6,6	0.00	-	-		
82	OHX	1	3694	-	0,6,6	0.00	-	-		
82	OHX	AS	209	-	0,6,6	0.00	-	-		
82	OHX	1	3590	-	0,6,6	0.00	-	-		
82	OHX	AR	3600	-	0,6,6	0.00	-	-		
82	OHX	1	3646	-	0,6,6	0.00	-	-		
82	OHX	1	3507	-	0,6,6	0.00	-	-		
82	OHX	1	3405	-	0,6,6	0.00	-	-		
82	OHX	AR	3674	-	0,6,6	0.00	-	-		
82	OHX	sR	1954	-	0,6,6	0.00	-	-		
82	OHX	1	3699	-	0,6,6	0.00	-	-		
82	OHX	1	3618	-	0,6,6	0.00	-	-		
82	OHX	AR	3648	-	0,6,6	0.00	-	-		
82	OHX	1	3705	-	0,6,6	0.00	-	-		
82	OHX	AR	3626	-	0,6,6	0.00	-	-		
82	OHX	AR	3490	-	0,6,6	0.00	-	-		
82	OHX	AR	3673	-	0,6,6	0.00	-	-		
82	OHX	1	3644	-	0,6,6	0.00	-	-		
82	OHX	1	3629	-	0,6,6	0.00	-	-		
82	OHX	AR	3656	-	0,6,6	0.00	-	-		
82	OHX	AR	3659	-	0,6,6	0.00	-	-		
82	OHX	A	1927	-	0,6,6	0.00	-	-		
82	OHX	1	3442	-	0,6,6	0.00	-	-		
82	OHX	CQ	201	-	0,6,6	0.00	-	-		
82	OHX	AR	3519	-	0,6,6	0.00	-	-		
82	OHX	1	3552	-	0,6,6	0.00	-	-		
82	OHX	CE	402	-	0,6,6	0.00	-	-		
82	OHX	AR	3559	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	GOL	AR	4262	-	5,5,5	0.28	0	5,5,5	0.37	0
82	OHX	A	1817	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3512	-	0,6,6	0.00	-	-	-	-
82	OHX	sR	1969	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3448	-	0,6,6	0.00	-	-	-	-
82	OHX	A	1919	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3551	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3588	82	0,6,6	0.00	-	-	-	-
82	OHX	AR	3403	-	0,6,6	0.00	-	-	-	-
82	OHX	A	1893	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3529	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3722	-	0,6,6	0.00	-	-	-	-
82	OHX	sR	1949	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3438	-	0,6,6	0.00	-	-	-	-
82	OHX	sR	1921	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3500	-	0,6,6	0.00	-	-	-	-
82	OHX	T	201	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3631	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3596	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3725	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3715	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3418	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3565	-	0,6,6	0.00	-	-	-	-
82	OHX	sR	1967	-	0,6,6	0.00	-	-	-	-
82	OHX	CL	302	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3683	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3695	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3553	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3598	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3623	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3643	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3492	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3664	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3672	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3441	-	0,6,6	0.00	-	-	-	-
82	OHX	sR	2043	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3471	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3420	-	0,6,6	0.00	-	-	-	-
82	OHX	sR	2037	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3658	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3478	-	0,6,6	0.00	-	-	-	-
82	OHX	AR	3653	-	0,6,6	0.00	-	-	-	-
82	OHX	1	3651	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3560	-	0,6,6	0.00	-	-		
82	OHX	1	3677	-	0,6,6	0.00	-	-		
82	OHX	1	3708	-	0,6,6	0.00	-	-		
82	OHX	AR	3573	-	0,6,6	0.00	-	-		
82	OHX	1	3723	-	0,6,6	0.00	-	-		
82	OHX	3	201	-	0,6,6	0.00	-	-		
82	OHX	sR	1939	-	0,6,6	0.00	-	-		
82	OHX	1	3527	-	0,6,6	0.00	-	-		
82	OHX	1	3510	-	0,6,6	0.00	-	-		
82	OHX	A	1871	-	0,6,6	0.00	-	-		
82	OHX	1	3697	82	0,6,6	0.00	-	-		
82	OHX	AR	3423	-	0,6,6	0.00	-	-		
82	OHX	sR	1919	-	0,6,6	0.00	-	-		
82	OHX	AR	3426	-	0,6,6	0.00	-	-		
82	OHX	sR	2020	-	0,6,6	0.00	-	-		
82	OHX	1	3502	-	0,6,6	0.00	-	-		
82	OHX	A	1837	-	0,6,6	0.00	-	-		
82	OHX	AR	3485	-	0,6,6	0.00	-	-		
82	OHX	AR	3501	-	0,6,6	0.00	-	-		
82	OHX	A	1831	-	0,6,6	0.00	-	-		
82	OHX	A	1942	-	0,6,6	0.00	-	-		
82	OHX	AR	3689	-	0,6,6	0.00	-	-		
82	OHX	1	3669	-	0,6,6	0.00	-	-		
82	OHX	A	1924	-	0,6,6	0.00	-	-		
82	OHX	AR	3696	-	0,6,6	0.00	-	-		
82	OHX	sR	2001	-	0,6,6	0.00	-	-		
82	OHX	1	3531	-	0,6,6	0.00	-	-		
82	OHX	1	3604	-	0,6,6	0.00	-	-		
82	OHX	1	3670	-	0,6,6	0.00	-	-		
82	OHX	1	3563	-	0,6,6	0.00	-	-		
82	OHX	1	3449	-	0,6,6	0.00	-	-		
82	OHX	1	3451	-	0,6,6	0.00	-	-		
82	OHX	AR	3704	-	0,6,6	0.00	-	-		
82	OHX	AR	3557	-	0,6,6	0.00	-	-		
82	OHX	1	3545	-	0,6,6	0.00	-	-		
82	OHX	sR	2049	81	0,6,6	0.00	-	-		
82	OHX	1	3643	-	0,6,6	0.00	-	-		
82	OHX	AR	3410	-	0,6,6	0.00	-	-		
82	OHX	AR	3591	-	0,6,6	0.00	-	-		
82	OHX	AR	3728	-	0,6,6	0.00	-	-		
82	OHX	AR	3703	-	0,6,6	0.00	-	-		
82	OHX	AR	3537	-	0,6,6	0.00	-	-		
82	OHX	AR	3404	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	A	1930	-	0,6,6	0.00	-	-		
82	OHX	AR	3518	-	0,6,6	0.00	-	-		
82	OHX	AR	3614	-	0,6,6	0.00	-	-		
82	OHX	AR	3603	-	0,6,6	0.00	-	-		
82	OHX	A	1813	-	0,6,6	0.00	-	-		
82	OHX	1	3454	-	0,6,6	0.00	-	-		
82	OHX	sR	2028	-	0,6,6	0.00	-	-		
82	OHX	AR	3470	-	0,6,6	0.00	-	-		
82	OHX	A	1888	-	0,6,6	0.00	-	-		
82	OHX	AR	3450	-	0,6,6	0.00	-	-		
82	OHX	AR	3732	-	0,6,6	0.00	-	-		
82	OHX	AR	3572	-	0,6,6	0.00	-	-		
82	OHX	1	3435	-	0,6,6	0.00	-	-		
82	OHX	J	302	-	0,6,6	0.00	-	-		
82	OHX	v	301	-	0,6,6	0.00	-	-		
82	OHX	AR	3675	-	0,6,6	0.00	-	-		
82	OHX	AR	3544	-	0,6,6	0.00	-	-		
82	OHX	1	3401	-	0,6,6	0.00	-	-		
82	OHX	sR	1989	-	0,6,6	0.00	-	-		
82	OHX	d9	102	-	0,6,6	0.00	-	-		
82	OHX	AR	3521	-	0,6,6	0.00	-	-		
82	OHX	1	3692	-	0,6,6	0.00	-	-		
82	OHX	AR	3431	-	0,6,6	0.00	-	-		
82	OHX	1	3671	-	0,6,6	0.00	-	-		
82	OHX	AR	3538	-	0,6,6	0.00	-	-		
82	OHX	sR	1991	-	0,6,6	0.00	-	-		
82	OHX	AR	3547	-	0,6,6	0.00	-	-		
82	OHX	AE	201	-	0,6,6	0.00	-	-		
82	OHX	1	3491	-	0,6,6	0.00	-	-		
82	OHX	sR	2027	-	0,6,6	0.00	-	-		
82	OHX	AR	3480	-	0,6,6	0.00	-	-		
82	OHX	CK	201	-	0,6,6	0.00	-	-		
82	OHX	1	3406	-	0,6,6	0.00	-	-		
82	OHX	AR	3714	-	0,6,6	0.00	-	-		
82	OHX	1	3415	-	0,6,6	0.00	-	-		
82	OHX	sR	1907	-	0,6,6	0.00	-	-		
82	OHX	A	1929	-	0,6,6	0.00	-	-		
82	OHX	AR	3642	-	0,6,6	0.00	-	-		
82	OHX	1	3567	-	0,6,6	0.00	-	-		
82	OHX	Q	201	-	0,6,6	0.00	-	-		
82	OHX	AR	3734	-	0,6,6	0.00	-	-		
82	OHX	AC	101	-	0,6,6	0.00	-	-		
82	OHX	AR	3510	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	1988	-	0,6,6	0.00	-	-		
82	OHX	AR	3641	-	0,6,6	0.00	-	-		
82	OHX	1	3680	-	0,6,6	0.00	-	-		
82	OHX	AR	3727	-	0,6,6	0.00	-	-		
82	OHX	A	1887	-	0,6,6	0.00	-	-		
82	OHX	sR	2035	-	0,6,6	0.00	-	-		
82	OHX	1	3461	-	0,6,6	0.00	-	-		
82	OHX	AT	216	-	0,6,6	0.00	-	-		
82	OHX	A	1815	-	0,6,6	0.00	-	-		
82	OHX	sR	1941	-	0,6,6	0.00	-	-		
82	OHX	1	3547	-	0,6,6	0.00	-	-		
82	OHX	A	1867	-	0,6,6	0.00	-	-		
86	GOL	AR	4263	-	5,5,5	0.07	0	5,5,5	0.24	0
82	OHX	1	3429	-	0,6,6	0.00	-	-		
82	OHX	AR	3422	-	0,6,6	0.00	-	-		
82	OHX	1	3592	-	0,6,6	0.00	-	-		
82	OHX	4	213	-	0,6,6	0.00	-	-		
82	OHX	1	3445	-	0,6,6	0.00	-	-		
82	OHX	sR	2029	-	0,6,6	0.00	-	-		
82	OHX	1	3667	-	0,6,6	0.00	-	-		
82	OHX	AR	3532	-	0,6,6	0.00	-	-		
82	OHX	sR	1999	-	0,6,6	0.00	-	-		
82	OHX	sR	2013	-	0,6,6	0.00	-	-		
82	OHX	AR	3514	-	0,6,6	0.00	-	-		
82	OHX	sR	2032	-	0,6,6	0.00	-	-		
82	OHX	1	3475	-	0,6,6	0.00	-	-		
82	OHX	AR	3669	-	0,6,6	0.00	-	-		
82	OHX	1	3597	-	0,6,6	0.00	-	-		
82	OHX	A	1829	-	0,6,6	0.00	-	-		
82	OHX	sR	1937	-	0,6,6	0.00	-	-		
82	OHX	1	3689	-	0,6,6	0.00	-	-		
82	OHX	AR	3562	-	0,6,6	0.00	-	-		
82	OHX	sR	1932	-	0,6,6	0.00	-	-		
82	OHX	1	3439	-	0,6,6	0.00	-	-		
82	OHX	1	3436	-	0,6,6	0.00	-	-		
82	OHX	A	1849	-	0,6,6	0.00	-	-		
82	OHX	A	1851	-	0,6,6	0.00	-	-		
82	OHX	AR	3601	-	0,6,6	0.00	-	-		
82	OHX	AR	3655	-	0,6,6	0.00	-	-		
82	OHX	3	208	-	0,6,6	0.00	-	-		
82	OHX	AR	3534	-	0,6,6	0.00	-	-		
82	OHX	AR	3594	-	0,6,6	0.00	-	-		
82	OHX	1	3668	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3501	-	0,6,6	0.00	-	-		
82	OHX	DH	201	-	0,6,6	0.00	-	-		
82	OHX	1	3591	-	0,6,6	0.00	-	-		
82	OHX	1	3608	-	0,6,6	0.00	-	-		
82	OHX	1	3602	-	0,6,6	0.00	-	-		
82	OHX	sR	1935	-	0,6,6	0.00	-	-		
82	OHX	1	3455	-	0,6,6	0.00	-	-		
82	OHX	4	201	-	0,6,6	0.00	-	-		
82	OHX	r	301	-	0,6,6	0.00	-	-		
82	OHX	AR	3409	-	0,6,6	0.00	-	-		
82	OHX	1	3431	-	0,6,6	0.00	-	-		
82	OHX	1	3468	-	0,6,6	0.00	-	-		
82	OHX	1	3622	-	0,6,6	0.00	-	-		
82	OHX	sR	2042	-	0,6,6	0.00	-	-		
82	OHX	sR	2008	-	0,6,6	0.00	-	-		
82	OHX	AT	211	-	0,6,6	0.00	-	-		
82	OHX	AR	3496	-	0,6,6	0.00	-	-		
82	OHX	1	3466	-	0,6,6	0.00	-	-		
82	OHX	AR	3708	-	0,6,6	0.00	-	-		
82	OHX	1	3605	-	0,6,6	0.00	-	-		
82	OHX	1	3437	-	0,6,6	0.00	-	-		
82	OHX	A	1810	-	0,6,6	0.00	-	-		
82	OHX	sR	1975	-	0,6,6	0.00	-	-		
82	OHX	AR	3701	-	0,6,6	0.00	-	-		
82	OHX	AR	3692	-	0,6,6	0.00	-	-		
82	OHX	AR	3457	-	0,6,6	0.00	-	-		
82	OHX	sR	1958	-	0,6,6	0.00	-	-		
82	OHX	DQ	502	-	0,6,6	0.00	-	-		
82	OHX	AR	3726	-	0,6,6	0.00	-	-		
82	OHX	AR	3729	-	0,6,6	0.00	-	-		
82	OHX	AR	3694	-	0,6,6	0.00	-	-		
82	OHX	AR	3662	-	0,6,6	0.00	-	-		
82	OHX	AR	3556	-	0,6,6	0.00	-	-		
82	OHX	1	3498	-	0,6,6	0.00	-	-		
82	OHX	AR	3553	-	0,6,6	0.00	-	-		
82	OHX	1	3411	-	0,6,6	0.00	-	-		
82	OHX	1	3499	-	0,6,6	0.00	-	-		
82	OHX	d4	201	-	0,6,6	0.00	-	-		
82	OHX	1	3709	-	0,6,6	0.00	-	-		
82	OHX	1	3702	-	0,6,6	0.00	-	-		
82	OHX	A	1910	-	0,6,6	0.00	-	-		
82	OHX	1	3520	-	0,6,6	0.00	-	-		
82	OHX	1	3457	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3680	-	0,6,6	0.00	-	-		
82	OHX	sR	2038	-	0,6,6	0.00	-	-		
82	OHX	AR	3460	-	0,6,6	0.00	-	-		
82	OHX	1	3570	-	0,6,6	0.00	-	-		
82	OHX	1	3408	-	0,6,6	0.00	-	-		
82	OHX	1	3661	-	0,6,6	0.00	-	-		
82	OHX	A	1884	-	0,6,6	0.00	-	-		
82	OHX	A	1802	-	0,6,6	0.00	-	-		
82	OHX	sR	1985	-	0,6,6	0.00	-	-		
82	OHX	A	1897	47	0,6,6	0.00	-	-		
82	OHX	AR	3671	-	0,6,6	0.00	-	-		
82	OHX	1	3453	-	0,6,6	0.00	-	-		
82	OHX	1	3703	-	0,6,6	0.00	-	-		
82	OHX	1	3497	-	0,6,6	0.00	-	-		
82	OHX	1	3578	-	0,6,6	0.00	-	-		
82	OHX	A	1805	-	0,6,6	0.00	-	-		
82	OHX	AT	215	-	0,6,6	0.00	-	-		
82	OHX	AT	202	-	0,6,6	0.00	-	-		
82	OHX	sR	1980	-	0,6,6	0.00	-	-		
82	OHX	AR	3638	-	0,6,6	0.00	-	-		
82	OHX	1	3623	-	0,6,6	0.00	-	-		
82	OHX	AR	3445	-	0,6,6	0.00	-	-		
82	OHX	A	1894	-	0,6,6	0.00	-	-		
82	OHX	sR	1936	-	0,6,6	0.00	-	-		
82	OHX	AR	3584	-	0,6,6	0.00	-	-		
82	OHX	sR	2007	-	0,6,6	0.00	-	-		
82	OHX	AR	3523	-	0,6,6	0.00	-	-		
82	OHX	AR	3593	-	0,6,6	0.00	-	-		
82	OHX	AR	3599	-	0,6,6	0.00	-	-		
82	OHX	AR	3596	-	0,6,6	0.00	-	-		
82	OHX	1	3521	-	0,6,6	0.00	-	-		
82	OHX	sR	1979	-	0,6,6	0.00	-	-		
82	OHX	A	1895	-	0,6,6	0.00	-	-		
82	OHX	AT	213	-	0,6,6	0.00	-	-		
82	OHX	A	1861	-	0,6,6	0.00	-	-		
82	OHX	1	3657	-	0,6,6	0.00	-	-		
82	OHX	e	102	-	0,6,6	0.00	-	-		
82	OHX	1	3549	-	0,6,6	0.00	-	-		
82	OHX	AR	3417	-	0,6,6	0.00	-	-		
82	OHX	CE	401	-	0,6,6	0.00	-	-		
82	OHX	sR	1944	-	0,6,6	0.00	-	-		
82	OHX	AR	3723	82	0,6,6	0.00	-	-		
82	OHX	AR	3717	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3519	-	0,6,6	0.00	-	-		
82	OHX	sR	1995	-	0,6,6	0.00	-	-		
82	OHX	AR	3554	-	0,6,6	0.00	-	-		
82	OHX	AR	3452	-	0,6,6	0.00	-	-		
82	OHX	A	1821	-	0,6,6	0.00	-	-		
82	OHX	A	1846	-	0,6,6	0.00	-	-		
82	OHX	1	3681	-	0,6,6	0.00	-	-		
82	OHX	1	3579	-	0,6,6	0.00	-	-		
82	OHX	AR	3558	-	0,6,6	0.00	-	-		
82	OHX	A	1830	-	0,6,6	0.00	-	-		
82	OHX	AR	3526	82	0,6,6	0.00	-	-		
82	OHX	AR	3700	-	0,6,6	0.00	-	-		
82	OHX	Rb	401	-	0,6,6	0.00	-	-		
82	OHX	y	201	-	0,6,6	0.00	-	-		
82	OHX	AR	3604	-	0,6,6	0.00	-	-		
82	OHX	1	3432	-	0,6,6	0.00	-	-		
82	OHX	z	201	-	0,6,6	0.00	-	-		
82	OHX	AR	3477	-	0,6,6	0.00	-	-		
82	OHX	AS	210	-	0,6,6	0.00	-	-		
82	OHX	sR	2019	-	0,6,6	0.00	-	-		
82	OHX	AR	3619	-	0,6,6	0.00	-	-		
82	OHX	1	3490	-	0,6,6	0.00	-	-		
82	OHX	sR	1926	-	0,6,6	0.00	-	-		
82	OHX	1	3599	-	0,6,6	0.00	-	-		
82	OHX	A	1804	-	0,6,6	0.00	-	-		
82	OHX	1	3682	-	0,6,6	0.00	-	-		
82	OHX	sR	1978	-	0,6,6	0.00	-	-		
82	OHX	CX	201	-	0,6,6	0.00	-	-		
82	OHX	AR	3685	-	0,6,6	0.00	-	-		
82	OHX	A	1920	82	0,6,6	0.00	-	-		
82	OHX	AR	3625	-	0,6,6	0.00	-	-		
82	OHX	AR	3542	-	0,6,6	0.00	-	-		
82	OHX	AR	3414	-	0,6,6	0.00	-	-		
82	OHX	1	3467	-	0,6,6	0.00	-	-		
82	OHX	AT	208	-	0,6,6	0.00	-	-		
82	OHX	3	206	-	0,6,6	0.00	-	-		
82	OHX	sR	1966	-	0,6,6	0.00	-	-		
82	OHX	3	203	-	0,6,6	0.00	-	-		
82	OHX	AR	3447	-	0,6,6	0.00	-	-		
82	OHX	sR	1963	-	0,6,6	0.00	-	-		
82	OHX	A	1818	-	0,6,6	0.00	-	-		
82	OHX	AR	3563	-	0,6,6	0.00	-	-		
82	OHX	1	3529	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3606	-	0,6,6	0.00	-	-		
82	OHX	sR	1972	-	0,6,6	0.00	-	-		
82	OHX	sR	1955	-	0,6,6	0.00	-	-		
82	OHX	A	1809	82	0,6,6	0.00	-	-		
82	OHX	1	3444	-	0,6,6	0.00	-	-		
82	OHX	1	3625	-	0,6,6	0.00	-	-		
82	OHX	AR	3488	-	0,6,6	0.00	-	-		
82	OHX	sR	1976	-	0,6,6	0.00	-	-		
82	OHX	1	3575	-	0,6,6	0.00	-	-		
82	OHX	A	1926	-	0,6,6	0.00	-	-		
82	OHX	AR	3511	-	0,6,6	0.00	-	-		
82	OHX	1	3722	-	0,6,6	0.00	-	-		
82	OHX	1	3482	-	0,6,6	0.00	-	-		
82	OHX	AR	3451	-	0,6,6	0.00	-	-		
82	OHX	1	3672	-	0,6,6	0.00	-	-		
82	OHX	sR	1964	-	0,6,6	0.00	-	-		
82	OHX	AR	3712	-	0,6,6	0.00	-	-		
82	OHX	AR	3709	82	0,6,6	0.00	-	-		
82	OHX	sR	1983	-	0,6,6	0.00	-	-		
82	OHX	1	3713	-	0,6,6	0.00	-	-		
82	OHX	1	3666	-	0,6,6	0.00	-	-		
82	OHX	AR	3449	-	0,6,6	0.00	-	-		
82	OHX	A	1923	-	0,6,6	0.00	-	-		
82	OHX	1	3659	-	0,6,6	0.00	-	-		
82	OHX	AR	3471	-	0,6,6	0.00	-	-		
82	OHX	sR	2046	-	0,6,6	0.00	-	-		
82	OHX	A	1917	-	0,6,6	0.00	-	-		
82	OHX	1	3427	-	0,6,6	0.00	-	-		
82	OHX	c3	201	-	0,6,6	0.00	-	-		
82	OHX	AR	3612	-	0,6,6	0.00	-	-		
82	OHX	sR	2030	-	0,6,6	0.00	-	-		
82	OHX	1	3675	-	0,6,6	0.00	-	-		
82	OHX	AR	3491	-	0,6,6	0.00	-	-		
82	OHX	AR	3668	-	0,6,6	0.00	-	-		
82	OHX	AR	3436	-	0,6,6	0.00	-	-		
82	OHX	AR	3645	-	0,6,6	0.00	-	-		
82	OHX	AR	3446	-	0,6,6	0.00	-	-		
82	OHX	A	1866	-	0,6,6	0.00	-	-		
82	OHX	1	3492	-	0,6,6	0.00	-	-		
82	OHX	1	3704	-	0,6,6	0.00	-	-		
82	OHX	sR	1977	-	0,6,6	0.00	-	-		
82	OHX	AR	3430	-	0,6,6	0.00	-	-		
82	OHX	sR	2021	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	2036	-	0,6,6	0.00	-	-		
82	OHX	AR	3495	-	0,6,6	0.00	-	-		
82	OHX	sR	1947	-	0,6,6	0.00	-	-		
82	OHX	AR	3425	-	0,6,6	0.00	-	-		
82	OHX	1	3438	-	0,6,6	0.00	-	-		
82	OHX	1	3653	-	0,6,6	0.00	-	-		
82	OHX	AR	3621	-	0,6,6	0.00	-	-		
82	OHX	CX	202	-	0,6,6	0.00	-	-		
82	OHX	sR	2048	-	0,6,6	0.00	-	-		
82	OHX	A	1803	-	0,6,6	0.00	-	-		
82	OHX	1	3404	-	0,6,6	0.00	-	-		
82	OHX	A	1863	-	0,6,6	0.00	-	-		
82	OHX	AR	3421	-	0,6,6	0.00	-	-		
82	OHX	AR	3541	-	0,6,6	0.00	-	-		
82	OHX	1	3533	-	0,6,6	0.00	-	-		
82	OHX	AR	3533	-	0,6,6	0.00	-	-		
82	OHX	AR	3582	-	0,6,6	0.00	-	-		
82	OHX	CL	301	-	0,6,6	0.00	-	-		
82	OHX	A	1822	82	0,6,6	0.00	-	-		
82	OHX	AR	3736	-	0,6,6	0.00	-	-		
82	OHX	1	3652	-	0,6,6	0.00	-	-		
82	OHX	1	3434	-	0,6,6	0.00	-	-		
82	OHX	3	202	-	0,6,6	0.00	-	-		
82	OHX	sR	1971	-	0,6,6	0.00	-	-		
82	OHX	AR	3428	-	0,6,6	0.00	-	-		
82	OHX	AR	3583	-	0,6,6	0.00	-	-		
82	OHX	1	3628	-	0,6,6	0.00	-	-		
82	OHX	1	3627	-	0,6,6	0.00	-	-		
82	OHX	1	3446	-	0,6,6	0.00	-	-		
82	OHX	AS	203	-	0,6,6	0.00	-	-		
82	OHX	sR	1927	-	0,6,6	0.00	-	-		
82	OHX	A	1872	-	0,6,6	0.00	-	-		
82	OHX	1	3428	-	0,6,6	0.00	-	-		
82	OHX	sR	1909	-	0,6,6	0.00	-	-		
82	OHX	1	3518	-	0,6,6	0.00	-	-		
82	OHX	1	3508	-	0,6,6	0.00	-	-		
82	OHX	1	3662	-	0,6,6	0.00	-	-		
82	OHX	A	1841	-	0,6,6	0.00	-	-		
82	OHX	AR	3524	-	0,6,6	0.00	-	-		
82	OHX	AR	3718	-	0,6,6	0.00	-	-		
82	OHX	AR	3540	-	0,6,6	0.00	-	-		
82	OHX	AR	3640	-	0,6,6	0.00	-	-		
82	OHX	sR	1924	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3515	-	0,6,6	0.00	-	-		
82	OHX	AR	3474	-	0,6,6	0.00	-	-		
82	OHX	AR	3515	-	0,6,6	0.00	-	-		
82	OHX	1	3685	-	0,6,6	0.00	-	-		
82	OHX	AR	3411	-	0,6,6	0.00	-	-		
82	OHX	1	3721	1	0,6,6	0.00	-	-		
82	OHX	A	1939	-	0,6,6	0.00	-	-		
82	OHX	1	3641	-	0,6,6	0.00	-	-		
82	OHX	1	3607	-	0,6,6	0.00	-	-		
82	OHX	AR	3408	-	0,6,6	0.00	-	-		
82	OHX	1	3610	-	0,6,6	0.00	-	-		
82	OHX	AR	3478	-	0,6,6	0.00	-	-		
82	OHX	1	3633	-	0,6,6	0.00	-	-		
82	OHX	AR	3506	-	0,6,6	0.00	-	-		
82	OHX	sR	2044	-	0,6,6	0.00	-	-		
82	OHX	AR	3437	-	0,6,6	0.00	-	-		
82	OHX	1	3542	-	0,6,6	0.00	-	-		
82	OHX	1	3486	-	0,6,6	0.00	-	-		
82	OHX	1	3509	-	0,6,6	0.00	-	-		
82	OHX	AT	203	82	0,6,6	0.00	-	-		
82	OHX	AR	3629	-	0,6,6	0.00	-	-		
82	OHX	AR	3585	-	0,6,6	0.00	-	-		
82	OHX	AR	3720	-	0,6,6	0.00	-	-		
82	OHX	1	3402	-	0,6,6	0.00	-	-		
82	OHX	sR	1910	-	0,6,6	0.00	-	-		
82	OHX	sR	1934	-	0,6,6	0.00	-	-		
82	OHX	4	203	-	0,6,6	0.00	-	-		
82	OHX	AR	3697	-	0,6,6	0.00	-	-		
82	OHX	sR	2034	-	0,6,6	0.00	-	-		
82	OHX	A	1882	-	0,6,6	0.00	-	-		
82	OHX	sR	2012	-	0,6,6	0.00	-	-		
82	OHX	AR	3456	-	0,6,6	0.00	-	-		
84	G5B	1	4224	-	27,28,28	0.39	0	33,45,45	0.91	2 (6%)
82	OHX	A	1891	-	0,6,6	0.00	-	-		
82	OHX	sR	2009	-	0,6,6	0.00	-	-		
82	OHX	1	3616	-	0,6,6	0.00	-	-		
82	OHX	CO	201	-	0,6,6	0.00	-	-		
82	OHX	AR	3652	-	0,6,6	0.00	-	-		
82	OHX	AR	3574	-	0,6,6	0.00	-	-		
82	OHX	A	1905	-	0,6,6	0.00	-	-		
82	OHX	AR	3657	-	0,6,6	0.00	-	-		
82	OHX	A	1900	-	0,6,6	0.00	-	-		
82	OHX	sR	2031	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3479	-	0,6,6	0.00	-	-		
82	OHX	1	3561	-	0,6,6	0.00	-	-		
82	OHX	sR	2023	-	0,6,6	0.00	-	-		
82	OHX	A	1844	-	0,6,6	0.00	-	-		
82	OHX	AR	3531	-	0,6,6	0.00	-	-		
82	OHX	AR	3633	-	0,6,6	0.00	-	-		
82	OHX	A	1826	-	0,6,6	0.00	-	-		
82	OHX	sR	1916	-	0,6,6	0.00	-	-		
82	OHX	AR	3617	-	0,6,6	0.00	-	-		
82	OHX	AR	3527	-	0,6,6	0.00	-	-		
82	OHX	A	1853	-	0,6,6	0.00	-	-		
82	OHX	x	201	-	0,6,6	0.00	-	-		
82	OHX	AS	207	-	0,6,6	0.00	-	-		
82	OHX	1	3412	-	0,6,6	0.00	-	-		
82	OHX	AR	3539	-	0,6,6	0.00	-	-		
82	OHX	A	1857	-	0,6,6	0.00	-	-		
82	OHX	AR	3439	-	0,6,6	0.00	-	-		
82	OHX	sR	2025	-	0,6,6	0.00	-	-		
82	OHX	A	1843	-	0,6,6	0.00	-	-		
82	OHX	AR	3650	-	0,6,6	0.00	-	-		
82	OHX	AR	3647	-	0,6,6	0.00	-	-		
82	OHX	sR	1929	-	0,6,6	0.00	-	-		
82	OHX	A	1907	-	0,6,6	0.00	-	-		
82	OHX	1	3485	-	0,6,6	0.00	-	-		
82	OHX	sR	2005	-	0,6,6	0.00	-	-		
82	OHX	4	210	-	0,6,6	0.00	-	-		
82	OHX	A	1933	-	0,6,6	0.00	-	-		
82	OHX	A	1915	-	0,6,6	0.00	-	-		
82	OHX	1	3656	-	0,6,6	0.00	-	-		
82	OHX	1	3655	-	0,6,6	0.00	-	-		
82	OHX	1	3463	-	0,6,6	0.00	-	-		
82	OHX	A	1901	-	0,6,6	0.00	-	-		
82	OHX	A	1874	-	0,6,6	0.00	-	-		
82	OHX	AR	3698	-	0,6,6	0.00	-	-		
82	OHX	A	1858	-	0,6,6	0.00	-	-		
82	OHX	1	3690	82	0,6,6	0.00	-	-		
82	OHX	AS	204	-	0,6,6	0.00	-	-		
82	OHX	sR	1940	-	0,6,6	0.00	-	-		
82	OHX	AR	3738	-	0,6,6	0.00	-	-		
82	OHX	AT	212	82	0,6,6	0.00	-	-		
82	OHX	1	3472	-	0,6,6	0.00	-	-		
82	OHX	AR	3608	-	0,6,6	0.00	-	-		
82	OHX	1	3551	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3674	-	0,6,6	0.00	-	-		
82	OHX	AR	3586	-	0,6,6	0.00	-	-		
82	OHX	AT	206	-	0,6,6	0.00	-	-		
82	OHX	1	3688	-	0,6,6	0.00	-	-		
84	G5B	AR	4264	-	27,28,28	0.41	0	33,45,45	0.51	0
82	OHX	1	3626	-	0,6,6	0.00	-	-		
82	OHX	c8	201	-	0,6,6	0.00	-	-		
82	OHX	sR	1925	-	0,6,6	0.00	-	-		
82	OHX	1	3617	-	0,6,6	0.00	-	-		
82	OHX	1	3422	-	0,6,6	0.00	-	-		
82	OHX	sR	1952	-	0,6,6	0.00	-	-		
82	OHX	A	1937	-	0,6,6	0.00	-	-		
82	OHX	AR	3555	-	0,6,6	0.00	-	-		
82	OHX	1	3695	-	0,6,6	0.00	-	-		
82	OHX	1	3678	-	0,6,6	0.00	-	-		
82	OHX	A	1842	-	0,6,6	0.00	-	-		
82	OHX	AR	3730	-	0,6,6	0.00	-	-		
82	OHX	1	3523	-	0,6,6	0.00	-	-		
82	OHX	AR	3512	-	0,6,6	0.00	-	-		
82	OHX	1	3693	-	0,6,6	0.00	-	-		
82	OHX	A	1807	-	0,6,6	0.00	-	-		
82	OHX	A	1892	-	0,6,6	0.00	-	-		
82	OHX	sR	2018	-	0,6,6	0.00	-	-		
82	OHX	AR	3618	-	0,6,6	0.00	-	-		
82	OHX	AR	3453	-	0,6,6	0.00	-	-		
82	OHX	AR	3412	-	0,6,6	0.00	-	-		
82	OHX	CH	201	-	0,6,6	0.00	-	-		
82	OHX	AR	3509	-	0,6,6	0.00	-	-		
82	OHX	1	3524	-	0,6,6	0.00	-	-		
82	OHX	A	1840	-	0,6,6	0.00	-	-		
82	OHX	AR	3548	-	0,6,6	0.00	-	-		
82	OHX	AR	3639	-	0,6,6	0.00	-	-		
82	OHX	A	1852	-	0,6,6	0.00	-	-		
82	OHX	AR	3683	-	0,6,6	0.00	-	-		
82	OHX	sR	1943	-	0,6,6	0.00	-	-		
82	OHX	4	212	-	0,6,6	0.00	-	-		
82	OHX	AR	3440	-	0,6,6	0.00	-	-		
82	OHX	AR	3661	-	0,6,6	0.00	-	-		
82	OHX	AR	3610	-	0,6,6	0.00	-	-		
82	OHX	AR	3418	-	0,6,6	0.00	-	-		
82	OHX	1	3664	-	0,6,6	0.00	-	-		
82	OHX	AR	3615	-	0,6,6	0.00	-	-		
82	OHX	sR	1953	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	CP	501	-	0,6,6	0.00	-	-		
82	OHX	AR	3592	-	0,6,6	0.00	-	-		
82	OHX	1	3691	-	0,6,6	0.00	-	-		
82	OHX	sR	1942	-	0,6,6	0.00	-	-		
82	OHX	1	3719	-	0,6,6	0.00	-	-		
82	OHX	1	3470	-	0,6,6	0.00	-	-		
82	OHX	AR	3721	-	0,6,6	0.00	-	-		
82	OHX	1	3493	-	0,6,6	0.00	-	-		
82	OHX	1	3700	-	0,6,6	0.00	-	-		
82	OHX	1	3687	-	0,6,6	0.00	-	-		
82	OHX	1	3556	-	0,6,6	0.00	-	-		
82	OHX	1	3600	-	0,6,6	0.00	-	-		
82	OHX	AR	3568	-	0,6,6	0.00	-	-		
82	OHX	sR	1928	-	0,6,6	0.00	-	-		
82	OHX	AR	3442	-	0,6,6	0.00	-	-		
82	OHX	AR	3463	-	0,6,6	0.00	-	-		
82	OHX	A	1836	-	0,6,6	0.00	-	-		
82	OHX	AR	3567	-	0,6,6	0.00	-	-		
82	OHX	CM	201	-	0,6,6	0.00	-	-		
82	OHX	1	3572	-	0,6,6	0.00	-	-		
82	OHX	A	1932	-	0,6,6	0.00	-	-		
82	OHX	1	3410	-	0,6,6	0.00	-	-		
