



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:28 PM UTC

PDB ID : 4U3M / pdb_00004u3m
Title : Crystal structure of Anisomycin bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-22
Resolution : 3.00 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

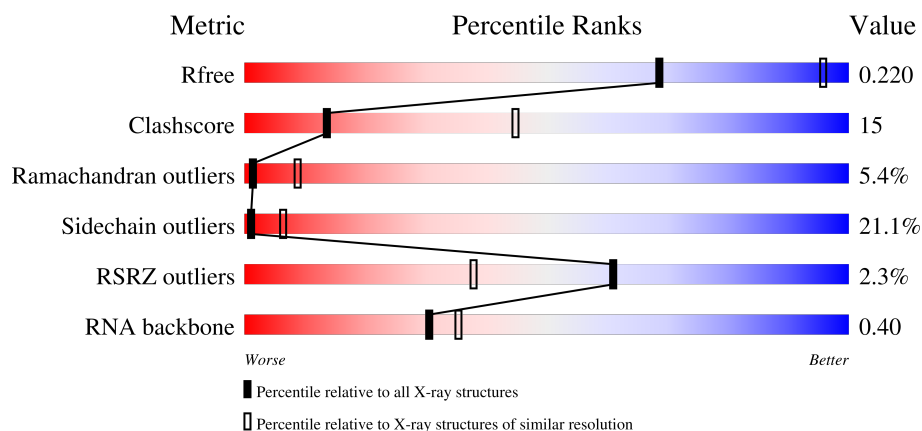
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	2% 40% 42% 15% .
1	6	1800	2% 44% 41% 14%
2	S0	251	4% 34% 35% 12% . 18%
2	s0	251	2% 34% 35% 11% . 18%

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Mol	Chain	Length	Quality of chain
3	S1	254	
3	s1	254	
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	

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Mol	Chain	Length	Quality of chain
15	c3	150	
16	C4	136	
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	

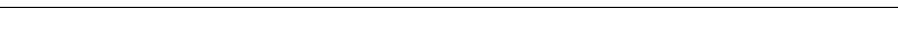
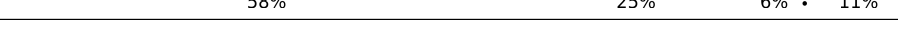
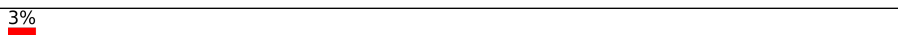
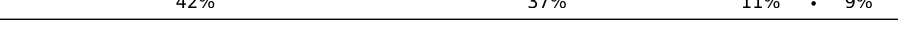
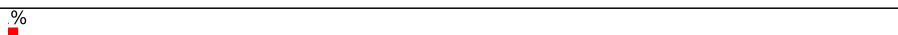
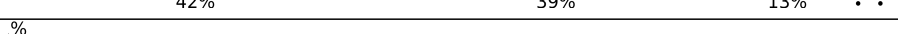
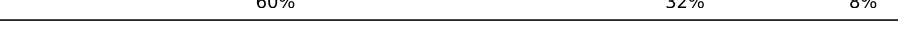
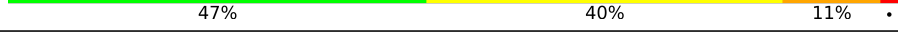
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Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	

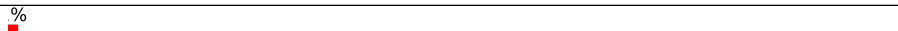
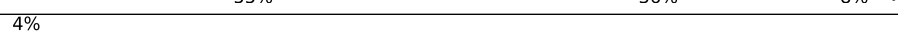
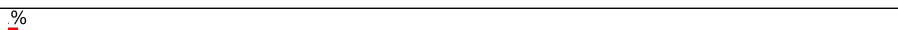
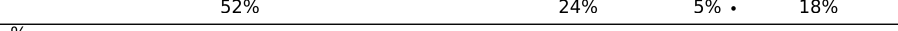
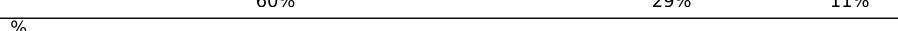
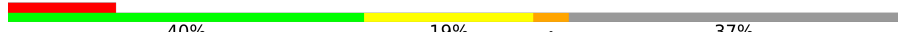
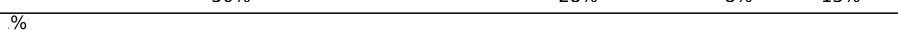
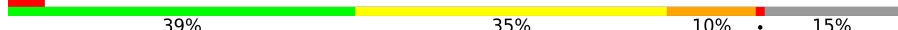
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Mol	Chain	Length	Quality of chain
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	

