



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:52 PM UTC

PDB ID : 4U56 / pdb_00004u56
Title : Crystal structure of Blasticidin S bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

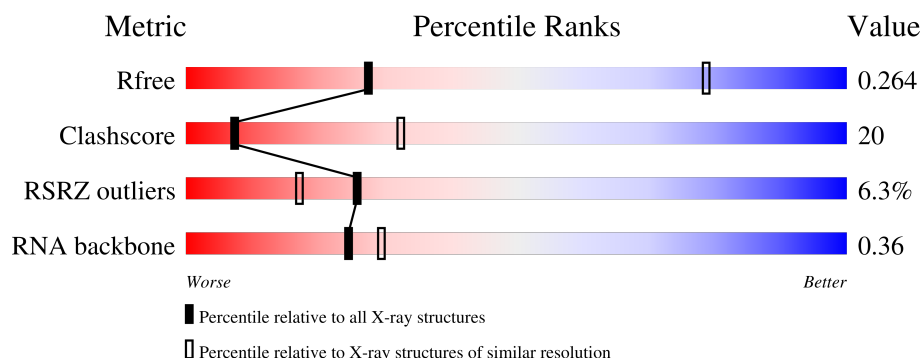
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)
RNA backbone	3983	1186 (3.92-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2	1800	5% 29% 49% 20% .
1	6	1800	4% 33% 49% 18%
2	S0	251	4% 36% 45% 18%
2	s0	251	2% 33% 47% 18%
3	S1	254	8% 37% 47% 16%
3	s1	254	2% 46% 39% 15%

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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	

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Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	

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Mol	Chain	Length	Quality of chain
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	

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Mol	Chain	Length	Quality of chain
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	

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Mol	Chain	Length	Quality of chain
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	

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Mol	Chain	Length	Quality of chain
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	120	
70	o4	120	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	

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Mol	Chain	Length	Quality of chain
79	q3	91	
80	e0	62	
81	p0	311	
82	m2	160	
83	p1	47	
84	p2	46	

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
85	MG	1	3586	-	-	-	X
85	MG	1	3780	-	-	-	X
85	MG	1	3800	-	-	-	X
85	MG	1	4217	-	-	-	X
85	MG	2	1914	-	-	-	X
85	MG	2	1915	-	-	-	X
85	MG	2	1924	-	-	-	X
85	MG	2	1933	-	-	-	X
85	MG	2	1936	-	-	-	X
85	MG	2	1950	-	-	-	X
85	MG	2	1959	-	-	-	X
85	MG	2	1980	-	-	-	X
85	MG	2	1987	-	-	-	X
85	MG	3	214	-	-	-	X
85	MG	5	3438	-	-	-	X
85	MG	5	3525	-	-	-	X
85	MG	5	3751	-	-	-	X
85	MG	6	1924	-	-	-	X
85	MG	6	1939	-	-	-	X
85	MG	6	1945	-	-	-	X
85	MG	6	1950	-	-	-	X
85	MG	6	1960	-	-	-	X
85	MG	6	2028	-	-	-	X
85	MG	m1	201	-	-	-	X
86	OHX	1	3951	-	-	X	-
86	OHX	1	3965	-	-	X	-
86	OHX	1	3998	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	4023	-	-	X	-
86	OHX	1	4027	-	-	X	-
86	OHX	1	4040	-	-	X	-
86	OHX	1	4050	-	-	X	-
86	OHX	1	4143	-	-	X	-
86	OHX	1	4153	-	-	X	-
86	OHX	1	4160	-	-	X	-
86	OHX	1	4169	-	-	X	-
86	OHX	1	4178	-	-	X	-
86	OHX	1	4194	-	-	X	-
86	OHX	2	2031	-	-	X	-
86	OHX	2	2043	-	-	X	-
86	OHX	2	2074	-	-	X	-
86	OHX	2	2098	-	-	X	-
86	OHX	2	2131	-	-	X	-
86	OHX	2	2146	-	-	X	-
86	OHX	2	2162	-	-	X	-
86	OHX	5	3935	-	-	X	-
86	OHX	5	3966	-	-	X	-
86	OHX	5	3971	-	-	X	-
86	OHX	5	3994	-	-	X	-
86	OHX	5	3995	-	-	X	-
86	OHX	5	4004	-	-	X	-
86	OHX	5	4014	-	-	X	-
86	OHX	5	4029	-	-	X	-
86	OHX	5	4060	-	-	X	-
86	OHX	5	4085	-	-	X	-
86	OHX	5	4193	-	-	X	-
86	OHX	5	4195	-	-	X	-
86	OHX	5	4212	-	-	X	-
86	OHX	5	4228	-	-	X	-
86	OHX	5	4232	-	-	X	-
86	OHX	5	4238	-	-	X	-
86	OHX	6	2059	-	-	X	-
86	OHX	6	2120	-	-	X	-
86	OHX	6	2147	-	-	X	-
86	OHX	6	2171	-	-	X	-
86	OHX	7	220	-	-	X	-
86	OHX	7	228	-	-	X	-
86	OHX	8	216	-	-	X	-
86	OHX	8	223	-	-	X	-
86	OHX	O1	202	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	O7	104	-	-	X	-
87	ZN	Q2	501	-	-	X	-

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 411214 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1750	Total	C	N	O	P	0	0	0
			37283	16668	6591	12274	1750			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S1	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
5	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S6	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

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

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			773	500	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
c0	89	ALA	GLY	conflict	UNP Q08745

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	147	ALA	GLY	conflict	UNP P0CX47
c1	147	ALA	GLY	conflict	UNP P0CX47

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	104	ALA	GLY	conflict	UNP P48589
C2	110	ALA	GLY	conflict	UNP P48589
c2	104	ALA	GLY	conflict	UNP P48589
c2	110	ALA	GLY	conflict	UNP P48589

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	C3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C5	137	SER	ARG	conflict	UNP Q01855
c5	137	SER	ARG	conflict	UNP Q01855

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	C8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	C9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
21	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	D0	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	D1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	D2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	D4	134	Total	C	N	O	0	0	0
			1073	676	208	189			
26	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	D5	70	Total	C	N	O	0	0	0
			563	360	104	99			
27	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

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

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	D8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
33	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2441	1544	419	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	652	221	231				
35	sM	104	Total	C	N	O		0	0	0
			679	402	140	137				

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	l3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	l4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	l6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	l9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	M0	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
47	m0	213	Total	C	N	O	S	0	0	0
			1722	1094	325	297	6			

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	M1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
48	m1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O	0	0	0
			1543	962	315	266			
49	m3	194	Total	C	N	O	0	0	0
			1548	965	316	267			

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
52	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	M7	183	Total	C	N	O		0	0	0
			1420	882	281	257				
53	m7	155	Total	C	N	O		0	0	0
			1227	764	238	225				

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	M8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	m8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O		0	0	0
			1521	935	326	260				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	m9	188	Total	C	N	O	0	0	0
			1521	935	326	260			

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	N1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
57	n1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O	0	0	0
			796	516	131	149			
58	n2	98	Total	C	N	O	0	0	0
			778	505	127	146			

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	N3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
59	n3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
60	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O	0	0	0
			993	625	192	176			
62	n6	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	N7	135	Total	C	N	O	0	0	0
			1092	710	202	180			
63	n7	135	Total	C	N	O	0	0	0
			1092	710	202	180			

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	N8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	n8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	N9	58	Total	C	N	O	0	0	0
			462	289	100	73			
65	n9	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	o0	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	O1	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
67	o1	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	O2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	O3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	o3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	O4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	o4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	121	LYS	-	expression tag	UNP P87262
o4	121	LYS	-	expression tag	UNP P87262

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	O5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	o5	119	Total	C	N	O	S	0	0	0
			965	612	185	167	1			

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	O7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
73	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	0	0	0
			612	391	115	106			
74	o8	77	Total	C	N	O	0	0	0
			608	388	114	106			

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	O9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
75	o9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
78	q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	Q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 82 is a protein called unknown protein chain m2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
82	m2	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 83 is a protein called unknown protein chain p1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
83	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			

- Molecule 84 is a protein called unknown protein chain p2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
84	p2	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	122	Total	Mg	0	0
			122	122		
85	S4	1	Total	Mg	0	0
			1	1		
85	S8	1	Total	Mg	0	0
			1	1		
85	C1	1	Total	Mg	0	0
			1	1		
85	D0	1	Total	Mg	0	0
			1	1		
85	D3	1	Total	Mg	0	0
			1	1		
85	D4	1	Total	Mg	0	0
			1	1		
85	SM	1	Total	Mg	0	0
			1	1		
85	1	462	Total	Mg	0	0
			462	462		
85	3	15	Total	Mg	0	0
			15	15		
85	4	23	Total	Mg	0	0
			23	23		
85	L2	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L3	4	Total 4	Mg 4	0	0
85	L4	3	Total 3	Mg 3	0	0
85	L7	2	Total 2	Mg 2	0	0
85	L8	1	Total 1	Mg 1	0	0
85	M0	3	Total 3	Mg 3	0	0
85	M1	1	Total 1	Mg 1	0	0
85	M3	2	Total 2	Mg 2	0	0
85	M5	2	Total 2	Mg 2	0	0
85	M6	1	Total 1	Mg 1	0	0
85	M7	5	Total 5	Mg 5	0	0
85	M9	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0
85	N3	3	Total 3	Mg 3	0	0
85	N5	1	Total 1	Mg 1	0	0
85	N6	2	Total 2	Mg 2	0	0
85	N8	5	Total 5	Mg 5	0	0
85	O1	1	Total 1	Mg 1	0	0
85	O2	2	Total 2	Mg 2	0	0
85	O5	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	Q2	1	Total 1	Mg 1	0	0

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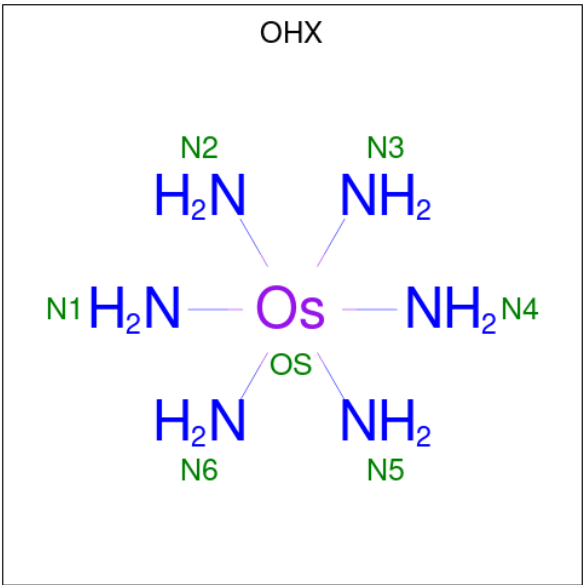
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	6	147	Total 147	Mg 147	0	0
85	s1	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	c1	1	Total 1	Mg 1	0	0
85	c4	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0
85	d0	1	Total 1	Mg 1	0	0
85	d3	3	Total 3	Mg 3	0	0
85	d6	1	Total 1	Mg 1	0	0
85	sM	1	Total 1	Mg 1	0	0
85	5	495	Total 495	Mg 495	0	0
85	7	17	Total 17	Mg 17	0	0
85	8	14	Total 14	Mg 14	0	0
85	l2	3	Total 3	Mg 3	0	0
85	l3	3	Total 3	Mg 3	0	0
85	l4	1	Total 1	Mg 1	0	0
85	l5	3	Total 3	Mg 3	0	0
85	l7	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	m0	1	Total 1	Mg 1	0	0
85	m1	1	Total 1	Mg 1	0	0
85	m4	1	Total 1	Mg 1	0	0
85	m5	5	Total 5	Mg 5	0	0
85	m6	2	Total 2	Mg 2	0	0
85	m7	6	Total 6	Mg 6	0	0
85	n0	1	Total 1	Mg 1	0	0
85	n3	1	Total 1	Mg 1	0	0
85	n6	2	Total 2	Mg 2	0	0
85	n8	3	Total 3	Mg 3	0	0
85	n9	2	Total 2	Mg 2	0	0
85	o3	2	Total 2	Mg 2	0	0
85	o4	3	Total 3	Mg 3	0	0
85	o7	1	Total 1	Mg 1	0	0
85	q0	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0

- Molecule 86 is osmium (III) hexammine (CCD ID: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	C3	1	Total	N	Os	0	0
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86	C5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	D3	1	Total	N	Os	0	0
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86	D9	1	Total	N	Os	0	0
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86	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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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	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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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	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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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	L3	1	Total	N	Os	0	0
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86	L4	1	Total	N	Os	0	0
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86	M0	1	Total	N	Os	0	0
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86	M5	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M9	1	Total	N	Os	0	0
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86	O1	1	Total	N	Os	0	0
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86	O3	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	Q2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	n1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

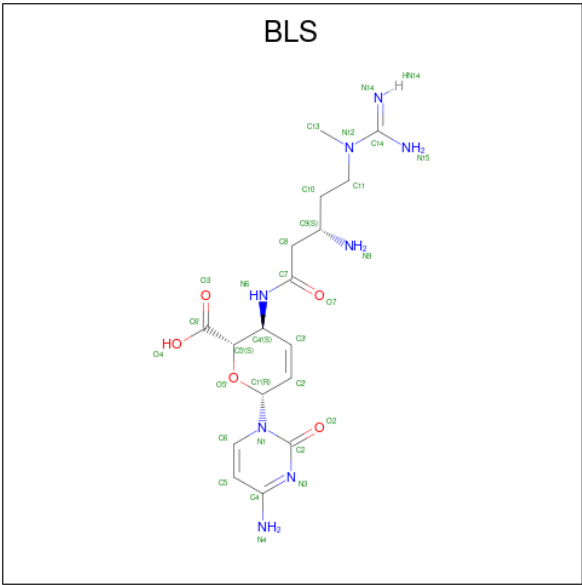
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	D6	1	Total	Zn	0	0
			1	1		
87	D7	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	o7	1	Total	Zn	0	0
			1	1		
87	q0	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q2	1	Total	Zn	0	0
			1	1		
87	q3	1	Total	Zn	0	0
			1	1		

- Molecule 88 is BLASTICIDIN S (CCD ID: BLS) (formula: C₁₇H₂₆N₈O₅).

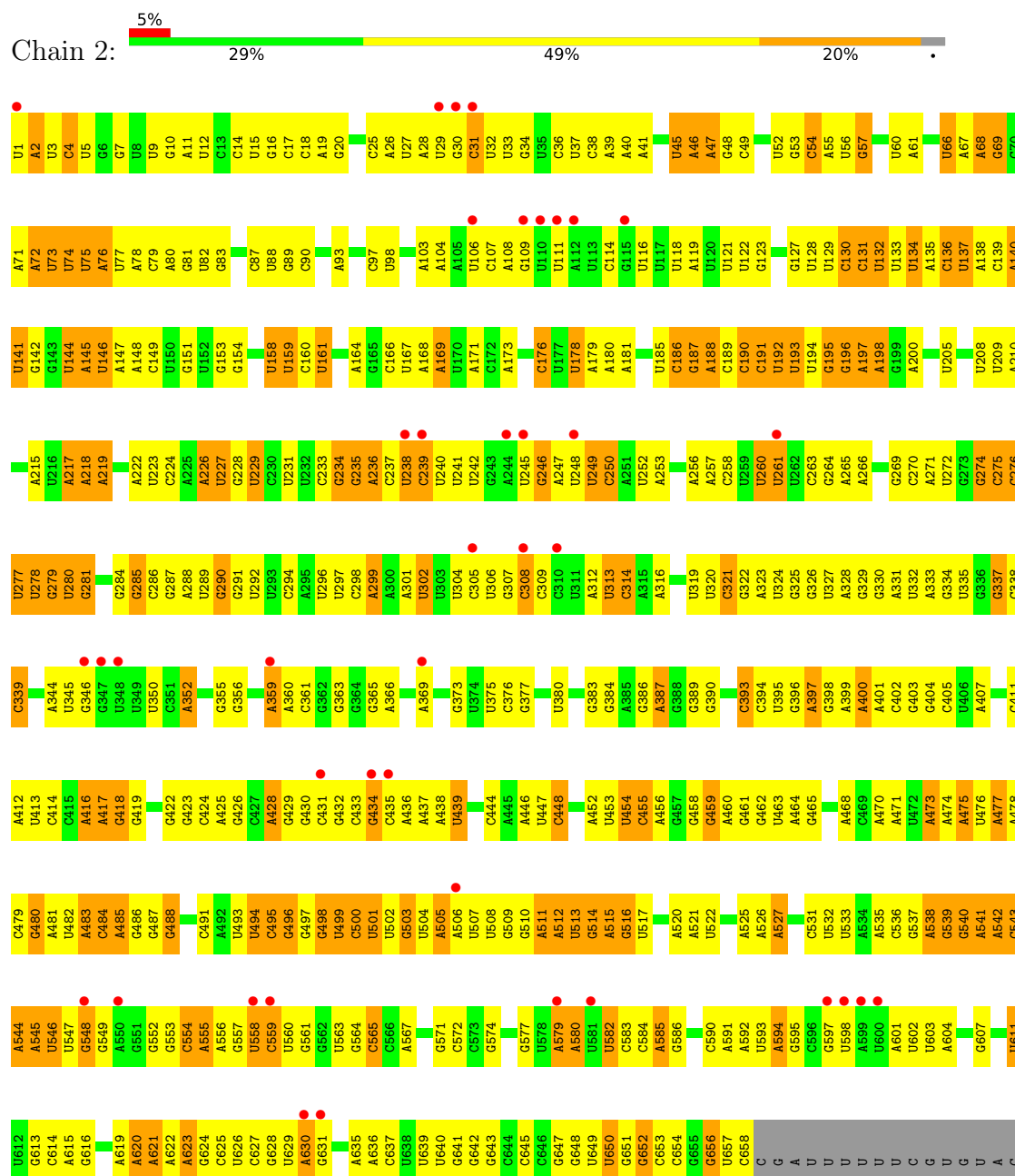


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total	C	N	O	0	0
			30	17	8	5		
88	5	1	Total	C	N	O	0	0
			30	17	8	5		

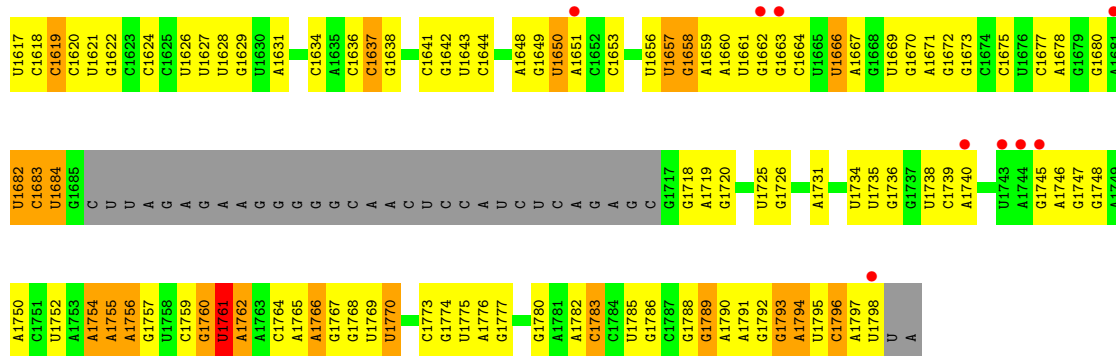
3 Residue-property plots

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

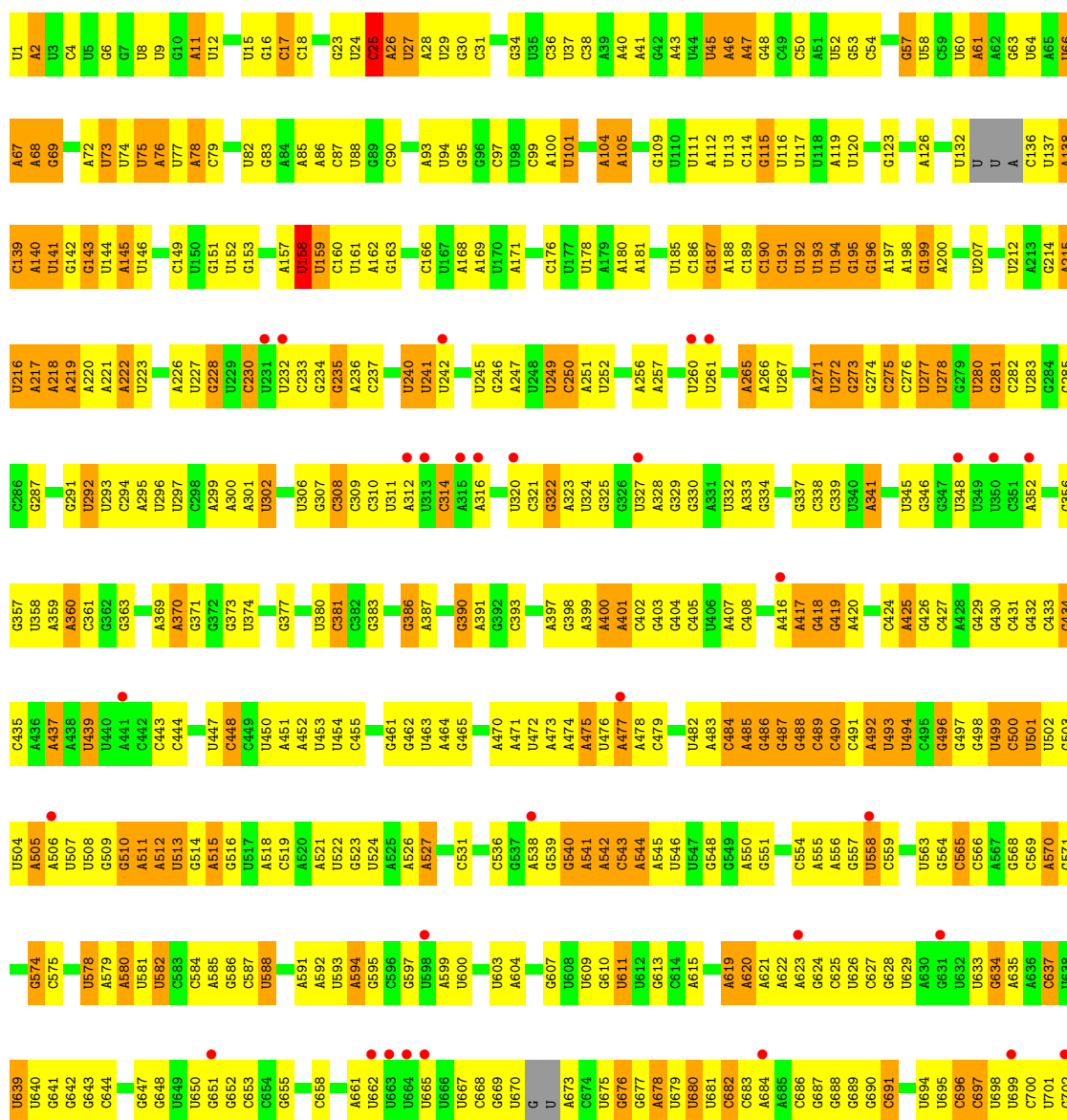
- Molecule 1: 18S ribosomal RNA



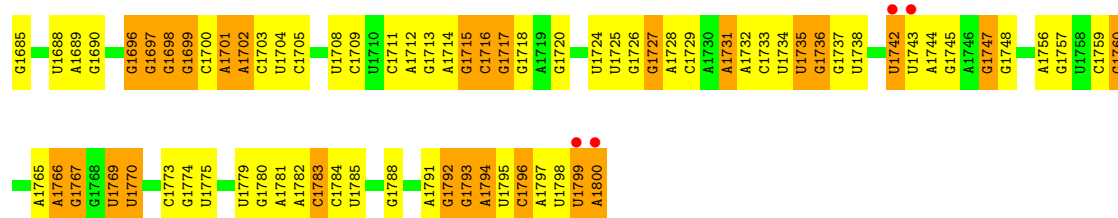
A1555	C1490	G1281	C1216	A1152	C1077	A1003	U932	A863	A799	C736	U
A1556	U1491	G1284	A1217	G1153	C1078	U1004	A933	U864	U800	A737	G676
U1557	U1492	C1285	A1218	G1154	U1080	A1005	C934	A865	G801	A678	G677
U1558	A1493	U1286	A1219	G1155	U1081	G1008	U935	G866	G802	G739	A679
U1559		U1287		G1156	C1082	U1009	G936	G867	A803	A740	U679
U1560	U1497	G1288	C1222	A1157	C1083	C1010	G937	G868	U805	A741	U680
U1561	G1498	U1289	A1223	C1158	G1086	G1011	G938	A869	U806	U742	U681
G1562	G1499	U1290	A1224	A1159	A1088	U1012		C870	A806	U743	U682
C1500	C1501	U1291	A1225	G1160	A1089	A1013	A941	G871	A807	U744	G683
U1430	C1431	G1292	A1226	C1161	A1088	G1014	G942	G872	U808	U745	A684
U1432	U1433	G1293	A1227	C1162	A1089	U1015		U873	A809	U746	A685
G1433	U1434	U1294	G1228	G1163	A1091	U1016	U947	G876	G810	U747	G686
U1436	U1437	A1295	G1229	G1164	A1092	U1017	G948		A811	U748	G687
U1437		A1296	A1230	G1165	A1092	U1018	C949	G877	A812	U749	G688
U1509	U1510	U1297	U1232	G1166	A1093	U1019	C950	A881	U813	U750	G689
U1511	U1512	U1298	U1233	A1167	A1094	A1021	A951	U882	A814	U751	
U1513	U1514	U1299	G1233	U1168	U1095	C1022	A952	G885	G815	A752	C692
U1515	U1516	A1300	A1234	G1169	U1097	C1022	A955	U886	G816	A753	U693
U1517	U1518	U1303	C1235	G1172	U1098			A887	A817	A754	U694
U1519	U1520	U1307	A1238	G1173	U1098	A1026	U958	U888	C818	A755	U695
U1521	U1522	G1307	U1239	C1174	G1100	A1027	U959	U889	U820		C696
U1523	U1524	G1308	U1240	U1175	G1101	C1028	U960	A891	U821	U759	C697
U1525	U1526	U1309	A1241	G1176	G1102			A892	U822	U760	U699
U1527	U1528	U1310	G1242	C1177	U1103	U1031	U964	U893	G823	G761	C700
U1529	U1530	A1312	G1243	G1178	U1104	G1032	U965	U894	G824	A762	U701
U1531	U1532	U1313	A1244	C1180	U1106	C1033	A966	G895	U825	G763	G702
U1533	U1534	U1314	G1245	G1181	U1107	A1036	A967	U896	U826	U764	G703
U1535	U1536	U1315	C1246	U1182	G1108	C1037	U968	C897	U827	G765	G704
U1537	U1538	G1316	U1247	G1183	G1109	U1038	C969	A898	U828	U766	U705
U1539	U1540	C1317	U1248	A1184	G1114	A1039	A970	G899	A829	U767	A706
U1541	U1542	U1320	U1250	U1185		G1040	A973	A900	U830	C768	A707
U1543	U1544	A1321	U1251	U1186	A1125	G1041	A974	G901	U831	A769	C708
U1545	U1546	U1322	U1252	U1187	G1126	G1042	C975	G902	U832	A771	C709
U1547	U1548	U1323	U1253	G1188	G1127	A1043	G976	A905	G834	G772	U710
U1549	U1550	G1324	G1255	U1191	C1128		A977	A906	U835	C773	U711
U1551	U1552	A1325	A1256	C1192	U1129	U1052	A978	A907		A774	G712
U1553	U1554	U1326	U1257	G1193	G1130	G1053	A979	U908	G838	G775	A713
U1555	U1556	C1327	U1258	G1194	A1131	U1054	G980	U909	U839		U714
U1557	U1558	G1328	G1261	G1195	A1132	U1058	U981	U912	U843	G778	U715
U1559	U1560	U1329	U1262	G1196	A1133	U1059	U982	G914	U844	U779	C716
U1561	U1562	A1330		G1197	C1134	U1060	A983	A915	G845	A780	U717
U1563	U1564	U1331	G1265	G1198	A1137	U1061	G986	U916	U846	U781	U718
U1565	U1566	A1332	U1266	G1199	A1138	A1062	G987	U917	G847	U782	G720
U1567	U1568	U1333	G1267	G1200	A1139	U1063	A988	U918	C948	G783	U721
U1569	U1570	C1334	U1268	G1201	A1140	U1064	U989	A919	U850	C784	G722
U1571	U1572	U1335	U1269	A1202	G1141	G991	C990	U920	U851	U785	G723
U1573	U1574	U1336	G1270	A1203	A1142	A1065	A992	U921	G852	G787	U724
U1575	U1576	A1337		G1207	A1143	C1066	A993	G924	G853	A788	U725
U1577	U1578	U1338	G1273	A1208	U1144	C1067	G984	A925	U854	A789	C726
U1579	U1580	A1339	C1274	C1209	U1145	C1068	A995	G926	A855	U792	U727
U1581	U1582	U1340	U1275	G1210	U1146	A1069	A996	A927	A856	A793	U728
U1583	U1584	U1341	U1276	A1211	A1147		G997	C927	U857	U794	G730
U1585	U1586	U1342	G1277	G1212	C1148			U928	G858	U795	G731
U1587	U1588	A1343	U1278	U1213	G1149	G1073	C1000	A929	U861	A796	G732
U1589	U1590	U1344	G1279	G1214	U1150	C1074	A1001	G931		G797	A733
U1591	U1592	U1345	C1280	C1215	A1151	C1075	A930	C931		C798	A734
U1593	U1594	U1346				A1076					C735



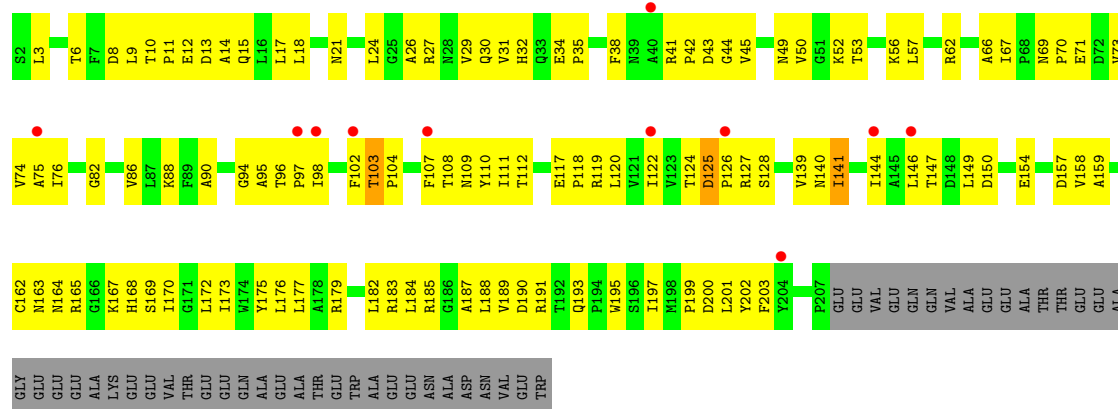
● Molecule 1: 18S ribosomal RNA



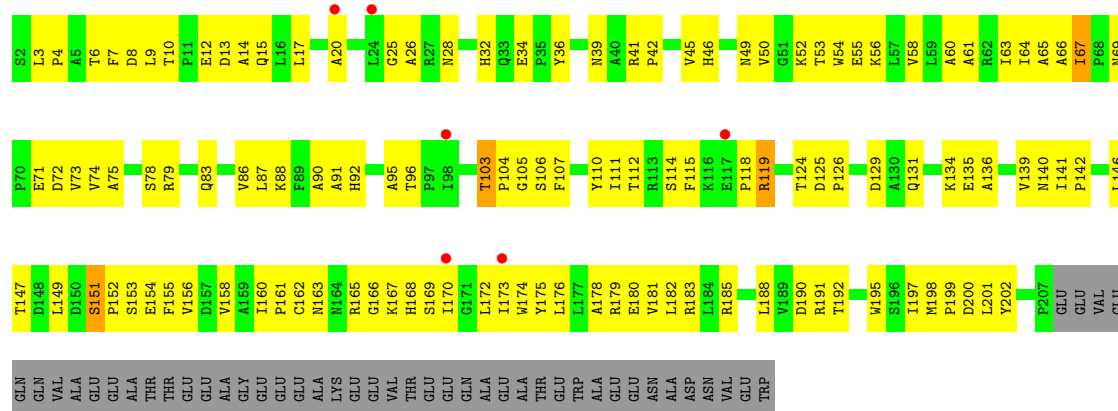




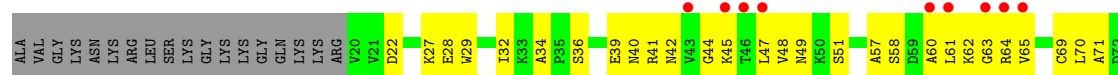
• Molecule 2: 40S ribosomal protein S0-A

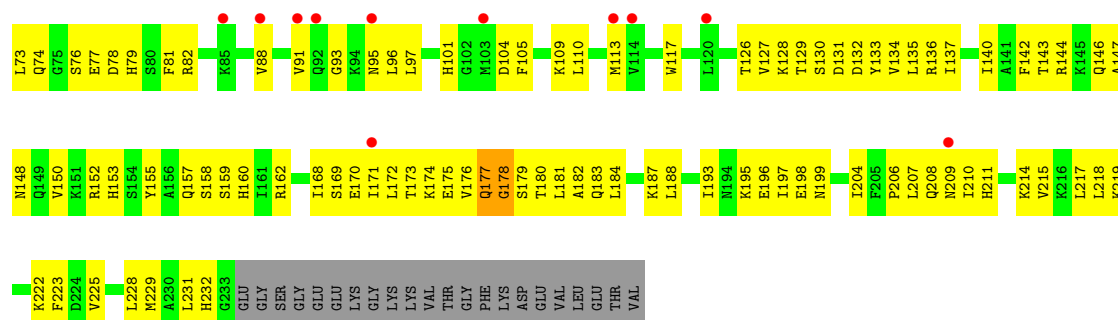


• Molecule 2: 40S ribosomal protein S0-A

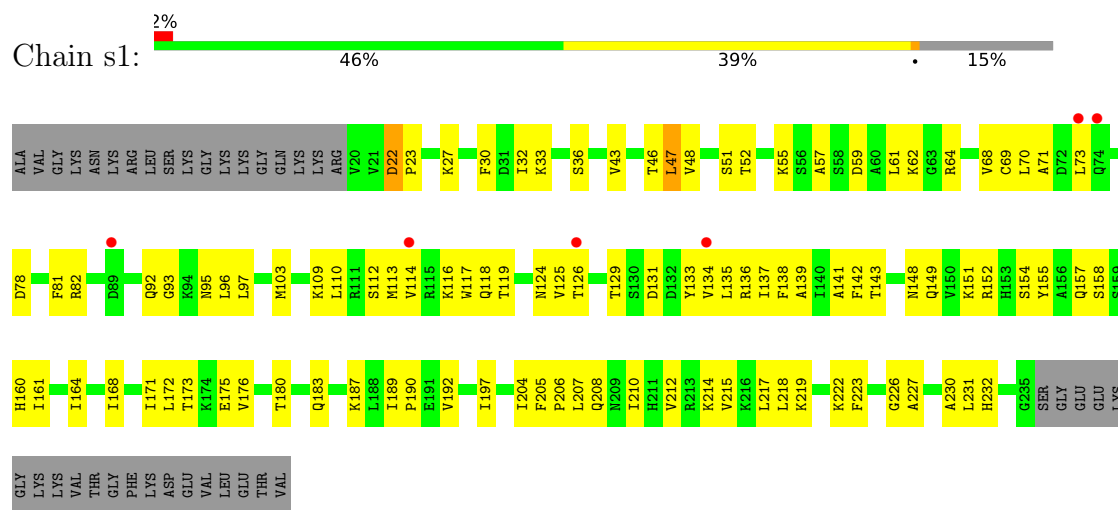


• Molecule 3: 40S ribosomal protein S1-A

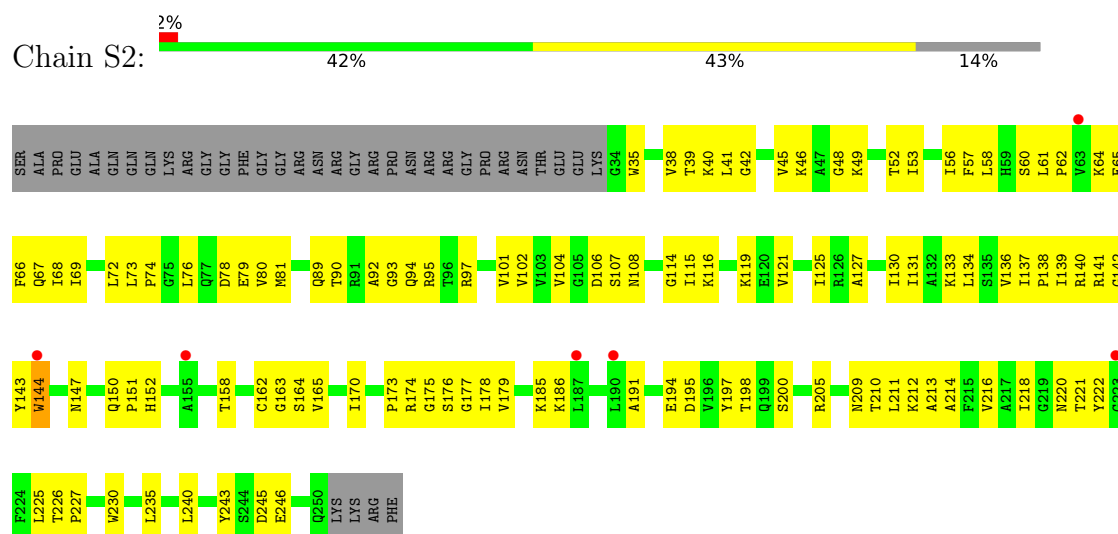




• Molecule 3: 40S ribosomal protein S1-A

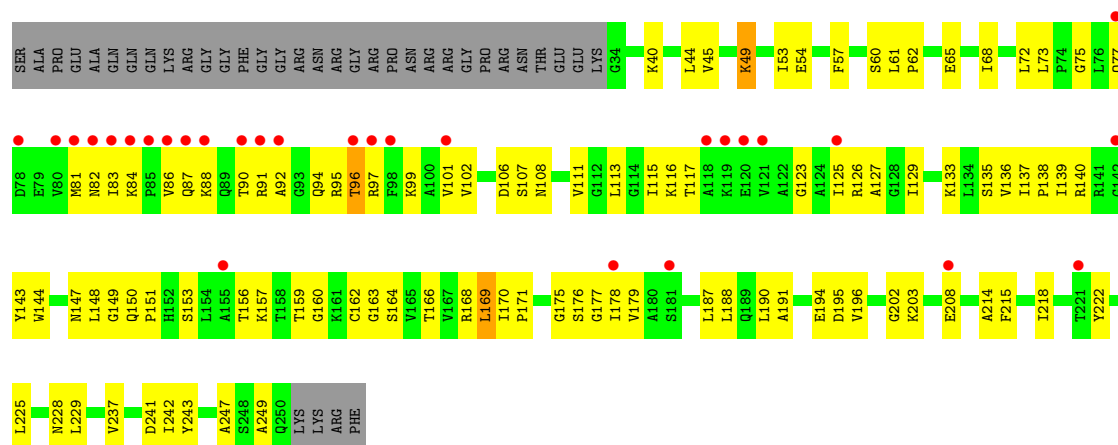


• Molecule 4: 40S ribosomal protein S2

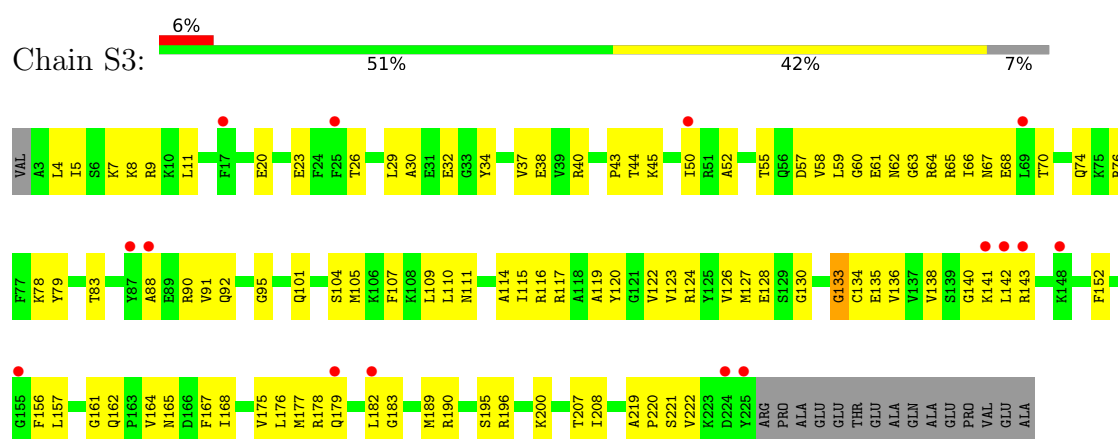


• Molecule 4: 40S ribosomal protein S2

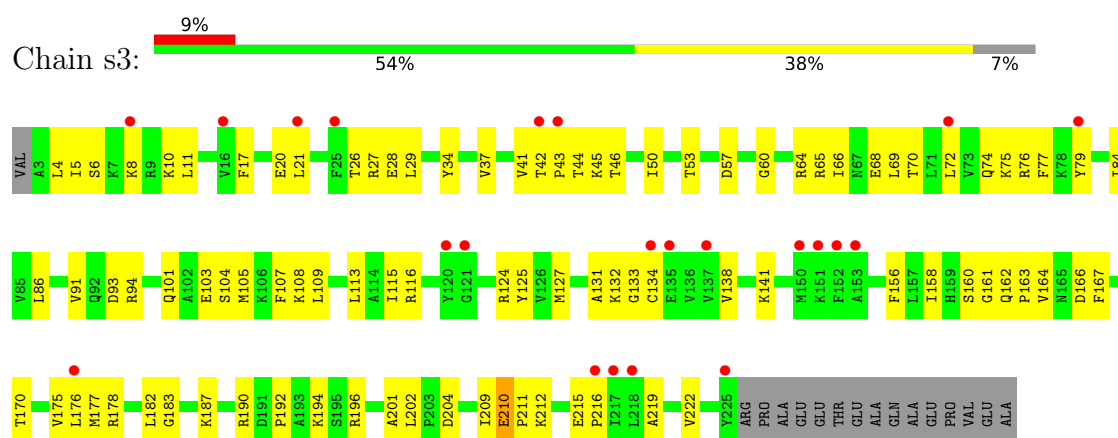




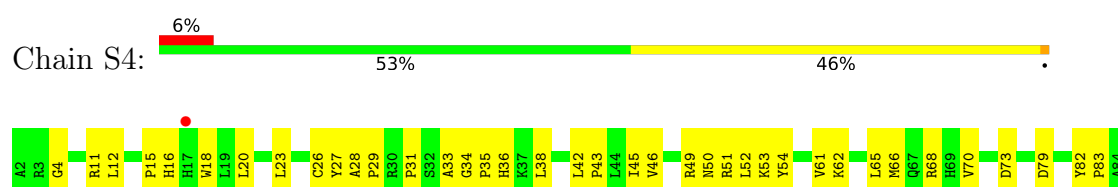
• Molecule 5: 40S ribosomal protein S3

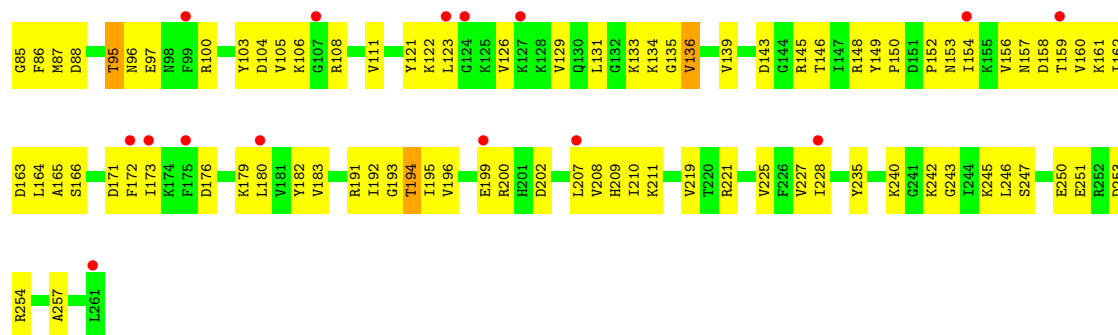


• Molecule 5: 40S ribosomal protein S3

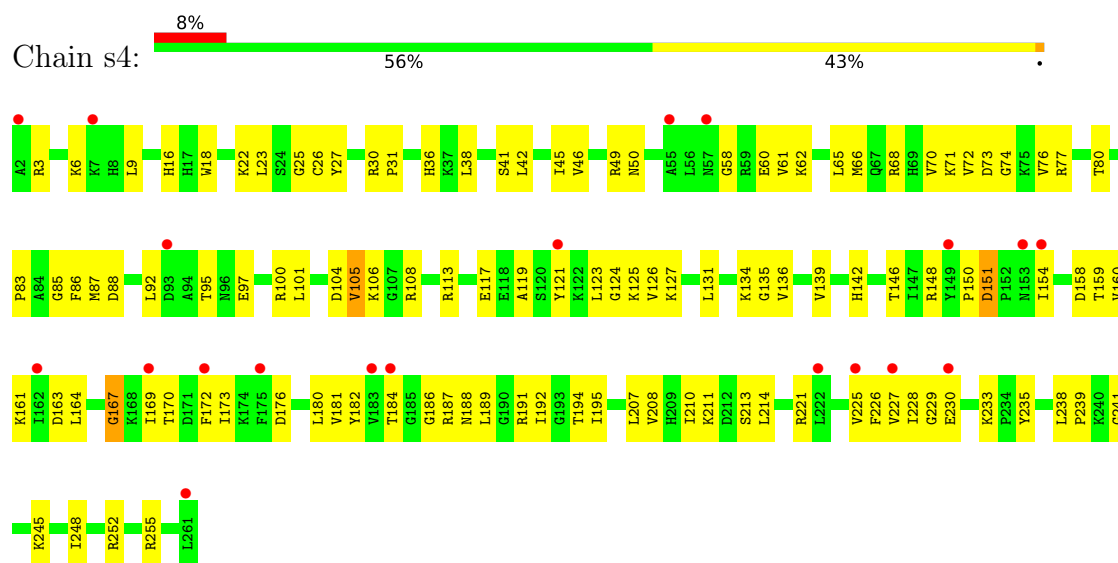


• Molecule 6: 40S ribosomal protein S4-A

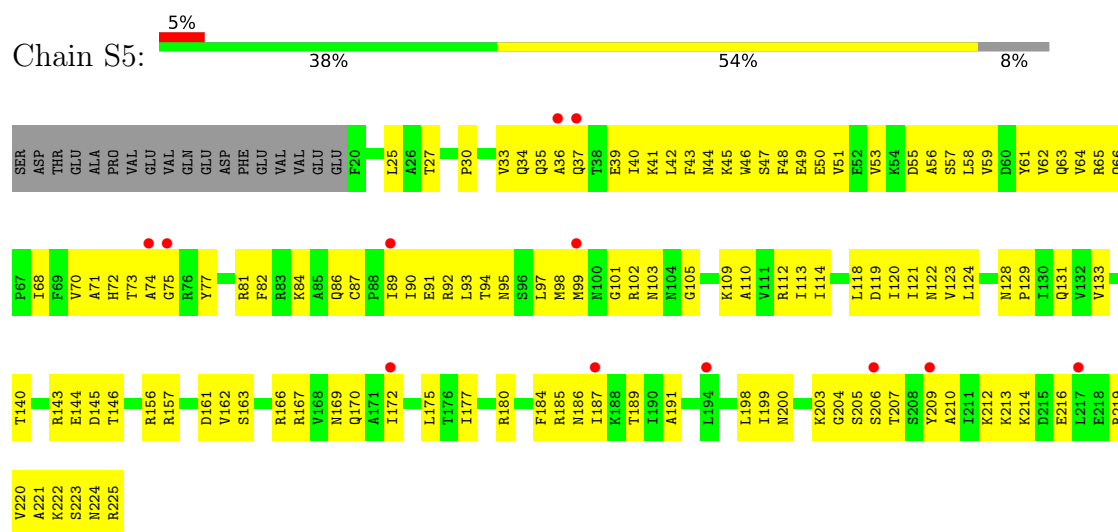




• Molecule 6: 40S ribosomal protein S4-A

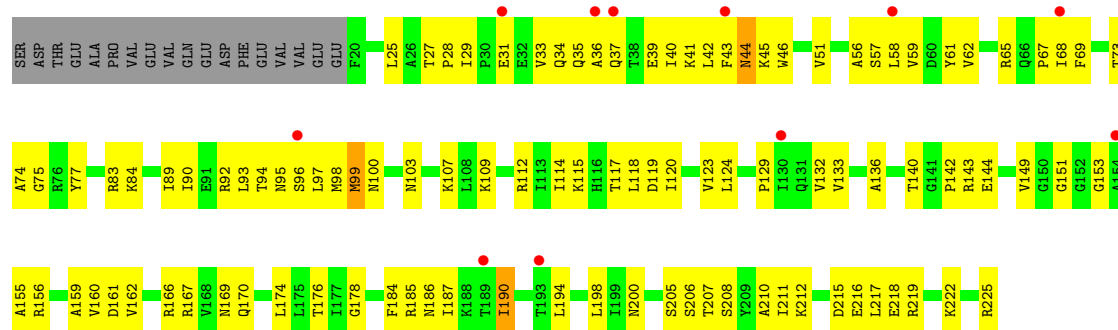


• Molecule 7: 40S ribosomal protein S5

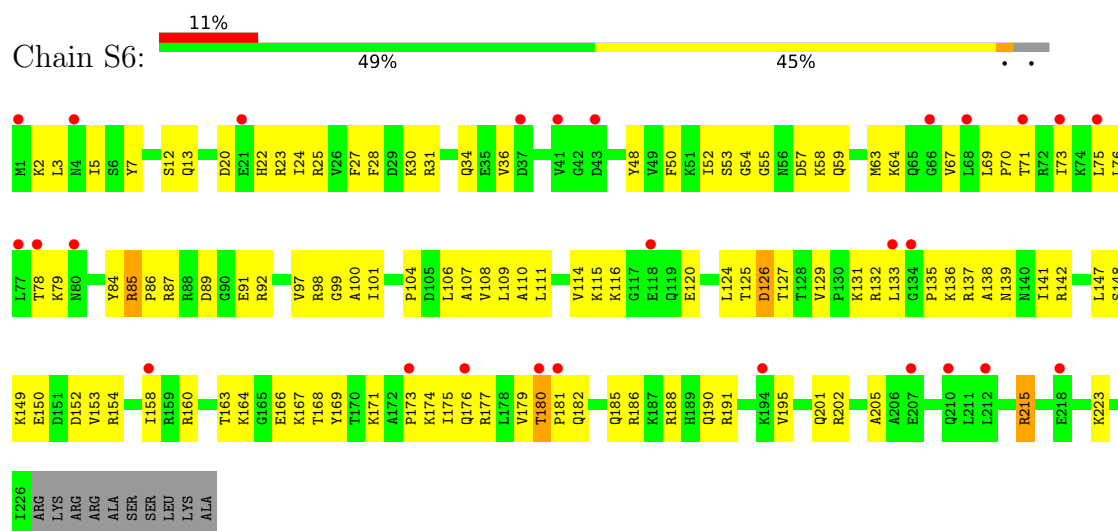


• Molecule 7: 40S ribosomal protein S5

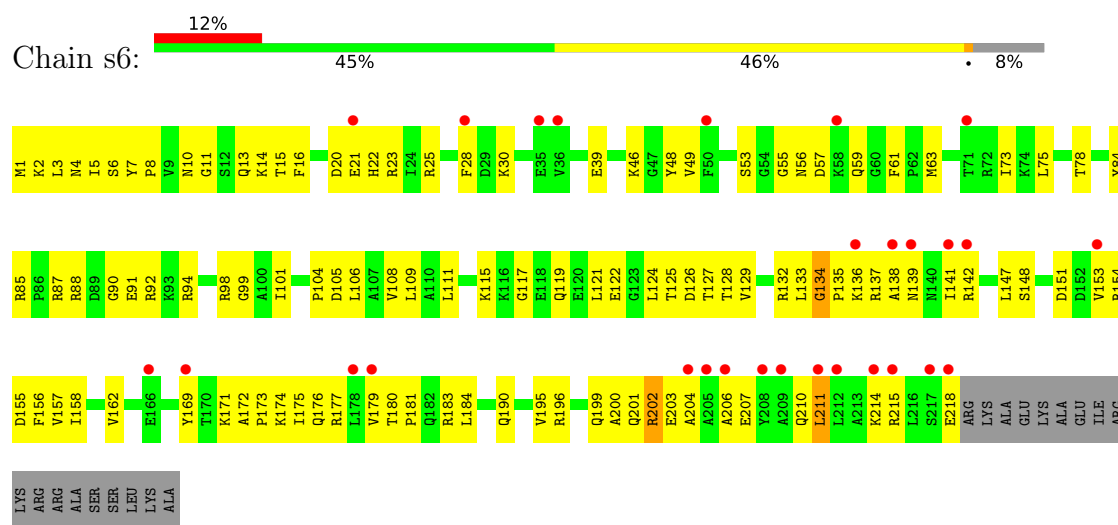




• Molecule 8: 40S ribosomal protein S6-A

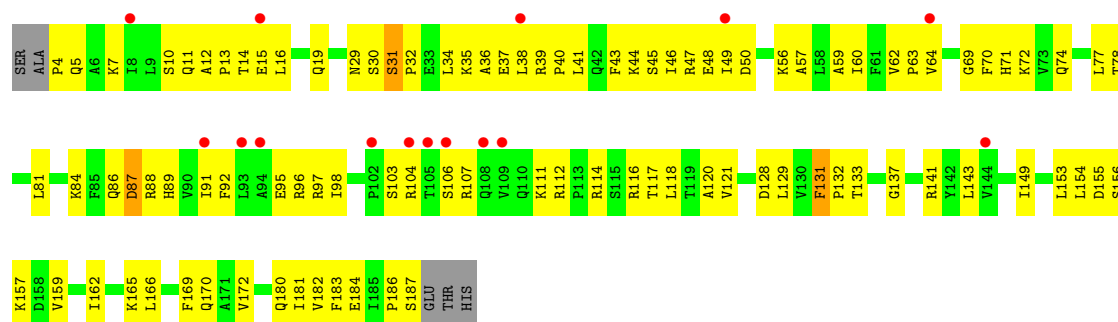


• Molecule 8: 40S ribosomal protein S6-A

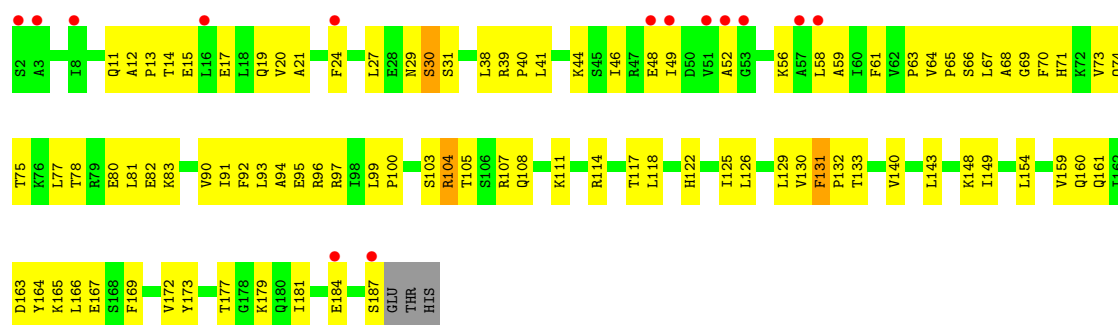


• Molecule 9: 40S ribosomal protein S7-A

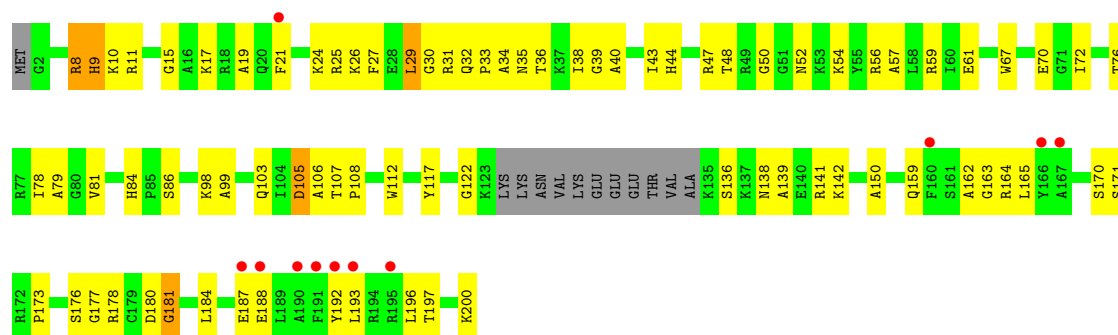




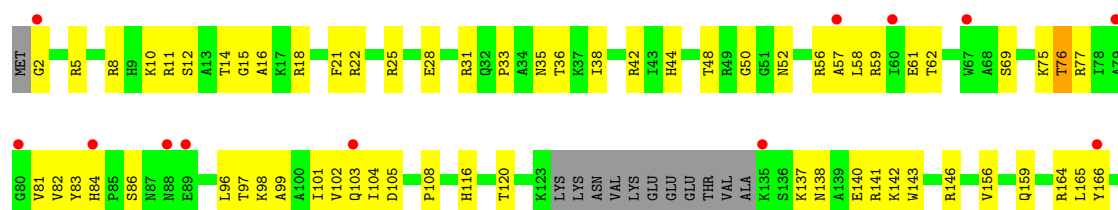
• Molecule 9: 40S ribosomal protein S7-A