82	OHX	sR	2004	-	0,6,6	0.00	-	-		
82	OHX	AR	3475	-	0,6,6	0.00	-	-		
82	OHX	s1	301	-	0,6,6	0.00	-	-		
82	OHX	sR	2014	-	0,6,6	0.00	-	-		
82	OHX	A	1854	-	0,6,6	0.00	-	-		
82	OHX	sR	1996	-	0,6,6	0.00	-	-		
82	OHX	A	1941	47	0,6,6	0.00	-	-		
82	OHX	AR	3407	-	0,6,6	0.00	-	-		
82	OHX	A	1859	-	0,6,6	0.00	-	-		
82	OHX	1	3544	-	0,6,6	0.00	-	-		
82	OHX	1	3488	-	0,6,6	0.00	-	-		
82	OHX	AR	3605	-	0,6,6	0.00	-	-		
82	OHX	1	3450	-	0,6,6	0.00	-	-		
82	OHX	1	3464	-	0,6,6	0.00	-	-		
82	OHX	A	1833	-	0,6,6	0.00	-	-		
82	OHX	4	208	-	0,6,6	0.00	-	-		
82	OHX	4	209	-	0,6,6	0.00	-	-		
82	OHX	1	3582	-	0,6,6	0.00	-	-		
82	OHX	AR	3580	-	0,6,6	0.00	-	-		
82	OHX	1	3536	-	0,6,6	0.00	-	-		
82	OHX	AR	3609	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3555	-	0,6,6	0.00	-	-		
82	OHX	1	3525	-	0,6,6	0.00	-	-		
82	OHX	AR	3679	-	0,6,6	0.00	-	-		
82	OHX	A	1886	-	0,6,6	0.00	-	-		
82	OHX	3	205	-	0,6,6	0.00	-	-		
82	OHX	A	1865	-	0,6,6	0.00	-	-		
82	OHX	sR	1968	-	0,6,6	0.00	-	-		
82	OHX	1	3426	-	0,6,6	0.00	-	-		
82	OHX	sR	1961	-	0,6,6	0.00	-	-		
82	OHX	1	3496	-	0,6,6	0.00	-	-		
82	OHX	AR	3624	-	0,6,6	0.00	-	-		
82	OHX	A	1828	-	0,6,6	0.00	-	-		
82	OHX	AR	3681	-	0,6,6	0.00	-	-		
82	OHX	AR	3590	-	0,6,6	0.00	-	-		
82	OHX	AR	3520	-	0,6,6	0.00	-	-		
82	OHX	A	1904	-	0,6,6	0.00	-	-		
82	OHX	1	3637	-	0,6,6	0.00	-	-		
82	OHX	1	3489	-	0,6,6	0.00	-	-		
82	OHX	AR	3486	-	0,6,6	0.00	-	-		
82	OHX	1	3663	-	0,6,6	0.00	-	-		
82	OHX	AT	207	-	0,6,6	0.00	-	-		
82	OHX	1	3603	-	0,6,6	0.00	-	-		
82	OHX	AR	3670	-	0,6,6	0.00	-	-		
82	OHX	1	3528	-	0,6,6	0.00	-	-		
82	OHX	1	3514	-	0,6,6	0.00	-	-		
82	OHX	AR	3713	-	0,6,6	0.00	-	-		
82	OHX	AR	3507	-	0,6,6	0.00	-	-		
82	OHX	sR	1984	-	0,6,6	0.00	-	-		
82	OHX	AR	3688	-	0,6,6	0.00	-	-		
82	OHX	sR	1981	-	0,6,6	0.00	-	-		
82	OHX	AR	3607	-	0,6,6	0.00	-	-		
82	OHX	1	3717	-	0,6,6	0.00	-	-		
82	OHX	1	3487	-	0,6,6	0.00	-	-		
82	OHX	CG	301	-	0,6,6	0.00	-	-		
82	OHX	1	3473	-	0,6,6	0.00	-	-		
82	OHX	AR	3578	-	0,6,6	0.00	-	-		
82	OHX	2	201	-	0,6,6	0.00	-	-		
82	OHX	sR	2022	-	0,6,6	0.00	-	-		
82	OHX	1	3649	-	0,6,6	0.00	-	-		
82	OHX	AR	3616	-	0,6,6	0.00	-	-		
82	OHX	1	3686	-	0,6,6	0.00	-	-		
82	OHX	sR	2016	-	0,6,6	0.00	-	-		
82	OHX	1	3583	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3459	-	0,6,6	0.00	-	-		
82	OHX	AR	3462	-	0,6,6	0.00	-	-		
82	OHX	1	3413	-	0,6,6	0.00	-	-		
82	OHX	AR	3444	-	0,6,6	0.00	-	-		
82	OHX	A	1814	-	0,6,6	0.00	-	-		
82	OHX	A	1918	-	0,6,6	0.00	-	-		
82	OHX	AR	3552	-	0,6,6	0.00	-	-		
82	OHX	A	1847	-	0,6,6	0.00	-	-		
82	OHX	1	3707	-	0,6,6	0.00	-	-		
82	OHX	sR	1974	-	0,6,6	0.00	-	-		
82	OHX	1	3589	-	0,6,6	0.00	-	-		
82	OHX	AR	3711	-	0,6,6	0.00	-	-		
82	OHX	1	3414	-	0,6,6	0.00	-	-		
82	OHX	AT	210	-	0,6,6	0.00	-	-		
82	OHX	sR	1915	-	0,6,6	0.00	-	-		
82	OHX	sR	1920	-	0,6,6	0.00	-	-		
82	OHX	AR	3569	-	0,6,6	0.00	-	-		
82	OHX	1	3543	-	0,6,6	0.00	-	-		
82	OHX	k	401	-	0,6,6	0.00	-	-		
82	OHX	3	209	-	0,6,6	0.00	-	-		
82	OHX	A	1935	-	0,6,6	0.00	-	-		
82	OHX	1	3624	-	0,6,6	0.00	-	-		
82	OHX	l	401	-	0,6,6	0.00	-	-		
82	OHX	1	3645	-	0,6,6	0.00	-	-		
82	OHX	AR	3454	-	0,6,6	0.00	-	-		
82	OHX	AR	3483	-	0,6,6	0.00	-	-		
82	OHX	1	3465	-	0,6,6	0.00	-	-		
82	OHX	AR	3602	-	0,6,6	0.00	-	-		
82	OHX	A	1825	-	0,6,6	0.00	-	-		
82	OHX	1	3407	-	0,6,6	0.00	-	-		
82	OHX	A	1925	-	0,6,6	0.00	-	-		
82	OHX	1	3639	-	0,6,6	0.00	-	-		
82	OHX	AR	3543	-	0,6,6	0.00	-	-		
82	OHX	AR	3564	-	0,6,6	0.00	-	-		
82	OHX	1	3712	-	0,6,6	0.00	-	-		
82	OHX	1	3460	-	0,6,6	0.00	-	-		
82	OHX	A	1916	-	0,6,6	0.00	-	-		
82	OHX	1	3716	-	0,6,6	0.00	-	-		
82	OHX	1	3546	-	0,6,6	0.00	-	-		
82	OHX	AP	502	-	0,6,6	0.00	-	-		
82	OHX	A	1921	-	0,6,6	0.00	-	-		
82	OHX	1	3559	-	0,6,6	0.00	-	-		
82	OHX	1	3676	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	A	1855	-	0,6,6	0.00	-	-		
82	OHX	1	3619	-	0,6,6	0.00	-	-		
82	OHX	1	3660	-	0,6,6	0.00	-	-		
82	OHX	AR	3484	-	0,6,6	0.00	-	-		
82	OHX	A	1869	-	0,6,6	0.00	-	-		
82	OHX	1	3665	-	0,6,6	0.00	-	-		
82	OHX	AR	3622	-	0,6,6	0.00	-	-		
82	OHX	AR	3504	-	0,6,6	0.00	-	-		
82	OHX	1	3424	-	0,6,6	0.00	-	-		
82	OHX	1	3609	-	0,6,6	0.00	-	-		
82	OHX	A	1875	-	0,6,6	0.00	-	-		
82	OHX	A	1928	-	0,6,6	0.00	-	-		
82	OHX	A	1908	-	0,6,6	0.00	-	-		
82	OHX	1	3647	-	0,6,6	0.00	-	-		
82	OHX	h	401	-	0,6,6	0.00	-	-		
82	OHX	sR	2003	-	0,6,6	0.00	-	-		
82	OHX	1	3539	-	0,6,6	0.00	-	-		
82	OHX	AR	3733	-	0,6,6	0.00	-	-		
82	OHX	AR	3434	-	0,6,6	0.00	-	-		
82	OHX	AR	3611	-	0,6,6	0.00	-	-		
82	OHX	AR	3702	-	0,6,6	0.00	-	-		
82	OHX	AR	3560	-	0,6,6	0.00	-	-		
82	OHX	AR	3546	-	0,6,6	0.00	-	-		
82	OHX	1	3537	82	0,6,6	0.00	-	-		
82	OHX	s8	301	-	0,6,6	0.00	-	-		
82	OHX	AR	3693	-	0,6,6	0.00	-	-		
82	OHX	1	3587	-	0,6,6	0.00	-	-		
82	OHX	1	3505	-	0,6,6	0.00	-	-		
82	OHX	AR	3636	-	0,6,6	0.00	-	-		
82	OHX	AR	3716	-	0,6,6	0.00	-	-		
82	OHX	sR	1997	-	0,6,6	0.00	-	-		
82	OHX	A	1898	-	0,6,6	0.00	-	-		
82	OHX	1	3558	-	0,6,6	0.00	-	-		
82	OHX	AR	3513	-	0,6,6	0.00	-	-		
82	OHX	1	3534	-	0,6,6	0.00	-	-		
82	OHX	A	1922	-	0,6,6	0.00	-	-		
82	OHX	AR	3530	-	0,6,6	0.00	-	-		
82	OHX	A	1864	-	0,6,6	0.00	-	-		
82	OHX	AR	3577	-	0,6,6	0.00	-	-		
82	OHX	1	3443	-	0,6,6	0.00	-	-		
82	OHX	AS	205	-	0,6,6	0.00	-	-		
82	OHX	1	3568	-	0,6,6	0.00	-	-		
82	OHX	AT	214	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AS	208	-	0,6,6	0.00	-	-		
82	OHX	1	3511	-	0,6,6	0.00	-	-		
82	OHX	1	3504	-	0,6,6	0.00	-	-		
82	OHX	1	3593	-	0,6,6	0.00	-	-		
82	OHX	1	3562	-	0,6,6	0.00	-	-		
82	OHX	1	3632	-	0,6,6	0.00	-	-		
82	OHX	1	3458	-	0,6,6	0.00	-	-		
82	OHX	sR	2002	-	0,6,6	0.00	-	-		
82	OHX	sR	2015	-	0,6,6	0.00	-	-		
82	OHX	sR	2041	-	0,6,6	0.00	-	-		
82	OHX	1	3571	-	0,6,6	0.00	-	-		
82	OHX	AR	3497	-	0,6,6	0.00	-	-		
82	OHX	sR	1901	-	0,6,6	0.00	-	-		
82	OHX	AR	3489	-	0,6,6	0.00	-	-		
82	OHX	AR	3660	-	0,6,6	0.00	-	-		
82	OHX	A	1835	-	0,6,6	0.00	-	-		
82	OHX	AR	3628	-	0,6,6	0.00	-	-		
82	OHX	A	1848	-	0,6,6	0.00	-	-		
82	OHX	sR	1918	-	0,6,6	0.00	-	-		
82	OHX	A	1845	-	0,6,6	0.00	-	-		
82	OHX	AR	3651	-	0,6,6	0.00	-	-		
82	OHX	w	201	-	0,6,6	0.00	-	-		
82	OHX	1	3698	-	0,6,6	0.00	-	-		
82	OHX	4	202	-	0,6,6	0.00	-	-		
82	OHX	A	1902	-	0,6,6	0.00	-	-		
82	OHX	sR	1946	-	0,6,6	0.00	-	-		
82	OHX	4	211	-	0,6,6	0.00	-	-		
82	OHX	AR	3481	-	0,6,6	0.00	-	-		
82	OHX	1	3714	-	0,6,6	0.00	-	-		
82	OHX	A	1824	-	0,6,6	0.00	-	-		
82	OHX	1	3595	-	0,6,6	0.00	-	-		
82	OHX	1	3684	-	0,6,6	0.00	-	-		
82	OHX	AT	209	-	0,6,6	0.00	-	-		
82	OHX	A	1877	-	0,6,6	0.00	-	-		
82	OHX	A	1878	-	0,6,6	0.00	-	-		
82	OHX	1	3650	-	0,6,6	0.00	-	-		
82	OHX	A	1823	-	0,6,6	0.00	-	-		
82	OHX	sR	2000	-	0,6,6	0.00	-	-		
82	OHX	1	3469	-	0,6,6	0.00	-	-		
82	OHX	sR	1917	-	0,6,6	0.00	-	-		
82	OHX	AR	3466	-	0,6,6	0.00	-	-		
82	OHX	AR	3635	-	0,6,6	0.00	-	-		
82	OHX	AR	3598	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3441	-	0,6,6	0.00	-	-		
82	OHX	AR	3566	-	0,6,6	0.00	-	-		
82	OHX	AR	3710	-	0,6,6	0.00	-	-		
82	OHX	A	1940	-	0,6,6	0.00	-	-		
82	OHX	sR	1948	-	0,6,6	0.00	-	-		
82	OHX	AR	3561	-	0,6,6	0.00	-	-		
82	OHX	AR	3589	-	0,6,6	0.00	-	-		
82	OHX	sR	1922	-	0,6,6	0.00	-	-		
82	OHX	AR	3476	-	0,6,6	0.00	-	-		
82	OHX	A	1812	-	0,6,6	0.00	-	-		
82	OHX	AR	3468	-	0,6,6	0.00	-	-		
82	OHX	AR	3499	-	0,6,6	0.00	-	-		
82	OHX	A	1868	-	0,6,6	0.00	-	-		
82	OHX	AR	3433	-	0,6,6	0.00	-	-		
82	OHX	AS	202	-	0,6,6	0.00	-	-		
82	OHX	1	3416	-	0,6,6	0.00	-	-		
82	OHX	AR	3632	-	0,6,6	0.00	-	-		
82	OHX	AR	3550	-	0,6,6	0.00	-	-		
82	OHX	1	3554	-	0,6,6	0.00	-	-		
82	OHX	sR	1906	-	0,6,6	0.00	-	-		
82	OHX	1	3621	-	0,6,6	0.00	-	-		
82	OHX	A	1879	-	0,6,6	0.00	-	-		
82	OHX	1	3503	-	0,6,6	0.00	-	-		
82	OHX	sR	1970	-	0,6,6	0.00	-	-		
82	OHX	AR	3443	82	0,6,6	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	G5B	1	4224	-	-	1/8/62/62	0/3/3/3
86	GOL	AR	4263	-	-	0/4/4/4	-
86	GOL	AR	4262	-	-	2/4/4/4	-
84	G5B	AR	4264	-	-	1/8/62/62	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	1	4224	G5B	C11-C6-C5	-3.63	109.39	114.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	1	4224	G5B	C11-C6-C9	2.28	117.03	113.71

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	AR	4262	GOL	C1-C2-C3-O3
86	AR	4262	GOL	O2-C2-C3-O3
84	1	4224	G5B	C6-C11-C16-O1
84	AR	4264	G5B	C6-C11-C16-O1

There are no ring outliers.

540 monomers are involved in 924 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3663	OHX	1	0
82	A	1911	OHX	1	0
82	DD	101	OHX	1	0
82	AR	3706	OHX	1	0
82	AR	3677	OHX	1	0
82	1	3566	OHX	4	0
82	AR	3448	OHX	1	0
82	1	3613	OHX	2	0
82	AR	3576	OHX	1	0
82	AR	3691	OHX	9	0
82	AR	3467	OHX	1	0
82	1	3526	OHX	2	0
82	1	3440	OHX	1	0
82	AR	3406	OHX	3	0
82	AR	3427	OHX	1	0
82	1	3513	OHX	1	0
82	1	3456	OHX	1	0
82	1	3581	OHX	2	0
82	AR	3465	OHX	1	0
82	AR	3684	OHX	3	0
82	AR	3565	OHX	1	0
82	AR	3719	OHX	1	0
82	AR	3473	OHX	1	0
82	AR	3644	OHX	3	0
82	AR	3570	OHX	1	0
82	A	1839	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	3417	OHX	3	0
82	A	1856	OHX	1	0
82	A	1934	OHX	2	0
82	AK	102	OHX	5	0
82	AR	3581	OHX	3	0
82	1	3540	OHX	1	0
82	DG	201	OHX	1	0
82	AT	205	OHX	1	0
82	AR	3419	OHX	3	0
82	A	1931	OHX	1	0
82	1	3576	OHX	1	0
82	1	3573	OHX	1	0
82	AR	3435	OHX	1	0
82	AR	3493	OHX	2	0
82	1	3494	OHX	1	0
82	CF	401	OHX	4	0
82	AT	204	OHX	1	0
82	1	3483	OHX	1	0
82	AR	3525	OHX	1	0
82	1	3574	OHX	1	0
82	CG	303	OHX	1	0
82	AR	3424	OHX	1	0
82	1	3462	OHX	1	0
82	AR	3455	OHX	1	0
82	AR	3472	OHX	1	0
82	4	206	OHX	1	0
82	AK	103	OHX	1	0
82	AR	3469	OHX	1	0
82	CG	302	OHX	6	0
82	1	3530	OHX	1	0
82	AR	3597	OHX	4	0
82	AR	3637	OHX	1	0
82	1	3630	OHX	1	0
82	1	3569	OHX	1	0
82	AR	3620	OHX	1	0
82	1	3711	OHX	2	0
82	1	3517	OHX	3	0
82	A	1876	OHX	7	0
82	A	1903	OHX	1	0
82	AR	3678	OHX	1	0
82	AR	3479	OHX	9	0
82	1	3710	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	A	1896	OHX	1	0
82	1	3614	OHX	1	0
82	1	3585	OHX	2	0
82	1	3403	OHX	2	0
82	1	3580	OHX	2	0
82	A	1881	OHX	2	0
82	A	1870	OHX	2	0
82	1	3648	OHX	1	0
82	AR	3571	OHX	3	0
82	A	1850	OHX	1	0
82	4	214	OHX	1	0
82	1	3459	OHX	2	0
82	A	1936	OHX	5	0
82	A	1883	OHX	2	0
82	1	3673	OHX	8	0
82	1	3535	OHX	2	0
82	1	3706	OHX	1	0
82	AR	3676	OHX	2	0
82	AR	3401	OHX	1	0
82	AR	3508	OHX	1	0
82	A	1862	OHX	2	0
82	4	205	OHX	1	0
82	1	3611	OHX	1	0
82	AR	3579	OHX	3	0
82	1	3409	OHX	2	0
82	1	3522	OHX	3	0
82	A	1873	OHX	3	0
82	AR	3503	OHX	7	0
82	AR	3461	OHX	1	0
82	1	3516	OHX	3	0
82	3	207	OHX	2	0
82	1	3481	OHX	1	0
82	AR	3649	OHX	1	0
82	1	3577	OHX	4	0
82	AR	3735	OHX	3	0
82	AR	3687	OHX	1	0
82	AR	3505	OHX	2	0
82	1	3631	OHX	1	0
82	1	3612	OHX	1	0
82	1	3476	OHX	1	0
82	1	3532	OHX	2	0
82	AR	3402	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	3541	OHX	2	0
82	A	1885	OHX	1	0
82	1	3477	OHX	1	0
82	1	3425	OHX	4	0
82	AR	3458	OHX	4	0
82	A	1820	OHX	1	0
82	AR	3536	OHX	4	0
82	AR	3405	OHX	1	0
82	AT	201	OHX	2	0
82	AR	3517	OHX	1	0
82	AR	3587	OHX	1	0
82	AG	201	OHX	1	0
82	AR	3606	OHX	1	0
82	AR	3654	OHX	2	0
82	A	1801	OHX	2	0
82	4	207	OHX	1	0
82	1	3474	OHX	2	0
82	1	3694	OHX	1	0
82	AS	209	OHX	8	0
82	1	3590	OHX	4	0
82	AR	3600	OHX	2	0
82	1	3646	OHX	1	0
82	1	3405	OHX	4	0
82	AR	3674	OHX	2	0
82	1	3699	OHX	1	0
82	1	3618	OHX	2	0
82	AR	3648	OHX	2	0
82	1	3705	OHX	4	0
82	AR	3626	OHX	1	0
82	AR	3490	OHX	1	0
82	1	3629	OHX	1	0
82	AR	3659	OHX	1	0
82	A	1927	OHX	1	0
82	1	3442	OHX	1	0
82	CQ	201	OHX	1	0
82	CE	402	OHX	1	0
82	AR	3559	OHX	2	0
82	A	1817	OHX	3	0
82	A	1919	OHX	2	0
82	AR	3551	OHX	1	0
82	1	3588	OHX	6	0
82	AR	3403	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3529	OHX	2	0
82	AR	3438	OHX	1	0
82	1	3500	OHX	2	0
82	T	201	OHX	2	0
82	AR	3631	OHX	1	0
82	AR	3725	OHX	4	0
82	1	3418	OHX	2	0
82	1	3683	OHX	6	0
82	AR	3695	OHX	1	0
82	1	3553	OHX	6	0
82	1	3598	OHX	1	0
82	AR	3623	OHX	1	0
82	AR	3643	OHX	1	0
82	AR	3492	OHX	1	0
82	AR	3672	OHX	1	0
82	1	3441	OHX	1	0
82	AR	3420	OHX	2	0
82	1	3478	OHX	2	0
82	AR	3653	OHX	2	0
82	1	3560	OHX	1	0
82	1	3677	OHX	4	0
82	1	3708	OHX	1	0
82	1	3723	OHX	4	0
82	3	201	OHX	1	0
82	1	3510	OHX	1	0
82	A	1871	OHX	1	0
82	1	3697	OHX	7	0
82	AR	3423	OHX	1	0
82	1	3502	OHX	1	0
82	A	1837	OHX	1	0
82	AR	3485	OHX	1	0
82	AR	3501	OHX	2	0
82	A	1831	OHX	1	0
82	A	1942	OHX	2	0
82	AR	3696	OHX	5	0
82	1	3531	OHX	1	0
82	1	3604	OHX	1	0
82	1	3670	OHX	1	0
82	1	3563	OHX	1	0
82	1	3449	OHX	1	0
82	1	3451	OHX	2	0
82	AR	3704	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3557	OHX	1	0
82	1	3643	OHX	1	0
82	AR	3591	OHX	1	0
82	AR	3728	OHX	7	0
82	AR	3404	OHX	1	0
82	A	1930	OHX	1	0
82	A	1813	OHX	1	0
82	1	3454	OHX	1	0
82	AR	3470	OHX	1	0
82	A	1888	OHX	2	0
82	AR	3572	OHX	2	0
82	J	302	OHX	2	0
82	1	3401	OHX	2	0
82	AR	3521	OHX	1	0
82	1	3692	OHX	1	0
82	AR	3538	OHX	6	0
82	AR	3547	OHX	1	0
82	AE	201	OHX	9	0
82	1	3491	OHX	1	0
82	AR	3714	OHX	1	0
82	1	3567	OHX	2	0
82	Q	201	OHX	1	0
82	AR	3734	OHX	2	0
82	AC	101	OHX	2	0
82	AR	3510	OHX	2	0
82	AR	3641	OHX	2	0
82	AR	3727	OHX	1	0
82	A	1887	OHX	1	0
82	1	3461	OHX	1	0
82	AT	216	OHX	2	0
82	A	1815	OHX	1	0
82	1	3547	OHX	2	0
82	A	1867	OHX	5	0
82	AR	3422	OHX	1	0
82	1	3592	OHX	1	0
82	1	3667	OHX	4	0
82	AR	3514	OHX	2	0
82	AR	3669	OHX	3	0
82	1	3689	OHX	1	0
82	AR	3562	OHX	2	0
82	1	3439	OHX	1	0
82	A	1851	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3601	OHX	1	0
82	AR	3655	OHX	1	0
82	AR	3534	OHX	1	0
82	1	3668	OHX	2	0
82	1	3501	OHX	1	0
82	1	3591	OHX	1	0
82	AR	3409	OHX	2	0
82	1	3468	OHX	2	0
82	AT	211	OHX	2	0
82	AR	3708	OHX	1	0
82	1	3437	OHX	1	0
82	A	1810	OHX	2	0
82	AR	3692	OHX	5	0
82	DQ	502	OHX	4	0
82	AR	3694	OHX	2	0
82	AR	3556	OHX	1	0
82	1	3498	OHX	2	0
82	1	3411	OHX	1	0
82	A	1910	OHX	1	0
82	1	3520	OHX	1	0
82	1	3457	OHX	1	0
82	AR	3680	OHX	1	0
82	AR	3460	OHX	1	0
82	1	3408	OHX	1	0
82	1	3661	OHX	1	0
82	A	1884	OHX	1	0
82	A	1897	OHX	4	0
82	1	3703	OHX	1	0
82	1	3497	OHX	1	0
82	1	3578	OHX	4	0
82	AT	202	OHX	1	0
82	AR	3638	OHX	2	0
82	1	3623	OHX	2	0
82	AR	3445	OHX	1	0
82	A	1894	OHX	1	0
82	AR	3584	OHX	4	0
82	AR	3523	OHX	9	0
82	AR	3593	OHX	6	0
82	AR	3596	OHX	1	0
82	1	3521	OHX	1	0
82	A	1895	OHX	1	0
82	AT	213	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	A	1861	OHX	2	0
82	CE	401	OHX	3	0
82	AR	3723	OHX	6	0
82	AR	3717	OHX	1	0
82	1	3519	OHX	1	0
82	1	3681	OHX	4	0
82	1	3579	OHX	2	0
82	AR	3558	OHX	6	0
82	A	1830	OHX	1	0
82	AR	3526	OHX	4	0
82	AR	3700	OHX	1	0
82	AR	3604	OHX	1	0
82	AR	3477	OHX	1	0
82	AR	3619	OHX	1	0
82	1	3490	OHX	1	0
82	A	1804	OHX	3	0
82	1	3682	OHX	6	0
82	AR	3685	OHX	3	0
82	A	1920	OHX	5	0
82	AR	3542	OHX	3	0
82	AR	3414	OHX	1	0
82	1	3467	OHX	4	0
82	AT	208	OHX	2	0
82	A	1818	OHX	1	0
82	A	1809	OHX	7	0
82	1	3444	OHX	1	0
82	AR	3488	OHX	1	0
82	A	1926	OHX	3	0
82	1	3722	OHX	5	0
82	1	3482	OHX	1	0
82	AR	3451	OHX	2	0
82	AR	3709	OHX	11	0
82	1	3713	OHX	1	0
82	1	3666	OHX	2	0
82	AR	3449	OHX	1	0
82	A	1923	OHX	1	0
82	AR	3471	OHX	1	0
82	1	3427	OHX	1	0
82	AR	3612	OHX	2	0
82	1	3675	OHX	1	0
82	AR	3668	OHX	1	0
82	AR	3436	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3645	OHX	2	0
82	AR	3446	OHX	1	0
82	A	1866	OHX	1	0
82	AR	3425	OHX	1	0
82	1	3438	OHX	1	0
82	1	3653	OHX	1	0
82	AR	3621	OHX	1	0
82	CX	202	OHX	1	0
82	A	1803	OHX	1	0
82	A	1863	OHX	4	0
82	AR	3421	OHX	1	0
82	AR	3541	OHX	1	0
82	1	3533	OHX	1	0
82	AR	3533	OHX	2	0
82	AR	3582	OHX	1	0
82	CL	301	OHX	6	0
82	A	1822	OHX	7	0
82	AR	3736	OHX	4	0
82	1	3652	OHX	1	0
82	1	3434	OHX	1	0
82	AR	3583	OHX	1	0
82	1	3628	OHX	1	0
82	1	3627	OHX	1	0
82	AS	203	OHX	8	0
82	A	1872	OHX	1	0
82	1	3428	OHX	1	0
82	1	3518	OHX	1	0
82	1	3508	OHX	2	0
82	1	3662	OHX	3	0
82	A	1841	OHX	1	0
82	AR	3474	OHX	1	0
82	AR	3515	OHX	1	0
82	1	3721	OHX	4	0
82	A	1939	OHX	1	0
82	1	3641	OHX	2	0
82	AR	3408	OHX	2	0
82	AR	3478	OHX	1	0
82	AR	3506	OHX	1	0
82	AR	3437	OHX	1	0
82	1	3486	OHX	1	0
82	1	3509	OHX	7	0
82	AT	203	OHX	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3629	OHX	1	0
82	AR	3720	OHX	2	0
82	1	3402	OHX	1	0
82	AR	3697	OHX	1	0
82	A	1882	OHX	1	0
84	1	4224	G5B	1	0
82	AR	3574	OHX	1	0
82	AR	3657	OHX	1	0
82	A	1900	OHX	1	0
82	1	3561	OHX	1	0
82	A	1844	OHX	2	0
82	AR	3531	OHX	2	0
82	AR	3617	OHX	1	0
82	AR	3527	OHX	1	0
82	A	1853	OHX	6	0
82	1	3412	OHX	1	0
82	A	1843	OHX	3	0
82	AR	3650	OHX	2	0
82	AR	3647	OHX	1	0
82	A	1907	OHX	2	0
82	4	210	OHX	1	0
82	A	1933	OHX	1	0
82	1	3656	OHX	1	0
82	A	1874	OHX	1	0
82	AR	3698	OHX	1	0
82	1	3690	OHX	4	0
82	AS	204	OHX	1	0
82	AR	3738	OHX	3	0
82	AT	212	OHX	11	0
82	1	3472	OHX	1	0
82	1	3551	OHX	2	0
82	1	3688	OHX	1	0
82	1	3617	OHX	4	0
82	1	3695	OHX	1	0
82	1	3678	OHX	1	0
82	A	1842	OHX	1	0
82	AR	3730	OHX	2	0
82	1	3693	OHX	2	0
82	A	1892	OHX	2	0
82	AR	3412	OHX	2	0
82	CH	201	OHX	2	0
82	AR	3509	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	A	1840	OHX	1	0
82	AR	3639	OHX	2	0
82	A	1852	OHX	1	0
82	AR	3683	OHX	4	0
82	AR	3440	OHX	1	0
82	AR	3610	OHX	1	0
82	AR	3418	OHX	3	0
82	1	3664	OHX	1	0
82	AR	3615	OHX	1	0
82	CP	501	OHX	1	0
82	1	3691	OHX	1	0
82	1	3719	OHX	8	0
82	1	3493	OHX	4	0
82	1	3700	OHX	1	0
82	1	3687	OHX	2	0
82	1	3600	OHX	1	0
82	AR	3568	OHX	1	0
82	AR	3442	OHX	1	0
82	AR	3463	OHX	5	0
82	A	1836	OHX	1	0
82	AR	3567	OHX	2	0
82	1	3410	OHX	1	0
82	A	1854	OHX	1	0
82	A	1941	OHX	6	0
82	AR	3407	OHX	1	0
82	A	1859	OHX	1	0
82	AR	3605	OHX	1	0
82	1	3450	OHX	1	0
82	1	3464	OHX	1	0
82	1	3536	OHX	3	0
82	AR	3609	OHX	1	0
82	A	1886	OHX	5	0
82	3	205	OHX	1	0
82	A	1865	OHX	1	0
82	1	3426	OHX	1	0
82	AR	3624	OHX	1	0
82	AR	3590	OHX	1	0
82	AR	3520	OHX	1	0
82	1	3637	OHX	1	0
82	AR	3486	OHX	4	0
82	1	3663	OHX	1	0
82	AT	207	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	3603	OHX	1	0
82	1	3528	OHX	1	0
82	AR	3688	OHX	1	0
82	1	3487	OHX	2	0
82	CG	301	OHX	1	0
82	1	3473	OHX	1	0
82	1	3649	OHX	1	0
82	AR	3616	OHX	1	0
82	1	3686	OHX	1	0
82	1	3583	OHX	1	0
82	AR	3462	OHX	1	0
82	1	3413	OHX	1	0
82	AR	3444	OHX	1	0
82	A	1814	OHX	2	0
82	AR	3552	OHX	2	0
82	A	1847	OHX	1	0
82	1	3589	OHX	2	0
82	AR	3711	OHX	1	0
82	1	3414	OHX	2	0
82	AT	210	OHX	3	0
82	AR	3569	OHX	4	0
82	A	1935	OHX	1	0
82	1	3624	OHX	3	0
82	1	3645	OHX	1	0
82	AR	3483	OHX	1	0
82	A	1825	OHX	2	0
82	1	3407	OHX	2	0
82	AR	3564	OHX	1	0
82	1	3712	OHX	1	0
82	1	3460	OHX	2	0
82	A	1916	OHX	2	0
82	AP	502	OHX	3	0
82	1	3676	OHX	1	0
82	A	1855	OHX	1	0
82	1	3660	OHX	3	0
82	AR	3484	OHX	2	0
82	AR	3622	OHX	1	0
82	AR	3504	OHX	6	0
82	1	3424	OHX	1	0
82	A	1928	OHX	1	0
82	A	1908	OHX	1	0
82	1	3647	OHX	1	0

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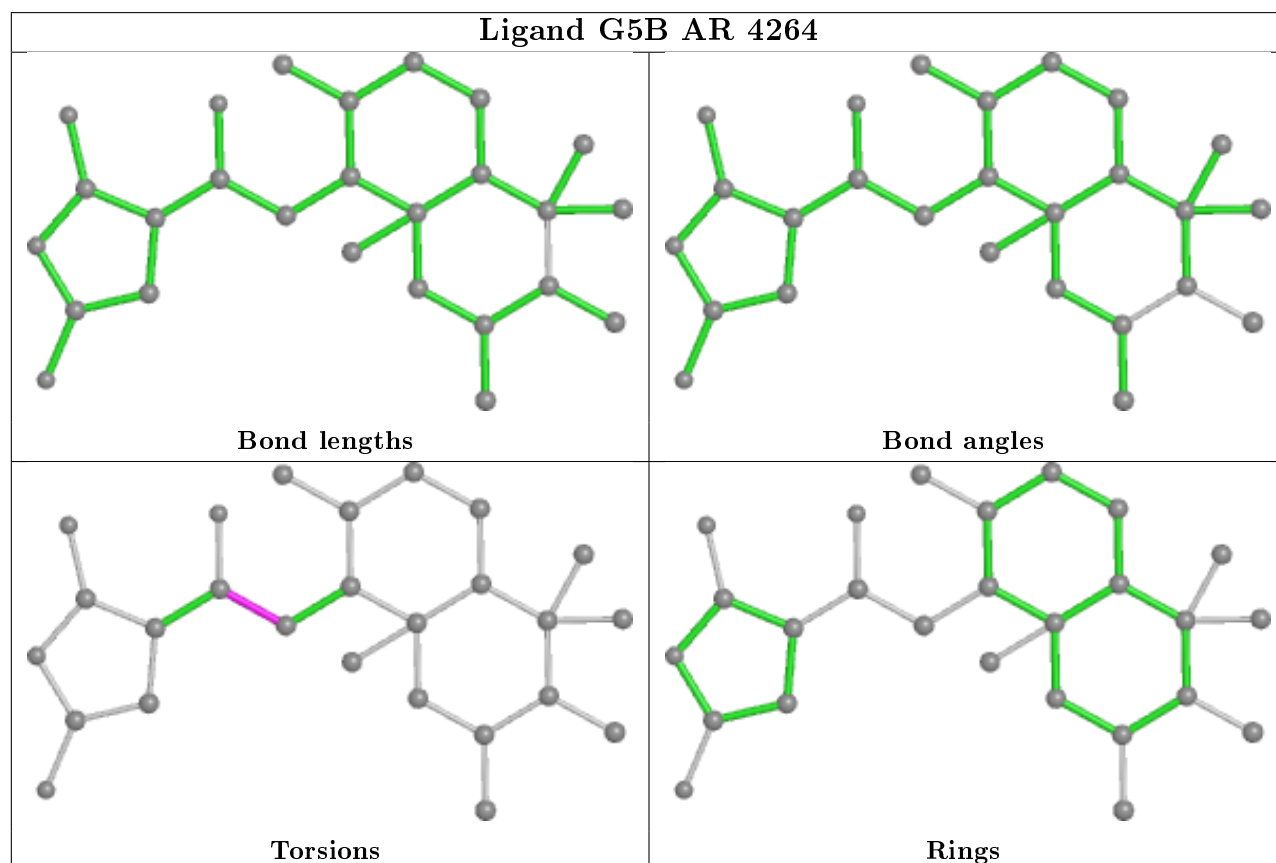
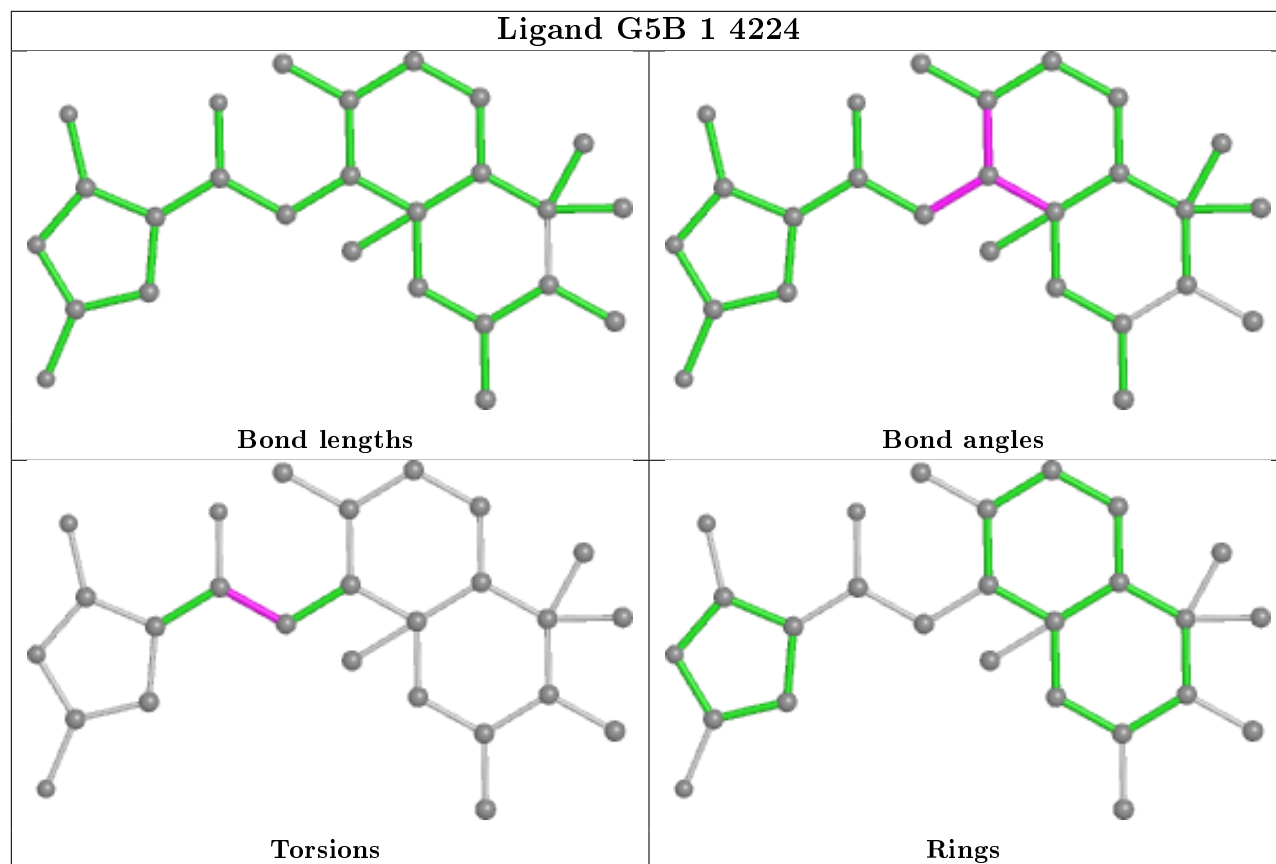
Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	3539	OHX	1	0
82	AR	3733	OHX	3	0
82	AR	3434	OHX	1	0
82	AR	3611	OHX	1	0
82	AR	3702	OHX	2	0
82	1	3537	OHX	6	0
82	AR	3693	OHX	7	0
82	1	3505	OHX	6	0
82	AR	3636	OHX	1	0
82	AR	3716	OHX	1	0
82	A	1898	OHX	1	0
82	AR	3513	OHX	7	0
82	AR	3530	OHX	4	0
82	A	1864	OHX	1	0
82	AR	3577	OHX	2	0
82	1	3443	OHX	2	0
82	AS	205	OHX	2	0
82	1	3568	OHX	1	0
82	AT	214	OHX	1	0
82	1	3511	OHX	1	0
82	1	3504	OHX	1	0
82	1	3562	OHX	6	0
82	1	3632	OHX	1	0
82	AR	3497	OHX	1	0
82	AR	3489	OHX	1	0
82	AR	3628	OHX	1	0
82	4	202	OHX	2	0
82	A	1902	OHX	1	0
82	AR	3481	OHX	1	0
82	1	3714	OHX	2	0
82	1	3595	OHX	2	0
82	1	3684	OHX	1	0
82	AT	209	OHX	1	0
82	A	1877	OHX	1	0
82	1	3650	OHX	1	0
82	A	1823	OHX	3	0
82	1	3469	OHX	1	0
82	AR	3466	OHX	1	0
82	AR	3598	OHX	5	0
82	AR	3441	OHX	2	1
82	AR	3561	OHX	1	0
82	AR	3589	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3468	OHX	1	0
82	A	1868	OHX	2	0
82	AR	3433	OHX	1	0
82	AS	202	OHX	1	0
82	1	3416	OHX	2	0
82	AR	3632	OHX	3	0
82	AR	3550	OHX	1	0
82	1	3554	OHX	1	0
82	1	3621	OHX	1	0
82	AR	3443	OHX	6	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	s0	1
58	c0	1
47	A	1
14	t	1
52	s4	1
52	F	1
7	CG	1

The worst 5 of 7 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	9.26
1	A	1716:C	O3'	1717:G	P	4.20
1	t	132:ALA	C	133:PRO	N	1.75
1	F	82:TYR	C	83:PRO	N	1.18
1	s0	160:ILE	C	161:PRO	N	1.16

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	3149/3396 (92%)	-0.03	116 (3%) 41 21	20, 42, 104, 200	0
1	AR	3147/3396 (92%)	-0.03	97 (3%) 49 26	21, 40, 100, 196	0
2	3	121/121 (100%)	-0.31	0 100 100	34, 58, 70, 71	0
2	AS	121/121 (100%)	-0.31	0 100 100	27, 43, 53, 56	0
3	4	158/158 (100%)	-0.23	2 (1%) 77 59	24, 40, 73, 107	0
3	AT	158/158 (100%)	-0.17	2 (1%) 77 59	29, 48, 78, 95	0
4	CD	252/254 (99%)	-0.28	3 (1%) 79 61	25, 40, 57, 64	0
4	j	252/254 (99%)	-0.28	0 100 100	25, 39, 53, 62	0
5	CE	386/387 (99%)	-0.31	2 (0%) 91 81	22, 33, 43, 76	0
5	k	386/387 (99%)	-0.28	1 (0%) 94 88	28, 44, 54, 64	0
6	CF	361/362 (99%)	-0.38	1 (0%) 94 88	25, 39, 53, 67	0
6	l	361/362 (99%)	-0.36	0 100 100	21, 34, 49, 56	0
7	CG	296/297 (99%)	-0.09	7 (2%) 59 37	34, 44, 64, 79	0
7	m	296/297 (99%)	-0.02	3 (1%) 82 67	41, 61, 74, 95	0
8	CH	156/176 (88%)	-0.28	1 (0%) 89 78	33, 41, 58, 70	0
8	n	156/176 (88%)	-0.35	0 100 100	33, 37, 49, 62	0
9	CI	222/244 (90%)	-0.37	3 (1%) 75 56	26, 31, 61, 93	0
9	o	222/244 (90%)	-0.37	3 (1%) 75 56	27, 33, 52, 79	0
10	CJ	233/256 (91%)	0.58	20 (8%) 10 4	54, 64, 94, 103	0
10	p	233/256 (91%)	-0.01	9 (3%) 39 20	45, 57, 85, 93	0