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Mol	Chain	Length	Quality of chain
54	M8	185	
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	

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Mol	Chain	Length	Quality of chain
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
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	

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Mol	Chain	Length	Quality of chain
79	Q3	91	
79	q3	91	
80	e0	62	
81	e1	76	
82	m2	160	
83	p0	311	
84	p1	47	
85	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
86	MG	1	3652	-	-	-	X
86	MG	1	3672	-	-	-	X
86	MG	1	3676	-	-	-	X
86	MG	1	3723	-	-	-	X
86	MG	1	3819	-	-	-	X
86	MG	2	1915	-	-	-	X
86	MG	2	1928	-	-	-	X
86	MG	2	1953	-	-	-	X
86	MG	2	1959	-	-	-	X
86	MG	2	1968	-	-	-	X
86	MG	2	1975	-	-	-	X
86	MG	2	1990	-	-	-	X
86	MG	2	2019	-	-	-	X
86	MG	4	222	-	-	-	X
86	MG	5	3790	-	-	-	X
86	MG	5	3887	-	-	-	X
86	MG	5	3891	-	-	-	X
86	MG	6	1924	-	-	-	X
86	MG	6	1933	-	-	-	X
86	MG	6	2026	-	-	-	X
86	MG	6	2036	-	-	-	X
86	MG	6	2037	-	-	-	X
86	MG	6	2042	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	S2	301	-	-	-	X
87	OHX	1	3961	-	-	X	-
87	OHX	1	3963	-	-	X	-
87	OHX	1	3975	-	-	X	-
87	OHX	1	4007	-	-	X	-
87	OHX	1	4023	-	-	X	-
87	OHX	1	4032	-	-	X	-
87	OHX	1	4036	-	-	X	-
87	OHX	1	4047	-	-	X	-
87	OHX	1	4048	-	-	X	-
87	OHX	1	4059	-	-	X	-
87	OHX	1	4060	-	-	X	-
87	OHX	1	4061	-	-	X	-
87	OHX	1	4084	-	-	X	-
87	OHX	1	4088	-	-	X	-
87	OHX	1	4144	-	-	X	-
87	OHX	1	4151	-	-	X	-
87	OHX	1	4159	-	-	X	-
87	OHX	1	4161	-	-	X	-
87	OHX	1	4168	-	-	X	-
87	OHX	1	4177	-	-	X	-
87	OHX	1	4186	-	-	X	-
87	OHX	1	4203	-	-	X	-
87	OHX	2	2031	-	-	X	-
87	OHX	2	2044	-	-	X	-
87	OHX	2	2075	-	-	X	-
87	OHX	2	2089	-	-	X	-
87	OHX	2	2090	-	-	X	-
87	OHX	2	2095	-	-	X	-
87	OHX	2	2096	-	-	X	-
87	OHX	2	2099	-	-	X	-
87	OHX	2	2109	-	-	X	-
87	OHX	2	2116	-	-	X	-
87	OHX	2	2132	-	-	X	-
87	OHX	2	2147	-	-	X	-
87	OHX	2	2163	-	-	X	-
87	OHX	5	3947	-	-	X	-
87	OHX	5	3967	-	-	X	-
87	OHX	5	3978	-	-	X	-
87	OHX	5	3983	-	-	X	-
87	OHX	5	4005	-	-	X	-
87	OHX	5	4006	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	5	4016	-	-	X	-
87	OHX	5	4026	-	-	X	-
87	OHX	5	4041	-	-	X	-
87	OHX	5	4061	-	-	X	-
87	OHX	5	4072	-	-	X	-
87	OHX	5	4096	-	-	X	-
87	OHX	5	4101	-	-	X	-
87	OHX	5	4150	-	-	X	-
87	OHX	5	4200	-	-	X	-
87	OHX	5	4206	-	-	X	-
87	OHX	5	4207	-	-	X	-
87	OHX	5	4208	-	-	X	-
87	OHX	5	4211	-	-	X	-
87	OHX	5	4221	-	-	X	-
87	OHX	5	4224	-	-	X	-
87	OHX	5	4231	-	-	X	-
87	OHX	5	4241	-	-	X	-
87	OHX	5	4243	-	-	X	-
87	OHX	5	4245	-	-	X	-
87	OHX	5	4250	-	-	X	-
87	OHX	6	2057	-	-	X	-
87	OHX	6	2118	-	-	X	-
87	OHX	6	2123	-	-	X	-
87	OHX	6	2145	-	-	X	-
87	OHX	6	2169	-	-	X	-
87	OHX	7	217	-	-	X	-
87	OHX	7	224	-	-	X	-
87	OHX	8	214	-	-	X	-
87	OHX	8	221	-	-	X	-
87	OHX	8	222	-	-	X	-
87	OHX	O1	202	-	-	X	-
87	OHX	O7	104	-	-	X	-
88	ZN	Q2	501	-	-	X	-