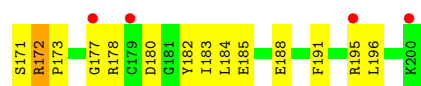


• Molecule 10: 40S ribosomal protein S8-A

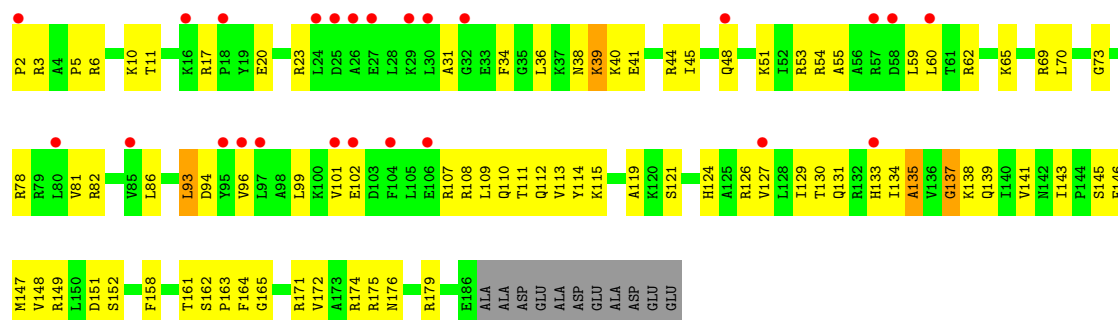


• Molecule 10: 40S ribosomal protein S8-A

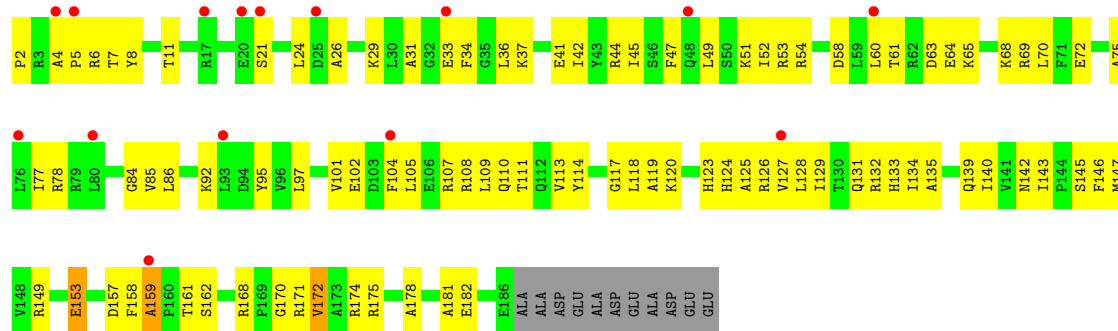




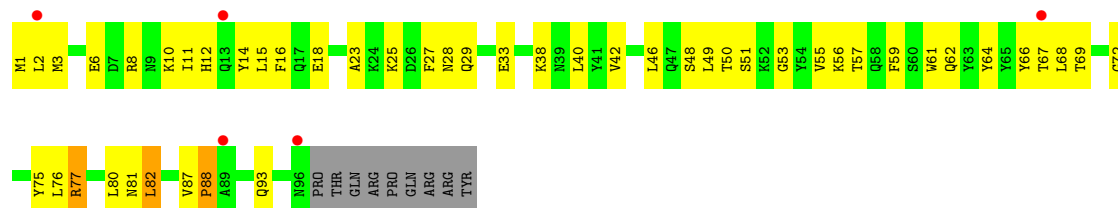
• Molecule 11: 40S ribosomal protein S9-A



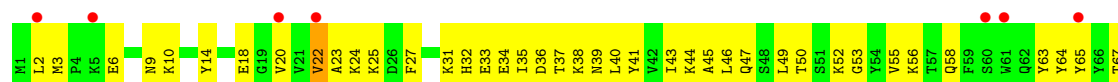
• Molecule 11: 40S ribosomal protein S9-A

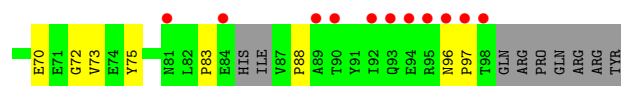


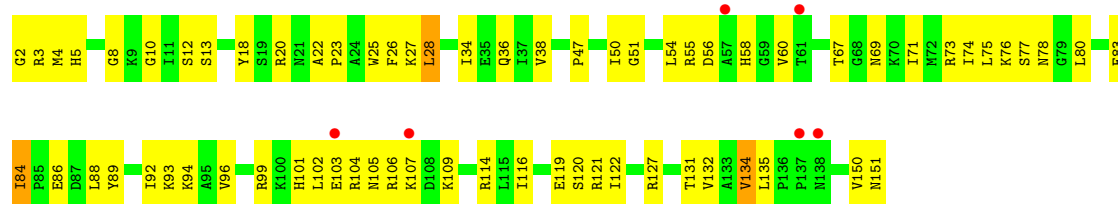
• Molecule 12: 40S ribosomal protein S10-A



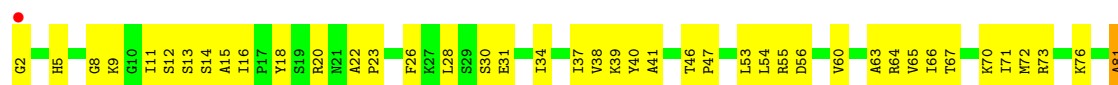
• Molecule 12: 40S ribosomal protein S10-A



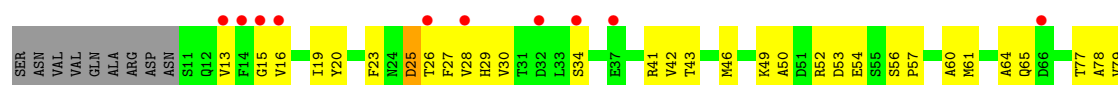




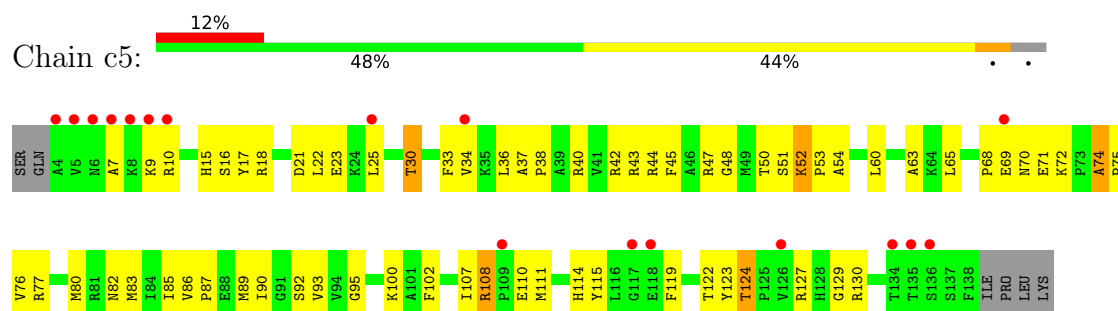
• Molecule 15: 40S ribosomal protein S13



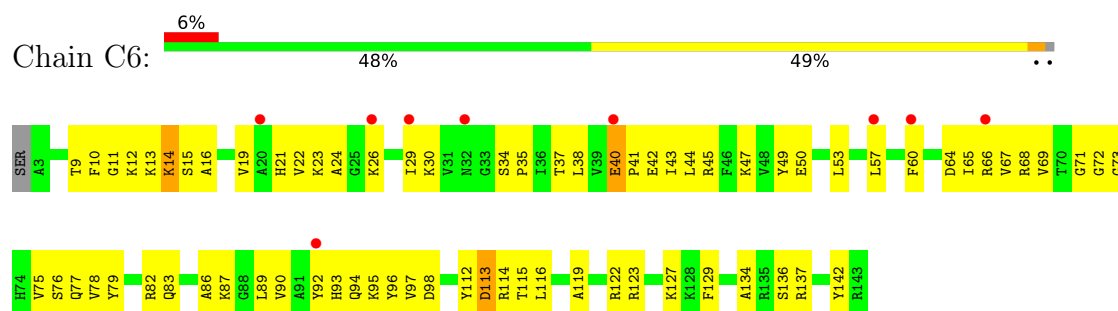
• Molecule 16: 40S ribosomal protein S14-A



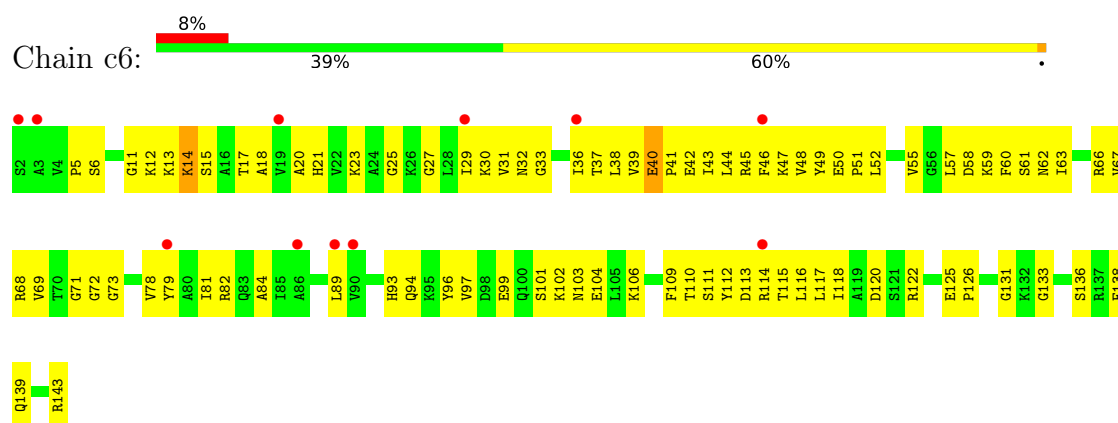
- Molecule 17: 40S ribosomal protein S15



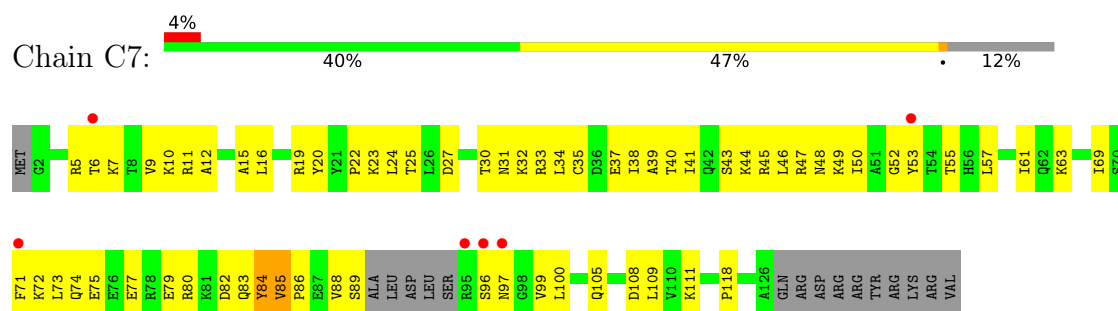
- Molecule 18: 40S ribosomal protein S16-A



- Molecule 18: 40S ribosomal protein S16-A

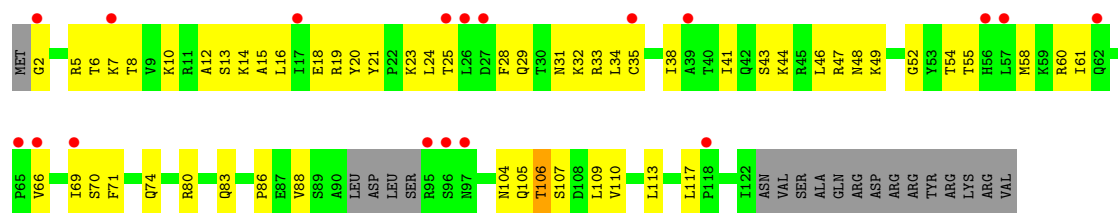


- Molecule 19: 40S ribosomal protein S17-A

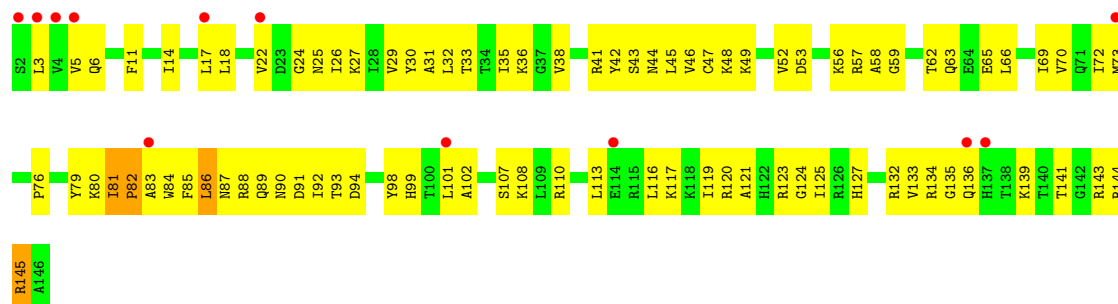


- Molecule 19: 40S ribosomal protein S17-A

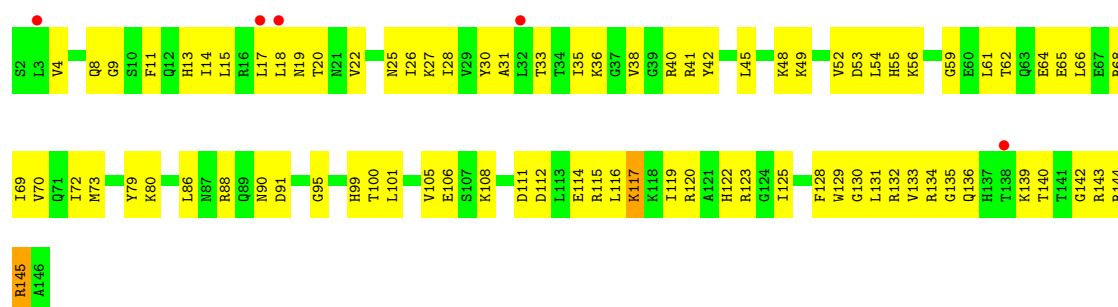




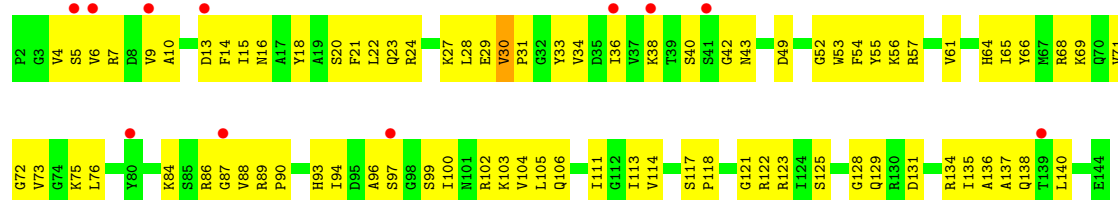
• Molecule 20: 40S ribosomal protein S18-A



• Molecule 20: 40S ribosomal protein S18-A

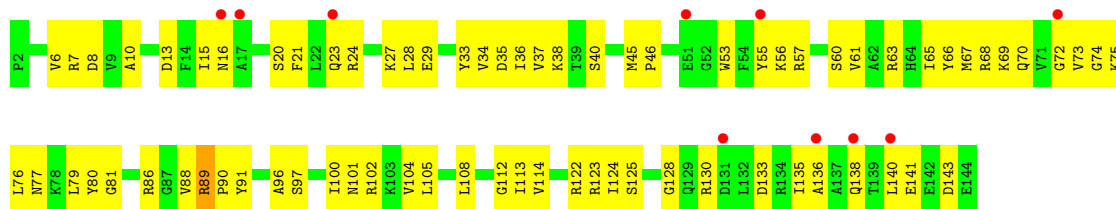


• Molecule 21: 40S ribosomal protein S19-A

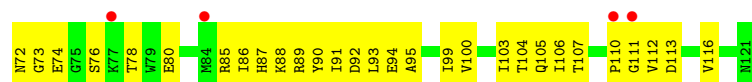
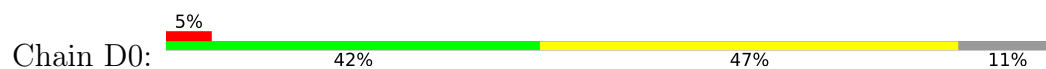


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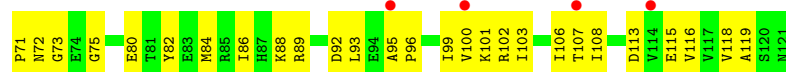
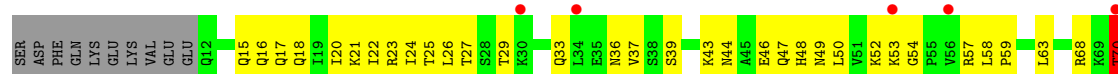
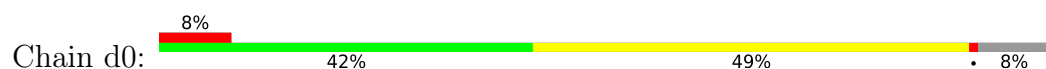




• Molecule 22: 40S ribosomal protein S20



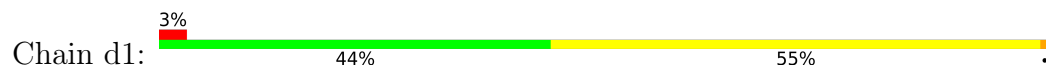
• Molecule 22: 40S ribosomal protein S20



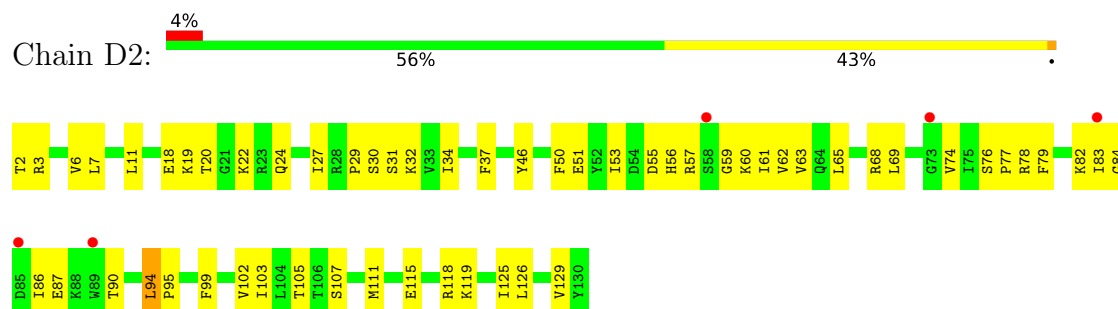
• Molecule 23: 40S ribosomal protein S21-A



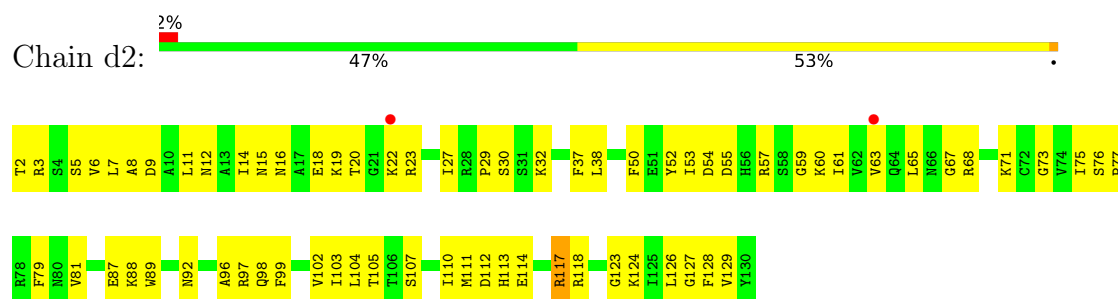
• Molecule 23: 40S ribosomal protein S21-A



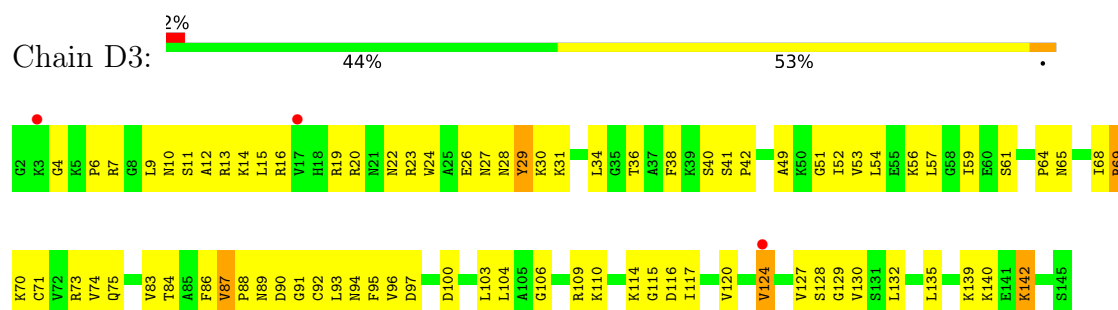
- Molecule 24: 40S ribosomal protein S22-A



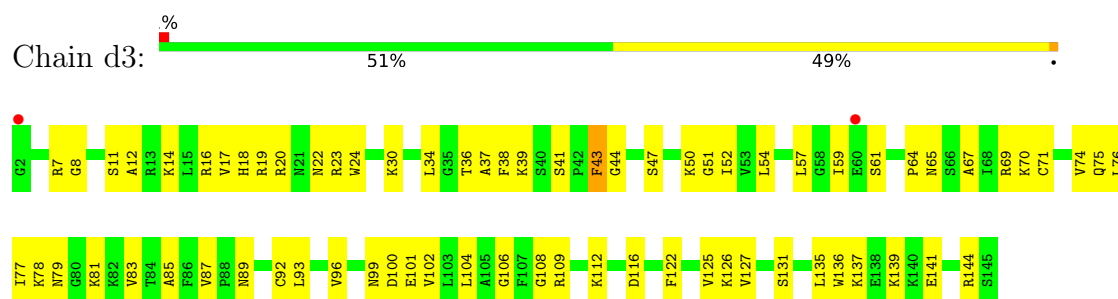
- Molecule 24: 40S ribosomal protein S22-A



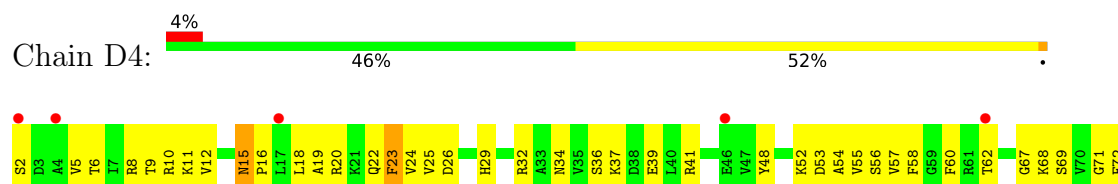
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 25: 40S ribosomal protein S23-A

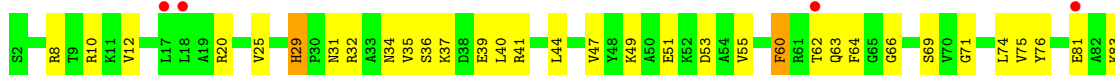


- Molecule 26: 40S ribosomal protein S24-A

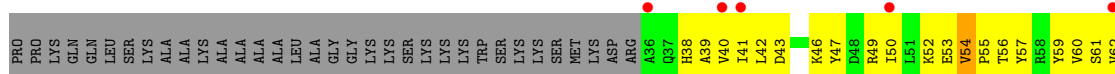
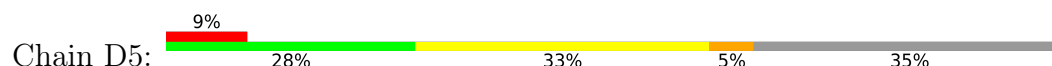




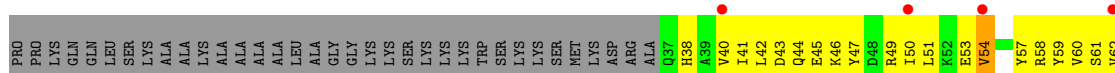
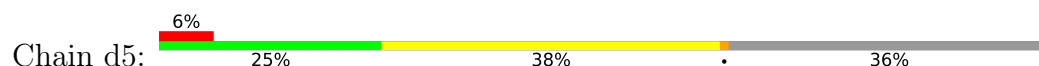
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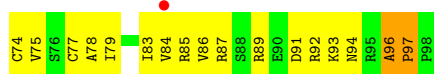
• Molecule 27: 40S ribosomal protein S25-A



• Molecule 27: 40S ribosomal protein S25-A

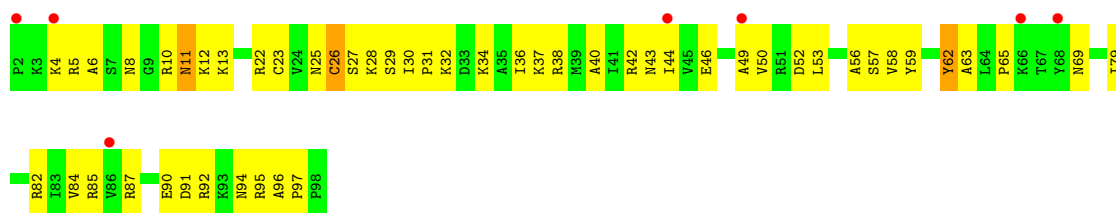


• Molecule 28: 40S ribosomal protein S26-B

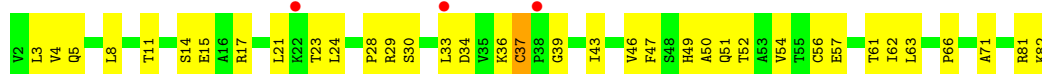


• Molecule 28: 40S ribosomal protein S26-B





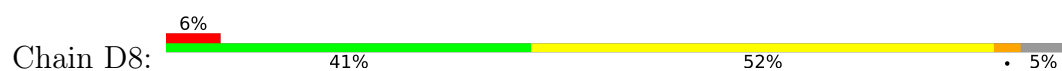
- Molecule 29: 40S ribosomal protein S27-A



- Molecule 29: 40S ribosomal protein S27-A



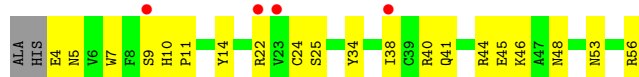
- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A



- Molecule 31: 40S ribosomal protein S29-A

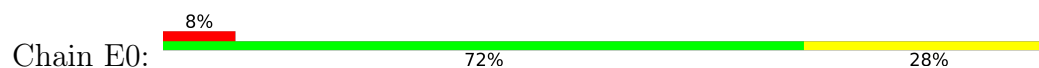


- Molecule 31: 40S ribosomal protein S29-A

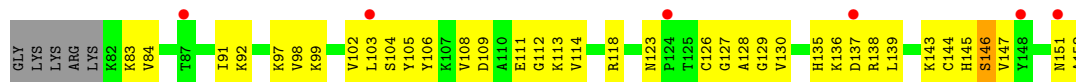




- Molecule 32: 40S ribosomal protein S30-A



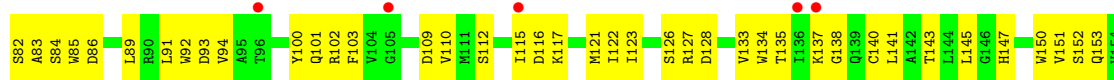
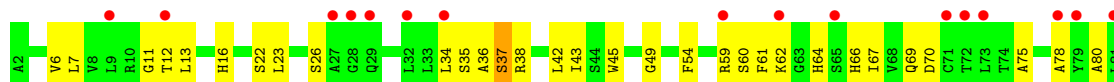
- Molecule 33: Ubiquitin-40S ribosomal protein S31



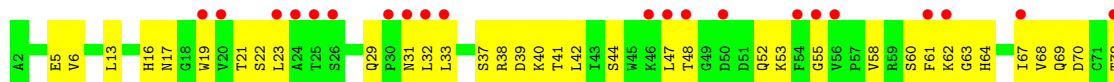
- Molecule 33: Ubiquitin-40S ribosomal protein S31

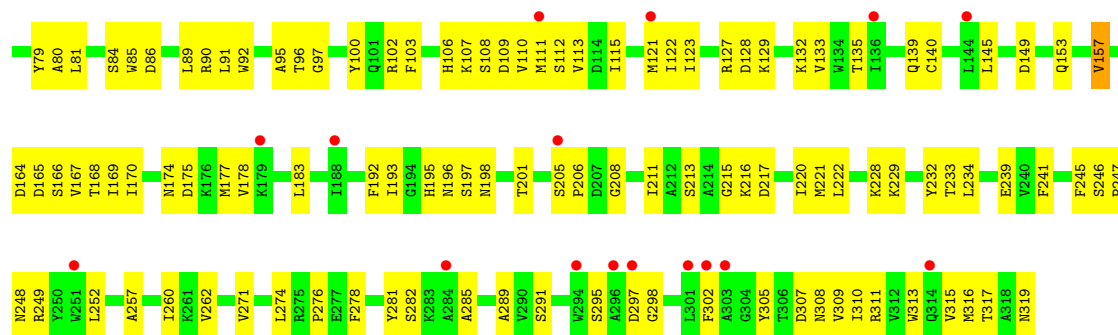


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

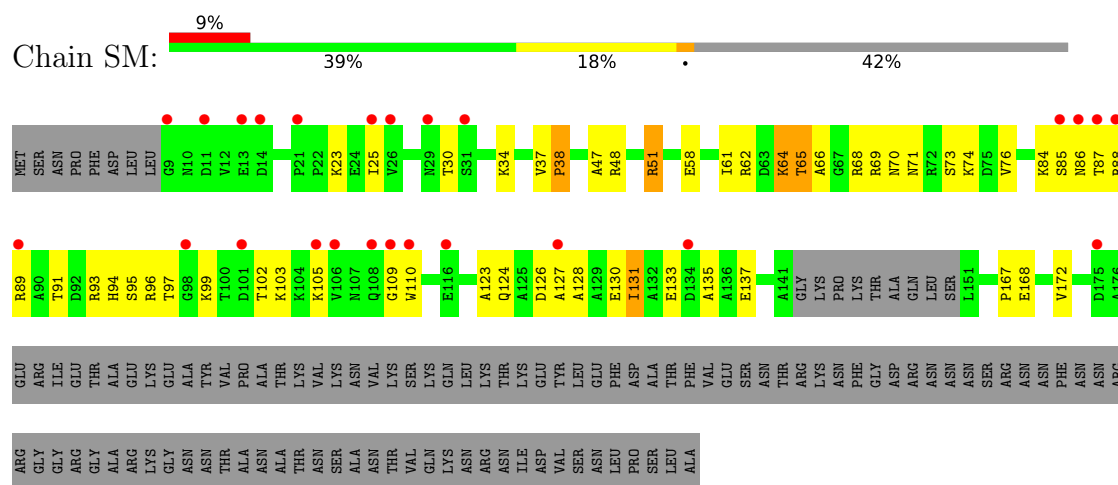


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

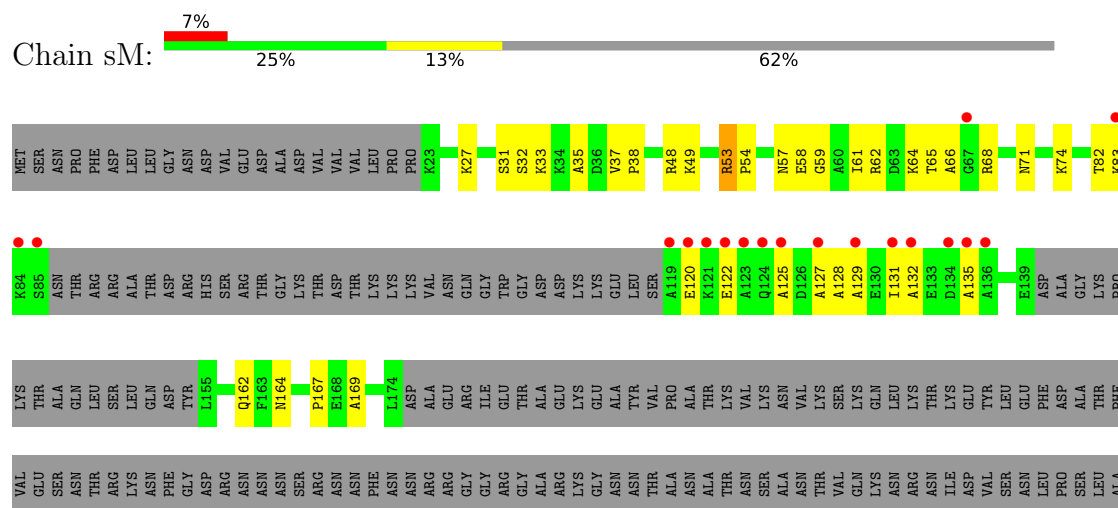




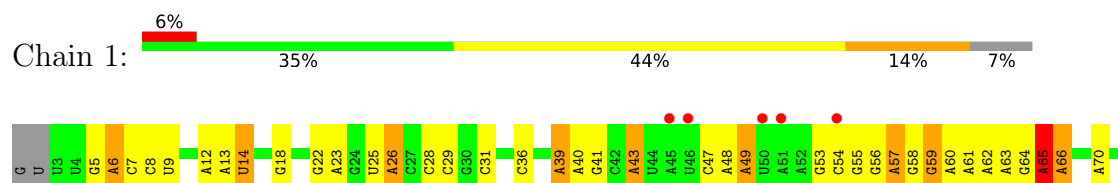
• Molecule 35: Suppressor protein STM1



• Molecule 35: Suppressor protein STM1



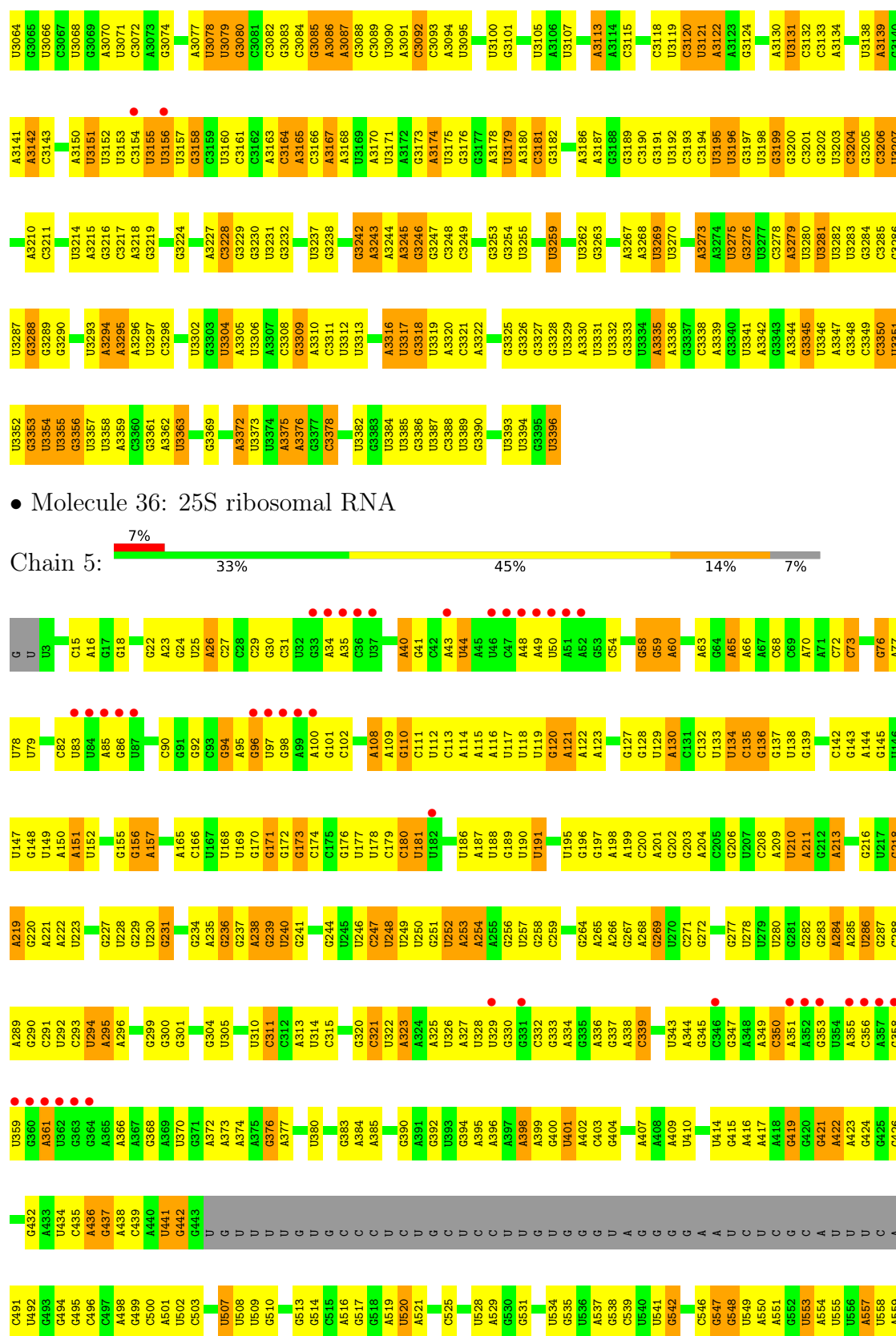
• Molecule 36: 25S ribosomal RNA

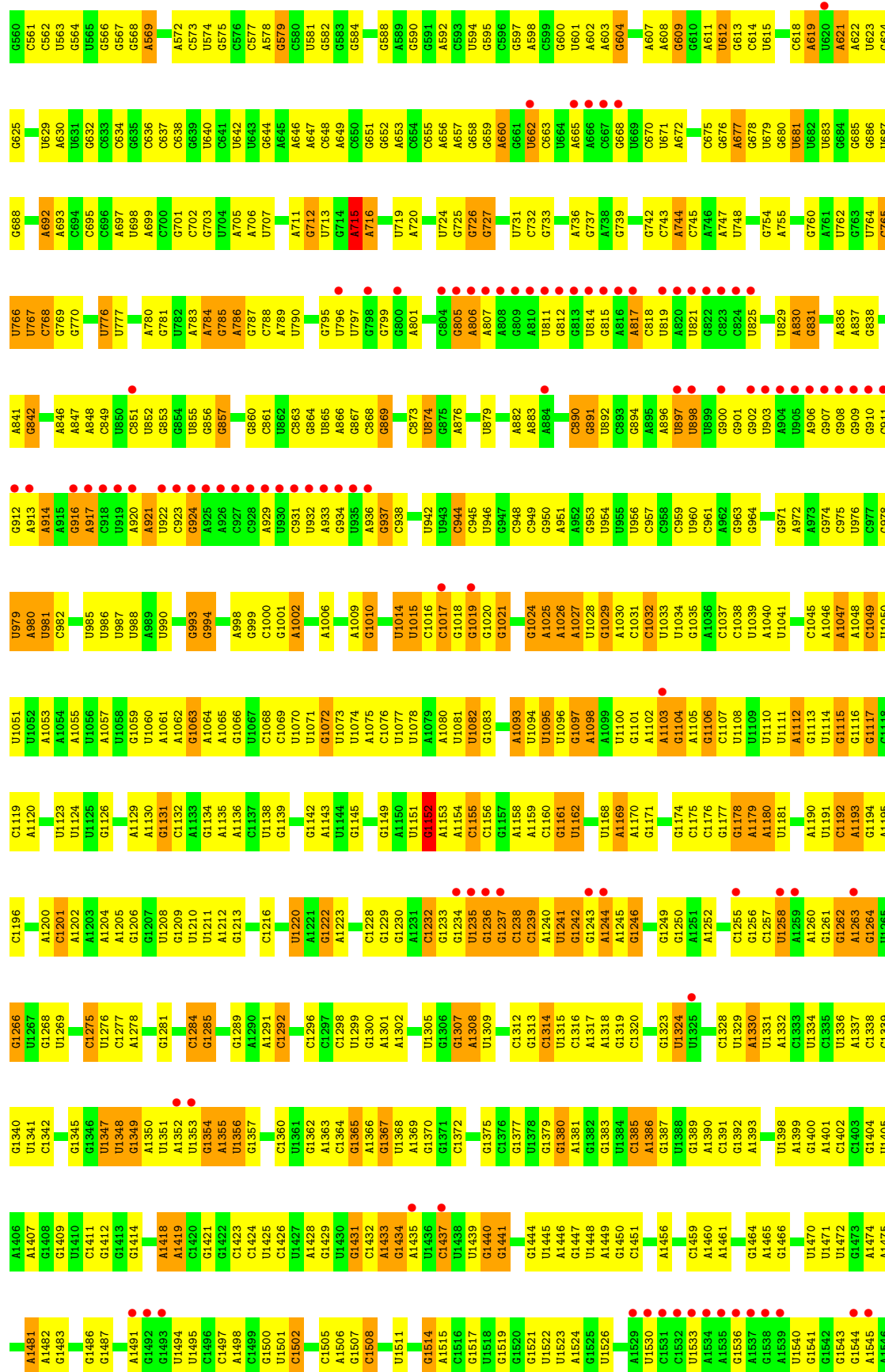




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U	A1244	A1317	A1381	A1452	G1513	C1578	A1643	U1717	G1789	C1856	C1943	C	U
U	A1245	A1318	G1382	A1453	G1514	C1579	C1644	G1718	U1790	C1857	U1944	C	G
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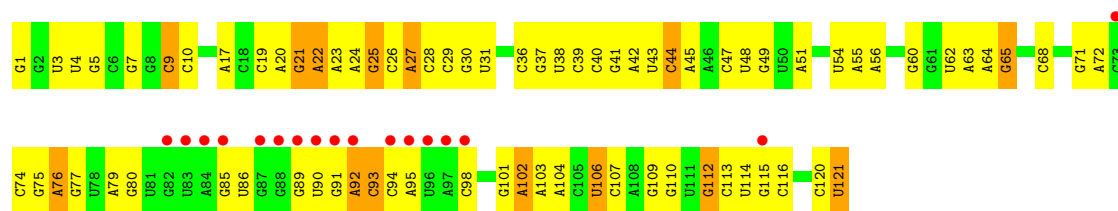
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C2852	U2924	C2852	C2774	U2631	U2553	U	A2423	C2361	U2282	A2219	A2147
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	A2991	U2843	U2767	A2695	C2622	C	C	U2417	U2274	U2274	A2213
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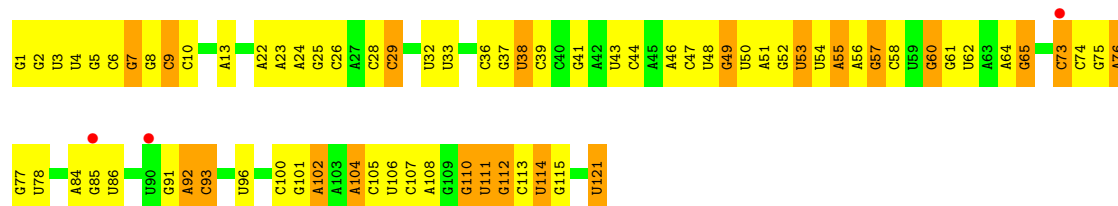