11	CK	191/191 (100%)	-0.27	3 (1%) 72 51	33, 39, 53, 62	0
11	q	191/191 (100%)	0.02	4 (2%) 63 43	42, 52, 62, 72	0
12	CL	211/221 (95%)	-0.21	4 (1%) 66 46	26, 39, 62, 90	0
12	r	211/221 (95%)	-0.10	2 (0%) 84 69	29, 42, 73, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CM	169/174 (97%)	-0.22	2 (1%) 79 61	36, 51, 65, 76	0
13	s	169/174 (97%)	-0.00	0 100 100	51, 67, 76, 82	0
14	CN	193/199 (96%)	0.06	5 (2%) 56 33	26, 49, 80, 95	0
14	t	193/199 (96%)	-0.15	2 (1%) 82 67	23, 41, 73, 95	0
15	CO	136/138 (98%)	-0.42	1 (0%) 87 75	31, 36, 53, 68	0
15	u	136/138 (98%)	-0.28	1 (0%) 87 75	34, 42, 53, 60	0
16	CP	203/204 (99%)	-0.25	0 100 100	28, 44, 53, 57	0
16	v	203/204 (99%)	-0.34	0 100 100	24, 37, 46, 51	0
17	CQ	197/199 (98%)	-0.37	3 (1%) 73 54	23, 26, 51, 56	0
17	w	197/199 (98%)	-0.40	0 100 100	27, 33, 48, 50	0
18	CR	183/184 (99%)	0.95	27 (14%) 2 1	25, 31, 109, 140	0
18	x	183/184 (99%)	0.06	9 (4%) 29 14	28, 35, 76, 106	0
19	CS	185/186 (99%)	-0.25	0 100 100	28, 39, 47, 53	0
19	y	185/186 (99%)	-0.35	0 100 100	27, 36, 48, 65	0
20	CT	188/189 (99%)	0.17	11 (5%) 22 10	38, 49, 119, 134	0
20	z	188/189 (99%)	0.25	8 (4%) 35 17	43, 55, 125, 139	0
21	0	172/172 (100%)	-0.37	1 (0%) 89 78	33, 40, 50, 54	0
21	CU	172/172 (100%)	-0.39	1 (0%) 89 78	28, 32, 40, 48	0
22	2	159/160 (99%)	-0.20	1 (0%) 89 78	27, 40, 73, 80	0
22	CV	159/160 (99%)	-0.23	0 100 100	24, 34, 67, 73	0
23	5	100/121 (82%)	0.47	5 (5%) 28 13	71, 82, 89, 95	0
23	CW	100/121 (82%)	0.76	10 (10%) 7 2	60, 70, 76, 90	0
24	6	136/137 (99%)	-0.24	1 (0%) 87 75	31, 40, 48, 52	0
24	CX	136/137 (99%)	-0.13	3 (2%) 62 41	24, 32, 42, 45	0
25	7	98/155 (63%)	1.03	25 (25%) 0 0	40, 52, 124, 127	0
25	CY	124/155 (80%)	0.03	7 (5%) 24 11	32, 64, 109, 125	0
26	8	121/142 (85%)	-0.17	1 (0%) 86 72	36, 46, 59, 90	0
26	CZ	121/142 (85%)	0.02	6 (4%) 28 13	38, 49, 68, 78	0
27	9	126/127 (99%)	-0.07	1 (0%) 86 72	27, 42, 51, 54	0
27	DA	124/127 (97%)	-0.08	1 (0%) 86 72	32, 49, 60, 64	0
28	AA	135/136 (99%)	0.04	0 100 100	55, 65, 79, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	135/136 (99%)	0.04	0 100 100	61, 73, 92, 99	0
29	AB	148/149 (99%)	-0.30	0 100 100	20, 36, 52, 60	0
29	DC	148/149 (99%)	-0.33	1 (0%) 87 75	22, 41, 54, 56	0
30	AC	58/59 (98%)	-0.01	4 (6%) 16 7	24, 43, 85, 97	0
30	DD	58/59 (98%)	-0.20	2 (3%) 45 24	23, 42, 64, 70	0
31	AD	97/105 (92%)	0.11	5 (5%) 27 12	53, 60, 77, 81	0
31	DE	97/105 (92%)	0.23	5 (5%) 27 12	53, 63, 79, 82	0
32	AE	109/113 (96%)	0.04	4 (3%) 41 21	40, 51, 74, 86	0
32	DF	109/113 (96%)	0.08	2 (1%) 68 47	33, 42, 69, 85	0
33	AF	127/130 (97%)	-0.16	3 (2%) 59 37	22, 34, 41, 51	0
33	DG	127/130 (97%)	-0.15	3 (2%) 59 37	22, 39, 47, 56	0
34	AG	106/107 (99%)	-0.41	0 100 100	28, 32, 49, 54	0
34	DH	106/107 (99%)	-0.34	0 100 100	26, 32, 57, 70	0
35	AH	112/121 (92%)	0.00	3 (2%) 54 31	38, 52, 86, 95	0
35	DI	112/121 (92%)	-0.13	0 100 100	39, 55, 86, 95	0
36	AI	119/120 (99%)	-0.18	1 (0%) 86 72	34, 48, 55, 59	0
36	DJ	119/120 (99%)	-0.04	2 (1%) 70 49	44, 54, 65, 72	0
37	AJ	99/100 (99%)	0.06	4 (4%) 38 19	39, 48, 71, 84	0
37	DK	99/100 (99%)	-0.10	4 (4%) 38 19	46, 56, 72, 85	0
38	AK	87/88 (98%)	-0.30	1 (1%) 80 64	25, 30, 47, 66	0
38	DL	87/88 (98%)	-0.08	2 (2%) 60 39	26, 33, 58, 86	0
39	AL	77/78 (98%)	0.29	2 (2%) 56 33	59, 70, 85, 89	0
39	DM	77/78 (98%)	1.09	16 (20%) 1 0	60, 70, 81, 86	0
40	AM	50/51 (98%)	-0.23	1 (2%) 65 44	33, 36, 43, 46	0
40	DN	50/51 (98%)	-0.30	0 100 100	35, 39, 48, 52	0
41	AN	52/128 (40%)	0.02	2 (3%) 40 20	39, 44, 53, 56	0
41	DO	52/128 (40%)	-0.22	1 (1%) 66 46	28, 30, 41, 48	0
42	AO	25/25 (100%)	0.03	0 100 100	48, 50, 54, 55	0
42	DP	25/25 (100%)	-0.41	0 100 100	34, 39, 46, 49	0
43	AP	105/106 (99%)	0.10	2 (1%) 66 46	26, 41, 62, 77	0
43	DQ	105/106 (99%)	0.06	0 100 100	27, 38, 52, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
44	AQ	91/92 (98%)	-0.26	0	100 100	32, 40, 50, 55	0
44	DR	91/92 (98%)	-0.40	0	100 100	30, 40, 51, 60	0
45	i	159/273 (58%)	0.67	20 (12%)	3 1	47, 77, 123, 128	0
45	sM	63/273 (23%)	0.71	8 (12%)	3 1	48, 76, 88, 91	0
46	p0	143/312 (45%)	0.84	17 (11%)	4 2	73, 90, 152, 161	0
47	A	1781/1797 (99%)	0.29	115 (6%)	18 8	47, 77, 163, 229	0
48	B	206/252 (81%)	0.32	12 (5%)	23 10	82, 94, 103, 116	0
48	s0	206/252 (81%)	-0.17	0	100 100	60, 73, 85, 89	0
49	C	214/255 (83%)	0.91	35 (16%)	1 1	84, 110, 135, 144	0
49	s1	216/255 (84%)	0.12	8 (3%)	41 21	53, 65, 92, 107	0
50	D	217/254 (85%)	-0.15	1 (0%)	91 81	61, 74, 88, 95	0
50	s2	217/254 (85%)	-0.10	5 (2%)	60 39	46, 57, 68, 77	0
51	E	223/240 (92%)	0.25	11 (4%)	29 14	67, 79, 105, 113	0
51	s3	223/240 (92%)	0.30	9 (4%)	38 19	62, 85, 103, 108	0
52	F	260/261 (99%)	0.24	6 (2%)	60 39	58, 74, 83, 101	0
52	s4	260/261 (99%)	-0.06	4 (1%)	73 54	42, 60, 73, 100	0
53	G	206/225 (91%)	0.45	15 (7%)	15 6	85, 101, 112, 120	0
53	s5	206/225 (91%)	0.25	7 (3%)	45 24	64, 82, 97, 101	0
54	H	226/236 (95%)	0.39	15 (6%)	18 7	57, 86, 105, 114	0
54	s6	218/236 (92%)	0.16	6 (2%)	53 30	43, 68, 84, 99	0
55	I	184/190 (96%)	0.45	11 (5%)	21 10	73, 99, 127, 132	0
55	s7	186/190 (97%)	0.36	8 (4%)	35 17	54, 85, 117, 126	0
56	J	188/200 (94%)	0.13	5 (2%)	54 31	50, 61, 94, 105	0
56	s8	188/200 (94%)	0.08	6 (3%)	47 25	39, 57, 96, 108	0
57	K	185/197 (93%)	0.45	12 (6%)	18 8	68, 83, 118, 149	0
57	s9	185/197 (93%)	0.04	6 (3%)	47 25	54, 65, 89, 113	0
58	L	96/105 (91%)	0.10	0	100 100	72, 91, 115, 130	0
58	c0	96/105 (91%)	1.03	17 (17%)	1 0	82, 110, 128, 145	0
59	M	155/156 (99%)	0.32	16 (10%)	6 2	51, 59, 92, 101	0
59	c1	146/156 (93%)	-0.01	5 (3%)	45 24	39, 52, 76, 97	0
60	N	124/143 (86%)	1.52	35 (28%)	0 0	114, 126, 146, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	c2	124/143 (86%)	2.50	63 (50%) 0 0	148, 162, 179, 183	0
61	O	150/151 (99%)	-0.04	2 (1%) 77 59	58, 73, 84, 88	0
61	c3	150/151 (99%)	-0.25	0 100 100	45, 57, 70, 83	0
62	P	127/138 (92%)	0.29	8 (6%) 20 8	59, 112, 126, 127	0
62	c4	128/138 (92%)	-0.11	0 100 100	38, 69, 76, 78	0
63	Q	124/142 (87%)	0.38	9 (7%) 15 6	67, 80, 105, 127	0
63	c5	135/142 (95%)	0.50	11 (8%) 12 5	68, 80, 99, 109	0
64	R	141/143 (98%)	0.57	13 (9%) 9 3	72, 94, 99, 101	0
64	c6	142/143 (99%)	0.33	5 (3%) 44 23	58, 76, 88, 102	0
65	S	120/136 (88%)	0.44	11 (9%) 9 3	81, 94, 112, 114	0
65	c7	117/136 (86%)	0.14	2 (1%) 70 49	66, 77, 95, 101	0
66	T	145/146 (99%)	0.58	13 (8%) 9 3	66, 89, 111, 118	0
66	c8	145/146 (99%)	0.37	16 (11%) 5 2	60, 74, 95, 104	0
67	U	143/144 (99%)	0.31	6 (4%) 36 18	76, 90, 103, 110	0
67	c9	143/144 (99%)	0.09	0 100 100	60, 70, 86, 94	0
68	V	107/121 (88%)	0.96	22 (20%) 1 0	64, 96, 118, 123	0
68	d0	110/121 (90%)	0.80	20 (18%) 1 0	61, 89, 122, 132	0
69	W	87/87 (100%)	-0.06	1 (1%) 80 64	77, 82, 95, 102	0
69	d1	87/87 (100%)	-0.20	1 (1%) 80 64	55, 62, 79, 85	0
70	X	129/130 (99%)	-0.12	0 100 100	59, 69, 76, 86	0
70	d2	129/130 (99%)	-0.28	0 100 100	43, 52, 58, 66	0
71	Y	144/145 (99%)	0.03	2 (1%) 75 56	50, 55, 63, 70	0
71	d3	144/145 (99%)	-0.09	0 100 100	38, 42, 53, 59	0
72	Z	134/135 (99%)	0.44	8 (5%) 21 10	64, 85, 97, 104	0
72	d4	134/135 (99%)	0.08	5 (3%) 41 21	49, 67, 78, 96	0
73	a	70/108 (64%)	1.05	13 (18%) 1 0	97, 109, 116, 118	0
73	d5	69/108 (63%)	0.66	11 (15%) 1 1	75, 92, 101, 103	0
74	b	97/119 (81%)	0.54	8 (8%) 11 4	61, 75, 126, 131	0
74	d6	97/119 (81%)	-0.16	1 (1%) 82 67	43, 52, 78, 85	0
75	c	81/82 (98%)	0.43	6 (7%) 14 5	72, 84, 112, 115	0
75	d7	81/82 (98%)	0.24	5 (6%) 20 9	53, 67, 97, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	d	63/67 (94%)	1.36	16 (25%) 0 0	95, 110, 118, 122	0
76	d8	63/67 (94%)	1.46	16 (25%) 0 0	79, 91, 100, 107	0
77	d9	53/56 (94%)	0.26	2 (3%) 40 20	61, 69, 100, 105	0
77	e	53/56 (94%)	-0.04	1 (1%) 66 46	66, 70, 85, 89	0
78	e0	62/63 (98%)	0.53	5 (8%) 12 5	44, 66, 84, 91	0
78	f	60/63 (95%)	0.83	8 (13%) 3 1	53, 83, 111, 113	0
79	e1	51/152 (33%)	1.54	17 (33%) 0 0	128, 142, 157, 160	0
79	g	71/152 (46%)	0.99	13 (18%) 1 0	87, 107, 119, 121	0
80	Rb	318/319 (99%)	0.49	26 (8%) 11 4	83, 95, 103, 111	0
80	h	318/319 (99%)	0.42	21 (6%) 18 7	88, 100, 113, 125	0
81	sR	1783/1800 (99%)	0.21	94 (5%) 26 12	33, 64, 134, 203	0
All	All	33026/35567 (92%)	0.08	1381 (4%) 36 18	20, 55, 110, 229	0

The worst 5 of 1381 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	CR	179	GLN	16.5
18	CR	161	ALA	16.0
18	CR	162	GLU	15.0
18	CR	160	ALA	13.1
47	A	1694	A	12.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	sR	2188	1/1	0.13	0.68	120,120,120,120	0
83	MG	AR	4112	1/1	0.26	0.46	73,73,73,73	0
83	MG	A	2012	1/1	0.35	0.99	83,83,83,83	0
83	MG	A	2001	1/1	0.45	0.71	71,71,71,71	0
83	MG	1	4111	1/1	0.46	0.32	58,58,58,58	0
83	MG	3	211	1/1	0.48	0.49	39,39,39,39	0
83	MG	AR	3953	1/1	0.51	0.65	38,38,38,38	0
83	MG	1	4146	1/1	0.54	0.39	174,174,174,174	0
83	MG	AM	101	1/1	0.55	0.29	49,49,49,49	0
83	MG	AR	4046	1/1	0.56	0.30	43,43,43,43	0
83	MG	A	2018	1/1	0.56	1.03	80,80,80,80	0
83	MG	sR	2131	1/1	0.56	0.31	73,73,73,73	0
83	MG	AR	4223	1/1	0.57	0.41	29,29,29,29	0
83	MG	1	4047	1/1	0.57	0.35	46,46,46,46	0
83	MG	A	2062	1/1	0.59	1.26	82,82,82,82	0
83	MG	t	202	1/1	0.59	0.30	76,76,76,76	0
83	MG	sR	2137	1/1	0.60	0.44	66,66,66,66	0
83	MG	1	4094	1/1	0.62	0.28	104,104,104,104	0
83	MG	1	3931	1/1	0.62	1.04	68,68,68,68	0
83	MG	1	4158	1/1	0.62	0.57	91,91,91,91	0
83	MG	A	2010	1/1	0.62	0.73	102,102,102,102	0
83	MG	1	3728	1/1	0.63	0.47	57,57,57,57	0
83	MG	c6	201	1/1	0.63	0.45	76,76,76,76	0
83	MG	1	4080	1/1	0.64	0.37	38,38,38,38	0
83	MG	DA	201	1/1	0.64	0.44	52,52,52,52	0
83	MG	A	1962	1/1	0.65	0.44	58,58,58,58	0
83	MG	A	2005	1/1	0.65	0.45	65,65,65,65	0
83	MG	AT	230	1/1	0.65	0.72	61,61,61,61	0
83	MG	6	202	1/1	0.65	0.29	58,58,58,58	0
83	MG	AR	3895	1/1	0.66	0.41	39,39,39,39	0
83	MG	A	2021	1/1	0.66	0.62	86,86,86,86	0
83	MG	DN	101	1/1	0.66	0.29	49,49,49,49	0
83	MG	A	1946	1/1	0.66	0.61	70,70,70,70	0
83	MG	1	3992	1/1	0.67	0.53	41,41,41,41	0
83	MG	w	202	1/1	0.67	0.25	40,40,40,40	0
83	MG	A	2057	1/1	0.67	0.28	109,109,109,109	0
83	MG	AR	3830	1/1	0.67	0.42	48,48,48,48	0
83	MG	sR	2164	1/1	0.67	0.41	43,43,43,43	0
83	MG	AR	3865	1/1	0.68	0.34	43,43,43,43	0
83	MG	sR	2180	1/1	0.68	0.61	59,59,59,59	0
83	MG	A	2009	1/1	0.68	0.21	79,79,79,79	0
83	MG	1	4142	1/1	0.68	0.38	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AR	3823	1/1	0.68	0.32	38,38,38,38	0
83	MG	A	2058	1/1	0.68	0.67	76,76,76,76	0
83	MG	AR	4014	1/1	0.69	0.33	27,27,27,27	0
83	MG	AR	3934	1/1	0.69	0.44	33,33,33,33	0
83	MG	s8	302	1/1	0.69	0.34	45,45,45,45	0
83	MG	AR	4006	1/1	0.70	0.12	76,76,76,76	0
83	MG	1	4133	1/1	0.70	0.32	41,41,41,41	0
83	MG	AR	3804	1/1	0.70	0.38	88,88,88,88	0
83	MG	AS	225	1/1	0.70	0.32	45,45,45,45	0
83	MG	A	1986	1/1	0.71	0.35	58,58,58,58	0
83	MG	AR	3752	1/1	0.71	0.55	50,50,50,50	0
83	MG	AT	228	1/1	0.71	0.49	46,46,46,46	0
83	MG	A	1954	1/1	0.71	0.50	62,62,62,62	0
83	MG	AR	4142	1/1	0.71	0.37	36,36,36,36	0
83	MG	sR	2157	1/1	0.71	0.80	42,42,42,42	0
83	MG	sR	2138	1/1	0.71	0.33	45,45,45,45	0
83	MG	CK	202	1/1	0.71	0.23	36,36,36,36	0
83	MG	AR	4222	1/1	0.71	0.50	30,30,30,30	0
83	MG	1	4077	1/1	0.71	0.34	42,42,42,42	0
83	MG	1	4029	1/1	0.71	0.92	59,59,59,59	0
83	MG	1	4204	1/1	0.72	0.38	54,54,54,54	0
83	MG	AR	4016	1/1	0.72	0.42	51,51,51,51	0
83	MG	1	3960	1/1	0.72	0.31	38,38,38,38	0
83	MG	AR	4235	1/1	0.72	0.71	38,38,38,38	0
83	MG	AR	4189	1/1	0.72	0.24	53,53,53,53	0
83	MG	A	2025	1/1	0.72	0.93	75,75,75,75	0
83	MG	1	4161	1/1	0.72	0.29	45,45,45,45	0
83	MG	3	217	1/1	0.72	0.56	53,53,53,53	0
83	MG	AR	3988	1/1	0.72	0.36	37,37,37,37	0
83	MG	1	4036	1/1	0.72	0.32	43,43,43,43	0
83	MG	AR	3994	1/1	0.73	0.40	48,48,48,48	0
83	MG	AR	4148	1/1	0.73	0.26	54,54,54,54	0
83	MG	DR	502	1/1	0.73	0.32	56,56,56,56	0
83	MG	AG	202	1/1	0.73	0.22	48,48,48,48	0
83	MG	1	3828	1/1	0.73	0.62	39,39,39,39	0
83	MG	1	4044	1/1	0.74	0.21	62,62,62,62	0
83	MG	CU	201	1/1	0.74	0.38	31,31,31,31	0
83	MG	AR	4260	1/1	0.74	0.42	33,33,33,33	0
83	MG	A	1969	1/1	0.74	0.58	51,51,51,51	0
83	MG	AR	4062	1/1	0.74	0.42	55,55,55,55	0
83	MG	AR	4182	1/1	0.74	0.24	41,41,41,41	0
83	MG	1	3849	1/1	0.74	0.24	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3859	1/1	0.74	0.35	35,35,35,35	0
83	MG	A	1988	1/1	0.74	0.69	77,77,77,77	0
83	MG	AR	3961	1/1	0.74	0.48	51,51,51,51	0
83	MG	AR	3742	1/1	0.74	0.20	34,34,34,34	0
83	MG	AR	3969	1/1	0.74	0.52	50,50,50,50	0
83	MG	1	4143	1/1	0.74	0.56	23,23,23,23	0
83	MG	1	4171	1/1	0.75	0.32	23,23,23,23	0
83	MG	AR	4088	1/1	0.75	0.20	39,39,39,39	0
83	MG	A	2068	1/1	0.75	0.49	67,67,67,67	0
83	MG	1	4062	1/1	0.75	0.20	71,71,71,71	0
83	MG	AR	3807	1/1	0.75	0.14	95,95,95,95	0
83	MG	1	4084	1/1	0.75	0.23	33,33,33,33	0
83	MG	AR	3816	1/1	0.75	0.26	47,47,47,47	0
83	MG	sR	2073	1/1	0.75	1.05	96,96,96,96	0
83	MG	1	3826	1/1	0.75	0.31	64,64,64,64	0
83	MG	AF	201	1/1	0.76	0.38	23,23,23,23	0
83	MG	1	4205	1/1	0.76	0.71	44,44,44,44	0
83	MG	AR	4025	1/1	0.76	0.28	37,37,37,37	0
83	MG	1	3803	1/1	0.76	0.49	35,35,35,35	0
83	MG	1	3745	1/1	0.76	0.28	55,55,55,55	0
83	MG	sR	2135	1/1	0.76	0.26	70,70,70,70	0
83	MG	1	3731	1/1	0.76	0.45	33,33,33,33	0
83	MG	A	2031	1/1	0.76	0.40	64,64,64,64	0
83	MG	1	4093	1/1	0.76	0.31	41,41,41,41	0
83	MG	1	4099	1/1	0.76	0.28	45,45,45,45	0
83	MG	sR	2154	1/1	0.76	0.49	43,43,43,43	0
83	MG	1	4164	1/1	0.76	0.23	47,47,47,47	0
83	MG	AR	4084	1/1	0.76	0.45	38,38,38,38	0
83	MG	AR	3987	1/1	0.76	0.13	35,35,35,35	0
83	MG	AR	4227	1/1	0.76	0.33	36,36,36,36	0
83	MG	AR	4109	1/1	0.76	0.29	74,74,74,74	0
83	MG	CD	301	1/1	0.77	0.60	40,40,40,40	0
83	MG	1	4160	1/1	0.77	0.34	54,54,54,54	0
83	MG	AS	219	1/1	0.77	0.20	48,48,48,48	0
83	MG	AR	4246	1/1	0.77	0.85	49,49,49,49	0
83	MG	AR	3829	1/1	0.77	0.39	44,44,44,44	0
83	MG	AR	3946	1/1	0.77	0.11	44,44,44,44	0
83	MG	sR	2079	1/1	0.77	0.63	63,63,63,63	0
83	MG	sR	2113	1/1	0.77	0.44	57,57,57,57	0
83	MG	A	2061	1/1	0.77	0.92	77,77,77,77	0
83	MG	sR	2118	1/1	0.77	0.17	52,52,52,52	0
83	MG	AR	4180	1/1	0.77	0.33	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	CD	303	1/1	0.77	0.34	31,31,31,31	0
83	MG	s	300	1/1	0.77	0.37	64,64,64,64	0
83	MG	AR	3834	1/1	0.77	0.25	21,21,21,21	0
83	MG	1	4210	1/1	0.78	0.68	58,58,58,58	0
83	MG	sR	2088	1/1	0.78	0.54	82,82,82,82	0
83	MG	AR	4090	1/1	0.78	0.39	46,46,46,46	0
83	MG	AR	3893	1/1	0.78	0.39	30,30,30,30	0
83	MG	AR	4247	1/1	0.78	0.32	39,39,39,39	0
83	MG	1	3956	1/1	0.78	0.26	24,24,24,24	0
83	MG	1	4003	1/1	0.78	0.38	54,54,54,54	0
83	MG	1	4051	1/1	0.78	0.21	44,44,44,44	0
83	MG	AR	4146	1/1	0.78	0.19	69,69,69,69	0
83	MG	1	3958	1/1	0.78	0.52	51,51,51,51	0
83	MG	1	3783	1/1	0.78	0.36	59,59,59,59	0
83	MG	sR	2107	1/1	0.78	0.75	51,51,51,51	0
83	MG	CM	202	1/1	0.78	0.23	52,52,52,52	0
83	MG	1	4136	1/1	0.78	0.46	41,41,41,41	0
83	MG	AR	3841	1/1	0.78	0.31	31,31,31,31	0
83	MG	AR	4091	1/1	0.78	0.77	48,48,48,48	0
83	MG	AR	4145	1/1	0.78	0.33	34,34,34,34	0
83	MG	AR	4113	1/1	0.79	0.54	61,61,61,61	0
83	MG	CR	207	1/1	0.79	0.25	37,37,37,37	0
83	MG	AR	3810	1/1	0.79	0.20	28,28,28,28	0
83	MG	DR	503	1/1	0.79	0.29	54,54,54,54	0
83	MG	AR	4117	1/1	0.79	0.21	29,29,29,29	0
83	MG	1	3959	1/1	0.79	0.32	61,61,61,61	0
83	MG	z	202	1/1	0.79	0.18	50,50,50,50	0
83	MG	1	3801	1/1	0.79	0.36	31,31,31,31	0
83	MG	sR	2148	1/1	0.79	0.30	62,62,62,62	0
83	MG	AR	4060	1/1	0.79	0.40	66,66,66,66	0
85	ZN	c	101	1/1	0.79	0.28	119,119,119,119	0
83	MG	1	3818	1/1	0.79	0.35	54,54,54,54	0
83	MG	AR	3794	1/1	0.79	0.64	25,25,25,25	0
83	MG	AR	4009	1/1	0.79	0.21	29,29,29,29	0
83	MG	sR	2140	1/1	0.79	0.34	45,45,45,45	0
83	MG	AR	4087	1/1	0.79	0.24	49,49,49,49	0
83	MG	AR	4199	1/1	0.79	0.45	41,41,41,41	0
83	MG	A	2016	1/1	0.79	0.36	61,61,61,61	0
83	MG	1	4008	1/1	0.79	0.62	72,72,72,72	0
83	MG	sM	301	1/1	0.79	0.17	37,37,37,37	0
83	MG	sR	2128	1/1	0.79	0.50	58,58,58,58	0
83	MG	AR	4137	1/1	0.79	0.39	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AT	225	1/1	0.79	0.48	50,50,50,50	0
83	MG	1	3962	1/1	0.79	0.42	49,49,49,49	0
83	MG	1	3940	1/1	0.79	0.14	52,52,52,52	0
83	MG	AR	4056	1/1	0.79	0.15	82,82,82,82	0
83	MG	CF	403	1/1	0.79	0.23	38,38,38,38	0
83	MG	d5	201	1/1	0.79	0.18	74,74,74,74	0
83	MG	sR	2069	1/1	0.80	0.55	55,55,55,55	0
83	MG	1	3752	1/1	0.80	0.37	31,31,31,31	0
83	MG	CG	306	1/1	0.80	0.34	52,52,52,52	0
83	MG	1	4106	1/1	0.80	0.27	33,33,33,33	0
83	MG	AR	4089	1/1	0.80	0.65	26,26,26,26	0
83	MG	AR	4085	1/1	0.80	0.34	40,40,40,40	0
83	MG	AR	4105	1/1	0.80	0.52	62,62,62,62	0
83	MG	sR	2141	1/1	0.80	0.23	37,37,37,37	0
83	MG	AR	4160	1/1	0.80	0.29	31,31,31,31	0
83	MG	1	4059	1/1	0.80	0.34	42,42,42,42	0
83	MG	AR	4029	1/1	0.80	0.29	52,52,52,52	0
83	MG	sR	2189	1/1	0.80	0.61	64,64,64,64	0
83	MG	AR	4206	1/1	0.80	0.37	33,33,33,33	0
83	MG	AR	4167	1/1	0.80	0.26	49,49,49,49	0
83	MG	1	3864	1/1	0.80	0.53	50,50,50,50	0
83	MG	1	3780	1/1	0.80	0.69	50,50,50,50	0
83	MG	A	1961	1/1	0.80	0.53	61,61,61,61	0
83	MG	1	3970	1/1	0.80	0.43	41,41,41,41	0
83	MG	AR	3802	1/1	0.80	0.38	31,31,31,31	0
83	MG	AR	4238	1/1	0.80	0.22	30,30,30,30	0
83	MG	AR	3982	1/1	0.80	0.44	61,61,61,61	0
83	MG	AR	4002	1/1	0.80	0.18	61,61,61,61	0
83	MG	sR	2159	1/1	0.80	0.56	95,95,95,95	0
83	MG	A	2032	1/1	0.80	0.20	81,81,81,81	0
83	MG	CE	403	1/1	0.80	0.52	21,21,21,21	0
83	MG	A	1947	1/1	0.81	0.69	53,53,53,53	0
83	MG	AR	3976	1/1	0.81	0.72	49,49,49,49	0
83	MG	AR	3743	1/1	0.81	0.36	29,29,29,29	0
83	MG	AR	4110	1/1	0.81	0.37	55,55,55,55	0
83	MG	1	3939	1/1	0.81	0.30	30,30,30,30	0
83	MG	AR	3980	1/1	0.81	0.24	40,40,40,40	0
83	MG	1	4002	1/1	0.81	0.36	48,48,48,48	0
83	MG	1	3966	1/1	0.81	0.35	36,36,36,36	0
83	MG	AS	218	1/1	0.81	0.31	50,50,50,50	0
83	MG	AR	4191	1/1	0.81	0.57	44,44,44,44	0
83	MG	1	4199	1/1	0.81	0.39	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	4048	1/1	0.81	0.51	43,43,43,43	0
83	MG	1	4027	1/1	0.81	0.47	39,39,39,39	0
83	MG	1	4175	1/1	0.81	0.28	22,22,22,22	0
83	MG	AR	4215	1/1	0.81	0.19	35,35,35,35	0
83	MG	AR	3769	1/1	0.81	0.32	33,33,33,33	0
83	MG	1	3991	1/1	0.81	0.15	65,65,65,65	0
83	MG	A	2004	1/1	0.81	0.43	51,51,51,51	0
83	MG	AR	3831	1/1	0.81	0.37	38,38,38,38	0
83	MG	1	3878	1/1	0.81	0.45	27,27,27,27	0
83	MG	1	3837	1/1	0.81	0.47	24,24,24,24	0
83	MG	1	4173	1/1	0.81	0.18	27,27,27,27	0
83	MG	A	2030	1/1	0.81	0.36	90,90,90,90	0
83	MG	sR	2132	1/1	0.81	0.27	38,38,38,38	0
83	MG	AR	4022	1/1	0.81	0.35	41,41,41,41	0
83	MG	1	3974	1/1	0.81	0.47	62,62,62,62	0
83	MG	r	303	1/1	0.82	0.32	37,37,37,37	0
83	MG	A	1985	1/1	0.82	0.33	63,63,63,63	0
83	MG	1	3949	1/1	0.82	0.40	63,63,63,63	0
83	MG	AR	4229	1/1	0.82	0.62	44,44,44,44	0
83	MG	AR	4190	1/1	0.82	0.24	32,32,32,32	0
83	MG	1	3954	1/1	0.82	0.31	34,34,34,34	0
83	MG	AR	3931	1/1	0.82	0.15	38,38,38,38	0
83	MG	sR	2095	1/1	0.82	0.57	48,48,48,48	0
83	MG	CK	203	1/1	0.82	0.29	38,38,38,38	0
83	MG	AR	4131	1/1	0.82	0.26	54,54,54,54	0
83	MG	A	1960	1/1	0.82	0.93	53,53,53,53	0
83	MG	1	4096	1/1	0.82	0.68	47,47,47,47	0
83	MG	1	4018	1/1	0.82	0.45	36,36,36,36	0
83	MG	A	1950	1/1	0.82	0.36	65,65,65,65	0
83	MG	sR	2114	1/1	0.82	0.30	71,71,71,71	0
83	MG	AR	3824	1/1	0.82	0.48	37,37,37,37	0
83	MG	1	4038	1/1	0.82	0.34	33,33,33,33	0
83	MG	1	4167	1/1	0.82	0.37	55,55,55,55	0
83	MG	1	3763	1/1	0.82	0.56	26,26,26,26	0
83	MG	AR	3753	1/1	0.82	0.22	26,26,26,26	0
83	MG	1	3868	1/1	0.82	0.55	34,34,34,34	0
83	MG	AR	3955	1/1	0.82	0.27	53,53,53,53	0
83	MG	A	1968	1/1	0.82	0.34	82,82,82,82	0
83	MG	1	3846	1/1	0.83	0.34	61,61,61,61	0
83	MG	AR	4237	1/1	0.83	0.30	34,34,34,34	0
83	MG	1	4089	1/1	0.83	0.53	38,38,38,38	0
83	MG	AR	3936	1/1	0.83	0.21	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AR	4168	1/1	0.83	0.13	56,56,56,56	0
83	MG	AR	3903	1/1	0.83	0.36	25,25,25,25	0
83	MG	1	3934	1/1	0.83	0.30	32,32,32,32	0
83	MG	AR	4015	1/1	0.83	0.37	42,42,42,42	0
83	MG	1	3809	1/1	0.83	0.26	31,31,31,31	0
83	MG	1	3792	1/1	0.83	0.54	35,35,35,35	0
83	MG	AR	4151	1/1	0.83	0.15	60,60,60,60	0
83	MG	AR	4093	1/1	0.83	0.27	39,39,39,39	0
83	MG	AR	3896	1/1	0.83	0.41	23,23,23,23	0
83	MG	sR	2053	1/1	0.83	0.54	66,66,66,66	0
83	MG	1	4021	1/1	0.83	0.58	62,62,62,62	0
83	MG	A	2037	1/1	0.83	0.35	64,64,64,64	0
83	MG	1	4049	1/1	0.83	0.48	37,37,37,37	0
83	MG	AR	4234	1/1	0.83	0.42	20,20,20,20	0
83	MG	sR	2052	1/1	0.83	0.52	38,38,38,38	0
83	MG	4	219	1/1	0.83	0.58	39,39,39,39	0
83	MG	AR	3840	1/1	0.83	0.56	33,33,33,33	0
83	MG	AR	4107	1/1	0.83	0.34	27,27,27,27	0
83	MG	AR	4216	1/1	0.83	0.24	38,38,38,38	0
83	MG	sR	2196	1/1	0.83	0.44	62,62,62,62	0
83	MG	AR	4023	1/1	0.83	0.37	38,38,38,38	0
83	MG	1	4052	1/1	0.83	0.36	38,38,38,38	0
83	MG	AR	4018	1/1	0.83	0.20	36,36,36,36	0
83	MG	1	4213	1/1	0.83	0.49	30,30,30,30	0
83	MG	sR	2063	1/1	0.83	0.33	64,64,64,64	0
83	MG	1	4108	1/1	0.83	0.25	60,60,60,60	0
83	MG	A	2007	1/1	0.83	0.46	87,87,87,87	0
83	MG	AR	3937	1/1	0.83	0.34	33,33,33,33	0
83	MG	1	4004	1/1	0.83	0.20	33,33,33,33	0
83	MG	1	4141	1/1	0.83	0.35	36,36,36,36	0