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411204 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 rRNA.

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-B.

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 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	6	GLU	GLN	conflict	UNP P46784
C0	7	ASP	GLU	conflict	UNP P46784
C0	89	ALA	GLY	conflict	UNP P46784
c0	6	GLU	GLN	conflict	UNP P46784
c0	7	ASP	GLU	conflict	UNP P46784
c0	89	ALA	GLY	conflict	UNP P46784

- 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			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

- 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
			680	403	140	137			

- Molecule 36 is a RNA chain called 25s rRNA.

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 5.8s rRNA.

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 rRNA.

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			
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			

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

- 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	S	0	0	0
			1420	882	281	257				
53	m7	155	Total	C	N	O	S	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	S	0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O	S	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 82 is a protein called UNKNOWN PROTEIN 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 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 84 is a protein called UNKNOWN PROTEIN p1.

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

- Molecule 85 is a protein called UNKNOWN PROTEIN p2.

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

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	2	124	Total	Mg	0	0
			124	124		
86	S2	2	Total	Mg	0	0
			2	2		
86	S8	1	Total	Mg	0	0
			1	1		
86	D3	1	Total	Mg	0	0
			1	1		
86	SM	1	Total	Mg	0	0
			1	1		
86	1	474	Total	Mg	0	0
			474	474		
86	3	14	Total	Mg	0	0
			14	14		
86	4	23	Total	Mg	0	0
			23	23		
86	L2	1	Total	Mg	0	0
			1	1		
86	L3	2	Total	Mg	0	0
			2	2		
86	L4	1	Total	Mg	0	0
			1	1		
86	L5	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	2	Total 2	Mg 2	0	0
86	L8	1	Total 1	Mg 1	0	0
86	M0	2	Total 2	Mg 2	0	0
86	M1	1	Total 1	Mg 1	0	0
86	M3	3	Total 3	Mg 3	0	0
86	M5	2	Total 2	Mg 2	0	0
86	M6	1	Total 1	Mg 1	0	0
86	M7	5	Total 5	Mg 5	0	0
86	M9	1	Total 1	Mg 1	0	0
86	N0	1	Total 1	Mg 1	0	0
86	N3	3	Total 3	Mg 3	0	0
86	N5	1	Total 1	Mg 1	0	0
86	N6	1	Total 1	Mg 1	0	0
86	N8	4	Total 4	Mg 4	0	0
86	O1	1	Total 1	Mg 1	0	0
86	O4	1	Total 1	Mg 1	0	0
86	O7	2	Total 2	Mg 2	0	0
86	Q2	1	Total 1	Mg 1	0	0
86	6	145	Total 145	Mg 145	0	0
86	s1	1	Total 1	Mg 1	0	0
86	s8	2	Total 2	Mg 2	0	0