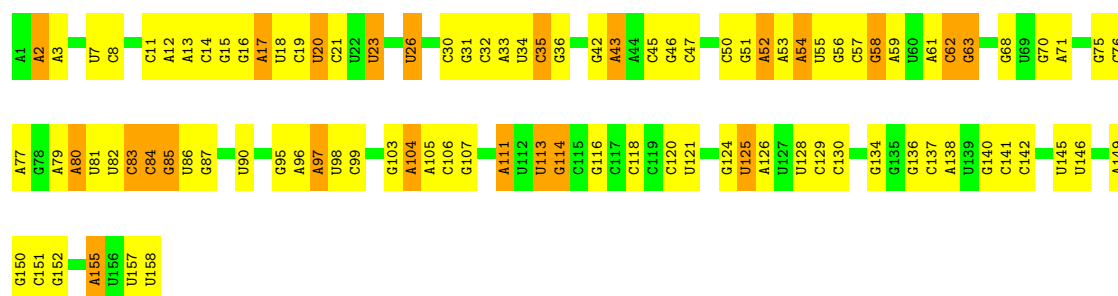




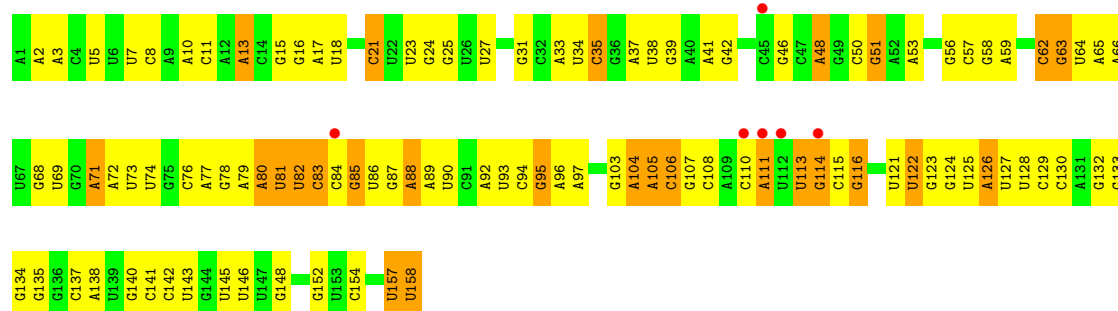
● Molecule 37: 5S ribosomal RNA



● Molecule 38: 5.8S ribosomal RNA

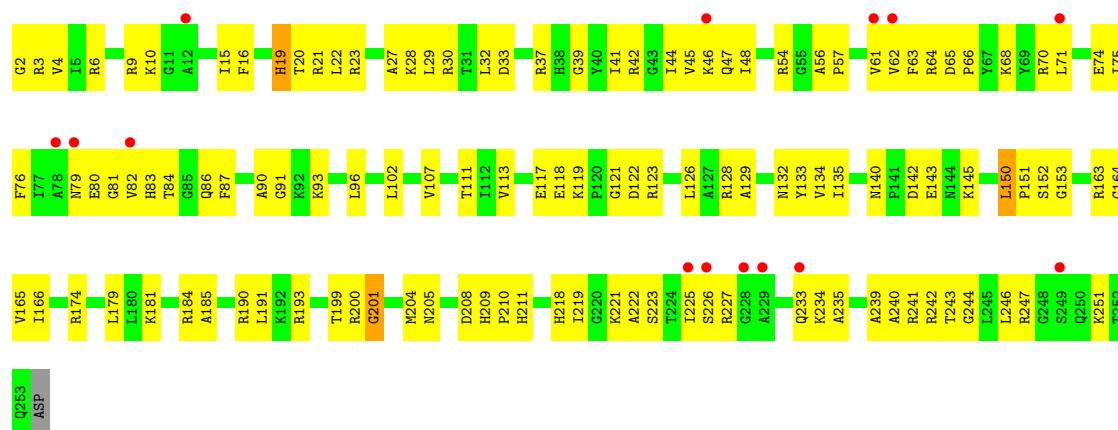


● Molecule 38: 5.8S ribosomal RNA

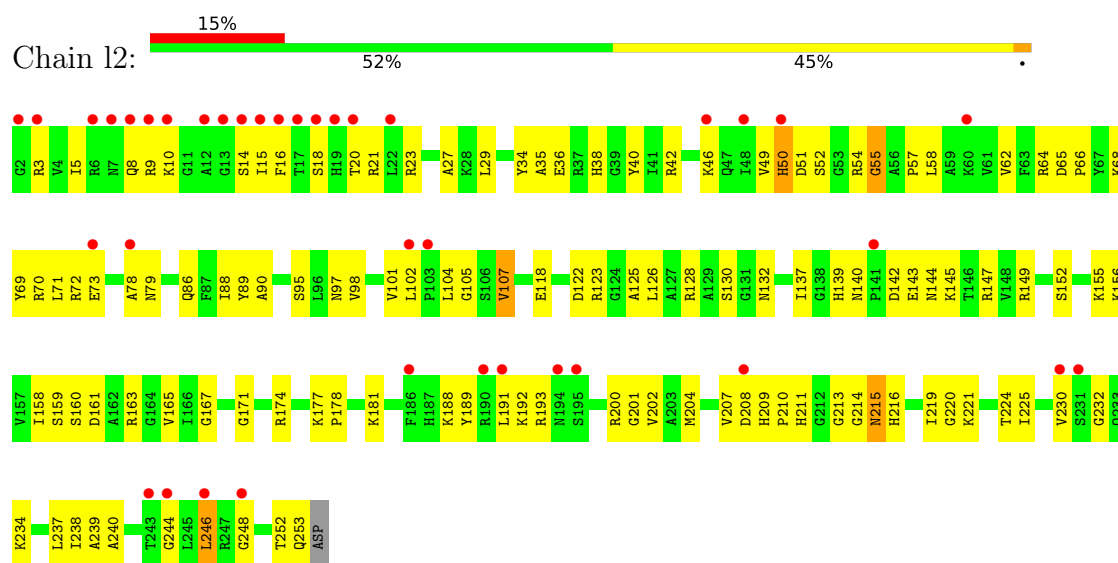


● Molecule 39: 60S ribosomal protein L2-A

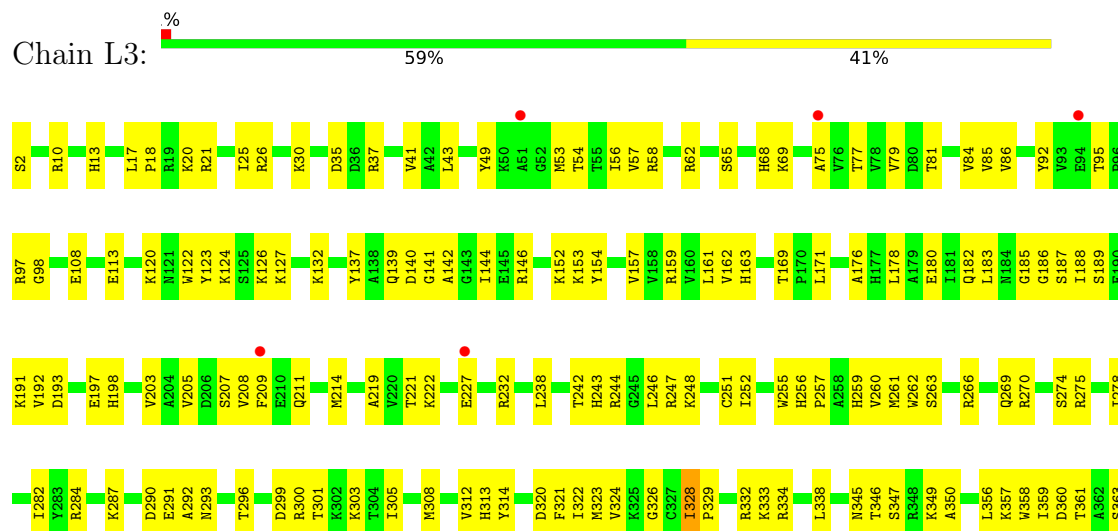




• Molecule 39: 60S ribosomal protein L2-A

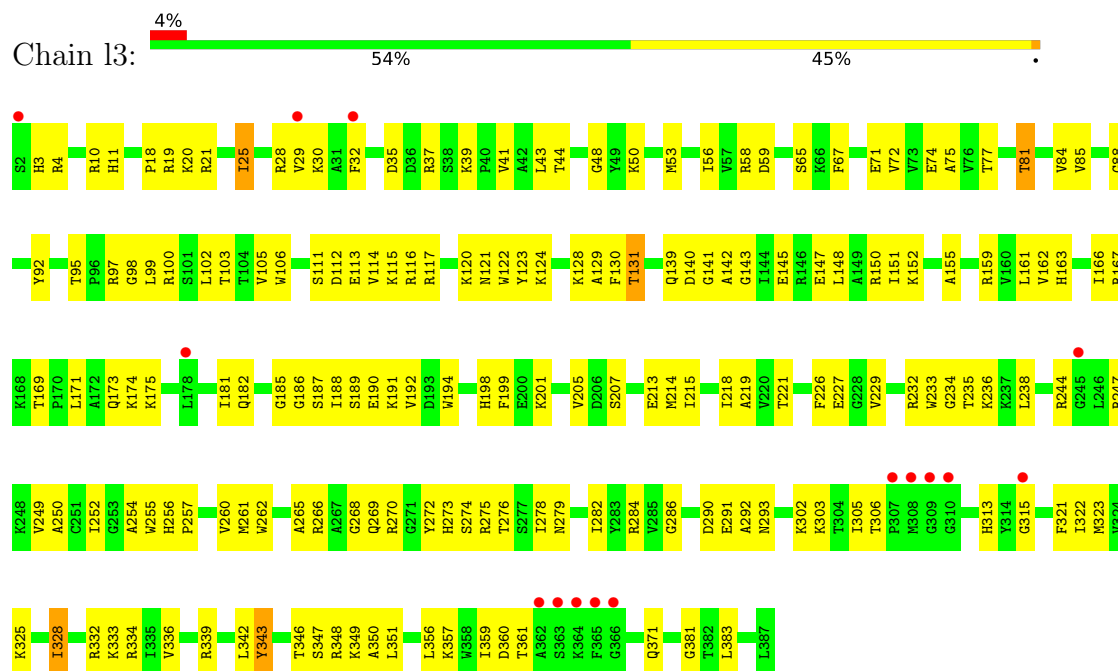


• Molecule 40: 60S ribosomal protein L3

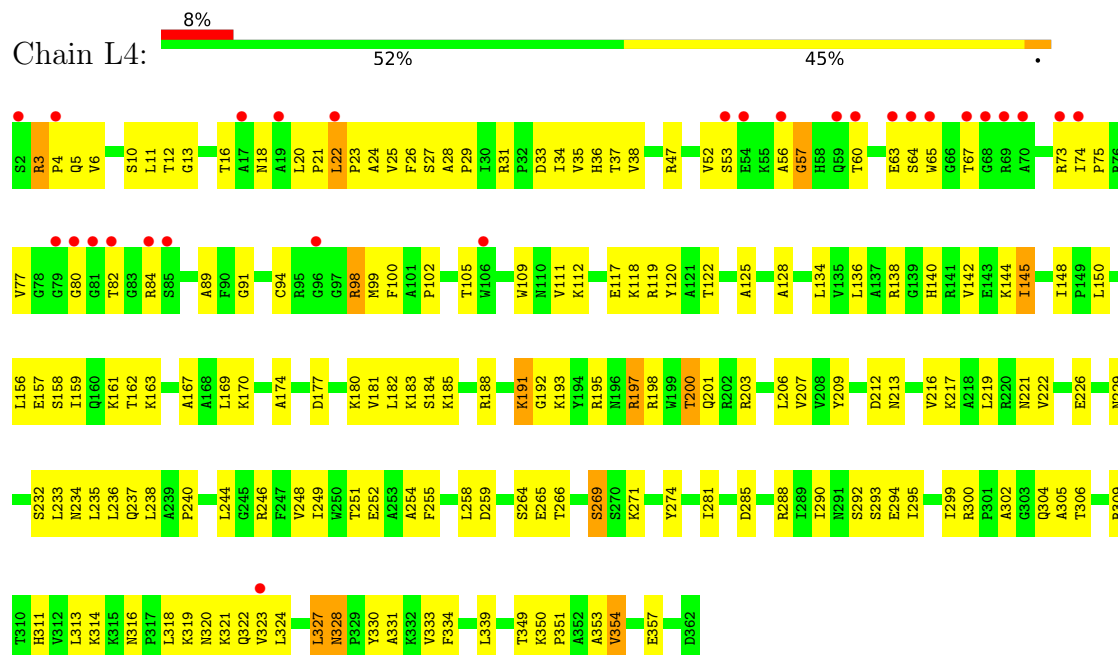




• Molecule 40: 60S ribosomal protein L3

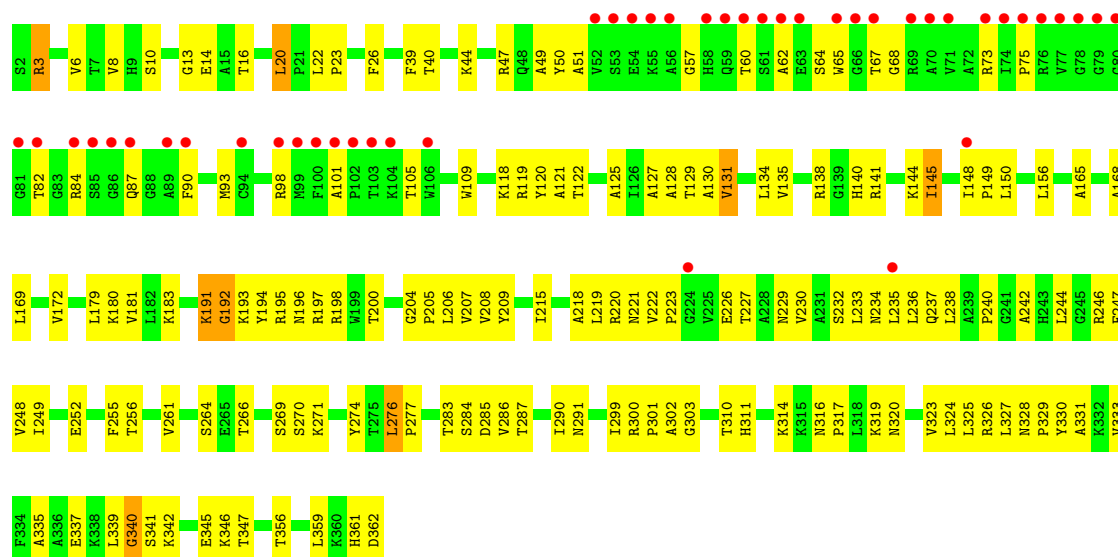


• Molecule 41: 60S ribosomal protein L4-A

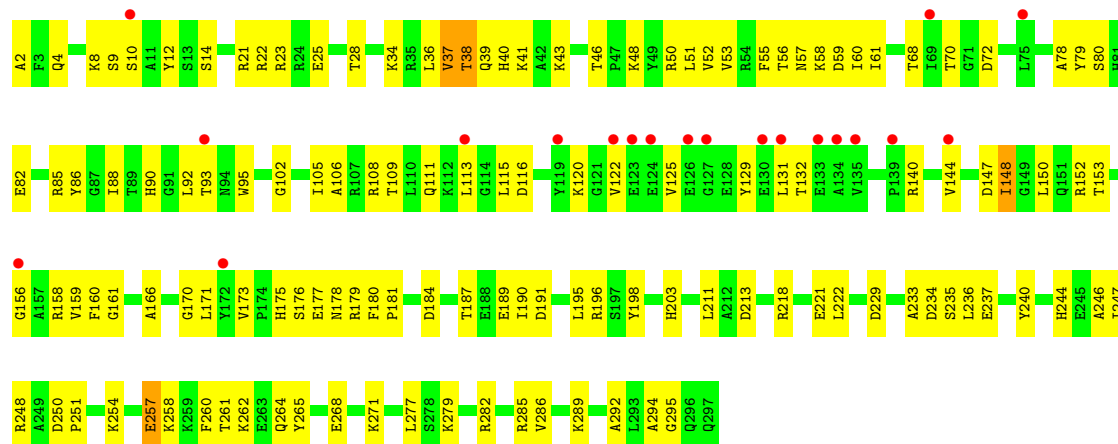


• Molecule 41: 60S ribosomal protein L4-A

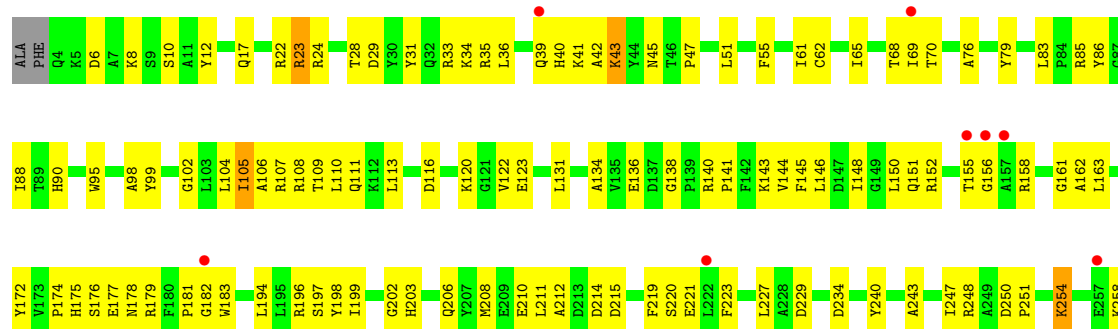




• Molecule 42: 60S ribosomal protein L5

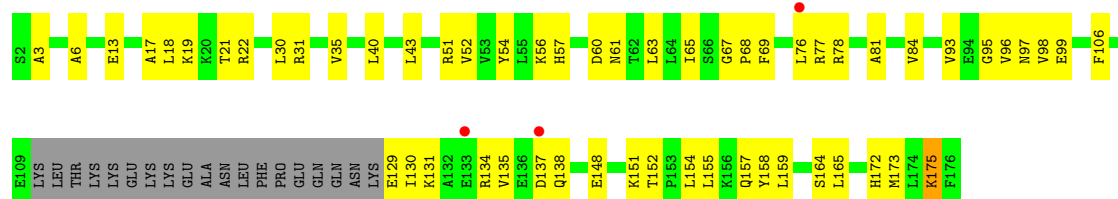


• Molecule 42: 60S ribosomal protein L5

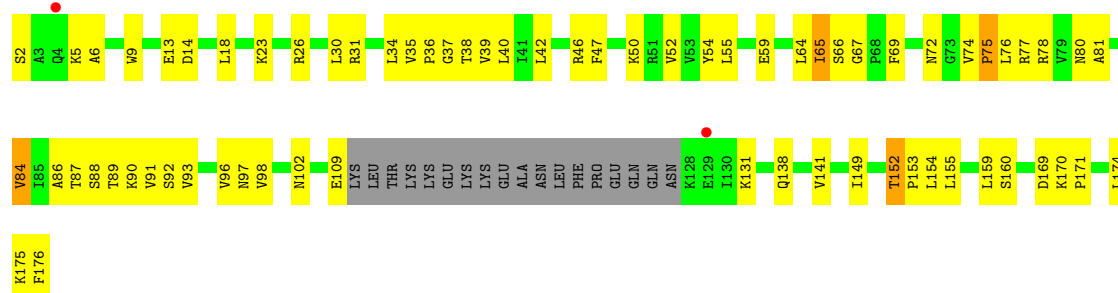




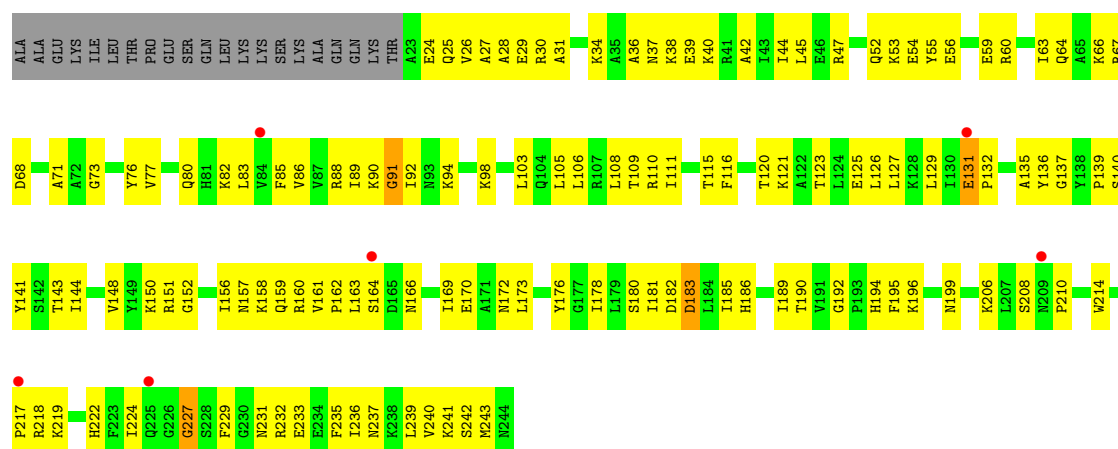
• Molecule 43: 60S ribosomal protein L6-A



• Molecule 43: 60S ribosomal protein L6-A

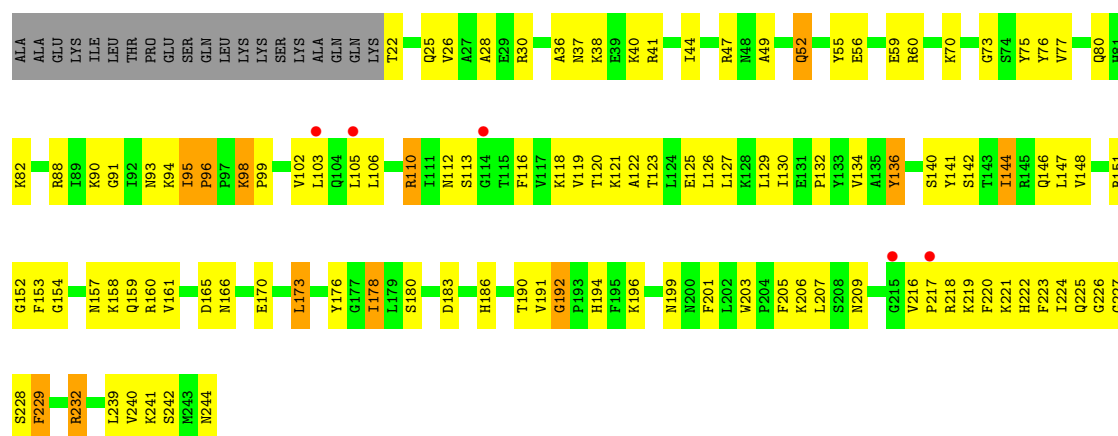


• Molecule 44: 60S ribosomal protein L7-A

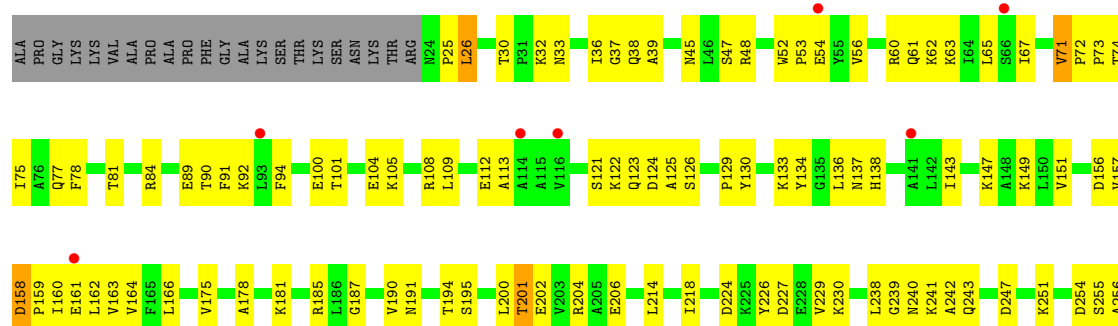


• Molecule 44: 60S ribosomal protein L7-A

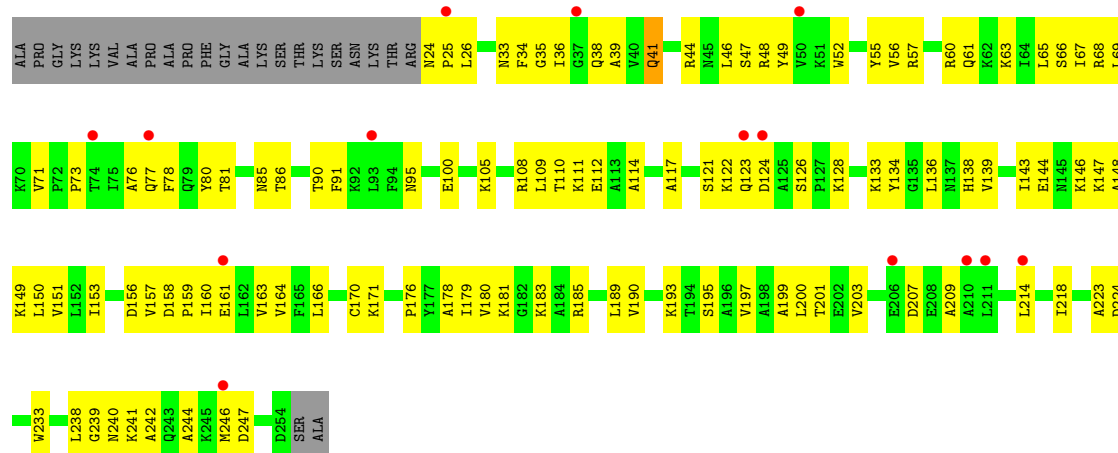




• Molecule 45: 60S ribosomal protein L8-A

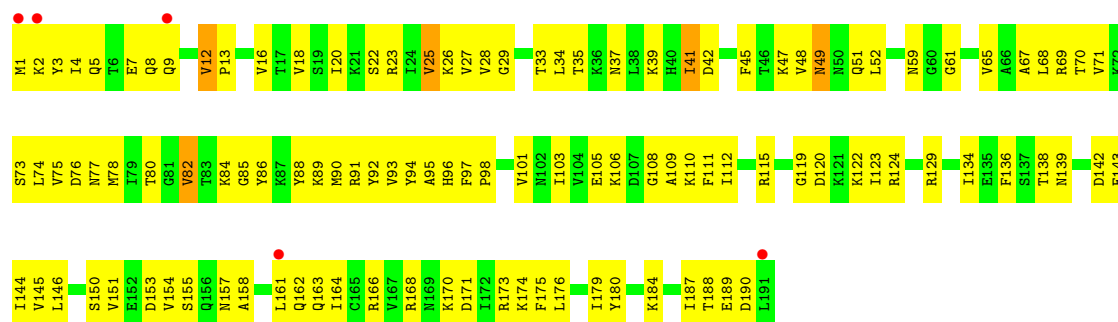


• Molecule 45: 60S ribosomal protein L8-A

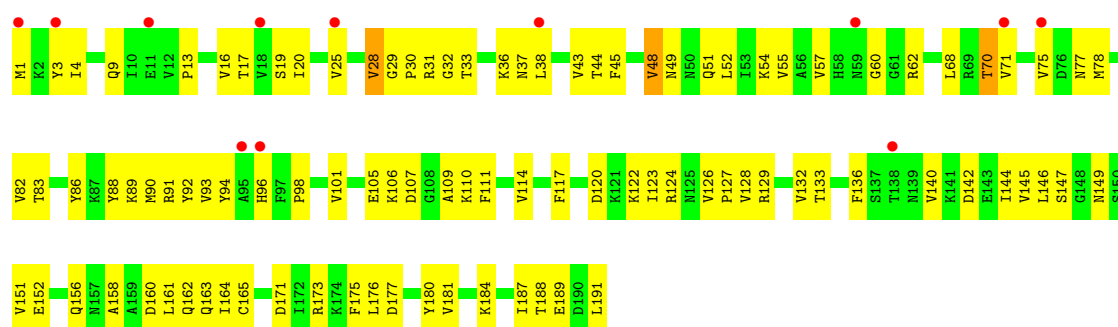


• Molecule 46: 60S ribosomal protein L9-A

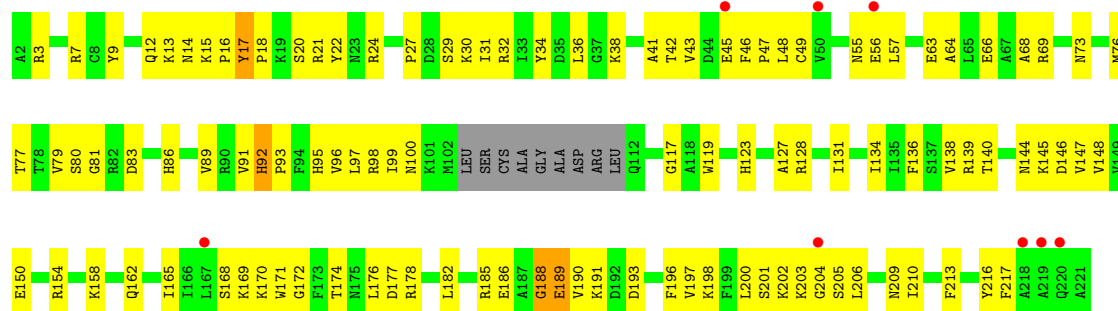




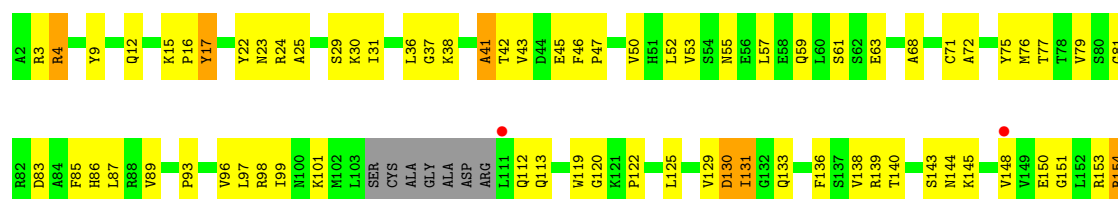
• Molecule 46: 60S ribosomal protein L9-A



• Molecule 47: 60S ribosomal protein L10



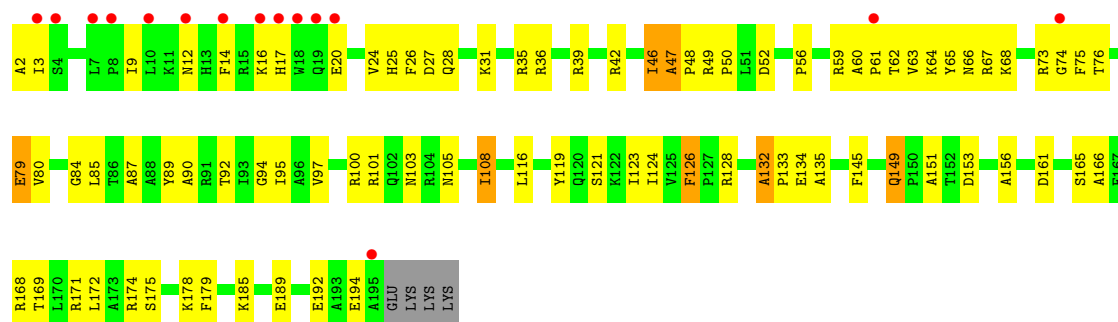
• Molecule 47: 60S ribosomal protein L10



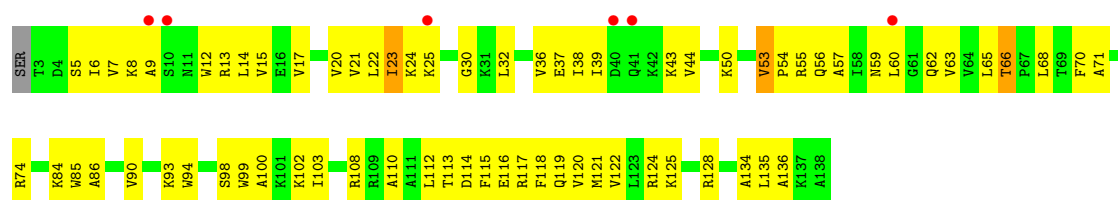


• Molecule 48: 60S ribosomal protein L11-B

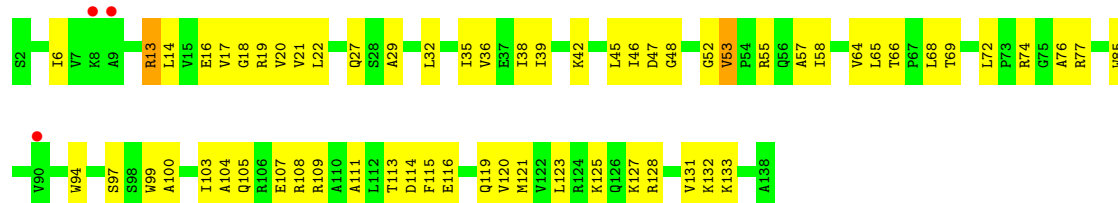




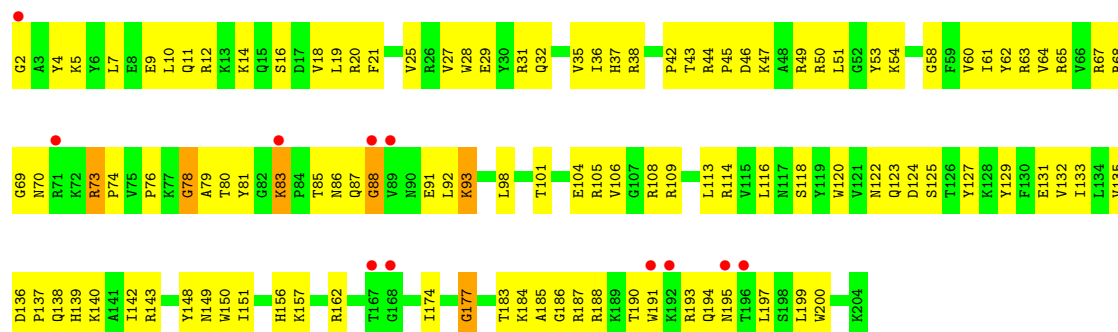
• Molecule 50: 60S ribosomal protein L14-A



• Molecule 50: 60S ribosomal protein L14-A

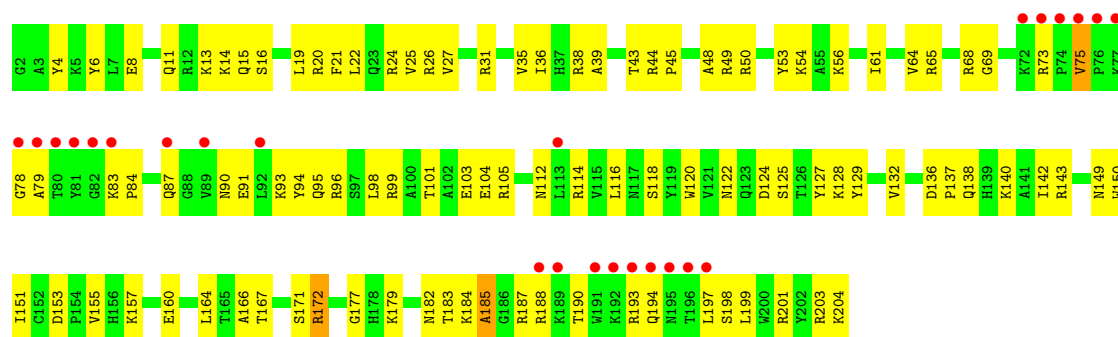


• Molecule 51: 60S ribosomal protein L15-A

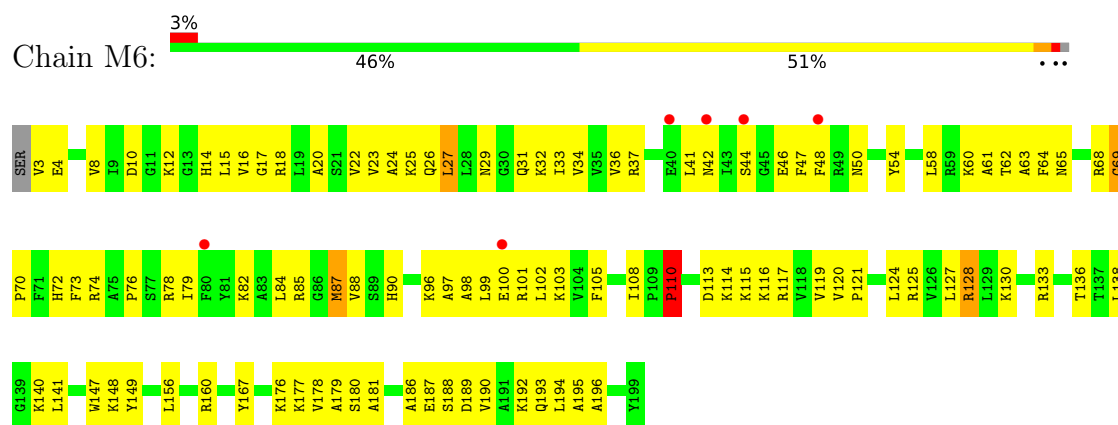


• Molecule 51: 60S ribosomal protein L15-A

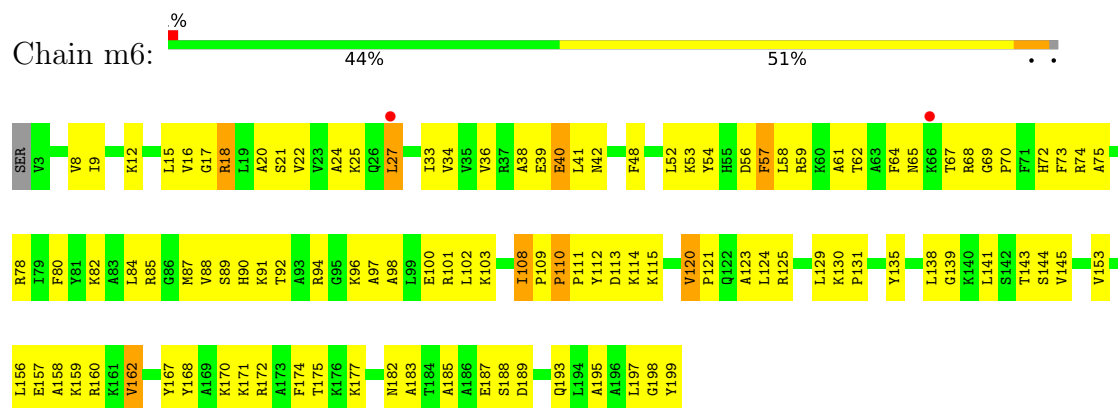




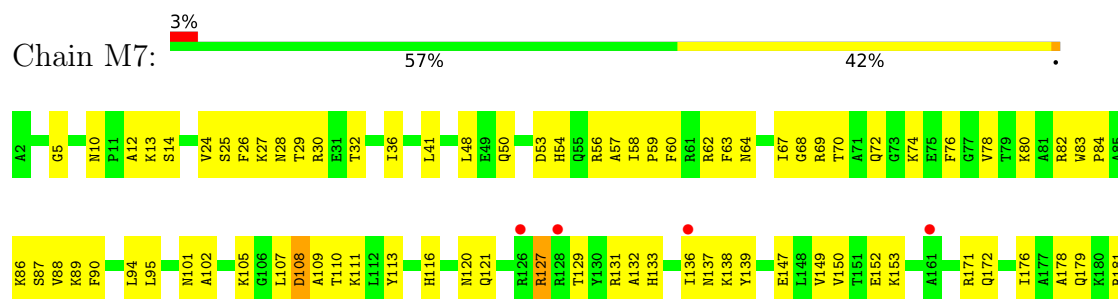
• Molecule 52: 60S ribosomal protein L16-A



• Molecule 52: 60S ribosomal protein L16-A

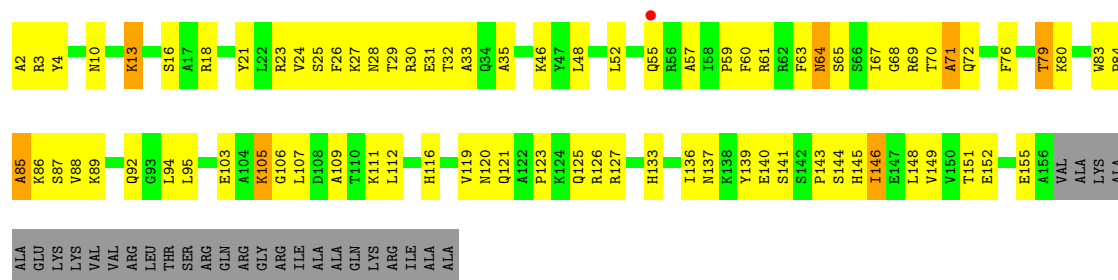
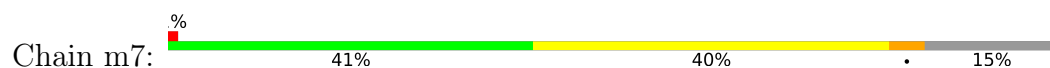


• Molecule 53: 60S ribosomal protein L17-A

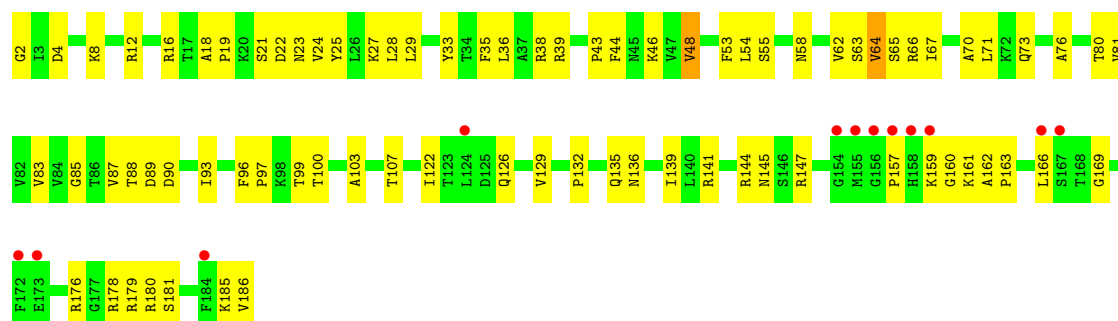




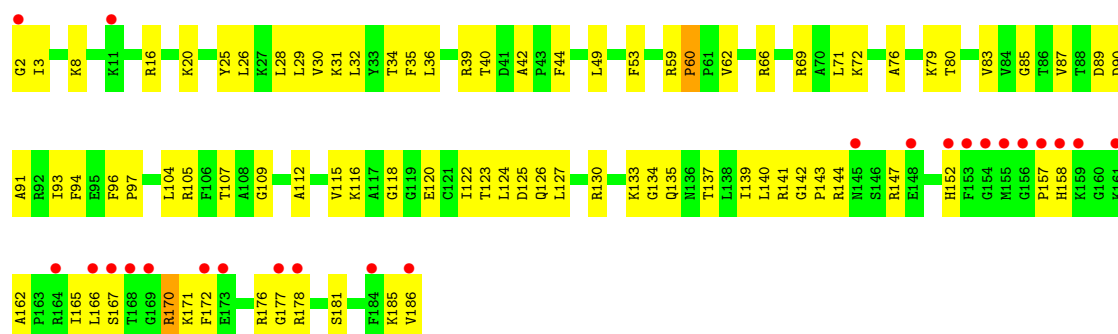
• Molecule 53: 60S ribosomal protein L17-A



• Molecule 54: 60S ribosomal protein L18-A

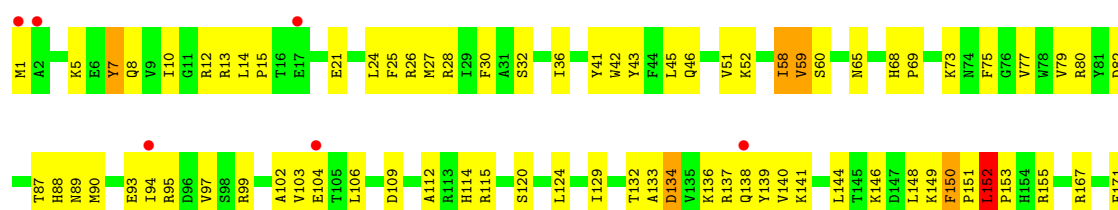


• Molecule 54: 60S ribosomal protein L18-A



• Molecule 55: 60S ribosomal protein L19-A





Y172

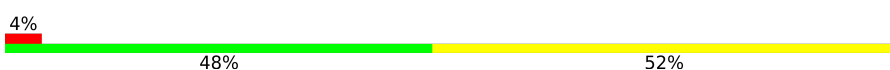
- Molecule 57: 60S ribosomal protein L21-A

Chain N1: 

G2 K3 S4 Y7 R8 T11 R12 Q103 Y13 F105 M14 R17 D18 F19 H22 G23 L27 Y30 L31 D38 N45 G46 S47 L48 Q49 R50 G51 H54 K55 F56 Y57 V64 V65 K69 G73 V74 L75 L76 N77 K78 M79 R83 Y84 L85 S86 K87 R88 L89 N90

L91 R92 V93 E94 I96 R102 Q103 E104 F105 L106 V109 K110 A111 N112 K115 R116 A121 V126 Q127 L128 Q131 P132 A133 Q134 P135 R136 R139 T143 Q149 T150 L151 A152 P153 V154 P155 Y156 F159 I160

- Molecule 57: 60S ribosomal protein L21-A

Chain n1: 

G2 Y7 R8 R12 Y13 F15 Q16 R17 D18 F19 H22 L27 S28 T29 Y30 K32 V33 Y34 D38 L39 V40 D41 N45 G46 S47 T49 Q49 K50 M52 P53 H54 K55 Q58 T61 G62 V63 V64 V67 T68 K69 S70 S71 V72 L75 L76 M79

V80 G81 R82 R83 Y84 S86 K87 R88 L89 N90 R92 H95 I96 K97 H98 S99 K100 C101 R102 Q103 V104 F105 L106 L107 R108 V109 K110 A111 N112 Q122 G123 V124 A125 Y126 Q127 L128 K129 R130 Q131 P132 A133 Q134 P135 R136 R139 T143 V147 P148 Q149 V154 P155 Y156

E157 T158 F159 I160

- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 

ALA PRO ASN THR SER ARG LYS Q9 Q10 I11 V17 S20 S21 P22 T23 V27 F28 D29 P30 A31 S32 S33 I41 K42 V43 N49 L50 G51 N52 A53 V54 T55 V56 D59 G60 T61 V62 V63 V64 V65 T68 A69 K70 F71 S72 L79 T80 K81 K82 Y83 L84 K85

K86 L89 R90 D91 SER Y92 I93 R94 F95 V96 S97 T98 K99 E102 D18 Y103 S20 R104 L105 A106 F107 Y108 G109 VAL THR PRO GLU GLU ASP ASP GLU

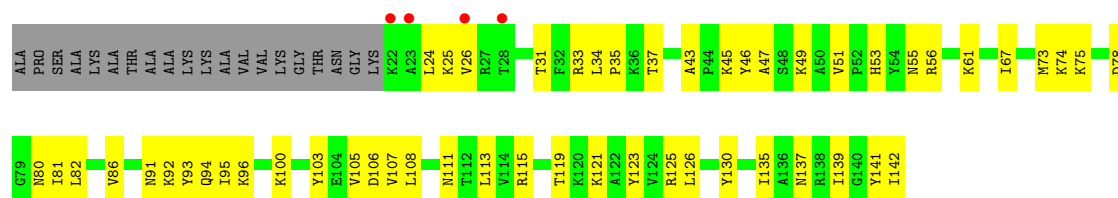
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 

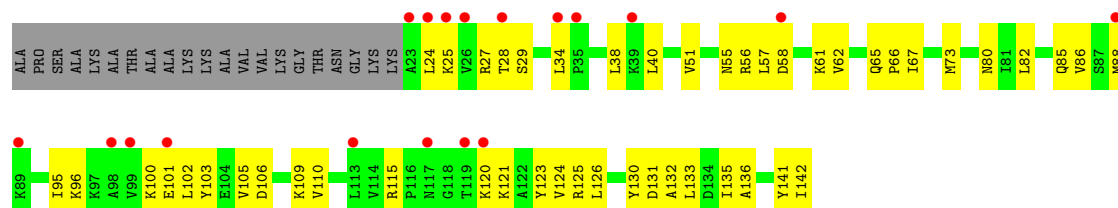
ALA PRO ASN THR SER ARG LYS I11 F15 T16 V17 D18 V19 P22 S21 S22 T23 E24 V27 F28 Y33 A34 K35 D39 K42 A46 N49 L50 G51 R52 T55 V56 T57 E58 D59 V63 T64 V65 F71 K77 K81 K82 N87 Q88 L89

R90 D91 I93 R94 F95 V96 N101 E102 Y103 R104 F107 Y108 VAL THR P22 Q23 GLU ASP GLU GLU ASP GLU ASP GLU

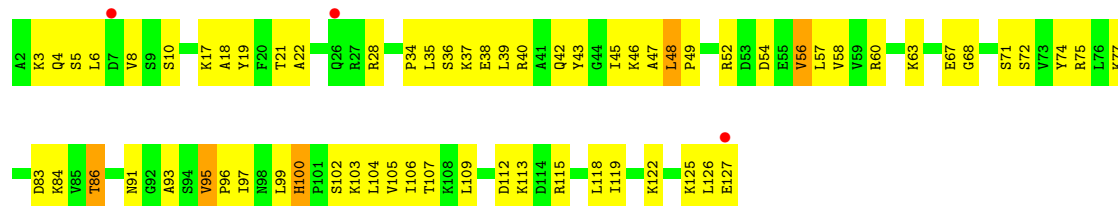
- Molecule 59: 60S ribosomal protein L23-A



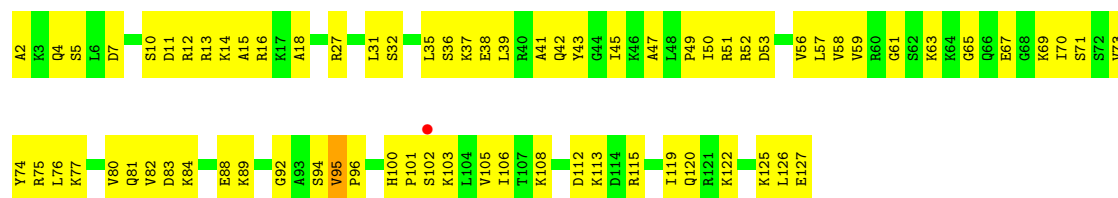
• Molecule 61: 60S ribosomal protein L25



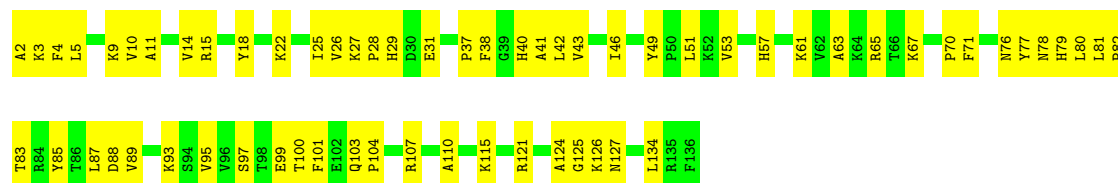
• Molecule 62: 60S ribosomal protein L26-A



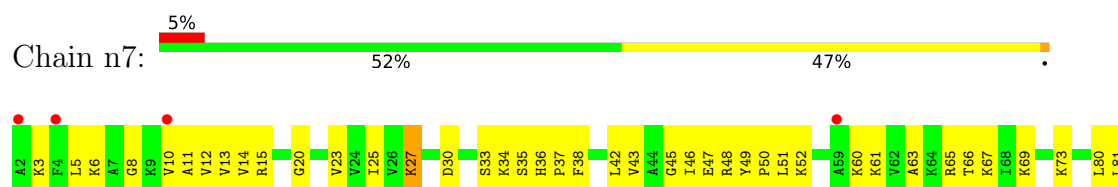
• Molecule 62: 60S ribosomal protein L26-A



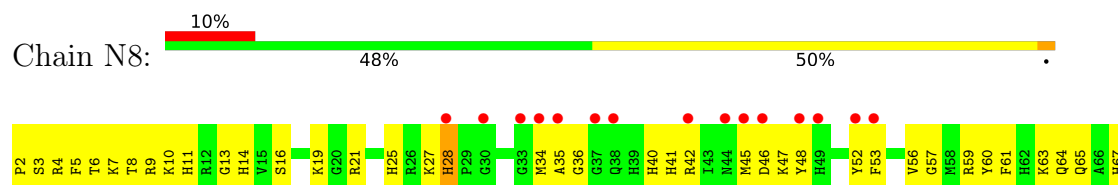
• Molecule 63: 60S ribosomal protein L27-A



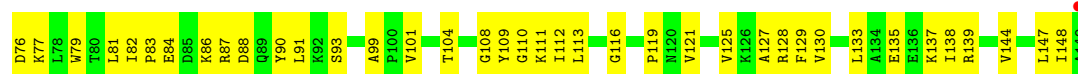
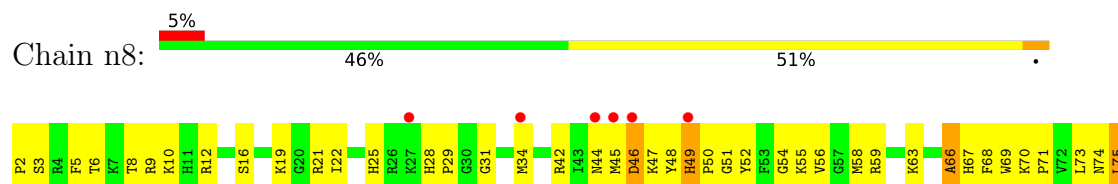
• Molecule 63: 60S ribosomal protein L27-A



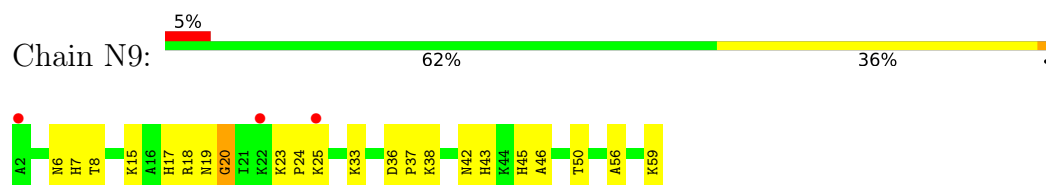
• Molecule 64: 60S ribosomal protein L28



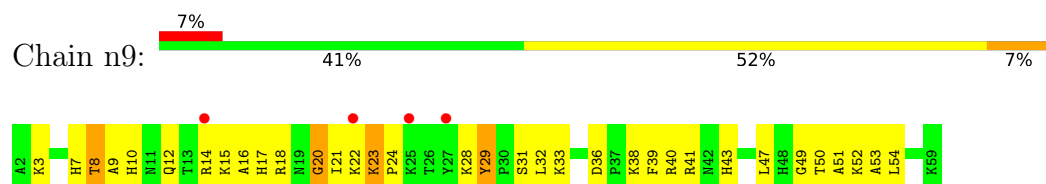
• Molecule 64: 60S ribosomal protein L28



• Molecule 65: 60S ribosomal protein L29

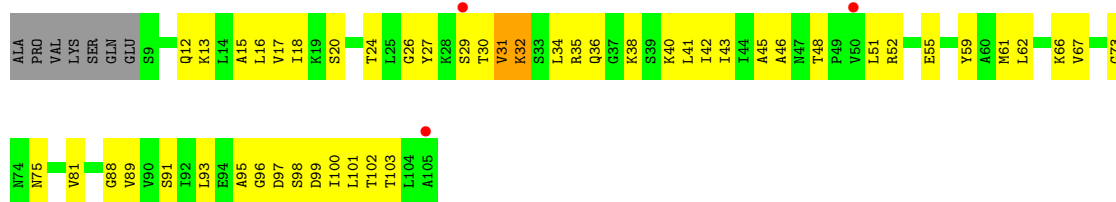


• Molecule 65: 60S ribosomal protein L29

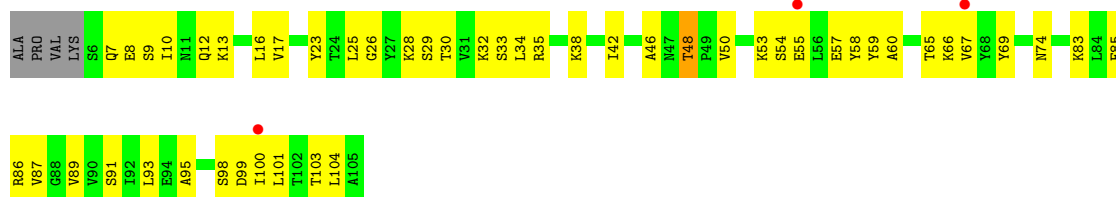


• Molecule 66: 60S ribosomal protein L30

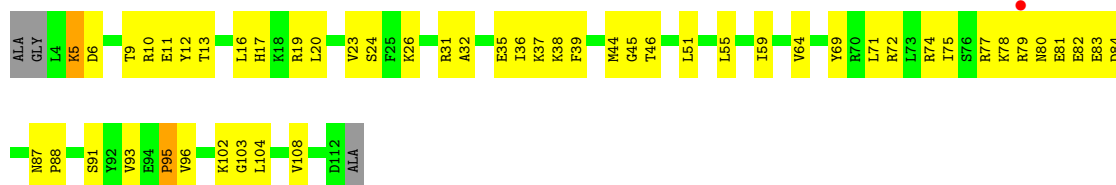




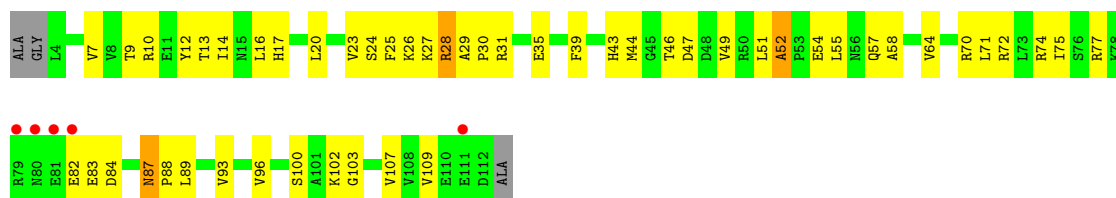
• Molecule 66: 60S ribosomal protein L30



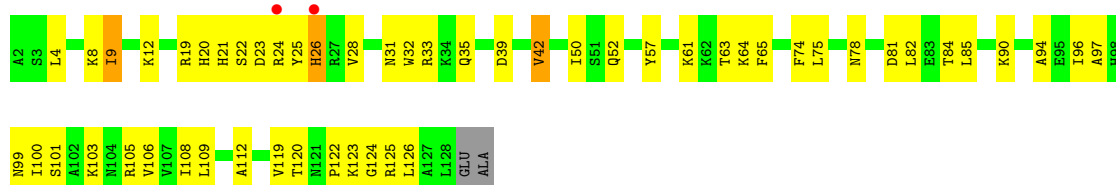
• Molecule 67: 60S ribosomal protein L31-A



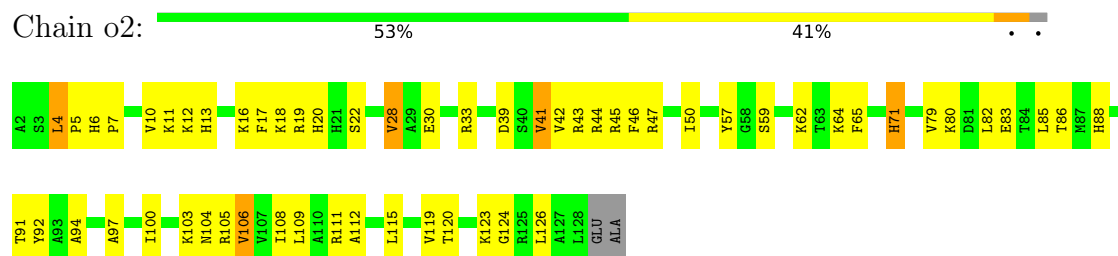
• Molecule 67: 60S ribosomal protein L31-A



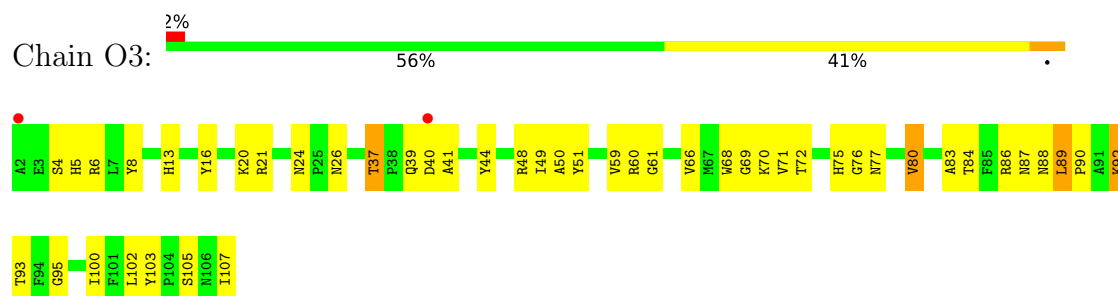
• Molecule 68: 60S ribosomal protein L32



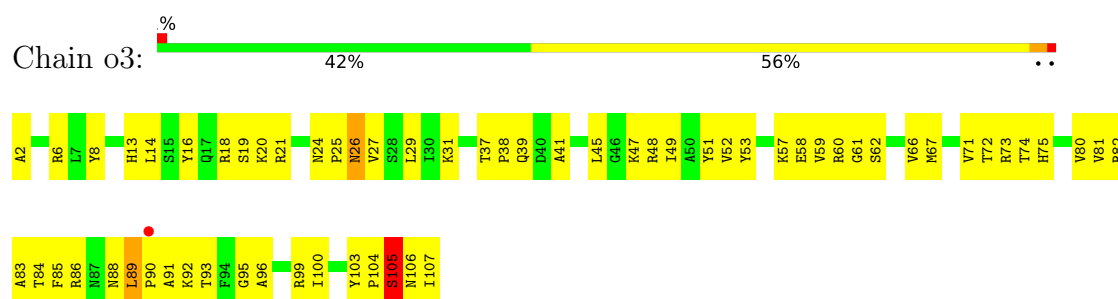
- Molecule 68: 60S ribosomal protein L32



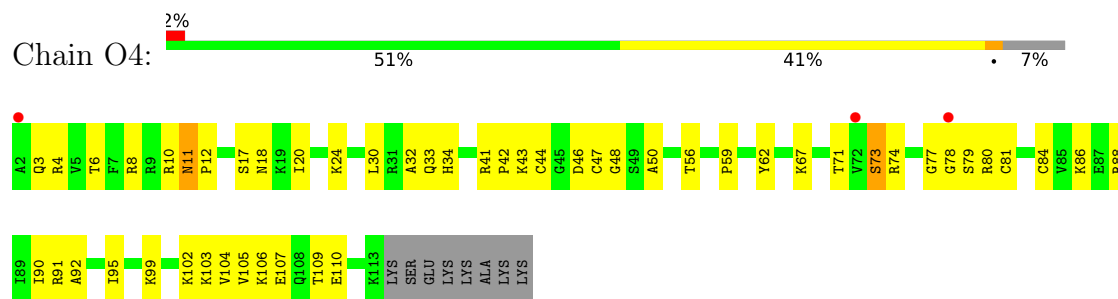
- Molecule 69: 60S ribosomal protein L33-A



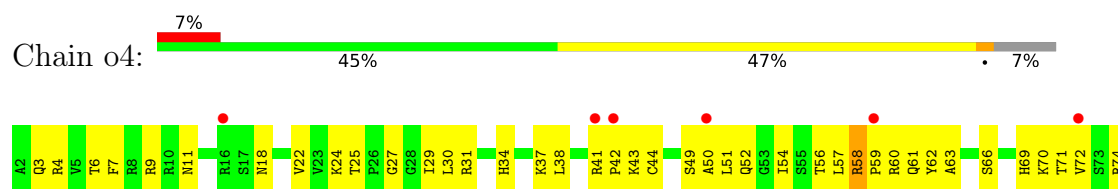
- Molecule 69: 60S ribosomal protein L33-A