83	MG	1	4022	1/1	0.84	0.33	37,37,37,37	0
83	MG	1	3986	1/1	0.84	0.33	42,42,42,42	0
83	MG	CR	202	1/1	0.84	0.34	28,28,28,28	0
83	MG	AR	3985	1/1	0.84	0.26	61,61,61,61	0
83	MG	sR	2183	1/1	0.84	0.51	34,34,34,34	0
83	MG	d9	103	1/1	0.84	0.69	94,94,94,94	0
83	MG	DD	102	1/1	0.84	0.33	29,29,29,29	0
83	MG	AS	214	1/1	0.84	0.55	55,55,55,55	0
83	MG	1	4180	1/1	0.84	0.82	52,52,52,52	0
83	MG	sR	2116	1/1	0.84	0.47	66,66,66,66	0
83	MG	AR	4155	1/1	0.84	0.19	27,27,27,27	0
83	MG	1	3973	1/1	0.84	0.37	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	4162	1/1	0.84	0.25	35,35,35,35	0
83	MG	AR	4030	1/1	0.84	0.32	36,36,36,36	0
83	MG	1	3881	1/1	0.84	0.09	41,41,41,41	0
83	MG	sR	2136	1/1	0.84	0.58	63,63,63,63	0
83	MG	AR	4214	1/1	0.84	0.36	26,26,26,26	0
83	MG	1	3877	1/1	0.84	0.38	45,45,45,45	0
83	MG	1	3808	1/1	0.84	0.27	42,42,42,42	0
83	MG	1	4067	1/1	0.84	0.26	59,59,59,59	0
83	MG	CX	204	1/1	0.84	0.23	33,33,33,33	0
83	MG	1	4145	1/1	0.84	0.26	32,32,32,32	0
83	MG	AR	4193	1/1	0.84	0.50	65,65,65,65	0
83	MG	AR	4048	1/1	0.84	0.22	44,44,44,44	0
83	MG	1	4079	1/1	0.84	0.21	47,47,47,47	0
83	MG	AR	3932	1/1	0.84	0.16	37,37,37,37	0
82	OHX	A	1938	7/7	0.84	0.52	106,106,106,106	0
83	MG	AT	217	1/1	0.84	0.32	29,29,29,29	0
83	MG	1	3744	1/1	0.84	0.34	70,70,70,70	0
83	MG	1	4028	1/1	0.84	0.42	38,38,38,38	0
83	MG	DC	203	1/1	0.84	0.32	28,28,28,28	0
83	MG	AR	3958	1/1	0.84	0.39	23,23,23,23	0
83	MG	CR	204	1/1	0.84	0.20	40,40,40,40	0
83	MG	AR	4158	1/1	0.84	0.27	37,37,37,37	0
83	MG	AR	4027	1/1	0.84	0.98	57,57,57,57	0
83	MG	AR	4122	1/1	0.84	0.24	41,41,41,41	0
82	OHX	AR	3662	7/7	0.85	0.39	137,137,137,137	0
83	MG	1	3936	1/1	0.85	0.37	45,45,45,45	0
83	MG	AR	3745	1/1	0.85	0.24	36,36,36,36	0
83	MG	4	232	1/1	0.85	0.26	60,60,60,60	0
83	MG	1	4211	1/1	0.85	0.32	29,29,29,29	0
83	MG	A	2008	1/1	0.85	0.64	54,54,54,54	0
83	MG	s8	303	1/1	0.85	0.27	42,42,42,42	0
83	MG	1	4159	1/1	0.85	0.24	33,33,33,33	0
83	MG	sR	2070	1/1	0.85	0.65	38,38,38,38	0
83	MG	AR	3814	1/1	0.85	0.48	30,30,30,30	0
83	MG	AR	4143	1/1	0.85	0.42	33,33,33,33	0
83	MG	1	3791	1/1	0.85	0.20	43,43,43,43	0
83	MG	AR	4039	1/1	0.85	0.65	73,73,73,73	0
83	MG	A	2033	1/1	0.85	0.85	53,53,53,53	0
83	MG	1	3742	1/1	0.85	0.44	37,37,37,37	0
83	MG	AR	3761	1/1	0.85	0.45	47,47,47,47	0
83	MG	1	3952	1/1	0.85	0.22	65,65,65,65	0
83	MG	AR	3921	1/1	0.85	0.73	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3810	1/1	0.85	0.45	41,41,41,41	0
83	MG	1	3972	1/1	0.85	0.28	56,56,56,56	0
83	MG	sR	2201	1/1	0.85	0.15	62,62,62,62	0
83	MG	4	220	1/1	0.85	0.45	29,29,29,29	0
83	MG	AR	4128	1/1	0.85	0.30	36,36,36,36	0
83	MG	AR	3803	1/1	0.85	0.41	50,50,50,50	0
83	MG	AR	3975	1/1	0.85	0.26	31,31,31,31	0
83	MG	AR	3890	1/1	0.85	0.62	31,31,31,31	0
83	MG	1	4013	1/1	0.85	0.22	31,31,31,31	0
83	MG	AR	3945	1/1	0.85	0.31	27,27,27,27	0
83	MG	x	205	1/1	0.85	0.19	36,36,36,36	0
83	MG	4	215	1/1	0.85	0.47	41,41,41,41	0
82	OHX	AR	3732	7/7	0.85	0.38	181,181,181,181	0
83	MG	A	1990	1/1	0.85	0.75	56,56,56,56	0
83	MG	sR	2182	1/1	0.85	0.53	37,37,37,37	0
83	MG	1	4107	1/1	0.85	0.43	47,47,47,47	0
83	MG	A	2038	1/1	0.85	0.56	65,65,65,65	0
82	OHX	A	1937	7/7	0.85	0.41	130,130,130,130	0
83	MG	CF	402	1/1	0.85	0.28	27,27,27,27	0
83	MG	AR	4248	1/1	0.85	0.35	31,31,31,31	0
83	MG	AR	4203	1/1	0.85	0.33	50,50,50,50	0
83	MG	1	4223	1/1	0.85	0.33	34,34,34,34	0
83	MG	1	4065	1/1	0.85	0.46	53,53,53,53	0
83	MG	3	213	1/1	0.86	0.49	32,32,32,32	0
83	MG	v	305	1/1	0.86	0.78	39,39,39,39	0
83	MG	AR	4133	1/1	0.86	0.14	59,59,59,59	0
83	MG	1	4019	1/1	0.86	0.31	40,40,40,40	0
83	MG	AR	4253	1/1	0.86	0.51	38,38,38,38	0
83	MG	A	2014	1/1	0.86	0.42	67,67,67,67	0
83	MG	A	1956	1/1	0.86	0.64	59,59,59,59	0
83	MG	A	2054	1/1	0.86	0.63	44,44,44,44	0
83	MG	AR	3779	1/1	0.86	0.37	21,21,21,21	0
83	MG	sR	2059	1/1	0.86	0.34	46,46,46,46	0
83	MG	1	3771	1/1	0.86	0.43	39,39,39,39	0
83	MG	1	4068	1/1	0.86	0.46	43,43,43,43	0
83	MG	1	4010	1/1	0.86	0.52	31,31,31,31	0
83	MG	4	234	1/1	0.86	0.48	31,31,31,31	0
83	MG	1	3755	1/1	0.86	0.51	37,37,37,37	0
83	MG	DE	201	1/1	0.86	0.17	55,55,55,55	0
83	MG	4	230	1/1	0.86	0.22	37,37,37,37	0
83	MG	AR	3768	1/1	0.86	0.49	76,76,76,76	0
83	MG	1	4083	1/1	0.86	0.28	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	4207	1/1	0.86	0.59	38,38,38,38	0
83	MG	sR	2120	1/1	0.86	0.50	50,50,50,50	0
83	MG	1	3814	1/1	0.86	0.27	42,42,42,42	0
83	MG	sR	2067	1/1	0.86	0.44	61,61,61,61	0
83	MG	AR	4034	1/1	0.86	0.17	55,55,55,55	0
83	MG	AR	3974	1/1	0.86	0.57	44,44,44,44	0
83	MG	1	4169	1/1	0.86	0.17	34,34,34,34	0
83	MG	1	3821	1/1	0.86	0.38	39,39,39,39	0
83	MG	1	4192	1/1	0.86	0.30	29,29,29,29	0
83	MG	3	218	1/1	0.86	0.58	56,56,56,56	0
83	MG	CR	205	1/1	0.86	0.28	28,28,28,28	0
83	MG	sR	2123	1/1	0.86	0.61	55,55,55,55	0
83	MG	d4	203	1/1	0.86	0.32	66,66,66,66	0
83	MG	AR	4178	1/1	0.86	0.15	46,46,46,46	0
83	MG	A	1948	1/1	0.86	0.34	49,49,49,49	0
83	MG	1	3906	1/1	0.86	0.39	33,33,33,33	0
83	MG	1	4046	1/1	0.86	0.36	27,27,27,27	0
83	MG	sR	2064	1/1	0.86	0.56	47,47,47,47	0
83	MG	A	2027	1/1	0.86	0.31	55,55,55,55	0
83	MG	AR	4198	1/1	0.86	0.31	40,40,40,40	0
83	MG	1	4116	1/1	0.86	0.42	40,40,40,40	0
83	MG	AR	3905	1/1	0.86	0.37	25,25,25,25	0
83	MG	AT	221	1/1	0.86	0.37	32,32,32,32	0
83	MG	1	4134	1/1	0.86	0.43	24,24,24,24	0
83	MG	AR	4118	1/1	0.86	0.77	70,70,70,70	0
83	MG	sR	2152	1/1	0.86	0.21	48,48,48,48	0
83	MG	AR	3747	1/1	0.86	0.29	37,37,37,37	0
83	MG	o	301	1/1	0.86	0.40	34,34,34,34	0
83	MG	1	3788	1/1	0.86	0.19	30,30,30,30	0
83	MG	1	3975	1/1	0.86	0.24	38,38,38,38	0
83	MG	1	3802	1/1	0.86	0.34	39,39,39,39	0
83	MG	DC	204	1/1	0.86	0.32	33,33,33,33	0
83	MG	AR	3889	1/1	0.86	0.39	38,38,38,38	0
83	MG	AR	3933	1/1	0.86	0.24	57,57,57,57	0
83	MG	A	1970	1/1	0.86	0.94	77,77,77,77	0
83	MG	A	2013	1/1	0.86	0.57	68,68,68,68	0
83	MG	4	227	1/1	0.86	0.32	52,52,52,52	0
83	MG	AR	4028	1/1	0.86	0.14	29,29,29,29	0
83	MG	1	4163	1/1	0.86	0.31	44,44,44,44	0
83	MG	AR	4075	1/1	0.86	0.43	50,50,50,50	0
83	MG	1	3989	1/1	0.86	0.35	41,41,41,41	0
82	OHX	A	1939	7/7	0.87	0.28	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3967	1/1	0.87	0.40	54,54,54,54	0
83	MG	1	3916	1/1	0.87	0.66	59,59,59,59	0
83	MG	AR	3990	1/1	0.87	0.34	26,26,26,26	0
83	MG	1	4070	1/1	0.87	0.38	54,54,54,54	0
83	MG	AR	4104	1/1	0.87	0.21	86,86,86,86	0
83	MG	AR	4250	1/1	0.87	0.24	49,49,49,49	0
83	MG	AR	4251	1/1	0.87	0.55	39,39,39,39	0
83	MG	AR	3876	1/1	0.87	0.48	31,31,31,31	0
83	MG	sR	2077	1/1	0.87	0.37	50,50,50,50	0
83	MG	AR	4058	1/1	0.87	0.23	45,45,45,45	0
83	MG	1	4197	1/1	0.87	0.34	26,26,26,26	0
83	MG	1	3795	1/1	0.87	0.17	33,33,33,33	0
83	MG	AR	3773	1/1	0.87	0.43	30,30,30,30	0
83	MG	AR	3789	1/1	0.87	0.33	29,29,29,29	0
83	MG	sR	2058	1/1	0.87	0.42	90,90,90,90	0
83	MG	A	1951	1/1	0.87	0.66	65,65,65,65	0
83	MG	AR	4138	1/1	0.87	0.21	40,40,40,40	0
83	MG	v	307	1/1	0.87	0.50	34,34,34,34	0
83	MG	d6	202	1/1	0.87	0.27	43,43,43,43	0
83	MG	A	2028	1/1	0.87	0.56	60,60,60,60	0
83	MG	AR	4184	1/1	0.87	0.25	44,44,44,44	0
83	MG	A	1981	1/1	0.87	0.42	61,61,61,61	0
83	MG	AR	4245	1/1	0.87	0.58	43,43,43,43	0
83	MG	AR	4011	1/1	0.87	0.25	27,27,27,27	0
83	MG	AR	4208	1/1	0.87	0.59	52,52,52,52	0
83	MG	1	4206	1/1	0.87	0.66	36,36,36,36	0
83	MG	AR	4202	1/1	0.87	1.05	72,72,72,72	0
83	MG	1	3876	1/1	0.87	0.59	29,29,29,29	0
83	MG	c4	201	1/1	0.87	0.46	46,46,46,46	0
83	MG	sR	2103	1/1	0.87	0.53	38,38,38,38	0
83	MG	1	4055	1/1	0.87	0.56	31,31,31,31	0
83	MG	A	1978	1/1	0.87	0.42	51,51,51,51	0
83	MG	1	3981	1/1	0.87	0.53	35,35,35,35	0
83	MG	AR	4020	1/1	0.87	0.53	40,40,40,40	0
83	MG	AR	4001	1/1	0.87	0.31	24,24,24,24	0
83	MG	AR	3939	1/1	0.87	0.48	26,26,26,26	0
83	MG	1	3827	1/1	0.87	0.46	21,21,21,21	0
83	MG	AR	3792	1/1	0.87	0.37	29,29,29,29	0
83	MG	AR	4188	1/1	0.87	0.49	31,31,31,31	0
83	MG	1	4042	1/1	0.87	0.24	37,37,37,37	0
83	MG	A	2002	1/1	0.87	0.56	94,94,94,94	0
83	MG	l	404	1/1	0.87	0.23	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	DA	202	1/1	0.87	0.40	39,39,39,39	0
83	MG	sR	2185	1/1	0.87	0.55	46,46,46,46	0
83	MG	1	4135	1/1	0.87	0.27	46,46,46,46	0
83	MG	A	1989	1/1	0.87	0.33	54,54,54,54	0
83	MG	A	2045	1/1	0.88	0.57	49,49,49,49	0
83	MG	AR	3924	1/1	0.88	0.43	35,35,35,35	0
83	MG	AR	4212	1/1	0.88	0.53	30,30,30,30	0
83	MG	c1	202	1/1	0.88	0.30	42,42,42,42	0
83	MG	1	4144	1/1	0.88	0.24	27,27,27,27	0
83	MG	AR	4013	1/1	0.88	0.26	42,42,42,42	0
83	MG	c9	201	1/1	0.88	0.55	65,65,65,65	0
82	OHX	sR	2018	7/7	0.88	0.29	136,136,136,136	0
83	MG	sR	2194	1/1	0.88	0.45	83,83,83,83	0
83	MG	AR	3880	1/1	0.88	0.44	26,26,26,26	0
83	MG	1	4195	1/1	0.88	0.70	42,42,42,42	0
83	MG	AR	3991	1/1	0.88	0.61	35,35,35,35	0
83	MG	sR	2061	1/1	0.88	0.63	47,47,47,47	0
83	MG	sR	2174	1/1	0.88	0.61	81,81,81,81	0
83	MG	1	4040	1/1	0.88	0.49	79,79,79,79	0
83	MG	AR	3806	1/1	0.88	0.33	30,30,30,30	0
83	MG	1	3729	1/1	0.88	0.76	59,59,59,59	0
83	MG	1	4074	1/1	0.88	0.62	46,46,46,46	0
83	MG	AR	4031	1/1	0.88	0.27	26,26,26,26	0
83	MG	AT	227	1/1	0.88	0.50	51,51,51,51	0
83	MG	1	4020	1/1	0.88	0.45	48,48,48,48	0
83	MG	A	2064	1/1	0.88	0.55	68,68,68,68	0
83	MG	1	3999	1/1	0.88	0.48	36,36,36,36	0
83	MG	CQ	203	1/1	0.88	0.39	27,27,27,27	0
83	MG	1	3816	1/1	0.88	0.61	53,53,53,53	0
83	MG	1	4157	1/1	0.88	0.20	41,41,41,41	0
83	MG	1	4098	1/1	0.88	0.19	39,39,39,39	0
83	MG	1	3774	1/1	0.88	0.30	35,35,35,35	0
83	MG	sR	2202	1/1	0.88	1.02	49,49,49,49	0
83	MG	AR	4173	1/1	0.88	0.49	30,30,30,30	0
83	MG	sR	2065	1/1	0.88	1.41	64,64,64,64	0
83	MG	1	4181	1/1	0.88	0.75	44,44,44,44	0
83	MG	AR	3771	1/1	0.88	0.32	68,68,68,68	0
83	MG	sR	2081	1/1	0.88	0.60	63,63,63,63	0
83	MG	AR	4038	1/1	0.88	0.18	41,41,41,41	0
83	MG	AR	3862	1/1	0.88	0.51	38,38,38,38	0
83	MG	1	3769	1/1	0.88	0.50	37,37,37,37	0
83	MG	1	3961	1/1	0.88	0.30	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AR	4181	1/1	0.88	0.22	29,29,29,29	0
83	MG	1	3854	1/1	0.88	0.69	54,54,54,54	0
83	MG	A	2053	1/1	0.88	0.75	46,46,46,46	0
83	MG	CR	203	1/1	0.88	0.69	93,93,93,93	0
83	MG	AR	4221	1/1	0.88	0.66	44,44,44,44	0
83	MG	1	3935	1/1	0.88	0.34	36,36,36,36	0
83	MG	1	3946	1/1	0.88	0.18	30,30,30,30	0
83	MG	A	2000	1/1	0.88	1.10	69,69,69,69	0
83	MG	e	103	1/1	0.88	0.54	81,81,81,81	0
83	MG	3	221	1/1	0.88	0.66	74,74,74,74	0
83	MG	1	3945	1/1	0.88	0.22	55,55,55,55	0
83	MG	1	4129	1/1	0.88	0.19	46,46,46,46	0
83	MG	sR	2191	1/1	0.88	0.34	75,75,75,75	0
83	MG	sR	2163	1/1	0.88	0.78	49,49,49,49	0
83	MG	AR	3744	1/1	0.88	0.41	32,32,32,32	0
83	MG	A	2029	1/1	0.88	0.40	59,59,59,59	0
83	MG	1	4026	1/1	0.88	0.27	32,32,32,32	0
82	OHX	1	3720	7/7	0.88	0.29	112,112,112,112	0
83	MG	AR	4045	1/1	0.88	0.29	38,38,38,38	0
83	MG	AR	3964	1/1	0.88	0.65	79,79,79,79	0
83	MG	1	3947	1/1	0.88	0.48	36,36,36,36	0
83	MG	AR	4147	1/1	0.88	0.21	46,46,46,46	0
83	MG	d4	204	1/1	0.88	0.43	57,57,57,57	0
83	MG	sR	2111	1/1	0.88	0.52	78,78,78,78	0
83	MG	1	4100	1/1	0.88	0.35	56,56,56,56	0
83	MG	1	4151	1/1	0.88	0.41	28,28,28,28	0
83	MG	A	2060	1/1	0.88	0.72	49,49,49,49	0
83	MG	AR	4066	1/1	0.88	0.34	58,58,58,58	0
83	MG	1	4039	1/1	0.89	0.33	33,33,33,33	0
83	MG	AR	4126	1/1	0.89	0.40	32,32,32,32	0
83	MG	1	3767	1/1	0.89	0.24	62,62,62,62	0
82	OHX	sR	2047	7/7	0.89	0.29	127,127,127,127	0
83	MG	3	210	1/1	0.89	0.31	60,60,60,60	0
83	MG	AR	3952	1/1	0.89	0.25	40,40,40,40	0
83	MG	CX	205	1/1	0.89	0.22	31,31,31,31	0
82	OHX	A	1919	7/7	0.89	0.35	117,117,117,117	0
83	MG	AR	3858	1/1	0.89	0.41	22,22,22,22	0
83	MG	AR	3801	1/1	0.89	0.43	44,44,44,44	0
83	MG	4	237	1/1	0.89	0.57	39,39,39,39	0
83	MG	A	1996	1/1	0.89	0.72	101,101,101,101	0
82	OHX	AS	210	7/7	0.89	0.33	112,112,112,112	0
83	MG	1	4060	1/1	0.89	0.38	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	j	302	1/1	0.89	0.31	28,28,28,28	0
83	MG	AR	3836	1/1	0.89	0.31	38,38,38,38	0
83	MG	1	4176	1/1	0.89	0.63	43,43,43,43	0
82	OHX	A	1853	7/7	0.89	0.35	112,112,112,112	0
83	MG	A	2006	1/1	0.89	0.31	108,108,108,108	0
83	MG	AR	4162	1/1	0.89	0.23	23,23,23,23	0
83	MG	AR	3949	1/1	0.89	0.15	40,40,40,40	0
83	MG	sR	2106	1/1	0.89	0.67	44,44,44,44	0
83	MG	A	2046	1/1	0.89	0.28	96,96,96,96	0
83	MG	A	2065	1/1	0.89	0.46	51,51,51,51	0
83	MG	AR	4036	1/1	0.89	0.42	44,44,44,44	0
83	MG	1	3762	1/1	0.89	0.29	39,39,39,39	0
83	MG	1	4105	1/1	0.89	0.29	48,48,48,48	0
83	MG	CE	405	1/1	0.89	0.28	28,28,28,28	0
83	MG	v	306	1/1	0.89	0.50	43,43,43,43	0
83	MG	1	3747	1/1	0.89	0.22	29,29,29,29	0
83	MG	A	2039	1/1	0.89	0.68	59,59,59,59	0
83	MG	A	2023	1/1	0.89	0.55	62,62,62,62	0
83	MG	AR	4017	1/1	0.89	0.22	61,61,61,61	0
83	MG	1	4191	1/1	0.89	0.63	37,37,37,37	0
83	MG	1	3875	1/1	0.89	0.56	29,29,29,29	0
83	MG	J	303	1/1	0.89	0.36	51,51,51,51	0
83	MG	AR	4057	1/1	0.89	0.26	25,25,25,25	0
83	MG	AF	202	1/1	0.89	0.23	24,24,24,24	0
83	MG	H	301	1/1	0.89	0.32	82,82,82,82	0
83	MG	1	4081	1/1	0.89	0.17	49,49,49,49	0
82	OHX	sR	2045	7/7	0.89	0.36	139,139,139,139	0
83	MG	AR	3906	1/1	0.89	0.40	31,31,31,31	0
83	MG	1	3768	1/1	0.89	0.26	55,55,55,55	0
83	MG	sR	2177	1/1	0.89	0.74	50,50,50,50	0
83	MG	1	3930	1/1	0.89	0.97	44,44,44,44	0
83	MG	AR	4049	1/1	0.89	0.27	45,45,45,45	0
83	MG	1	4035	1/1	0.89	0.17	42,42,42,42	0
83	MG	AT	219	1/1	0.89	0.25	46,46,46,46	0
83	MG	AR	3786	1/1	0.89	0.43	43,43,43,43	0
83	MG	1	3834	1/1	0.89	0.48	18,18,18,18	0
83	MG	1	4064	1/1	0.89	0.24	30,30,30,30	0
83	MG	AR	3944	1/1	0.89	0.18	26,26,26,26	0
83	MG	AR	4032	1/1	0.89	0.19	47,47,47,47	0
83	MG	AR	3778	1/1	0.89	0.36	32,32,32,32	0
83	MG	sR	2179	1/1	0.89	0.56	51,51,51,51	0
83	MG	CP	502	1/1	0.89	0.51	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AR	4000	1/1	0.89	0.35	47,47,47,47	0
83	MG	A	1965	1/1	0.89	0.77	54,54,54,54	0
83	MG	CP	505	1/1	0.89	0.52	40,40,40,40	0
83	MG	A	2036	1/1	0.89	0.23	48,48,48,48	0
83	MG	A	1995	1/1	0.89	0.15	81,81,81,81	0
83	MG	1	3957	1/1	0.89	0.21	54,54,54,54	0
83	MG	1	4092	1/1	0.89	0.30	30,30,30,30	0
83	MG	1	3994	1/1	0.89	0.40	28,28,28,28	0
82	OHX	A	1930	7/7	0.89	0.24	193,193,193,193	0
83	MG	AR	3854	1/1	0.89	0.47	30,30,30,30	0
83	MG	AR	3851	1/1	0.89	0.27	25,25,25,25	0
83	MG	AR	3963	1/1	0.89	0.16	37,37,37,37	0
83	MG	AR	3751	1/1	0.89	0.58	27,27,27,27	0
83	MG	3	220	1/1	0.89	0.23	42,42,42,42	0
83	MG	1	4001	1/1	0.89	0.21	29,29,29,29	0
83	MG	AR	3938	1/1	0.89	0.33	39,39,39,39	0
83	MG	x	204	1/1	0.89	0.21	33,33,33,33	0
83	MG	4	216	1/1	0.90	0.80	48,48,48,48	0
83	MG	AR	4124	1/1	0.90	0.45	70,70,70,70	0
83	MG	1	4034	1/1	0.90	0.12	46,46,46,46	0
83	MG	1	4005	1/1	0.90	0.56	40,40,40,40	0
83	MG	AR	3972	1/1	0.90	0.20	44,44,44,44	0
83	MG	AR	4252	1/1	0.90	0.53	26,26,26,26	0
83	MG	A	2017	1/1	0.90	0.22	60,60,60,60	0
83	MG	AR	3957	1/1	0.90	0.50	36,36,36,36	0
83	MG	AR	3843	1/1	0.90	0.44	24,24,24,24	0
83	MG	AR	3762	1/1	0.90	0.33	33,33,33,33	0
83	MG	AR	4026	1/1	0.90	0.28	34,34,34,34	0
83	MG	AS	227	1/1	0.90	0.43	38,38,38,38	0
83	MG	1	4109	1/1	0.90	0.30	45,45,45,45	0
83	MG	1	4058	1/1	0.90	0.34	28,28,28,28	0
82	OHX	AR	3712	7/7	0.90	0.46	104,104,104,104	0
83	MG	1	3911	1/1	0.90	0.44	29,29,29,29	0
83	MG	AT	223	1/1	0.90	0.30	55,55,55,55	0
83	MG	AR	4236	1/1	0.90	0.32	34,34,34,34	0
83	MG	AR	4242	1/1	0.90	0.65	41,41,41,41	0
83	MG	1	3971	1/1	0.90	0.26	39,39,39,39	0
83	MG	AR	4132	1/1	0.90	0.26	29,29,29,29	0
83	MG	1	4082	1/1	0.90	0.45	29,29,29,29	0
83	MG	sR	2133	1/1	0.90	0.35	65,65,65,65	0
83	MG	AR	3746	1/1	0.90	0.24	24,24,24,24	0
83	MG	AR	4050	1/1	0.90	0.23	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3886	1/1	0.90	0.52	22,22,22,22	0
82	OHX	1	3709	7/7	0.90	0.43	127,127,127,127	0
83	MG	A	1953	1/1	0.90	0.62	53,53,53,53	0
83	MG	A	1952	1/1	0.90	0.54	53,53,53,53	0
83	MG	1	3900	1/1	0.90	0.42	21,21,21,21	0
83	MG	AR	4064	1/1	0.90	0.27	36,36,36,36	0
83	MG	sR	2186	1/1	0.90	0.28	41,41,41,41	0
83	MG	sR	2057	1/1	0.90	0.28	43,43,43,43	0
83	MG	AB	208	1/1	0.90	0.38	45,45,45,45	0
83	MG	1	4069	1/1	0.90	0.23	40,40,40,40	0
83	MG	1	3995	1/1	0.90	0.38	40,40,40,40	0
83	MG	AR	3867	1/1	0.90	0.62	46,46,46,46	0
83	MG	1	4131	1/1	0.90	0.30	22,22,22,22	0
83	MG	AR	3775	1/1	0.90	0.32	42,42,42,42	0
83	MG	AR	3983	1/1	0.90	0.26	25,25,25,25	0
83	MG	sR	2066	1/1	0.90	0.45	48,48,48,48	0
83	MG	sR	2119	1/1	0.90	0.35	63,63,63,63	0
83	MG	sR	2130	1/1	0.90	0.20	68,68,68,68	0
83	MG	1	3825	1/1	0.90	0.89	59,59,59,59	0
83	MG	d3	201	1/1	0.90	0.37	48,48,48,48	0
83	MG	1	4168	1/1	0.90	0.52	36,36,36,36	0
83	MG	sR	2170	1/1	0.90	0.74	54,54,54,54	0
82	OHX	1	3710	7/7	0.90	0.40	106,106,106,106	0
83	MG	AR	4067	1/1	0.90	0.40	31,31,31,31	0
83	MG	1	3982	1/1	0.90	0.25	26,26,26,26	0
82	OHX	AR	3530	7/7	0.90	0.27	69,69,69,69	0
83	MG	sR	2199	1/1	0.90	0.57	65,65,65,65	0
82	OHX	sR	2041	7/7	0.90	0.48	92,92,92,92	0
83	MG	1	3905	1/1	0.90	0.40	39,39,39,39	0
83	MG	AR	4051	1/1	0.90	0.26	46,46,46,46	0
83	MG	AR	3767	1/1	0.90	0.17	22,22,22,22	0
83	MG	AR	4139	1/1	0.90	0.14	127,127,127,127	0
83	MG	1	3773	1/1	0.90	0.15	29,29,29,29	0
83	MG	sR	2178	1/1	0.90	0.24	45,45,45,45	0
83	MG	sR	2146	1/1	0.90	0.23	71,71,71,71	0
82	OHX	1	3701	7/7	0.90	0.38	103,103,103,103	0
83	MG	AR	4207	1/1	0.90	0.79	43,43,43,43	0
83	MG	1	3750	1/1	0.90	0.33	23,23,23,23	0
83	MG	AK	104	1/1	0.90	0.28	47,47,47,47	0
83	MG	4	236	1/1	0.90	0.49	42,42,42,42	0
83	MG	sR	2153	1/1	0.90	0.26	39,39,39,39	0
83	MG	1	3998	1/1	0.90	0.43	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AR	3852	1/1	0.90	0.53	46,46,46,46	0
83	MG	sR	2127	1/1	0.90	0.57	50,50,50,50	0
83	MG	1	4000	1/1	0.90	0.37	43,43,43,43	0
83	MG	A	1997	1/1	0.90	0.43	88,88,88,88	0
83	MG	AR	3774	1/1	0.90	0.46	32,32,32,32	0
83	MG	1	3796	1/1	0.90	0.43	28,28,28,28	0
83	MG	AR	4217	1/1	0.90	0.58	42,42,42,42	0
83	MG	1	3888	1/1	0.90	0.38	39,39,39,39	0
83	MG	AR	4063	1/1	0.90	0.24	29,29,29,29	0
82	OHX	AR	3682	7/7	0.90	0.38	121,121,121,121	0
83	MG	DQ	505	1/1	0.90	0.17	34,34,34,34	0
82	OHX	AR	3729	7/7	0.90	0.21	114,114,114,114	0
82	OHX	AR	3721	7/7	0.90	0.37	118,118,118,118	0
83	MG	1	3754	1/1	0.90	0.46	39,39,39,39	0
83	MG	sR	2087	1/1	0.90	0.82	62,62,62,62	0
83	MG	AK	105	1/1	0.90	0.61	33,33,33,33	0
83	MG	AR	4197	1/1	0.90	0.09	48,48,48,48	0
83	MG	AR	4154	1/1	0.90	0.42	34,34,34,34	0
83	MG	CP	504	1/1	0.90	0.80	48,48,48,48	0
83	MG	AR	3954	1/1	0.90	0.51	28,28,28,28	0
83	MG	6	203	1/1	0.90	0.49	40,40,40,40	0
83	MG	sR	2117	1/1	0.90	0.20	49,49,49,49	0
83	MG	sR	2076	1/1	0.90	0.76	55,55,55,55	0
83	MG	sR	2129	1/1	0.90	0.31	39,39,39,39	0
83	MG	1	3772	1/1	0.90	0.35	23,23,23,23	0
83	MG	AR	4135	1/1	0.90	0.23	25,25,25,25	0
83	MG	AR	3740	1/1	0.90	0.32	24,24,24,24	0
83	MG	AR	3886	1/1	0.90	0.67	35,35,35,35	0
83	MG	AR	4102	1/1	0.90	0.27	32,32,32,32	0
83	MG	sR	2105	1/1	0.90	1.04	56,56,56,56	0
83	MG	sR	2083	1/1	0.90	0.93	56,56,56,56	0
83	MG	AR	4136	1/1	0.90	0.19	34,34,34,34	0
82	OHX	1	3687	7/7	0.90	0.33	116,116,116,116	0
83	MG	1	3794	1/1	0.90	0.31	45,45,45,45	0
83	MG	AR	4115	1/1	0.90	0.15	47,47,47,47	0
83	MG	CE	404	1/1	0.90	0.31	22,22,22,22	0
83	MG	1	4215	1/1	0.90	0.49	38,38,38,38	0
83	MG	sR	2090	1/1	0.91	0.44	30,30,30,30	0
83	MG	1	3882	1/1	0.91	0.52	45,45,45,45	0
83	MG	AR	4076	1/1	0.91	0.21	51,51,51,51	0
82	OHX	1	3691	7/7	0.91	0.37	154,154,154,154	0
82	OHX	A	1932	7/7	0.91	0.23	215,215,215,215	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	A	1885	7/7	0.91	0.35	96,96,96,96	0
83	MG	1	3987	1/1	0.91	0.32	30,30,30,30	0
83	MG	A	2049	1/1	0.91	0.20	54,54,54,54	0
82	OHX	A	1846	7/7	0.91	0.21	126,126,126,126	0
83	MG	1	3993	1/1	0.91	0.50	57,57,57,57	0
83	MG	A	1984	1/1	0.91	0.49	66,66,66,66	0
83	MG	3	216	1/1	0.91	0.30	38,38,38,38	0
83	MG	1	3758	1/1	0.91	0.26	40,40,40,40	0
83	MG	1	3730	1/1	0.91	0.45	78,78,78,78	0
83	MG	AR	4210	1/1	0.91	0.30	33,33,33,33	0
82	OHX	sR	2021	7/7	0.91	0.31	137,137,137,137	0
83	MG	1	3933	1/1	0.91	0.28	35,35,35,35	0
83	MG	AR	4077	1/1	0.91	0.22	47,47,47,47	0
82	OHX	CG	302	7/7	0.91	0.36	107,107,107,107	0
82	OHX	AR	3687	7/7	0.91	0.33	136,136,136,136	0
83	MG	AR	4240	1/1	0.91	0.17	33,33,33,33	0
83	MG	AR	4021	1/1	0.91	0.41	35,35,35,35	0
83	MG	1	3743	1/1	0.91	0.51	41,41,41,41	0
83	MG	1	4154	1/1	0.91	0.24	38,38,38,38	0
82	OHX	1	3652	7/7	0.91	0.34	76,76,76,76	0
83	MG	r	302	1/1	0.91	0.33	35,35,35,35	0
83	MG	CR	201	1/1	0.91	0.45	26,26,26,26	0
83	MG	1	3867	1/1	0.91	0.55	31,31,31,31	0
83	MG	1	4165	1/1	0.91	0.22	33,33,33,33	0
83	MG	AR	3856	1/1	0.91	0.28	33,33,33,33	0
83	MG	1	3805	1/1	0.91	0.29	33,33,33,33	0
83	MG	1	3851	1/1	0.91	0.37	24,24,24,24	0
83	MG	F	301	1/1	0.91	0.51	62,62,62,62	0
83	MG	3	215	1/1	0.91	0.39	59,59,59,59	0
83	MG	1	3976	1/1	0.91	0.31	24,24,24,24	0
83	MG	AR	3828	1/1	0.91	0.48	25,25,25,25	0
83	MG	1	3979	1/1	0.91	0.65	31,31,31,31	0
83	MG	1	3776	1/1	0.91	0.34	29,29,29,29	0
83	MG	DC	201	1/1	0.91	0.30	20,20,20,20	0
83	MG	4	218	1/1	0.91	0.43	55,55,55,55	0
83	MG	3	222	1/1	0.91	0.52	27,27,27,27	0
83	MG	AR	4170	1/1	0.91	0.34	31,31,31,31	0
83	MG	AR	4019	1/1	0.91	0.12	31,31,31,31	0
82	OHX	AR	3711	7/7	0.91	0.40	133,133,133,133	0
83	MG	1	4202	1/1	0.91	0.39	43,43,43,43	0