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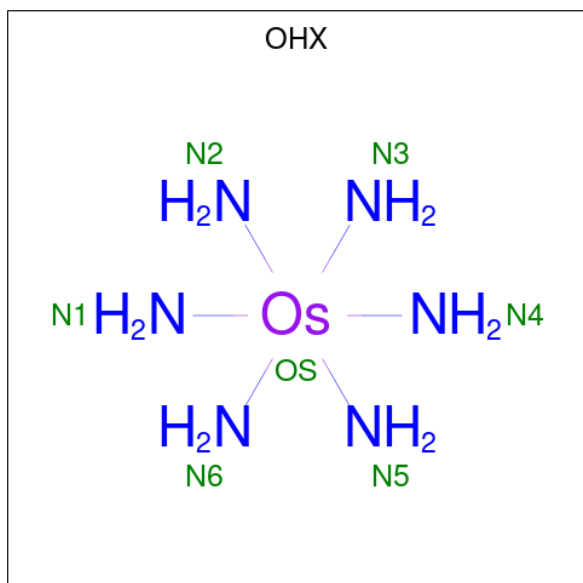
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	c1	2	Total 2	Mg 2	0	0
86	c7	2	Total 2	Mg 2	0	0
86	c8	1	Total 1	Mg 1	0	0
86	c9	1	Total 1	Mg 1	0	0
86	d3	2	Total 2	Mg 2	0	0
86	d4	1	Total 1	Mg 1	0	0
86	d6	1	Total 1	Mg 1	0	0
86	sM	2	Total 2	Mg 2	0	0
86	5	507	Total 507	Mg 507	0	0
86	7	15	Total 15	Mg 15	0	0
86	8	12	Total 12	Mg 12	0	0
86	l2	2	Total 2	Mg 2	0	0
86	l3	2	Total 2	Mg 2	0	0
86	l4	1	Total 1	Mg 1	0	0
86	l5	3	Total 3	Mg 3	0	0
86	l7	1	Total 1	Mg 1	0	0
86	m1	1	Total 1	Mg 1	0	0
86	m5	4	Total 4	Mg 4	0	0
86	m6	1	Total 1	Mg 1	0	0
86	m7	5	Total 5	Mg 5	0	0
86	n0	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	n3	2	Total 2	Mg 2	0	0
86	n6	2	Total 2	Mg 2	0	0
86	n8	4	Total 4	Mg 4	0	0
86	n9	1	Total 1	Mg 1	0	0
86	o1	2	Total 2	Mg 2	0	0
86	o3	1	Total 1	Mg 1	0	0
86	o4	1	Total 1	Mg 1	0	0
86	q0	1	Total 1	Mg 1	0	0
86	q1	1	Total 1	Mg 1	0	0
86	q3	1	Total 1	Mg 1	0	0

- Molecule 87 is osmium (III) hexammine (CCD ID: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	S8	1	Total	N	Os	0	0
			7	6	1		
87	C3	1	Total	N	Os	0	0
			7	6	1		
87	C5	1	Total	N	Os	0	0
			7	6	1		
87	C8	1	Total	N	Os	0	0
			7	6	1		
87	D9	1	Total	N	Os	0	0
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87	SR	1	Total	N	Os	0	0
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			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	3	1	Total	N	Os	0	0
			7	6	1		
87	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L4	1	Total	N	Os	0	0
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87	M0	1	Total	N	Os	0	0
			7	6	1		
87	M5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	M7	1	Total	N	Os	0	0
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87	M7	1	Total	N	Os	0	0
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87	M8	1	Total	N	Os	0	0
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87	M9	1	Total	N	Os	0	0
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87	N9	1	Total	N	Os	0	0
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87	O1	1	Total	N	Os	0	0
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87	O2	1	Total	N	Os	0	0
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87	O3	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
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87	Q2	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	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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87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	s1	1	Total 7	N 6	Os 1	0	0
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87	s4	1	Total 7	N 6	Os 1	0	0
87	s8	1	Total 7	N 6	Os 1	0	0
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87	c5	1	Total 7	N 6	Os 1	0	0
87	c8	1	Total 7	N 6	Os 1	0	0
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87	d9	1	Total 7	N 6	Os 1	0	0
87	sR	1	Total 7	N 6	Os 1	0	0
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87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
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87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		