- Molecule 70: 60S ribosomal protein L34-A

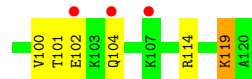
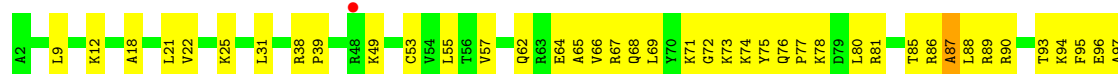


- Molecule 70: 60S ribosomal protein L34-A

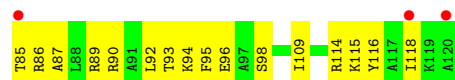
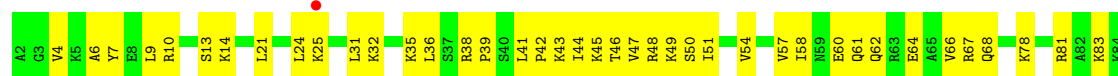




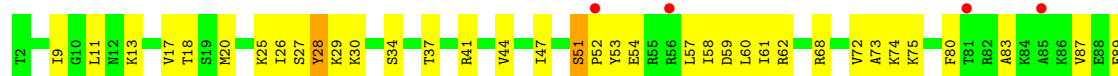
• Molecule 71: 60S ribosomal protein L35-A



• Molecule 71: 60S ribosomal protein L35-A



• Molecule 72: 60S ribosomal protein L36-A

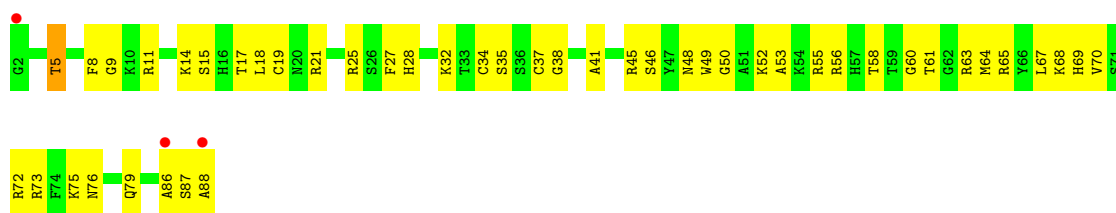


• Molecule 72: 60S ribosomal protein L36-A

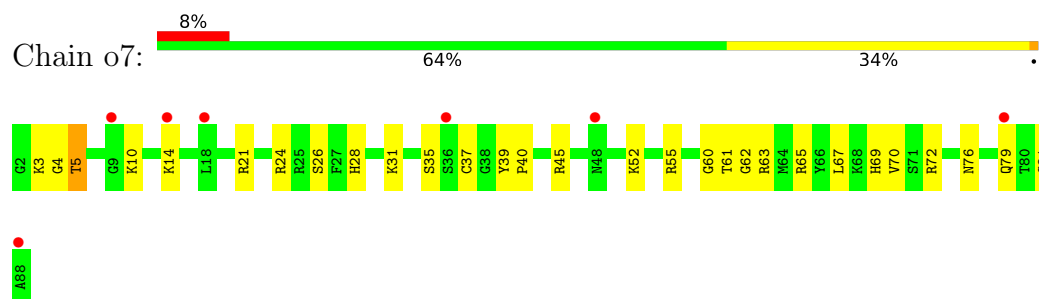


• Molecule 73: 60S ribosomal protein L37-A

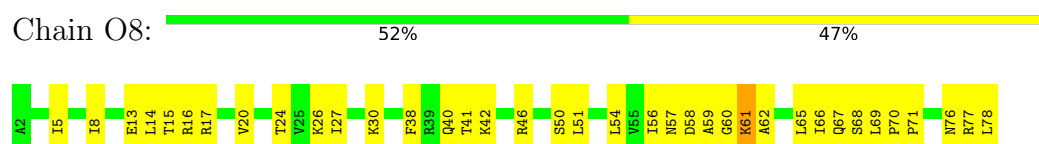




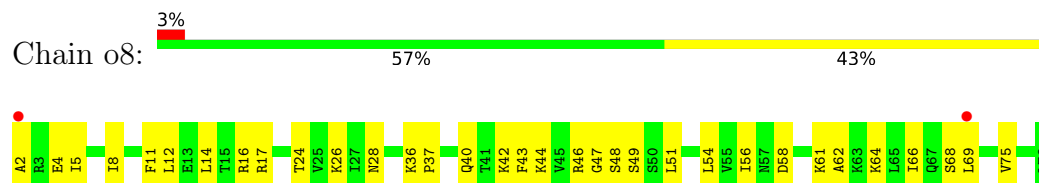
- Molecule 73: 60S ribosomal protein L37-A



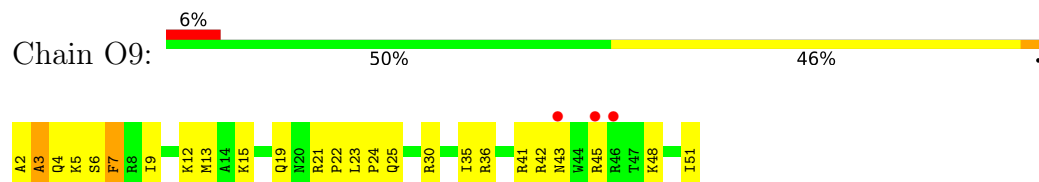
- Molecule 74: 60S ribosomal protein L38



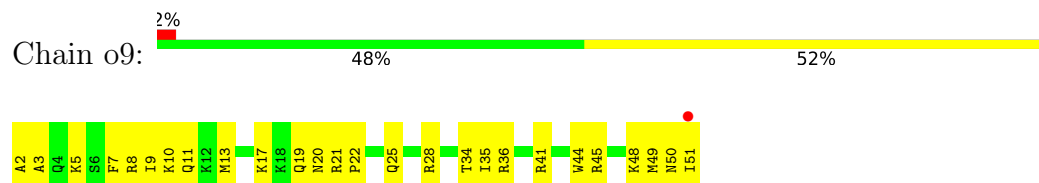
- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39

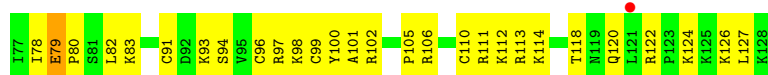


- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40

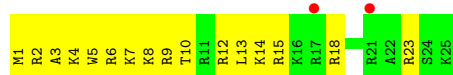




- Molecule 76: Ubiquitin-60S ribosomal protein L40



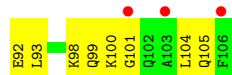
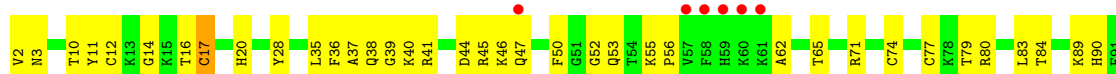
- Molecule 77: 60S ribosomal protein L41-A



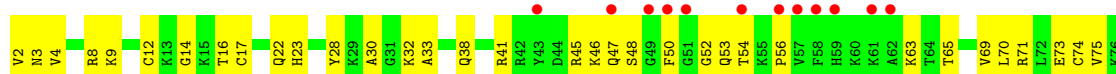
- Molecule 77: 60S ribosomal protein L41-A



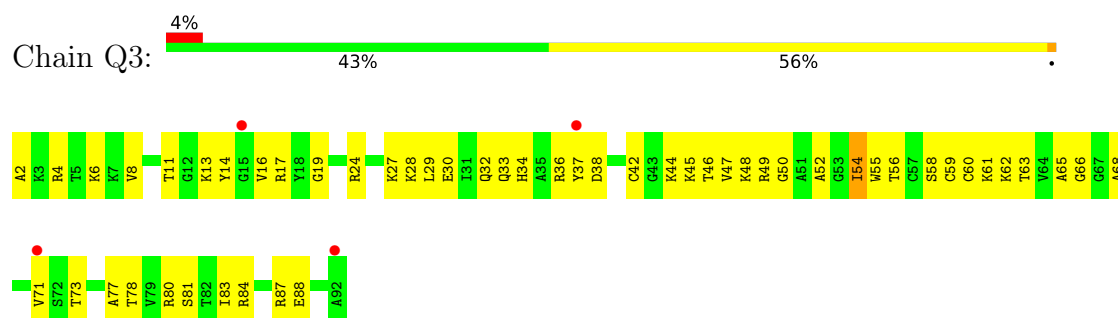
- Molecule 78: 60S ribosomal protein L42-A



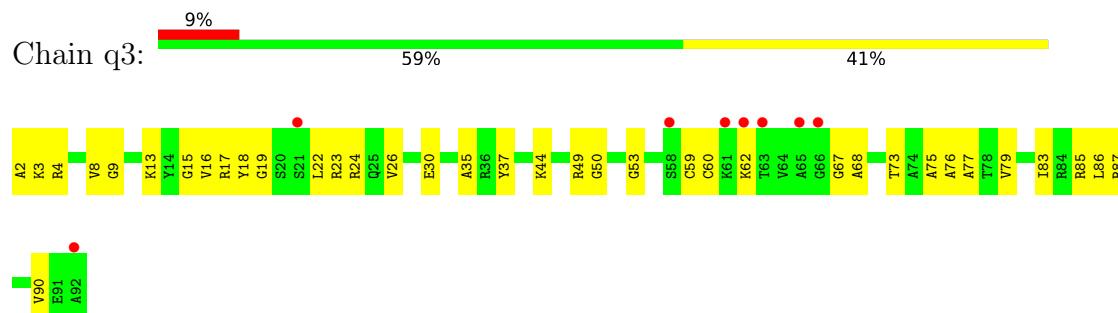
- Molecule 78: 60S ribosomal protein L42-A



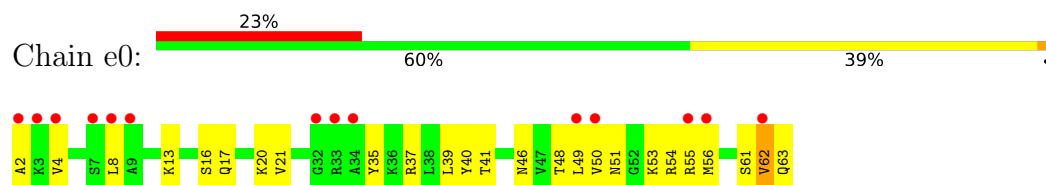
- Molecule 79: 60S ribosomal protein L43-A



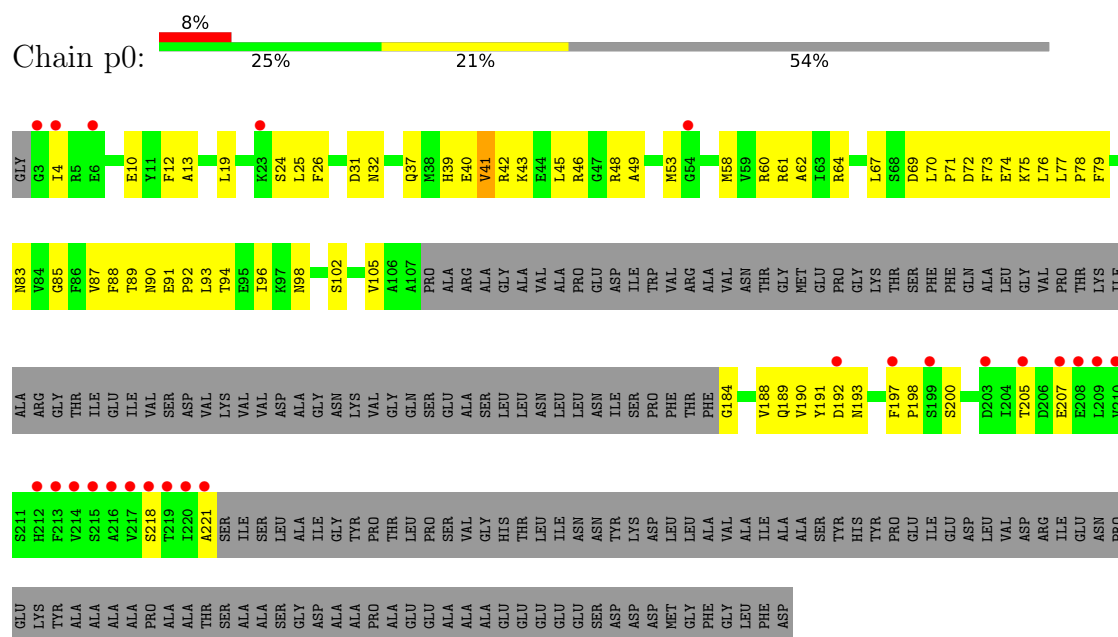
• Molecule 79: 60S ribosomal protein L43-A



• Molecule 80: 40S ribosomal protein S30-A



• Molecule 81: 60S acidic ribosomal protein P0



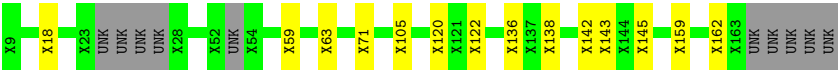
• Molecule 82: unknown protein chain m2

Chain m2:

85%

9%

6%

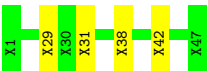


● Molecule 83: unknown protein chain p1

Chain p1:

91%

9%



● Molecule 84: unknown protein chain p2

Chain p2:

96%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.64Å 286.76Å 303.26Å 90.00° 98.72° 90.00°	Depositor
Resolution (Å)	299.76 – 3.45 299.76 – 3.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (299.76-3.45) 99.9 (299.76-3.45)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.196 , 0.260 0.203 , 0.264	Depositor DCC
R_{free} test set	19267 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	93.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 135.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	411214	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2	0.41	0/41698	0.62	2/64972 (0.0%)
1	6	0.45	0/42765	0.64	6/66634 (0.0%)
2	S0	0.61	0/1617	1.12	10/2215 (0.5%)
2	s0	0.63	0/1623	1.16	13/2222 (0.6%)
3	S1	0.51	0/1735	0.97	4/2335 (0.2%)
3	s1	0.63	0/1748	1.04	6/2352 (0.3%)
4	S2	0.60	0/1665	1.11	8/2263 (0.4%)
4	s2	0.74	0/1665	1.20	13/2263 (0.6%)
5	S3	0.63	0/1759	1.02	3/2368 (0.1%)
5	s3	0.58	0/1759	1.01	8/2368 (0.3%)
6	S4	0.63	0/2109	1.03	6/2839 (0.2%)
6	s4	0.64	0/2109	1.05	6/2839 (0.2%)
7	S5	0.54	0/1629	0.97	7/2202 (0.3%)
7	s5	0.60	0/1629	1.04	6/2202 (0.3%)
8	S6	0.62	0/1823	1.03	8/2439 (0.3%)
8	s6	0.71	0/1779	1.12	13/2379 (0.5%)
9	S7	0.57	0/1506	1.03	3/2028 (0.1%)
9	s7	0.60	0/1516	1.08	7/2043 (0.3%)
10	S8	0.71	0/1514	1.07	6/2021 (0.3%)
10	s8	0.70	0/1514	1.05	6/2021 (0.3%)
11	S9	0.60	0/1519	1.03	6/2035 (0.3%)
11	s9	0.67	0/1519	1.15	10/2035 (0.5%)
12	C0	0.57	0/790	1.09	7/1069 (0.7%)
12	c0	0.52	0/777	1.08	6/1049 (0.6%)
13	C1	0.73	0/1240	1.10	4/1675 (0.2%)
13	c1	0.72	0/1194	1.14	6/1610 (0.4%)
14	C2	0.59	0/900	0.99	1/1224 (0.1%)
14	c2	0.45	0/900	0.96	2/1224 (0.2%)
15	C3	0.67	0/1215	1.05	7/1638 (0.4%)
15	c3	0.71	1/1215 (0.1%)	1.08	9/1638 (0.5%)
16	C4	0.56	0/901	1.08	8/1217 (0.7%)
16	c4	0.66	0/960	1.10	6/1290 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.68	0/998	1.08	3/1341 (0.2%)
17	c5	0.63	0/1060	1.18	9/1426 (0.6%)
18	C6	0.61	0/1125	1.04	6/1510 (0.4%)
18	c6	0.62	0/1131	1.06	3/1518 (0.2%)
19	C7	0.65	0/935	1.02	1/1254 (0.1%)
19	c7	0.58	0/914	1.13	3/1224 (0.2%)
20	C8	0.58	0/1211	1.07	5/1628 (0.3%)
20	c8	0.60	0/1211	1.01	4/1628 (0.2%)
21	C9	0.54	0/1130	0.90	3/1517 (0.2%)
21	c9	0.65	0/1130	1.05	6/1517 (0.4%)
22	D0	0.60	0/865	1.05	1/1169 (0.1%)
22	d0	0.59	0/892	1.11	5/1205 (0.4%)
23	D1	0.57	0/693	0.98	2/935 (0.2%)
23	d1	0.66	0/693	1.02	3/935 (0.3%)
24	D2	0.62	0/1038	1.10	7/1395 (0.5%)
24	d2	0.73	0/1038	1.06	4/1395 (0.3%)
25	D3	0.76	0/1139	1.14	10/1518 (0.7%)
25	d3	0.90	0/1139	1.15	3/1518 (0.2%)
26	D4	0.57	0/1087	1.00	5/1449 (0.3%)
26	d4	0.67	0/1087	1.06	3/1449 (0.2%)
27	D5	0.57	0/571	1.10	3/768 (0.4%)
27	d5	0.56	0/566	1.08	3/761 (0.4%)
28	D6	0.64	0/782	1.07	5/1047 (0.5%)
28	d6	0.69	0/782	1.15	3/1047 (0.3%)
29	D7	0.54	0/620	0.99	2/838 (0.2%)
29	d7	0.62	0/620	1.28	7/838 (0.8%)
30	D8	0.51	0/499	1.01	4/670 (0.6%)
30	d8	0.54	0/499	0.93	0/670
31	D9	0.57	0/452	1.00	1/600 (0.2%)
31	d9	0.63	0/452	1.06	0/600
32	E0	0.64	0/483	0.96	0/643
33	E1	0.61	0/577	1.13	4/770 (0.5%)
33	e1	0.59	0/619	1.13	5/822 (0.6%)
34	SR	0.54	0/2494	0.97	5/3393 (0.1%)
34	sR	0.53	0/2495	0.88	1/3395 (0.0%)
35	SM	0.74	1/1113 (0.1%)	1.12	8/1502 (0.5%)
35	sM	0.66	0/682	1.28	6/921 (0.7%)
36	1	0.59	0/75394	0.76	17/117545 (0.0%)
36	5	0.59	0/75414	0.76	6/117575 (0.0%)
37	3	0.55	0/2883	0.69	0/4491
37	7	0.59	0/2883	0.78	0/4491
38	4	0.57	0/3746	0.73	0/5832
38	8	0.50	0/3746	0.66	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.88	0/1948	1.17	9/2617 (0.3%)
39	l2	0.80	0/1946	1.19	7/2614 (0.3%)
40	L3	0.90	0/3146	1.18	4/4228 (0.1%)
40	l3	0.99	3/3146 (0.1%)	1.20	16/4228 (0.4%)
41	L4	0.98	1/2800 (0.0%)	1.30	25/3790 (0.7%)
41	l4	0.93	0/2800	1.27	21/3790 (0.6%)
42	L5	0.72	0/2425	1.06	3/3271 (0.1%)
42	l5	0.85	0/2408	1.25	17/3248 (0.5%)
43	L6	0.94	0/1260	1.22	4/1694 (0.2%)
43	l6	0.97	0/1269	1.27	10/1705 (0.6%)
44	L7	1.03	0/1821	1.29	13/2451 (0.5%)
44	l7	1.04	1/1828 (0.1%)	1.39	26/2461 (1.1%)
45	L8	0.68	0/1836	1.16	12/2481 (0.5%)
45	l8	0.60	0/1795	1.02	2/2429 (0.1%)
46	L9	0.84	0/1539	1.11	5/2073 (0.2%)
46	l9	0.93	0/1539	1.18	6/2073 (0.3%)
47	M0	0.95	3/1741 (0.2%)	1.22	9/2335 (0.4%)
47	m0	0.93	1/1758 (0.1%)	1.21	8/2358 (0.3%)
48	M1	0.68	0/1374	1.03	3/1842 (0.2%)
48	m1	0.85	0/1374	1.15	8/1842 (0.4%)
49	M3	0.92	0/1568	1.21	7/2106 (0.3%)
49	m3	0.82	0/1573	1.28	12/2113 (0.6%)
50	M4	1.03	1/1068 (0.1%)	1.34	10/1438 (0.7%)
50	m4	1.03	1/1074 (0.1%)	1.26	10/1446 (0.7%)
51	M5	0.92	0/1757	1.30	14/2354 (0.6%)
51	m5	0.75	0/1757	1.13	10/2354 (0.4%)
52	M6	1.02	1/1585 (0.1%)	1.26	10/2128 (0.5%)
52	m6	1.19	4/1585 (0.3%)	1.39	16/2128 (0.8%)
53	M7	0.95	0/1443	1.19	4/1944 (0.2%)
53	m7	1.04	1/1250 (0.1%)	1.26	9/1683 (0.5%)
54	M8	1.00	2/1465 (0.1%)	1.24	4/1965 (0.2%)
54	m8	0.90	0/1465	1.24	9/1965 (0.5%)
55	M9	0.76	0/1538	1.11	7/2050 (0.3%)
55	m9	0.73	0/1538	1.04	4/2050 (0.2%)
56	N0	0.99	3/1481 (0.2%)	1.21	10/1990 (0.5%)
56	n0	1.07	1/1481 (0.1%)	1.28	10/1990 (0.5%)
57	N1	0.90	0/1300	1.17	4/1743 (0.2%)
57	n1	0.97	1/1300 (0.1%)	1.19	0/1743
58	N2	0.57	0/812	0.96	1/1099 (0.1%)
58	n2	0.57	0/794	0.99	3/1076 (0.3%)
59	N3	0.92	1/1018 (0.1%)	1.21	2/1369 (0.1%)
59	n3	1.02	0/1018	1.27	3/1369 (0.2%)
60	N4	0.81	0/712	1.35	8/958 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.82	0/1052	1.22	10/1398 (0.7%)
61	N5	0.79	0/979	1.10	2/1321 (0.2%)
61	n5	0.72	0/974	1.07	3/1314 (0.2%)
62	N6	0.88	0/1004	1.30	12/1341 (0.9%)
62	n6	0.79	0/1004	1.14	2/1341 (0.1%)
63	N7	0.61	0/1118	1.03	2/1497 (0.1%)
63	n7	0.58	0/1118	1.01	4/1497 (0.3%)
64	N8	0.89	1/1204 (0.1%)	1.21	5/1612 (0.3%)
64	n8	0.89	2/1204 (0.2%)	1.26	13/1612 (0.8%)
65	N9	0.90	0/473	1.19	3/629 (0.5%)
65	n9	0.88	0/473	1.51	8/629 (1.3%)
66	O0	0.59	0/751	1.04	3/1008 (0.3%)
66	o0	0.63	0/775	1.04	3/1040 (0.3%)
67	O1	0.79	0/890	1.14	3/1196 (0.3%)
67	o1	0.85	0/897	1.18	6/1205 (0.5%)
68	O2	1.02	0/1041	1.25	6/1394 (0.4%)
68	o2	1.06	3/1041 (0.3%)	1.29	7/1394 (0.5%)
69	O3	1.07	0/868	1.37	12/1168 (1.0%)
69	o3	1.09	1/868 (0.1%)	1.24	7/1168 (0.6%)
70	O4	0.75	0/890	1.15	3/1189 (0.3%)
70	o4	0.69	0/890	1.14	4/1189 (0.3%)
71	O5	0.81	0/978	1.14	4/1301 (0.3%)
71	o5	0.72	0/974	1.05	2/1297 (0.2%)
72	O6	0.84	1/778 (0.1%)	1.08	3/1034 (0.3%)
72	o6	0.72	0/777	1.06	2/1033 (0.2%)
73	O7	0.92	0/696	1.24	3/923 (0.3%)
73	o7	0.78	0/696	1.19	3/923 (0.3%)
74	O8	0.60	0/618	1.03	2/826 (0.2%)
74	o8	0.60	0/614	1.04	1/822 (0.1%)
75	O9	0.84	0/443	1.13	2/588 (0.3%)
75	o9	0.81	0/443	1.05	0/588
76	Q0	0.90	1/423 (0.2%)	1.24	2/562 (0.4%)
76	q0	1.05	0/423	1.35	2/562 (0.4%)
77	Q1	0.79	0/234	1.09	0/300
77	q1	0.70	0/234	1.06	1/300 (0.3%)
78	Q2	0.92	1/860 (0.1%)	1.15	4/1136 (0.4%)
78	q2	0.83	0/860	1.08	0/1136
79	Q3	0.86	0/701	1.16	2/934 (0.2%)
79	q3	0.82	0/701	1.07	0/934
80	e0	0.64	0/499	1.10	1/665 (0.2%)
81	p0	0.59	0/1091	1.00	1/1472 (0.1%)
All	All	0.65	37/430072 (0.0%)	0.90	907/631360 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	S1	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
10	S8	0	1
11	S9	0	1
16	C4	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	1
20	c8	0	1
22	d0	0	1
26	d4	0	1
27	D5	0	2
33	E1	0	1
39	L2	0	1
39	l2	0	1
40	L3	0	1
40	l3	0	1
42	L5	0	1
43	L6	0	1
44	l7	0	1
45	L8	0	1
47	M0	0	1
48	M1	0	1
48	m1	0	1
50	M4	0	1
52	M6	0	1
56	n0	0	2
64	n8	0	1
65	N9	0	1
67	O1	0	1
69	o3	0	1
80	e0	0	1
All	All	0	37

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	m7	146	ILE	CA-CB	-7.84	1.44	1.54
47	M0	165	ILE	CA-CB	7.43	1.63	1.54
52	m6	9	ILE	CA-CB	-7.00	1.46	1.54
56	n0	58	ILE	CA-CB	-6.96	1.46	1.53
78	Q2	17	CYS	CB-SG	6.60	2.03	1.81

The worst 5 of 907 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	M5	83	LYS	CA-C-N	-17.15	101.39	120.94
51	M5	83	LYS	C-N-CA	-17.15	101.39	120.94
60	N4	80	ARG	CA-C-N	14.68	138.19	119.84
60	N4	80	ARG	C-N-CA	14.68	138.19	119.84
50	M4	30	GLY	N-CA-C	-13.62	98.27	114.48

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
3	S1	177	GLN	Peptide
9	S7	131	PHE	Peptide
10	S8	8	ARG	Peptide
11	S9	137	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18758	1144	1
1	6	38238	0	19241	1149	0
2	S0	1577	0	1567	104	0
2	s0	1583	0	1578	101	0
3	S1	1709	0	1784	123	0
3	s1	1722	0	1793	81	0
4	S2	1635	0	1723	94	0
4	s2	1635	0	1723	84	0
5	S3	1734	0	1817	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	s3	1734	0	1817	79	0
6	S4	2068	0	2154	110	0
6	s4	2068	0	2154	107	0
7	S5	1609	0	1675	112	0
7	s5	1609	0	1675	102	0
8	S6	1799	0	1879	108	0
8	s6	1755	0	1846	97	0
9	S7	1481	0	1572	90	0
9	s7	1491	0	1578	72	0
10	S8	1489	0	1525	79	0
10	s8	1489	0	1525	68	0
11	S9	1494	0	1573	75	0
11	s9	1494	0	1573	96	0
12	C0	773	0	729	42	0
12	c0	762	0	699	41	0
13	C1	1214	0	1259	72	0
13	c1	1168	0	1231	48	0
14	C2	892	0	891	47	0
14	c2	892	0	891	33	0
15	C3	1192	0	1255	71	0
15	c3	1192	0	1255	71	0
16	C4	891	0	883	63	0
16	c4	949	0	985	55	0
17	C5	977	0	1002	54	0
17	c5	1039	0	1050	71	0
18	C6	1105	0	1166	72	0
18	c6	1111	0	1171	74	0
19	C7	926	0	930	62	0
19	c7	906	0	909	51	0
20	C8	1192	0	1222	79	0
20	c8	1192	0	1222	76	0
21	C9	1112	0	1124	79	0
21	c9	1112	0	1124	70	0
22	D0	855	0	917	57	0
22	d0	882	0	939	51	0
23	D1	684	0	672	39	0
23	d1	684	0	672	55	0
24	D2	1021	0	1060	56	0
24	d2	1021	0	1060	58	0
25	D3	1121	0	1196	66	0
25	d3	1121	0	1196	67	0
26	D4	1073	0	1132	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	d4	1073	0	1132	50	0
27	D5	563	0	603	40	0
27	d5	558	0	598	32	0
28	D6	769	0	814	78	0
28	d6	769	0	814	55	0
29	D7	610	0	631	34	0
29	d7	610	0	632	27	0
30	D8	497	0	535	30	0
30	d8	497	0	535	26	0
31	D9	442	0	428	20	0
31	d9	442	0	428	27	0
32	E0	475	0	525	16	0
33	E1	566	0	602	42	0
33	e1	608	0	656	33	0
34	SR	2441	0	2397	133	0
34	sR	2442	0	2392	116	0
35	SM	1104	0	996	59	0
35	sM	679	0	603	30	0
36	1	67355	0	33845	1716	0
36	5	67376	0	33855	1722	1
37	3	2579	0	1304	80	0
37	7	2579	0	1303	73	0
38	4	3353	0	1695	84	0
38	8	3353	0	1695	98	0
39	L2	1914	0	1981	105	0
39	l2	1912	0	1976	110	0
40	L3	3075	0	3142	143	0
40	l3	3075	0	3142	172	0
41	L4	2748	0	2859	164	0
41	l4	2748	0	2859	147	0
42	L5	2375	0	2325	129	0
42	l5	2359	0	2311	125	0
43	L6	1239	0	1326	50	0
43	l6	1248	0	1339	66	0
44	L7	1784	0	1862	111	0
44	l7	1791	0	1869	101	0
45	L8	1804	0	1877	92	0
45	l8	1763	0	1819	96	0
46	L9	1518	0	1587	105	0
46	l9	1518	0	1587	86	0
47	M0	1705	0	1736	95	0
47	m0	1722	0	1755	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	M1	1353	0	1383	73	0
48	m1	1353	0	1383	72	0
49	M3	1543	0	1608	86	0
49	m3	1548	0	1613	91	0
50	M4	1053	0	1149	63	0
50	m4	1059	0	1154	59	0
51	M5	1720	0	1779	111	0
51	m5	1720	0	1779	108	0
52	M6	1555	0	1659	107	0
52	m6	1555	0	1659	105	0
53	M7	1420	0	1437	77	0
53	m7	1227	0	1236	80	0
54	M8	1441	0	1543	80	0
54	m8	1441	0	1543	66	0
55	M9	1521	0	1616	95	0
55	m9	1521	0	1617	62	0
56	N0	1445	0	1487	86	0
56	n0	1445	0	1487	83	0
57	N1	1276	0	1323	66	0
57	n1	1276	0	1323	86	0
58	N2	796	0	812	39	0
58	n2	778	0	791	28	0
59	N3	1003	0	1048	76	0
59	n3	1003	0	1048	41	0
60	N4	699	0	640	29	0
60	n4	1038	0	1071	45	0
61	N5	964	0	1025	45	0
61	n5	959	0	1023	47	0
62	N6	993	0	1081	52	0
62	n6	993	0	1081	63	0
63	N7	1092	0	1155	50	0
63	n7	1092	0	1155	55	0
64	N8	1173	0	1215	72	0
64	n8	1173	0	1215	73	0
65	N9	462	0	491	18	0
65	n9	462	0	491	35	0
66	O0	743	0	797	41	0
66	o0	767	0	816	45	0
67	O1	876	0	912	43	0
67	o1	883	0	918	43	0
68	O2	1020	0	1090	59	0
68	o2	1020	0	1090	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	O3	850	0	880	43	0
69	o3	850	0	880	48	0
70	O4	880	0	945	56	0
70	o4	880	0	945	61	0
71	O5	969	0	1078	39	0
71	o5	965	0	1067	50	0
72	O6	771	0	849	44	0
72	o6	770	0	846	41	0
73	O7	681	0	683	51	0
73	o7	681	0	683	32	0
74	O8	612	0	682	36	0
74	o8	608	0	671	32	0
75	O9	436	0	475	25	0
75	o9	436	0	475	22	0
76	Q0	417	0	457	27	0
76	q0	417	0	456	23	0
77	Q1	233	0	284	21	0
77	q1	233	0	284	16	0
78	Q2	847	0	916	40	0
78	q2	847	0	914	49	0
79	Q3	694	0	734	48	0
79	q3	694	0	734	34	0
80	e0	491	0	542	22	0
81	p0	1076	0	1040	52	0
82	m2	750	0	179	7	0
83	p1	235	0	50	2	0
84	p2	230	0	51	2	0
85	1	462	0	0	0	0
85	2	122	0	0	0	0
85	3	15	0	0	0	0
85	4	23	0	0	0	0
85	5	495	0	0	0	0
85	6	147	0	0	0	0
85	7	17	0	0	0	0
85	8	14	0	0	0	0
85	C1	1	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	D4	1	0	0	0	0
85	L2	2	0	0	0	0
85	L3	4	0	0	0	0
85	L4	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L7	2	0	0	0	0
85	L8	1	0	0	0	0
85	M0	3	0	0	0	0
85	M1	1	0	0	0	0
85	M3	2	0	0	0	0
85	M5	2	0	0	0	0
85	M6	1	0	0	0	0
85	M7	5	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	3	0	0	0	0
85	N5	1	0	0	0	0
85	N6	2	0	0	0	0
85	N8	5	0	0	0	0
85	O1	1	0	0	0	0
85	O2	2	0	0	0	0
85	O5	1	0	0	0	0
85	O7	2	0	0	0	0
85	Q2	1	0	0	0	0
85	S4	1	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c4	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	1	0	0	0	0
85	c9	1	0	0	0	0
85	d0	1	0	0	0	0
85	d3	3	0	0	0	0
85	d6	1	0	0	0	0
85	l2	3	0	0	0	0
85	l3	3	0	0	0	0
85	l4	1	0	0	0	0
85	l5	3	0	0	0	0
85	l7	1	0	0	0	0
85	l9	1	0	0	0	0
85	m0	1	0	0	0	0
85	m1	1	0	0	0	0
85	m4	1	0	0	0	0
85	m5	5	0	0	0	0
85	m6	2	0	0	0	0
85	m7	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	n0	1	0	0	0	0
85	n3	1	0	0	0	0
85	n6	2	0	0	0	0
85	n8	3	0	0	0	0
85	n9	2	0	0	0	0
85	o3	2	0	0	0	0
85	o4	3	0	0	0	0
85	o7	1	0	0	0	0
85	q0	2	0	0	0	0
85	q1	1	0	0	0	0
85	s1	1	0	0	0	0
85	s8	1	0	0	0	0
85	sM	1	0	0	0	0
86	1	2478	0	0	204	0
86	2	1106	0	0	106	0
86	3	70	0	0	4	0
86	4	105	0	0	6	0
86	5	2492	0	0	217	0
86	6	1113	0	0	108	0
86	7	84	0	0	12	0
86	8	105	0	0	10	0
86	C3	7	0	0	0	0
86	C5	7	0	0	2	0
86	C8	7	0	0	0	0
86	D3	7	0	0	2	0
86	D9	7	0	0	0	0
86	L3	14	0	0	2	0
86	L4	7	0	0	2	0
86	M0	7	0	0	1	0
86	M5	7	0	0	1	0
86	M7	14	0	0	2	0
86	M9	7	0	0	1	0
86	N9	7	0	0	0	0
86	O1	7	0	0	7	0
86	O3	7	0	0	1	0
86	O7	14	0	0	8	0
86	Q2	7	0	0	2	0
86	S8	7	0	0	0	0
86	SR	7	0	0	0	0
86	c3	7	0	0	1	0
86	c5	7	0	0	1	0
86	c8	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	14	0	0	1	0
86	l4	14	0	0	0	0
86	l5	21	0	0	1	0
86	l9	7	0	0	0	0
86	m0	14	0	0	2	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	1	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	n1	7	0	0	1	0
86	n3	7	0	0	0	0
86	n9	7	0	0	1	0
86	o3	7	0	0	1	0
86	o7	7	0	0	1	0
86	q2	7	0	0	3	0
86	s1	14	0	0	2	0
86	s4	7	0	0	0	0
86	s8	7	0	0	1	0
86	s9	7	0	0	1	0
86	sR	7	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	1	0
87	Q2	1	0	0	2	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	1	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
88	1	30	0	24	2	0
88	5	30	0	25	2	0
All	All	411214	0	297334	14070	1

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 20.

The worst 5 of 14070 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)
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.03	1.47
78:Q2:17:CYS:CB	87:Q2:501:ZN:ZN	0.98	1.42
78:Q2:17:CYS:SG	87:Q2:501:ZN:ZN	1.30	1.18
36:5:2273:G:O6	86:5:4193:OHX:N5	1.90	1.05
40:l3:41:VAL:HA	40:l3:185:GLY:HA3	1.37	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1353:U:O2'	36:5:3165:A:OP1[2_546]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	544 (31%)	51 (2%)
1	6	1793/1800 (99%)	495 (27%)	48 (2%)
36	1	3145/3396 (92%)	783 (24%)	86 (2%)
36	5	3145/3396 (92%)	804 (25%)	77 (2%)
37	3	120/121 (99%)	20 (16%)	0
37	7	120/121 (99%)	28 (23%)	2 (1%)
38	4	157/158 (99%)	42 (26%)	3 (1%)
38	8	157/158 (99%)	44 (28%)	2 (1%)
All	All	10384/10950 (94%)	2760 (26%)	269 (2%)

5 of 2760 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	10	G
1	2	25	C
1	2	26	A

5 of 269 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	2116	G
36	5	2374	C
36	5	3330	A
36	1	2249	G
36	1	2112	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2557 ligands modelled in this entry, 1423 are monoatomic - leaving 1134 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	$\# Z > 2$
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	1	3860	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	n1	201	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	c8	202	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	D3	202	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	m4	202	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	1	4204	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	M7	206	-	0,6,6	-	-	-		
86	OHX	m7	207	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	14	402	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	1	3861	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	l3	405	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	L3	405	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	O1	202	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	5	3892	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	6	2204	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	1	3862	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	5	3898	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	5	3895	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	L3	406	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	6	2190	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	2	2178	-	0,6,6	-	-	-		
86	OHX	7	228	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	3	225	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
88	BLS	5	4248	-	30,31,31	1.35	3 (10%)	30,43,43	0.90	1 (3%)
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	1	3859	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	L4	404	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	4	238	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	5	4195	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	M0	304	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	s8	302	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	5	3894	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	5	4246	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	m0	303	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	1	3857	-	0,6,6	-	-	-		
86	OHX	n3	202	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	5	3893	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	5	4233	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	Q2	503	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	l5	305	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	M7	207	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	O7	105	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	6	2046	-	0,6,6	-	-	-		
86	OHX	1	3864	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	1	3863	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	15	306	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	15	304	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	m6	203	-	0,6,6	-	-	-		
86	OHX	5	3896	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	O7	104	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	2	2179	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	m5	306	-	0,6,6	-	-	-		
86	OHX	7	227	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	4	237	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	5	3899	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	14	403	-	0,6,6	-	-	-		
86	OHX	o7	103	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	1	3858	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
88	BLS	1	4211	-	30,31,31	1.74	5 (16%)	30,43,43	1.61	8 (26%)
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	n9	103	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	19	202	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	O3	201	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	5	4232	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	5	3897	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	o3	203	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2180	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	7	229	-	0,6,6	-	-	-		
86	OHX	m1	202	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	BLS	1	4211	-	-	3/25/38/38	0/2/2/2
88	BLS	5	4248	-	-	9/25/38/38	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4211	BLS	C1'-N1	-5.06	1.40	1.48
88	5	4248	BLS	C11-N12	-4.97	1.36	1.47
88	1	4211	BLS	C2-N3	-3.27	1.29	1.36
88	1	4211	BLS	C11-N12	3.11	1.53	1.47
88	1	4211	BLS	C5-C4	2.98	1.49	1.42

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4211	BLS	C4-N3-C2	3.95	126.48	120.26
88	5	4248	BLS	N15-C14-N12	-3.04	115.32	118.64
88	1	4211	BLS	N15-C14-N12	-2.75	115.63	118.64
88	1	4211	BLS	O5'-C5'-C6'	-2.62	97.94	106.14
88	1	4211	BLS	C1'-N1-C2	2.46	121.68	117.94

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	1	4211	BLS	C11-C10-C9-C8
88	1	4211	BLS	C11-C10-C9-N9
88	5	4248	BLS	C3'-C4'-N6-C7
88	5	4248	BLS	C4'-C5'-C6'-O4
88	5	4248	BLS	C4'-C5'-C6'-O3

There are no ring outliers.

476 monomers are involved in 714 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4075	OHX	1	0
86	6	2088	OHX	1	0
86	1	4001	OHX	2	0
86	2	2026	OHX	2	0
86	1	3860	OHX	1	0
86	1	3976	OHX	1	0
86	5	4222	OHX	1	0
86	6	2091	OHX	1	0
86	n1	201	OHX	1	0
86	6	2201	OHX	1	0
86	5	4095	OHX	1	0
86	5	3995	OHX	6	0
86	5	4239	OHX	1	0
86	6	2100	OHX	2	0
86	5	3966	OHX	6	0
86	5	3955	OHX	3	0
86	1	4140	OHX	2	0
86	1	4124	OHX	2	0
86	5	4105	OHX	2	0
86	1	4130	OHX	1	0
86	7	218	OHX	2	0
86	1	3873	OHX	1	0
86	5	4014	OHX	7	0
86	D3	202	OHX	2	0
86	6	2130	OHX	1	0
86	l3	404	OHX	1	0
86	2	2050	OHX	1	0
86	5	3932	OHX	1	0
86	7	223	OHX	1	0
86	5	4173	OHX	1	0
86	6	2147	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2165	OHX	1	0
86	1	4201	OHX	1	0
86	1	4131	OHX	1	0
86	2	2167	OHX	1	0
86	2	2131	OHX	5	0
86	m0	302	OHX	1	0
86	1	3897	OHX	2	0
86	2	2173	OHX	1	0
86	2	2165	OHX	1	0
86	6	2049	OHX	1	0
86	5	4074	OHX	1	0
86	2	2104	OHX	1	0
86	8	222	OHX	1	0
86	1	4155	OHX	1	0
86	6	2057	OHX	1	0
86	6	2192	OHX	3	0
86	5	3975	OHX	1	0
86	3	218	OHX	1	0
86	M7	206	OHX	1	0
86	6	2098	OHX	1	0
86	6	2143	OHX	2	0
86	1	3899	OHX	1	0
86	2	2092	OHX	2	0
86	1	3977	OHX	1	0
86	1	4195	OHX	1	0
86	6	2163	OHX	1	0
86	5	4049	OHX	1	0
86	1	4121	OHX	1	0
86	1	3958	OHX	1	0
86	2	2130	OHX	1	0
86	2	2140	OHX	1	0
86	6	2105	OHX	2	0
86	1	3871	OHX	1	0
86	1	3865	OHX	1	0
86	c5	201	OHX	1	0
86	1	4040	OHX	7	0
86	1	4103	OHX	1	0
86	1	4172	OHX	1	0
86	5	3992	OHX	1	0
86	1	4132	OHX	1	0
86	6	2188	OHX	1	0
86	5	3935	OHX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4207	OHX	1	0
86	5	4126	OHX	2	0
86	5	4029	OHX	4	0
86	1	3955	OHX	1	0
86	5	4234	OHX	1	0
86	5	4209	OHX	1	0
86	5	3952	OHX	1	0
86	2	2134	OHX	1	0
86	5	4179	OHX	1	0
86	2	2072	OHX	1	0
86	1	4128	OHX	2	0
86	5	3910	OHX	2	0
86	5	4047	OHX	1	0
86	1	3931	OHX	1	0
86	L3	405	OHX	1	0
86	1	3876	OHX	2	0
86	8	215	OHX	1	0
86	6	2175	OHX	1	0
86	5	4068	OHX	1	0
86	6	2104	OHX	2	0
86	1	4057	OHX	1	0
86	5	4082	OHX	1	0
86	1	4147	OHX	2	0
86	5	4180	OHX	1	0
86	5	4188	OHX	1	0
86	1	3991	OHX	1	0
86	1	4205	OHX	1	0
86	1	4038	OHX	1	0
86	2	2034	OHX	1	0
86	5	3980	OHX	1	0
86	2	2046	OHX	2	0
86	6	2122	OHX	1	0
86	8	216	OHX	5	0
86	5	4033	OHX	1	0
86	1	3966	OHX	1	0
86	5	4097	OHX	2	0
86	O1	202	OHX	7	0
86	1	3919	OHX	2	0
86	4	232	OHX	1	0
86	1	3924	OHX	2	0
86	6	2093	OHX	1	0
86	5	4238	OHX	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4162	OHX	1	0
86	1	3965	OHX	6	0
86	1	3994	OHX	2	0
86	6	2062	OHX	1	0
86	5	4214	OHX	1	0
86	5	4088	OHX	2	0
86	5	3892	OHX	2	0
86	6	2204	OHX	1	0
86	6	2137	OHX	1	0
86	5	4155	OHX	1	0
86	1	3862	OHX	3	0
86	6	2124	OHX	1	0
86	5	4228	OHX	7	0
86	1	3881	OHX	1	0
86	1	3879	OHX	2	0
86	6	2047	OHX	1	0
86	5	3982	OHX	1	0
86	s9	201	OHX	1	0
86	5	3903	OHX	1	0
86	5	3930	OHX	1	0
86	1	4137	OHX	1	0
86	6	2125	OHX	2	0
86	5	4161	OHX	1	0
86	2	2077	OHX	2	0
86	2	2075	OHX	1	0
86	2	2081	OHX	1	0
86	2	2155	OHX	1	0
86	2	2053	OHX	2	0
86	6	2178	OHX	2	0
86	2	2063	OHX	2	0
86	6	2053	OHX	1	0
86	1	4029	OHX	1	0
86	1	3882	OHX	1	0
86	5	4004	OHX	4	0
86	5	4133	OHX	1	0
86	5	3898	OHX	1	0
86	1	4144	OHX	1	0
86	1	3883	OHX	1	0
86	1	4070	OHX	1	0
86	5	3962	OHX	2	0
86	6	2086	OHX	1	0
86	5	3925	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	8	219	OHX	1	0
86	2	2157	OHX	3	0
86	5	3959	OHX	1	0
86	5	4124	OHX	1	0
86	1	4003	OHX	1	0
86	5	3895	OHX	1	0
86	1	3974	OHX	1	0
86	1	4008	OHX	1	0
86	5	4017	OHX	2	0
86	L3	406	OHX	1	0
86	6	2123	OHX	1	0
86	2	2129	OHX	2	0
86	q2	502	OHX	3	0
86	6	2190	OHX	3	0
86	5	3968	OHX	1	0
86	3	221	OHX	1	0
86	7	228	OHX	6	0
86	5	4083	OHX	1	0
86	1	4178	OHX	4	0
86	1	4165	OHX	1	0
86	2	2043	OHX	6	0
86	2	2091	OHX	2	0
86	1	4161	OHX	1	0
86	5	4048	OHX	1	0
86	6	2144	OHX	1	0
88	5	4248	BLS	2	0
86	2	2159	OHX	1	0
86	6	2074	OHX	2	0
86	5	3996	OHX	1	0
86	6	2159	OHX	3	0
86	1	3936	OHX	1	0
86	2	2103	OHX	2	0
86	L4	404	OHX	2	0
86	6	2071	OHX	2	0
86	5	4195	OHX	5	0
86	3	224	OHX	1	0
86	1	4167	OHX	1	0
86	6	2092	OHX	1	0
86	5	3953	OHX	2	0
86	5	3928	OHX	1	0
86	1	3908	OHX	1	0
86	5	4157	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4189	OHX	2	0
86	5	4212	OHX	6	0
86	2	2138	OHX	1	0
86	1	3884	OHX	1	0
86	2	2074	OHX	4	0
86	1	3971	OHX	2	0
86	5	4172	OHX	1	0
86	1	3867	OHX	1	0
86	1	4134	OHX	1	0
86	2	2044	OHX	2	0
86	5	3940	OHX	1	0
86	1	4190	OHX	1	0
86	M0	304	OHX	1	0
86	5	4106	OHX	1	0
86	5	4154	OHX	2	0
86	5	4043	OHX	1	0
86	5	4114	OHX	1	0
86	5	4136	OHX	1	0
86	5	3904	OHX	1	0
86	5	4145	OHX	1	0
86	2	2061	OHX	1	0
86	s8	302	OHX	1	0
86	5	3926	OHX	1	0
86	1	3940	OHX	1	0
86	5	3894	OHX	1	0
86	5	3972	OHX	1	0
86	5	4028	OHX	1	0
86	1	3926	OHX	1	0
86	1	3950	OHX	1	0
86	2	2116	OHX	1	0
86	1	4086	OHX	1	0
86	1	4194	OHX	7	0
86	5	3971	OHX	8	0
86	5	4138	OHX	3	0
86	5	4128	OHX	1	0
86	5	4006	OHX	1	0
86	6	2055	OHX	1	0
86	2	2055	OHX	1	0
86	8	229	OHX	1	0
86	6	2184	OHX	3	0
86	5	4022	OHX	1	0
86	1	4081	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3909	OHX	3	0
86	4	234	OHX	1	0
86	1	4078	OHX	1	0
86	6	2149	OHX	1	0
86	6	2102	OHX	1	0
86	5	3991	OHX	1	0
86	m0	303	OHX	1	0
86	6	2126	OHX	2	0
86	6	2109	OHX	1	0
86	7	220	OHX	7	0
86	2	2041	OHX	1	0
86	1	4042	OHX	2	0
86	1	3886	OHX	1	0
86	7	222	OHX	1	0
86	1	3952	OHX	1	0
86	1	3877	OHX	1	0
86	2	2120	OHX	3	0
86	5	3965	OHX	2	0
86	1	3857	OHX	1	0
86	5	3946	OHX	1	0
86	6	2202	OHX	1	0
86	2	2069	OHX	1	0
86	4	236	OHX	1	0
86	5	3989	OHX	1	0
86	1	3932	OHX	1	0
86	5	4000	OHX	2	0
86	2	2126	OHX	1	0
86	5	4229	OHX	1	0
86	2	2107	OHX	2	0
86	2	2040	OHX	1	0
86	5	4192	OHX	1	0
86	5	3969	OHX	1	0
86	5	3994	OHX	5	0
86	5	4211	OHX	1	0
86	1	4027	OHX	6	0
86	6	2061	OHX	3	0
86	6	2077	OHX	1	0
86	c3	201	OHX	1	0
86	5	3912	OHX	1	0
86	1	3878	OHX	1	0
86	1	4136	OHX	1	0
86	1	3998	OHX	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2162	OHX	4	0
86	2	2066	OHX	1	0
86	2	2036	OHX	2	0
86	6	2157	OHX	1	0
86	1	4039	OHX	2	0
86	1	4153	OHX	6	0
86	6	2106	OHX	1	0
86	6	2112	OHX	1	0
86	5	3943	OHX	1	0
86	5	4193	OHX	10	0
86	1	3970	OHX	1	0
86	8	223	OHX	5	0
86	2	2097	OHX	1	0
86	1	4052	OHX	2	0
86	Q2	503	OHX	2	0
86	4	229	OHX	2	0
86	1	4051	OHX	1	0
86	1	4012	OHX	1	0
86	5	4244	OHX	1	0
86	5	4113	OHX	1	0
86	5	4100	OHX	2	0
86	2	2105	OHX	1	0
86	M5	303	OHX	1	0
86	2	2073	OHX	2	0
86	5	4046	OHX	1	0
86	5	4061	OHX	1	0
86	5	4008	OHX	2	0
86	5	3900	OHX	1	0
86	1	4014	OHX	1	0
86	6	2138	OHX	2	0
86	6	2083	OHX	1	0
86	5	3984	OHX	2	0
86	2	2106	OHX	1	0
86	M7	207	OHX	1	0
86	1	4080	OHX	2	0
86	7	221	OHX	1	0
86	2	2029	OHX	1	0
86	6	2111	OHX	2	0
86	2	2085	OHX	1	0
86	O7	105	OHX	1	0
86	6	2068	OHX	1	0
86	1	4177	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2095	OHX	1	0
86	5	4190	OHX	1	0
86	5	3901	OHX	1	0
86	6	2120	OHX	7	0
86	2	2023	OHX	1	0
86	1	3933	OHX	1	0
86	6	2114	OHX	1	0
86	1	4152	OHX	1	0
86	1	3894	OHX	2	0
86	6	2171	OHX	7	0
86	5	4040	OHX	1	0
86	1	4200	OHX	3	0
86	5	4092	OHX	1	0
86	2	2099	OHX	1	0
86	C5	201	OHX	2	0
86	6	2046	OHX	1	0
86	1	3864	OHX	1	0
86	5	3905	OHX	2	0
86	6	2128	OHX	1	0
86	2	2149	OHX	1	0
86	6	2107	OHX	1	0
86	2	2025	OHX	1	0
86	5	3920	OHX	1	0
86	1	3927	OHX	2	0
86	1	4118	OHX	2	0
86	5	4182	OHX	1	0
86	2	2031	OHX	8	0
86	5	3908	OHX	1	0
86	5	4112	OHX	1	0
86	1	4023	OHX	6	0
86	5	3917	OHX	1	0
86	1	3917	OHX	1	0
86	6	2183	OHX	1	0
86	6	2103	OHX	1	0
86	2	2108	OHX	1	0
86	l5	304	OHX	1	0
86	1	4160	OHX	4	0
86	5	3949	OHX	2	0
86	5	4163	OHX	1	0
86	6	2070	OHX	1	0
86	6	2079	OHX	1	0
86	2	2143	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2179	OHX	1	0
86	6	2182	OHX	1	0
86	1	3997	OHX	2	0
86	1	3988	OHX	2	0
86	2	2038	OHX	2	0
86	5	4175	OHX	1	0
86	1	4092	OHX	1	0
86	6	2075	OHX	1	0
86	5	4218	OHX	2	0
86	5	4187	OHX	1	0
86	6	2096	OHX	2	0
86	O7	104	OHX	7	0
86	5	4023	OHX	1	0
86	6	2073	OHX	1	0
86	5	4230	OHX	1	0
86	1	3957	OHX	3	0
86	5	4194	OHX	2	0
86	1	3905	OHX	1	0
86	2	2096	OHX	1	0
86	1	4141	OHX	2	0
86	5	3938	OHX	1	0
86	6	2146	OHX	1	0
86	1	4191	OHX	1	0
86	1	4139	OHX	1	0
86	1	4059	OHX	2	0
86	5	4069	OHX	1	0
86	6	2195	OHX	1	0
86	5	4087	OHX	2	0
86	1	4050	OHX	5	0
86	m5	306	OHX	1	0
86	1	4036	OHX	1	0
86	s1	302	OHX	2	0
86	2	2089	OHX	3	0
86	1	3874	OHX	1	0
86	5	3950	OHX	3	0
86	1	3920	OHX	2	0
86	5	3963	OHX	1	0
86	5	4045	OHX	1	0
86	1	3961	OHX	1	0
86	5	3899	OHX	1	0
86	3	216	OHX	1	0
86	5	4164	OHX	1	0

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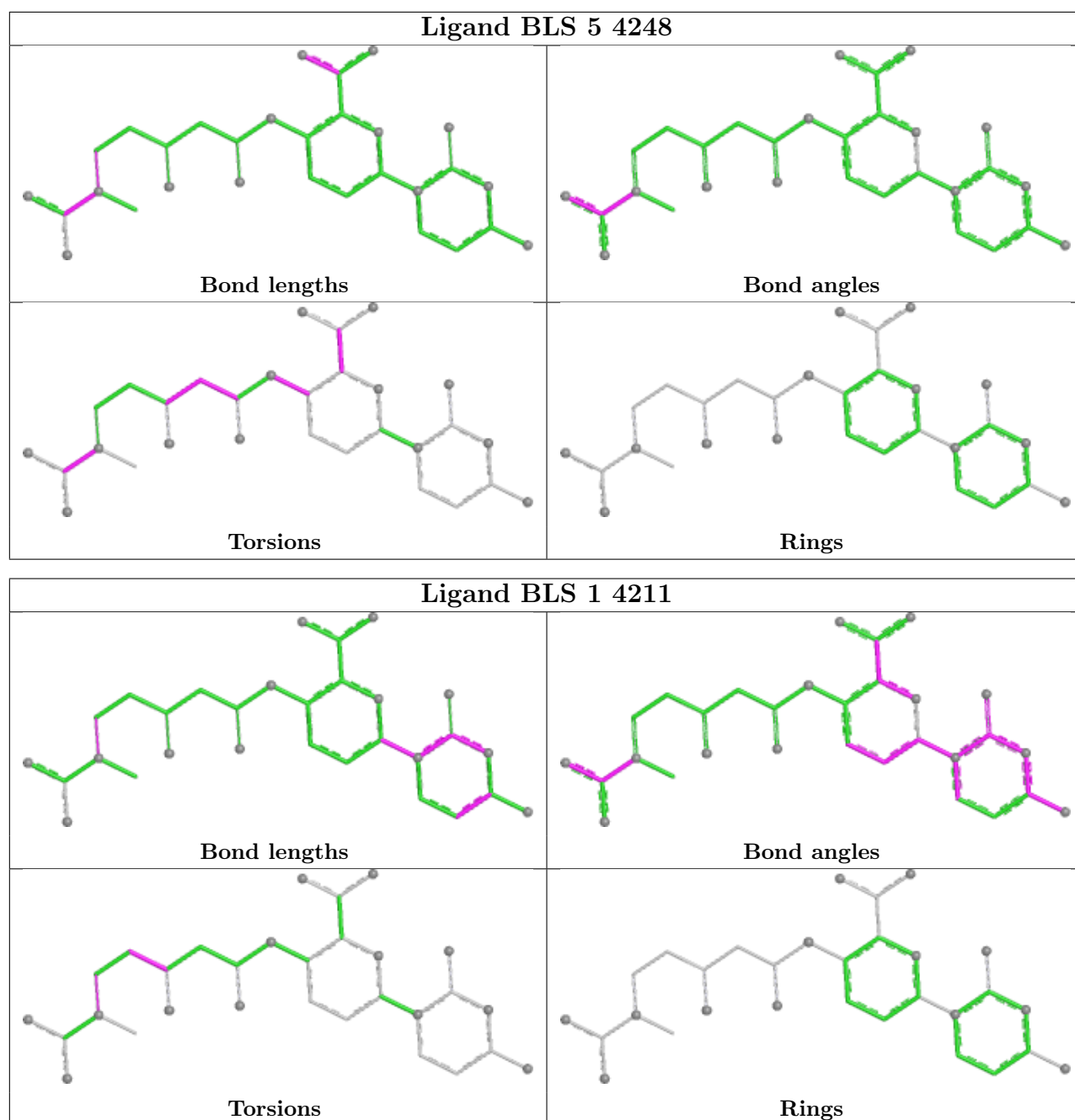
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	o7	103	OHX	1	0
86	2	2024	OHX	1	0
86	2	2146	OHX	6	0
86	1	3979	OHX	1	0
86	2	2110	OHX	3	0
86	5	4066	OHX	1	0
86	1	3996	OHX	1	0
86	5	3902	OHX	2	0
86	M9	202	OHX	1	0
86	1	3962	OHX	1	0
86	6	2154	OHX	1	0
86	1	4089	OHX	1	0
86	1	4129	OHX	1	0
86	5	4186	OHX	2	0
86	1	3935	OHX	2	0
86	2	2045	OHX	1	0
86	1	4180	OHX	1	0
88	1	4211	BLS	2	0
86	5	3947	OHX	1	0
86	1	3947	OHX	1	0
86	1	4005	OHX	1	0
86	n9	103	OHX	1	0
86	1	4166	OHX	1	0
86	5	4018	OHX	2	0
86	1	4048	OHX	1	0
86	6	2065	OHX	1	0
86	6	2189	OHX	1	0
86	5	4206	OHX	1	0
86	1	4135	OHX	2	0
86	O3	201	OHX	1	0
86	8	228	OHX	1	0
86	2	2160	OHX	1	0
86	1	4034	OHX	2	0
86	4	226	OHX	1	0
86	5	4232	OHX	4	0
86	5	4104	OHX	1	0
86	2	2168	OHX	1	0
86	1	4025	OHX	1	0
86	1	4065	OHX	1	0
86	2	2057	OHX	2	0
86	2	2154	OHX	1	0
86	2	2098	OHX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2109	OHX	1	0
86	2	2122	OHX	1	0
86	1	4169	OHX	6	0
86	1	4076	OHX	2	0
86	6	2059	OHX	5	0
86	5	3897	OHX	1	0
86	1	3869	OHX	1	0
86	1	4138	OHX	1	0
86	1	4143	OHX	6	0
86	1	3951	OHX	5	0
86	1	4033	OHX	2	0
86	6	2136	OHX	2	0
86	5	3951	OHX	1	0
86	5	4142	OHX	1	0
86	5	4184	OHX	2	0
86	2	2115	OHX	1	0
86	o3	203	OHX	1	0
86	1	3982	OHX	1	0
86	6	2081	OHX	1	0
86	5	4060	OHX	4	0
86	5	4139	OHX	3	0
86	5	3929	OHX	1	0
86	5	4085	OHX	7	0
86	6	2117	OHX	2	0
86	5	4231	OHX	1	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](#)

There are no chain breaks in this entry.