83	MG	AH	201	1/1	0.91	0.48	49,49,49,49	0
83	MG	AS	226	1/1	0.91	0.29	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AR	4127	1/1	0.91	0.25	37,37,37,37	0
83	MG	D	301	1/1	0.91	0.68	66,66,66,66	0
83	MG	1	4006	1/1	0.91	0.26	38,38,38,38	0
82	OHX	s1	301	7/7	0.91	0.45	126,126,126,126	0
83	MG	AR	4010	1/1	0.91	0.59	66,66,66,66	0
82	OHX	sR	1960	7/7	0.91	0.24	92,92,92,92	0
83	MG	AR	3996	1/1	0.91	0.30	21,21,21,21	0
83	MG	sR	2203	1/1	0.91	0.61	42,42,42,42	0
82	OHX	AR	3519	7/7	0.91	0.15	122,122,122,122	0
83	MG	1	3727	1/1	0.91	0.24	31,31,31,31	0
83	MG	AR	3793	1/1	0.91	0.37	36,36,36,36	0
83	MG	A	2066	1/1	0.91	0.80	58,58,58,58	0
83	MG	AR	3993	1/1	0.91	0.27	39,39,39,39	0
83	MG	1	4033	1/1	0.91	0.26	30,30,30,30	0
83	MG	A	1982	1/1	0.91	0.21	57,57,57,57	0
82	OHX	sR	2042	7/7	0.91	0.35	118,118,118,118	0
82	OHX	AR	3642	7/7	0.91	0.28	101,101,101,101	0
83	MG	AR	4239	1/1	0.91	0.41	30,30,30,30	0
83	MG	4	235	1/1	0.91	0.16	30,30,30,30	0
83	MG	A	2063	1/1	0.91	0.77	76,76,76,76	0
83	MG	AR	4200	1/1	0.91	0.25	70,70,70,70	0
83	MG	4	231	1/1	0.91	0.32	35,35,35,35	0
82	OHX	A	1921	7/7	0.91	0.29	140,140,140,140	0
83	MG	j	301	1/1	0.91	0.36	25,25,25,25	0
83	MG	1	4177	1/1	0.91	0.50	66,66,66,66	0
83	MG	AR	3756	1/1	0.91	0.33	27,27,27,27	0
83	MG	1	3990	1/1	0.91	0.63	36,36,36,36	0
83	MG	1	3778	1/1	0.91	0.40	31,31,31,31	0
83	MG	1	4187	1/1	0.91	0.20	34,34,34,34	0
83	MG	1	3872	1/1	0.91	0.48	37,37,37,37	0
82	OHX	AS	208	7/7	0.91	0.28	115,115,115,115	0
83	MG	A	2003	1/1	0.91	0.45	55,55,55,55	0
83	MG	AR	4074	1/1	0.91	0.45	36,36,36,36	0
82	OHX	A	1871	7/7	0.91	0.20	116,116,116,116	0
83	MG	1	4086	1/1	0.91	0.15	28,28,28,28	0
82	OHX	AR	3724	7/7	0.91	0.41	115,115,115,115	0
83	MG	1	4216	1/1	0.91	0.59	44,44,44,44	0
83	MG	AR	4258	1/1	0.91	0.60	26,26,26,26	0
83	MG	1	3969	1/1	0.91	0.16	35,35,35,35	0
83	MG	CD	302	1/1	0.91	0.57	27,27,27,27	0
83	MG	sR	2074	1/1	0.91	0.55	41,41,41,41	0
83	MG	AR	3780	1/1	0.91	0.42	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3731	7/7	0.91	0.35	135,135,135,135	0
83	MG	1	4024	1/1	0.91	0.36	33,33,33,33	0
83	MG	1	3964	1/1	0.91	0.34	30,30,30,30	0
83	MG	AR	3749	1/1	0.91	0.53	32,32,32,32	0
83	MG	AT	222	1/1	0.92	0.48	39,39,39,39	0
83	MG	AR	3875	1/1	0.92	0.38	29,29,29,29	0
83	MG	AR	3901	1/1	0.92	0.43	42,42,42,42	0
83	MG	AR	3827	1/1	0.92	0.20	22,22,22,22	0
83	MG	AR	4012	1/1	0.92	0.24	29,29,29,29	0
83	MG	1	4071	1/1	0.92	0.12	39,39,39,39	0
83	MG	AR	3748	1/1	0.92	0.24	44,44,44,44	0
83	MG	AR	3821	1/1	0.92	0.61	23,23,23,23	0
83	MG	1	4172	1/1	0.92	0.38	42,42,42,42	0
83	MG	1	3941	1/1	0.92	0.19	45,45,45,45	0
83	MG	1	3738	1/1	0.92	0.64	51,51,51,51	0
83	MG	AR	4086	1/1	0.92	0.13	38,38,38,38	0
83	MG	AR	3978	1/1	0.92	0.32	41,41,41,41	0
82	OHX	A	1934	7/7	0.92	0.48	103,103,103,103	0
83	MG	AR	3891	1/1	0.92	0.42	25,25,25,25	0
83	MG	sR	2200	1/1	0.92	0.25	36,36,36,36	0
82	OHX	4	212	7/7	0.92	0.35	112,112,112,112	0
83	MG	1	4011	1/1	0.92	0.66	45,45,45,45	0
83	MG	3	219	1/1	0.92	0.15	63,63,63,63	0
83	MG	AB	204	1/1	0.92	0.26	25,25,25,25	0
83	MG	x	203	1/1	0.92	0.18	27,27,27,27	0
82	OHX	A	1881	7/7	0.92	0.21	173,173,173,173	0
83	MG	sR	2126	1/1	0.92	0.31	62,62,62,62	0
85	ZN	d7	101	1/1	0.92	0.20	108,108,108,108	0
83	MG	AR	3966	1/1	0.92	0.39	70,70,70,70	0
83	MG	AR	3920	1/1	0.92	0.30	24,24,24,24	0
83	MG	AR	3797	1/1	0.92	0.36	23,23,23,23	0
83	MG	AR	3776	1/1	0.92	0.30	52,52,52,52	0
83	MG	AR	3759	1/1	0.92	0.27	29,29,29,29	0
83	MG	AR	3965	1/1	0.92	0.27	30,30,30,30	0
82	OHX	sR	2048	7/7	0.92	0.36	112,112,112,112	0
83	MG	1	3823	1/1	0.92	0.45	36,36,36,36	0
82	OHX	AR	3649	7/7	0.92	0.31	101,101,101,101	0
83	MG	sR	2181	1/1	0.92	0.47	44,44,44,44	0
83	MG	1	4056	1/1	0.92	0.21	27,27,27,27	0
83	MG	1	3921	1/1	0.92	0.48	31,31,31,31	0
83	MG	1	3857	1/1	0.92	0.23	23,23,23,23	0
82	OHX	A	1909	7/7	0.92	0.26	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3853	1/1	0.92	0.82	31,31,31,31	0
83	MG	AR	4108	1/1	0.92	0.41	24,24,24,24	0
82	OHX	z	201	7/7	0.92	0.39	123,123,123,123	0
83	MG	1	3948	1/1	0.92	0.49	40,40,40,40	0
83	MG	AR	4121	1/1	0.92	0.27	26,26,26,26	0
83	MG	A	1944	1/1	0.92	0.41	36,36,36,36	0
83	MG	A	2022	1/1	0.92	0.50	53,53,53,53	0
83	MG	AP	503	1/1	0.92	0.11	52,52,52,52	0
83	MG	1	4121	1/1	0.92	0.30	39,39,39,39	0
83	MG	sR	2071	1/1	0.92	0.82	47,47,47,47	0
83	MG	1	3965	1/1	0.92	0.17	36,36,36,36	0
83	MG	4	229	1/1	0.92	0.22	45,45,45,45	0
82	OHX	A	1912	7/7	0.92	0.35	125,125,125,125	0
83	MG	DH	202	1/1	0.92	0.57	29,29,29,29	0
83	MG	sR	2144	1/1	0.92	0.20	51,51,51,51	0
83	MG	1	4188	1/1	0.92	0.53	41,41,41,41	0
83	MG	1	4193	1/1	0.92	0.48	35,35,35,35	0
83	MG	DC	202	1/1	0.92	0.38	41,41,41,41	0
82	OHX	1	3718	7/7	0.92	0.43	94,94,94,94	0
82	OHX	AR	3700	7/7	0.92	0.35	106,106,106,106	0
83	MG	AR	3785	1/1	0.92	0.21	36,36,36,36	0
83	MG	1	3950	1/1	0.92	0.28	31,31,31,31	0
82	OHX	A	1908	7/7	0.92	0.24	122,122,122,122	0
83	MG	1	3840	1/1	0.92	0.43	31,31,31,31	0
82	OHX	AR	3727	7/7	0.92	0.39	107,107,107,107	0
83	MG	t	203	1/1	0.92	0.35	22,22,22,22	0
82	OHX	sR	1969	7/7	0.92	0.19	91,91,91,91	0
83	MG	1	3910	1/1	0.92	0.72	40,40,40,40	0
83	MG	1	4217	1/1	0.92	0.25	50,50,50,50	0
82	OHX	AR	3713	7/7	0.92	0.40	121,121,121,121	0
83	MG	AR	3763	1/1	0.92	0.36	36,36,36,36	0
82	OHX	J	301	7/7	0.92	0.32	106,106,106,106	0
83	MG	1	4124	1/1	0.92	0.20	29,29,29,29	0
83	MG	1	3873	1/1	0.92	0.41	28,28,28,28	0
83	MG	AB	205	1/1	0.92	0.45	26,26,26,26	0
83	MG	A	1949	1/1	0.92	0.67	53,53,53,53	0
83	MG	sR	2060	1/1	0.92	0.32	69,69,69,69	0
83	MG	1	4045	1/1	0.92	0.20	33,33,33,33	0
83	MG	t	201	1/1	0.92	0.19	39,39,39,39	0
83	MG	sR	2078	1/1	0.92	0.34	48,48,48,48	0
83	MG	1	3786	1/1	0.92	0.43	22,22,22,22	0
83	MG	1	4057	1/1	0.92	0.26	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AR	4044	1/1	0.92	0.24	42,42,42,42	0
83	MG	AR	4177	1/1	0.92	0.28	33,33,33,33	0
83	MG	sR	2156	1/1	0.92	0.61	51,51,51,51	0
83	MG	AR	3967	1/1	0.92	0.21	42,42,42,42	0
82	OHX	sR	2036	7/7	0.92	0.41	118,118,118,118	0
82	OHX	CS	201	1/7	0.92	0.05	137,137,137,137	0
83	MG	AR	4169	1/1	0.92	0.20	29,29,29,29	0
83	MG	AR	4003	1/1	0.92	0.62	38,38,38,38	0
83	MG	DI	201	1/1	0.92	0.39	53,53,53,53	0
83	MG	AR	4042	1/1	0.92	0.29	33,33,33,33	0
83	MG	AR	3848	1/1	0.92	0.47	36,36,36,36	0
83	MG	AR	4037	1/1	0.92	0.21	29,29,29,29	0
83	MG	sR	2155	1/1	0.92	0.21	44,44,44,44	0
83	MG	1	3852	1/1	0.92	0.34	43,43,43,43	0
83	MG	AR	3923	1/1	0.92	0.38	31,31,31,31	0
83	MG	A	2020	1/1	0.92	0.41	78,78,78,78	0
83	MG	1	3869	1/1	0.92	0.33	42,42,42,42	0
83	MG	sR	2147	1/1	0.92	0.33	45,45,45,45	0
82	OHX	AR	3703	7/7	0.92	0.35	99,99,99,99	0
83	MG	1	4152	1/1	0.92	0.20	40,40,40,40	0
83	MG	AR	4033	1/1	0.92	0.33	25,25,25,25	0
83	MG	AR	3872	1/1	0.92	0.38	29,29,29,29	0
83	MG	1	4122	1/1	0.92	0.33	38,38,38,38	0
83	MG	A	2034	1/1	0.92	0.70	73,73,73,73	0
83	MG	1	4179	1/1	0.92	0.52	34,34,34,34	0
83	MG	AR	4068	1/1	0.92	0.52	28,28,28,28	0
83	MG	AR	4005	1/1	0.92	0.12	27,27,27,27	0
82	OHX	CM	201	7/7	0.92	0.37	120,120,120,120	0
83	MG	A	2067	1/1	0.92	0.85	56,56,56,56	0
83	MG	A	1945	1/1	0.92	0.63	47,47,47,47	0
83	MG	AR	3820	1/1	0.92	0.14	53,53,53,53	0
83	MG	1	4117	1/1	0.92	0.18	54,54,54,54	0
82	OHX	sR	2027	7/7	0.93	0.33	114,114,114,114	0
83	MG	1	3885	1/1	0.93	0.61	32,32,32,32	0
83	MG	AB	201	1/1	0.93	0.23	20,20,20,20	0
83	MG	AR	4098	1/1	0.93	0.33	33,33,33,33	0
82	OHX	sR	2002	7/7	0.93	0.32	97,97,97,97	0
86	GOL	AR	4262	6/6	0.93	0.28	27,27,27,27	0
83	MG	AR	4070	1/1	0.93	0.35	27,27,27,27	0
83	MG	1	3968	1/1	0.93	0.54	28,28,28,28	0
82	OHX	sR	2006	7/7	0.93	0.28	121,121,121,121	0
83	MG	AS	223	1/1	0.93	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	sR	2172	1/1	0.93	0.27	70,70,70,70	0
82	OHX	AR	3641	7/7	0.93	0.28	104,104,104,104	0
82	OHX	1	3712	7/7	0.93	0.48	99,99,99,99	0
83	MG	AR	4205	1/1	0.93	0.18	30,30,30,30	0
82	OHX	AR	3677	7/7	0.93	0.31	117,117,117,117	0
83	MG	AR	3947	1/1	0.93	0.14	34,34,34,34	0
83	MG	1	3836	1/1	0.93	0.39	27,27,27,27	0
83	MG	AR	3861	1/1	0.93	0.48	23,23,23,23	0
82	OHX	1	3698	7/7	0.93	0.38	131,131,131,131	0
83	MG	sR	2198	1/1	0.93	0.49	60,60,60,60	0
83	MG	AR	4219	1/1	0.93	0.57	39,39,39,39	0
83	MG	sR	2122	1/1	0.93	0.36	48,48,48,48	0
83	MG	AR	3863	1/1	0.93	0.46	30,30,30,30	0
83	MG	1	3914	1/1	0.93	0.56	28,28,28,28	0
83	MG	CU	202	1/1	0.93	0.27	32,32,32,32	0
83	MG	1	4153	1/1	0.93	0.24	42,42,42,42	0
83	MG	AR	3760	1/1	0.93	0.22	36,36,36,36	0
82	OHX	sR	2044	7/7	0.93	0.36	126,126,126,126	0
83	MG	AR	3770	1/1	0.93	0.32	40,40,40,40	0
83	MG	1	4218	1/1	0.93	0.16	23,23,23,23	0
82	OHX	sR	1990	7/7	0.93	0.36	103,103,103,103	0
82	OHX	1	3486	7/7	0.93	0.20	73,73,73,73	0
83	MG	1	4119	1/1	0.93	0.18	44,44,44,44	0
83	MG	AR	4004	1/1	0.93	0.34	35,35,35,35	0
82	OHX	AR	3633	7/7	0.93	0.20	142,142,142,142	0
82	OHX	CF	401	7/7	0.93	0.35	107,107,107,107	0
83	MG	AR	3960	1/1	0.93	0.21	41,41,41,41	0
82	OHX	sR	2040	7/7	0.93	0.46	111,111,111,111	0
83	MG	AR	4224	1/1	0.93	0.29	28,28,28,28	0
82	OHX	A	1926	7/7	0.93	0.38	115,115,115,115	0
83	MG	AR	3822	1/1	0.93	0.14	38,38,38,38	0
83	MG	1	4041	1/1	0.93	0.21	27,27,27,27	0
82	OHX	AR	3657	7/7	0.93	0.32	82,82,82,82	0
82	OHX	4	213	7/7	0.93	0.33	109,109,109,109	0
83	MG	1	4174	1/1	0.93	0.54	27,27,27,27	0
82	OHX	1	3708	7/7	0.93	0.36	110,110,110,110	0
83	MG	AR	4101	1/1	0.93	0.17	27,27,27,27	0
83	MG	AR	3941	1/1	0.93	0.50	23,23,23,23	0
83	MG	CR	206	1/1	0.93	0.43	33,33,33,33	0
83	MG	1	4104	1/1	0.93	0.17	39,39,39,39	0
83	MG	1	4156	1/1	0.93	0.12	46,46,46,46	0
82	OHX	AR	3697	7/7	0.93	0.43	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3736	1/1	0.93	0.30	30,30,30,30	0
83	MG	1	4095	1/1	0.93	0.15	38,38,38,38	0
83	MG	AR	3930	1/1	0.93	0.14	37,37,37,37	0
83	MG	AR	3811	1/1	0.93	0.24	44,44,44,44	0
82	OHX	AR	3650	7/7	0.93	0.37	103,103,103,103	0
83	MG	AB	207	1/1	0.93	0.19	29,29,29,29	0
83	MG	AR	3943	1/1	0.93	0.29	43,43,43,43	0
82	OHX	CO	201	7/7	0.93	0.39	148,148,148,148	0
83	MG	AR	3777	1/1	0.93	0.41	28,28,28,28	0
83	MG	s4	302	1/1	0.93	0.38	47,47,47,47	0
83	MG	1	3775	1/1	0.93	0.40	37,37,37,37	0
83	MG	1	3996	1/1	0.93	0.31	21,21,21,21	0
83	MG	1	3734	1/1	0.93	0.46	24,24,24,24	0
83	MG	1	3985	1/1	0.93	0.11	39,39,39,39	0
83	MG	A	1993	1/1	0.93	0.72	74,74,74,74	0
83	MG	1	3860	1/1	0.93	0.70	46,46,46,46	0
83	MG	sR	2151	1/1	0.93	0.39	48,48,48,48	0
83	MG	AR	4078	1/1	0.93	0.41	34,34,34,34	0
83	MG	1	4196	1/1	0.93	0.63	29,29,29,29	0
82	OHX	sR	1932	7/7	0.93	0.17	88,88,88,88	0
83	MG	AR	3912	1/1	0.93	0.90	38,38,38,38	0
83	MG	1	4043	1/1	0.93	0.19	35,35,35,35	0
83	MG	AR	4241	1/1	0.93	0.49	25,25,25,25	0
83	MG	DQ	504	1/1	0.93	0.12	31,31,31,31	0
83	MG	d4	202	1/1	0.93	0.35	43,43,43,43	0
83	MG	1	4198	1/1	0.93	0.19	29,29,29,29	0
83	MG	AR	3950	1/1	0.93	0.35	32,32,32,32	0
82	OHX	1	3608	7/7	0.93	0.27	96,96,96,96	0
82	OHX	AR	3607	7/7	0.93	0.19	124,124,124,124	0
82	OHX	AR	3715	7/7	0.93	0.30	111,111,111,111	0
83	MG	1	3789	1/1	0.93	0.70	40,40,40,40	0
83	MG	AR	4052	1/1	0.93	0.34	39,39,39,39	0
83	MG	sR	2056	1/1	0.93	0.37	61,61,61,61	0
82	OHX	AR	3566	7/7	0.93	0.22	100,100,100,100	0
82	OHX	sR	1966	7/7	0.93	0.19	101,101,101,101	0
83	MG	1	4113	1/1	0.93	0.20	43,43,43,43	0
82	OHX	sR	2037	7/7	0.93	0.35	114,114,114,114	0
83	MG	1	3915	1/1	0.93	0.45	45,45,45,45	0
83	MG	1	4190	1/1	0.93	0.50	21,21,21,21	0
83	MG	AR	4196	1/1	0.93	0.17	29,29,29,29	0
83	MG	AR	4185	1/1	0.93	0.21	29,29,29,29	0
82	OHX	A	1918	7/7	0.93	0.33	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	sR	2092	1/1	0.93	0.81	58,58,58,58	0
83	MG	A	2059	1/1	0.93	0.85	69,69,69,69	0
83	MG	CO	202	1/1	0.93	0.22	34,34,34,34	0
83	MG	4	233	1/1	0.93	0.43	52,52,52,52	0
82	OHX	1	3666	7/7	0.93	0.49	86,86,86,86	0
82	OHX	A	1925	7/7	0.93	0.28	149,149,149,149	0
83	MG	AR	4176	1/1	0.93	0.20	28,28,28,28	0
83	MG	1	3726	1/1	0.93	0.65	40,40,40,40	0
83	MG	AT	226	1/1	0.93	0.17	38,38,38,38	0
83	MG	sR	2168	1/1	0.93	0.58	48,48,48,48	0
82	OHX	1	3700	7/7	0.93	0.40	111,111,111,111	0
82	OHX	1	3717	7/7	0.93	0.37	117,117,117,117	0
83	MG	sR	2096	1/1	0.93	0.58	37,37,37,37	0
83	MG	1	3953	1/1	0.93	0.18	39,39,39,39	0
83	MG	1	3858	1/1	0.93	0.48	26,26,26,26	0
83	MG	1	3929	1/1	0.93	0.09	47,47,47,47	0
83	MG	1	3756	1/1	0.93	0.67	38,38,38,38	0
83	MG	1	4053	1/1	0.93	0.32	34,34,34,34	0
83	MG	1	4091	1/1	0.93	0.23	42,42,42,42	0
83	MG	c1	203	1/1	0.93	0.33	51,51,51,51	0
83	MG	A	1958	1/1	0.93	0.41	47,47,47,47	0
82	OHX	sR	2019	7/7	0.93	0.38	113,113,113,113	0
83	MG	sR	2091	1/1	0.93	0.38	38,38,38,38	0
83	MG	1	4014	1/1	0.93	0.44	33,33,33,33	0
83	MG	1	3740	1/1	0.93	0.14	43,43,43,43	0
83	MG	sR	2158	1/1	0.93	0.20	57,57,57,57	0
83	MG	AR	4163	1/1	0.93	0.31	38,38,38,38	0
82	OHX	sR	1977	7/7	0.93	0.20	104,104,104,104	0
83	MG	sR	2075	1/1	0.93	0.61	42,42,42,42	0
83	MG	AS	224	1/1	0.93	0.55	36,36,36,36	0
83	MG	1	3908	1/1	0.93	0.38	35,35,35,35	0
83	MG	sR	2190	1/1	0.93	0.41	53,53,53,53	0
83	MG	AR	4083	1/1	0.93	0.22	47,47,47,47	0
83	MG	AR	3818	1/1	0.93	0.62	50,50,50,50	0
82	OHX	AR	3725	7/7	0.93	0.41	111,111,111,111	0
83	MG	A	2019	1/1	0.93	0.29	51,51,51,51	0
83	MG	1	3737	1/1	0.93	0.50	35,35,35,35	0
82	OHX	AR	3702	7/7	0.93	0.36	82,82,82,82	0
83	MG	A	2052	1/1	0.93	0.58	66,66,66,66	0
83	MG	AR	3860	1/1	0.93	0.48	29,29,29,29	0
82	OHX	1	3668	7/7	0.93	0.42	79,79,79,79	0
83	MG	sR	2104	1/1	0.93	0.57	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3659	7/7	0.93	0.35	95,95,95,95	0
83	MG	AS	216	1/1	0.93	0.34	37,37,37,37	0
82	OHX	1	3716	7/7	0.93	0.41	112,112,112,112	0
83	MG	sR	2112	1/1	0.94	0.43	50,50,50,50	0
82	OHX	1	3603	7/7	0.94	0.31	85,85,85,85	0
83	MG	b	202	1/1	0.94	0.46	63,63,63,63	0
83	MG	1	4007	1/1	0.94	0.21	28,28,28,28	0
83	MG	sR	2192	1/1	0.94	0.52	41,41,41,41	0
82	OHX	AR	3603	7/7	0.94	0.34	85,85,85,85	0
83	MG	Y	201	1/1	0.94	0.15	50,50,50,50	0
83	MG	AR	3998	1/1	0.94	0.37	36,36,36,36	0
82	OHX	CG	303	7/7	0.94	0.42	105,105,105,105	0
83	MG	A	2015	1/1	0.94	0.43	75,75,75,75	0
83	MG	AR	3914	1/1	0.94	0.45	32,32,32,32	0
83	MG	AR	3795	1/1	0.94	0.34	22,22,22,22	0
83	MG	sR	2166	1/1	0.94	0.21	56,56,56,56	0
83	MG	AR	3790	1/1	0.94	0.28	27,27,27,27	0
83	MG	AR	4209	1/1	0.94	0.30	44,44,44,44	0
83	MG	1	4088	1/1	0.94	0.25	86,86,86,86	0
83	MG	A	1999	1/1	0.94	0.45	55,55,55,55	0
83	MG	CG	304	1/1	0.94	0.53	35,35,35,35	0
83	MG	AR	4159	1/1	0.94	0.15	30,30,30,30	0
83	MG	AR	3825	1/1	0.94	0.25	43,43,43,43	0
83	MG	AR	4043	1/1	0.94	0.17	51,51,51,51	0
82	OHX	1	3645	7/7	0.94	0.33	99,99,99,99	0
83	MG	CR	208	1/1	0.94	0.39	31,31,31,31	0
86	GOL	AR	4263	6/6	0.94	0.36	40,40,40,40	0
83	MG	CJ	301	1/1	0.94	0.44	68,68,68,68	0
83	MG	AR	4040	1/1	0.94	0.49	30,30,30,30	0
82	OHX	sR	2034	7/7	0.94	0.39	110,110,110,110	0
82	OHX	1	3665	7/7	0.94	0.36	107,107,107,107	0
83	MG	sR	2051	1/1	0.94	0.38	46,46,46,46	0
83	MG	A	1964	1/1	0.94	0.64	60,60,60,60	0
83	MG	AR	3809	1/1	0.94	0.32	37,37,37,37	0
82	OHX	sR	2013	7/7	0.94	0.34	83,83,83,83	0
82	OHX	A	1877	7/7	0.94	0.31	118,118,118,118	0
83	MG	1	4166	1/1	0.94	0.19	34,34,34,34	0
83	MG	1	3804	1/1	0.94	0.12	59,59,59,59	0
83	MG	AR	4081	1/1	0.94	0.29	35,35,35,35	0
82	OHX	AR	3716	7/7	0.94	0.24	120,120,120,120	0
83	MG	AR	4255	1/1	0.94	0.45	48,48,48,48	0
83	MG	1	3782	1/1	0.94	0.40	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AR	4183	1/1	0.94	0.37	36,36,36,36	0
82	OHX	sR	2025	7/7	0.94	0.33	110,110,110,110	0
83	MG	A	1972	1/1	0.94	0.29	59,59,59,59	0
83	MG	1	4032	1/1	0.94	0.13	63,63,63,63	0
82	OHX	sR	2029	7/7	0.94	0.40	86,86,86,86	0
82	OHX	A	1915	7/7	0.94	0.35	125,125,125,125	0
83	MG	AR	4080	1/1	0.94	0.17	43,43,43,43	0
83	MG	A	1974	1/1	0.94	0.61	54,54,54,54	0
83	MG	c8	202	1/1	0.94	0.56	68,68,68,68	0
83	MG	1	4102	1/1	0.94	0.18	31,31,31,31	0
83	MG	sR	2098	1/1	0.94	0.43	38,38,38,38	0
83	MG	AR	3942	1/1	0.94	0.32	25,25,25,25	0
82	OHX	sR	1972	7/7	0.94	0.35	110,110,110,110	0
83	MG	1	3819	1/1	0.94	0.23	69,69,69,69	0
82	OHX	AR	3726	7/7	0.94	0.39	105,105,105,105	0
83	MG	1	4101	1/1	0.94	0.23	69,69,69,69	0
83	MG	1	3892	1/1	0.94	0.37	23,23,23,23	0
83	MG	AR	3874	1/1	0.94	0.38	30,30,30,30	0
83	MG	AR	3902	1/1	0.94	0.49	21,21,21,21	0
82	OHX	1	3597	7/7	0.94	0.35	100,100,100,100	0
83	MG	AR	3832	1/1	0.94	0.31	30,30,30,30	0
83	MG	A	1966	1/1	0.94	0.59	75,75,75,75	0
83	MG	AS	229	1/1	0.94	0.24	43,43,43,43	0
83	MG	1	3932	1/1	0.94	0.58	52,52,52,52	0
83	MG	1	4148	1/1	0.94	0.24	31,31,31,31	0
83	MG	A	1980	1/1	0.94	0.56	55,55,55,55	0
83	MG	AR	4225	1/1	0.94	0.38	45,45,45,45	0
82	OHX	1	3702	7/7	0.94	0.26	162,162,162,162	0
83	MG	A	2024	1/1	0.94	0.77	53,53,53,53	0
83	MG	v	304	1/1	0.94	0.25	37,37,37,37	0
82	OHX	A	1818	7/7	0.94	0.15	80,80,80,80	0
83	MG	1	3741	1/1	0.94	0.28	25,25,25,25	0
83	MG	AR	3918	1/1	0.94	0.44	25,25,25,25	0
83	MG	1	4123	1/1	0.94	0.23	30,30,30,30	0
82	OHX	sR	1980	7/7	0.94	0.45	76,76,76,76	0
83	MG	AR	3910	1/1	0.94	0.57	36,36,36,36	0
82	OHX	s4	301	7/7	0.94	0.24	118,118,118,118	0
83	MG	sR	2089	1/1	0.94	0.30	41,41,41,41	0
82	OHX	AR	3678	7/7	0.94	0.46	111,111,111,111	0
82	OHX	1	3675	7/7	0.94	0.34	111,111,111,111	0
83	MG	A	1987	1/1	0.94	0.47	60,60,60,60	0
82	OHX	1	3655	7/7	0.94	0.37	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3980	1/1	0.94	0.39	36,36,36,36	0
83	MG	1	4209	1/1	0.94	0.33	34,34,34,34	0
83	MG	AR	4165	1/1	0.94	0.51	38,38,38,38	0
83	MG	AS	212	1/1	0.94	0.41	25,25,25,25	0
83	MG	1	4075	1/1	0.94	0.41	25,25,25,25	0
83	MG	1	3889	1/1	0.94	0.42	25,25,25,25	0
82	OHX	AR	3735	7/7	0.94	0.35	85,85,85,85	0
83	MG	1	3988	1/1	0.94	0.49	63,63,63,63	0
83	MG	AR	4114	1/1	0.94	0.31	64,64,64,64	0
83	MG	A	2047	1/1	0.94	0.36	60,60,60,60	0
82	OHX	1	3614	7/7	0.94	0.35	111,111,111,111	0
82	OHX	AR	3500	7/7	0.94	0.16	90,90,90,90	0
82	OHX	3	208	7/7	0.94	0.22	112,112,112,112	0
83	MG	1	3984	1/1	0.94	0.30	36,36,36,36	0
82	OHX	AR	3710	7/7	0.94	0.38	112,112,112,112	0
83	MG	1	3797	1/1	0.94	0.33	24,24,24,24	0
83	MG	AR	4007	1/1	0.94	0.25	35,35,35,35	0
83	MG	1	4066	1/1	0.94	0.27	26,26,26,26	0
83	MG	4	217	1/1	0.94	0.53	41,41,41,41	0
83	MG	1	3748	1/1	0.94	0.28	32,32,32,32	0
83	MG	sR	2121	1/1	0.94	0.28	45,45,45,45	0
83	MG	1	4200	1/1	0.94	0.49	29,29,29,29	0
82	OHX	AR	3571	7/7	0.94	0.30	76,76,76,76	0
83	MG	1	3781	1/1	0.94	0.37	20,20,20,20	0
83	MG	4	224	1/1	0.94	0.32	36,36,36,36	0
83	MG	1	3766	1/1	0.94	0.34	21,21,21,21	0
82	OHX	AR	3737	7/7	0.94	0.25	58,58,58,58	0
83	MG	A	1979	1/1	0.94	0.61	53,53,53,53	0
83	MG	AT	218	1/1	0.94	0.53	31,31,31,31	0
83	MG	1	4015	1/1	0.94	0.17	38,38,38,38	0
83	MG	AR	3864	1/1	0.94	0.42	25,25,25,25	0
82	OHX	1	3669	7/7	0.94	0.34	112,112,112,112	0
82	OHX	AR	3719	7/7	0.94	0.42	83,83,83,83	0
83	MG	AR	4140	1/1	0.94	0.13	27,27,27,27	0
82	OHX	A	1870	7/7	0.94	0.28	92,92,92,92	0
83	MG	AR	4065	1/1	0.94	0.36	32,32,32,32	0
82	OHX	A	1917	7/7	0.94	0.21	115,115,115,115	0
83	MG	sR	2197	1/1	0.94	0.52	38,38,38,38	0
82	OHX	A	1851	7/7	0.94	0.17	111,111,111,111	0
83	MG	1	3764	1/1	0.94	0.35	28,28,28,28	0
83	MG	AR	4171	1/1	0.94	0.28	34,34,34,34	0
83	MG	1	3870	1/1	0.94	0.27	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	A	1906	7/7	0.94	0.29	160,160,160,160	0
83	MG	A	2055	1/1	0.94	0.65	40,40,40,40	0
82	OHX	1	3692	7/7	0.94	0.40	83,83,83,83	0
83	MG	AR	4144	1/1	0.94	0.28	39,39,39,39	0
83	MG	sR	2125	1/1	0.94	0.30	42,42,42,42	0
83	MG	sR	2054	1/1	0.94	0.68	47,47,47,47	0
83	MG	AR	4134	1/1	0.94	0.18	27,27,27,27	0
83	MG	sR	2187	1/1	0.94	0.38	43,43,43,43	0
82	OHX	1	3648	7/7	0.94	0.42	98,98,98,98	0
83	MG	x	206	1/1	0.94	0.16	30,30,30,30	0
82	OHX	AR	3661	7/7	0.94	0.28	109,109,109,109	0
83	MG	AR	3788	1/1	0.94	0.31	24,24,24,24	0
83	MG	A	2056	1/1	0.94	0.78	36,36,36,36	0
82	OHX	A	1936	7/7	0.94	0.28	123,123,123,123	0
83	MG	AR	4254	1/1	0.94	0.38	34,34,34,34	0
83	MG	AR	4249	1/1	0.94	0.57	42,42,42,42	0
83	MG	A	1991	1/1	0.94	0.68	80,80,80,80	0
83	MG	sR	2084	1/1	0.94	0.37	61,61,61,61	0
83	MG	AR	4226	1/1	0.94	0.50	22,22,22,22	0
83	MG	AR	4079	1/1	0.94	0.27	46,46,46,46	0
82	OHX	sR	2005	7/7	0.94	0.33	83,83,83,83	0
83	MG	AR	4149	1/1	0.94	0.21	37,37,37,37	0
83	MG	AR	4172	1/1	0.94	1.16	31,31,31,31	0
83	MG	x	202	1/1	0.94	0.43	29,29,29,29	0
82	OHX	sR	1984	7/7	0.94	0.24	90,90,90,90	0
82	OHX	1	3601	7/7	0.94	0.29	94,94,94,94	0
83	MG	sR	2050	1/1	0.94	0.58	40,40,40,40	0
82	OHX	1	3618	7/7	0.94	0.16	170,170,170,170	0
82	OHX	AR	3600	7/7	0.94	0.28	110,110,110,110	0
83	MG	1	3732	1/1	0.94	0.43	33,33,33,33	0
82	OHX	1	3671	7/7	0.94	0.30	115,115,115,115	0
82	OHX	1	3707	7/7	0.94	0.32	111,111,111,111	0
83	MG	DP	101	1/1	0.94	0.35	38,38,38,38	0
83	MG	AR	4055	1/1	0.94	0.57	29,29,29,29	0
82	OHX	4	214	7/7	0.94	0.23	106,106,106,106	0
83	MG	AR	3948	1/1	0.94	0.62	35,35,35,35	0
83	MG	1	3735	1/1	0.94	0.53	39,39,39,39	0
82	OHX	1	3499	7/7	0.94	0.17	89,89,89,89	0
82	OHX	A	1893	7/7	0.94	0.31	111,111,111,111	0
83	MG	DO	202	1/1	0.94	0.28	37,37,37,37	0
83	MG	AR	3989	1/1	0.94	0.21	36,36,36,36	0
83	MG	3	212	1/1	0.94	0.63	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	1	3724	1/7	0.94	0.16	143,143,143,143	0