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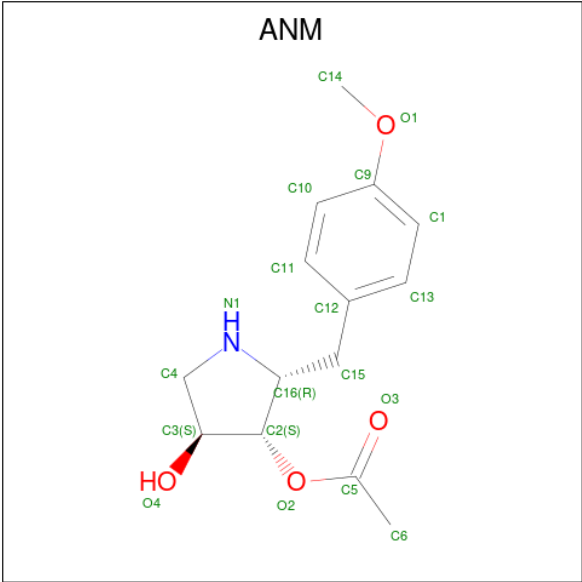
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l9	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m1	1	Total	N	Os	0	0
			7	6	1		
87	m4	1	Total	N	Os	0	0
			7	6	1		
87	m5	1	Total	N	Os	0	0
			7	6	1		
87	m6	1	Total	N	Os	0	0
			7	6	1		
87	m7	1	Total	N	Os	0	0
			7	6	1		
87	m8	1	Total	N	Os	0	0
			7	6	1		
87	n3	1	Total	N	Os	0	0
			7	6	1		
87	n9	1	Total	N	Os	0	0
			7	6	1		
87	o2	1	Total	N	Os	0	0
			7	6	1		
87	o3	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o9	1	Total	N	Os	0	0
			7	6	1		
87	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	D6	1	Total 1	Zn 1	0	0
88	D7	1	Total 1	Zn 1	0	0
88	D9	1	Total 1	Zn 1	0	0
88	E1	1	Total 1	Zn 1	0	0
88	O7	1	Total 1	Zn 1	0	0
88	Q0	1	Total 1	Zn 1	0	0
88	Q2	1	Total 1	Zn 1	0	0
88	Q3	1	Total 1	Zn 1	0	0
88	d6	1	Total 1	Zn 1	0	0
88	d7	1	Total 1	Zn 1	0	0
88	d9	1	Total 1	Zn 1	0	0
88	e1	1	Total 1	Zn 1	0	0
88	o7	1	Total 1	Zn 1	0	0
88	q0	1	Total 1	Zn 1	0	0
88	q2	1	Total 1	Zn 1	0	0
88	q3	1	Total 1	Zn 1	0	0