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	2	1750/1800 (97%)	0.18	96 (5%) 30 19	61, 94, 179, 258	0
1	6	1795/1800 (99%)	0.13	72 (4%) 42 25	51, 84, 200, 293	0
2	S0	206/251 (82%)	0.50	11 (5%) 32 20	102, 118, 131, 153	0
2	s0	206/251 (82%)	0.36	6 (2%) 53 32	85, 103, 119, 128	0
3	S1	214/254 (84%)	0.70	20 (9%) 14 10	103, 132, 156, 161	0
3	s1	216/254 (85%)	0.22	6 (2%) 55 33	77, 92, 120, 138	0
4	S2	217/253 (85%)	0.34	6 (2%) 55 33	78, 96, 115, 139	0
4	s2	217/253 (85%)	0.78	29 (13%) 7 6	63, 80, 106, 123	0
5	S3	223/239 (93%)	0.49	15 (6%) 24 16	79, 97, 128, 158	0
5	s3	223/239 (93%)	0.63	22 (9%) 13 9	83, 107, 137, 152	0
6	S4	260/260 (100%)	0.53	16 (6%) 26 17	69, 91, 105, 128	0
6	s4	260/260 (100%)	0.55	20 (7%) 19 14	59, 86, 103, 125	0
7	S5	206/224 (91%)	0.71	12 (5%) 29 18	96, 118, 140, 155	0
7	s5	206/224 (91%)	0.66	11 (5%) 32 20	75, 99, 130, 154	0
8	S6	226/236 (95%)	0.77	27 (11%) 9 7	69, 99, 127, 139	0
8	s6	218/236 (92%)	0.72	28 (12%) 7 7	58, 83, 114, 141	0
9	S7	184/189 (97%)	0.61	15 (8%) 17 13	92, 123, 146, 151	0
9	s7	186/189 (98%)	0.53	14 (7%) 20 14	80, 113, 142, 151	0
10	S8	188/200 (94%)	0.49	11 (5%) 28 18	60, 77, 123, 136	0
10	s8	188/200 (94%)	0.49	16 (8%) 16 12	54, 81, 135, 154	0
11	S9	185/196 (94%)	0.88	25 (13%) 7 6	89, 102, 138, 173	0
11	s9	185/196 (94%)	0.59	15 (8%) 18 13	69, 88, 131, 167	0
12	C0	96/105 (91%)	0.47	5 (5%) 33 20	83, 104, 134, 152	0
12	c0	96/105 (91%)	0.90	18 (18%) 3 4	95, 129, 149, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	0.70	13 (8%) 17 12	65, 80, 140, 148	0
13	c1	146/155 (94%)	0.77	16 (10%) 10 8	62, 79, 118, 142	0
14	C2	124/142 (87%)	1.12	20 (16%) 4 5	124, 142, 161, 171	0
14	c2	124/142 (87%)	0.92	13 (10%) 11 9	169, 188, 204, 211	0
15	C3	150/150 (100%)	0.39	6 (4%) 42 25	72, 94, 112, 115	0
15	c3	150/150 (100%)	0.27	5 (3%) 49 29	68, 85, 104, 122	0
16	C4	127/136 (93%)	1.10	22 (17%) 4 4	74, 135, 153, 161	0
16	c4	128/136 (94%)	0.51	3 (2%) 61 38	72, 92, 102, 107	0
17	C5	124/141 (87%)	0.36	2 (1%) 70 46	74, 92, 132, 145	0
17	c5	135/141 (95%)	1.08	17 (12%) 8 7	81, 102, 135, 190	0
18	C6	141/142 (99%)	0.65	9 (6%) 25 17	84, 113, 122, 128	0
18	c6	142/142 (100%)	0.65	11 (7%) 19 14	72, 93, 112, 135	0
19	C7	120/136 (88%)	0.42	6 (5%) 34 20	96, 117, 143, 147	0
19	c7	117/136 (86%)	0.76	18 (15%) 5 5	85, 102, 128, 141	0
20	C8	145/145 (100%)	0.62	12 (8%) 17 13	73, 102, 133, 142	0
20	c8	145/145 (100%)	0.51	5 (3%) 48 29	77, 89, 114, 130	0
21	C9	143/143 (100%)	0.82	11 (7%) 19 14	88, 104, 127, 141	0
21	c9	143/143 (100%)	0.64	10 (6%) 22 15	72, 85, 110, 134	0
22	D0	107/120 (89%)	0.60	6 (5%) 30 19	83, 115, 147, 151	0
22	d0	110/120 (91%)	0.70	9 (8%) 17 13	74, 109, 160, 202	0
23	D1	87/87 (100%)	0.34	4 (4%) 37 21	99, 107, 126, 139	0
23	d1	87/87 (100%)	0.28	3 (3%) 48 29	77, 88, 113, 129	0
24	D2	129/129 (100%)	0.36	5 (3%) 43 25	77, 89, 97, 104	0
24	d2	129/129 (100%)	0.12	2 (1%) 70 46	64, 75, 86, 99	0
25	D3	144/144 (100%)	0.26	3 (2%) 63 39	58, 70, 81, 106	0
25	d3	144/144 (100%)	0.10	2 (1%) 73 49	48, 58, 71, 90	0
26	D4	134/134 (100%)	0.40	5 (3%) 45 27	75, 103, 123, 132	0
26	d4	134/134 (100%)	0.61	17 (12%) 8 7	62, 85, 103, 139	0
27	D5	70/107 (65%)	0.79	10 (14%) 6 6	112, 130, 146, 148	0
27	d5	69/107 (64%)	0.69	6 (8%) 16 11	84, 114, 130, 133	0
28	D6	97/97 (100%)	0.62	4 (4%) 41 24	80, 100, 161, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.47	7 (7%) 21 15	65, 79, 105, 114	0
29	D7	81/81 (100%)	0.35	3 (3%) 45 27	90, 107, 150, 157	0
29	d7	81/81 (100%)	0.24	2 (2%) 58 35	81, 96, 135, 149	0
30	D8	63/66 (95%)	0.68	4 (6%) 26 17	110, 129, 144, 147	0
30	d8	63/66 (95%)	0.40	3 (4%) 35 21	92, 116, 134, 147	0
31	D9	53/55 (96%)	0.70	4 (7%) 20 14	80, 85, 105, 113	0
31	d9	53/55 (96%)	1.16	16 (30%) 1 2	74, 83, 126, 148	0
32	E0	60/60 (100%)	0.58	5 (8%) 17 13	76, 100, 140, 147	0
33	E1	71/76 (93%)	0.65	6 (8%) 16 12	99, 123, 139, 143	0
33	e1	76/76 (100%)	1.01	7 (9%) 14 10	127, 158, 172, 178	0
34	SR	318/318 (100%)	0.58	23 (7%) 21 15	69, 123, 149, 180	0
34	sR	318/318 (100%)	0.83	37 (11%) 9 7	103, 125, 145, 168	0
35	SM	159/273 (58%)	0.82	25 (15%) 5 5	64, 96, 142, 152	0
35	sM	104/273 (38%)	0.86	18 (17%) 4 4	67, 103, 179, 188	0
36	1	3149/3396 (92%)	0.04	196 (6%) 26 17	31, 56, 144, 283	0
36	5	3150/3396 (92%)	0.07	241 (7%) 19 14	32, 58, 136, 278	0
37	3	121/121 (100%)	0.27	17 (14%) 6 6	43, 68, 84, 89	0
37	7	121/121 (100%)	-0.03	3 (2%) 58 35	40, 58, 74, 85	0
38	4	158/158 (100%)	-0.35	0 100 100	40, 60, 104, 160	0
38	8	158/158 (100%)	-0.13	6 (3%) 44 26	45, 71, 119, 144	0
39	L2	252/253 (99%)	0.35	14 (5%) 30 19	42, 55, 74, 83	0
39	l2	252/253 (99%)	0.79	38 (15%) 5 5	45, 63, 86, 101	0
40	L3	386/386 (100%)	-0.02	5 (1%) 75 51	36, 54, 73, 110	0
40	l3	386/386 (100%)	0.10	15 (3%) 43 25	33, 45, 61, 97	0
41	L4	361/361 (100%)	0.29	28 (7%) 19 13	35, 48, 64, 77	0
41	l4	361/361 (100%)	0.59	45 (12%) 8 7	41, 53, 76, 91	0
42	L5	296/296 (100%)	0.34	20 (6%) 23 16	52, 74, 96, 122	0
42	l5	294/296 (99%)	0.32	15 (5%) 33 20	44, 62, 93, 138	0
43	L6	156/175 (89%)	0.11	3 (1%) 66 42	41, 49, 76, 95	0
43	l6	157/175 (89%)	-0.02	2 (1%) 75 51	41, 50, 74, 89	0
44	L7	222/243 (91%)	0.17	6 (2%) 56 33	34, 43, 82, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	-0.04	5 (2%) 62 39	33, 41, 84, 138	0
45	L8	233/255 (91%)	0.25	7 (3%) 52 31	65, 81, 122, 138	0
45	l8	231/255 (90%)	0.47	14 (6%) 27 17	79, 95, 132, 141	0
46	L9	191/191 (100%)	0.14	5 (2%) 57 34	49, 59, 71, 92	0
46	l9	191/191 (100%)	0.31	12 (6%) 26 17	40, 49, 74, 111	0
47	M0	211/220 (95%)	0.17	8 (3%) 44 26	39, 50, 85, 123	0
47	m0	213/220 (96%)	0.13	6 (2%) 55 33	40, 60, 90, 105	0
48	M1	169/173 (97%)	0.43	9 (5%) 32 20	57, 77, 93, 106	0
48	m1	169/173 (97%)	0.24	4 (2%) 59 37	47, 65, 81, 95	0
49	M3	193/198 (97%)	0.07	11 (5%) 29 18	43, 59, 106, 135	0
49	m3	194/198 (97%)	0.36	15 (7%) 19 14	49, 70, 116, 144	0
50	M4	136/137 (99%)	0.02	6 (4%) 39 23	43, 50, 66, 81	0
50	m4	137/137 (100%)	-0.07	3 (2%) 62 39	36, 45, 69, 82	0
51	M5	203/203 (100%)	0.34	11 (5%) 31 19	37, 54, 66, 73	0
51	m5	203/203 (100%)	0.62	25 (12%) 8 7	52, 66, 80, 88	0
52	M6	197/198 (99%)	-0.03	6 (3%) 52 31	34, 41, 64, 68	0
52	m6	197/198 (99%)	0.01	2 (1%) 79 56	29, 35, 63, 71	0
53	M7	183/183 (100%)	0.11	5 (2%) 56 33	41, 49, 119, 148	0
53	m7	155/183 (84%)	-0.12	1 (0%) 85 66	36, 46, 60, 95	0
54	M8	185/185 (100%)	0.33	12 (6%) 25 17	40, 49, 70, 86	0
54	m8	185/185 (100%)	0.50	24 (12%) 7 6	46, 54, 64, 69	0
55	M9	188/188 (100%)	0.34	13 (6%) 23 15	53, 73, 156, 164	0
55	m9	188/188 (100%)	0.49	19 (10%) 12 9	56, 71, 148, 159	0
56	N0	172/172 (100%)	0.12	5 (2%) 53 32	40, 49, 62, 68	0
56	n0	172/172 (100%)	-0.02	6 (3%) 47 28	34, 42, 56, 71	0
57	N1	159/159 (100%)	0.35	8 (5%) 34 20	41, 52, 101, 110	0
57	n1	159/159 (100%)	0.14	6 (3%) 44 26	39, 48, 91, 102	0
58	N2	100/120 (83%)	0.52	6 (6%) 27 17	85, 104, 119, 154	0
58	n2	98/120 (81%)	0.22	1 (1%) 79 56	80, 94, 107, 115	0
59	N3	136/136 (100%)	0.20	3 (2%) 62 39	39, 52, 67, 81	0
59	n3	136/136 (100%)	0.08	4 (2%) 53 32	33, 45, 64, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	0.84	16 (16%) 4 4	50, 68, 177, 185	0
60	n4	135/155 (87%)	0.63	9 (6%) 24 16	44, 90, 137, 154	0
61	N5	121/141 (85%)	0.23	4 (3%) 49 29	50, 65, 87, 134	0
61	n5	120/141 (85%)	0.53	18 (15%) 5 5	57, 74, 101, 109	0
62	N6	126/126 (100%)	0.07	3 (2%) 59 37	47, 59, 72, 85	0
62	n6	126/126 (100%)	0.12	1 (0%) 82 61	50, 66, 87, 97	0
63	N7	135/135 (100%)	0.12	0 100 100	74, 93, 114, 129	0
63	n7	135/135 (100%)	0.50	7 (5%) 33 20	91, 105, 124, 135	0
64	N8	148/148 (100%)	0.32	15 (10%) 12 9	40, 49, 77, 92	0
64	n8	148/148 (100%)	0.17	7 (4%) 36 21	42, 58, 81, 86	0
65	N9	58/58 (100%)	0.35	3 (5%) 33 20	51, 60, 102, 108	0
65	n9	58/58 (100%)	0.34	4 (6%) 23 15	47, 60, 90, 104	0
66	O0	97/104 (93%)	0.12	3 (3%) 51 31	74, 84, 116, 122	0
66	o0	100/104 (96%)	0.19	3 (3%) 52 31	79, 90, 123, 130	0
67	O1	109/112 (97%)	0.05	1 (0%) 81 58	50, 64, 105, 135	0
67	o1	109/112 (97%)	0.33	5 (4%) 37 21	45, 57, 103, 130	0
68	O2	127/129 (98%)	0.04	2 (1%) 70 46	33, 45, 62, 81	0
68	o2	127/129 (98%)	-0.03	0 100 100	35, 50, 65, 87	0
69	O3	106/106 (100%)	-0.08	2 (1%) 66 42	35, 42, 64, 73	0
69	o3	106/106 (100%)	-0.09	1 (0%) 81 58	31, 40, 68, 88	0
70	O4	112/120 (93%)	0.20	3 (2%) 56 33	53, 71, 108, 125	0
70	o4	112/120 (93%)	0.53	8 (7%) 22 15	59, 81, 123, 135	0
71	O5	119/119 (100%)	0.24	4 (3%) 48 29	47, 68, 77, 81	0
71	o5	119/119 (100%)	0.11	4 (3%) 48 29	60, 76, 92, 102	0
72	O6	99/99 (100%)	0.21	4 (4%) 42 25	58, 70, 99, 119	0
72	o6	99/99 (100%)	0.08	0 100 100	66, 83, 112, 135	0
73	O7	87/87 (100%)	0.24	3 (3%) 48 29	41, 50, 82, 107	0
73	o7	87/87 (100%)	0.30	7 (8%) 18 13	52, 58, 92, 128	0
74	O8	77/77 (100%)	0.02	0 100 100	76, 91, 115, 128	0
74	o8	77/77 (100%)	0.23	2 (2%) 57 34	86, 99, 111, 115	0
75	O9	50/50 (100%)	0.10	3 (6%) 27 17	49, 56, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	0.23	1 (2%) 65 41	57, 62, 74, 91	0
76	Q0	52/52 (100%)	-0.17	1 (1%) 66 42	46, 53, 82, 94	0
76	q0	52/52 (100%)	-0.27	0 100 100	34, 42, 58, 69	0
77	Q1	25/25 (100%)	0.12	2 (8%) 18 13	59, 63, 68, 70	0
77	q1	25/25 (100%)	-0.15	0 100 100	53, 59, 73, 87	0
78	Q2	105/105 (100%)	0.37	9 (8%) 16 12	44, 62, 90, 129	0
78	q2	105/105 (100%)	0.58	12 (11%) 10 7	54, 64, 86, 114	0
79	Q3	91/91 (100%)	0.10	4 (4%) 39 23	49, 59, 82, 100	0
79	q3	91/91 (100%)	0.41	8 (8%) 15 11	48, 63, 79, 89	0
80	e0	62/62 (100%)	0.99	14 (22%) 2 3	63, 86, 124, 155	0
81	p0	143/311 (45%)	0.97	24 (16%) 4 4	89, 108, 197, 216	0
82	m2	0/160	-	-	-	-
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35346 (93%)	0.30	2084 (6%) 26 17	29, 75, 140, 293	0

The worst 5 of 2084 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	l4	62	ALA	12.6
17	c5	4	ALA	11.2
60	N4	75	THR	11.0
41	l4	63	GLU	10.9
41	l4	65	TRP	9.7