83	MG	AR	3817	1/1	0.94	0.30	51,51,51,51	0
83	MG	1	4110	1/1	0.94	0.28	26,26,26,26	0
82	OHX	1	3714	7/7	0.94	0.48	112,112,112,112	0
83	MG	1	4114	1/1	0.94	0.23	58,58,58,58	0
83	MG	AR	3884	1/1	0.94	0.31	38,38,38,38	0
83	MG	1	4012	1/1	0.94	0.32	30,30,30,30	0
83	MG	1	3833	1/1	0.94	0.41	28,28,28,28	0
83	MG	k	402	1/1	0.94	0.35	30,30,30,30	0
82	OHX	sR	2046	7/7	0.94	0.37	112,112,112,112	0
83	MG	AR	3815	1/1	0.94	0.34	21,21,21,21	0
83	MG	1	4016	1/1	0.94	0.39	29,29,29,29	0
82	OHX	A	1924	7/7	0.94	0.29	126,126,126,126	0
82	OHX	AR	3529	7/7	0.94	0.26	80,80,80,80	0
83	MG	1	3920	1/1	0.94	0.44	20,20,20,20	0
83	MG	AR	3868	1/1	0.94	0.24	24,24,24,24	0
83	MG	AR	3741	1/1	0.94	0.70	50,50,50,50	0
83	MG	DL	102	1/1	0.94	0.41	27,27,27,27	0
83	MG	AR	3784	1/1	0.94	0.57	29,29,29,29	0
83	MG	4	226	1/1	0.94	0.38	42,42,42,42	0
83	MG	AR	3812	1/1	0.94	0.61	41,41,41,41	0
83	MG	1	3924	1/1	0.94	0.40	22,22,22,22	0
83	MG	A	2051	1/1	0.94	0.66	50,50,50,50	0
83	MG	l	403	1/1	0.94	0.25	25,25,25,25	0
83	MG	1	3903	1/1	0.94	0.61	29,29,29,29	0
83	MG	1	4201	1/1	0.94	0.65	33,33,33,33	0
82	OHX	AR	3705	7/7	0.94	0.36	97,97,97,97	0
83	MG	AR	4152	1/1	0.94	0.27	25,25,25,25	0
82	OHX	1	3690	7/7	0.94	0.36	123,123,123,123	0
83	MG	AR	4244	1/1	0.94	0.57	28,28,28,28	0
83	MG	A	2042	1/1	0.94	0.15	81,81,81,81	0
83	MG	1	3944	1/1	0.94	0.46	52,52,52,52	0
83	MG	sR	2082	1/1	0.94	0.29	70,70,70,70	0
83	MG	AR	3838	1/1	0.94	0.40	31,31,31,31	0
82	OHX	1	3604	7/7	0.94	0.32	101,101,101,101	0
83	MG	1	3822	1/1	0.94	0.24	28,28,28,28	0
82	OHX	AR	3508	7/7	0.94	0.17	91,91,91,91	0
82	OHX	1	3552	7/7	0.95	0.21	103,103,103,103	0
82	OHX	A	1873	7/7	0.95	0.22	121,121,121,121	0
83	MG	1	3835	1/1	0.95	0.33	38,38,38,38	0
83	MG	1	3951	1/1	0.95	0.22	28,28,28,28	0
82	OHX	AR	3667	7/7	0.95	0.26	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	1	3689	7/7	0.95	0.43	115,115,115,115	0
83	MG	A	1975	1/1	0.95	0.53	55,55,55,55	0
82	OHX	sR	2028	7/7	0.95	0.35	73,73,73,73	0
82	OHX	AR	3655	7/7	0.95	0.27	110,110,110,110	0
83	MG	AB	203	1/1	0.95	0.20	40,40,40,40	0
82	OHX	AR	3684	7/7	0.95	0.31	108,108,108,108	0
83	MG	1	3847	1/1	0.95	0.51	30,30,30,30	0
83	MG	1	4130	1/1	0.95	0.15	48,48,48,48	0
83	MG	AT	224	1/1	0.95	0.23	37,37,37,37	0
82	OHX	1	3609	7/7	0.95	0.25	105,105,105,105	0
83	MG	sR	2134	1/1	0.95	0.20	40,40,40,40	0
82	OHX	1	3660	7/7	0.95	0.36	117,117,117,117	0
83	MG	AR	3799	1/1	0.95	0.34	35,35,35,35	0
82	OHX	AR	3708	7/7	0.95	0.39	103,103,103,103	0
82	OHX	1	3670	7/7	0.95	0.27	83,83,83,83	0
83	MG	AR	3805	1/1	0.95	0.32	27,27,27,27	0
82	OHX	A	1855	7/7	0.95	0.15	97,97,97,97	0
82	OHX	AR	3706	7/7	0.95	0.27	112,112,112,112	0
82	OHX	A	1899	7/7	0.95	0.38	100,100,100,100	0
83	MG	A	2041	1/1	0.95	0.39	71,71,71,71	0
83	MG	1	3751	1/1	0.95	0.14	50,50,50,50	0
82	OHX	sR	2039	7/7	0.95	0.35	118,118,118,118	0
83	MG	AR	4053	1/1	0.95	0.29	33,33,33,33	0
83	MG	AR	4047	1/1	0.95	0.32	52,52,52,52	0
83	MG	1	4009	1/1	0.95	0.39	40,40,40,40	0
82	OHX	1	3554	7/7	0.95	0.26	91,91,91,91	0
82	OHX	AR	3658	7/7	0.95	0.37	98,98,98,98	0
82	OHX	A	1922	7/7	0.95	0.40	85,85,85,85	0
83	MG	AR	4061	1/1	0.95	0.35	32,32,32,32	0
83	MG	1	4214	1/1	0.95	0.70	33,33,33,33	0
82	OHX	AT	214	7/7	0.95	0.32	98,98,98,98	0
83	MG	sR	2094	1/1	0.95	0.45	59,59,59,59	0
82	OHX	AR	3676	7/7	0.95	0.40	109,109,109,109	0
83	MG	AR	3992	1/1	0.95	0.35	23,23,23,23	0
82	OHX	1	3711	7/7	0.95	0.46	95,95,95,95	0
83	MG	4	225	1/1	0.95	0.28	40,40,40,40	0
83	MG	1	3842	1/1	0.95	0.66	32,32,32,32	0
83	MG	AR	3791	1/1	0.95	0.53	32,32,32,32	0
82	OHX	1	3659	7/7	0.95	0.29	118,118,118,118	0
83	MG	AS	215	1/1	0.95	0.60	26,26,26,26	0
83	MG	AR	4100	1/1	0.95	0.36	23,23,23,23	0
83	MG	AR	3959	1/1	0.95	0.25	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AT	231	1/1	0.95	0.51	30,30,30,30	0
83	MG	A	1976	1/1	0.95	0.80	67,67,67,67	0
83	MG	sR	2068	1/1	0.95	0.54	35,35,35,35	0
83	MG	sR	2109	1/1	0.95	0.72	71,71,71,71	0
82	OHX	1	3650	7/7	0.95	0.25	98,98,98,98	0
83	MG	1	4221	1/1	0.95	0.49	41,41,41,41	0
83	MG	AR	3808	1/1	0.95	0.30	29,29,29,29	0
82	OHX	A	1931	7/7	0.95	0.42	87,87,87,87	0
83	MG	AR	4157	1/1	0.95	0.10	31,31,31,31	0
82	OHX	A	1940	7/7	0.95	0.23	128,128,128,128	0
82	OHX	AR	3722	7/7	0.95	0.23	120,120,120,120	0
82	OHX	CL	302	7/7	0.95	0.24	88,88,88,88	0
83	MG	A	2071	1/1	0.95	0.41	56,56,56,56	0
83	MG	sM	302	1/1	0.95	0.26	38,38,38,38	0
83	MG	1	3787	1/1	0.95	0.38	21,21,21,21	0
82	OHX	sR	2049	7/7	0.95	0.30	72,72,72,72	0
82	OHX	AR	3707	7/7	0.95	0.25	149,149,149,149	0
83	MG	1	3923	1/1	0.95	0.40	33,33,33,33	0
82	OHX	1	3594	7/7	0.95	0.16	120,120,120,120	0
82	OHX	AR	3606	7/7	0.95	0.26	73,73,73,73	0
83	MG	sR	2175	1/1	0.95	0.20	82,82,82,82	0
83	MG	AR	4035	1/1	0.95	0.13	41,41,41,41	0
83	MG	AR	3798	1/1	0.95	0.20	25,25,25,25	0
82	OHX	AR	3668	7/7	0.95	0.34	71,71,71,71	0
83	MG	CI	301	1/1	0.95	0.19	29,29,29,29	0
82	OHX	1	3530	7/7	0.95	0.10	128,128,128,128	0
82	OHX	1	3653	7/7	0.95	0.25	105,105,105,105	0
83	MG	CQ	202	1/1	0.95	0.08	33,33,33,33	0
82	OHX	1	3622	7/7	0.95	0.27	100,100,100,100	0
82	OHX	sR	2033	7/7	0.95	0.34	97,97,97,97	0
82	OHX	AR	3652	7/7	0.95	0.29	110,110,110,110	0
83	MG	1	4078	1/1	0.95	0.56	36,36,36,36	0
83	MG	AR	3844	1/1	0.95	0.32	44,44,44,44	0
83	MG	1	4140	1/1	0.95	0.31	43,43,43,43	0
82	OHX	1	3656	7/7	0.95	0.48	114,114,114,114	0
83	MG	AR	4123	1/1	0.95	0.30	28,28,28,28	0
83	MG	1	3977	1/1	0.95	0.29	42,42,42,42	0
82	OHX	A	1896	7/7	0.95	0.28	101,101,101,101	0
83	MG	AS	221	1/1	0.95	0.74	37,37,37,37	0
83	MG	sR	2097	1/1	0.95	0.52	44,44,44,44	0
82	OHX	AR	3674	7/7	0.95	0.50	110,110,110,110	0
83	MG	sR	2184	1/1	0.95	0.38	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3583	7/7	0.95	0.19	86,86,86,86	0
82	OHX	AR	3698	7/7	0.95	0.38	103,103,103,103	0
83	MG	AR	3885	1/1	0.95	0.46	40,40,40,40	0
82	OHX	AR	3540	7/7	0.95	0.24	88,88,88,88	0
82	OHX	1	3705	7/7	0.95	0.25	74,74,74,74	0
82	OHX	1	3673	7/7	0.95	0.35	101,101,101,101	0
82	OHX	AR	3648	7/7	0.95	0.30	81,81,81,81	0
82	OHX	1	3706	7/7	0.95	0.44	106,106,106,106	0
82	OHX	A	1854	7/7	0.95	0.25	97,97,97,97	0
83	MG	AR	4097	1/1	0.95	0.44	32,32,32,32	0
82	OHX	AR	3720	7/7	0.95	0.33	137,137,137,137	0
83	MG	AR	3883	1/1	0.95	0.59	43,43,43,43	0
83	MG	AR	3882	1/1	0.95	0.41	25,25,25,25	0
82	OHX	AR	3701	7/7	0.95	0.30	114,114,114,114	0
83	MG	1	3918	1/1	0.95	0.59	19,19,19,19	0
83	MG	AR	4228	1/1	0.95	0.35	26,26,26,26	0
83	MG	AR	4141	1/1	0.95	0.18	82,82,82,82	0
83	MG	1	4115	1/1	0.95	0.23	32,32,32,32	0
83	MG	1	3880	1/1	0.95	0.43	30,30,30,30	0
82	OHX	c5	201	7/7	0.95	0.29	130,130,130,130	0
82	OHX	sR	2024	7/7	0.95	0.38	121,121,121,121	0
82	OHX	1	3640	7/7	0.95	0.36	95,95,95,95	0
82	OHX	1	3661	7/7	0.95	0.31	83,83,83,83	0
82	OHX	AR	3630	7/7	0.95	0.30	120,120,120,120	0
83	MG	sR	2173	1/1	0.95	0.50	58,58,58,58	0
82	OHX	1	3454	7/7	0.95	0.15	91,91,91,91	0
83	MG	1	3926	1/1	0.95	0.26	31,31,31,31	0
83	MG	AR	4150	1/1	0.95	0.15	36,36,36,36	0
83	MG	AS	211	1/1	0.95	0.59	36,36,36,36	0
83	MG	AS	220	1/1	0.95	0.32	41,41,41,41	0
83	MG	sR	2108	1/1	0.95	0.60	40,40,40,40	0
83	MG	AR	4194	1/1	0.95	0.51	52,52,52,52	0
83	MG	AR	3892	1/1	0.95	0.51	40,40,40,40	0
83	MG	1	3765	1/1	0.95	0.32	36,36,36,36	0
83	MG	AR	4059	1/1	0.95	0.31	33,33,33,33	0
83	MG	sR	2149	1/1	0.95	0.15	64,64,64,64	0
83	MG	AR	3962	1/1	0.95	0.36	30,30,30,30	0
82	OHX	AR	3610	7/7	0.95	0.27	78,78,78,78	0
82	OHX	AR	3626	7/7	0.95	0.22	119,119,119,119	0
83	MG	AR	4096	1/1	0.95	0.14	31,31,31,31	0
82	OHX	AR	3544	7/7	0.95	0.10	127,127,127,127	0
82	OHX	1	3699	7/7	0.95	0.39	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3955	1/1	0.95	0.33	23,23,23,23	0
83	MG	AR	3881	1/1	0.95	0.47	57,57,57,57	0
82	OHX	1	3644	7/7	0.95	0.24	134,134,134,134	0
83	MG	1	3739	1/1	0.95	0.39	29,29,29,29	0
83	MG	sR	2086	1/1	0.95	0.32	35,35,35,35	0
82	OHX	r	301	7/7	0.95	0.19	74,74,74,74	0
83	MG	1	3832	1/1	0.95	0.62	31,31,31,31	0
83	MG	1	3942	1/1	0.95	0.54	41,41,41,41	0
83	MG	1	3806	1/1	0.95	0.60	36,36,36,36	0
83	MG	1	3866	1/1	0.95	0.48	32,32,32,32	0
82	OHX	AR	3624	7/7	0.95	0.23	109,109,109,109	0
82	OHX	AR	3605	7/7	0.95	0.15	118,118,118,118	0
83	MG	1	3798	1/1	0.95	0.55	22,22,22,22	0
83	MG	1	3815	1/1	0.95	0.23	28,28,28,28	0
82	OHX	AR	3622	7/7	0.95	0.29	114,114,114,114	0
82	OHX	AR	3631	7/7	0.95	0.21	108,108,108,108	0
83	MG	sR	2093	1/1	0.95	0.63	40,40,40,40	0
82	OHX	AP	502	7/7	0.95	0.28	63,63,63,63	0
82	OHX	1	3715	7/7	0.95	0.10	140,140,140,140	0
83	MG	sR	2139	1/1	0.95	1.21	59,59,59,59	0
83	MG	1	4212	1/1	0.95	0.49	42,42,42,42	0
82	OHX	A	1927	7/7	0.95	0.27	132,132,132,132	0
82	OHX	A	1904	7/7	0.95	0.36	94,94,94,94	0
82	OHX	1	3557	7/7	0.95	0.19	109,109,109,109	0
82	OHX	AR	3664	7/7	0.95	0.28	96,96,96,96	0
82	OHX	1	3462	7/7	0.95	0.15	80,80,80,80	0
82	OHX	1	3663	7/7	0.95	0.17	84,84,84,84	0
83	MG	A	1957	1/1	0.95	0.85	63,63,63,63	0
83	MG	AR	4256	1/1	0.95	0.19	26,26,26,26	0
83	MG	AR	4054	1/1	0.95	0.17	44,44,44,44	0
83	MG	AR	3837	1/1	0.95	0.22	24,24,24,24	0
83	MG	A	2026	1/1	0.95	0.25	59,59,59,59	0
82	OHX	A	1941	7/7	0.95	0.38	78,78,78,78	0
82	OHX	AR	3663	7/7	0.95	0.33	102,102,102,102	0
82	OHX	1	3676	7/7	0.95	0.33	113,113,113,113	0
83	MG	1	3896	1/1	0.95	0.41	25,25,25,25	0
83	MG	AB	206	1/1	0.95	0.34	22,22,22,22	0
82	OHX	sR	2000	7/7	0.95	0.21	107,107,107,107	0
83	MG	1	4112	1/1	0.95	0.25	36,36,36,36	0
83	MG	AR	3855	1/1	0.95	0.44	23,23,23,23	0
83	MG	AR	3970	1/1	0.95	0.32	33,33,33,33	0
82	OHX	A	1875	7/7	0.95	0.14	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3730	7/7	0.95	0.50	109,109,109,109	0
83	MG	1	3807	1/1	0.95	0.23	28,28,28,28	0
82	OHX	AR	3557	7/7	0.95	0.24	77,77,77,77	0
83	MG	A	1973	1/1	0.95	0.71	67,67,67,67	0
83	MG	AR	3984	1/1	0.95	0.14	32,32,32,32	0
83	MG	AR	3758	1/1	0.95	0.20	76,76,76,76	0
82	OHX	AR	3728	7/7	0.95	0.33	100,100,100,100	0
82	OHX	sR	1940	7/7	0.95	0.12	105,105,105,105	0
82	OHX	A	1923	7/7	0.95	0.32	123,123,123,123	0
82	OHX	AR	3696	7/7	0.95	0.40	91,91,91,91	0
83	MG	AR	3995	1/1	0.95	0.52	40,40,40,40	0
83	MG	1	3841	1/1	0.95	0.63	33,33,33,33	0
83	MG	1	3899	1/1	0.95	0.54	17,17,17,17	0
82	OHX	1	3672	7/7	0.95	0.31	114,114,114,114	0
82	OHX	AR	3587	7/7	0.95	0.18	107,107,107,107	0
83	MG	O	202	1/1	0.95	0.88	59,59,59,59	0
83	MG	1	3779	1/1	0.95	0.49	45,45,45,45	0
82	OHX	sR	2026	7/7	0.95	0.34	116,116,116,116	0
82	OHX	1	3696	7/7	0.95	0.40	138,138,138,138	0
82	OHX	c3	201	7/7	0.95	0.28	113,113,113,113	0
83	MG	4	228	1/1	0.95	0.25	28,28,28,28	0
82	OHX	1	3550	7/7	0.95	0.12	125,125,125,125	0
82	OHX	sR	1989	7/7	0.95	0.20	100,100,100,100	0
83	MG	1	3793	1/1	0.95	0.70	51,51,51,51	0
82	OHX	1	3610	7/7	0.95	0.41	91,91,91,91	0
83	MG	1	3829	1/1	0.95	0.32	22,22,22,22	0
82	OHX	1	3561	7/7	0.95	0.28	84,84,84,84	0
83	MG	1	3862	1/1	0.95	0.47	32,32,32,32	0
82	OHX	sR	2035	7/7	0.95	0.40	107,107,107,107	0
82	OHX	A	1888	7/7	0.95	0.22	90,90,90,90	0
82	OHX	1	3695	7/7	0.95	0.39	120,120,120,120	0
83	MG	AR	4201	1/1	0.95	0.19	37,37,37,37	0
83	MG	1	4097	1/1	0.95	0.33	39,39,39,39	0
82	OHX	1	3628	7/7	0.96	0.26	111,111,111,111	0
82	OHX	AR	3699	7/7	0.96	0.42	109,109,109,109	0
82	OHX	A	1928	7/7	0.96	0.27	118,118,118,118	0
82	OHX	J	302	7/7	0.96	0.31	125,125,125,125	0
82	OHX	3	206	7/7	0.96	0.18	98,98,98,98	0
82	OHX	3	203	7/7	0.96	0.14	75,75,75,75	0
82	OHX	AR	3623	7/7	0.96	0.36	98,98,98,98	0
82	OHX	sR	2032	7/7	0.96	0.23	118,118,118,118	0
82	OHX	AR	3636	7/7	0.96	0.33	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	A	1849	7/7	0.96	0.23	103,103,103,103	0
82	OHX	1	3606	7/7	0.96	0.21	95,95,95,95	0
82	OHX	CK	201	7/7	0.96	0.28	97,97,97,97	0
83	MG	1	4147	1/1	0.96	0.32	56,56,56,56	0
83	MG	1	4063	1/1	0.96	0.28	52,52,52,52	0
82	OHX	sR	1955	7/7	0.96	0.13	133,133,133,133	0
82	OHX	AR	3734	7/7	0.96	0.35	64,64,64,64	0
83	MG	AR	3826	1/1	0.96	0.61	24,24,24,24	0
82	OHX	sR	1961	7/7	0.96	0.18	86,86,86,86	0
83	MG	A	1967	1/1	0.96	0.96	64,64,64,64	0
82	OHX	AR	3570	7/7	0.96	0.16	96,96,96,96	0
83	MG	AR	3977	1/1	0.96	0.54	32,32,32,32	0
82	OHX	AR	3539	7/7	0.96	0.16	106,106,106,106	0
82	OHX	A	1858	7/7	0.96	0.16	127,127,127,127	0
83	MG	AR	3878	1/1	0.96	0.37	24,24,24,24	0
83	MG	1	4203	1/1	0.96	0.47	35,35,35,35	0
82	OHX	AR	3532	7/7	0.96	0.22	69,69,69,69	0
82	OHX	1	3595	7/7	0.96	0.49	110,110,110,110	0
83	MG	1	4120	1/1	0.96	0.36	31,31,31,31	0
83	MG	1	3912	1/1	0.96	0.51	20,20,20,20	0
82	OHX	AR	3638	7/7	0.96	0.39	100,100,100,100	0
82	OHX	AR	3601	7/7	0.96	0.25	89,89,89,89	0
82	OHX	AR	3714	7/7	0.96	0.35	109,109,109,109	0
82	OHX	1	3516	7/7	0.96	0.23	81,81,81,81	0
82	OHX	1	3723	7/7	0.96	0.29	72,72,72,72	0
83	MG	CI	302	1/1	0.96	0.41	35,35,35,35	0
83	MG	1	4118	1/1	0.96	0.26	38,38,38,38	0
82	OHX	A	1895	7/7	0.96	0.31	110,110,110,110	0
83	MG	AR	3871	1/1	0.96	0.45	39,39,39,39	0
84	G5B	1	4224	26/26	0.96	0.20	27,27,27,27	0
83	MG	A	2050	1/1	0.96	0.71	39,39,39,39	0
82	OHX	sR	1950	7/7	0.96	0.15	104,104,104,104	0
83	MG	A	2035	1/1	0.96	0.27	87,87,87,87	0
82	OHX	A	1913	7/7	0.96	0.20	111,111,111,111	0
82	OHX	AR	3717	7/7	0.96	0.33	95,95,95,95	0
82	OHX	1	3469	7/7	0.96	0.13	80,80,80,80	0
83	MG	sR	2099	1/1	0.96	0.81	63,63,63,63	0
82	OHX	e	102	7/7	0.96	0.33	110,110,110,110	0
82	OHX	1	3697	7/7	0.96	0.28	74,74,74,74	0
83	MG	1	3784	1/1	0.96	0.45	28,28,28,28	0
83	MG	1	3902	1/1	0.96	0.50	20,20,20,20	0
82	OHX	1	3620	7/7	0.96	0.31	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3898	1/1	0.96	0.63	33,33,33,33	0
83	MG	1	3820	1/1	0.96	0.22	33,33,33,33	0
82	OHX	AR	3609	7/7	0.96	0.30	76,76,76,76	0
82	OHX	1	3674	7/7	0.96	0.37	113,113,113,113	0
82	OHX	sR	2011	7/7	0.96	0.33	110,110,110,110	0
82	OHX	AR	3619	7/7	0.96	0.32	76,76,76,76	0
83	MG	1	4185	1/1	0.96	0.40	24,24,24,24	0
85	ZN	e1	501	1/1	0.96	0.04	136,136,136,136	0
83	MG	1	3725	1/1	0.96	0.52	32,32,32,32	0
83	MG	AR	3887	1/1	0.96	0.75	43,43,43,43	0
82	OHX	1	3688	7/7	0.96	0.27	100,100,100,100	0
83	MG	AR	4161	1/1	0.96	0.17	32,32,32,32	0
82	OHX	1	3627	7/7	0.96	0.36	97,97,97,97	0
82	OHX	1	3479	7/7	0.96	0.13	88,88,88,88	0
83	MG	AR	4116	1/1	0.96	0.34	23,23,23,23	0
82	OHX	1	3629	7/7	0.96	0.25	113,113,113,113	0
83	MG	AR	3842	1/1	0.96	0.30	35,35,35,35	0
83	MG	6	201	1/1	0.96	0.48	25,25,25,25	0
82	OHX	AR	3611	7/7	0.96	0.36	90,90,90,90	0
82	OHX	1	3704	7/7	0.96	0.41	99,99,99,99	0
82	OHX	1	3643	7/7	0.96	0.28	100,100,100,100	0
82	OHX	sR	2007	7/7	0.96	0.19	111,111,111,111	0
82	OHX	AR	3718	7/7	0.96	0.33	134,134,134,134	0
83	MG	1	3759	1/1	0.96	0.35	32,32,32,32	0
82	OHX	A	1883	7/7	0.96	0.27	101,101,101,101	0
82	OHX	A	1914	7/7	0.96	0.26	125,125,125,125	0
82	OHX	1	3722	7/7	0.96	0.35	58,58,58,58	0
82	OHX	sR	1954	7/7	0.96	0.17	127,127,127,127	0
82	OHX	sR	1994	7/7	0.96	0.27	104,104,104,104	0
82	OHX	sR	2022	7/7	0.96	0.42	91,91,91,91	0
82	OHX	sR	1976	7/7	0.96	0.17	115,115,115,115	0
82	OHX	sR	2017	7/7	0.96	0.29	100,100,100,100	0
83	MG	1	4090	1/1	0.96	0.12	27,27,27,27	0
82	OHX	1	3542	7/7	0.96	0.21	96,96,96,96	0
82	OHX	AR	3618	7/7	0.96	0.25	114,114,114,114	0
83	MG	sR	2145	1/1	0.96	0.50	89,89,89,89	0
83	MG	s2	301	1/1	0.96	0.19	48,48,48,48	0
82	OHX	sR	1979	7/7	0.96	0.27	101,101,101,101	0
83	MG	AR	3898	1/1	0.96	0.83	26,26,26,26	0
82	OHX	AR	3666	7/7	0.96	0.19	143,143,143,143	0
82	OHX	sR	1993	7/7	0.96	0.25	93,93,93,93	0
82	OHX	1	3625	7/7	0.96	0.25	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	1	3613	7/7	0.96	0.40	87,87,87,87	0
82	OHX	AR	3574	7/7	0.96	0.23	103,103,103,103	0
82	OHX	1	3667	7/7	0.96	0.26	103,103,103,103	0
82	OHX	CE	402	7/7	0.96	0.40	112,112,112,112	0
83	MG	1	3770	1/1	0.96	0.15	36,36,36,36	0
82	OHX	CG	301	7/7	0.96	0.23	109,109,109,109	0
83	MG	4	221	1/1	0.96	0.58	27,27,27,27	0
82	OHX	A	1910	7/7	0.96	0.32	97,97,97,97	0
82	OHX	AR	3547	7/7	0.96	0.28	64,64,64,64	0
83	MG	CK	204	1/1	0.96	0.26	32,32,32,32	0
83	MG	AR	4232	1/1	0.96	0.52	49,49,49,49	0
82	OHX	sR	1949	7/7	0.96	0.15	104,104,104,104	0
83	MG	A	2048	1/1	0.96	0.46	60,60,60,60	0
82	OHX	1	3546	7/7	0.96	0.14	107,107,107,107	0
83	MG	1	3760	1/1	0.96	0.30	38,38,38,38	0
82	OHX	AR	3621	7/7	0.96	0.31	95,95,95,95	0
82	OHX	1	3596	7/7	0.96	0.36	99,99,99,99	0
82	OHX	A	1882	7/7	0.96	0.25	88,88,88,88	0
83	MG	1	3909	1/1	0.96	0.76	41,41,41,41	0
82	OHX	sR	1962	7/7	0.96	0.31	102,102,102,102	0
82	OHX	AR	3505	7/7	0.96	0.15	82,82,82,82	0
82	OHX	AR	3686	7/7	0.96	0.33	86,86,86,86	0
83	MG	A	2069	1/1	0.96	0.51	58,58,58,58	0
82	OHX	A	1900	7/7	0.96	0.29	110,110,110,110	0
82	OHX	sR	2023	7/7	0.96	0.32	122,122,122,122	0
83	MG	1	3893	1/1	0.96	0.43	22,22,22,22	0
82	OHX	h	401	7/7	0.96	0.19	134,134,134,134	0
83	MG	AT	229	1/1	0.96	0.47	31,31,31,31	0
83	MG	1	4186	1/1	0.96	0.25	22,22,22,22	0
82	OHX	AR	3672	7/7	0.96	0.27	102,102,102,102	0
82	OHX	AR	3637	7/7	0.96	0.22	103,103,103,103	0
83	MG	sR	2100	1/1	0.96	0.58	61,61,61,61	0
83	MG	AR	4230	1/1	0.96	0.48	35,35,35,35	0
82	OHX	sR	2010	7/7	0.96	0.36	107,107,107,107	0
82	OHX	sR	2043	7/7	0.96	0.28	120,120,120,120	0
83	MG	1	4189	1/1	0.96	0.46	18,18,18,18	0
82	OHX	AR	3640	7/7	0.96	0.41	90,90,90,90	0
83	MG	AR	4218	1/1	0.96	0.48	21,21,21,21	0
83	MG	AR	3765	1/1	0.96	0.47	35,35,35,35	0
83	MG	1	3978	1/1	0.96	0.37	28,28,28,28	0
83	MG	AR	3973	1/1	0.96	0.15	26,26,26,26	0
82	OHX	1	3633	7/7	0.96	0.35	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AR	4111	1/1	0.96	0.24	38,38,38,38	0
82	OHX	AR	3653	7/7	0.96	0.35	82,82,82,82	0
83	MG	1	3844	1/1	0.96	0.50	35,35,35,35	0
83	MG	AR	4211	1/1	0.96	0.21	29,29,29,29	0
83	MG	AR	4120	1/1	0.96	0.14	40,40,40,40	0
82	OHX	1	3616	7/7	0.96	0.26	114,114,114,114	0
82	OHX	sR	2009	7/7	0.96	0.20	85,85,85,85	0
82	OHX	A	1905	7/7	0.96	0.28	118,118,118,118	0
83	MG	AR	3951	1/1	0.96	0.25	70,70,70,70	0
83	MG	1	4031	1/1	0.96	0.42	24,24,24,24	0
82	OHX	AR	3551	7/7	0.96	0.21	83,83,83,83	0
82	OHX	sR	1998	7/7	0.96	0.31	107,107,107,107	0
82	OHX	1	3513	7/7	0.96	0.16	80,80,80,80	0
82	OHX	1	3480	7/7	0.96	0.15	69,69,69,69	0
83	MG	AR	3981	1/1	0.96	0.28	80,80,80,80	0
82	OHX	AR	3613	7/7	0.96	0.39	106,106,106,106	0
82	OHX	sR	2004	7/7	0.96	0.31	105,105,105,105	0
82	OHX	A	1933	7/7	0.96	0.47	117,117,117,117	0
83	MG	1	4219	1/1	0.96	0.19	31,31,31,31	0
83	MG	AR	3999	1/1	0.96	0.25	27,27,27,27	0
82	OHX	A	1942	7/7	0.96	0.27	111,111,111,111	0
83	MG	AR	3915	1/1	0.96	0.54	32,32,32,32	0
82	OHX	AS	209	7/7	0.96	0.25	74,74,74,74	0
82	OHX	1	3635	7/7	0.96	0.21	107,107,107,107	0
82	OHX	A	1874	7/7	0.96	0.11	136,136,136,136	0
82	OHX	sR	1973	7/7	0.96	0.19	105,105,105,105	0
83	MG	AR	4072	1/1	0.96	0.21	29,29,29,29	0
82	OHX	sR	2008	7/7	0.96	0.17	106,106,106,106	0
83	MG	1	3817	1/1	0.96	0.33	25,25,25,25	0
83	MG	AR	3928	1/1	0.96	0.82	34,34,34,34	0
83	MG	AR	3986	1/1	0.96	0.38	46,46,46,46	0
82	OHX	1	3693	7/7	0.96	0.32	90,90,90,90	0
84	G5B	AR	4264	26/26	0.96	0.20	29,29,29,29	0
82	OHX	1	3626	7/7	0.96	0.23	109,109,109,109	0
83	MG	CP	503	1/1	0.96	0.10	35,35,35,35	0
82	OHX	AR	3595	7/7	0.96	0.28	79,79,79,79	0
82	OHX	c8	201	7/7	0.96	0.17	115,115,115,115	0
82	OHX	1	3605	7/7	0.96	0.29	105,105,105,105	0
83	MG	sR	2110	1/1	0.96	0.31	39,39,39,39	0
82	OHX	A	1836	7/7	0.96	0.15	84,84,84,84	0
83	MG	AR	3873	1/1	0.96	0.24	41,41,41,41	0
82	OHX	sR	1975	7/7	0.96	0.23	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3690	7/7	0.96	0.31	81,81,81,81	0
83	MG	1	3733	1/1	0.96	0.42	28,28,28,28	0
83	MG	1	3919	1/1	0.96	0.64	22,22,22,22	0
82	OHX	A	1859	7/7	0.96	0.18	107,107,107,107	0
82	OHX	AR	3639	7/7	0.96	0.36	92,92,92,92	0
83	MG	AR	3888	1/1	0.96	0.65	25,25,25,25	0
82	OHX	4	208	7/7	0.96	0.28	79,79,79,79	0
83	MG	AR	3869	1/1	0.96	0.34	26,26,26,26	0
83	MG	CG	305	1/1	0.96	0.18	49,49,49,49	0
83	MG	AR	4213	1/1	0.96	0.39	25,25,25,25	0
82	OHX	AR	3665	7/7	0.96	0.28	117,117,117,117	0
83	MG	A	1959	1/1	0.96	0.48	55,55,55,55	0
82	OHX	1	3664	7/7	0.96	0.31	94,94,94,94	0
83	MG	AR	3911	1/1	0.96	0.53	26,26,26,26	0
83	MG	d3	202	1/1	0.96	0.27	41,41,41,41	0
82	OHX	1	3579	7/7	0.96	0.24	82,82,82,82	0
82	OHX	1	3646	7/7	0.96	0.24	103,103,103,103	0
83	MG	A	1977	1/1	0.96	0.70	57,57,57,57	0
82	OHX	AR	3694	7/7	0.96	0.38	86,86,86,86	0
82	OHX	sR	2031	7/7	0.96	0.33	110,110,110,110	0
83	MG	1	3824	1/1	0.96	0.36	25,25,25,25	0
83	MG	1	4023	1/1	0.96	0.16	82,82,82,82	0
82	OHX	x	201	7/7	0.96	0.41	101,101,101,101	0
83	MG	1	3785	1/1	0.96	0.45	18,18,18,18	0
82	OHX	sR	1971	7/7	0.96	0.20	102,102,102,102	0
83	MG	sR	2085	1/1	0.96	0.52	37,37,37,37	0
83	MG	1	3811	1/1	0.96	0.50	32,32,32,32	0
82	OHX	sR	2038	7/7	0.96	0.40	125,125,125,125	0
83	MG	AR	3968	1/1	0.96	0.55	40,40,40,40	0
82	OHX	4	209	7/7	0.96	0.19	116,116,116,116	0
82	OHX	3	209	7/7	0.96	0.26	118,118,118,118	0
83	MG	AR	4233	1/1	0.96	0.45	57,57,57,57	0
83	MG	1	3928	1/1	0.96	0.21	33,33,33,33	0
82	OHX	AR	3646	7/7	0.96	0.30	98,98,98,98	0
82	OHX	AR	3602	7/7	0.96	0.17	104,104,104,104	0
83	MG	AR	3782	1/1	0.96	0.20	35,35,35,35	0
83	MG	1	4194	1/1	0.96	0.31	38,38,38,38	0