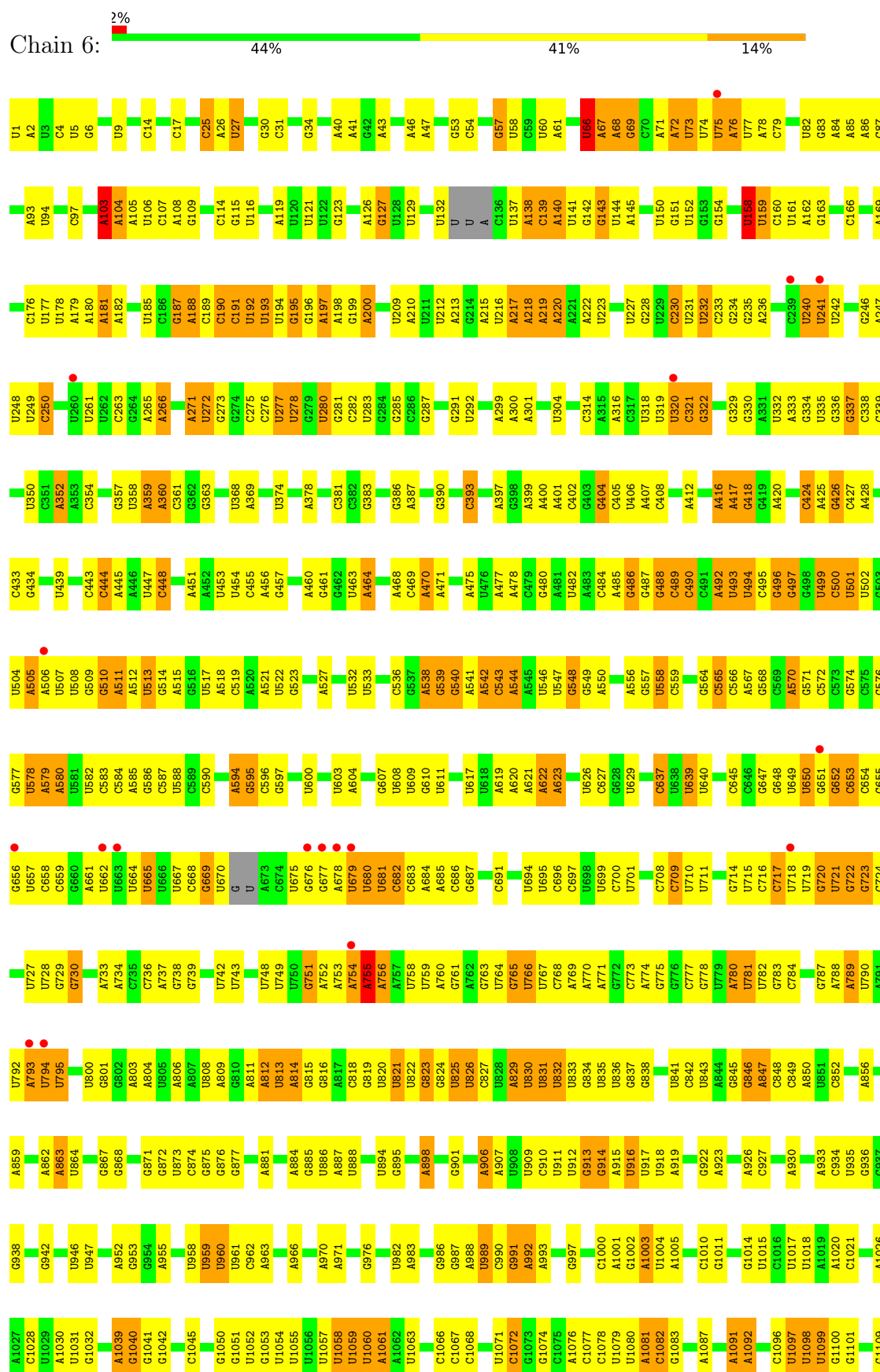
- Molecule 89 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).