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 oligosaccharides 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(Å ²)	Q<0.9
85	MG	1	3810	1/1	-0.11	0.32	133,133,133,133	0
85	MG	2	1963	1/1	-0.02	0.20	175,175,175,175	0
85	MG	2	2003	1/1	0.05	0.31	119,119,119,119	0
85	MG	6	2039	1/1	0.06	0.37	112,112,112,112	0
85	MG	2	1968	1/1	0.10	0.39	137,137,137,137	0
85	MG	2	1959	1/1	0.17	0.45	96,96,96,96	0
85	MG	6	1923	1/1	0.20	0.39	115,115,115,115	0
85	MG	1	3800	1/1	0.28	0.42	180,180,180,180	0
85	MG	1	3695	1/1	0.31	0.21	81,81,81,81	0
85	MG	6	1998	1/1	0.33	0.39	109,109,109,109	0
85	MG	2	1994	1/1	0.35	0.35	125,125,125,125	0
85	MG	6	1939	1/1	0.36	0.43	90,90,90,90	0
85	MG	5	3875	1/1	0.39	0.40	97,97,97,97	0
85	MG	2	1987	1/1	0.40	0.41	105,105,105,105	0
85	MG	6	2002	1/1	0.41	0.35	84,84,84,84	0
85	MG	2	1953	1/1	0.41	0.39	107,107,107,107	0
85	MG	5	3815	1/1	0.41	0.23	114,114,114,114	0
85	MG	2	2016	1/1	0.41	0.33	84,84,84,84	0
85	MG	2	1954	1/1	0.42	0.34	101,101,101,101	0
85	MG	2	2022	1/1	0.43	0.23	134,134,134,134	0
85	MG	1	3419	1/1	0.44	0.38	86,86,86,86	0
85	MG	2	1980	1/1	0.45	0.42	69,69,69,69	0
85	MG	2	1928	1/1	0.46	0.39	97,97,97,97	0
85	MG	M3	202	1/1	0.48	0.24	108,108,108,108	0
85	MG	5	3703	1/1	0.48	0.36	103,103,103,103	0
85	MG	2	1951	1/1	0.49	0.39	96,96,96,96	0
85	MG	6	1964	1/1	0.49	0.18	80,80,80,80	0
85	MG	1	3844	1/1	0.50	0.20	95,95,95,95	0
85	MG	5	3751	1/1	0.50	0.40	107,107,107,107	0
85	MG	2	1944	1/1	0.50	0.22	68,68,68,68	0
85	MG	5	3466	1/1	0.50	0.33	102,102,102,102	0
85	MG	2	1977	1/1	0.51	0.32	85,85,85,85	0
85	MG	6	2045	1/1	0.52	0.38	98,98,98,98	0
85	MG	2	1915	1/1	0.52	0.45	73,73,73,73	0
85	MG	2	1966	1/1	0.52	0.33	85,85,85,85	0
85	MG	6	1979	1/1	0.53	0.13	81,81,81,81	0
85	MG	2	2006	1/1	0.53	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1990	1/1	0.54	0.20	110,110,110,110	0
85	MG	5	3806	1/1	0.54	0.20	81,81,81,81	0
85	MG	5	3879	1/1	0.54	0.34	79,79,79,79	0
85	MG	5	3705	1/1	0.55	0.28	100,100,100,100	0
85	MG	5	3449	1/1	0.55	0.18	67,67,67,67	0
85	MG	5	3629	1/1	0.56	0.38	90,90,90,90	0
85	MG	1	3637	1/1	0.57	0.34	63,63,63,63	0
85	MG	2	2000	1/1	0.58	0.34	91,91,91,91	0
85	MG	1	3760	1/1	0.58	0.10	60,60,60,60	0
85	MG	2	1969	1/1	0.59	0.34	89,89,89,89	0
85	MG	6	1960	1/1	0.59	0.45	76,76,76,76	0
85	MG	2	1937	1/1	0.59	0.30	66,66,66,66	0
85	MG	6	1971	1/1	0.60	0.31	75,75,75,75	0
85	MG	2	1948	1/1	0.60	0.29	91,91,91,91	0
85	MG	2	1984	1/1	0.61	0.24	76,76,76,76	0
85	MG	6	1909	1/1	0.61	0.33	109,109,109,109	0
85	MG	6	1981	1/1	0.62	0.28	90,90,90,90	0
85	MG	1	3418	1/1	0.62	0.28	91,91,91,91	0
85	MG	2	1909	1/1	0.62	0.40	73,73,73,73	0
85	MG	5	3494	1/1	0.62	0.34	42,42,42,42	0
85	MG	5	3827	1/1	0.62	0.15	48,48,48,48	0
85	MG	6	2014	1/1	0.62	0.17	149,149,149,149	0
85	MG	1	3722	1/1	0.62	0.16	68,68,68,68	0
85	MG	6	1995	1/1	0.63	0.33	77,77,77,77	0
85	MG	6	1965	1/1	0.63	0.31	82,82,82,82	0
85	MG	5	3469	1/1	0.63	0.24	121,121,121,121	0
85	MG	M1	201	1/1	0.63	0.28	64,64,64,64	0
85	MG	5	3763	1/1	0.63	0.16	104,104,104,104	0
86	OHX	1	4183	7/7	0.63	0.17	201,201,201,201	0
85	MG	2	1939	1/1	0.64	0.34	73,73,73,73	0
85	MG	5	3677	1/1	0.64	0.30	89,89,89,89	0
85	MG	6	1932	1/1	0.64	0.32	81,81,81,81	0
85	MG	1	3492	1/1	0.64	0.26	84,84,84,84	0
85	MG	2	1961	1/1	0.64	0.31	65,65,65,65	0
85	MG	6	1962	1/1	0.64	0.28	95,95,95,95	0
85	MG	5	3766	1/1	0.65	0.23	102,102,102,102	0
85	MG	6	1949	1/1	0.65	0.29	58,58,58,58	0
85	MG	2	2019	1/1	0.65	0.36	70,70,70,70	0
85	MG	6	1919	1/1	0.65	0.30	68,68,68,68	0
85	MG	5	3850	1/1	0.65	0.26	83,83,83,83	0
85	MG	2	1914	1/1	0.65	0.42	59,59,59,59	0
85	MG	6	1902	1/1	0.65	0.31	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	o4	203	1/1	0.65	0.16	59,59,59,59	0
85	MG	6	1907	1/1	0.65	0.28	79,79,79,79	0
85	MG	2	1917	1/1	0.66	0.38	61,61,61,61	0
85	MG	6	1904	1/1	0.66	0.37	73,73,73,73	0
85	MG	6	2029	1/1	0.66	0.27	105,105,105,105	0
85	MG	5	3630	1/1	0.67	0.36	54,54,54,54	0
85	MG	6	1950	1/1	0.67	0.44	65,65,65,65	0
85	MG	2	1933	1/1	0.67	0.42	74,74,74,74	0
85	MG	1	3586	1/1	0.67	0.40	51,51,51,51	0
85	MG	1	3604	1/1	0.67	0.14	81,81,81,81	0
85	MG	2	1930	1/1	0.68	0.31	74,74,74,74	0
85	MG	6	1992	1/1	0.68	0.21	58,58,58,58	0
85	MG	6	2034	1/1	0.68	0.25	94,94,94,94	0
85	MG	D0	201	1/1	0.68	0.39	72,72,72,72	0
85	MG	2	2002	1/1	0.68	0.14	102,102,102,102	0
85	MG	5	3775	1/1	0.68	0.15	66,66,66,66	0
85	MG	2	1996	1/1	0.68	0.29	98,98,98,98	0
86	OHX	5	4230	7/7	0.68	0.19	178,178,178,178	0
85	MG	1	3668	1/1	0.69	0.26	73,73,73,73	0
85	MG	3	201	1/1	0.69	0.30	66,66,66,66	0
85	MG	5	3525	1/1	0.69	0.50	64,64,64,64	0
85	MG	6	1922	1/1	0.69	0.25	78,78,78,78	0
85	MG	2	1936	1/1	0.69	0.41	60,60,60,60	0
85	MG	5	3673	1/1	0.69	0.13	98,98,98,98	0
85	MG	2	1924	1/1	0.69	0.46	83,83,83,83	0
85	MG	1	3632	1/1	0.69	0.28	70,70,70,70	0
85	MG	7	201	1/1	0.69	0.39	47,47,47,47	0
85	MG	2	1972	1/1	0.69	0.30	95,95,95,95	0
85	MG	1	3648	1/1	0.69	0.33	95,95,95,95	0
85	MG	6	1953	1/1	0.69	0.22	63,63,63,63	0
85	MG	6	1938	1/1	0.70	0.39	65,65,65,65	0
85	MG	1	3814	1/1	0.70	0.20	51,51,51,51	0
85	MG	5	3797	1/1	0.70	0.12	174,174,174,174	0
85	MG	3	209	1/1	0.70	0.39	56,56,56,56	0
85	MG	2	1952	1/1	0.70	0.11	108,108,108,108	0
85	MG	5	3825	1/1	0.70	0.16	85,85,85,85	0
85	MG	6	1951	1/1	0.70	0.33	64,64,64,64	0
85	MG	6	2006	1/1	0.71	0.28	69,69,69,69	0
85	MG	2	1992	1/1	0.71	0.15	66,66,66,66	0
85	MG	7	210	1/1	0.71	0.36	51,51,51,51	0
85	MG	5	3713	1/1	0.71	0.32	62,62,62,62	0
85	MG	5	3721	1/1	0.71	0.14	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1926	1/1	0.71	0.35	92,92,92,92	0
85	MG	5	3681	1/1	0.72	0.39	94,94,94,94	0
85	MG	2	1986	1/1	0.72	0.22	74,74,74,74	0
85	MG	1	3780	1/1	0.72	0.43	49,49,49,49	0
85	MG	1	3544	1/1	0.72	0.22	59,59,59,59	0
85	MG	5	3808	1/1	0.72	0.17	69,69,69,69	0
85	MG	1	3752	1/1	0.72	0.18	106,106,106,106	0
85	MG	6	2021	1/1	0.72	0.14	94,94,94,94	0
85	MG	6	1967	1/1	0.72	0.33	76,76,76,76	0
85	MG	2	1970	1/1	0.73	0.28	69,69,69,69	0
85	MG	6	1993	1/1	0.73	0.35	62,62,62,62	0
85	MG	5	3478	1/1	0.73	0.30	71,71,71,71	0
85	MG	2	1983	1/1	0.73	0.32	74,74,74,74	0
85	MG	6	1918	1/1	0.73	0.36	43,43,43,43	0
85	MG	1	3526	1/1	0.73	0.36	48,48,48,48	0
85	MG	6	2005	1/1	0.73	0.31	80,80,80,80	0
85	MG	2	2018	1/1	0.73	0.27	73,73,73,73	0
85	MG	2	1941	1/1	0.73	0.24	71,71,71,71	0
85	MG	1	3757	1/1	0.73	0.17	52,52,52,52	0
85	MG	5	3877	1/1	0.73	0.15	64,64,64,64	0
85	MG	2	1976	1/1	0.73	0.30	62,62,62,62	0
85	MG	2	1950	1/1	0.73	0.41	88,88,88,88	0
85	MG	6	2036	1/1	0.73	0.31	74,74,74,74	0
85	MG	6	1945	1/1	0.73	0.48	73,73,73,73	0
85	MG	2	1978	1/1	0.73	0.39	83,83,83,83	0
86	OHX	1	4186	7/7	0.73	0.20	167,167,167,167	0
85	MG	6	1991	1/1	0.73	0.34	79,79,79,79	0
85	MG	5	3658	1/1	0.74	0.37	61,61,61,61	0
85	MG	5	3799	1/1	0.74	0.26	99,99,99,99	0
85	MG	6	1987	1/1	0.74	0.19	76,76,76,76	0
85	MG	5	3728	1/1	0.74	0.25	73,73,73,73	0
85	MG	L8	301	1/1	0.74	0.20	69,69,69,69	0
85	MG	7	217	1/1	0.74	0.36	74,74,74,74	0
85	MG	m1	201	1/1	0.74	0.42	63,63,63,63	0
85	MG	o4	202	1/1	0.74	0.25	79,79,79,79	0
85	MG	5	3541	1/1	0.74	0.30	78,78,78,78	0
86	OHX	1	4123	7/7	0.74	0.16	180,180,180,180	0
85	MG	S4	301	1/1	0.74	0.18	71,71,71,71	0
85	MG	1	3746	1/1	0.74	0.18	62,62,62,62	0
86	OHX	6	2191	7/7	0.74	0.16	192,192,192,192	0
85	MG	5	3869	1/1	0.74	0.38	46,46,46,46	0
85	MG	6	1976	1/1	0.75	0.27	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	8	209	1/1	0.75	0.28	87,87,87,87	0
85	MG	1	3856	1/1	0.75	0.20	65,65,65,65	0
85	MG	2	1971	1/1	0.75	0.23	76,76,76,76	0
85	MG	6	1966	1/1	0.75	0.20	82,82,82,82	0
86	OHX	2	2160	7/7	0.75	0.19	162,162,162,162	0
85	MG	6	1990	1/1	0.75	0.31	75,75,75,75	0
85	MG	2	2020	1/1	0.75	0.22	50,50,50,50	0
85	MG	5	3548	1/1	0.75	0.37	60,60,60,60	0
85	MG	c9	201	1/1	0.75	0.17	65,65,65,65	0
86	OHX	5	4229	7/7	0.75	0.16	180,180,180,180	0
85	MG	2	1993	1/1	0.75	0.23	77,77,77,77	0
85	MG	2	1955	1/1	0.76	0.28	72,72,72,72	0
85	MG	1	3761	1/1	0.76	0.20	64,64,64,64	0
85	MG	6	1985	1/1	0.76	0.28	82,82,82,82	0
85	MG	5	3741	1/1	0.76	0.37	47,47,47,47	0
85	MG	5	3744	1/1	0.76	0.35	54,54,54,54	0
85	MG	1	3768	1/1	0.76	0.13	68,68,68,68	0
85	MG	6	1989	1/1	0.76	0.18	88,88,88,88	0
85	MG	8	208	1/1	0.76	0.08	76,76,76,76	0
85	MG	1	3772	1/1	0.76	0.12	68,68,68,68	0
85	MG	2	1929	1/1	0.76	0.38	65,65,65,65	0
85	MG	5	3796	1/1	0.76	0.12	77,77,77,77	0
85	MG	2	1908	1/1	0.76	0.24	78,78,78,78	0
85	MG	6	2044	1/1	0.76	0.27	84,84,84,84	0
85	MG	2	1962	1/1	0.76	0.26	76,76,76,76	0
86	OHX	1	4138	7/7	0.76	0.20	167,167,167,167	0
85	MG	2	1931	1/1	0.76	0.35	61,61,61,61	0
85	MG	5	3418	1/1	0.76	0.37	31,31,31,31	0
85	MG	5	3695	1/1	0.76	0.17	72,72,72,72	0
86	OHX	5	4137	7/7	0.76	0.16	178,178,178,178	0
86	OHX	5	4155	7/7	0.76	0.19	161,161,161,161	0
86	OHX	5	4183	7/7	0.76	0.14	195,195,195,195	0
85	MG	1	3839	1/1	0.76	0.20	54,54,54,54	0
85	MG	1	3663	1/1	0.76	0.40	80,80,80,80	0
85	MG	6	1994	1/1	0.77	0.13	56,56,56,56	0
85	MG	2	1935	1/1	0.77	0.31	55,55,55,55	0
85	MG	5	3680	1/1	0.77	0.36	67,67,67,67	0
85	MG	5	3781	1/1	0.77	0.15	61,61,61,61	0
85	MG	2	1946	1/1	0.77	0.18	92,92,92,92	0
85	MG	12	301	1/1	0.77	0.24	43,43,43,43	0
85	MG	1	3703	1/1	0.77	0.16	49,49,49,49	0
85	MG	5	3492	1/1	0.77	0.29	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	2003	1/1	0.77	0.24	74,74,74,74	0
85	MG	5	3706	1/1	0.77	0.23	44,44,44,44	0
85	MG	5	3810	1/1	0.77	0.11	43,43,43,43	0
85	MG	6	1924	1/1	0.77	0.41	46,46,46,46	0
85	MG	5	3719	1/1	0.77	0.22	66,66,66,66	0
85	MG	1	3797	1/1	0.77	0.19	67,67,67,67	0
85	MG	6	2007	1/1	0.77	0.07	64,64,64,64	0
85	MG	5	3858	1/1	0.77	0.24	78,78,78,78	0
85	MG	5	3732	1/1	0.77	0.38	80,80,80,80	0
85	MG	d6	102	1/1	0.77	0.31	71,71,71,71	0
86	OHX	5	4202	7/7	0.77	0.18	172,172,172,172	0
86	OHX	5	4217	7/7	0.77	0.16	179,179,179,179	0
85	MG	6	1934	1/1	0.77	0.24	61,61,61,61	0
85	MG	5	3430	1/1	0.77	0.24	73,73,73,73	0
86	OHX	5	4236	7/7	0.77	0.13	250,250,250,250	0
85	MG	1	3416	1/1	0.78	0.27	44,44,44,44	0
85	MG	6	1933	1/1	0.78	0.33	86,86,86,86	0
86	OHX	2	2149	7/7	0.78	0.13	199,199,199,199	0
86	OHX	2	2159	7/7	0.78	0.15	184,184,184,184	0
85	MG	2	1979	1/1	0.78	0.25	62,62,62,62	0
85	MG	5	3855	1/1	0.78	0.10	48,48,48,48	0
85	MG	5	3756	1/1	0.78	0.26	45,45,45,45	0
85	MG	1	4217	1/1	0.78	0.42	47,47,47,47	0
85	MG	6	2206	1/1	0.78	0.22	80,80,80,80	0
86	OHX	6	2183	7/7	0.78	0.15	177,177,177,177	0
85	MG	5	3498	1/1	0.78	0.31	29,29,29,29	0
85	MG	1	3581	1/1	0.78	0.37	48,48,48,48	0
85	MG	6	1940	1/1	0.78	0.30	60,60,60,60	0
86	OHX	5	4160	7/7	0.78	0.15	208,208,208,208	0
85	MG	5	3710	1/1	0.78	0.26	48,48,48,48	0
85	MG	1	3636	1/1	0.78	0.23	55,55,55,55	0
85	MG	5	3599	1/1	0.78	0.17	53,53,53,53	0
85	MG	6	2031	1/1	0.78	0.17	67,67,67,67	0
85	MG	5	3448	1/1	0.78	0.16	52,52,52,52	0
85	MG	3	215	1/1	0.78	0.28	46,46,46,46	0
86	OHX	m4	202	7/7	0.78	0.12	223,223,223,223	0
85	MG	1	3426	1/1	0.79	0.15	44,44,44,44	0
85	MG	6	2028	1/1	0.79	0.42	80,80,80,80	0
85	MG	1	3597	1/1	0.79	0.15	31,31,31,31	0
85	MG	6	2030	1/1	0.79	0.18	93,93,93,93	0
85	MG	Q2	502	1/1	0.79	0.19	77,77,77,77	0
85	MG	1	3845	1/1	0.79	0.13	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3506	1/1	0.79	0.34	41,41,41,41	0
85	MG	5	3512	1/1	0.79	0.26	51,51,51,51	0
85	MG	1	3483	1/1	0.79	0.26	50,50,50,50	0
86	OHX	M9	202	7/7	0.79	0.13	185,185,185,185	0
86	OHX	6	2136	7/7	0.79	0.16	168,168,168,168	0
85	MG	SM	301	1/1	0.79	0.33	55,55,55,55	0
85	MG	5	3739	1/1	0.79	0.33	68,68,68,68	0
85	MG	2	1932	1/1	0.79	0.28	68,68,68,68	0
85	MG	6	2001	1/1	0.79	0.19	58,58,58,58	0
85	MG	6	1942	1/1	0.79	0.32	42,42,42,42	0
85	MG	6	1910	1/1	0.79	0.32	55,55,55,55	0
85	MG	5	3645	1/1	0.79	0.21	103,103,103,103	0
86	OHX	5	4214	7/7	0.79	0.17	165,165,165,165	0
85	MG	2	1989	1/1	0.79	0.39	61,61,61,61	0
85	MG	3	214	1/1	0.79	0.43	49,49,49,49	0
85	MG	1	3575	1/1	0.79	0.30	24,24,24,24	0
85	MG	2	1975	1/1	0.79	0.39	77,77,77,77	0
86	OHX	m1	202	7/7	0.79	0.16	180,180,180,180	0
85	MG	6	2020	1/1	0.79	0.12	128,128,128,128	0
85	MG	6	1997	1/1	0.80	0.13	73,73,73,73	0
85	MG	6	2035	1/1	0.80	0.11	79,79,79,79	0
85	MG	2	1901	1/1	0.80	0.39	77,77,77,77	0
85	MG	2	1964	1/1	0.80	0.24	96,96,96,96	0
85	MG	1	3596	1/1	0.80	0.28	43,43,43,43	0
85	MG	1	3435	1/1	0.80	0.24	51,51,51,51	0
86	OHX	1	4172	7/7	0.80	0.15	177,177,177,177	0
85	MG	1	3466	1/1	0.80	0.26	45,45,45,45	0
85	MG	D4	201	1/1	0.80	0.34	72,72,72,72	0
86	OHX	1	4188	7/7	0.80	0.13	176,176,176,176	0
85	MG	2	1957	1/1	0.80	0.24	79,79,79,79	0
85	MG	5	3624	1/1	0.80	0.25	69,69,69,69	0
85	MG	5	3405	1/1	0.80	0.18	57,57,57,57	0
85	MG	1	3410	1/1	0.80	0.29	51,51,51,51	0
85	MG	6	1954	1/1	0.80	0.42	42,42,42,42	0
85	MG	5	3438	1/1	0.80	0.43	47,47,47,47	0
85	MG	6	1929	1/1	0.80	0.21	66,66,66,66	0
85	MG	5	3773	1/1	0.80	0.12	81,81,81,81	0
86	OHX	5	4191	7/7	0.80	0.14	190,190,190,190	0
85	MG	8	207	1/1	0.80	0.24	62,62,62,62	0
85	MG	N3	203	1/1	0.80	0.11	41,41,41,41	0
85	MG	2	1958	1/1	0.80	0.31	90,90,90,90	0
86	OHX	5	4223	7/7	0.80	0.21	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3848	1/1	0.80	0.32	51,51,51,51	0
85	MG	5	3472	1/1	0.80	0.42	40,40,40,40	0
85	MG	m4	201	1/1	0.80	0.19	49,49,49,49	0
85	MG	m5	301	1/1	0.80	0.12	42,42,42,42	0
85	MG	2	1974	1/1	0.80	0.19	71,71,71,71	0
86	OHX	m7	207	7/7	0.80	0.17	160,160,160,160	0
85	MG	5	3633	1/1	0.81	0.12	45,45,45,45	0
85	MG	1	3666	1/1	0.81	0.12	89,89,89,89	0
85	MG	1	3827	1/1	0.81	0.32	45,45,45,45	0
85	MG	5	3793	1/1	0.81	0.11	78,78,78,78	0
85	MG	5	3671	1/1	0.81	0.18	52,52,52,52	0
85	MG	4	204	1/1	0.81	0.27	79,79,79,79	0
86	OHX	2	2163	7/7	0.81	0.14	183,183,183,183	0
86	OHX	2	2175	7/7	0.81	0.13	198,198,198,198	0
86	OHX	2	2176	7/7	0.81	0.15	169,169,169,169	0
86	OHX	2	2180	7/7	0.81	0.16	186,186,186,186	0
85	MG	5	3465	1/1	0.81	0.25	60,60,60,60	0
85	MG	5	3803	1/1	0.81	0.17	76,76,76,76	0
85	MG	6	1968	1/1	0.81	0.21	64,64,64,64	0
86	OHX	1	4174	7/7	0.81	0.15	177,177,177,177	0
85	MG	4	222	1/1	0.81	0.24	80,80,80,80	0
85	MG	5	3686	1/1	0.81	0.26	69,69,69,69	0
85	MG	2	1943	1/1	0.81	0.23	74,74,74,74	0
86	OHX	1	4191	7/7	0.81	0.15	165,165,165,165	0
85	MG	2	1949	1/1	0.81	0.23	59,59,59,59	0
85	MG	5	3479	1/1	0.81	0.07	46,46,46,46	0
85	MG	6	2038	1/1	0.81	0.34	96,96,96,96	0
85	MG	1	3473	1/1	0.81	0.30	79,79,79,79	0
85	MG	1	3401	1/1	0.81	0.41	42,42,42,42	0
85	MG	1	3793	1/1	0.81	0.22	89,89,89,89	0
85	MG	6	1959	1/1	0.81	0.40	47,47,47,47	0
85	MG	6	2011	1/1	0.81	0.31	65,65,65,65	0
86	OHX	5	4190	7/7	0.81	0.18	165,165,165,165	0
85	MG	1	3583	1/1	0.81	0.37	33,33,33,33	0
85	MG	sM	301	1/1	0.81	0.17	51,51,51,51	0
85	MG	5	3558	1/1	0.81	0.30	36,36,36,36	0
85	MG	7	211	1/1	0.81	0.34	43,43,43,43	0
86	OHX	5	4219	7/7	0.81	0.16	176,176,176,176	0
85	MG	5	3598	1/1	0.81	0.24	48,48,48,48	0
86	OHX	5	4225	7/7	0.81	0.15	177,177,177,177	0
85	MG	2	1991	1/1	0.81	0.19	100,100,100,100	0
85	MG	5	3415	1/1	0.81	0.24	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3757	1/1	0.81	0.31	49,49,49,49	0
86	OHX	14	403	7/7	0.81	0.16	175,175,175,175	0
85	MG	1	3493	1/1	0.81	0.24	48,48,48,48	0
85	MG	5	3765	1/1	0.81	0.10	79,79,79,79	0
85	MG	6	2022	1/1	0.81	0.25	83,83,83,83	0
85	MG	7	216	1/1	0.82	0.24	74,74,74,74	0
85	MG	5	3592	1/1	0.82	0.38	44,44,44,44	0
86	OHX	1	4190	7/7	0.82	0.16	165,165,165,165	0
85	MG	1	3630	1/1	0.82	0.19	79,79,79,79	0
86	OHX	1	4198	7/7	0.82	0.19	160,160,160,160	0
85	MG	1	3408	1/1	0.82	0.27	30,30,30,30	0
85	MG	1	3485	1/1	0.82	0.28	41,41,41,41	0
85	MG	1	3454	1/1	0.82	0.42	63,63,63,63	0
86	OHX	6	2185	7/7	0.82	0.12	203,203,203,203	0
85	MG	L2	301	1/1	0.82	0.17	40,40,40,40	0
86	OHX	6	2199	7/7	0.82	0.16	178,178,178,178	0
85	MG	L4	401	1/1	0.82	0.11	98,98,98,98	0
86	OHX	5	4149	7/7	0.82	0.20	146,146,146,146	0
85	MG	5	3636	1/1	0.82	0.31	70,70,70,70	0
85	MG	2	2001	1/1	0.82	0.25	91,91,91,91	0
85	MG	1	3522	1/1	0.82	0.22	44,44,44,44	0
85	MG	1	3593	1/1	0.82	0.32	30,30,30,30	0
85	MG	M7	204	1/1	0.82	0.17	42,42,42,42	0
85	MG	5	3857	1/1	0.82	0.20	58,58,58,58	0
85	MG	6	2026	1/1	0.82	0.25	88,88,88,88	0
86	OHX	2	2164	7/7	0.82	0.16	172,172,172,172	0
85	MG	5	3866	1/1	0.82	0.23	34,34,34,34	0
85	MG	1	3853	1/1	0.82	0.11	153,153,153,153	0
86	OHX	2	2177	7/7	0.82	0.13	202,202,202,202	0
86	OHX	5	4226	7/7	0.82	0.17	154,154,154,154	0
85	MG	2	1982	1/1	0.82	0.30	76,76,76,76	0
85	MG	5	3536	1/1	0.82	0.27	38,38,38,38	0
86	OHX	5	4234	7/7	0.82	0.14	171,171,171,171	0
86	OHX	5	4235	7/7	0.82	0.14	204,204,204,204	0
85	MG	1	3542	1/1	0.82	0.25	51,51,51,51	0
85	MG	5	3698	1/1	0.82	0.23	64,64,64,64	0
85	MG	1	3543	1/1	0.82	0.28	57,57,57,57	0
86	OHX	1	4176	7/7	0.82	0.15	165,165,165,165	0
85	MG	1	3613	1/1	0.82	0.28	66,66,66,66	0
86	OHX	1	4185	7/7	0.83	0.16	155,155,155,155	0
85	MG	6	1911	1/1	0.83	0.27	87,87,87,87	0
85	MG	5	3634	1/1	0.83	0.31	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	2043	1/1	0.83	0.14	52,52,52,52	0
85	MG	1	3626	1/1	0.83	0.09	65,65,65,65	0
86	OHX	1	4197	7/7	0.83	0.16	162,162,162,162	0
85	MG	1	3469	1/1	0.83	0.13	48,48,48,48	0
86	OHX	4	236	7/7	0.83	0.14	166,166,166,166	0
85	MG	6	1921	1/1	0.83	0.39	62,62,62,62	0
85	MG	5	3772	1/1	0.83	0.34	82,82,82,82	0
86	OHX	6	2148	7/7	0.83	0.15	157,157,157,157	0
86	OHX	6	2156	7/7	0.83	0.11	203,203,203,203	0
86	OHX	6	2178	7/7	0.83	0.14	171,171,171,171	0
85	MG	8	204	1/1	0.83	0.26	60,60,60,60	0
85	MG	M0	301	1/1	0.83	0.13	88,88,88,88	0
85	MG	5	3502	1/1	0.83	0.34	61,61,61,61	0
85	MG	2	1995	1/1	0.83	0.26	57,57,57,57	0
86	OHX	s1	303	7/7	0.83	0.14	180,180,180,180	0
86	OHX	s9	201	7/7	0.83	0.17	160,160,160,160	0
85	MG	5	3510	1/1	0.83	0.24	63,63,63,63	0
85	MG	14	401	1/1	0.83	0.10	59,59,59,59	0
85	MG	1	3707	1/1	0.83	0.20	43,43,43,43	0
85	MG	5	3688	1/1	0.83	0.10	48,48,48,48	0
85	MG	6	2023	1/1	0.83	0.20	62,62,62,62	0
85	MG	5	3532	1/1	0.83	0.25	44,44,44,44	0
85	MG	5	3411	1/1	0.83	0.21	45,45,45,45	0
86	OHX	2	2127	7/7	0.83	0.14	174,174,174,174	0
86	OHX	5	4208	7/7	0.83	0.14	175,175,175,175	0
85	MG	1	3710	1/1	0.83	0.37	78,78,78,78	0
86	OHX	5	4216	7/7	0.83	0.15	165,165,165,165	0
85	MG	1	3476	1/1	0.83	0.22	44,44,44,44	0
85	MG	2	2008	1/1	0.83	0.44	55,55,55,55	0
86	OHX	5	4220	7/7	0.83	0.14	177,177,177,177	0
85	MG	5	3822	1/1	0.83	0.33	68,68,68,68	0
85	MG	5	3572	1/1	0.83	0.39	41,41,41,41	0
85	MG	1	3643	1/1	0.83	0.28	76,76,76,76	0
85	MG	5	3836	1/1	0.83	0.23	53,53,53,53	0
85	MG	6	1903	1/1	0.83	0.24	45,45,45,45	0
85	MG	5	3724	1/1	0.83	0.20	57,57,57,57	0
85	MG	1	3414	1/1	0.83	0.27	39,39,39,39	0
85	MG	5	3619	1/1	0.83	0.23	48,48,48,48	0
86	OHX	5	4239	7/7	0.83	0.13	193,193,193,193	0
86	OHX	5	4244	7/7	0.83	0.15	157,157,157,157	0
86	OHX	5	4245	7/7	0.83	0.15	175,175,175,175	0
86	OHX	14	402	7/7	0.83	0.13	182,182,182,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3863	1/1	0.83	0.32	43,43,43,43	0
85	MG	2	1938	1/1	0.83	0.30	67,67,67,67	0
85	MG	1	3842	1/1	0.83	0.12	40,40,40,40	0
85	MG	1	3407	1/1	0.83	0.18	51,51,51,51	0
85	MG	5	3641	1/1	0.84	0.29	43,43,43,43	0
85	MG	4	212	1/1	0.84	0.17	62,62,62,62	0
86	OHX	M7	207	7/7	0.84	0.16	159,159,159,159	0
85	MG	5	3655	1/1	0.84	0.12	51,51,51,51	0
85	MG	2	2017	1/1	0.84	0.41	83,83,83,83	0
85	MG	5	3500	1/1	0.84	0.19	48,48,48,48	0
85	MG	2	1999	1/1	0.84	0.24	79,79,79,79	0
86	OHX	6	2172	7/7	0.84	0.14	165,165,165,165	0
85	MG	l5	302	1/1	0.84	0.19	71,71,71,71	0
85	MG	l5	303	1/1	0.84	0.16	63,63,63,63	0
85	MG	5	3504	1/1	0.84	0.28	37,37,37,37	0
86	OHX	6	2188	7/7	0.84	0.15	170,170,170,170	0
86	OHX	6	2189	7/7	0.84	0.14	176,176,176,176	0
85	MG	s1	301	1/1	0.84	0.15	93,93,93,93	0
86	OHX	6	2193	7/7	0.84	0.12	209,209,209,209	0
85	MG	5	3507	1/1	0.84	0.33	38,38,38,38	0
86	OHX	6	2204	7/7	0.84	0.14	173,173,173,173	0
85	MG	m7	204	1/1	0.84	0.12	40,40,40,40	0
85	MG	1	3496	1/1	0.84	0.23	42,42,42,42	0
86	OHX	5	4135	7/7	0.84	0.13	173,173,173,173	0
85	MG	1	3720	1/1	0.84	0.12	50,50,50,50	0
86	OHX	2	2099	7/7	0.84	0.14	170,170,170,170	0
85	MG	1	3471	1/1	0.84	0.14	37,37,37,37	0
85	MG	1	3841	1/1	0.84	0.14	51,51,51,51	0
85	MG	5	3700	1/1	0.84	0.19	60,60,60,60	0
85	MG	5	3701	1/1	0.84	0.27	50,50,50,50	0
86	OHX	2	2161	7/7	0.84	0.14	175,175,175,175	0
86	OHX	5	4200	7/7	0.84	0.15	162,162,162,162	0
86	OHX	5	4201	7/7	0.84	0.14	181,181,181,181	0
85	MG	1	3472	1/1	0.84	0.23	28,28,28,28	0
85	MG	2	1942	1/1	0.84	0.15	80,80,80,80	0
85	MG	1	3654	1/1	0.84	0.27	45,45,45,45	0
85	MG	1	3657	1/1	0.84	0.15	68,68,68,68	0
85	MG	5	3433	1/1	0.84	0.16	86,86,86,86	0
85	MG	2	1907	1/1	0.84	0.35	48,48,48,48	0
86	OHX	1	4122	7/7	0.84	0.14	167,167,167,167	0
85	MG	5	3593	1/1	0.84	0.34	36,36,36,36	0
85	MG	5	3597	1/1	0.84	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	4156	7/7	0.84	0.13	176,176,176,176	0
86	OHX	1	4166	7/7	0.84	0.13	179,179,179,179	0
86	OHX	1	4167	7/7	0.84	0.15	176,176,176,176	0
85	MG	1	3855	1/1	0.84	0.40	72,72,72,72	0
85	MG	2	1956	1/1	0.84	0.16	59,59,59,59	0
85	MG	1	3770	1/1	0.84	0.20	61,61,61,61	0
86	OHX	1	4182	7/7	0.84	0.14	180,180,180,180	0
86	OHX	5	4241	7/7	0.84	0.15	177,177,177,177	0
86	OHX	5	4242	7/7	0.84	0.16	175,175,175,175	0
85	MG	5	3622	1/1	0.84	0.26	64,64,64,64	0
85	MG	1	3623	1/1	0.84	0.27	36,36,36,36	0
86	OHX	8	225	7/7	0.84	0.15	162,162,162,162	0
85	MG	1	3672	1/1	0.84	0.17	68,68,68,68	0
85	MG	1	3786	1/1	0.84	0.14	58,58,58,58	0
86	OHX	l5	306	7/7	0.84	0.14	170,170,170,170	0
85	MG	1	3456	1/1	0.84	0.24	46,46,46,46	0
85	MG	4	201	1/1	0.84	0.18	61,61,61,61	0
85	MG	1	3696	1/1	0.84	0.24	49,49,49,49	0
87	ZN	D7	101	1/1	0.84	0.19	176,176,176,176	0
86	OHX	1	4203	7/7	0.85	0.17	151,151,151,151	0
85	MG	5	3770	1/1	0.85	0.31	68,68,68,68	0
86	OHX	L4	404	7/7	0.85	0.14	160,160,160,160	0
85	MG	2	1997	1/1	0.85	0.15	93,93,93,93	0
85	MG	S8	301	1/1	0.85	0.21	68,68,68,68	0
86	OHX	6	2106	7/7	0.85	0.15	151,151,151,151	0
85	MG	6	2041	1/1	0.85	0.22	72,72,72,72	0
85	MG	5	3669	1/1	0.85	0.19	68,68,68,68	0
85	MG	1	3557	1/1	0.85	0.33	39,39,39,39	0
86	OHX	6	2170	7/7	0.85	0.13	176,176,176,176	0
85	MG	1	3659	1/1	0.85	0.16	48,48,48,48	0
86	OHX	6	2174	7/7	0.85	0.17	161,161,161,161	0
85	MG	1	3605	1/1	0.85	0.36	69,69,69,69	0
85	MG	m6	201	1/1	0.85	0.12	32,32,32,32	0
86	OHX	6	2184	7/7	0.85	0.14	164,164,164,164	0
85	MG	6	1956	1/1	0.85	0.42	60,60,60,60	0
86	OHX	6	2186	7/7	0.85	0.14	166,166,166,166	0
85	MG	1	3612	1/1	0.85	0.13	47,47,47,47	0
85	MG	c4	201	1/1	0.85	0.24	58,58,58,58	0
85	MG	c8	201	1/1	0.85	0.50	68,68,68,68	0
86	OHX	2	2115	7/7	0.85	0.12	178,178,178,178	0
85	MG	5	3692	1/1	0.85	0.25	66,66,66,66	0
86	OHX	6	2203	7/7	0.85	0.17	173,173,173,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2134	7/7	0.85	0.15	157,157,157,157	0
86	OHX	2	2137	7/7	0.85	0.13	182,182,182,182	0
86	OHX	2	2139	7/7	0.85	0.14	192,192,192,192	0
86	OHX	5	4038	7/7	0.85	0.53	120,120,120,120	0
86	OHX	2	2147	7/7	0.85	0.12	205,205,205,205	0
85	MG	3	211	1/1	0.85	0.27	69,69,69,69	0
85	MG	1	3571	1/1	0.85	0.31	38,38,38,38	0
85	MG	1	3617	1/1	0.85	0.32	50,50,50,50	0
85	MG	1	3787	1/1	0.85	0.73	48,48,48,48	0
86	OHX	5	4174	7/7	0.85	0.13	177,177,177,177	0
86	OHX	5	4178	7/7	0.85	0.13	168,168,168,168	0
85	MG	5	3408	1/1	0.85	0.10	46,46,46,46	0
85	MG	1	3692	1/1	0.85	0.12	52,52,52,52	0
85	MG	5	3851	1/1	0.85	0.08	50,50,50,50	0
86	OHX	5	4199	7/7	0.85	0.14	160,160,160,160	0
85	MG	1	3619	1/1	0.85	0.11	48,48,48,48	0
85	MG	5	3589	1/1	0.85	0.29	48,48,48,48	0
86	OHX	2	2179	7/7	0.85	0.16	168,168,168,168	0
86	OHX	5	4205	7/7	0.85	0.15	167,167,167,167	0
85	MG	1	3517	1/1	0.85	0.39	22,22,22,22	0
86	OHX	5	4209	7/7	0.85	0.18	141,141,141,141	0
86	OHX	1	4091	7/7	0.85	0.12	165,165,165,165	0
86	OHX	1	4096	7/7	0.85	0.12	181,181,181,181	0
85	MG	5	3860	1/1	0.85	0.17	48,48,48,48	0
85	MG	6	1969	1/1	0.85	0.10	65,65,65,65	0
86	OHX	1	4136	7/7	0.85	0.14	156,156,156,156	0
86	OHX	1	4137	7/7	0.85	0.17	154,154,154,154	0
85	MG	1	3701	1/1	0.85	0.14	54,54,54,54	0
85	MG	5	3434	1/1	0.85	0.26	38,38,38,38	0
85	MG	1	3578	1/1	0.85	0.16	55,55,55,55	0
85	MG	1	3705	1/1	0.85	0.17	51,51,51,51	0
86	OHX	1	4168	7/7	0.85	0.16	162,162,162,162	0
85	MG	1	3428	1/1	0.85	0.35	37,37,37,37	0
85	MG	5	3461	1/1	0.85	0.15	37,37,37,37	0
85	MG	7	202	1/1	0.85	0.26	52,52,52,52	0
86	OHX	1	4179	7/7	0.85	0.15	157,157,157,157	0
85	MG	7	206	1/1	0.85	0.28	26,26,26,26	0
85	MG	5	3627	1/1	0.85	0.39	84,84,84,84	0
85	MG	6	1936	1/1	0.85	0.36	43,43,43,43	0
86	OHX	7	229	7/7	0.85	0.14	156,156,156,156	0
85	MG	7	215	1/1	0.85	0.18	44,44,44,44	0
85	MG	2	2010	1/1	0.85	0.45	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3539	1/1	0.85	0.24	29,29,29,29	0
85	MG	1	3587	1/1	0.85	0.30	46,46,46,46	0
86	OHX	1	4195	7/7	0.85	0.15	156,156,156,156	0
85	MG	1	3640	1/1	0.85	0.18	45,45,45,45	0
85	MG	2	2011	1/1	0.85	0.31	67,67,67,67	0
86	OHX	1	4200	7/7	0.85	0.14	162,162,162,162	0
87	ZN	d7	101	1/1	0.85	0.14	160,160,160,160	0
85	MG	l3	402	1/1	0.86	0.14	59,59,59,59	0
86	OHX	1	4204	7/7	0.86	0.15	158,158,158,158	0
86	OHX	4	235	7/7	0.86	0.13	168,168,168,168	0
85	MG	l3	403	1/1	0.86	0.49	39,39,39,39	0
86	OHX	L3	406	7/7	0.86	0.12	175,175,175,175	0
85	MG	1	3514	1/1	0.86	0.33	30,30,30,30	0
85	MG	6	1957	1/1	0.86	0.36	64,64,64,64	0
85	MG	6	1999	1/1	0.86	0.12	65,65,65,65	0
85	MG	6	2205	1/1	0.86	0.38	65,65,65,65	0
85	MG	1	3616	1/1	0.86	0.19	69,69,69,69	0
85	MG	1	3515	1/1	0.86	0.31	38,38,38,38	0
85	MG	5	3780	1/1	0.86	0.12	43,43,43,43	0
86	OHX	6	2167	7/7	0.86	0.10	194,194,194,194	0
85	MG	5	3656	1/1	0.86	0.24	40,40,40,40	0
85	MG	5	3789	1/1	0.86	0.12	82,82,82,82	0
85	MG	1	3840	1/1	0.86	0.28	59,59,59,59	0
86	OHX	6	2175	7/7	0.86	0.13	181,181,181,181	0
85	MG	q0	3601	1/1	0.86	0.13	63,63,63,63	0
86	OHX	6	2181	7/7	0.86	0.16	167,167,167,167	0
85	MG	q1	101	1/1	0.86	0.29	50,50,50,50	0
85	MG	5	3660	1/1	0.86	0.15	44,44,44,44	0
85	MG	5	3666	1/1	0.86	0.13	39,39,39,39	0
86	OHX	2	2124	7/7	0.86	0.12	172,172,172,172	0
85	MG	1	3580	1/1	0.86	0.31	43,43,43,43	0
85	MG	5	3800	1/1	0.86	0.08	42,42,42,42	0
86	OHX	6	2190	7/7	0.86	0.13	174,174,174,174	0
85	MG	5	3670	1/1	0.86	0.18	48,48,48,48	0
85	MG	2	1923	1/1	0.86	0.36	61,61,61,61	0
85	MG	1	3405	1/1	0.86	0.33	96,96,96,96	0
86	OHX	6	2200	7/7	0.86	0.14	174,174,174,174	0
86	OHX	2	2148	7/7	0.86	0.17	144,144,144,144	0
85	MG	1	3457	1/1	0.86	0.14	66,66,66,66	0
86	OHX	2	2153	7/7	0.86	0.12	186,186,186,186	0
85	MG	5	3514	1/1	0.86	0.22	43,43,43,43	0
85	MG	5	3519	1/1	0.86	0.24	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1906	1/1	0.86	0.21	62,62,62,62	0
86	OHX	2	2162	7/7	0.86	0.13	190,190,190,190	0
85	MG	5	3687	1/1	0.86	0.09	49,49,49,49	0
85	MG	5	3530	1/1	0.86	0.32	35,35,35,35	0
86	OHX	2	2172	7/7	0.86	0.14	174,174,174,174	0
85	MG	5	3847	1/1	0.86	0.13	83,83,83,83	0
85	MG	1	3633	1/1	0.86	0.31	71,71,71,71	0
86	OHX	5	4179	7/7	0.86	0.16	141,141,141,141	0
85	MG	6	1970	1/1	0.86	0.10	72,72,72,72	0
85	MG	5	3852	1/1	0.86	0.14	100,100,100,100	0
85	MG	1	3777	1/1	0.86	0.22	63,63,63,63	0
86	OHX	1	4058	7/7	0.86	0.15	154,154,154,154	0
85	MG	5	3543	1/1	0.86	0.29	53,53,53,53	0
85	MG	1	3486	1/1	0.86	0.21	35,35,35,35	0
86	OHX	1	4107	7/7	0.86	0.15	167,167,167,167	0
86	OHX	1	4121	7/7	0.86	0.17	143,143,143,143	0
86	OHX	5	4207	7/7	0.86	0.14	164,164,164,164	0
85	MG	5	3554	1/1	0.86	0.14	36,36,36,36	0
85	MG	1	3785	1/1	0.86	0.07	66,66,66,66	0
86	OHX	1	4134	7/7	0.86	0.13	166,166,166,166	0
85	MG	6	2027	1/1	0.86	0.28	66,66,66,66	0
85	MG	5	3588	1/1	0.86	0.34	39,39,39,39	0
85	MG	5	3871	1/1	0.86	0.21	28,28,28,28	0
86	OHX	1	4145	7/7	0.86	0.13	173,173,173,173	0
86	OHX	5	4221	7/7	0.86	0.14	167,167,167,167	0
86	OHX	1	4149	7/7	0.86	0.14	168,168,168,168	0
85	MG	5	3873	1/1	0.86	0.09	32,32,32,32	0
86	OHX	1	4165	7/7	0.86	0.16	141,141,141,141	0
85	MG	5	3874	1/1	0.86	0.19	56,56,56,56	0
85	MG	2	1905	1/1	0.86	0.34	70,70,70,70	0
86	OHX	5	4232	7/7	0.86	0.15	175,175,175,175	0
85	MG	1	3704	1/1	0.86	0.09	63,63,63,63	0
85	MG	5	3443	1/1	0.86	0.23	33,33,33,33	0
85	MG	2	2013	1/1	0.86	0.28	57,57,57,57	0
86	OHX	5	4237	7/7	0.86	0.16	162,162,162,162	0
85	MG	5	3725	1/1	0.86	0.08	41,41,41,41	0
85	MG	7	205	1/1	0.86	0.14	75,75,75,75	0
85	MG	5	3726	1/1	0.86	0.27	60,60,60,60	0
85	MG	6	1948	1/1	0.86	0.33	59,59,59,59	0
85	MG	6	1908	1/1	0.86	0.27	56,56,56,56	0
86	OHX	7	227	7/7	0.86	0.14	171,171,171,171	0
85	MG	5	3611	1/1	0.86	0.24	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1912	1/1	0.86	0.26	71,71,71,71	0
85	MG	1	3568	1/1	0.86	0.33	43,43,43,43	0
85	MG	6	1952	1/1	0.86	0.35	64,64,64,64	0
86	OHX	15	305	7/7	0.86	0.14	166,166,166,166	0
86	OHX	1	4192	7/7	0.86	0.12	183,183,183,183	0
85	MG	5	3470	1/1	0.86	0.28	44,44,44,44	0
86	OHX	1	4196	7/7	0.86	0.14	175,175,175,175	0
85	MG	1	3513	1/1	0.86	0.35	41,41,41,41	0
85	MG	5	3760	1/1	0.86	0.42	43,43,43,43	0
85	MG	6	1916	1/1	0.86	0.25	65,65,65,65	0
86	OHX	1	4090	7/7	0.87	0.14	158,158,158,158	0
85	MG	2	1947	1/1	0.87	0.33	54,54,54,54	0
85	MG	5	3675	1/1	0.87	0.25	54,54,54,54	0
85	MG	6	1978	1/1	0.87	0.29	53,53,53,53	0
85	MG	5	3787	1/1	0.87	0.16	62,62,62,62	0
85	MG	5	3788	1/1	0.87	0.09	57,57,57,57	0
85	MG	2	1913	1/1	0.87	0.38	78,78,78,78	0
86	OHX	1	4125	7/7	0.87	0.13	165,165,165,165	0
86	OHX	1	4130	7/7	0.87	0.14	134,134,134,134	0
85	MG	5	3550	1/1	0.87	0.14	49,49,49,49	0
85	MG	1	3854	1/1	0.87	0.22	56,56,56,56	0
85	MG	6	1984	1/1	0.87	0.16	90,90,90,90	0
85	MG	8	210	1/1	0.87	0.26	65,65,65,65	0
85	MG	5	3567	1/1	0.87	0.26	37,37,37,37	0
86	OHX	1	4146	7/7	0.87	0.11	180,180,180,180	0
86	OHX	5	4134	7/7	0.87	0.17	155,155,155,155	0
85	MG	5	3571	1/1	0.87	0.24	37,37,37,37	0
86	OHX	5	4136	7/7	0.87	0.15	160,160,160,160	0
86	OHX	1	4154	7/7	0.87	0.12	176,176,176,176	0
85	MG	1	3631	1/1	0.87	0.17	70,70,70,70	0
86	OHX	5	4154	7/7	0.87	0.17	137,137,137,137	0
86	OHX	1	4164	7/7	0.87	0.15	137,137,137,137	0
86	OHX	5	4159	7/7	0.87	0.12	172,172,172,172	0
85	MG	1	3721	1/1	0.87	0.15	48,48,48,48	0
85	MG	5	3462	1/1	0.87	0.10	53,53,53,53	0
85	MG	1	3600	1/1	0.87	0.22	40,40,40,40	0
85	MG	1	3528	1/1	0.87	0.24	79,79,79,79	0
86	OHX	5	4182	7/7	0.87	0.16	144,144,144,144	0
85	MG	3	207	1/1	0.87	0.35	53,53,53,53	0
85	MG	5	3823	1/1	0.87	0.15	86,86,86,86	0
85	MG	m5	302	1/1	0.87	0.13	56,56,56,56	0
85	MG	1	3802	1/1	0.87	0.18	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4181	7/7	0.87	0.16	160,160,160,160	0
85	MG	1	3807	1/1	0.87	0.12	45,45,45,45	0
85	MG	m7	206	1/1	0.87	0.27	58,58,58,58	0
86	OHX	5	4203	7/7	0.87	0.11	192,192,192,192	0
86	OHX	1	4184	7/7	0.87	0.14	164,164,164,164	0
85	MG	n6	202	1/1	0.87	0.35	47,47,47,47	0
85	MG	5	3830	1/1	0.87	0.19	44,44,44,44	0
85	MG	5	3832	1/1	0.87	0.16	55,55,55,55	0
86	OHX	5	4213	7/7	0.87	0.13	165,165,165,165	0
85	MG	5	3835	1/1	0.87	0.17	60,60,60,60	0
86	OHX	5	4215	7/7	0.87	0.09	204,204,204,204	0
85	MG	5	3473	1/1	0.87	0.27	60,60,60,60	0
85	MG	5	3842	1/1	0.87	0.27	74,74,74,74	0
86	OHX	5	4218	7/7	0.87	0.12	170,170,170,170	0
85	MG	3	213	1/1	0.87	0.24	59,59,59,59	0
85	MG	1	3676	1/1	0.87	0.19	64,64,64,64	0
85	MG	1	3683	1/1	0.87	0.18	103,103,103,103	0
86	OHX	5	4222	7/7	0.87	0.12	184,184,184,184	0
85	MG	1	3531	1/1	0.87	0.11	37,37,37,37	0
85	MG	1	3829	1/1	0.87	0.16	57,57,57,57	0
86	OHX	1	4201	7/7	0.87	0.15	158,158,158,158	0
85	MG	1	3508	1/1	0.87	0.18	39,39,39,39	0
86	OHX	2	2140	7/7	0.87	0.14	173,173,173,173	0
85	MG	1	3427	1/1	0.87	0.24	56,56,56,56	0
85	MG	5	3859	1/1	0.87	0.11	51,51,51,51	0
85	MG	6	1963	1/1	0.87	0.23	58,58,58,58	0
85	MG	5	3862	1/1	0.87	0.26	51,51,51,51	0
85	MG	1	3403	1/1	0.87	0.15	41,41,41,41	0
85	MG	5	3638	1/1	0.87	0.16	59,59,59,59	0
85	MG	L3	404	1/1	0.87	0.17	57,57,57,57	0
86	OHX	6	2134	7/7	0.87	0.12	153,153,153,153	0
85	MG	2	1973	1/1	0.87	0.19	75,75,75,75	0
85	MG	L4	403	1/1	0.87	0.22	36,36,36,36	0
86	OHX	6	2150	7/7	0.87	0.13	172,172,172,172	0
85	MG	2	1967	1/1	0.87	0.33	62,62,62,62	0
86	OHX	6	2160	7/7	0.87	0.15	158,158,158,158	0
85	MG	1	3565	1/1	0.87	0.21	35,35,35,35	0
85	MG	5	3764	1/1	0.87	0.16	79,79,79,79	0
85	MG	5	3522	1/1	0.87	0.32	28,28,28,28	0
85	MG	6	1935	1/1	0.87	0.21	86,86,86,86	0
85	MG	1	3846	1/1	0.87	0.14	33,33,33,33	0
85	MG	5	3420	1/1	0.87	0.10	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2179	7/7	0.87	0.12	174,174,174,174	0
85	MG	6	1975	1/1	0.87	0.14	68,68,68,68	0
86	OHX	1	4083	7/7	0.87	0.17	150,150,150,150	0
85	MG	2	1965	1/1	0.88	0.30	51,51,51,51	0
85	MG	2	1904	1/1	0.88	0.30	55,55,55,55	0
85	MG	5	3586	1/1	0.88	0.30	71,71,71,71	0
85	MG	6	1973	1/1	0.88	0.17	70,70,70,70	0
85	MG	5	3716	1/1	0.88	0.14	55,55,55,55	0
85	MG	1	3649	1/1	0.88	0.10	66,66,66,66	0
86	OHX	2	2169	7/7	0.88	0.13	182,182,182,182	0
86	OHX	2	2171	7/7	0.88	0.13	167,167,167,167	0
85	MG	5	3591	1/1	0.88	0.26	34,34,34,34	0
86	OHX	2	2174	7/7	0.88	0.12	169,169,169,169	0
85	MG	5	3723	1/1	0.88	0.31	84,84,84,84	0
85	MG	1	3450	1/1	0.88	0.11	42,42,42,42	0
85	MG	5	3455	1/1	0.88	0.20	43,43,43,43	0
85	MG	1	3622	1/1	0.88	0.27	82,82,82,82	0
85	MG	1	3506	1/1	0.88	0.14	36,36,36,36	0
85	MG	5	3731	1/1	0.88	0.10	39,39,39,39	0
86	OHX	1	4068	7/7	0.88	0.35	122,122,122,122	0
86	OHX	1	4077	7/7	0.88	0.12	164,164,164,164	0
86	OHX	6	2194	7/7	0.88	0.12	196,196,196,196	0
86	OHX	6	2198	7/7	0.88	0.14	171,171,171,171	0
85	MG	6	2032	1/1	0.88	0.12	58,58,58,58	0
86	OHX	1	4088	7/7	0.88	0.11	165,165,165,165	0
85	MG	5	3603	1/1	0.88	0.18	35,35,35,35	0
85	MG	5	3604	1/1	0.88	0.16	55,55,55,55	0
86	OHX	1	4093	7/7	0.88	0.11	175,175,175,175	0
85	MG	5	3878	1/1	0.88	0.30	65,65,65,65	0
85	MG	1	3789	1/1	0.88	0.25	60,60,60,60	0
86	OHX	5	4094	7/7	0.88	0.14	149,149,149,149	0
86	OHX	1	4116	7/7	0.88	0.14	164,164,164,164	0
85	MG	5	3884	1/1	0.88	0.14	33,33,33,33	0
85	MG	1	3662	1/1	0.88	0.09	40,40,40,40	0
85	MG	5	3755	1/1	0.88	0.11	74,74,74,74	0
86	OHX	5	4146	7/7	0.88	0.15	145,145,145,145	0
86	OHX	5	4147	7/7	0.88	0.12	165,165,165,165	0
86	OHX	5	4148	7/7	0.88	0.17	140,140,140,140	0
85	MG	7	204	1/1	0.88	0.30	50,50,50,50	0
85	MG	5	3620	1/1	0.88	0.34	48,48,48,48	0
85	MG	M9	201	1/1	0.88	0.12	68,68,68,68	0
85	MG	6	1943	1/1	0.88	0.31	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1925	1/1	0.88	0.38	69,69,69,69	0
86	OHX	5	4164	7/7	0.88	0.14	160,160,160,160	0
85	MG	6	1946	1/1	0.88	0.25	61,61,61,61	0
86	OHX	1	4139	7/7	0.88	0.11	153,153,153,153	0
85	MG	2	2007	1/1	0.88	0.35	79,79,79,79	0
86	OHX	5	4181	7/7	0.88	0.15	153,153,153,153	0
85	MG	5	3484	1/1	0.88	0.21	53,53,53,53	0
85	MG	3	203	1/1	0.88	0.10	73,73,73,73	0
85	MG	5	3493	1/1	0.88	0.17	40,40,40,40	0
85	MG	2	1988	1/1	0.88	0.14	64,64,64,64	0
86	OHX	5	4197	7/7	0.88	0.12	166,166,166,166	0
86	OHX	1	4157	7/7	0.88	0.12	179,179,179,179	0
85	MG	5	3774	1/1	0.88	0.26	96,96,96,96	0
85	MG	1	3608	1/1	0.88	0.08	45,45,45,45	0
85	MG	1	3610	1/1	0.88	0.23	37,37,37,37	0
85	MG	l3	401	1/1	0.88	0.37	26,26,26,26	0
85	MG	1	3753	1/1	0.88	0.22	48,48,48,48	0
86	OHX	1	4170	7/7	0.88	0.10	200,200,200,200	0
85	MG	1	3815	1/1	0.88	0.16	72,72,72,72	0
85	MG	1	3756	1/1	0.88	0.24	61,61,61,61	0
85	MG	1	3679	1/1	0.88	0.09	46,46,46,46	0
86	OHX	1	4177	7/7	0.88	0.15	165,165,165,165	0
85	MG	d0	201	1/1	0.88	0.21	75,75,75,75	0
85	MG	1	3458	1/1	0.88	0.22	34,34,34,34	0
85	MG	4	205	1/1	0.88	0.12	46,46,46,46	0
85	MG	4	208	1/1	0.88	0.21	43,43,43,43	0
85	MG	5	3407	1/1	0.88	0.17	48,48,48,48	0
85	MG	5	3801	1/1	0.88	0.12	39,39,39,39	0
85	MG	5	3802	1/1	0.88	0.09	82,82,82,82	0
85	MG	5	3523	1/1	0.88	0.31	57,57,57,57	0
85	MG	1	3411	1/1	0.88	0.10	35,35,35,35	0
85	MG	n8	202	1/1	0.88	0.20	52,52,52,52	0
85	MG	4	213	1/1	0.88	0.13	57,57,57,57	0
86	OHX	5	4227	7/7	0.88	0.10	216,216,216,216	0
86	OHX	1	4193	7/7	0.88	0.15	157,157,157,157	0
85	MG	4	216	1/1	0.88	0.19	44,44,44,44	0
85	MG	5	3682	1/1	0.88	0.11	49,49,49,49	0
85	MG	5	3820	1/1	0.88	0.32	45,45,45,45	0
86	OHX	2	2067	7/7	0.88	0.10	194,194,194,194	0
85	MG	5	3685	1/1	0.88	0.28	46,46,46,46	0
85	MG	1	3694	1/1	0.88	0.10	59,59,59,59	0
85	MG	5	3419	1/1	0.88	0.12	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4240	7/7	0.88	0.15	164,164,164,164	0
85	MG	6	1928	1/1	0.88	0.16	61,61,61,61	0
86	OHX	1	4206	7/7	0.88	0.14	161,161,161,161	0
86	OHX	5	4243	7/7	0.88	0.14	171,171,171,171	0
85	MG	5	3423	1/1	0.88	0.20	74,74,74,74	0
86	OHX	2	2136	7/7	0.88	0.13	164,164,164,164	0
85	MG	5	3694	1/1	0.88	0.50	41,41,41,41	0
85	MG	5	3425	1/1	0.88	0.19	45,45,45,45	0
86	OHX	M7	206	7/7	0.88	0.20	135,135,135,135	0
85	MG	1	3615	1/1	0.88	0.12	72,72,72,72	0
86	OHX	2	2145	7/7	0.88	0.13	166,166,166,166	0
85	MG	5	3431	1/1	0.88	0.12	40,40,40,40	0
85	MG	6	1931	1/1	0.88	0.20	53,53,53,53	0
85	MG	5	3849	1/1	0.88	0.29	45,45,45,45	0
85	MG	5	3568	1/1	0.88	0.25	34,34,34,34	0
86	OHX	2	2157	7/7	0.88	0.16	138,138,138,138	0
86	OHX	6	2152	7/7	0.88	0.14	177,177,177,177	0
86	OHX	2	2158	7/7	0.88	0.09	278,278,278,278	0
88	BLS	1	4211	30/30	0.88	0.11	52,52,52,52	0
88	BLS	5	4248	30/30	0.88	0.12	52,52,52,52	0
85	MG	7	214	1/1	0.89	0.08	81,81,81,81	0
85	MG	1	3754	1/1	0.89	0.10	56,56,56,56	0
85	MG	5	3639	1/1	0.89	0.11	41,41,41,41	0
86	OHX	1	4095	7/7	0.89	0.15	147,147,147,147	0
85	MG	s8	301	1/1	0.89	0.29	57,57,57,57	0
86	OHX	1	4103	7/7	0.89	0.12	161,161,161,161	0
85	MG	5	3501	1/1	0.89	0.28	37,37,37,37	0
85	MG	2	1916	1/1	0.89	0.20	61,61,61,61	0
86	OHX	6	2195	7/7	0.89	0.11	183,183,183,183	0
85	MG	1	3497	1/1	0.89	0.17	39,39,39,39	0
85	MG	1	3533	1/1	0.89	0.26	47,47,47,47	0
85	MG	5	3784	1/1	0.89	0.14	78,78,78,78	0
85	MG	6	1996	1/1	0.89	0.09	67,67,67,67	0
85	MG	M5	302	1/1	0.89	0.23	55,55,55,55	0
86	OHX	1	4133	7/7	0.89	0.13	154,154,154,154	0
85	MG	M7	201	1/1	0.89	0.37	69,69,69,69	0
86	OHX	c3	201	7/7	0.89	0.11	182,182,182,182	0
85	MG	5	3513	1/1	0.89	0.21	34,34,34,34	0
85	MG	1	3628	1/1	0.89	0.15	37,37,37,37	0
86	OHX	5	4115	7/7	0.89	0.14	139,139,139,139	0
86	OHX	5	4132	7/7	0.89	0.15	161,161,161,161	0
85	MG	1	3765	1/1	0.89	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	N3	201	1/1	0.89	0.20	35,35,35,35	0
85	MG	5	3409	1/1	0.89	0.09	36,36,36,36	0
85	MG	1	3499	1/1	0.89	0.24	73,73,73,73	0
86	OHX	5	4142	7/7	0.89	0.17	138,138,138,138	0
86	OHX	5	4144	7/7	0.89	0.12	167,167,167,167	0
85	MG	1	3590	1/1	0.89	0.21	35,35,35,35	0
85	MG	1	3541	1/1	0.89	0.27	41,41,41,41	0
85	MG	2	2021	1/1	0.89	0.19	89,89,89,89	0
85	MG	m7	202	1/1	0.89	0.19	35,35,35,35	0
86	OHX	5	4151	7/7	0.89	0.12	168,168,168,168	0
85	MG	5	3807	1/1	0.89	0.12	62,62,62,62	0
85	MG	1	3478	1/1	0.89	0.21	79,79,79,79	0
85	MG	5	3422	1/1	0.89	0.13	45,45,45,45	0
85	MG	6	2013	1/1	0.89	0.16	82,82,82,82	0
85	MG	1	3481	1/1	0.89	0.15	62,62,62,62	0
86	OHX	5	4171	7/7	0.89	0.13	160,160,160,160	0
85	MG	6	2019	1/1	0.89	0.11	59,59,59,59	0
86	OHX	5	4176	7/7	0.89	0.12	169,169,169,169	0
85	MG	1	3549	1/1	0.89	0.34	37,37,37,37	0
85	MG	1	3550	1/1	0.89	0.40	38,38,38,38	0
85	MG	5	3699	1/1	0.89	0.08	49,49,49,49	0
86	OHX	2	2092	7/7	0.89	0.13	172,172,172,172	0
85	MG	1	3647	1/1	0.89	0.13	56,56,56,56	0
86	OHX	1	4180	7/7	0.89	0.12	167,167,167,167	0
85	MG	1	3791	1/1	0.89	0.10	53,53,53,53	0
86	OHX	2	2119	7/7	0.89	0.13	161,161,161,161	0
85	MG	5	3441	1/1	0.89	0.20	38,38,38,38	0
85	MG	5	3576	1/1	0.89	0.38	45,45,45,45	0