82	OHX	1	3632	7/7	0.96	0.29	90,90,90,90	0
85	ZN	g	501	1/1	0.96	0.08	102,102,102,102	0
82	OHX	AR	3695	7/7	0.96	0.46	107,107,107,107	0
83	MG	1	3753	1/1	0.96	0.40	40,40,40,40	0
82	OHX	AR	3704	7/7	0.96	0.34	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	4073	1/1	0.96	0.28	41,41,41,41	0
82	OHX	1	3637	7/7	0.96	0.28	91,91,91,91	0
82	OHX	sR	2014	7/7	0.96	0.41	93,93,93,93	0
82	OHX	AR	3599	7/7	0.96	0.24	93,93,93,93	0
83	MG	AR	3926	1/1	0.96	0.34	25,25,25,25	0
82	OHX	AR	3688	7/7	0.96	0.39	97,97,97,97	0
82	OHX	sR	1981	7/7	0.96	0.32	88,88,88,88	0
82	OHX	sR	1992	7/7	0.96	0.21	94,94,94,94	0
83	MG	AR	4129	1/1	0.96	0.23	38,38,38,38	0
83	MG	AR	4094	1/1	0.96	0.29	68,68,68,68	0
82	OHX	sR	2015	7/7	0.96	0.35	90,90,90,90	0
82	OHX	AR	3546	7/7	0.96	0.17	83,83,83,83	0
83	MG	AR	3757	1/1	0.96	0.36	58,58,58,58	0
83	MG	1	3907	1/1	0.96	0.53	28,28,28,28	0
83	MG	9	201	1/1	0.96	0.39	34,34,34,34	0
82	OHX	1	3505	7/7	0.96	0.24	74,74,74,74	0
82	OHX	AR	3580	7/7	0.96	0.10	135,135,135,135	0
82	OHX	A	1894	7/7	0.96	0.20	118,118,118,118	0
83	MG	1	3838	1/1	0.96	0.49	20,20,20,20	0
82	OHX	1	3686	7/7	0.96	0.53	121,121,121,121	0
83	MG	A	1998	1/1	0.96	0.26	58,58,58,58	0
82	OHX	sR	1919	7/7	0.96	0.15	73,73,73,73	0
82	OHX	1	3593	7/7	0.96	0.20	99,99,99,99	0
82	OHX	1	3551	7/7	0.96	0.23	91,91,91,91	0
82	OHX	sR	2020	7/7	0.96	0.26	111,111,111,111	0
82	OHX	A	1831	7/7	0.96	0.11	105,105,105,105	0
82	OHX	A	1935	7/7	0.96	0.35	122,122,122,122	0
82	OHX	AR	3689	7/7	0.96	0.21	105,105,105,105	0
82	OHX	AR	3651	7/7	0.96	0.34	90,90,90,90	0
82	OHX	sR	2001	7/7	0.96	0.28	83,83,83,83	0
82	OHX	AR	3573	7/7	0.96	0.22	90,90,90,90	0
83	MG	AR	3857	1/1	0.96	0.58	21,21,21,21	0
82	OHX	1	3444	7/7	0.96	0.20	66,66,66,66	0
82	OHX	1	3483	7/7	0.96	0.13	95,95,95,95	0
82	OHX	1	3485	7/7	0.96	0.13	82,82,82,82	0
83	MG	1	3831	1/1	0.96	0.33	31,31,31,31	0
82	OHX	AR	3594	7/7	0.96	0.26	88,88,88,88	0
82	OHX	AR	3561	7/7	0.96	0.13	106,106,106,106	0
82	OHX	1	3496	7/7	0.96	0.16	74,74,74,74	0
83	MG	AR	3859	1/1	0.96	0.33	34,34,34,34	0
82	OHX	1	3713	7/7	0.96	0.22	105,105,105,105	0
82	OHX	AT	216	7/7	0.96	0.36	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3496	7/7	0.96	0.15	86,86,86,86	0
82	OHX	1	3562	7/7	0.96	0.29	99,99,99,99	0
82	OHX	1	3619	7/7	0.96	0.24	102,102,102,102	0
82	OHX	4	211	7/7	0.96	0.28	87,87,87,87	0
83	MG	sR	2101	1/1	0.96	0.49	57,57,57,57	0
82	OHX	sR	2030	7/7	0.96	0.43	95,95,95,95	0
83	MG	1	3749	1/1	0.97	0.28	37,37,37,37	0
83	MG	A	1983	1/1	0.97	0.57	57,57,57,57	0
82	OHX	1	3538	7/7	0.97	0.19	90,90,90,90	0
82	OHX	AR	3644	7/7	0.97	0.32	103,103,103,103	0
82	OHX	AR	3692	7/7	0.97	0.27	83,83,83,83	0
82	OHX	3	201	7/7	0.97	0.11	76,76,76,76	0
82	OHX	1	3615	7/7	0.97	0.30	98,98,98,98	0
82	OHX	sR	1939	7/7	0.97	0.12	91,91,91,91	0
82	OHX	sR	1991	7/7	0.97	0.34	95,95,95,95	0
83	MG	AR	4164	1/1	0.97	0.18	36,36,36,36	0
83	MG	1	3777	1/1	0.97	0.37	38,38,38,38	0
82	OHX	A	1884	7/7	0.97	0.17	86,86,86,86	0
82	OHX	A	1880	7/7	0.97	0.28	119,119,119,119	0
82	OHX	1	3600	7/7	0.97	0.31	78,78,78,78	0
83	MG	A	2070	1/1	0.97	0.30	76,76,76,76	0
83	MG	AR	3935	1/1	0.97	0.34	31,31,31,31	0
82	OHX	1	3490	7/7	0.97	0.16	70,70,70,70	0
82	OHX	1	3577	7/7	0.97	0.20	81,81,81,81	0
83	MG	AB	202	1/1	0.97	0.33	22,22,22,22	0
82	OHX	1	3563	7/7	0.97	0.21	99,99,99,99	0
82	OHX	l	401	7/7	0.97	0.35	106,106,106,106	0
82	OHX	A	1891	7/7	0.97	0.17	122,122,122,122	0
82	OHX	A	1920	7/7	0.97	0.25	98,98,98,98	0
82	OHX	1	3545	7/7	0.97	0.13	93,93,93,93	0
82	OHX	AR	3680	7/7	0.97	0.39	93,93,93,93	0
82	OHX	AT	208	7/7	0.97	0.26	85,85,85,85	0
82	OHX	1	3642	7/7	0.97	0.34	107,107,107,107	0
83	MG	AS	217	1/1	0.97	0.09	52,52,52,52	0
82	OHX	AR	3525	7/7	0.97	0.21	76,76,76,76	0
82	OHX	A	1897	7/7	0.97	0.26	119,119,119,119	0
83	MG	1	4025	1/1	0.97	0.33	42,42,42,42	0
82	OHX	AR	3535	7/7	0.97	0.23	81,81,81,81	0
82	OHX	AR	3534	7/7	0.97	0.11	106,106,106,106	0
83	MG	sR	2142	1/1	0.97	0.20	65,65,65,65	0
82	OHX	1	3585	7/7	0.97	0.20	103,103,103,103	0
82	OHX	y	201	7/7	0.97	0.26	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3894	1/1	0.97	0.39	19,19,19,19	0
82	OHX	1	3535	7/7	0.97	0.21	74,74,74,74	0
82	OHX	AR	3596	7/7	0.97	0.27	81,81,81,81	0
83	MG	1	3761	1/1	0.97	0.33	24,24,24,24	0
83	MG	1	3855	1/1	0.97	0.39	21,21,21,21	0
83	MG	AR	3781	1/1	0.97	0.28	22,22,22,22	0
83	MG	1	4050	1/1	0.97	0.32	25,25,25,25	0
82	OHX	A	1861	7/7	0.97	0.18	110,110,110,110	0
82	OHX	sR	1965	7/7	0.97	0.22	82,82,82,82	0
82	OHX	AG	201	7/7	0.97	0.27	83,83,83,83	0
82	OHX	1	3493	7/7	0.97	0.13	85,85,85,85	0
83	MG	AR	4103	1/1	0.97	0.29	36,36,36,36	0
82	OHX	A	1869	7/7	0.97	0.32	108,108,108,108	0
83	MG	AR	3839	1/1	0.97	0.36	24,24,24,24	0
82	OHX	1	3641	7/7	0.97	0.25	92,92,92,92	0
83	MG	1	3799	1/1	0.97	0.30	64,64,64,64	0
82	OHX	1	3501	7/7	0.97	0.09	105,105,105,105	0
82	OHX	1	3572	7/7	0.97	0.24	91,91,91,91	0
83	MG	1	3812	1/1	0.97	0.48	32,32,32,32	0
82	OHX	AR	3538	7/7	0.97	0.28	89,89,89,89	0
82	OHX	AR	3565	7/7	0.97	0.24	89,89,89,89	0
82	OHX	1	3529	7/7	0.97	0.25	74,74,74,74	0
83	MG	AR	3904	1/1	0.97	0.52	26,26,26,26	0
82	OHX	1	3636	7/7	0.97	0.27	93,93,93,93	0
82	OHX	1	3500	7/7	0.97	0.20	73,73,73,73	0
82	OHX	AR	3681	7/7	0.97	0.29	94,94,94,94	0
83	MG	AR	3850	1/1	0.97	0.58	22,22,22,22	0
82	OHX	1	3482	7/7	0.97	0.10	105,105,105,105	0
83	MG	1	3879	1/1	0.97	0.58	24,24,24,24	0
82	OHX	1	3623	7/7	0.97	0.27	120,120,120,120	0
83	MG	A	1992	1/1	0.97	0.21	52,52,52,52	0
83	MG	sR	2167	1/1	0.97	0.32	63,63,63,63	0
83	MG	AS	213	1/1	0.97	0.41	47,47,47,47	0
83	MG	AR	3894	1/1	0.97	0.51	22,22,22,22	0
83	MG	1	3938	1/1	0.97	0.28	36,36,36,36	0
83	MG	AR	4082	1/1	0.97	0.27	25,25,25,25	0
83	MG	sR	2195	1/1	0.97	0.23	58,58,58,58	0
82	OHX	1	3719	7/7	0.97	0.22	93,93,93,93	0
82	OHX	AR	3548	7/7	0.97	0.20	85,85,85,85	0
83	MG	1	3757	1/1	0.97	0.44	26,26,26,26	0
82	OHX	A	1866	7/7	0.97	0.22	100,100,100,100	0
82	OHX	sR	1995	7/7	0.97	0.24	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3597	7/7	0.97	0.25	86,86,86,86	0
82	OHX	sR	1978	7/7	0.97	0.31	81,81,81,81	0
82	OHX	1	3649	7/7	0.97	0.28	83,83,83,83	0
82	OHX	A	1865	7/7	0.97	0.21	103,103,103,103	0
82	OHX	sR	1985	7/7	0.97	0.17	116,116,116,116	0
82	OHX	AR	3473	7/7	0.97	0.14	62,62,62,62	0
82	OHX	AR	3549	7/7	0.97	0.27	73,73,73,73	0
82	OHX	AR	3457	7/7	0.97	0.14	70,70,70,70	0
82	OHX	AR	3592	7/7	0.97	0.41	78,78,78,78	0
82	OHX	1	3540	7/7	0.97	0.22	78,78,78,78	0
83	MG	AR	4195	1/1	0.97	0.47	28,28,28,28	0
83	MG	1	3983	1/1	0.97	0.24	27,27,27,27	0
83	MG	1	3901	1/1	0.97	0.14	22,22,22,22	0
82	OHX	CL	301	7/7	0.97	0.16	97,97,97,97	0
82	OHX	1	3541	7/7	0.97	0.28	78,78,78,78	0
83	MG	AR	4008	1/1	0.97	0.52	37,37,37,37	0
82	OHX	AR	3515	7/7	0.97	0.09	123,123,123,123	0
82	OHX	AR	3428	7/7	0.97	0.20	57,57,57,57	0
82	OHX	AR	3567	7/7	0.97	0.20	122,122,122,122	0
83	MG	AR	3916	1/1	0.97	0.65	37,37,37,37	0
82	OHX	AR	3582	7/7	0.97	0.26	95,95,95,95	0
82	OHX	sR	2016	7/7	0.97	0.31	89,89,89,89	0
82	OHX	1	3679	7/7	0.97	0.32	106,106,106,106	0
82	OHX	3	207	7/7	0.97	0.20	97,97,97,97	0
83	MG	AR	3796	1/1	0.97	0.43	24,24,24,24	0
82	OHX	1	3662	7/7	0.97	0.30	88,88,88,88	0
83	MG	1	3895	1/1	0.97	0.59	38,38,38,38	0
82	OHX	1	3582	7/7	0.97	0.24	86,86,86,86	0
82	OHX	AR	3598	7/7	0.97	0.35	98,98,98,98	0
82	OHX	AT	213	7/7	0.97	0.27	106,106,106,106	0
82	OHX	3	205	7/7	0.97	0.20	94,94,94,94	0
82	OHX	1	3694	7/7	0.97	0.34	81,81,81,81	0
82	OHX	1	3631	7/7	0.97	0.33	82,82,82,82	0
82	OHX	1	3721	7/7	0.97	0.27	55,55,55,55	0
82	OHX	1	3458	7/7	0.97	0.12	64,64,64,64	0
82	OHX	1	3612	7/7	0.97	0.26	87,87,87,87	0
83	MG	AR	4095	1/1	0.97	0.46	37,37,37,37	0
82	OHX	1	3532	7/7	0.97	0.32	79,79,79,79	0
83	MG	AT	220	1/1	0.97	0.59	37,37,37,37	0
82	OHX	1	3508	7/7	0.97	0.14	81,81,81,81	0
83	MG	1	4128	1/1	0.97	0.15	75,75,75,75	0
83	MG	AR	4243	1/1	0.97	0.27	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	A	1955	1/1	0.97	1.56	71,71,71,71	0
82	OHX	AT	212	7/7	0.97	0.26	93,93,93,93	0
83	MG	1	4222	1/1	0.97	0.52	32,32,32,32	0
82	OHX	sR	1958	7/7	0.97	0.18	84,84,84,84	0
82	OHX	AR	3673	7/7	0.97	0.33	103,103,103,103	0
82	OHX	1	3651	7/7	0.97	0.27	109,109,109,109	0
82	OHX	A	1844	7/7	0.97	0.13	109,109,109,109	0
83	MG	sR	2176	1/1	0.97	0.36	63,63,63,63	0
83	MG	AR	3907	1/1	0.97	0.53	27,27,27,27	0
82	OHX	1	3592	7/7	0.97	0.18	129,129,129,129	0
83	MG	1	3884	1/1	0.97	0.52	33,33,33,33	0
83	MG	1	3874	1/1	0.97	0.40	35,35,35,35	0
82	OHX	4	207	7/7	0.97	0.24	92,92,92,92	0
82	OHX	A	1911	7/7	0.97	0.46	99,99,99,99	0
83	MG	AR	3927	1/1	0.97	0.60	35,35,35,35	0
82	OHX	1	3507	7/7	0.97	0.10	98,98,98,98	0
83	MG	1	3839	1/1	0.97	0.56	18,18,18,18	0
83	MG	1	3848	1/1	0.97	0.44	22,22,22,22	0
82	OHX	A	1863	7/7	0.97	0.20	114,114,114,114	0
83	MG	AR	3846	1/1	0.97	0.65	30,30,30,30	0
82	OHX	A	1833	7/7	0.97	0.21	90,90,90,90	0
82	OHX	1	3657	7/7	0.97	0.30	89,89,89,89	0
83	MG	AR	4125	1/1	0.97	0.53	26,26,26,26	0
82	OHX	AR	3536	7/7	0.97	0.23	76,76,76,76	0
83	MG	AR	4220	1/1	0.97	0.30	38,38,38,38	0
82	OHX	1	3589	7/7	0.97	0.25	69,69,69,69	0
83	MG	4	222	1/1	0.97	0.39	22,22,22,22	0
83	MG	1	3927	1/1	0.97	0.45	31,31,31,31	0
82	OHX	1	3587	7/7	0.97	0.25	76,76,76,76	0
82	OHX	AR	3460	7/7	0.97	0.14	53,53,53,53	0
83	MG	AR	4071	1/1	0.97	0.42	28,28,28,28	0
83	MG	AR	3971	1/1	0.97	0.45	30,30,30,30	0
82	OHX	AR	3671	7/7	0.97	0.41	97,97,97,97	0
83	MG	AR	3909	1/1	0.97	0.54	22,22,22,22	0
83	MG	AR	3879	1/1	0.97	0.53	33,33,33,33	0
82	OHX	1	3524	7/7	0.97	0.27	78,78,78,78	0
83	MG	1	3843	1/1	0.97	0.52	27,27,27,27	0
82	OHX	AR	3543	7/7	0.97	0.20	99,99,99,99	0
83	MG	AR	4259	1/1	0.97	0.50	44,44,44,44	0
82	OHX	A	1845	7/7	0.97	0.14	110,110,110,110	0
82	OHX	AT	215	7/7	0.97	0.25	108,108,108,108	0
82	OHX	AR	3709	7/7	0.97	0.25	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3616	7/7	0.97	0.22	83,83,83,83	0
82	OHX	1	3591	7/7	0.97	0.33	88,88,88,88	0
83	MG	AR	3847	1/1	0.97	0.46	22,22,22,22	0
82	OHX	AR	3475	7/7	0.97	0.10	84,84,84,84	0
83	MG	1	3856	1/1	0.97	0.64	31,31,31,31	0
83	MG	sR	2162	1/1	0.97	0.15	25,25,25,25	0
82	OHX	AR	3593	7/7	0.97	0.34	74,74,74,74	0
82	OHX	1	3471	7/7	0.97	0.13	69,69,69,69	0
82	OHX	1	3571	7/7	0.97	0.19	103,103,103,103	0
83	MG	AR	3922	1/1	0.97	0.39	22,22,22,22	0
83	MG	AR	4099	1/1	0.97	0.13	45,45,45,45	0
82	OHX	1	3536	7/7	0.97	0.15	95,95,95,95	0
82	OHX	A	1886	7/7	0.97	0.35	123,123,123,123	0
83	MG	1	3861	1/1	0.97	0.79	26,26,26,26	0
82	OHX	sR	1987	7/7	0.97	0.32	117,117,117,117	0
83	MG	1	3917	1/1	0.97	0.48	22,22,22,22	0
82	OHX	1	3548	7/7	0.97	0.17	99,99,99,99	0
83	MG	AR	3929	1/1	0.97	0.70	30,30,30,30	0
83	MG	1	3890	1/1	0.97	0.56	27,27,27,27	0
83	MG	AR	3997	1/1	0.97	0.15	22,22,22,22	0
82	OHX	Rb	401	7/7	0.97	0.26	127,127,127,127	0
82	OHX	1	3565	7/7	0.97	0.20	103,103,103,103	0
83	MG	AR	3835	1/1	0.97	0.52	28,28,28,28	0
82	OHX	AR	3670	7/7	0.97	0.21	99,99,99,99	0
82	OHX	A	1903	7/7	0.97	0.25	113,113,113,113	0
82	OHX	AR	3617	7/7	0.97	0.23	87,87,87,87	0
82	OHX	AR	3476	7/7	0.97	0.13	71,71,71,71	0
82	OHX	AR	3620	7/7	0.97	0.24	86,86,86,86	0
82	OHX	AR	3635	7/7	0.97	0.21	96,96,96,96	0
82	OHX	1	3473	7/7	0.97	0.10	86,86,86,86	0
83	MG	1	3887	1/1	0.97	0.39	42,42,42,42	0
82	OHX	1	3638	7/7	0.97	0.16	116,116,116,116	0
82	OHX	AR	3628	7/7	0.97	0.26	100,100,100,100	0
82	OHX	1	3534	7/7	0.97	0.26	82,82,82,82	0
83	MG	AR	3764	1/1	0.97	0.34	31,31,31,31	0
82	OHX	DQ	502	7/7	0.97	0.26	64,64,64,64	0
83	MG	sR	2102	1/1	0.97	0.42	42,42,42,42	0
82	OHX	A	1847	7/7	0.97	0.24	90,90,90,90	0
82	OHX	A	1902	7/7	0.97	0.34	91,91,91,91	0
83	MG	AR	3979	1/1	0.97	0.30	37,37,37,37	0
82	OHX	sR	1986	7/7	0.97	0.33	87,87,87,87	0
82	OHX	AT	210	7/7	0.97	0.26	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	1	3684	7/7	0.97	0.40	110,110,110,110	0
82	OHX	AR	3685	7/7	0.97	0.29	89,89,89,89	0
83	MG	AR	3739	1/1	0.97	0.16	45,45,45,45	0
82	OHX	AR	3632	7/7	0.97	0.21	83,83,83,83	0
82	OHX	AR	3625	7/7	0.97	0.24	106,106,106,106	0
82	OHX	A	1843	7/7	0.97	0.23	83,83,83,83	0
82	OHX	sR	1997	7/7	0.97	0.24	117,117,117,117	0
82	OHX	1	3683	7/7	0.97	0.27	82,82,82,82	0
82	OHX	AR	3614	7/7	0.97	0.19	96,96,96,96	0
82	OHX	A	1901	7/7	0.97	0.27	115,115,115,115	0
83	MG	AR	3813	1/1	0.97	0.10	64,64,64,64	0
82	OHX	1	3430	7/7	0.97	0.18	62,62,62,62	0
82	OHX	AR	3589	7/7	0.97	0.24	96,96,96,96	0
82	OHX	A	1817	7/7	0.97	0.12	76,76,76,76	0
82	OHX	1	3599	7/7	0.97	0.14	117,117,117,117	0
83	MG	AR	3849	1/1	0.97	0.59	24,24,24,24	0
82	OHX	A	1864	7/7	0.97	0.24	92,92,92,92	0
82	OHX	AR	3643	7/7	0.97	0.42	94,94,94,94	0
82	OHX	1	3682	7/7	0.97	0.21	77,77,77,77	0
83	MG	1	4132	1/1	0.97	0.72	27,27,27,27	0
82	OHX	d9	102	7/7	0.97	0.38	125,125,125,125	0
82	OHX	A	1879	7/7	0.97	0.20	114,114,114,114	0
83	MG	AR	4106	1/1	0.97	0.26	27,27,27,27	0
83	MG	A	2043	1/1	0.97	0.50	63,63,63,63	0
82	OHX	A	1868	7/7	0.97	0.17	93,93,93,93	0
82	OHX	sR	1999	7/7	0.97	0.25	98,98,98,98	0
82	OHX	s8	301	7/7	0.97	0.37	127,127,127,127	0
82	OHX	sR	1983	7/7	0.97	0.13	112,112,112,112	0
82	OHX	1	3654	7/7	0.97	0.17	114,114,114,114	0
82	OHX	T	201	7/7	0.97	0.11	91,91,91,91	0
82	OHX	A	1929	7/7	0.97	0.28	116,116,116,116	0
82	OHX	A	1857	7/7	0.97	0.27	93,93,93,93	0
82	OHX	Q	201	7/7	0.97	0.26	131,131,131,131	0
83	MG	3	214	1/1	0.97	0.55	31,31,31,31	0
82	OHX	AR	3541	7/7	0.97	0.16	99,99,99,99	0
82	OHX	AR	3584	7/7	0.97	0.21	77,77,77,77	0
82	OHX	AS	207	7/7	0.97	0.14	101,101,101,101	0
82	OHX	1	3586	7/7	0.97	0.18	104,104,104,104	0
83	MG	sR	2161	1/1	0.97	0.17	53,53,53,53	0
83	MG	A	1943	1/1	0.97	1.25	72,72,72,72	0
83	MG	sR	2062	1/1	0.97	0.51	32,32,32,32	0
83	MG	AR	3877	1/1	0.97	0.37	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	sR	1951	7/7	0.97	0.15	102,102,102,102	0
82	OHX	A	1848	7/7	0.97	0.09	106,106,106,106	0
82	OHX	1	3647	7/7	0.97	0.18	93,93,93,93	0
82	OHX	1	3526	7/7	0.97	0.13	110,110,110,110	0
82	OHX	1	3658	7/7	0.97	0.28	114,114,114,114	0
82	OHX	sR	1946	7/7	0.97	0.21	85,85,85,85	0
83	MG	AR	4187	1/1	0.97	0.13	25,25,25,25	0
83	MG	d3	203	1/1	0.97	0.25	40,40,40,40	0
83	MG	1	4072	1/1	0.97	0.13	32,32,32,32	0
82	OHX	AR	3555	7/7	0.97	0.26	80,80,80,80	0
83	MG	1	3925	1/1	0.97	0.44	26,26,26,26	0
83	MG	1	4182	1/1	0.97	0.54	31,31,31,31	0
82	OHX	1	3549	7/7	0.97	0.27	80,80,80,80	0
83	MG	sR	2169	1/1	0.97	0.23	40,40,40,40	0
83	MG	1	4054	1/1	0.97	0.19	51,51,51,51	0
82	OHX	AR	3467	7/7	0.97	0.12	85,85,85,85	0
82	OHX	A	1807	7/7	0.97	0.13	83,83,83,83	0
82	OHX	A	1837	7/7	0.97	0.12	102,102,102,102	0
82	OHX	AR	3545	7/7	0.97	0.25	98,98,98,98	0
82	OHX	AR	3468	7/7	0.97	0.14	64,64,64,64	0
82	OHX	A	1821	7/7	0.97	0.12	95,95,95,95	0
82	OHX	1	3560	7/7	0.97	0.15	102,102,102,102	0
82	OHX	1	3495	7/7	0.97	0.12	97,97,97,97	0
82	OHX	A	1898	7/7	0.97	0.29	115,115,115,115	0
82	OHX	1	3573	7/7	0.97	0.26	81,81,81,81	0
82	OHX	AR	3736	7/7	0.97	0.31	53,53,53,53	0
82	OHX	AR	3494	7/7	0.98	0.22	71,71,71,71	0
82	OHX	AR	3516	7/7	0.98	0.15	70,70,70,70	0
82	OHX	AR	3441	7/7	0.98	0.11	65,65,65,65	0
83	MG	AR	3787	1/1	0.98	0.41	53,53,53,53	0
82	OHX	AR	3445	7/7	0.98	0.11	67,67,67,67	0
83	MG	CL	303	1/1	0.98	0.56	26,26,26,26	0
82	OHX	CE	401	7/7	0.98	0.14	76,76,76,76	0
83	MG	sR	2055	1/1	0.98	0.58	42,42,42,42	0
82	OHX	AR	3723	7/7	0.98	0.19	74,74,74,74	0
82	OHX	1	3519	7/7	0.98	0.14	94,94,94,94	0
82	OHX	AR	3523	7/7	0.98	0.25	74,74,74,74	0
82	OHX	AR	3504	7/7	0.98	0.21	55,55,55,55	0
82	OHX	sR	1988	7/7	0.98	0.24	104,104,104,104	0
82	OHX	AR	3433	7/7	0.98	0.14	53,53,53,53	0
82	OHX	A	1872	7/7	0.98	0.09	125,125,125,125	0
83	MG	AR	3956	1/1	0.98	0.45	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	A	1887	7/7	0.98	0.22	114,114,114,114	0
82	OHX	AR	3459	7/7	0.98	0.11	69,69,69,69	0
83	MG	1	3863	1/1	0.98	0.48	22,22,22,22	0
82	OHX	c1	201	7/7	0.98	0.34	101,101,101,101	0
82	OHX	AR	3452	7/7	0.98	0.12	92,92,92,92	0
82	OHX	A	1834	7/7	0.98	0.12	111,111,111,111	0
83	MG	AR	3754	1/1	0.98	0.21	23,23,23,23	0
82	OHX	AR	3524	7/7	0.98	0.12	84,84,84,84	0
82	OHX	AT	211	7/7	0.98	0.14	108,108,108,108	0
82	OHX	AR	3470	7/7	0.98	0.09	74,74,74,74	0
83	MG	AR	4119	1/1	0.98	0.10	36,36,36,36	0
82	OHX	1	3445	7/7	0.98	0.09	71,71,71,71	0
82	OHX	AR	3526	7/7	0.98	0.24	82,82,82,82	0
83	MG	1	4037	1/1	0.98	0.32	30,30,30,30	0
82	OHX	A	1806	7/7	0.98	0.14	78,78,78,78	0
82	OHX	AR	3447	7/7	0.98	0.12	54,54,54,54	0
82	OHX	1	3588	7/7	0.98	0.22	110,110,110,110	0
83	MG	1	3871	1/1	0.98	0.17	37,37,37,37	0
82	OHX	AR	3518	7/7	0.98	0.16	80,80,80,80	0
82	OHX	AT	205	7/7	0.98	0.14	80,80,80,80	0
83	MG	v	303	1/1	0.98	0.32	27,27,27,27	0
82	OHX	1	3518	7/7	0.98	0.26	72,72,72,72	0
82	OHX	1	3583	7/7	0.98	0.23	83,83,83,83	0
82	OHX	d4	201	7/7	0.98	0.26	116,116,116,116	0
82	OHX	AR	3499	7/7	0.98	0.10	82,82,82,82	0
82	OHX	1	3498	7/7	0.98	0.17	76,76,76,76	0
82	OHX	1	3575	7/7	0.98	0.26	85,85,85,85	0
82	OHX	sR	1941	7/7	0.98	0.12	81,81,81,81	0
82	OHX	AR	3464	7/7	0.98	0.11	72,72,72,72	0
82	OHX	1	3489	7/7	0.98	0.10	78,78,78,78	0
82	OHX	1	3476	7/7	0.98	0.19	68,68,68,68	0
82	OHX	3	204	7/7	0.98	0.17	75,75,75,75	0
82	OHX	AR	3552	7/7	0.98	0.23	78,78,78,78	0
82	OHX	1	3607	7/7	0.98	0.24	94,94,94,94	0
82	OHX	1	3502	7/7	0.98	0.14	74,74,74,74	0
83	MG	AR	3819	1/1	0.98	0.47	34,34,34,34	0
82	OHX	AT	204	7/7	0.98	0.15	78,78,78,78	0
82	OHX	sR	1926	7/7	0.98	0.09	85,85,85,85	0
82	OHX	k	401	7/7	0.98	0.20	87,87,87,87	0
82	OHX	v	302	7/7	0.98	0.24	85,85,85,85	0
83	MG	AR	3908	1/1	0.98	0.74	33,33,33,33	0
82	OHX	sR	1963	7/7	0.98	0.23	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AR	4261	1/1	0.98	0.33	29,29,29,29	0
82	OHX	AR	3491	7/7	0.98	0.11	77,77,77,77	0
82	OHX	1	3553	7/7	0.98	0.24	85,85,85,85	0
82	OHX	1	3452	7/7	0.98	0.10	77,77,77,77	0
82	OHX	AR	3563	7/7	0.98	0.11	110,110,110,110	0
83	MG	CY	201	1/1	0.98	0.17	69,69,69,69	0
82	OHX	4	206	7/7	0.98	0.27	78,78,78,78	0
82	OHX	sR	1947	7/7	0.98	0.09	93,93,93,93	0
82	OHX	1	3544	7/7	0.98	0.20	97,97,97,97	0
82	OHX	AR	3456	7/7	0.98	0.17	70,70,70,70	0
82	OHX	sR	1944	7/7	0.98	0.08	103,103,103,103	0
82	OHX	1	3522	7/7	0.98	0.17	79,79,79,79	0
82	OHX	AR	3569	7/7	0.98	0.18	90,90,90,90	0
82	OHX	sR	1918	7/7	0.98	0.12	67,67,67,67	0
82	OHX	1	3681	7/7	0.98	0.31	96,96,96,96	0
82	OHX	A	1830	7/7	0.98	0.12	87,87,87,87	0
82	OHX	A	1809	7/7	0.98	0.23	94,94,94,94	0
82	OHX	sR	1936	7/7	0.98	0.12	75,75,75,75	0
82	OHX	AR	3477	7/7	0.98	0.12	79,79,79,79	0
82	OHX	1	3578	7/7	0.98	0.29	79,79,79,79	0
82	OHX	1	3576	7/7	0.98	0.23	74,74,74,74	0
82	OHX	1	3520	7/7	0.98	0.13	81,81,81,81	0
82	OHX	AR	3489	7/7	0.98	0.11	94,94,94,94	0
82	OHX	AR	3448	7/7	0.98	0.11	72,72,72,72	0
83	MG	sR	2193	1/1	0.98	0.54	37,37,37,37	0
82	OHX	1	3478	7/7	0.98	0.11	70,70,70,70	0
83	MG	1	3790	1/1	0.98	0.31	48,48,48,48	0
82	OHX	1	3511	7/7	0.98	0.21	67,67,67,67	0
82	OHX	AR	3469	7/7	0.98	0.12	72,72,72,72	0
82	OHX	CQ	201	7/7	0.98	0.12	70,70,70,70	0
83	MG	AR	3940	1/1	0.98	0.30	25,25,25,25	0
82	OHX	sR	1964	7/7	0.98	0.16	97,97,97,97	0
82	OHX	AS	203	7/7	0.98	0.16	72,72,72,72	0
82	OHX	AT	209	7/7	0.98	0.14	95,95,95,95	0
82	OHX	AR	3431	7/7	0.98	0.10	58,58,58,58	0
82	OHX	AR	3590	7/7	0.98	0.19	94,94,94,94	0
82	OHX	1	3624	7/7	0.98	0.25	82,82,82,82	0
83	MG	1	4150	1/1	0.98	0.10	41,41,41,41	0
82	OHX	AR	3463	7/7	0.98	0.09	72,72,72,72	0
82	OHX	AR	3522	7/7	0.98	0.22	85,85,85,85	0
82	OHX	A	1878	7/7	0.98	0.17	120,120,120,120	0
82	OHX	1	3447	7/7	0.98	0.11	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3559	7/7	0.98	0.23	78,78,78,78	0
82	OHX	1	3569	7/7	0.98	0.20	70,70,70,70	0
83	MG	1	3813	1/1	0.98	0.21	30,30,30,30	0
82	OHX	1	3492	7/7	0.98	0.11	86,86,86,86	0
82	OHX	AR	3482	7/7	0.98	0.10	66,66,66,66	0
82	OHX	AR	3629	7/7	0.98	0.30	98,98,98,98	0
82	OHX	A	1827	7/7	0.98	0.08	96,96,96,96	0
82	OHX	A	1820	7/7	0.98	0.10	81,81,81,81	0
83	MG	1	3904	1/1	0.98	0.57	33,33,33,33	0
82	OHX	A	1841	7/7	0.98	0.12	106,106,106,106	0
83	MG	A	1963	1/1	0.98	0.46	48,48,48,48	0
82	OHX	1	3630	7/7	0.98	0.32	114,114,114,114	0
82	OHX	1	3564	7/7	0.98	0.24	82,82,82,82	0
82	OHX	sR	2012	7/7	0.98	0.19	106,106,106,106	0
82	OHX	1	3598	7/7	0.98	0.29	73,73,73,73	0
83	MG	AR	3899	1/1	0.98	0.53	26,26,26,26	0
82	OHX	1	3556	7/7	0.98	0.21	111,111,111,111	0
82	OHX	sR	1982	7/7	0.98	0.31	114,114,114,114	0
82	OHX	A	1876	7/7	0.98	0.29	89,89,89,89	0
82	OHX	A	1838	7/7	0.98	0.20	78,78,78,78	0
83	MG	A	1971	1/1	0.98	0.70	61,61,61,61	0
82	OHX	A	1835	7/7	0.98	0.18	107,107,107,107	0
82	OHX	sR	1967	7/7	0.98	0.22	98,98,98,98	0
82	OHX	CX	202	7/7	0.98	0.26	81,81,81,81	0
83	MG	1	4220	1/1	0.98	0.10	45,45,45,45	0
82	OHX	1	3467	7/7	0.98	0.07	84,84,84,84	0
83	MG	AR	3917	1/1	0.98	0.69	35,35,35,35	0
82	OHX	AR	3509	7/7	0.98	0.10	101,101,101,101	0
82	OHX	1	3525	7/7	0.98	0.24	86,86,86,86	0
83	MG	1	3963	1/1	0.98	0.29	30,30,30,30	0
83	MG	1	3922	1/1	0.98	0.59	22,22,22,22	0
82	OHX	A	1824	7/7	0.98	0.10	91,91,91,91	0
83	MG	AS	222	1/1	0.98	0.35	45,45,45,45	0
82	OHX	AR	3579	7/7	0.98	0.34	94,94,94,94	0
83	MG	AR	3845	1/1	0.98	0.42	23,23,23,23	0