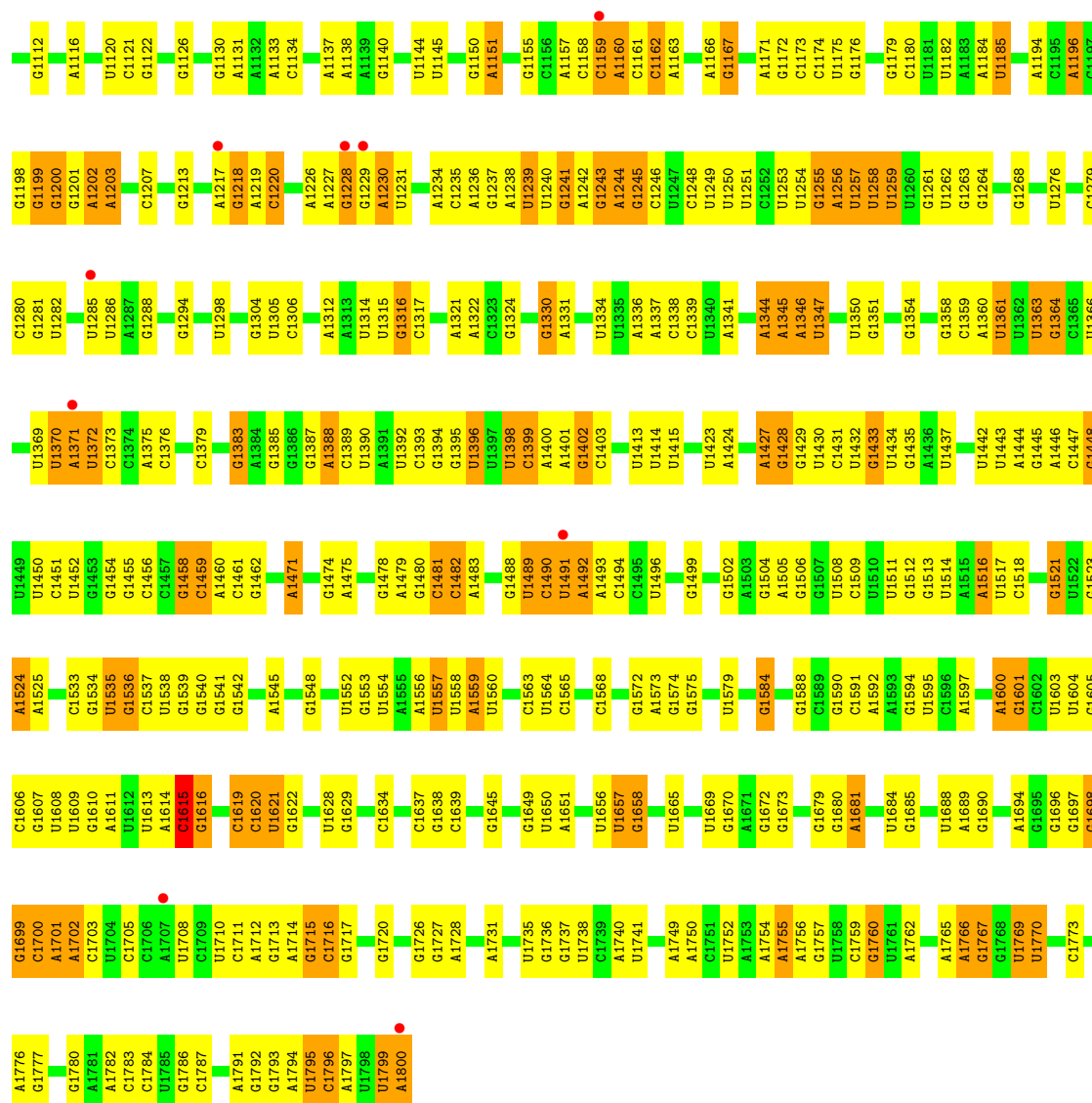


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			19	14	1	4		
89	5	1	Total	C	N	O	0	0
			19	14	1	4		