85	MG	5	3839	1/1	0.89	0.21	46,46,46,46	0
86	OHX	2	2135	7/7	0.89	0.13	160,160,160,160	0
85	MG	5	3581	1/1	0.89	0.27	46,46,46,46	0
86	OHX	5	4204	7/7	0.89	0.17	150,150,150,150	0
85	MG	2	2005	1/1	0.89	0.27	67,67,67,67	0
85	MG	1	3448	1/1	0.89	0.29	34,34,34,34	0
85	MG	1	3719	1/1	0.89	0.41	52,52,52,52	0
86	OHX	2	2142	7/7	0.89	0.13	163,163,163,163	0
86	OHX	5	4211	7/7	0.89	0.14	165,165,165,165	0
85	MG	2	1920	1/1	0.89	0.15	68,68,68,68	0
85	MG	1	3805	1/1	0.89	0.13	50,50,50,50	0
85	MG	4	202	1/1	0.89	0.33	49,49,49,49	0
85	MG	5	3595	1/1	0.89	0.33	41,41,41,41	0
86	OHX	1	4199	7/7	0.89	0.12	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2152	7/7	0.89	0.13	166,166,166,166	0
85	MG	1	3806	1/1	0.89	0.08	41,41,41,41	0
86	OHX	1	4202	7/7	0.89	0.13	163,163,163,163	0
86	OHX	2	2154	7/7	0.89	0.11	172,172,172,172	0
85	MG	1	3520	1/1	0.89	0.25	25,25,25,25	0
85	MG	1	3574	1/1	0.89	0.09	35,35,35,35	0
86	OHX	1	4209	7/7	0.89	0.14	162,162,162,162	0
86	OHX	1	4210	7/7	0.89	0.14	171,171,171,171	0
85	MG	4	211	1/1	0.89	0.15	80,80,80,80	0
85	MG	1	3730	1/1	0.89	0.10	45,45,45,45	0
86	OHX	4	238	7/7	0.89	0.15	159,159,159,159	0
85	MG	5	3736	1/1	0.89	0.12	45,45,45,45	0
85	MG	5	3867	1/1	0.89	0.23	43,43,43,43	0
85	MG	5	3737	1/1	0.89	0.14	41,41,41,41	0
85	MG	1	3453	1/1	0.89	0.26	53,53,53,53	0
85	MG	1	3826	1/1	0.89	0.27	32,32,32,32	0
85	MG	1	3749	1/1	0.89	0.14	68,68,68,68	0
86	OHX	6	2127	7/7	0.89	0.13	149,149,149,149	0
85	MG	5	3748	1/1	0.89	0.13	47,47,47,47	0
85	MG	5	3750	1/1	0.89	0.11	51,51,51,51	0
85	MG	5	3481	1/1	0.89	0.20	57,57,57,57	0
85	MG	5	3754	1/1	0.89	0.25	54,54,54,54	0
85	MG	1	3525	1/1	0.89	0.33	31,31,31,31	0
86	OHX	6	2153	7/7	0.89	0.12	169,169,169,169	0
85	MG	5	3626	1/1	0.89	0.14	49,49,49,49	0
85	MG	5	3486	1/1	0.89	0.17	40,40,40,40	0
86	OHX	8	228	7/7	0.89	0.14	154,154,154,154	0
86	OHX	8	229	7/7	0.89	0.14	161,161,161,161	0
86	OHX	13	405	7/7	0.89	0.12	170,170,170,170	0
86	OHX	1	4031	7/7	0.89	0.14	156,156,156,156	0
85	MG	5	3490	1/1	0.89	0.19	47,47,47,47	0
86	OHX	1	4063	7/7	0.89	0.14	155,155,155,155	0
85	MG	1	3836	1/1	0.89	0.29	59,59,59,59	0
86	OHX	1	4071	7/7	0.89	0.14	154,154,154,154	0
86	OHX	1	4074	7/7	0.89	0.13	155,155,155,155	0
86	OHX	1	4075	7/7	0.89	0.15	150,150,150,150	0
86	OHX	6	2180	7/7	0.89	0.14	164,164,164,164	0
85	MG	1	3838	1/1	0.89	0.10	49,49,49,49	0
85	MG	2	1921	1/1	0.89	0.45	61,61,61,61	0
85	MG	5	3497	1/1	0.89	0.24	48,48,48,48	0
85	MG	1	3404	1/1	0.90	0.29	73,73,73,73	0
85	MG	5	3587	1/1	0.90	0.28	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	2015	1/1	0.90	0.09	51,51,51,51	0
85	MG	1	3470	1/1	0.90	0.16	44,44,44,44	0
86	OHX	6	2177	7/7	0.90	0.15	143,143,143,143	0
85	MG	5	3590	1/1	0.90	0.23	30,30,30,30	0
85	MG	5	3735	1/1	0.90	0.19	49,49,49,49	0
86	OHX	2	2178	7/7	0.90	0.11	192,192,192,192	0
85	MG	2	1940	1/1	0.90	0.18	74,74,74,74	0
85	MG	1	3620	1/1	0.90	0.24	48,48,48,48	0
86	OHX	D9	102	7/7	0.90	0.13	164,164,164,164	0
85	MG	5	3457	1/1	0.90	0.28	35,35,35,35	0
85	MG	O1	201	1/1	0.90	0.26	64,64,64,64	0
85	MG	1	3790	1/1	0.90	0.76	38,38,38,38	0
86	OHX	1	4065	7/7	0.90	0.13	140,140,140,140	0
85	MG	5	3885	1/1	0.90	0.09	89,89,89,89	0
85	MG	5	3888	1/1	0.90	0.23	61,61,61,61	0
86	OHX	1	4073	7/7	0.90	0.14	147,147,147,147	0
85	MG	5	3745	1/1	0.90	0.28	53,53,53,53	0
85	MG	5	3464	1/1	0.90	0.09	38,38,38,38	0
85	MG	6	2024	1/1	0.90	0.16	74,74,74,74	0
85	MG	6	1901	1/1	0.90	0.39	55,55,55,55	0
85	MG	1	3661	1/1	0.90	0.23	60,60,60,60	0
85	MG	1	3588	1/1	0.90	0.34	47,47,47,47	0
85	MG	5	3471	1/1	0.90	0.15	46,46,46,46	0
85	MG	1	3796	1/1	0.90	0.23	57,57,57,57	0
85	MG	1	3728	1/1	0.90	0.11	86,86,86,86	0
85	MG	1	3589	1/1	0.90	0.18	83,83,83,83	0
86	OHX	d4	201	7/7	0.90	0.10	174,174,174,174	0
86	OHX	d9	102	7/7	0.90	0.12	179,179,179,179	0
86	OHX	1	4097	7/7	0.90	0.12	165,165,165,165	0
86	OHX	5	4072	7/7	0.90	0.42	120,120,120,120	0
86	OHX	5	4091	7/7	0.90	0.11	172,172,172,172	0
85	MG	1	3745	1/1	0.90	0.20	50,50,50,50	0
86	OHX	5	4095	7/7	0.90	0.12	152,152,152,152	0
86	OHX	5	4111	7/7	0.90	0.10	172,172,172,172	0
86	OHX	5	4113	7/7	0.90	0.12	154,154,154,154	0
85	MG	8	203	1/1	0.90	0.11	68,68,68,68	0
86	OHX	1	4108	7/7	0.90	0.17	140,140,140,140	0
86	OHX	5	4133	7/7	0.90	0.11	151,151,151,151	0
86	OHX	1	4114	7/7	0.90	0.12	157,157,157,157	0
85	MG	2	2015	1/1	0.90	0.37	57,57,57,57	0
85	MG	8	205	1/1	0.90	0.12	56,56,56,56	0
85	MG	1	3521	1/1	0.90	0.19	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3768	1/1	0.90	0.13	34,34,34,34	0
85	MG	5	3769	1/1	0.90	0.22	60,60,60,60	0
85	MG	6	1914	1/1	0.90	0.25	57,57,57,57	0
85	MG	8	211	1/1	0.90	0.47	49,49,49,49	0
85	MG	6	1915	1/1	0.90	0.40	64,64,64,64	0
85	MG	1	3494	1/1	0.90	0.16	50,50,50,50	0
85	MG	6	1974	1/1	0.90	0.17	61,61,61,61	0
86	OHX	5	4153	7/7	0.90	0.13	155,155,155,155	0
85	MG	6	2042	1/1	0.90	0.25	71,71,71,71	0
85	MG	1	3673	1/1	0.90	0.11	40,40,40,40	0
86	OHX	5	4156	7/7	0.90	0.14	151,151,151,151	0
86	OHX	1	4142	7/7	0.90	0.11	171,171,171,171	0
85	MG	1	3812	1/1	0.90	0.13	45,45,45,45	0
85	MG	5	3783	1/1	0.90	0.07	35,35,35,35	0
86	OHX	5	4166	7/7	0.90	0.11	184,184,184,184	0
86	OHX	5	4170	7/7	0.90	0.14	174,174,174,174	0
85	MG	6	1920	1/1	0.90	0.32	44,44,44,44	0
85	MG	5	3651	1/1	0.90	0.12	44,44,44,44	0
85	MG	1	3561	1/1	0.90	0.26	37,37,37,37	0
86	OHX	5	4177	7/7	0.90	0.11	162,162,162,162	0
85	MG	6	1980	1/1	0.90	0.27	57,57,57,57	0
86	OHX	1	4160	7/7	0.90	0.10	185,185,185,185	0
85	MG	m5	304	1/1	0.90	0.23	50,50,50,50	0
85	MG	m5	305	1/1	0.90	0.20	87,87,87,87	0
85	MG	5	3657	1/1	0.90	0.28	51,51,51,51	0
85	MG	1	3430	1/1	0.90	0.24	42,42,42,42	0
85	MG	1	3817	1/1	0.90	0.21	70,70,70,70	0
85	MG	4	207	1/1	0.90	0.34	35,35,35,35	0
85	MG	n3	201	1/1	0.90	0.29	24,24,24,24	0
85	MG	1	3821	1/1	0.90	0.13	31,31,31,31	0
86	OHX	1	4175	7/7	0.90	0.07	246,246,246,246	0
85	MG	1	3822	1/1	0.90	0.26	56,56,56,56	0
85	MG	n9	101	1/1	0.90	0.09	40,40,40,40	0
85	MG	6	1930	1/1	0.90	0.39	54,54,54,54	0
85	MG	1	3824	1/1	0.90	0.22	43,43,43,43	0
85	MG	5	3674	1/1	0.90	0.21	43,43,43,43	0
85	MG	5	3517	1/1	0.90	0.35	30,30,30,30	0
85	MG	1	3434	1/1	0.90	0.13	41,41,41,41	0
85	MG	4	214	1/1	0.90	0.14	45,45,45,45	0
85	MG	1	3477	1/1	0.90	0.11	98,98,98,98	0
86	OHX	2	2107	7/7	0.90	0.13	154,154,154,154	0
86	OHX	2	2111	7/7	0.90	0.10	179,179,179,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2112	7/7	0.90	0.12	158,158,158,158	0
85	MG	5	3818	1/1	0.90	0.11	41,41,41,41	0
86	OHX	2	2118	7/7	0.90	0.11	158,158,158,158	0
85	MG	4	220	1/1	0.90	0.11	44,44,44,44	0
86	OHX	2	2122	7/7	0.90	0.11	170,170,170,170	0
85	MG	5	3821	1/1	0.90	0.21	32,32,32,32	0
85	MG	1	3501	1/1	0.90	0.46	54,54,54,54	0
86	OHX	2	2133	7/7	0.90	0.10	180,180,180,180	0
86	OHX	5	4224	7/7	0.90	0.08	212,212,212,212	0
85	MG	5	3531	1/1	0.90	0.20	59,59,59,59	0
85	MG	1	3831	1/1	0.90	0.17	34,34,34,34	0
85	MG	1	3832	1/1	0.90	0.23	64,64,64,64	0
85	MG	5	3828	1/1	0.90	0.08	43,43,43,43	0
85	MG	1	3639	1/1	0.90	0.19	49,49,49,49	0
85	MG	1	3766	1/1	0.90	0.11	60,60,60,60	0
85	MG	5	3544	1/1	0.90	0.46	51,51,51,51	0
86	OHX	2	2143	7/7	0.90	0.16	148,148,148,148	0
86	OHX	2	2144	7/7	0.90	0.10	182,182,182,182	0
86	OHX	4	234	7/7	0.90	0.14	133,133,133,133	0
85	MG	5	3546	1/1	0.90	0.36	49,49,49,49	0
85	MG	5	3547	1/1	0.90	0.27	51,51,51,51	0
85	MG	1	3413	1/1	0.90	0.24	66,66,66,66	0
85	MG	5	3845	1/1	0.90	0.17	102,102,102,102	0
86	OHX	2	2150	7/7	0.90	0.12	175,175,175,175	0
85	MG	5	3549	1/1	0.90	0.23	29,29,29,29	0
85	MG	5	3421	1/1	0.90	0.29	45,45,45,45	0
86	OHX	5	4247	7/7	0.90	0.10	188,188,188,188	0
85	MG	1	3641	1/1	0.90	0.07	54,54,54,54	0
86	OHX	2	2156	7/7	0.90	0.08	262,262,262,262	0
86	OHX	8	224	7/7	0.90	0.12	172,172,172,172	0
86	OHX	6	2116	7/7	0.90	0.13	159,159,159,159	0
86	OHX	8	227	7/7	0.90	0.13	150,150,150,150	0
86	OHX	6	2124	7/7	0.90	0.13	161,161,161,161	0
85	MG	6	2004	1/1	0.90	0.11	101,101,101,101	0
85	MG	5	3707	1/1	0.90	0.18	72,72,72,72	0
85	MG	1	3534	1/1	0.90	0.18	52,52,52,52	0
86	OHX	6	2144	7/7	0.90	0.12	159,159,159,159	0
85	MG	1	3775	1/1	0.90	0.19	49,49,49,49	0
85	MG	M5	301	1/1	0.90	0.20	39,39,39,39	0
85	MG	6	2010	1/1	0.90	0.09	61,61,61,61	0
85	MG	1	3462	1/1	0.90	0.14	61,61,61,61	0
86	OHX	6	2154	7/7	0.90	0.10	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3579	1/1	0.90	0.32	33,33,33,33	0
86	OHX	2	2166	7/7	0.90	0.11	177,177,177,177	0
85	MG	1	3421	1/1	0.90	0.16	37,37,37,37	0
86	OHX	6	2168	7/7	0.90	0.15	151,151,151,151	0
85	MG	5	3552	1/1	0.91	0.16	39,39,39,39	0
85	MG	1	3714	1/1	0.91	0.09	82,82,82,82	0
86	OHX	1	4111	7/7	0.91	0.13	146,146,146,146	0
85	MG	5	3451	1/1	0.91	0.33	43,43,43,43	0
85	MG	5	3691	1/1	0.91	0.16	44,44,44,44	0
85	MG	5	3562	1/1	0.91	0.23	31,31,31,31	0
86	OHX	6	2192	7/7	0.91	0.11	173,173,173,173	0
85	MG	1	3715	1/1	0.91	0.08	41,41,41,41	0
85	MG	n8	201	1/1	0.91	0.11	37,37,37,37	0
85	MG	1	3489	1/1	0.91	0.10	59,59,59,59	0
86	OHX	6	2196	7/7	0.91	0.09	183,183,183,183	0
86	OHX	1	4128	7/7	0.91	0.13	142,142,142,142	0
85	MG	5	3697	1/1	0.91	0.17	59,59,59,59	0
86	OHX	1	4131	7/7	0.91	0.14	141,141,141,141	0
85	MG	3	212	1/1	0.91	0.15	65,65,65,65	0
85	MG	1	3491	1/1	0.91	0.10	52,52,52,52	0
86	OHX	1	4135	7/7	0.91	0.17	131,131,131,131	0
86	OHX	s4	301	7/7	0.91	0.12	168,168,168,168	0
85	MG	o7	101	1/1	0.91	0.15	47,47,47,47	0
85	MG	1	3460	1/1	0.91	0.21	28,28,28,28	0
85	MG	1	3474	1/1	0.91	0.16	41,41,41,41	0
85	MG	C1	201	1/1	0.91	0.16	69,69,69,69	0
86	OHX	1	4141	7/7	0.91	0.12	174,174,174,174	0
86	OHX	5	4050	7/7	0.91	0.13	140,140,140,140	0
86	OHX	2	2079	7/7	0.91	0.08	193,193,193,193	0
86	OHX	5	4082	7/7	0.91	0.14	138,138,138,138	0
86	OHX	1	4143	7/7	0.91	0.12	155,155,155,155	0
85	MG	5	3585	1/1	0.91	0.25	25,25,25,25	0
85	MG	6	2033	1/1	0.91	0.20	70,70,70,70	0
86	OHX	5	4097	7/7	0.91	0.20	125,125,125,125	0
86	OHX	5	4100	7/7	0.91	0.15	129,129,129,129	0
86	OHX	5	4106	7/7	0.91	0.11	155,155,155,155	0
85	MG	1	3809	1/1	0.91	0.08	53,53,53,53	0
85	MG	6	1917	1/1	0.91	0.35	67,67,67,67	0
86	OHX	5	4114	7/7	0.91	0.14	142,142,142,142	0
85	MG	1	3463	1/1	0.91	0.23	53,53,53,53	0
86	OHX	5	4119	7/7	0.91	0.10	176,176,176,176	0
86	OHX	5	4123	7/7	0.91	0.12	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4127	7/7	0.91	0.09	211,211,211,211	0
85	MG	5	3714	1/1	0.91	0.18	63,63,63,63	0
86	OHX	1	4158	7/7	0.91	0.12	155,155,155,155	0
86	OHX	1	4159	7/7	0.91	0.10	169,169,169,169	0
85	MG	5	3848	1/1	0.91	0.19	63,63,63,63	0
86	OHX	1	4162	7/7	0.91	0.09	211,211,211,211	0
85	MG	1	3733	1/1	0.91	0.14	53,53,53,53	0
86	OHX	5	4139	7/7	0.91	0.14	134,134,134,134	0
85	MG	5	3474	1/1	0.91	0.12	92,92,92,92	0
86	OHX	5	4143	7/7	0.91	0.14	158,158,158,158	0
85	MG	5	3475	1/1	0.91	0.35	50,50,50,50	0
85	MG	1	3736	1/1	0.91	0.35	55,55,55,55	0
86	OHX	2	2129	7/7	0.91	0.10	218,218,218,218	0
85	MG	1	3740	1/1	0.91	0.17	50,50,50,50	0
85	MG	1	3576	1/1	0.91	0.36	28,28,28,28	0
86	OHX	1	4173	7/7	0.91	0.16	143,143,143,143	0
85	MG	1	3442	1/1	0.91	0.18	54,54,54,54	0
85	MG	1	3747	1/1	0.91	0.09	34,34,34,34	0
85	MG	5	3600	1/1	0.91	0.19	39,39,39,39	0
85	MG	6	1927	1/1	0.91	0.28	81,81,81,81	0
85	MG	1	3443	1/1	0.91	0.19	47,47,47,47	0
85	MG	5	3605	1/1	0.91	0.27	36,36,36,36	0
86	OHX	5	4161	7/7	0.91	0.13	154,154,154,154	0
86	OHX	5	4162	7/7	0.91	0.11	161,161,161,161	0
86	OHX	5	4163	7/7	0.91	0.10	162,162,162,162	0
85	MG	1	3500	1/1	0.91	0.28	28,28,28,28	0
85	MG	5	3738	1/1	0.91	0.10	61,61,61,61	0
85	MG	5	3617	1/1	0.91	0.24	39,39,39,39	0
85	MG	4	218	1/1	0.91	0.08	67,67,67,67	0
85	MG	1	3624	1/1	0.91	0.20	39,39,39,39	0
85	MG	1	3828	1/1	0.91	0.32	41,41,41,41	0
85	MG	1	3482	1/1	0.91	0.15	48,48,48,48	0
85	MG	5	3625	1/1	0.91	0.14	43,43,43,43	0
85	MG	1	3675	1/1	0.91	0.16	42,42,42,42	0
85	MG	5	3880	1/1	0.91	0.23	61,61,61,61	0
85	MG	5	3883	1/1	0.91	0.17	36,36,36,36	0
85	MG	1	3504	1/1	0.91	0.18	32,32,32,32	0
86	OHX	5	4188	7/7	0.91	0.13	143,143,143,143	0
85	MG	1	3629	1/1	0.91	0.09	34,34,34,34	0
85	MG	5	3887	1/1	0.91	0.06	135,135,135,135	0
85	MG	6	1937	1/1	0.91	0.15	56,56,56,56	0
86	OHX	5	4198	7/7	0.91	0.16	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3680	1/1	0.91	0.14	50,50,50,50	0
85	MG	5	3509	1/1	0.91	0.14	44,44,44,44	0
85	MG	1	3447	1/1	0.91	0.11	41,41,41,41	0
85	MG	5	3637	1/1	0.91	0.07	30,30,30,30	0
86	OHX	2	2165	7/7	0.91	0.09	197,197,197,197	0
85	MG	1	3687	1/1	0.91	0.10	28,28,28,28	0
86	OHX	2	2167	7/7	0.91	0.10	172,172,172,172	0
86	OHX	5	4206	7/7	0.91	0.30	126,126,126,126	0
86	OHX	1	4207	7/7	0.91	0.16	154,154,154,154	0
86	OHX	1	4208	7/7	0.91	0.10	185,185,185,185	0
85	MG	7	207	1/1	0.91	0.17	45,45,45,45	0
85	MG	6	2000	1/1	0.91	0.10	108,108,108,108	0
86	OHX	3	222	7/7	0.91	0.10	160,160,160,160	0
86	OHX	3	224	7/7	0.91	0.13	157,157,157,157	0
85	MG	6	1941	1/1	0.91	0.19	46,46,46,46	0
85	MG	7	212	1/1	0.91	0.14	63,63,63,63	0
85	MG	7	213	1/1	0.91	0.08	59,59,59,59	0
86	OHX	4	237	7/7	0.91	0.12	168,168,168,168	0
85	MG	5	3644	1/1	0.91	0.05	31,31,31,31	0
85	MG	5	3412	1/1	0.91	0.25	45,45,45,45	0
85	MG	5	3646	1/1	0.91	0.21	71,71,71,71	0
85	MG	5	3649	1/1	0.91	0.27	69,69,69,69	0
85	MG	1	3688	1/1	0.91	0.17	43,43,43,43	0
86	OHX	C3	201	7/7	0.91	0.10	174,174,174,174	0
86	OHX	6	2099	7/7	0.91	0.10	197,197,197,197	0
85	MG	1	3689	1/1	0.91	0.15	45,45,45,45	0
86	OHX	1	3995	7/7	0.91	0.13	135,135,135,135	0
85	MG	5	3778	1/1	0.91	0.18	43,43,43,43	0
86	OHX	6	2126	7/7	0.91	0.18	136,136,136,136	0
86	OHX	1	4053	7/7	0.91	0.14	145,145,145,145	0
86	OHX	5	4233	7/7	0.91	0.10	169,169,169,169	0
86	OHX	6	2131	7/7	0.91	0.10	172,172,172,172	0
86	OHX	6	2133	7/7	0.91	0.10	169,169,169,169	0
86	OHX	1	4057	7/7	0.91	0.10	165,165,165,165	0
85	MG	1	3507	1/1	0.91	0.33	20,20,20,20	0
86	OHX	5	4238	7/7	0.91	0.26	125,125,125,125	0
86	OHX	6	2138	7/7	0.91	0.13	138,138,138,138	0
86	OHX	6	2141	7/7	0.91	0.10	181,181,181,181	0
85	MG	1	3429	1/1	0.91	0.16	52,52,52,52	0
85	MG	1	3511	1/1	0.91	0.34	25,25,25,25	0
85	MG	1	3548	1/1	0.91	0.19	46,46,46,46	0
85	MG	5	3786	1/1	0.91	0.58	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3449	1/1	0.91	0.33	50,50,50,50	0
86	OHX	5	4246	7/7	0.91	0.12	166,166,166,166	0
85	MG	1	3487	1/1	0.91	0.31	61,61,61,61	0
85	MG	5	3538	1/1	0.91	0.24	32,32,32,32	0
86	OHX	1	4076	7/7	0.91	0.14	139,139,139,139	0
86	OHX	6	2163	7/7	0.91	0.11	161,161,161,161	0
86	OHX	6	2164	7/7	0.91	0.09	214,214,214,214	0
85	MG	N5	201	1/1	0.91	0.21	69,69,69,69	0
86	OHX	1	4079	7/7	0.91	0.10	161,161,161,161	0
85	MG	N8	205	1/1	0.91	0.24	39,39,39,39	0
85	MG	1	3553	1/1	0.91	0.29	42,42,42,42	0
86	OHX	6	2173	7/7	0.91	0.13	164,164,164,164	0
85	MG	5	3545	1/1	0.91	0.30	50,50,50,50	0
85	MG	5	3676	1/1	0.91	0.10	40,40,40,40	0
86	OHX	6	2176	7/7	0.91	0.14	132,132,132,132	0
86	OHX	m0	303	7/7	0.91	0.13	145,145,145,145	0
85	MG	O2	201	1/1	0.91	0.11	36,36,36,36	0
85	MG	1	3554	1/1	0.91	0.21	50,50,50,50	0
85	MG	1	3488	1/1	0.91	0.19	36,36,36,36	0
85	MG	1	3560	1/1	0.91	0.24	50,50,50,50	0
86	OHX	1	4100	7/7	0.91	0.13	143,143,143,143	0
86	OHX	1	4102	7/7	0.91	0.14	142,142,142,142	0
85	MG	1	3711	1/1	0.91	0.20	40,40,40,40	0
85	MG	1	3530	1/1	0.92	0.28	42,42,42,42	0
85	MG	5	3551	1/1	0.92	0.35	46,46,46,46	0
86	OHX	6	2197	7/7	0.92	0.11	163,163,163,163	0
85	MG	5	3826	1/1	0.92	0.10	48,48,48,48	0
86	OHX	2	2075	7/7	0.92	0.13	151,151,151,151	0
86	OHX	2	2077	7/7	0.92	0.11	161,161,161,161	0
86	OHX	6	2201	7/7	0.92	0.11	173,173,173,173	0
85	MG	5	3444	1/1	0.92	0.30	36,36,36,36	0
85	MG	5	3446	1/1	0.92	0.17	43,43,43,43	0
85	MG	5	3556	1/1	0.92	0.14	53,53,53,53	0
86	OHX	2	2101	7/7	0.92	0.12	158,158,158,158	0
86	OHX	s8	302	7/7	0.92	0.10	193,193,193,193	0
85	MG	4	203	1/1	0.92	0.31	53,53,53,53	0
86	OHX	1	4144	7/7	0.92	0.12	159,159,159,159	0
85	MG	1	3818	1/1	0.92	0.10	51,51,51,51	0
85	MG	5	3565	1/1	0.92	0.36	32,32,32,32	0
86	OHX	5	4031	7/7	0.92	0.10	145,145,145,145	0
85	MG	1	3601	1/1	0.92	0.27	46,46,46,46	0
86	OHX	1	4150	7/7	0.92	0.13	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4065	7/7	0.92	0.12	150,150,150,150	0
85	MG	1	3763	1/1	0.92	0.18	45,45,45,45	0
86	OHX	5	4076	7/7	0.92	0.13	136,136,136,136	0
86	OHX	1	4155	7/7	0.92	0.12	148,148,148,148	0
86	OHX	5	4087	7/7	0.92	0.14	137,137,137,137	0
86	OHX	5	4090	7/7	0.92	0.11	144,144,144,144	0
85	MG	1	3577	1/1	0.92	0.29	39,39,39,39	0
86	OHX	2	2121	7/7	0.92	0.10	170,170,170,170	0
85	MG	1	3825	1/1	0.92	0.24	23,23,23,23	0
85	MG	5	3573	1/1	0.92	0.18	18,18,18,18	0
86	OHX	2	2125	7/7	0.92	0.11	155,155,155,155	0
86	OHX	5	4101	7/7	0.92	0.13	141,141,141,141	0
86	OHX	5	4104	7/7	0.92	0.14	137,137,137,137	0
86	OHX	1	4161	7/7	0.92	0.12	153,153,153,153	0
86	OHX	5	4108	7/7	0.92	0.18	135,135,135,135	0
85	MG	1	3708	1/1	0.92	0.19	66,66,66,66	0
85	MG	1	3767	1/1	0.92	0.10	64,64,64,64	0
85	MG	1	3441	1/1	0.92	0.20	24,24,24,24	0
85	MG	4	215	1/1	0.92	0.10	69,69,69,69	0
86	OHX	5	4118	7/7	0.92	0.11	165,165,165,165	0
85	MG	5	3708	1/1	0.92	0.20	48,48,48,48	0
86	OHX	5	4122	7/7	0.92	0.11	150,150,150,150	0
85	MG	5	3856	1/1	0.92	0.08	49,49,49,49	0
85	MG	5	3467	1/1	0.92	0.23	40,40,40,40	0
86	OHX	5	4128	7/7	0.92	0.14	141,141,141,141	0
86	OHX	5	4130	7/7	0.92	0.14	143,143,143,143	0
86	OHX	2	2138	7/7	0.92	0.11	159,159,159,159	0
85	MG	1	3769	1/1	0.92	0.13	66,66,66,66	0
85	MG	6	1977	1/1	0.92	0.15	53,53,53,53	0
85	MG	4	217	1/1	0.92	0.11	56,56,56,56	0
85	MG	5	3718	1/1	0.92	0.15	28,28,28,28	0
85	MG	6	1925	1/1	0.92	0.22	52,52,52,52	0
85	MG	5	3864	1/1	0.92	0.13	46,46,46,46	0
86	OHX	5	4140	7/7	0.92	0.12	160,160,160,160	0
85	MG	2	1918	1/1	0.92	0.35	57,57,57,57	0
85	MG	6	2040	1/1	0.92	0.28	59,59,59,59	0
85	MG	2	1922	1/1	0.92	0.34	65,65,65,65	0
85	MG	5	3476	1/1	0.92	0.26	30,30,30,30	0
85	MG	5	3596	1/1	0.92	0.42	28,28,28,28	0
85	MG	1	3635	1/1	0.92	0.10	60,60,60,60	0
85	MG	1	3837	1/1	0.92	0.20	49,49,49,49	0
86	OHX	1	4187	7/7	0.92	0.10	171,171,171,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2155	7/7	0.92	0.11	164,164,164,164	0
85	MG	5	3480	1/1	0.92	0.16	49,49,49,49	0
85	MG	6	1986	1/1	0.92	0.07	51,51,51,51	0
85	MG	1	3444	1/1	0.92	0.12	50,50,50,50	0
86	OHX	5	4157	7/7	0.92	0.13	140,140,140,140	0
86	OHX	5	4158	7/7	0.92	0.14	141,141,141,141	0
85	MG	6	1988	1/1	0.92	0.09	58,58,58,58	0
85	MG	5	3489	1/1	0.92	0.32	59,59,59,59	0
85	MG	1	3779	1/1	0.92	0.09	50,50,50,50	0
85	MG	5	3612	1/1	0.92	0.11	54,54,54,54	0
85	MG	5	3886	1/1	0.92	0.24	64,64,64,64	0
85	MG	5	3613	1/1	0.92	0.16	42,42,42,42	0
86	OHX	5	4165	7/7	0.92	0.08	203,203,203,203	0
85	MG	5	3614	1/1	0.92	0.18	54,54,54,54	0
86	OHX	5	4167	7/7	0.92	0.21	126,126,126,126	0
86	OHX	5	4169	7/7	0.92	0.13	157,157,157,157	0
85	MG	5	3889	1/1	0.92	0.24	56,56,56,56	0
85	MG	5	4252	1/1	0.92	0.14	40,40,40,40	0
85	MG	1	3585	1/1	0.92	0.22	29,29,29,29	0
86	OHX	2	2170	7/7	0.92	0.11	162,162,162,162	0
86	OHX	1	4205	7/7	0.92	0.15	146,146,146,146	0
85	MG	1	3678	1/1	0.92	0.08	43,43,43,43	0
85	MG	1	3503	1/1	0.92	0.38	46,46,46,46	0
86	OHX	5	4180	7/7	0.92	0.12	147,147,147,147	0
85	MG	c7	201	1/1	0.92	0.24	61,61,61,61	0
85	MG	1	3480	1/1	0.92	0.20	33,33,33,33	0
85	MG	1	3681	1/1	0.92	0.33	53,53,53,53	0
86	OHX	5	4184	7/7	0.92	0.14	149,149,149,149	0
86	OHX	5	4186	7/7	0.92	0.13	147,147,147,147	0
86	OHX	5	4187	7/7	0.92	0.14	146,146,146,146	0
85	MG	7	209	1/1	0.92	0.08	65,65,65,65	0
86	OHX	3	223	7/7	0.92	0.10	173,173,173,173	0
85	MG	1	3682	1/1	0.92	0.12	36,36,36,36	0
86	OHX	5	4192	7/7	0.92	0.12	146,146,146,146	0
86	OHX	5	4194	7/7	0.92	0.12	147,147,147,147	0
86	OHX	5	4195	7/7	0.92	0.11	148,148,148,148	0
86	OHX	5	4196	7/7	0.92	0.13	144,144,144,144	0
86	OHX	4	231	7/7	0.92	0.13	136,136,136,136	0
85	MG	d3	201	1/1	0.92	0.14	49,49,49,49	0
85	MG	5	3503	1/1	0.92	0.26	30,30,30,30	0
85	MG	1	3847	1/1	0.92	0.15	77,77,77,77	0
85	MG	5	3631	1/1	0.92	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3972	7/7	0.92	0.13	130,130,130,130	0
85	MG	1	3734	1/1	0.92	0.20	54,54,54,54	0
86	OHX	1	4015	7/7	0.92	0.12	140,140,140,140	0
85	MG	1	3567	1/1	0.92	0.25	24,24,24,24	0
86	OHX	1	4037	7/7	0.92	0.11	154,154,154,154	0
86	OHX	1	4038	7/7	0.92	0.25	122,122,122,122	0
86	OHX	1	4044	7/7	0.92	0.14	136,136,136,136	0
85	MG	5	3508	1/1	0.92	0.24	28,28,28,28	0
86	OHX	5	4210	7/7	0.92	0.08	221,221,221,221	0
86	OHX	6	2111	7/7	0.92	0.11	152,152,152,152	0
85	MG	1	3422	1/1	0.92	0.33	39,39,39,39	0
85	MG	5	3771	1/1	0.92	0.26	54,54,54,54	0
86	OHX	1	4062	7/7	0.92	0.13	136,136,136,136	0
85	MG	1	3741	1/1	0.92	0.19	31,31,31,31	0
85	MG	1	3743	1/1	0.92	0.14	54,54,54,54	0
86	OHX	1	4066	7/7	0.92	0.11	154,154,154,154	0
85	MG	5	3640	1/1	0.92	0.16	64,64,64,64	0
85	MG	1	4215	1/1	0.92	0.48	41,41,41,41	0
85	MG	1	3645	1/1	0.92	0.20	37,37,37,37	0
85	MG	5	3414	1/1	0.92	0.21	36,36,36,36	0
85	MG	8	213	1/1	0.92	0.26	69,69,69,69	0
86	OHX	6	2146	7/7	0.92	0.11	160,160,160,160	0
86	OHX	6	2147	7/7	0.92	0.13	141,141,141,141	0
85	MG	8	214	1/1	0.92	0.25	37,37,37,37	0
85	MG	1	3804	1/1	0.92	0.16	53,53,53,53	0
86	OHX	6	2151	7/7	0.92	0.14	144,144,144,144	0
85	MG	5	3648	1/1	0.92	0.15	46,46,46,46	0
86	OHX	5	4231	7/7	0.92	0.12	157,157,157,157	0
85	MG	5	3417	1/1	0.92	0.18	33,33,33,33	0
86	OHX	1	4087	7/7	0.92	0.13	142,142,142,142	0
85	MG	1	3569	1/1	0.92	0.23	41,41,41,41	0
86	OHX	6	2157	7/7	0.92	0.14	163,163,163,163	0
86	OHX	6	2158	7/7	0.92	0.11	163,163,163,163	0
85	MG	5	3654	1/1	0.92	0.21	35,35,35,35	0
86	OHX	6	2162	7/7	0.92	0.13	147,147,147,147	0
85	MG	O5	201	1/1	0.92	0.15	56,56,56,56	0
85	MG	5	3528	1/1	0.92	0.17	27,27,27,27	0
86	OHX	6	2165	7/7	0.92	0.11	165,165,165,165	0
86	OHX	6	2166	7/7	0.92	0.10	169,169,169,169	0
85	MG	O7	102	1/1	0.92	0.14	66,66,66,66	0
85	MG	6	2008	1/1	0.92	0.26	64,64,64,64	0
86	OHX	6	2169	7/7	0.92	0.11	176,176,176,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3621	1/1	0.92	0.09	56,56,56,56	0
86	OHX	1	4098	7/7	0.92	0.11	166,166,166,166	0
86	OHX	7	226	7/7	0.92	0.13	132,132,132,132	0
85	MG	5	3664	1/1	0.92	0.11	44,44,44,44	0
85	MG	5	3533	1/1	0.92	0.28	30,30,30,30	0
85	MG	1	3693	1/1	0.92	0.17	55,55,55,55	0
86	OHX	1	4105	7/7	0.92	0.10	156,156,156,156	0
85	MG	2	2009	1/1	0.92	0.24	56,56,56,56	0
85	MG	5	3539	1/1	0.92	0.26	28,28,28,28	0
85	MG	5	3428	1/1	0.92	0.13	29,29,29,29	0
86	OHX	1	4113	7/7	0.92	0.12	148,148,148,148	0
85	MG	1	3652	1/1	0.92	0.16	40,40,40,40	0
85	MG	1	3811	1/1	0.92	0.17	44,44,44,44	0
86	OHX	1	4117	7/7	0.92	0.10	170,170,170,170	0
85	MG	6	2018	1/1	0.92	0.27	46,46,46,46	0
85	MG	5	3813	1/1	0.92	0.26	63,63,63,63	0
85	MG	1	3594	1/1	0.92	0.22	38,38,38,38	0
85	MG	5	3678	1/1	0.92	0.11	41,41,41,41	0
86	OHX	1	4127	7/7	0.92	0.11	176,176,176,176	0
85	MG	5	3437	1/1	0.92	0.15	58,58,58,58	0
86	OHX	1	4129	7/7	0.92	0.12	157,157,157,157	0
85	MG	2	1960	1/1	0.92	0.29	69,69,69,69	0
85	MG	1	3461	1/1	0.92	0.20	32,32,32,32	0
86	OHX	1	3959	7/7	0.93	0.10	134,134,134,134	0
86	OHX	5	4093	7/7	0.93	0.10	166,166,166,166	0
85	MG	5	3831	1/1	0.93	0.21	36,36,36,36	0
85	MG	1	3718	1/1	0.93	0.10	74,74,74,74	0
86	OHX	1	3998	7/7	0.93	0.12	131,131,131,131	0
86	OHX	1	4004	7/7	0.93	0.11	148,148,148,148	0
85	MG	m5	303	1/1	0.93	0.12	53,53,53,53	0
86	OHX	5	4103	7/7	0.93	0.11	154,154,154,154	0
86	OHX	1	4022	7/7	0.93	0.12	131,131,131,131	0
86	OHX	1	4194	7/7	0.93	0.11	152,152,152,152	0
86	OHX	5	4107	7/7	0.93	0.12	154,154,154,154	0
85	MG	5	3403	1/1	0.93	0.17	34,34,34,34	0
86	OHX	5	4109	7/7	0.93	0.14	147,147,147,147	0
85	MG	5	3727	1/1	0.93	0.10	42,42,42,42	0
85	MG	5	3404	1/1	0.93	0.22	33,33,33,33	0
86	OHX	1	4041	7/7	0.93	0.26	126,126,126,126	0
85	MG	5	3729	1/1	0.93	0.34	47,47,47,47	0
86	OHX	1	4046	7/7	0.93	0.10	159,159,159,159	0
86	OHX	1	4048	7/7	0.93	0.10	161,161,161,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	4120	7/7	0.93	0.09	175,175,175,175	0
86	OHX	1	4051	7/7	0.93	0.20	121,121,121,121	0
85	MG	m7	203	1/1	0.93	0.10	48,48,48,48	0
86	OHX	5	4124	7/7	0.93	0.10	165,165,165,165	0
86	OHX	1	4055	7/7	0.93	0.11	147,147,147,147	0
85	MG	5	3843	1/1	0.93	0.08	47,47,47,47	0
86	OHX	5	4129	7/7	0.93	0.11	156,156,156,156	0
85	MG	1	3813	1/1	0.93	0.18	59,59,59,59	0
86	OHX	1	4059	7/7	0.93	0.13	149,149,149,149	0
85	MG	5	3406	1/1	0.93	0.20	36,36,36,36	0
85	MG	5	3734	1/1	0.93	0.09	64,64,64,64	0
85	MG	1	3437	1/1	0.93	0.14	50,50,50,50	0
85	MG	1	3538	1/1	0.93	0.29	55,55,55,55	0
86	OHX	1	4067	7/7	0.93	0.10	168,168,168,168	0
85	MG	M7	203	1/1	0.93	0.20	38,38,38,38	0
85	MG	n9	102	1/1	0.93	0.26	24,24,24,24	0
85	MG	1	3459	1/1	0.93	0.11	31,31,31,31	0
85	MG	1	3440	1/1	0.93	0.10	47,47,47,47	0
85	MG	5	3650	1/1	0.93	0.16	63,63,63,63	0
86	OHX	5	4145	7/7	0.93	0.11	166,166,166,166	0
85	MG	N0	201	1/1	0.93	0.22	45,45,45,45	0
85	MG	5	3488	1/1	0.93	0.20	49,49,49,49	0
86	OHX	1	4078	7/7	0.93	0.12	153,153,153,153	0
85	MG	1	3723	1/1	0.93	0.20	40,40,40,40	0
85	MG	5	3416	1/1	0.93	0.10	37,37,37,37	0
86	OHX	5	4152	7/7	0.93	0.11	156,156,156,156	0
86	OHX	1	4085	7/7	0.93	0.10	146,146,146,146	0
85	MG	5	3861	1/1	0.93	0.32	37,37,37,37	0
86	OHX	O3	201	7/7	0.93	0.13	137,137,137,137	0
86	OHX	6	2094	7/7	0.93	0.10	157,157,157,157	0
85	MG	6	2025	1/1	0.93	0.15	91,91,91,91	0
85	MG	5	3752	1/1	0.93	0.12	71,71,71,71	0
85	MG	1	3726	1/1	0.93	0.20	34,34,34,34	0
86	OHX	6	2112	7/7	0.93	0.11	128,128,128,128	0
85	MG	1	3686	1/1	0.93	0.18	46,46,46,46	0
86	OHX	6	2117	7/7	0.93	0.12	139,139,139,139	0
86	OHX	2	2102	7/7	0.93	0.10	166,166,166,166	0
86	OHX	2	2105	7/7	0.93	0.10	158,158,158,158	0
85	MG	5	3663	1/1	0.93	0.11	32,32,32,32	0
85	MG	5	3580	1/1	0.93	0.21	33,33,33,33	0
86	OHX	6	2132	7/7	0.93	0.13	157,157,157,157	0
86	OHX	5	4168	7/7	0.93	0.30	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3495	1/1	0.93	0.14	41,41,41,41	0
85	MG	5	3761	1/1	0.93	0.15	42,42,42,42	0
86	OHX	2	2116	7/7	0.93	0.11	160,160,160,160	0
86	OHX	5	4172	7/7	0.93	0.11	152,152,152,152	0
86	OHX	5	4173	7/7	0.93	0.14	136,136,136,136	0
86	OHX	1	4104	7/7	0.93	0.12	142,142,142,142	0
86	OHX	5	4175	7/7	0.93	0.08	183,183,183,183	0
86	OHX	6	2139	7/7	0.93	0.10	161,161,161,161	0
86	OHX	6	2140	7/7	0.93	0.10	165,165,165,165	0
85	MG	5	3583	1/1	0.93	0.31	33,33,33,33	0
85	MG	1	3651	1/1	0.93	0.13	45,45,45,45	0
85	MG	5	3876	1/1	0.93	0.28	33,33,33,33	0
86	OHX	1	4109	7/7	0.93	0.09	181,181,181,181	0
86	OHX	1	4110	7/7	0.93	0.12	155,155,155,155	0
85	MG	1	3731	1/1	0.93	0.24	60,60,60,60	0
86	OHX	2	2123	7/7	0.93	0.12	166,166,166,166	0
85	MG	1	3778	1/1	0.93	0.06	37,37,37,37	0
85	MG	O2	202	1/1	0.93	0.14	38,38,38,38	0
85	MG	1	3732	1/1	0.93	0.07	35,35,35,35	0
86	OHX	1	4120	7/7	0.93	0.10	168,168,168,168	0
85	MG	2	1985	1/1	0.93	0.13	67,67,67,67	0
86	OHX	2	2131	7/7	0.93	0.14	153,153,153,153	0
86	OHX	6	2159	7/7	0.93	0.12	137,137,137,137	0
86	OHX	2	2132	7/7	0.93	0.09	176,176,176,176	0
86	OHX	6	2161	7/7	0.93	0.11	156,156,156,156	0
86	OHX	1	4124	7/7	0.93	0.13	143,143,143,143	0
85	MG	1	3523	1/1	0.93	0.23	34,34,34,34	0
86	OHX	1	4126	7/7	0.93	0.10	169,169,169,169	0
85	MG	1	3573	1/1	0.93	0.24	29,29,29,29	0
85	MG	1	3524	1/1	0.93	0.23	24,24,24,24	0
85	MG	6	2037	1/1	0.93	0.35	52,52,52,52	0
85	MG	1	3546	1/1	0.93	0.25	45,45,45,45	0
85	MG	5	3684	1/1	0.93	0.14	51,51,51,51	0
85	MG	5	4249	1/1	0.93	0.32	38,38,38,38	0
85	MG	5	3779	1/1	0.93	0.19	56,56,56,56	0
85	MG	1	3742	1/1	0.93	0.19	43,43,43,43	0
85	MG	6	1905	1/1	0.93	0.30	56,56,56,56	0
85	MG	5	3782	1/1	0.93	0.13	65,65,65,65	0
85	MG	1	3484	1/1	0.93	0.31	41,41,41,41	0
86	OHX	2	2146	7/7	0.93	0.12	153,153,153,153	0
86	OHX	1	4140	7/7	0.93	0.14	145,145,145,145	0
85	MG	2	1998	1/1	0.93	0.09	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3690	1/1	0.93	0.24	58,58,58,58	0
85	MG	2	1902	1/1	0.93	0.22	52,52,52,52	0
86	OHX	6	2182	7/7	0.93	0.12	158,158,158,158	0
85	MG	1	3667	1/1	0.93	0.15	49,49,49,49	0
86	OHX	2	2151	7/7	0.93	0.08	201,201,201,201	0
85	MG	1	3748	1/1	0.93	0.22	47,47,47,47	0
85	MG	1	3529	1/1	0.93	0.20	29,29,29,29	0
86	OHX	6	2187	7/7	0.93	0.09	177,177,177,177	0
85	MG	5	3454	1/1	0.93	0.21	30,30,30,30	0
86	OHX	1	4151	7/7	0.93	0.13	154,154,154,154	0
85	MG	5	3526	1/1	0.93	0.30	41,41,41,41	0
85	MG	1	3669	1/1	0.93	0.23	37,37,37,37	0
85	MG	5	3616	1/1	0.93	0.13	56,56,56,56	0
86	OHX	5	4228	7/7	0.93	0.13	139,139,139,139	0
85	MG	4	221	1/1	0.93	0.07	58,58,58,58	0
85	MG	8	201	1/1	0.93	0.09	41,41,41,41	0
85	MG	8	202	1/1	0.93	0.29	46,46,46,46	0
85	MG	5	3702	1/1	0.93	0.17	52,52,52,52	0
85	MG	5	3458	1/1	0.93	0.12	30,30,30,30	0
85	MG	5	3704	1/1	0.93	0.17	57,57,57,57	0
86	OHX	1	4163	7/7	0.93	0.15	136,136,136,136	0
85	MG	5	3459	1/1	0.93	0.07	74,74,74,74	0
85	MG	1	3498	1/1	0.93	0.20	62,62,62,62	0
85	MG	5	3809	1/1	0.93	0.20	47,47,47,47	0
85	MG	1	3582	1/1	0.93	0.39	49,49,49,49	0
85	MG	1	3851	1/1	0.93	0.08	68,68,68,68	0
85	MG	1	3555	1/1	0.93	0.14	46,46,46,46	0
86	OHX	1	4171	7/7	0.93	0.11	155,155,155,155	0
85	MG	5	3540	1/1	0.93	0.19	34,34,34,34	0
85	MG	1	3808	1/1	0.93	0.07	67,67,67,67	0
86	OHX	2	2173	7/7	0.93	0.11	168,168,168,168	0
85	MG	1	3402	1/1	0.93	0.25	54,54,54,54	0
86	OHX	5	3957	7/7	0.93	0.27	101,101,101,101	0
86	OHX	5	3996	7/7	0.93	0.11	124,124,124,124	0
86	OHX	5	4010	7/7	0.93	0.11	166,166,166,166	0
85	MG	5	3717	1/1	0.93	0.17	52,52,52,52	0
86	OHX	8	219	7/7	0.93	0.11	149,149,149,149	0
86	OHX	8	221	7/7	0.93	0.10	147,147,147,147	0
86	OHX	5	4036	7/7	0.93	0.10	157,157,157,157	0
85	MG	5	3468	1/1	0.93	0.13	35,35,35,35	0
85	MG	5	3632	1/1	0.93	0.13	73,73,73,73	0
86	OHX	5	4054	7/7	0.93	0.09	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4057	7/7	0.93	0.10	148,148,148,148	0
86	OHX	5	4062	7/7	0.93	0.12	131,131,131,131	0
86	OHX	5	4063	7/7	0.93	0.10	160,160,160,160	0
85	MG	1	3558	1/1	0.93	0.27	28,28,28,28	0
86	OHX	15	304	7/7	0.93	0.09	166,166,166,166	0
86	OHX	5	4070	7/7	0.93	0.11	156,156,156,156	0
85	MG	5	3722	1/1	0.93	0.32	35,35,35,35	0
86	OHX	19	202	7/7	0.93	0.15	138,138,138,138	0
86	OHX	5	4073	7/7	0.93	0.10	152,152,152,152	0
85	MG	19	201	1/1	0.93	0.08	50,50,50,50	0
86	OHX	5	4081	7/7	0.93	0.10	151,151,151,151	0
86	OHX	S8	302	7/7	0.93	0.09	182,182,182,182	0
86	OHX	5	4086	7/7	0.93	0.13	133,133,133,133	0
85	MG	d3	203	1/1	0.93	0.11	49,49,49,49	0
86	OHX	5	4089	7/7	0.93	0.10	155,155,155,155	0
85	MG	2	2014	1/1	0.93	0.21	54,54,54,54	0
86	OHX	5	4096	7/7	0.94	0.10	162,162,162,162	0
85	MG	N8	203	1/1	0.94	0.10	46,46,46,46	0
85	MG	6	2009	1/1	0.94	0.09	58,58,58,58	0
86	OHX	1	4040	7/7	0.94	0.11	135,135,135,135	0
86	OHX	5	4102	7/7	0.94	0.12	143,143,143,143	0
85	MG	1	3758	1/1	0.94	0.16	61,61,61,61	0
85	MG	5	3499	1/1	0.94	0.13	42,42,42,42	0
86	OHX	1	4045	7/7	0.94	0.10	136,136,136,136	0
85	MG	1	3716	1/1	0.94	0.25	52,52,52,52	0
85	MG	5	3709	1/1	0.94	0.23	46,46,46,46	0
85	MG	5	3601	1/1	0.94	0.10	33,33,33,33	0
86	OHX	5	4110	7/7	0.94	0.12	145,145,145,145	0
85	MG	n6	201	1/1	0.94	0.23	54,54,54,54	0
86	OHX	5	4112	7/7	0.94	0.21	120,120,120,120	0
85	MG	5	3712	1/1	0.94	0.08	54,54,54,54	0
85	MG	6	2012	1/1	0.94	0.18	54,54,54,54	0
85	MG	1	3717	1/1	0.94	0.17	41,41,41,41	0
86	OHX	5	4116	7/7	0.94	0.09	157,157,157,157	0
86	OHX	5	4117	7/7	0.94	0.09	166,166,166,166	0
85	MG	1	3677	1/1	0.94	0.15	70,70,70,70	0
86	OHX	1	4060	7/7	0.94	0.24	126,126,126,126	0
85	MG	1	3642	1/1	0.94	0.25	42,42,42,42	0
85	MG	o3	202	1/1	0.94	0.23	38,38,38,38	0
85	MG	5	3840	1/1	0.94	0.11	58,58,58,58	0
85	MG	6	1955	1/1	0.94	0.37	51,51,51,51	0
86	OHX	5	4125	7/7	0.94	0.08	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3537	1/1	0.94	0.24	24,24,24,24	0
85	MG	O7	103	1/1	0.94	0.07	35,35,35,35	0
85	MG	5	3846	1/1	0.94	0.12	56,56,56,56	0
86	OHX	1	4072	7/7	0.94	0.10	153,153,153,153	0
85	MG	5	3615	1/1	0.94	0.07	48,48,48,48	0
86	OHX	2	2070	7/7	0.94	0.10	152,152,152,152	0
86	OHX	2	2073	7/7	0.94	0.11	135,135,135,135	0
86	OHX	2	2074	7/7	0.94	0.10	162,162,162,162	0
85	MG	1	3644	1/1	0.94	0.23	36,36,36,36	0
85	MG	1	3819	1/1	0.94	0.11	46,46,46,46	0
85	MG	5	3427	1/1	0.94	0.34	51,51,51,51	0
86	OHX	2	2080	7/7	0.94	0.10	165,165,165,165	0
86	OHX	5	4141	7/7	0.94	0.12	141,141,141,141	0
86	OHX	1	4084	7/7	0.94	0.28	107,107,107,107	0
86	OHX	2	2087	7/7	0.94	0.10	152,152,152,152	0
86	OHX	6	2113	7/7	0.94	0.10	148,148,148,148	0
86	OHX	1	4086	7/7	0.94	0.08	177,177,177,177	0
85	MG	2	1927	1/1	0.94	0.28	49,49,49,49	0
86	OHX	6	2118	7/7	0.94	0.10	164,164,164,164	0
86	OHX	6	2120	7/7	0.94	0.12	134,134,134,134	0
86	OHX	2	2097	7/7	0.94	0.10	172,172,172,172	0
85	MG	1	3562	1/1	0.94	0.06	39,39,39,39	0
86	OHX	2	2100	7/7	0.94	0.09	165,165,165,165	0
86	OHX	6	2129	7/7	0.94	0.10	160,160,160,160	0
86	OHX	1	4092	7/7	0.94	0.09	167,167,167,167	0
85	MG	5	3854	1/1	0.94	0.18	73,73,73,73	0
86	OHX	1	4094	7/7	0.94	0.12	134,134,134,134	0
85	MG	1	3518	1/1	0.94	0.19	40,40,40,40	0
86	OHX	6	2135	7/7	0.94	0.09	160,160,160,160	0
86	OHX	2	2103	7/7	0.94	0.08	204,204,204,204	0
86	OHX	2	2104	7/7	0.94	0.10	143,143,143,143	0
85	MG	5	3518	1/1	0.94	0.06	39,39,39,39	0
85	MG	5	3432	1/1	0.94	0.23	40,40,40,40	0
85	MG	5	3521	1/1	0.94	0.29	39,39,39,39	0
85	MG	1	3727	1/1	0.94	0.29	69,69,69,69	0
86	OHX	2	2113	7/7	0.94	0.10	179,179,179,179	0
85	MG	6	1906	1/1	0.94	0.18	45,45,45,45	0
85	MG	5	3436	1/1	0.94	0.18	48,48,48,48	0
86	OHX	2	2117	7/7	0.94	0.09	171,171,171,171	0
85	MG	1	3774	1/1	0.94	0.11	54,54,54,54	0
85	MG	5	3527	1/1	0.94	0.18	33,33,33,33	0
85	MG	4	209	1/1	0.94	0.07	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4112	7/7	0.94	0.10	147,147,147,147	0
85	MG	5	3529	1/1	0.94	0.23	41,41,41,41	0
85	MG	5	3743	1/1	0.94	0.12	54,54,54,54	0
86	OHX	1	4115	7/7	0.94	0.13	136,136,136,136	0
85	MG	1	3540	1/1	0.94	0.21	34,34,34,34	0
85	MG	5	3870	1/1	0.94	0.18	49,49,49,49	0
86	OHX	1	4119	7/7	0.94	0.10	164,164,164,164	0
85	MG	5	3442	1/1	0.94	0.10	40,40,40,40	0
86	OHX	2	2128	7/7	0.94	0.09	172,172,172,172	0
85	MG	5	3747	1/1	0.94	0.09	60,60,60,60	0
85	MG	1	3432	1/1	0.94	0.11	39,39,39,39	0
85	MG	5	3749	1/1	0.94	0.08	67,67,67,67	0
85	MG	2	1934	1/1	0.94	0.24	53,53,53,53	0
85	MG	5	3534	1/1	0.94	0.28	34,34,34,34	0
85	MG	5	3642	1/1	0.94	0.22	58,58,58,58	0
85	MG	5	3753	1/1	0.94	0.19	46,46,46,46	0
85	MG	6	1913	1/1	0.94	0.28	39,39,39,39	0
85	MG	2	1903	1/1	0.94	0.22	47,47,47,47	0
85	MG	1	3655	1/1	0.94	0.10	47,47,47,47	0
85	MG	1	3835	1/1	0.94	0.16	45,45,45,45	0
85	MG	5	3759	1/1	0.94	0.16	73,73,73,73	0
85	MG	5	3452	1/1	0.94	0.06	28,28,28,28	0
85	MG	1	3781	1/1	0.94	0.15	37,37,37,37	0
85	MG	1	3436	1/1	0.94	0.21	35,35,35,35	0
85	MG	1	3598	1/1	0.94	0.20	36,36,36,36	0
85	MG	5	4251	1/1	0.94	0.25	47,47,47,47	0
85	MG	1	3737	1/1	0.94	0.26	51,51,51,51	0
85	MG	1	3788	1/1	0.94	0.11	35,35,35,35	0
85	MG	1	3739	1/1	0.94	0.14	50,50,50,50	0
85	MG	L3	401	1/1	0.94	0.19	41,41,41,41	0
85	MG	L3	402	1/1	0.94	0.13	71,71,71,71	0
85	MG	5	3661	1/1	0.94	0.10	56,56,56,56	0
85	MG	L3	403	1/1	0.94	0.20	48,48,48,48	0
86	OHX	1	4148	7/7	0.94	0.12	157,157,157,157	0
85	MG	1	3660	1/1	0.94	0.14	56,56,56,56	0
85	MG	D3	201	1/1	0.94	0.15	54,54,54,54	0
85	MG	L4	402	1/1	0.94	0.09	74,74,74,74	0
86	OHX	1	4152	7/7	0.94	0.23	123,123,123,123	0
86	OHX	1	4153	7/7	0.94	0.11	139,139,139,139	0
85	MG	5	3557	1/1	0.94	0.32	38,38,38,38	0
85	MG	1	3698	1/1	0.94	0.09	43,43,43,43	0
85	MG	5	3672	1/1	0.94	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3561	1/1	0.94	0.31	24,24,24,24	0
85	MG	L7	301	1/1	0.94	0.08	39,39,39,39	0
85	MG	1	3699	1/1	0.94	0.32	48,48,48,48	0
85	MG	1	3490	1/1	0.94	0.19	36,36,36,36	0
85	MG	M0	303	1/1	0.94	0.10	41,41,41,41	0
85	MG	5	3569	1/1	0.94	0.30	24,24,24,24	0
85	MG	1	3799	1/1	0.94	0.28	44,44,44,44	0
86	OHX	2	2168	7/7	0.94	0.12	144,144,144,144	0
85	MG	1	3451	1/1	0.94	0.07	48,48,48,48	0
85	MG	5	3790	1/1	0.94	0.20	60,60,60,60	0
85	MG	1	3801	1/1	0.94	0.08	62,62,62,62	0
86	OHX	c5	201	7/7	0.94	0.09	181,181,181,181	0
85	MG	5	3574	1/1	0.94	0.24	30,30,30,30	0
85	MG	5	3575	1/1	0.94	0.18	30,30,30,30	0
86	OHX	5	3933	7/7	0.94	0.13	103,103,103,103	0
85	MG	1	3479	1/1	0.94	0.25	50,50,50,50	0
85	MG	1	3552	1/1	0.94	0.30	23,23,23,23	0
85	MG	5	3401	1/1	0.94	0.08	54,54,54,54	0
86	OHX	5	4021	7/7	0.94	0.16	115,115,115,115	0
86	OHX	5	4024	7/7	0.94	0.11	138,138,138,138	0
86	OHX	5	4030	7/7	0.94	0.09	157,157,157,157	0
85	MG	5	3402	1/1	0.94	0.09	54,54,54,54	0
85	MG	5	3482	1/1	0.94	0.31	54,54,54,54	0
86	OHX	5	4037	7/7	0.94	0.11	140,140,140,140	0
85	MG	1	3464	1/1	0.94	0.27	49,49,49,49	0
86	OHX	5	4043	7/7	0.94	0.25	121,121,121,121	0
86	OHX	5	4046	7/7	0.94	0.20	124,124,124,124	0
86	OHX	5	4047	7/7	0.94	0.13	127,127,127,127	0
85	MG	1	4212	1/1	0.94	0.10	34,34,34,34	0
86	OHX	1	4178	7/7	0.94	0.22	124,124,124,124	0
85	MG	5	3487	1/1	0.94	0.23	61,61,61,61	0
86	OHX	5	4059	7/7	0.94	0.12	137,137,137,137	0
86	OHX	7	228	7/7	0.94	0.12	142,142,142,142	0
85	MG	2	2012	1/1	0.94	0.15	66,66,66,66	0
86	OHX	C5	201	7/7	0.94	0.08	178,178,178,178	0
86	OHX	5	4064	7/7	0.94	0.12	141,141,141,141	0
86	OHX	8	223	7/7	0.94	0.11	153,153,153,153	0
85	MG	1	3638	1/1	0.94	0.09	62,62,62,62	0
86	OHX	5	4068	7/7	0.94	0.11	141,141,141,141	0
86	OHX	8	226	7/7	0.94	0.09	167,167,167,167	0
86	OHX	SR	401	7/7	0.94	0.08	196,196,196,196	0
86	OHX	5	4071	7/7	0.94	0.09	176,176,176,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3946	7/7	0.94	0.14	112,112,112,112	0
85	MG	17	301	1/1	0.94	0.09	42,42,42,42	0
86	OHX	1	3971	7/7	0.94	0.29	109,109,109,109	0
86	OHX	5	4079	7/7	0.94	0.10	135,135,135,135	0
85	MG	5	3811	1/1	0.94	0.06	70,70,70,70	0
86	OHX	1	3973	7/7	0.94	0.11	131,131,131,131	0
86	OHX	5	4083	7/7	0.94	0.15	132,132,132,132	0
86	OHX	1	3978	7/7	0.94	0.12	124,124,124,124	0
85	MG	1	3406	1/1	0.94	0.20	45,45,45,45	0
85	MG	5	3814	1/1	0.94	0.20	64,64,64,64	0
85	MG	5	3491	1/1	0.94	0.11	51,51,51,51	0
85	MG	2	2004	1/1	0.94	0.07	89,89,89,89	0
86	OHX	5	4092	7/7	0.94	0.11	147,147,147,147	0
87	ZN	Q2	501	1/1	0.94	0.14	87,87,87,87	0
85	MG	1	3516	1/1	0.94	0.26	35,35,35,35	0
86	OHX	1	4026	7/7	0.94	0.11	150,150,150,150	0
85	MG	5	3410	1/1	0.94	0.29	52,52,52,52	0
86	OHX	4	229	7/7	0.95	0.11	126,126,126,126	0
86	OHX	4	230	7/7	0.95	0.09	136,136,136,136	0
86	OHX	1	4082	7/7	0.95	0.10	151,151,151,151	0
86	OHX	4	232	7/7	0.95	0.07	166,166,166,166	0
85	MG	5	3653	1/1	0.95	0.09	60,60,60,60	0
85	MG	1	3468	1/1	0.95	0.15	29,29,29,29	0
85	MG	5	3439	1/1	0.95	0.24	35,35,35,35	0
85	MG	1	3433	1/1	0.95	0.15	49,49,49,49	0
85	MG	1	3744	1/1	0.95	0.08	41,41,41,41	0
86	OHX	L3	405	7/7	0.95	0.10	141,141,141,141	0
85	MG	1	3591	1/1	0.95	0.17	21,21,21,21	0
86	OHX	1	4089	7/7	0.95	0.08	161,161,161,161	0
86	OHX	5	4098	7/7	0.95	0.08	173,173,173,173	0
86	OHX	5	4099	7/7	0.95	0.08	163,163,163,163	0
85	MG	1	3834	1/1	0.95	0.11	54,54,54,54	0
85	MG	8	212	1/1	0.95	0.09	67,67,67,67	0
85	MG	5	3445	1/1	0.95	0.16	47,47,47,47	0
86	OHX	2	2141	7/7	0.95	0.07	202,202,202,202	0
86	OHX	6	2063	7/7	0.95	0.12	114,114,114,114	0
86	OHX	6	2076	7/7	0.95	0.11	133,133,133,133	0
86	OHX	6	2083	7/7	0.95	0.10	135,135,135,135	0
86	OHX	6	2084	7/7	0.95	0.09	156,156,156,156	0
86	OHX	6	2085	7/7	0.95	0.12	124,124,124,124	0
85	MG	5	3662	1/1	0.95	0.06	40,40,40,40	0