82	OHX	A	1839	7/7	0.98	0.08	105,105,105,105	0
83	MG	A	1994	1/1	0.98	0.77	86,86,86,86	0
82	OHX	AR	3493	7/7	0.98	0.11	77,77,77,77	0
82	OHX	sR	1931	7/7	0.98	0.10	79,79,79,79	0
83	MG	AR	3866	1/1	0.98	0.52	27,27,27,27	0
82	OHX	AR	3474	7/7	0.98	0.10	56,56,56,56	0
83	MG	1	4076	1/1	0.98	0.15	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	4087	1/1	0.98	0.35	24,24,24,24	0
83	MG	sR	2160	1/1	0.98	0.27	42,42,42,42	0
82	OHX	AR	3502	7/7	0.98	0.09	83,83,83,83	0
82	OHX	1	3539	7/7	0.98	0.21	87,87,87,87	0
82	OHX	A	1812	7/7	0.98	0.14	87,87,87,87	0
82	OHX	AR	3669	7/7	0.98	0.38	65,65,65,65	0
82	OHX	1	3527	7/7	0.98	0.13	92,92,92,92	0
82	OHX	AT	206	7/7	0.98	0.12	96,96,96,96	0
82	OHX	A	1890	7/7	0.98	0.29	100,100,100,100	0
82	OHX	1	3639	7/7	0.98	0.22	88,88,88,88	0
82	OHX	1	3611	7/7	0.98	0.24	91,91,91,91	0
82	OHX	1	3434	7/7	0.98	0.13	65,65,65,65	0
83	MG	1	4017	1/1	0.98	0.38	35,35,35,35	0
82	OHX	1	3555	7/7	0.98	0.23	87,87,87,87	0
83	MG	AR	3900	1/1	0.98	0.27	21,21,21,21	0
82	OHX	A	1832	7/7	0.98	0.18	98,98,98,98	0
82	OHX	AR	3484	7/7	0.98	0.23	75,75,75,75	0
82	OHX	AR	3461	7/7	0.98	0.11	57,57,57,57	0
82	OHX	1	3685	7/7	0.98	0.32	101,101,101,101	0
82	OHX	sR	1952	7/7	0.98	0.11	121,121,121,121	0
83	MG	1	4208	1/1	0.98	0.39	39,39,39,39	0
82	OHX	1	3416	7/7	0.98	0.14	56,56,56,56	0
82	OHX	sR	1916	7/7	0.98	0.11	63,63,63,63	0
83	MG	1	4126	1/1	0.98	0.31	21,21,21,21	0
83	MG	1	3830	1/1	0.98	0.49	37,37,37,37	0
82	OHX	A	1826	7/7	0.98	0.12	93,93,93,93	0
82	OHX	AR	3588	7/7	0.98	0.28	88,88,88,88	0
82	OHX	AR	3533	7/7	0.98	0.19	81,81,81,81	0
83	MG	1	3865	1/1	0.98	0.29	21,21,21,21	0
82	OHX	AR	3487	7/7	0.98	0.12	64,64,64,64	0
83	MG	1	4138	1/1	0.98	0.10	44,44,44,44	0
82	OHX	AR	3572	7/7	0.98	0.24	105,105,105,105	0
82	OHX	AR	3478	7/7	0.98	0.11	70,70,70,70	0
82	OHX	AR	3479	7/7	0.98	0.16	58,58,58,58	0
82	OHX	A	1850	7/7	0.98	0.19	95,95,95,95	0
82	OHX	AS	204	7/7	0.98	0.16	69,69,69,69	0
82	OHX	AR	3683	7/7	0.98	0.36	92,92,92,92	0
83	MG	AR	3783	1/1	0.98	0.34	34,34,34,34	0
82	OHX	1	3472	7/7	0.98	0.10	69,69,69,69	0
83	MG	DQ	503	1/1	0.98	0.09	34,34,34,34	0
82	OHX	AR	3585	7/7	0.98	0.30	78,78,78,78	0
83	MG	AR	4069	1/1	0.98	0.18	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3675	7/7	0.98	0.25	121,121,121,121	0
83	MG	AR	3913	1/1	0.98	0.44	26,26,26,26	0
83	MG	1	4155	1/1	0.98	0.12	42,42,42,42	0
82	OHX	AR	3615	7/7	0.98	0.31	73,73,73,73	0
82	OHX	1	3509	7/7	0.98	0.20	77,77,77,77	0
82	OHX	AR	3556	7/7	0.98	0.19	72,72,72,72	0
82	OHX	sR	1934	7/7	0.98	0.11	86,86,86,86	0
82	OHX	AR	3647	7/7	0.98	0.35	92,92,92,92	0
82	OHX	AR	3575	7/7	0.98	0.31	88,88,88,88	0
82	OHX	A	1842	7/7	0.98	0.22	88,88,88,88	0
82	OHX	1	3470	7/7	0.98	0.08	76,76,76,76	0
82	OHX	1	3523	7/7	0.98	0.22	82,82,82,82	0
82	OHX	AR	3512	7/7	0.98	0.11	85,85,85,85	0
82	OHX	AR	3562	7/7	0.98	0.28	90,90,90,90	0
82	OHX	A	1889	7/7	0.98	0.29	130,130,130,130	0
83	MG	1	3746	1/1	0.98	0.48	26,26,26,26	0
82	OHX	sR	1959	7/7	0.98	0.17	92,92,92,92	0
82	OHX	A	1840	7/7	0.98	0.22	99,99,99,99	0
82	OHX	sR	1928	7/7	0.98	0.10	101,101,101,101	0
82	OHX	AR	3656	7/7	0.98	0.32	104,104,104,104	0
82	OHX	O	201	7/7	0.98	0.18	125,125,125,125	0
82	OHX	AE	201	7/7	0.98	0.19	91,91,91,91	0
82	OHX	AR	3442	7/7	0.98	0.10	63,63,63,63	0
83	MG	AR	3870	1/1	0.98	0.60	21,21,21,21	0
82	OHX	1	3590	7/7	0.98	0.36	84,84,84,84	0
82	OHX	sR	1956	7/7	0.98	0.07	135,135,135,135	0
83	MG	CX	203	1/1	0.98	0.54	21,21,21,21	0
82	OHX	AR	3627	7/7	0.98	0.33	107,107,107,107	0
82	OHX	AR	3513	7/7	0.98	0.18	77,77,77,77	0
82	OHX	AR	3604	7/7	0.98	0.28	97,97,97,97	0
82	OHX	A	1862	7/7	0.98	0.26	91,91,91,91	0
82	OHX	1	3581	7/7	0.98	0.15	107,107,107,107	0
82	OHX	AR	3495	7/7	0.98	0.15	97,97,97,97	0
82	OHX	sR	1929	7/7	0.98	0.12	106,106,106,106	0
82	OHX	1	3487	7/7	0.98	0.16	68,68,68,68	0
82	OHX	AR	3558	7/7	0.98	0.17	78,78,78,78	0
82	OHX	1	3512	7/7	0.98	0.15	78,78,78,78	0
82	OHX	1	3451	7/7	0.98	0.10	75,75,75,75	0
82	OHX	AR	3679	7/7	0.98	0.32	88,88,88,88	0
83	MG	1	3850	1/1	0.98	0.35	25,25,25,25	0
82	OHX	1	3680	7/7	0.98	0.33	98,98,98,98	0
82	OHX	sR	1921	7/7	0.98	0.12	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	A	1828	7/7	0.98	0.15	86,86,86,86	0
82	OHX	AR	3503	7/7	0.98	0.23	73,73,73,73	0
82	OHX	4	210	7/7	0.98	0.23	103,103,103,103	0
83	MG	1	4183	1/1	0.98	0.41	20,20,20,20	0
82	OHX	sR	1938	7/7	0.98	0.10	90,90,90,90	0
82	OHX	1	3425	7/7	0.98	0.14	58,58,58,58	0
82	OHX	AR	3691	7/7	0.98	0.21	62,62,62,62	0
83	MG	AR	3853	1/1	0.98	0.58	21,21,21,21	0
82	OHX	AT	207	7/7	0.98	0.15	91,91,91,91	0
82	OHX	A	1907	7/7	0.98	0.22	88,88,88,88	0
82	OHX	1	3584	7/7	0.98	0.15	102,102,102,102	0
83	MG	A	2011	1/1	0.98	0.77	72,72,72,72	0
82	OHX	sR	1905	7/7	0.98	0.18	59,59,59,59	0
82	OHX	sR	1945	7/7	0.98	0.15	81,81,81,81	0
82	OHX	1	3547	7/7	0.98	0.24	90,90,90,90	0
83	MG	AR	3766	1/1	0.98	0.11	27,27,27,27	0
82	OHX	A	1867	7/7	0.98	0.20	82,82,82,82	0
82	OHX	1	3463	7/7	0.98	0.11	83,83,83,83	0
82	OHX	AR	3480	7/7	0.98	0.12	71,71,71,71	0
82	OHX	1	3617	7/7	0.98	0.22	96,96,96,96	0
83	MG	sR	2115	1/1	0.98	0.21	67,67,67,67	0
82	OHX	AR	3576	7/7	0.98	0.28	83,83,83,83	0
82	OHX	AK	102	7/7	0.98	0.08	71,71,71,71	0
82	OHX	1	3677	7/7	0.98	0.29	82,82,82,82	0
83	MG	sR	2143	1/1	0.98	0.14	48,48,48,48	0
83	MG	AR	3833	1/1	0.98	0.40	23,23,23,23	0
82	OHX	AR	3444	7/7	0.98	0.11	62,62,62,62	0
83	MG	AR	4130	1/1	0.98	0.08	26,26,26,26	0
82	OHX	sR	1933	7/7	0.98	0.12	70,70,70,70	0
82	OHX	sR	1974	7/7	0.98	0.19	83,83,83,83	0
82	OHX	AR	3514	7/7	0.98	0.18	81,81,81,81	0
83	MG	AR	3755	1/1	0.98	0.54	17,17,17,17	0
82	OHX	AR	3645	7/7	0.98	0.30	90,90,90,90	0
82	OHX	A	1829	7/7	0.98	0.16	82,82,82,82	0
82	OHX	1	3543	7/7	0.98	0.17	98,98,98,98	0
82	OHX	1	3439	7/7	0.98	0.11	64,64,64,64	0
82	OHX	A	1808	7/7	0.98	0.14	81,81,81,81	0
82	OHX	A	1916	7/7	0.98	0.19	130,130,130,130	0
82	OHX	1	3703	7/7	0.98	0.41	98,98,98,98	0
82	OHX	AS	206	7/7	0.98	0.13	84,84,84,84	0
82	OHX	1	3559	7/7	0.98	0.20	98,98,98,98	0
82	OHX	1	3602	7/7	0.98	0.17	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3560	7/7	0.98	0.18	100,100,100,100	0
82	OHX	1	3634	7/7	0.98	0.30	93,93,93,93	0
82	OHX	A	1813	7/7	0.98	0.15	83,83,83,83	0
83	MG	1	4127	1/1	0.98	0.14	51,51,51,51	0
82	OHX	AR	3564	7/7	0.98	0.24	76,76,76,76	0
82	OHX	AR	3634	7/7	0.98	0.31	91,91,91,91	0
83	MG	1	3997	1/1	0.98	0.15	56,56,56,56	0
82	OHX	1	3431	7/7	0.98	0.14	64,64,64,64	0
83	MG	AR	4231	1/1	0.98	0.33	36,36,36,36	0
82	OHX	A	1803	7/7	0.98	0.20	74,74,74,74	0
82	OHX	A	1892	7/7	0.98	0.26	100,100,100,100	0
82	OHX	sR	1970	7/7	0.98	0.25	90,90,90,90	0
82	OHX	sR	2003	7/7	0.98	0.24	83,83,83,83	0
82	OHX	A	1811	7/7	0.98	0.16	89,89,89,89	0
82	OHX	AR	3451	7/7	0.98	0.13	64,64,64,64	0
82	OHX	AR	3455	7/7	0.98	0.13	72,72,72,72	0
83	MG	1	3913	1/1	0.98	0.40	26,26,26,26	0
82	OHX	AR	3693	7/7	0.98	0.33	90,90,90,90	0
82	OHX	AR	3608	7/7	0.98	0.15	96,96,96,96	0
82	OHX	sR	1943	7/7	0.98	0.13	87,87,87,87	0
82	OHX	A	1822	7/7	0.98	0.12	77,77,77,77	0
82	OHX	AR	3586	7/7	0.98	0.17	81,81,81,81	0
82	OHX	A	1816	7/7	0.98	0.13	83,83,83,83	0
82	OHX	1	3506	7/7	0.98	0.19	73,73,73,73	0
82	OHX	A	1860	7/7	0.98	0.14	122,122,122,122	0
82	OHX	AR	3738	7/7	0.98	0.29	71,71,71,71	0
83	MG	1	4178	1/1	0.98	0.43	42,42,42,42	0
82	OHX	AR	3577	7/7	0.98	0.20	86,86,86,86	0
82	OHX	AR	3578	7/7	0.98	0.28	87,87,87,87	0
82	OHX	AR	3733	7/7	0.98	0.25	76,76,76,76	0
82	OHX	AR	3450	7/7	0.98	0.10	83,83,83,83	0
82	OHX	3	202	7/7	0.98	0.19	76,76,76,76	0
82	OHX	1	3448	7/7	0.98	0.13	67,67,67,67	0
82	OHX	AR	3521	7/7	0.98	0.24	74,74,74,74	0
82	OHX	1	3450	7/7	0.98	0.11	62,62,62,62	0
82	OHX	AR	3660	7/7	0.98	0.26	81,81,81,81	0
82	OHX	1	3558	7/7	0.98	0.20	74,74,74,74	0
82	OHX	sR	1996	7/7	0.98	0.33	102,102,102,102	0
82	OHX	AR	3528	7/7	0.98	0.14	81,81,81,81	0
82	OHX	1	3491	7/7	0.98	0.17	56,56,56,56	0
82	OHX	AS	205	7/7	0.98	0.09	79,79,79,79	0
83	MG	1	3891	1/1	0.98	0.57	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	1	3531	7/7	0.98	0.12	115,115,115,115	0
83	MG	1	3937	1/1	0.98	0.51	30,30,30,30	0
82	OHX	1	3537	7/7	0.98	0.24	78,78,78,78	0
82	OHX	AR	3497	7/7	0.98	0.17	69,69,69,69	0
82	OHX	1	3567	7/7	0.98	0.27	80,80,80,80	0
83	MG	sR	2165	1/1	0.98	0.15	85,85,85,85	0
83	MG	AR	4166	1/1	0.98	0.10	60,60,60,60	0
82	OHX	1	3457	7/7	0.98	0.10	57,57,57,57	0
82	OHX	AR	3654	7/7	0.98	0.27	83,83,83,83	0
82	OHX	4	204	7/7	0.98	0.12	90,90,90,90	0
82	OHX	AR	3537	7/7	0.98	0.11	67,67,67,67	0
82	OHX	AR	3553	7/7	0.98	0.11	104,104,104,104	0
82	OHX	A	1815	7/7	0.98	0.12	101,101,101,101	0
82	OHX	AR	3481	7/7	0.98	0.13	78,78,78,78	0
83	MG	AR	3925	1/1	0.98	0.52	22,22,22,22	0
82	OHX	1	3517	7/7	0.98	0.18	63,63,63,63	0
82	OHX	1	3580	7/7	0.98	0.18	95,95,95,95	0
82	OHX	AS	202	7/7	0.98	0.13	71,71,71,71	0
82	OHX	1	3570	7/7	0.98	0.19	92,92,92,92	0
82	OHX	A	1856	7/7	0.98	0.21	103,103,103,103	0
83	MG	sR	2080	1/1	0.98	0.19	42,42,42,42	0
82	OHX	1	3503	7/7	0.98	0.15	85,85,85,85	0
82	OHX	AR	3426	7/7	0.99	0.09	50,50,50,50	0
82	OHX	1	3449	7/7	0.99	0.11	76,76,76,76	0
82	OHX	1	3481	7/7	0.99	0.16	83,83,83,83	0
82	OHX	sR	1914	7/7	0.99	0.11	80,80,80,80	0
82	OHX	1	3494	7/7	0.99	0.13	73,73,73,73	0
82	OHX	1	3566	7/7	0.99	0.25	77,77,77,77	0
83	MG	AR	3800	1/1	0.99	0.54	22,22,22,22	0
82	OHX	sR	1924	7/7	0.99	0.07	78,78,78,78	0
82	OHX	sR	1968	7/7	0.99	0.21	82,82,82,82	0
83	MG	1	4149	1/1	0.99	0.14	26,26,26,26	0
82	OHX	AR	3404	7/7	0.99	0.15	40,40,40,40	0
82	OHX	sR	1930	7/7	0.99	0.13	64,64,64,64	0
85	ZN	b	201	1/1	0.99	0.11	71,71,71,71	0
82	OHX	1	3418	7/7	0.99	0.10	45,45,45,45	0
82	OHX	1	3436	7/7	0.99	0.08	60,60,60,60	0
82	OHX	AR	3612	7/7	0.99	0.19	63,63,63,63	0
82	OHX	AR	3472	7/7	0.99	0.09	66,66,66,66	0
82	OHX	AR	3591	7/7	0.99	0.20	83,83,83,83	0
82	OHX	sR	1942	7/7	0.99	0.12	85,85,85,85	0
83	MG	A	2040	1/1	0.99	0.20	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	1	3621	7/7	0.99	0.21	64,64,64,64	0
82	OHX	1	3419	7/7	0.99	0.11	55,55,55,55	0
83	MG	4	223	1/1	0.99	0.28	30,30,30,30	0
82	OHX	AK	103	7/7	0.99	0.11	73,73,73,73	0
82	OHX	sR	1935	7/7	0.99	0.15	71,71,71,71	0
83	MG	1	3845	1/1	0.99	0.15	26,26,26,26	0
82	OHX	AR	3430	7/7	0.99	0.08	55,55,55,55	0
82	OHX	1	3504	7/7	0.99	0.22	83,83,83,83	0
82	OHX	1	3440	7/7	0.99	0.12	70,70,70,70	0
82	OHX	sR	1948	7/7	0.99	0.14	80,80,80,80	0
82	OHX	1	3459	7/7	0.99	0.10	60,60,60,60	0
85	ZN	AP	501	1/1	0.99	0.03	54,54,54,54	0
82	OHX	AR	3511	7/7	0.99	0.15	69,69,69,69	0
82	OHX	AR	3401	7/7	0.99	0.20	37,37,37,37	0
83	MG	l	402	1/1	0.99	0.07	46,46,46,46	0
83	MG	1	3800	1/1	0.99	0.23	25,25,25,25	0
82	OHX	AR	3507	7/7	0.99	0.15	78,78,78,78	0
82	OHX	1	3404	7/7	0.99	0.20	45,45,45,45	0
82	OHX	4	205	7/7	0.99	0.20	94,94,94,94	0
82	OHX	1	3437	7/7	0.99	0.14	60,60,60,60	0
82	OHX	A	1814	7/7	0.99	0.11	76,76,76,76	0
82	OHX	A	1810	7/7	0.99	0.11	81,81,81,81	0
82	OHX	AR	3520	7/7	0.99	0.07	96,96,96,96	0
82	OHX	AR	3425	7/7	0.99	0.14	55,55,55,55	0
82	OHX	AS	201	7/7	0.99	0.10	67,67,67,67	0
82	OHX	AC	101	7/7	0.99	0.15	47,47,47,47	0
83	MG	AR	4024	1/1	0.99	0.10	42,42,42,42	0
83	MG	AR	3772	1/1	0.99	0.30	23,23,23,23	0
83	MG	A	2044	1/1	0.99	0.16	70,70,70,70	0
82	OHX	1	3414	7/7	0.99	0.14	52,52,52,52	0
82	OHX	1	3466	7/7	0.99	0.08	74,74,74,74	0
82	OHX	1	3477	7/7	0.99	0.08	82,82,82,82	0
82	OHX	sR	1907	7/7	0.99	0.14	59,59,59,59	0
82	OHX	AR	3486	7/7	0.99	0.12	69,69,69,69	0
82	OHX	AR	3436	7/7	0.99	0.09	57,57,57,57	0
82	OHX	AR	3483	7/7	0.99	0.13	59,59,59,59	0
82	OHX	sR	1902	7/7	0.99	0.19	59,59,59,59	0
82	OHX	sR	1913	7/7	0.99	0.11	64,64,64,64	0
82	OHX	1	3429	7/7	0.99	0.10	60,60,60,60	0
82	OHX	A	1825	7/7	0.99	0.07	104,104,104,104	0
83	MG	AR	4156	1/1	0.99	0.12	50,50,50,50	0
83	MG	AR	4204	1/1	0.99	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	1	3433	7/7	0.99	0.16	71,71,71,71	0
82	OHX	AR	3421	7/7	0.99	0.13	52,52,52,52	0
82	OHX	1	3528	7/7	0.99	0.08	102,102,102,102	0
82	OHX	1	3465	7/7	0.99	0.08	66,66,66,66	0
82	OHX	DG	201	7/7	0.99	0.18	68,68,68,68	0
82	OHX	1	3460	7/7	0.99	0.10	88,88,88,88	0
83	MG	1	4137	1/1	0.99	0.10	70,70,70,70	0
82	OHX	AR	3429	7/7	0.99	0.09	57,57,57,57	0
82	OHX	AR	3415	7/7	0.99	0.13	50,50,50,50	0
82	OHX	AR	3443	7/7	0.99	0.14	72,72,72,72	0
82	OHX	A	1852	7/7	0.99	0.28	92,92,92,92	0
82	OHX	w	201	7/7	0.99	0.11	80,80,80,80	0
82	OHX	AR	3440	7/7	0.99	0.09	70,70,70,70	0
82	OHX	sR	1911	7/7	0.99	0.14	65,65,65,65	0
82	OHX	sR	1953	7/7	0.99	0.12	91,91,91,91	0
83	MG	AR	4175	1/1	0.99	0.09	49,49,49,49	0
83	MG	AR	4041	1/1	0.99	0.17	69,69,69,69	0
82	OHX	AR	3498	7/7	0.99	0.06	95,95,95,95	0
82	OHX	AR	3510	7/7	0.99	0.07	49,49,49,49	0
82	OHX	sR	1904	7/7	0.99	0.12	61,61,61,61	0
82	OHX	1	3514	7/7	0.99	0.10	57,57,57,57	0
82	OHX	AR	3406	7/7	0.99	0.14	45,45,45,45	0
82	OHX	sR	1923	7/7	0.99	0.12	70,70,70,70	0
82	OHX	AR	3418	7/7	0.99	0.10	49,49,49,49	0
82	OHX	sR	1915	7/7	0.99	0.13	64,64,64,64	0
82	OHX	CH	201	7/7	0.99	0.16	43,43,43,43	0
82	OHX	AR	3411	7/7	0.99	0.18	52,52,52,52	0
82	OHX	AR	3568	7/7	0.99	0.23	82,82,82,82	0
83	MG	AR	4073	1/1	0.99	0.22	52,52,52,52	0
82	OHX	AR	3454	7/7	0.99	0.11	55,55,55,55	0
82	OHX	AR	3458	7/7	0.99	0.08	61,61,61,61	0
82	OHX	1	3464	7/7	0.99	0.08	62,62,62,62	0
82	OHX	1	3409	7/7	0.99	0.15	49,49,49,49	0
82	OHX	AR	3453	7/7	0.99	0.07	80,80,80,80	0
83	MG	AR	4174	1/1	0.99	0.15	28,28,28,28	0
82	OHX	AR	3446	7/7	0.99	0.07	59,59,59,59	0
82	OHX	AR	3405	7/7	0.99	0.16	41,41,41,41	0
82	OHX	1	3443	7/7	0.99	0.11	54,54,54,54	0
83	MG	AR	4186	1/1	0.99	0.61	23,23,23,23	0
82	OHX	1	3442	7/7	0.99	0.13	71,71,71,71	0
82	OHX	1	3568	7/7	0.99	0.10	115,115,115,115	0
82	OHX	sR	1903	7/7	0.99	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	sR	1910	7/7	0.99	0.13	52,52,52,52	0
82	OHX	1	3441	7/7	0.99	0.12	66,66,66,66	0
82	OHX	1	3411	7/7	0.99	0.12	49,49,49,49	0
82	OHX	4	203	7/7	0.99	0.12	71,71,71,71	0
83	MG	AS	228	1/1	0.99	0.29	44,44,44,44	0
82	OHX	1	3497	7/7	0.99	0.10	45,45,45,45	0
82	OHX	DH	201	7/7	0.99	0.11	82,82,82,82	0
82	OHX	A	1805	7/7	0.99	0.12	63,63,63,63	0
82	OHX	AT	202	7/7	0.99	0.09	57,57,57,57	0
83	MG	1	3897	1/1	0.99	0.61	26,26,26,26	0
83	MG	AR	3750	1/1	0.99	0.47	25,25,25,25	0
82	OHX	4	201	7/7	0.99	0.15	44,44,44,44	0
82	OHX	1	3474	7/7	0.99	0.07	78,78,78,78	0
82	OHX	4	202	7/7	0.99	0.11	61,61,61,61	0
82	OHX	A	1801	7/7	0.99	0.17	64,64,64,64	0
82	OHX	1	3432	7/7	0.99	0.10	61,61,61,61	0
82	OHX	1	3484	7/7	0.99	0.08	65,65,65,65	0
82	OHX	1	3424	7/7	0.99	0.14	63,63,63,63	0
82	OHX	AR	3407	7/7	0.99	0.18	44,44,44,44	0
85	ZN	AN	500	1/1	0.99	0.12	40,40,40,40	0
82	OHX	sR	1957	7/7	0.99	0.11	89,89,89,89	0
82	OHX	sR	1927	7/7	0.99	0.20	67,67,67,67	0
82	OHX	AR	3462	7/7	0.99	0.06	63,63,63,63	0
82	OHX	1	3678	7/7	0.99	0.17	94,94,94,94	0
82	OHX	AR	3517	7/7	0.99	0.16	76,76,76,76	0
85	ZN	DO	201	1/1	0.99	0.13	29,29,29,29	0
82	OHX	AR	3492	7/7	0.99	0.15	66,66,66,66	0
82	OHX	1	3521	7/7	0.99	0.13	87,87,87,87	0
82	OHX	1	3515	7/7	0.99	0.09	85,85,85,85	0
82	OHX	AR	3554	7/7	0.99	0.32	89,89,89,89	0
85	ZN	d6	201	1/1	0.99	0.12	44,44,44,44	0
83	MG	sR	2150	1/1	0.99	0.10	75,75,75,75	0
82	OHX	1	3407	7/7	0.99	0.12	40,40,40,40	0
82	OHX	AT	201	7/7	0.99	0.14	45,45,45,45	0
82	OHX	sR	1937	7/7	0.99	0.12	81,81,81,81	0
85	ZN	DQ	501	1/1	0.99	0.03	51,51,51,51	0
82	OHX	1	3574	7/7	0.99	0.18	100,100,100,100	0
83	MG	1	4184	1/1	0.99	0.53	28,28,28,28	0
85	ZN	d9	101	1/1	0.99	0.14	69,69,69,69	0
82	OHX	sR	1920	7/7	0.99	0.08	80,80,80,80	0
82	OHX	sR	1908	7/7	0.99	0.15	60,60,60,60	0
83	MG	1	3883	1/1	0.99	0.34	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	AR	3501	7/7	0.99	0.14	65,65,65,65	0
82	OHX	AR	3506	7/7	0.99	0.15	70,70,70,70	0
82	OHX	1	3427	7/7	0.99	0.12	59,59,59,59	0
82	OHX	AT	203	7/7	0.99	0.12	84,84,84,84	0
82	OHX	1	3417	7/7	0.99	0.14	49,49,49,49	0
82	OHX	AR	3527	7/7	0.99	0.10	88,88,88,88	0
82	OHX	1	3461	7/7	0.99	0.10	68,68,68,68	0
82	OHX	AR	3542	7/7	0.99	0.22	64,64,64,64	0
82	OHX	AR	3414	7/7	0.99	0.13	46,46,46,46	0
83	MG	1	4125	1/1	0.99	0.33	24,24,24,24	0
83	MG	sR	2072	1/1	0.99	0.34	61,61,61,61	0
83	MG	AR	3919	1/1	0.99	0.59	22,22,22,22	0
82	OHX	1	3406	7/7	0.99	0.17	45,45,45,45	0
82	OHX	A	1802	7/7	0.99	0.13	68,68,68,68	0
83	MG	1	4170	1/1	0.99	0.11	49,49,49,49	0
82	OHX	sR	1922	7/7	0.99	0.17	66,66,66,66	0
82	OHX	AR	3581	7/7	0.99	0.17	69,69,69,69	0
82	OHX	1	3435	7/7	0.99	0.08	51,51,51,51	0
82	OHX	1	3456	7/7	0.99	0.09	70,70,70,70	0
83	MG	AR	4192	1/1	0.99	0.16	37,37,37,37	0
83	MG	AR	4257	1/1	0.99	0.70	32,32,32,32	0
85	ZN	DR	501	1/1	0.99	0.11	49,49,49,49	0
82	OHX	AR	3485	7/7	0.99	0.15	69,69,69,69	0
82	OHX	sR	1901	7/7	0.99	0.16	47,47,47,47	0
82	OHX	AR	3434	7/7	0.99	0.14	72,72,72,72	0
82	OHX	AR	3437	7/7	0.99	0.08	56,56,56,56	0
82	OHX	AR	3412	7/7	0.99	0.11	47,47,47,47	0
82	OHX	AR	3531	7/7	0.99	0.15	61,61,61,61	0
82	OHX	1	3453	7/7	0.99	0.07	61,61,61,61	0
82	OHX	AR	3416	7/7	0.99	0.13	49,49,49,49	0
82	OHX	1	3510	7/7	0.99	0.18	64,64,64,64	0
82	OHX	1	3422	7/7	0.99	0.14	64,64,64,64	0
82	OHX	A	1819	7/7	0.99	0.09	81,81,81,81	0
82	OHX	A	1823	7/7	0.99	0.07	83,83,83,83	0
82	OHX	sR	1909	7/7	0.99	0.13	72,72,72,72	0
82	OHX	AR	3420	7/7	0.99	0.11	54,54,54,54	0
82	OHX	A	1804	7/7	0.99	0.12	70,70,70,70	0
83	MG	sR	2124	1/1	0.99	0.20	42,42,42,42	0
82	OHX	AR	3438	7/7	0.99	0.10	53,53,53,53	0
82	OHX	AR	3435	7/7	0.99	0.10	56,56,56,56	0
82	OHX	1	3488	7/7	0.99	0.14	69,69,69,69	0
82	OHX	DD	101	7/7	0.99	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	sR	1912	7/7	0.99	0.11	62,62,62,62	0
82	OHX	CP	501	7/7	0.99	0.17	94,94,94,94	0
82	OHX	1	3475	7/7	0.99	0.11	70,70,70,70	0
83	MG	AR	3897	1/1	0.99	0.52	25,25,25,25	0
82	OHX	AR	3466	7/7	0.99	0.11	74,74,74,74	0
82	OHX	1	3533	7/7	0.99	0.11	64,64,64,64	0
82	OHX	sR	1917	7/7	0.99	0.06	67,67,67,67	0
82	OHX	AR	3465	7/7	0.99	0.14	60,60,60,60	0
82	OHX	1	3455	7/7	0.99	0.09	68,68,68,68	0
82	OHX	1	3415	7/7	0.99	0.09	47,47,47,47	0
83	MG	1	3943	1/1	0.99	0.23	39,39,39,39	0
83	MG	sR	2171	1/1	0.99	0.09	71,71,71,71	0
82	OHX	sR	1925	7/7	0.99	0.10	67,67,67,67	0
82	OHX	AR	3419	7/7	0.99	0.11	49,49,49,49	0
82	OHX	CX	201	7/7	0.99	0.07	67,67,67,67	0
82	OHX	AR	3471	7/7	0.99	0.10	78,78,78,78	0
82	OHX	1	3446	7/7	0.99	0.09	64,64,64,64	0
82	OHX	2	201	7/7	0.99	0.12	53,53,53,53	0
82	OHX	AR	3439	7/7	0.99	0.12	66,66,66,66	0
85	ZN	e	101	1/1	0.99	0.10	70,70,70,70	0
82	OHX	AR	3550	7/7	0.99	0.17	91,91,91,91	0
82	OHX	AR	3449	7/7	0.99	0.08	75,75,75,75	0
82	OHX	AR	3488	7/7	0.99	0.09	72,72,72,72	0
83	MG	AR	4092	1/1	0.99	0.15	36,36,36,36	0
82	OHX	1	3410	7/7	1.00	0.12	46,46,46,46	0
82	OHX	1	3421	7/7	1.00	0.11	54,54,54,54	0
83	MG	1	4139	1/1	1.00	0.12	44,44,44,44	0
82	OHX	1	3408	7/7	1.00	0.12	49,49,49,49	0
82	OHX	1	3412	7/7	1.00	0.09	46,46,46,46	0
82	OHX	1	3402	7/7	1.00	0.14	40,40,40,40	0
82	OHX	AR	3402	7/7	1.00	0.15	33,33,33,33	0
82	OHX	AR	3410	7/7	1.00	0.12	35,35,35,35	0
82	OHX	AR	3417	7/7	1.00	0.11	55,55,55,55	0
82	OHX	1	3423	7/7	1.00	0.09	53,53,53,53	0
82	OHX	1	3401	7/7	1.00	0.15	33,33,33,33	0
83	MG	s1	302	1/1	1.00	0.12	63,63,63,63	0
82	OHX	n	201	7/7	1.00	0.14	43,43,43,43	0
82	OHX	1	3403	7/7	1.00	0.14	38,38,38,38	0
83	MG	1	4061	1/1	1.00	0.11	40,40,40,40	0
83	MG	1	4085	1/1	1.00	0.28	45,45,45,45	0
82	OHX	AR	3408	7/7	1.00	0.14	45,45,45,45	0
82	OHX	1	3405	7/7	1.00	0.13	39,39,39,39	0

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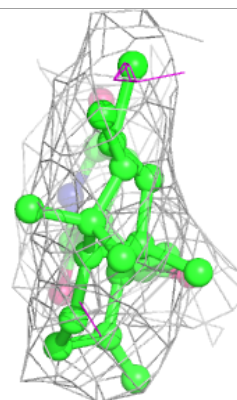
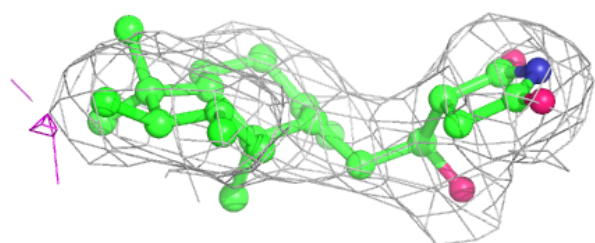
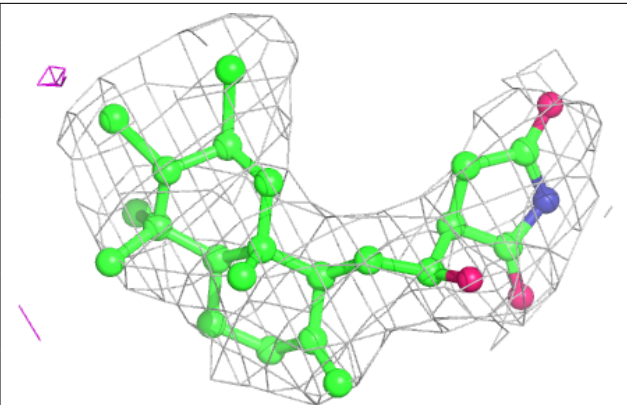
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	OHX	1	3468	7/7	1.00	0.10	46,46,46,46	0
83	MG	AR	4153	1/1	1.00	0.09	44,44,44,44	0
83	MG	1	4030	1/1	1.00	0.12	54,54,54,54	0
82	OHX	sR	1906	7/7	1.00	0.11	56,56,56,56	0
82	OHX	AR	3427	7/7	1.00	0.09	47,47,47,47	0
82	OHX	AR	3424	7/7	1.00	0.11	52,52,52,52	0
85	ZN	AK	101	1/1	1.00	0.11	27,27,27,27	0
83	MG	AR	4179	1/1	1.00	0.12	41,41,41,41	0
85	ZN	DL	101	1/1	1.00	0.12	35,35,35,35	0
82	OHX	AR	3409	7/7	1.00	0.15	44,44,44,44	0
82	OHX	AR	3403	7/7	1.00	0.15	34,34,34,34	0
82	OHX	1	3413	7/7	1.00	0.10	51,51,51,51	0
82	OHX	1	3428	7/7	1.00	0.06	55,55,55,55	0
82	OHX	1	3426	7/7	1.00	0.09	53,53,53,53	0
82	OHX	AR	3423	7/7	1.00	0.13	48,48,48,48	0
82	OHX	1	3420	7/7	1.00	0.12	53,53,53,53	0
82	OHX	AR	3432	7/7	1.00	0.09	48,48,48,48	0
82	OHX	1	3438	7/7	1.00	0.07	54,54,54,54	0
85	ZN	AQ	501	1/1	1.00	0.08	43,43,43,43	0
83	MG	1	4103	1/1	1.00	0.09	47,47,47,47	0
82	OHX	v	301	7/7	1.00	0.12	43,43,43,43	0
82	OHX	AR	3413	7/7	1.00	0.10	43,43,43,43	0
82	OHX	AR	3490	7/7	1.00	0.10	47,47,47,47	0
82	OHX	AR	3422	7/7	1.00	0.09	49,49,49,49	0

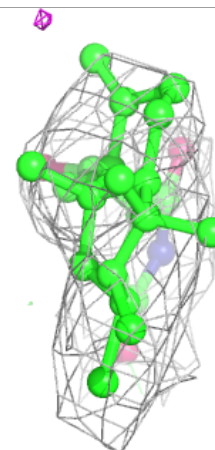
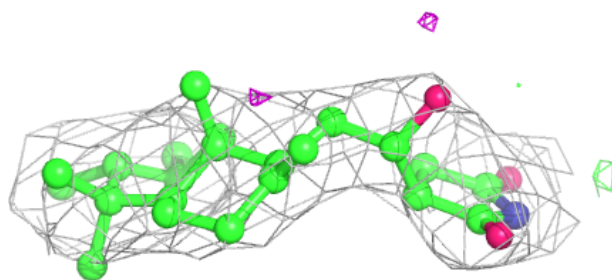
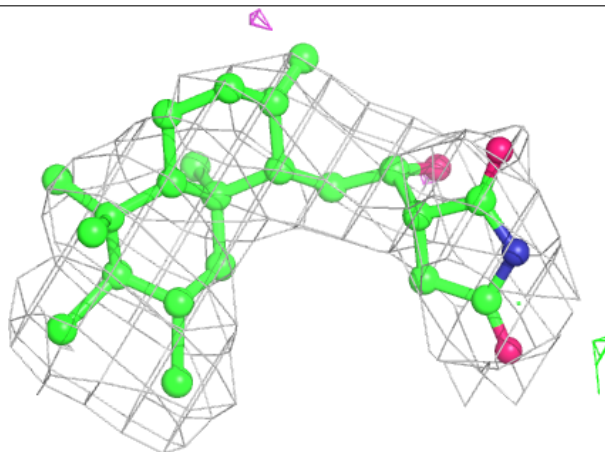
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G5B 1 4224:

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

**Electron density around G5B AR 4264:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.