85	MG	1	3709	1/1	0.95	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2102	7/7	0.95	0.11	133,133,133,133	0
86	OHX	6	2104	7/7	0.95	0.10	141,141,141,141	0
85	MG	12	303	1/1	0.95	0.13	46,46,46,46	0
85	MG	5	3838	1/1	0.95	0.08	31,31,31,31	0
85	MG	1	3425	1/1	0.95	0.13	69,69,69,69	0
85	MG	1	3646	1/1	0.95	0.09	50,50,50,50	0
86	OHX	6	2114	7/7	0.95	0.08	146,146,146,146	0
86	OHX	6	2115	7/7	0.95	0.11	147,147,147,147	0
85	MG	1	3792	1/1	0.95	0.06	47,47,47,47	0
86	OHX	5	4121	7/7	0.95	0.08	160,160,160,160	0
85	MG	1	3713	1/1	0.95	0.11	48,48,48,48	0
85	MG	5	3516	1/1	0.95	0.17	26,26,26,26	0
86	OHX	6	2119	7/7	0.95	0.09	151,151,151,151	0
85	MG	5	3453	1/1	0.95	0.31	45,45,45,45	0
86	OHX	6	2122	7/7	0.95	0.09	164,164,164,164	0
86	OHX	6	2123	7/7	0.95	0.11	135,135,135,135	0
86	OHX	1	4106	7/7	0.95	0.14	132,132,132,132	0
86	OHX	6	2125	7/7	0.95	0.11	166,166,166,166	0
86	OHX	5	4131	7/7	0.95	0.10	157,157,157,157	0
85	MG	1	3751	1/1	0.95	0.18	29,29,29,29	0
85	MG	1	3551	1/1	0.95	0.12	40,40,40,40	0
85	MG	5	3520	1/1	0.95	0.28	41,41,41,41	0
85	MG	2	1919	1/1	0.95	0.31	65,65,65,65	0
85	MG	2	1981	1/1	0.95	0.37	60,60,60,60	0
85	MG	4	219	1/1	0.95	0.25	43,43,43,43	0
86	OHX	5	4138	7/7	0.95	0.10	151,151,151,151	0
85	MG	1	3755	1/1	0.95	0.19	41,41,41,41	0
85	MG	2	1910	1/1	0.95	0.33	61,61,61,61	0
85	MG	1	3438	1/1	0.95	0.23	22,22,22,22	0
86	OHX	6	2137	7/7	0.95	0.10	148,148,148,148	0
85	MG	1	3653	1/1	0.95	0.18	42,42,42,42	0
85	MG	5	3602	1/1	0.95	0.09	38,38,38,38	0
86	OHX	1	4118	7/7	0.95	0.19	124,124,124,124	0
85	MG	1	3849	1/1	0.95	0.15	89,89,89,89	0
86	OHX	6	2143	7/7	0.95	0.09	166,166,166,166	0
85	MG	m7	205	1/1	0.95	0.39	44,44,44,44	0
85	MG	6	1961	1/1	0.95	0.10	50,50,50,50	0
85	MG	1	3759	1/1	0.95	0.22	47,47,47,47	0
85	MG	5	3689	1/1	0.95	0.08	55,55,55,55	0
85	MG	6	1912	1/1	0.95	0.23	52,52,52,52	0
85	MG	1	3685	1/1	0.95	0.10	37,37,37,37	0
85	MG	1	3579	1/1	0.95	0.23	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3535	1/1	0.95	0.16	42,42,42,42	0
85	MG	1	3475	1/1	0.95	0.19	43,43,43,43	0
86	OHX	6	2155	7/7	0.95	0.11	133,133,133,133	0
85	MG	5	3777	1/1	0.95	0.07	37,37,37,37	0
85	MG	o4	201	1/1	0.95	0.21	45,45,45,45	0
85	MG	1	3417	1/1	0.95	0.19	43,43,43,43	0
86	OHX	1	4132	7/7	0.95	0.15	122,122,122,122	0
85	MG	1	3607	1/1	0.95	0.14	45,45,45,45	0
85	MG	1	3452	1/1	0.95	0.17	37,37,37,37	0
85	MG	L7	302	1/1	0.95	0.23	47,47,47,47	0
85	MG	5	3542	1/1	0.95	0.10	43,43,43,43	0
86	OHX	2	2037	7/7	0.95	0.11	163,163,163,163	0
86	OHX	2	2050	7/7	0.95	0.18	123,123,123,123	0
86	OHX	2	2056	7/7	0.95	0.08	157,157,157,157	0
86	OHX	2	2062	7/7	0.95	0.08	151,151,151,151	0
86	OHX	2	2064	7/7	0.95	0.11	130,130,130,130	0
85	MG	5	3623	1/1	0.95	0.10	59,59,59,59	0
86	OHX	1	3903	7/7	0.95	0.19	103,103,103,103	0
86	OHX	6	2171	7/7	0.95	0.13	133,133,133,133	0
86	OHX	1	3943	7/7	0.95	0.11	132,132,132,132	0
85	MG	5	3477	1/1	0.95	0.19	62,62,62,62	0
86	OHX	1	3956	7/7	0.95	0.14	112,112,112,112	0
86	OHX	1	4147	7/7	0.95	0.11	128,128,128,128	0
85	MG	5	3785	1/1	0.95	0.11	39,39,39,39	0
86	OHX	1	3966	7/7	0.95	0.12	129,129,129,129	0
85	MG	1	3609	1/1	0.95	0.26	42,42,42,42	0
85	MG	5	3881	1/1	0.95	0.14	56,56,56,56	0
85	MG	6	1972	1/1	0.95	0.20	72,72,72,72	0
86	OHX	1	3977	7/7	0.95	0.25	111,111,111,111	0
85	MG	1	3423	1/1	0.95	0.17	48,48,48,48	0
86	OHX	1	3983	7/7	0.95	0.11	131,131,131,131	0
86	OHX	1	3988	7/7	0.95	0.24	122,122,122,122	0
86	OHX	5	4189	7/7	0.95	0.08	195,195,195,195	0
86	OHX	1	3994	7/7	0.95	0.28	113,113,113,113	0
85	MG	5	3628	1/1	0.95	0.10	30,30,30,30	0
86	OHX	2	2082	7/7	0.95	0.09	159,159,159,159	0
86	OHX	1	4000	7/7	0.95	0.10	137,137,137,137	0
86	OHX	1	4002	7/7	0.95	0.09	127,127,127,127	0
86	OHX	1	4003	7/7	0.95	0.10	142,142,142,142	0
86	OHX	2	2085	7/7	0.95	0.10	137,137,137,137	0
86	OHX	1	4005	7/7	0.95	0.10	148,148,148,148	0
86	OHX	1	4006	7/7	0.95	0.10	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4011	7/7	0.95	0.08	160,160,160,160	0
85	MG	M0	302	1/1	0.95	0.09	38,38,38,38	0
86	OHX	1	4017	7/7	0.95	0.08	162,162,162,162	0
86	OHX	1	4020	7/7	0.95	0.08	147,147,147,147	0
86	OHX	2	2090	7/7	0.95	0.09	159,159,159,159	0
86	OHX	1	4023	7/7	0.95	0.10	154,154,154,154	0
86	OHX	2	2091	7/7	0.95	0.13	134,134,134,134	0
85	MG	5	3791	1/1	0.95	0.11	42,42,42,42	0
86	OHX	1	4032	7/7	0.95	0.08	163,163,163,163	0
86	OHX	1	4033	7/7	0.95	0.11	144,144,144,144	0
86	OHX	1	4034	7/7	0.95	0.11	137,137,137,137	0
86	OHX	2	2093	7/7	0.95	0.08	173,173,173,173	0
86	OHX	2	2096	7/7	0.95	0.08	186,186,186,186	0
85	MG	1	3424	1/1	0.95	0.17	34,34,34,34	0
85	MG	5	3483	1/1	0.95	0.26	51,51,51,51	0
85	MG	5	3891	1/1	0.95	0.17	41,41,41,41	0
86	OHX	c8	202	7/7	0.95	0.09	163,163,163,163	0
85	MG	3	205	1/1	0.95	0.12	37,37,37,37	0
85	MG	5	4250	1/1	0.95	0.19	34,34,34,34	0
86	OHX	sR	401	7/7	0.95	0.08	182,182,182,182	0
85	MG	1	3771	1/1	0.95	0.12	40,40,40,40	0
86	OHX	1	4049	7/7	0.95	0.21	120,120,120,120	0
86	OHX	5	3959	7/7	0.95	0.12	112,112,112,112	0
86	OHX	5	3970	7/7	0.95	0.14	110,110,110,110	0
86	OHX	5	3984	7/7	0.95	0.27	108,108,108,108	0
86	OHX	5	3985	7/7	0.95	0.14	124,124,124,124	0
86	OHX	5	3987	7/7	0.95	0.09	150,150,150,150	0
86	OHX	5	3988	7/7	0.95	0.11	134,134,134,134	0
86	OHX	5	3992	7/7	0.95	0.10	122,122,122,122	0
86	OHX	5	3995	7/7	0.95	0.24	89,89,89,89	0
85	MG	1	3664	1/1	0.95	0.27	55,55,55,55	0
86	OHX	5	3999	7/7	0.95	0.09	135,135,135,135	0
86	OHX	5	4007	7/7	0.95	0.15	122,122,122,122	0
86	OHX	1	4052	7/7	0.95	0.11	136,136,136,136	0
86	OHX	5	4012	7/7	0.95	0.11	129,129,129,129	0
86	OHX	5	4016	7/7	0.95	0.11	132,132,132,132	0
86	OHX	5	4019	7/7	0.95	0.10	135,135,135,135	0
86	OHX	5	4020	7/7	0.95	0.23	118,118,118,118	0
86	OHX	1	4189	7/7	0.95	0.09	184,184,184,184	0
85	MG	5	3715	1/1	0.95	0.17	48,48,48,48	0
85	MG	5	3635	1/1	0.95	0.13	54,54,54,54	0
86	OHX	1	4056	7/7	0.95	0.08	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4033	7/7	0.95	0.27	112,112,112,112	0
86	OHX	5	4035	7/7	0.95	0.10	170,170,170,170	0
85	MG	7	203	1/1	0.95	0.13	23,23,23,23	0
85	MG	5	3553	1/1	0.95	0.30	43,43,43,43	0
85	MG	5	3805	1/1	0.95	0.07	44,44,44,44	0
86	OHX	5	4041	7/7	0.95	0.09	149,149,149,149	0
86	OHX	5	4042	7/7	0.95	0.09	133,133,133,133	0
85	MG	3	210	1/1	0.95	0.38	52,52,52,52	0
86	OHX	5	4044	7/7	0.95	0.08	151,151,151,151	0
86	OHX	8	217	7/7	0.95	0.17	126,126,126,126	0
86	OHX	1	4061	7/7	0.95	0.07	164,164,164,164	0
85	MG	5	3555	1/1	0.95	0.29	25,25,25,25	0
86	OHX	5	4048	7/7	0.95	0.11	126,126,126,126	0
85	MG	1	3697	1/1	0.95	0.15	50,50,50,50	0
85	MG	5	3426	1/1	0.95	0.09	46,46,46,46	0
86	OHX	5	4055	7/7	0.95	0.16	128,128,128,128	0
86	OHX	5	4056	7/7	0.95	0.10	142,142,142,142	0
85	MG	1	3510	1/1	0.95	0.19	37,37,37,37	0
86	OHX	2	2120	7/7	0.95	0.09	169,169,169,169	0
85	MG	6	1982	1/1	0.95	0.29	56,56,56,56	0
85	MG	1	3614	1/1	0.95	0.19	54,54,54,54	0
85	MG	M7	205	1/1	0.95	0.13	45,45,45,45	0
85	MG	1	3700	1/1	0.95	0.20	41,41,41,41	0
86	OHX	5	4066	7/7	0.95	0.10	148,148,148,148	0
85	MG	5	3817	1/1	0.95	0.08	43,43,43,43	0
86	OHX	5	4069	7/7	0.95	0.12	143,143,143,143	0
86	OHX	2	2126	7/7	0.95	0.10	158,158,158,158	0
85	MG	1	3545	1/1	0.95	0.14	43,43,43,43	0
85	MG	1	3467	1/1	0.95	0.11	48,48,48,48	0
86	OHX	m5	306	7/7	0.95	0.10	145,145,145,145	0
85	MG	N3	202	1/1	0.95	0.15	63,63,63,63	0
86	OHX	o7	103	7/7	0.95	0.25	126,126,126,126	0
85	MG	1	3670	1/1	0.95	0.10	36,36,36,36	0
86	OHX	5	4077	7/7	0.95	0.09	143,143,143,143	0
86	OHX	1	4080	7/7	0.95	0.10	150,150,150,150	0
86	OHX	3	225	7/7	0.95	0.10	165,165,165,165	0
86	OHX	4	226	7/7	0.95	0.22	112,112,112,112	0
86	OHX	1	4070	7/7	0.96	0.09	133,133,133,133	0
86	OHX	5	4074	7/7	0.96	0.08	141,141,141,141	0
86	OHX	5	4075	7/7	0.96	0.20	125,125,125,125	0
85	MG	5	3683	1/1	0.96	0.10	58,58,58,58	0
85	MG	5	3511	1/1	0.96	0.33	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4078	7/7	0.96	0.07	156,156,156,156	0
85	MG	3	204	1/1	0.96	0.36	34,34,34,34	0
86	OHX	5	4080	7/7	0.96	0.09	147,147,147,147	0
86	OHX	6	2065	7/7	0.96	0.10	146,146,146,146	0
86	OHX	6	2070	7/7	0.96	0.08	125,125,125,125	0
86	OHX	6	2071	7/7	0.96	0.15	108,108,108,108	0
86	OHX	5	4085	7/7	0.96	0.17	127,127,127,127	0
85	MG	1	3823	1/1	0.96	0.28	43,43,43,43	0
86	OHX	6	2077	7/7	0.96	0.16	111,111,111,111	0
86	OHX	5	4088	7/7	0.96	0.10	141,141,141,141	0
85	MG	3	206	1/1	0.96	0.30	25,25,25,25	0
85	MG	5	3515	1/1	0.96	0.26	24,24,24,24	0
85	MG	6	1926	1/1	0.96	0.16	51,51,51,51	0
86	OHX	6	2087	7/7	0.96	0.09	146,146,146,146	0
86	OHX	6	2091	7/7	0.96	0.08	140,140,140,140	0
85	MG	M3	201	1/1	0.96	0.05	45,45,45,45	0
86	OHX	6	2097	7/7	0.96	0.08	131,131,131,131	0
85	MG	5	3794	1/1	0.96	0.06	36,36,36,36	0
85	MG	5	3795	1/1	0.96	0.16	42,42,42,42	0
85	MG	5	3447	1/1	0.96	0.08	50,50,50,50	0
86	OHX	6	2105	7/7	0.96	0.10	138,138,138,138	0
85	MG	1	3536	1/1	0.96	0.22	44,44,44,44	0
86	OHX	6	2110	7/7	0.96	0.09	144,144,144,144	0
85	MG	5	3693	1/1	0.96	0.14	43,43,43,43	0
85	MG	3	208	1/1	0.96	0.06	50,50,50,50	0
85	MG	1	3702	1/1	0.96	0.08	69,69,69,69	0
85	MG	5	3696	1/1	0.96	0.14	37,37,37,37	0
85	MG	M6	201	1/1	0.96	0.05	43,43,43,43	0
85	MG	5	3804	1/1	0.96	0.16	47,47,47,47	0
85	MG	1	3729	1/1	0.96	0.19	61,61,61,61	0
85	MG	5	3524	1/1	0.96	0.09	22,22,22,22	0
85	MG	5	3607	1/1	0.96	0.17	46,46,46,46	0
85	MG	5	3608	1/1	0.96	0.23	45,45,45,45	0
86	OHX	6	2121	7/7	0.96	0.08	163,163,163,163	0
85	MG	5	3609	1/1	0.96	0.05	43,43,43,43	0
85	MG	5	3610	1/1	0.96	0.05	35,35,35,35	0
85	MG	M7	202	1/1	0.96	0.22	33,33,33,33	0
85	MG	c1	201	1/1	0.96	0.24	55,55,55,55	0
85	MG	5	3456	1/1	0.96	0.14	84,84,84,84	0
86	OHX	1	4099	7/7	0.96	0.09	138,138,138,138	0
86	OHX	6	2128	7/7	0.96	0.10	164,164,164,164	0
85	MG	1	3495	1/1	0.96	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3816	1/1	0.96	0.17	78,78,78,78	0
85	MG	1	3512	1/1	0.96	0.15	25,25,25,25	0
85	MG	1	3656	1/1	0.96	0.07	38,38,38,38	0
85	MG	5	3819	1/1	0.96	0.10	41,41,41,41	0
86	OHX	5	4126	7/7	0.96	0.09	127,127,127,127	0
85	MG	5	3460	1/1	0.96	0.17	33,33,33,33	0
85	MG	5	3618	1/1	0.96	0.17	62,62,62,62	0
85	MG	1	3830	1/1	0.96	0.23	64,64,64,64	0
85	MG	1	3794	1/1	0.96	0.15	63,63,63,63	0
85	MG	1	3706	1/1	0.96	0.26	36,36,36,36	0
85	MG	d3	202	1/1	0.96	0.11	63,63,63,63	0
85	MG	1	3833	1/1	0.96	0.19	31,31,31,31	0
85	MG	1	3762	1/1	0.96	0.08	102,102,102,102	0
85	MG	1	3798	1/1	0.96	0.09	41,41,41,41	0
86	OHX	6	2145	7/7	0.96	0.10	154,154,154,154	0
85	MG	N6	201	1/1	0.96	0.33	46,46,46,46	0
85	MG	N6	202	1/1	0.96	0.26	38,38,38,38	0
85	MG	1	3570	1/1	0.96	0.21	22,22,22,22	0
86	OHX	6	2149	7/7	0.96	0.11	127,127,127,127	0
85	MG	6	1947	1/1	0.96	0.21	40,40,40,40	0
85	MG	N8	204	1/1	0.96	0.10	35,35,35,35	0
85	MG	4	206	1/1	0.96	0.18	19,19,19,19	0
85	MG	1	3735	1/1	0.96	0.17	48,48,48,48	0
85	MG	1	3618	1/1	0.96	0.07	42,42,42,42	0
85	MG	1	3556	1/1	0.96	0.17	29,29,29,29	0
85	MG	4	210	1/1	0.96	0.08	54,54,54,54	0
85	MG	1	3603	1/1	0.96	0.38	45,45,45,45	0
85	MG	5	3733	1/1	0.96	0.27	28,28,28,28	0
86	OHX	5	4150	7/7	0.96	0.10	132,132,132,132	0
85	MG	1	3572	1/1	0.96	0.15	15,15,15,15	0
85	MG	1	3547	1/1	0.96	0.11	36,36,36,36	0
85	MG	o3	201	1/1	0.96	0.33	47,47,47,47	0
85	MG	1	3843	1/1	0.96	0.07	49,49,49,49	0
85	MG	6	1958	1/1	0.96	0.34	57,57,57,57	0
85	MG	1	3606	1/1	0.96	0.22	48,48,48,48	0
85	MG	5	3643	1/1	0.96	0.31	51,51,51,51	0
86	OHX	D3	202	7/7	0.96	0.12	114,114,114,114	0
85	MG	1	3420	1/1	0.96	0.11	40,40,40,40	0
85	MG	2	1945	1/1	0.96	0.12	76,76,76,76	0
85	MG	q0	3603	1/1	0.96	0.08	47,47,47,47	0
86	OHX	1	3913	7/7	0.96	0.13	123,123,123,123	0
86	OHX	1	3918	7/7	0.96	0.18	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3921	7/7	0.96	0.13	114,114,114,114	0
86	OHX	1	3934	7/7	0.96	0.15	109,109,109,109	0
86	OHX	1	3935	7/7	0.96	0.25	104,104,104,104	0
86	OHX	1	3938	7/7	0.96	0.11	120,120,120,120	0
86	OHX	1	3940	7/7	0.96	0.09	127,127,127,127	0
85	MG	1	3627	1/1	0.96	0.21	31,31,31,31	0
86	OHX	1	3945	7/7	0.96	0.10	125,125,125,125	0
85	MG	5	3647	1/1	0.96	0.10	39,39,39,39	0
86	OHX	1	3955	7/7	0.96	0.07	142,142,142,142	0
86	OHX	2	2039	7/7	0.96	0.10	112,112,112,112	0
86	OHX	2	2049	7/7	0.96	0.08	136,136,136,136	0
86	OHX	1	3964	7/7	0.96	0.10	131,131,131,131	0
86	OHX	1	3965	7/7	0.96	0.15	120,120,120,120	0
85	MG	5	3746	1/1	0.96	0.10	49,49,49,49	0
86	OHX	1	3970	7/7	0.96	0.20	103,103,103,103	0
86	OHX	2	2055	7/7	0.96	0.09	143,143,143,143	0
85	MG	5	3559	1/1	0.96	0.28	23,23,23,23	0
86	OHX	2	2061	7/7	0.96	0.09	144,144,144,144	0
86	OHX	1	3976	7/7	0.96	0.15	125,125,125,125	0
85	MG	1	3502	1/1	0.96	0.15	29,29,29,29	0
86	OHX	2	2063	7/7	0.96	0.20	128,128,128,128	0
86	OHX	5	4185	7/7	0.96	0.08	157,157,157,157	0
86	OHX	1	3981	7/7	0.96	0.09	136,136,136,136	0
85	MG	1	3509	1/1	0.96	0.14	34,34,34,34	0
86	OHX	1	3984	7/7	0.96	0.19	127,127,127,127	0
86	OHX	1	3985	7/7	0.96	0.09	139,139,139,139	0
86	OHX	1	3987	7/7	0.96	0.09	145,145,145,145	0
85	MG	5	3564	1/1	0.96	0.26	50,50,50,50	0
86	OHX	1	3990	7/7	0.96	0.19	121,121,121,121	0
86	OHX	1	3993	7/7	0.96	0.10	127,127,127,127	0
86	OHX	2	2068	7/7	0.96	0.11	133,133,133,133	0
85	MG	1	3850	1/1	0.96	0.34	53,53,53,53	0
85	MG	5	3566	1/1	0.96	0.17	30,30,30,30	0
86	OHX	1	3999	7/7	0.96	0.09	140,140,140,140	0
85	MG	5	3424	1/1	0.96	0.15	38,38,38,38	0
86	OHX	1	4001	7/7	0.96	0.13	123,123,123,123	0
85	MG	5	3868	1/1	0.96	0.36	31,31,31,31	0
86	OHX	2	2076	7/7	0.96	0.08	143,143,143,143	0
85	MG	1	3611	1/1	0.96	0.06	39,39,39,39	0
86	OHX	2	2078	7/7	0.96	0.11	145,145,145,145	0
85	MG	4	223	1/1	0.96	0.08	86,86,86,86	0
86	OHX	1	4008	7/7	0.96	0.09	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4009	7/7	0.96	0.08	143,143,143,143	0
86	OHX	1	4010	7/7	0.96	0.10	131,131,131,131	0
86	OHX	5	3954	7/7	0.96	0.13	119,119,119,119	0
86	OHX	5	3956	7/7	0.96	0.15	113,113,113,113	0
85	MG	5	3570	1/1	0.96	0.22	48,48,48,48	0
86	OHX	1	4013	7/7	0.96	0.08	146,146,146,146	0
86	OHX	5	3960	7/7	0.96	0.19	108,108,108,108	0
86	OHX	5	3964	7/7	0.96	0.20	105,105,105,105	0
86	OHX	5	3967	7/7	0.96	0.10	125,125,125,125	0
86	OHX	1	4014	7/7	0.96	0.09	131,131,131,131	0
86	OHX	5	3973	7/7	0.96	0.09	129,129,129,129	0
86	OHX	5	3974	7/7	0.96	0.18	107,107,107,107	0
85	MG	5	3872	1/1	0.96	0.06	40,40,40,40	0
86	OHX	1	4016	7/7	0.96	0.09	135,135,135,135	0
86	OHX	2	2083	7/7	0.96	0.11	146,146,146,146	0
86	OHX	1	4018	7/7	0.96	0.07	169,169,169,169	0
86	OHX	5	3989	7/7	0.96	0.18	122,122,122,122	0
86	OHX	2	2084	7/7	0.96	0.08	161,161,161,161	0
85	MG	5	3659	1/1	0.96	0.11	75,75,75,75	0
85	MG	1	3852	1/1	0.96	0.22	78,78,78,78	0
86	OHX	1	4024	7/7	0.96	0.08	156,156,156,156	0
86	OHX	5	4005	7/7	0.96	0.12	120,120,120,120	0
85	MG	5	3496	1/1	0.96	0.17	40,40,40,40	0
86	OHX	1	4028	7/7	0.96	0.10	130,130,130,130	0
86	OHX	5	4011	7/7	0.96	0.08	145,145,145,145	0
85	MG	1	3650	1/1	0.96	0.20	46,46,46,46	0
86	OHX	5	4015	7/7	0.96	0.08	144,144,144,144	0
85	MG	5	3762	1/1	0.96	0.13	58,58,58,58	0
85	MG	1	3674	1/1	0.96	0.20	54,54,54,54	0
86	OHX	2	2094	7/7	0.96	0.08	170,170,170,170	0
86	OHX	2	2095	7/7	0.96	0.09	159,159,159,159	0
86	OHX	5	4022	7/7	0.96	0.21	108,108,108,108	0
85	MG	1	3816	1/1	0.96	0.34	46,46,46,46	0
86	OHX	5	4025	7/7	0.96	0.07	166,166,166,166	0
86	OHX	5	4026	7/7	0.96	0.15	125,125,125,125	0
86	OHX	5	4029	7/7	0.96	0.09	138,138,138,138	0
85	MG	5	3665	1/1	0.96	0.24	51,51,51,51	0
86	OHX	2	2098	7/7	0.96	0.09	141,141,141,141	0
86	OHX	5	4032	7/7	0.96	0.07	149,149,149,149	0
86	OHX	1	4043	7/7	0.96	0.08	153,153,153,153	0
86	OHX	7	225	7/7	0.96	0.08	154,154,154,154	0
85	MG	1	3782	1/1	0.96	0.59	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3882	1/1	0.96	0.29	33,33,33,33	0
85	MG	5	3667	1/1	0.96	0.18	66,66,66,66	0
85	MG	5	3668	1/1	0.96	0.40	36,36,36,36	0
86	OHX	5	4039	7/7	0.96	0.09	148,148,148,148	0
86	OHX	8	218	7/7	0.96	0.08	153,153,153,153	0
86	OHX	5	4040	7/7	0.96	0.13	126,126,126,126	0
86	OHX	8	220	7/7	0.96	0.10	140,140,140,140	0
85	MG	5	3577	1/1	0.96	0.18	26,26,26,26	0
86	OHX	8	222	7/7	0.96	0.07	166,166,166,166	0
86	OHX	3	219	7/7	0.96	0.08	131,131,131,131	0
86	OHX	3	220	7/7	0.96	0.08	144,144,144,144	0
86	OHX	3	221	7/7	0.96	0.09	145,145,145,145	0
85	MG	5	3578	1/1	0.96	0.36	27,27,27,27	0
85	MG	1	3784	1/1	0.96	0.10	94,94,94,94	0
86	OHX	2	2106	7/7	0.96	0.11	129,129,129,129	0
85	MG	1	4213	1/1	0.96	0.07	35,35,35,35	0
86	OHX	5	4051	7/7	0.96	0.08	148,148,148,148	0
86	OHX	5	4053	7/7	0.96	0.08	134,134,134,134	0
86	OHX	2	2110	7/7	0.96	0.10	128,128,128,128	0
85	MG	5	3435	1/1	0.96	0.06	37,37,37,37	0
85	MG	5	3890	1/1	0.96	0.10	119,119,119,119	0
85	MG	1	4214	1/1	0.96	0.07	72,72,72,72	0
85	MG	5	3584	1/1	0.96	0.34	20,20,20,20	0
86	OHX	5	4061	7/7	0.96	0.08	139,139,139,139	0
85	MG	5	3505	1/1	0.96	0.19	31,31,31,31	0
85	MG	1	3412	1/1	0.96	0.15	42,42,42,42	0
85	MG	1	3820	1/1	0.96	0.13	57,57,57,57	0
86	OHX	1	4064	7/7	0.96	0.11	140,140,140,140	0
85	MG	5	3679	1/1	0.96	0.09	44,44,44,44	0
85	MG	1	3724	1/1	0.96	0.14	70,70,70,70	0
85	MG	5	3440	1/1	0.96	0.14	40,40,40,40	0
85	MG	1	3566	1/1	0.96	0.22	30,30,30,30	0
87	ZN	q2	501	1/1	0.96	0.13	98,98,98,98	0
86	OHX	M0	304	7/7	0.96	0.11	118,118,118,118	0
86	OHX	1	4069	7/7	0.96	0.08	133,133,133,133	0
85	MG	5	3711	1/1	0.97	0.26	72,72,72,72	0
86	OHX	6	2202	7/7	0.97	0.05	228,228,228,228	0
86	OHX	M5	303	7/7	0.97	0.09	130,130,130,130	0
85	MG	5	3429	1/1	0.97	0.06	41,41,41,41	0
85	MG	5	3824	1/1	0.97	0.10	56,56,56,56	0
85	MG	5	3652	1/1	0.97	0.18	37,37,37,37	0
86	OHX	O1	202	7/7	0.97	0.07	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3519	1/1	0.97	0.08	39,39,39,39	0
86	OHX	O7	104	7/7	0.97	0.10	112,112,112,112	0
86	OHX	O7	105	7/7	0.97	0.21	107,107,107,107	0
86	OHX	2	2108	7/7	0.97	0.07	170,170,170,170	0
86	OHX	1	4021	7/7	0.97	0.08	140,140,140,140	0
86	OHX	2	2109	7/7	0.97	0.06	152,152,152,152	0
85	MG	8	206	1/1	0.97	0.11	74,74,74,74	0
86	OHX	5	3915	7/7	0.97	0.14	83,83,83,83	0
86	OHX	6	2072	7/7	0.97	0.08	142,142,142,142	0
86	OHX	5	3944	7/7	0.97	0.18	117,117,117,117	0
86	OHX	5	3953	7/7	0.97	0.09	93,93,93,93	0
86	OHX	6	2073	7/7	0.97	0.06	157,157,157,157	0
86	OHX	6	2075	7/7	0.97	0.11	125,125,125,125	0
85	MG	5	3537	1/1	0.97	0.15	21,21,21,21	0
86	OHX	1	4025	7/7	0.97	0.17	126,126,126,126	0
85	MG	6	2017	1/1	0.97	0.05	33,33,33,33	0
86	OHX	5	3961	7/7	0.97	0.09	110,110,110,110	0
85	MG	1	3415	1/1	0.97	0.07	58,58,58,58	0
86	OHX	1	4029	7/7	0.97	0.06	163,163,163,163	0
86	OHX	5	3968	7/7	0.97	0.11	109,109,109,109	0
86	OHX	6	2086	7/7	0.97	0.07	138,138,138,138	0
86	OHX	5	3972	7/7	0.97	0.12	109,109,109,109	0
86	OHX	1	4030	7/7	0.97	0.18	111,111,111,111	0
86	OHX	6	2089	7/7	0.97	0.09	121,121,121,121	0
86	OHX	5	3976	7/7	0.97	0.19	116,116,116,116	0
86	OHX	5	3980	7/7	0.97	0.08	119,119,119,119	0
86	OHX	5	3983	7/7	0.97	0.17	120,120,120,120	0
86	OHX	2	2114	7/7	0.97	0.10	146,146,146,146	0
86	OHX	6	2092	7/7	0.97	0.11	126,126,126,126	0
86	OHX	5	3986	7/7	0.97	0.21	108,108,108,108	0
86	OHX	2	2035	7/7	0.97	0.12	112,112,112,112	0
86	OHX	6	2095	7/7	0.97	0.08	142,142,142,142	0
85	MG	1	3455	1/1	0.97	0.11	26,26,26,26	0
86	OHX	6	2098	7/7	0.97	0.06	181,181,181,181	0
86	OHX	5	3994	7/7	0.97	0.10	127,127,127,127	0
85	MG	1	3773	1/1	0.97	0.06	46,46,46,46	0
86	OHX	6	2100	7/7	0.97	0.07	192,192,192,192	0
86	OHX	5	3998	7/7	0.97	0.18	116,116,116,116	0
86	OHX	6	2101	7/7	0.97	0.08	124,124,124,124	0
86	OHX	5	4003	7/7	0.97	0.12	127,127,127,127	0
86	OHX	5	4004	7/7	0.97	0.09	129,129,129,129	0
86	OHX	1	4035	7/7	0.97	0.08	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4006	7/7	0.97	0.08	161,161,161,161	0
86	OHX	6	2103	7/7	0.97	0.07	144,144,144,144	0
86	OHX	5	4008	7/7	0.97	0.15	117,117,117,117	0
86	OHX	5	4009	7/7	0.97	0.08	134,134,134,134	0
86	OHX	2	2042	7/7	0.97	0.09	132,132,132,132	0
86	OHX	2	2045	7/7	0.97	0.10	127,127,127,127	0
86	OHX	1	4039	7/7	0.97	0.12	125,125,125,125	0
86	OHX	5	4013	7/7	0.97	0.09	138,138,138,138	0
86	OHX	5	4014	7/7	0.97	0.17	122,122,122,122	0
86	OHX	6	2107	7/7	0.97	0.10	130,130,130,130	0
86	OHX	6	2108	7/7	0.97	0.07	144,144,144,144	0
86	OHX	5	4017	7/7	0.97	0.15	125,125,125,125	0
86	OHX	5	4018	7/7	0.97	0.07	144,144,144,144	0
86	OHX	6	2109	7/7	0.97	0.08	131,131,131,131	0
86	OHX	2	2048	7/7	0.97	0.07	139,139,139,139	0
86	OHX	1	3889	7/7	0.97	0.10	87,87,87,87	0
86	OHX	1	4042	7/7	0.97	0.08	140,140,140,140	0
86	OHX	5	4023	7/7	0.97	0.17	105,105,105,105	0
86	OHX	1	3892	7/7	0.97	0.15	95,95,95,95	0
85	MG	5	3833	1/1	0.97	0.08	76,76,76,76	0
86	OHX	1	3907	7/7	0.97	0.09	110,110,110,110	0
86	OHX	5	4027	7/7	0.97	0.10	126,126,126,126	0
85	MG	5	3792	1/1	0.97	0.36	49,49,49,49	0
86	OHX	1	3914	7/7	0.97	0.13	103,103,103,103	0
86	OHX	2	2052	7/7	0.97	0.07	148,148,148,148	0
86	OHX	1	4050	7/7	0.97	0.07	164,164,164,164	0
86	OHX	2	2053	7/7	0.97	0.08	140,140,140,140	0
86	OHX	5	4034	7/7	0.97	0.08	151,151,151,151	0
86	OHX	1	3923	7/7	0.97	0.17	104,104,104,104	0
86	OHX	1	3925	7/7	0.97	0.10	118,118,118,118	0
86	OHX	1	4054	7/7	0.97	0.07	183,183,183,183	0
86	OHX	1	3928	7/7	0.97	0.09	115,115,115,115	0
86	OHX	1	3930	7/7	0.97	0.11	108,108,108,108	0
86	OHX	1	3931	7/7	0.97	0.14	104,104,104,104	0
86	OHX	1	3932	7/7	0.97	0.09	105,105,105,105	0
86	OHX	2	2054	7/7	0.97	0.08	132,132,132,132	0
85	MG	1	3725	1/1	0.97	0.18	39,39,39,39	0
86	OHX	6	2130	7/7	0.97	0.08	133,133,133,133	0
86	OHX	5	4045	7/7	0.97	0.15	126,126,126,126	0
85	MG	5	3837	1/1	0.97	0.21	56,56,56,56	0
86	OHX	5	4212	7/7	0.97	0.18	119,119,119,119	0
86	OHX	1	3939	7/7	0.97	0.09	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	4169	7/7	0.97	0.12	125,125,125,125	0
86	OHX	2	2057	7/7	0.97	0.09	126,126,126,126	0
86	OHX	1	3941	7/7	0.97	0.13	124,124,124,124	0
86	OHX	5	4052	7/7	0.97	0.07	161,161,161,161	0
86	OHX	1	3942	7/7	0.97	0.10	128,128,128,128	0
86	OHX	2	2059	7/7	0.97	0.08	130,130,130,130	0
86	OHX	2	2130	7/7	0.97	0.10	136,136,136,136	0
86	OHX	2	2060	7/7	0.97	0.08	138,138,138,138	0
86	OHX	1	3948	7/7	0.97	0.14	111,111,111,111	0
86	OHX	5	4058	7/7	0.97	0.06	170,170,170,170	0
86	OHX	1	3954	7/7	0.97	0.19	116,116,116,116	0
85	MG	1	3439	1/1	0.97	0.15	31,31,31,31	0
85	MG	1	3776	1/1	0.97	0.09	39,39,39,39	0
85	MG	5	3758	1/1	0.97	0.07	50,50,50,50	0
86	OHX	1	3960	7/7	0.97	0.14	112,112,112,112	0
86	OHX	1	3962	7/7	0.97	0.13	120,120,120,120	0
85	MG	5	3841	1/1	0.97	0.04	42,42,42,42	0
85	MG	N8	201	1/1	0.97	0.10	32,32,32,32	0
85	MG	l5	301	1/1	0.97	0.24	39,39,39,39	0
86	OHX	1	3967	7/7	0.97	0.07	135,135,135,135	0
86	OHX	1	3968	7/7	0.97	0.08	124,124,124,124	0
86	OHX	1	4081	7/7	0.97	0.06	192,192,192,192	0
85	MG	1	3795	1/1	0.97	0.07	67,67,67,67	0
86	OHX	2	2071	7/7	0.97	0.08	137,137,137,137	0
85	MG	2	1911	1/1	0.97	0.32	54,54,54,54	0
85	MG	5	3606	1/1	0.97	0.16	35,35,35,35	0
86	OHX	1	3974	7/7	0.97	0.23	98,98,98,98	0
85	MG	1	3671	1/1	0.97	0.14	83,83,83,83	0
85	MG	m0	301	1/1	0.97	0.06	35,35,35,35	0
85	MG	1	3684	1/1	0.97	0.22	49,49,49,49	0
86	OHX	1	3979	7/7	0.97	0.07	136,136,136,136	0
86	OHX	1	3980	7/7	0.97	0.09	138,138,138,138	0
85	MG	5	3730	1/1	0.97	0.19	48,48,48,48	0
86	OHX	5	4084	7/7	0.97	0.17	118,118,118,118	0
86	OHX	7	220	7/7	0.97	0.12	115,115,115,115	0
86	OHX	7	221	7/7	0.97	0.20	109,109,109,109	0
86	OHX	7	222	7/7	0.97	0.14	114,114,114,114	0
86	OHX	7	223	7/7	0.97	0.07	118,118,118,118	0
86	OHX	7	224	7/7	0.97	0.09	123,123,123,123	0
86	OHX	1	3982	7/7	0.97	0.14	116,116,116,116	0
85	MG	1	3559	1/1	0.97	0.22	28,28,28,28	0
85	MG	5	3767	1/1	0.97	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2081	7/7	0.97	0.07	167,167,167,167	0
86	OHX	1	3986	7/7	0.97	0.07	144,144,144,144	0
85	MG	1	3602	1/1	0.97	0.06	68,68,68,68	0
85	MG	6	1983	1/1	0.97	0.09	59,59,59,59	0
86	OHX	1	3989	7/7	0.97	0.08	149,149,149,149	0
86	OHX	1	4101	7/7	0.97	0.06	163,163,163,163	0
85	MG	1	3445	1/1	0.97	0.24	34,34,34,34	0
86	OHX	1	3991	7/7	0.97	0.07	171,171,171,171	0
86	OHX	3	216	7/7	0.97	0.11	108,108,108,108	0
86	OHX	3	217	7/7	0.97	0.09	127,127,127,127	0
85	MG	1	3783	1/1	0.97	0.10	81,81,81,81	0
86	OHX	2	2086	7/7	0.97	0.08	148,148,148,148	0
85	MG	m7	201	1/1	0.97	0.19	39,39,39,39	0
86	OHX	1	3996	7/7	0.97	0.14	115,115,115,115	0
86	OHX	2	2088	7/7	0.97	0.09	135,135,135,135	0
85	MG	1	3446	1/1	0.97	0.08	32,32,32,32	0
85	MG	5	3812	1/1	0.97	0.11	63,63,63,63	0
86	OHX	5	4105	7/7	0.97	0.20	110,110,110,110	0
85	MG	1	3592	1/1	0.97	0.40	20,20,20,20	0
86	OHX	4	227	7/7	0.97	0.07	135,135,135,135	0
86	OHX	4	228	7/7	0.97	0.08	141,141,141,141	0
85	MG	5	3450	1/1	0.97	0.15	38,38,38,38	0
86	OHX	m0	302	7/7	0.97	0.08	133,133,133,133	0
85	MG	3	202	1/1	0.97	0.06	42,42,42,42	0
85	MG	5	3740	1/1	0.97	0.08	73,73,73,73	0
85	MG	6	1944	1/1	0.97	0.29	33,33,33,33	0
86	OHX	4	233	7/7	0.97	0.07	152,152,152,152	0
86	OHX	m6	203	7/7	0.97	0.16	113,113,113,113	0
85	MG	5	3742	1/1	0.97	0.21	51,51,51,51	0
86	OHX	o3	203	7/7	0.97	0.16	124,124,124,124	0
86	OHX	1	4007	7/7	0.97	0.07	157,157,157,157	0
85	MG	5	3865	1/1	0.97	0.33	44,44,44,44	0
85	MG	1	3690	1/1	0.97	0.20	45,45,45,45	0
85	MG	n8	203	1/1	0.97	0.06	43,43,43,43	0
85	MG	1	3431	1/1	0.97	0.14	33,33,33,33	0
86	OHX	1	4012	7/7	0.97	0.08	142,142,142,142	0
85	MG	5	3621	1/1	0.97	0.05	38,38,38,38	0
86	OHX	2	2029	7/7	0.98	0.10	109,109,109,109	0
86	OHX	1	3949	7/7	0.98	0.10	115,115,115,115	0
86	OHX	5	3990	7/7	0.98	0.05	136,136,136,136	0
86	OHX	5	3991	7/7	0.98	0.07	115,115,115,115	0
86	OHX	1	4036	7/7	0.98	0.06	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3993	7/7	0.98	0.06	128,128,128,128	0
86	OHX	1	3950	7/7	0.98	0.10	113,113,113,113	0
86	OHX	1	3951	7/7	0.98	0.18	87,87,87,87	0
86	OHX	3	218	7/7	0.98	0.08	119,119,119,119	0
86	OHX	5	3997	7/7	0.98	0.11	114,114,114,114	0
86	OHX	1	3953	7/7	0.98	0.07	123,123,123,123	0
86	OHX	2	2031	7/7	0.98	0.08	127,127,127,127	0
86	OHX	5	4000	7/7	0.98	0.05	146,146,146,146	0
86	OHX	5	4001	7/7	0.98	0.08	96,96,96,96	0
86	OHX	5	4002	7/7	0.98	0.16	104,104,104,104	0
86	OHX	2	2033	7/7	0.98	0.10	121,121,121,121	0
85	MG	1	3803	1/1	0.98	0.09	42,42,42,42	0
86	OHX	1	3957	7/7	0.98	0.14	90,90,90,90	0
86	OHX	1	3958	7/7	0.98	0.09	115,115,115,115	0
85	MG	1	3564	1/1	0.98	0.17	33,33,33,33	0
86	OHX	4	225	7/7	0.98	0.09	86,86,86,86	0
86	OHX	6	2142	7/7	0.98	0.07	150,150,150,150	0
86	OHX	2	2038	7/7	0.98	0.08	114,114,114,114	0
86	OHX	1	4047	7/7	0.98	0.06	155,155,155,155	0
86	OHX	1	3961	7/7	0.98	0.07	137,137,137,137	0
85	MG	5	3720	1/1	0.98	0.11	42,42,42,42	0
86	OHX	1	3963	7/7	0.98	0.07	125,125,125,125	0
85	MG	5	3594	1/1	0.98	0.21	17,17,17,17	0
86	OHX	2	2044	7/7	0.98	0.09	120,120,120,120	0
85	MG	5	3413	1/1	0.98	0.15	31,31,31,31	0
86	OHX	2	2089	7/7	0.98	0.07	141,141,141,141	0
86	OHX	2	2046	7/7	0.98	0.06	137,137,137,137	0
86	OHX	1	3969	7/7	0.98	0.13	111,111,111,111	0
86	OHX	2	2047	7/7	0.98	0.06	127,127,127,127	0
85	MG	1	3625	1/1	0.98	0.06	41,41,41,41	0
85	MG	1	3634	1/1	0.98	0.04	66,66,66,66	0
85	MG	1	3409	1/1	0.98	0.16	25,25,25,25	0
86	OHX	2	2051	7/7	0.98	0.06	127,127,127,127	0
86	OHX	1	3975	7/7	0.98	0.07	129,129,129,129	0
86	OHX	C8	201	7/7	0.98	0.08	123,123,123,123	0
86	OHX	5	4028	7/7	0.98	0.10	125,125,125,125	0
85	MG	1	3750	1/1	0.98	0.06	36,36,36,36	0
85	MG	1	3527	1/1	0.98	0.29	23,23,23,23	0
85	MG	n0	201	1/1	0.98	0.05	40,40,40,40	0
86	OHX	1	3861	7/7	0.98	0.17	64,64,64,64	0
86	OHX	1	3872	7/7	0.98	0.13	75,75,75,75	0
86	OHX	1	3883	7/7	0.98	0.11	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3887	7/7	0.98	0.09	88,88,88,88	0
86	OHX	Q2	503	7/7	0.98	0.15	99,99,99,99	0
86	OHX	6	2050	7/7	0.98	0.09	89,89,89,89	0
86	OHX	6	2052	7/7	0.98	0.10	95,95,95,95	0
86	OHX	6	2053	7/7	0.98	0.11	97,97,97,97	0
86	OHX	5	4193	7/7	0.98	0.12	103,103,103,103	0
86	OHX	6	2054	7/7	0.98	0.14	101,101,101,101	0
86	OHX	6	2058	7/7	0.98	0.10	105,105,105,105	0
86	OHX	6	2060	7/7	0.98	0.08	103,103,103,103	0
86	OHX	6	2061	7/7	0.98	0.09	103,103,103,103	0
86	OHX	6	2062	7/7	0.98	0.08	109,109,109,109	0
86	OHX	1	3888	7/7	0.98	0.11	94,94,94,94	0
86	OHX	6	2064	7/7	0.98	0.07	127,127,127,127	0
85	MG	1	3665	1/1	0.98	0.24	35,35,35,35	0
86	OHX	6	2066	7/7	0.98	0.11	112,112,112,112	0
86	OHX	6	2067	7/7	0.98	0.11	108,108,108,108	0
86	OHX	6	2069	7/7	0.98	0.11	104,104,104,104	0
85	MG	L2	302	1/1	0.98	0.07	36,36,36,36	0
86	OHX	1	3896	7/7	0.98	0.08	88,88,88,88	0
86	OHX	1	3898	7/7	0.98	0.09	103,103,103,103	0
86	OHX	1	3900	7/7	0.98	0.10	94,94,94,94	0
86	OHX	1	3901	7/7	0.98	0.09	110,110,110,110	0
85	MG	1	3712	1/1	0.98	0.08	44,44,44,44	0
86	OHX	1	3992	7/7	0.98	0.05	165,165,165,165	0
86	OHX	6	2078	7/7	0.98	0.07	126,126,126,126	0
86	OHX	6	2079	7/7	0.98	0.11	120,120,120,120	0
86	OHX	6	2080	7/7	0.98	0.08	117,117,117,117	0
86	OHX	6	2082	7/7	0.98	0.07	128,128,128,128	0
86	OHX	1	3904	7/7	0.98	0.08	103,103,103,103	0
86	OHX	1	3906	7/7	0.98	0.10	94,94,94,94	0
86	OHX	2	2058	7/7	0.98	0.07	141,141,141,141	0
86	OHX	5	4067	7/7	0.98	0.11	126,126,126,126	0
86	OHX	1	3908	7/7	0.98	0.07	118,118,118,118	0
86	OHX	1	3997	7/7	0.98	0.07	135,135,135,135	0
86	OHX	6	2088	7/7	0.98	0.06	142,142,142,142	0
86	OHX	1	3909	7/7	0.98	0.10	109,109,109,109	0
86	OHX	6	2090	7/7	0.98	0.09	137,137,137,137	0
86	OHX	1	3910	7/7	0.98	0.08	107,107,107,107	0
86	OHX	1	3911	7/7	0.98	0.09	105,105,105,105	0
86	OHX	6	2093	7/7	0.98	0.06	145,145,145,145	0
86	OHX	s1	302	7/7	0.98	0.08	100,100,100,100	0
86	OHX	1	3912	7/7	0.98	0.07	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3798	1/1	0.98	0.08	37,37,37,37	0
86	OHX	6	2096	7/7	0.98	0.05	163,163,163,163	0
85	MG	7	208	1/1	0.98	0.06	44,44,44,44	0
86	OHX	1	3915	7/7	0.98	0.07	111,111,111,111	0
86	OHX	1	3916	7/7	0.98	0.12	79,79,79,79	0
86	OHX	1	3917	7/7	0.98	0.10	102,102,102,102	0
85	MG	N8	202	1/1	0.98	0.10	41,41,41,41	0
86	OHX	1	3919	7/7	0.98	0.10	121,121,121,121	0
85	MG	5	3776	1/1	0.98	0.04	39,39,39,39	0
86	OHX	5	3901	7/7	0.98	0.14	66,66,66,66	0
86	OHX	5	3903	7/7	0.98	0.12	76,76,76,76	0
86	OHX	1	3922	7/7	0.98	0.07	121,121,121,121	0
86	OHX	5	3919	7/7	0.98	0.11	82,82,82,82	0
86	OHX	5	3922	7/7	0.98	0.10	93,93,93,93	0
86	OHX	5	3924	7/7	0.98	0.08	85,85,85,85	0
86	OHX	5	3925	7/7	0.98	0.10	109,109,109,109	0
86	OHX	5	3927	7/7	0.98	0.07	93,93,93,93	0
86	OHX	5	3932	7/7	0.98	0.10	98,98,98,98	0
86	OHX	7	219	7/7	0.98	0.07	101,101,101,101	0
85	MG	1	3599	1/1	0.98	0.10	42,42,42,42	0
86	OHX	5	3934	7/7	0.98	0.08	104,104,104,104	0
86	OHX	5	3936	7/7	0.98	0.08	91,91,91,91	0
86	OHX	5	3937	7/7	0.98	0.09	102,102,102,102	0
86	OHX	5	3938	7/7	0.98	0.08	93,93,93,93	0
86	OHX	5	3939	7/7	0.98	0.08	89,89,89,89	0
86	OHX	5	3940	7/7	0.98	0.07	97,97,97,97	0
86	OHX	5	3942	7/7	0.98	0.07	108,108,108,108	0
86	OHX	5	3943	7/7	0.98	0.08	100,100,100,100	0
85	MG	1	3535	1/1	0.98	0.45	34,34,34,34	0
86	OHX	8	216	7/7	0.98	0.05	131,131,131,131	0
86	OHX	5	3945	7/7	0.98	0.07	116,116,116,116	0
86	OHX	5	3948	7/7	0.98	0.09	107,107,107,107	0
86	OHX	5	3949	7/7	0.98	0.10	101,101,101,101	0
86	OHX	5	3951	7/7	0.98	0.08	105,105,105,105	0
86	OHX	2	2065	7/7	0.98	0.07	142,142,142,142	0
86	OHX	1	3929	7/7	0.98	0.07	112,112,112,112	0
86	OHX	2	2066	7/7	0.98	0.06	155,155,155,155	0
85	MG	1	3505	1/1	0.98	0.26	35,35,35,35	0
86	OHX	5	3958	7/7	0.98	0.09	115,115,115,115	0
85	MG	1	3691	1/1	0.98	0.05	36,36,36,36	0
86	OHX	1	3933	7/7	0.98	0.09	112,112,112,112	0
86	OHX	1	4019	7/7	0.98	0.14	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3962	7/7	0.98	0.09	113,113,113,113	0
86	OHX	l3	404	7/7	0.98	0.12	117,117,117,117	0
86	OHX	5	3963	7/7	0.98	0.07	117,117,117,117	0
86	OHX	2	2069	7/7	0.98	0.07	139,139,139,139	0
86	OHX	5	3965	7/7	0.98	0.09	98,98,98,98	0
86	OHX	5	3966	7/7	0.98	0.09	92,92,92,92	0
85	MG	5	3829	1/1	0.98	0.20	58,58,58,58	0
86	OHX	1	3937	7/7	0.98	0.07	112,112,112,112	0
85	MG	5	3485	1/1	0.98	0.25	28,28,28,28	0
86	OHX	2	2072	7/7	0.98	0.06	157,157,157,157	0
85	MG	1	3658	1/1	0.98	0.08	35,35,35,35	0
85	MG	1	3532	1/1	0.98	0.36	33,33,33,33	0
86	OHX	5	3975	7/7	0.98	0.10	108,108,108,108	0
86	OHX	1	4027	7/7	0.98	0.14	121,121,121,121	0
86	OHX	5	3977	7/7	0.98	0.11	108,108,108,108	0
86	OHX	5	3978	7/7	0.98	0.08	110,110,110,110	0
86	OHX	n3	202	7/7	0.98	0.12	106,106,106,106	0
86	OHX	5	3979	7/7	0.98	0.13	107,107,107,107	0
85	MG	6	2016	1/1	0.98	0.10	82,82,82,82	0
86	OHX	q2	502	7/7	0.98	0.13	98,98,98,98	0
86	OHX	5	3981	7/7	0.98	0.06	130,130,130,130	0
87	ZN	E1	501	1/1	0.98	0.05	118,118,118,118	0
85	MG	5	3834	1/1	0.98	0.11	40,40,40,40	0
86	OHX	1	3944	7/7	0.98	0.11	114,114,114,114	0
87	ZN	e1	501	1/1	0.98	0.07	158,158,158,158	0
86	OHX	2	2025	7/7	0.98	0.11	97,97,97,97	0
86	OHX	2	2028	7/7	0.98	0.09	106,106,106,106	0
86	OHX	1	3947	7/7	0.98	0.13	113,113,113,113	0
86	OHX	5	3952	7/7	0.99	0.07	88,88,88,88	0
86	OHX	1	3891	7/7	0.99	0.07	93,93,93,93	0
85	MG	5	3463	1/1	0.99	0.09	38,38,38,38	0
86	OHX	5	3955	7/7	0.99	0.05	109,109,109,109	0
86	OHX	1	3893	7/7	0.99	0.06	97,97,97,97	0
86	OHX	1	3894	7/7	0.99	0.06	80,80,80,80	0
86	OHX	1	3895	7/7	0.99	0.07	85,85,85,85	0
85	MG	5	3844	1/1	0.99	0.09	54,54,54,54	0
86	OHX	1	3897	7/7	0.99	0.06	78,78,78,78	0
86	OHX	2	2040	7/7	0.99	0.05	108,108,108,108	0
86	OHX	1	3899	7/7	0.99	0.04	101,101,101,101	0
86	OHX	2	2041	7/7	0.99	0.06	113,113,113,113	0
86	OHX	4	224	7/7	0.99	0.07	65,65,65,65	0
85	MG	5	3560	1/1	0.99	0.32	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3902	7/7	0.99	0.07	92,92,92,92	0
86	OHX	2	2043	7/7	0.99	0.07	120,120,120,120	0
85	MG	1	4216	1/1	0.99	0.10	40,40,40,40	0
86	OHX	5	3969	7/7	0.99	0.05	119,119,119,119	0
86	OHX	1	3905	7/7	0.99	0.07	101,101,101,101	0
86	OHX	5	3971	7/7	0.99	0.11	101,101,101,101	0
85	MG	5	3582	1/1	0.99	0.32	28,28,28,28	0
85	MG	1	3465	1/1	0.99	0.10	47,47,47,47	0
85	MG	5	3563	1/1	0.99	0.10	32,32,32,32	0
85	MG	12	302	1/1	0.99	0.08	36,36,36,36	0
86	OHX	2	2023	7/7	0.99	0.12	84,84,84,84	0
86	OHX	2	2024	7/7	0.99	0.07	94,94,94,94	0
85	MG	1	3595	1/1	0.99	0.27	13,13,13,13	0
86	OHX	2	2026	7/7	0.99	0.08	98,98,98,98	0
86	OHX	2	2027	7/7	0.99	0.07	89,89,89,89	0
85	MG	1	3563	1/1	0.99	0.29	24,24,24,24	0
86	OHX	5	3982	7/7	0.99	0.07	100,100,100,100	0
85	MG	1	3584	1/1	0.99	0.18	24,24,24,24	0
86	OHX	2	2030	7/7	0.99	0.09	118,118,118,118	0
85	MG	5	3853	1/1	0.99	0.10	63,63,63,63	0
86	OHX	1	3857	7/7	0.99	0.11	52,52,52,52	0
86	OHX	1	3920	7/7	0.99	0.08	101,101,101,101	0
86	OHX	1	3860	7/7	0.99	0.09	64,64,64,64	0
86	OHX	2	2032	7/7	0.99	0.07	121,121,121,121	0
86	OHX	N9	101	7/7	0.99	0.08	72,72,72,72	0
86	OHX	1	3862	7/7	0.99	0.06	61,61,61,61	0
86	OHX	1	3924	7/7	0.99	0.07	96,96,96,96	0
86	OHX	1	3863	7/7	0.99	0.11	66,66,66,66	0
86	OHX	1	3926	7/7	0.99	0.06	108,108,108,108	0
86	OHX	1	3927	7/7	0.99	0.10	94,94,94,94	0
86	OHX	6	2046	7/7	0.99	0.10	66,66,66,66	0
86	OHX	6	2047	7/7	0.99	0.13	85,85,85,85	0
86	OHX	6	2048	7/7	0.99	0.08	83,83,83,83	0
86	OHX	6	2049	7/7	0.99	0.07	79,79,79,79	0
86	OHX	1	3864	7/7	0.99	0.06	63,63,63,63	0
86	OHX	6	2051	7/7	0.99	0.07	85,85,85,85	0
86	OHX	1	3865	7/7	0.99	0.07	69,69,69,69	0
86	OHX	1	3866	7/7	0.99	0.10	68,68,68,68	0
86	OHX	1	3867	7/7	0.99	0.06	67,67,67,67	0
86	OHX	6	2055	7/7	0.99	0.08	90,90,90,90	0
86	OHX	6	2057	7/7	0.99	0.07	111,111,111,111	0
86	OHX	1	3868	7/7	0.99	0.08	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2059	7/7	0.99	0.05	106,106,106,106	0
86	OHX	1	3869	7/7	0.99	0.07	80,80,80,80	0
86	OHX	1	3870	7/7	0.99	0.06	85,85,85,85	0
86	OHX	5	3892	7/7	0.99	0.14	57,57,57,57	0
86	OHX	5	3894	7/7	0.99	0.10	53,53,53,53	0
86	OHX	5	3895	7/7	0.99	0.11	58,58,58,58	0
86	OHX	5	3896	7/7	0.99	0.11	59,59,59,59	0
86	OHX	5	3897	7/7	0.99	0.06	68,68,68,68	0
86	OHX	7	218	7/7	0.99	0.07	96,96,96,96	0
86	OHX	5	3899	7/7	0.99	0.09	70,70,70,70	0
86	OHX	5	3900	7/7	0.99	0.07	73,73,73,73	0
85	MG	1	3738	1/1	0.99	0.09	40,40,40,40	0
86	OHX	5	3902	7/7	0.99	0.08	60,60,60,60	0
86	OHX	1	3936	7/7	0.99	0.05	111,111,111,111	0
86	OHX	5	3904	7/7	0.99	0.06	81,81,81,81	0
86	OHX	5	3905	7/7	0.99	0.08	77,77,77,77	0
86	OHX	5	3906	7/7	0.99	0.07	72,72,72,72	0
86	OHX	5	3907	7/7	0.99	0.08	71,71,71,71	0
86	OHX	5	3908	7/7	0.99	0.07	83,83,83,83	0
86	OHX	5	3910	7/7	0.99	0.07	70,70,70,70	0
86	OHX	8	215	7/7	0.99	0.07	68,68,68,68	0
86	OHX	5	3911	7/7	0.99	0.09	79,79,79,79	0
86	OHX	5	3912	7/7	0.99	0.07	92,92,92,92	0
86	OHX	5	3913	7/7	0.99	0.08	78,78,78,78	0
86	OHX	5	3914	7/7	0.99	0.08	84,84,84,84	0
86	OHX	1	3873	7/7	0.99	0.07	77,77,77,77	0
86	OHX	5	3916	7/7	0.99	0.09	89,89,89,89	0
86	OHX	5	3917	7/7	0.99	0.07	83,83,83,83	0
86	OHX	1	3874	7/7	0.99	0.07	87,87,87,87	0
86	OHX	5	3920	7/7	0.99	0.06	95,95,95,95	0
86	OHX	5	3921	7/7	0.99	0.07	89,89,89,89	0
86	OHX	1	3875	7/7	0.99	0.10	81,81,81,81	0
86	OHX	1	3876	7/7	0.99	0.05	73,73,73,73	0
86	OHX	6	2068	7/7	0.99	0.05	118,118,118,118	0
86	OHX	5	3926	7/7	0.99	0.05	85,85,85,85	0
86	OHX	1	3877	7/7	0.99	0.07	83,83,83,83	0
86	OHX	5	3928	7/7	0.99	0.07	93,93,93,93	0
86	OHX	5	3929	7/7	0.99	0.05	83,83,83,83	0
86	OHX	5	3930	7/7	0.99	0.10	86,86,86,86	0
86	OHX	5	3931	7/7	0.99	0.07	95,95,95,95	0
86	OHX	1	3878	7/7	0.99	0.08	86,86,86,86	0
86	OHX	1	3879	7/7	0.99	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3880	7/7	0.99	0.07	91,91,91,91	0
86	OHX	5	4049	7/7	0.99	0.07	124,124,124,124	0
86	OHX	5	3935	7/7	0.99	0.06	105,105,105,105	0
86	OHX	1	3881	7/7	0.99	0.07	87,87,87,87	0
86	OHX	6	2074	7/7	0.99	0.05	110,110,110,110	0
86	OHX	1	3882	7/7	0.99	0.08	76,76,76,76	0
86	OHX	2	2034	7/7	0.99	0.10	110,110,110,110	0
86	OHX	1	3884	7/7	0.99	0.08	73,73,73,73	0
86	OHX	n1	201	7/7	0.99	0.09	69,69,69,69	0
86	OHX	5	3941	7/7	0.99	0.06	100,100,100,100	0
86	OHX	n9	103	7/7	0.99	0.05	77,77,77,77	0
86	OHX	1	3885	7/7	0.99	0.08	83,83,83,83	0
85	MG	m6	202	1/1	0.99	0.05	39,39,39,39	0
86	OHX	2	2036	7/7	0.99	0.06	110,110,110,110	0
86	OHX	5	4060	7/7	0.99	0.06	130,130,130,130	0
86	OHX	6	2081	7/7	0.99	0.09	109,109,109,109	0
86	OHX	5	3946	7/7	0.99	0.05	84,84,84,84	0
86	OHX	5	3947	7/7	0.99	0.05	112,112,112,112	0
87	ZN	d9	101	1/1	0.99	0.04	87,87,87,87	0
86	OHX	1	3952	7/7	0.99	0.05	125,125,125,125	0
85	MG	1	3764	1/1	0.99	0.08	75,75,75,75	0
86	OHX	5	3950	7/7	0.99	0.09	96,96,96,96	0
86	OHX	1	3890	7/7	0.99	0.08	87,87,87,87	0
86	OHX	5	3893	7/7	1.00	0.08	51,51,51,51	0
87	ZN	D6	500	1/1	1.00	0.01	84,84,84,84	0
86	OHX	1	3859	7/7	1.00	0.07	55,55,55,55	0
87	ZN	D9	101	1/1	1.00	0.02	83,83,83,83	0
86	OHX	5	3909	7/7	1.00	0.04	74,74,74,74	0
87	ZN	O7	101	1/1	1.00	0.04	50,50,50,50	0
87	ZN	Q0	500	1/1	1.00	0.01	52,52,52,52	0
86	OHX	5	3918	7/7	1.00	0.04	68,68,68,68	0
87	ZN	Q3	501	1/1	1.00	0.03	72,72,72,72	0
87	ZN	d6	101	1/1	1.00	0.02	68,68,68,68	0
86	OHX	1	3858	7/7	1.00	0.06	62,62,62,62	0
86	OHX	1	3886	7/7	1.00	0.08	82,82,82,82	0
86	OHX	1	3871	7/7	1.00	0.05	69,69,69,69	0
87	ZN	o7	102	1/1	1.00	0.05	53,53,53,53	0
87	ZN	q0	3602	1/1	1.00	0.01	38,38,38,38	0
86	OHX	5	3898	7/7	1.00	0.05	69,69,69,69	0
87	ZN	q3	501	1/1	1.00	0.05	78,78,78,78	0
86	OHX	5	3923	7/7	1.00	0.04	81,81,81,81	0
86	OHX	6	2056	7/7	1.00	0.05	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.