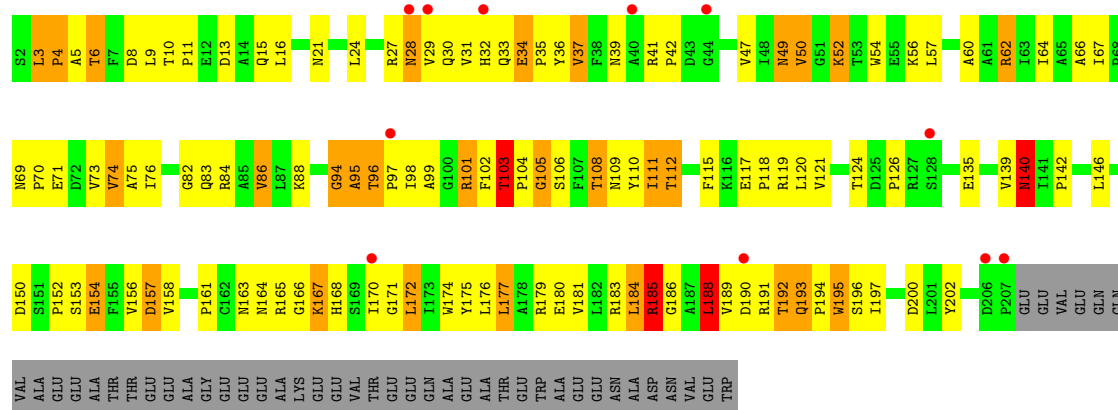
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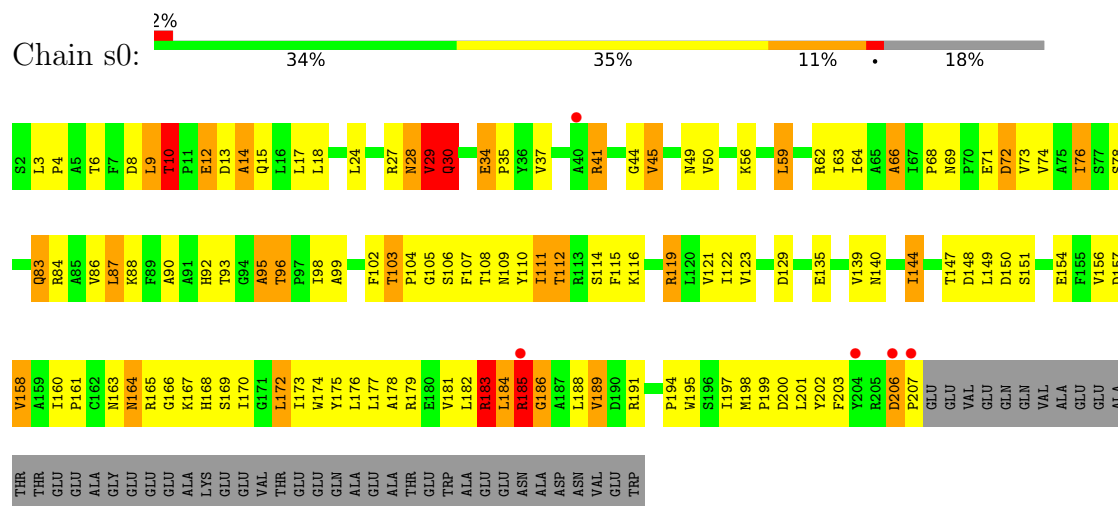




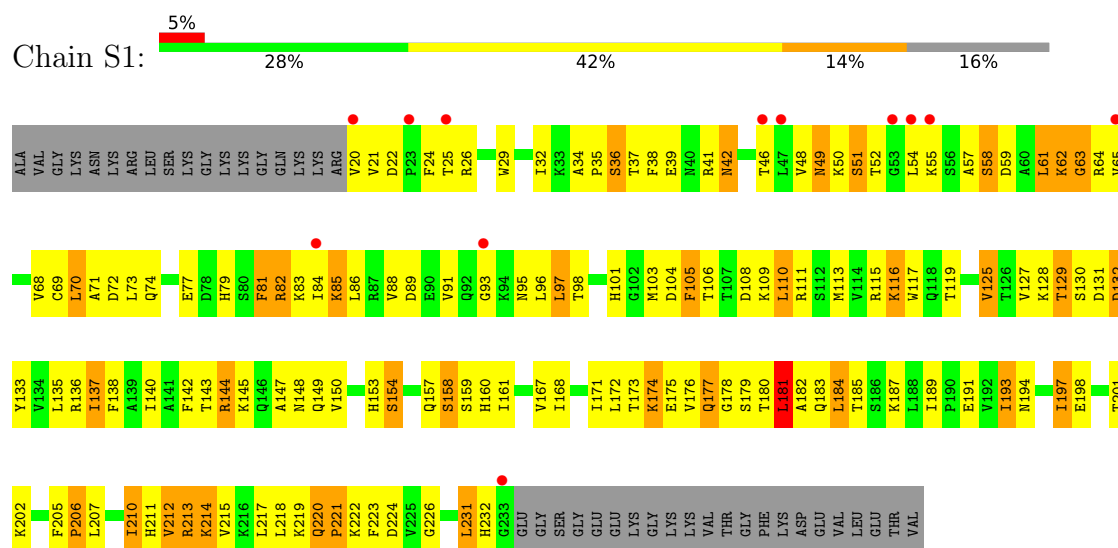
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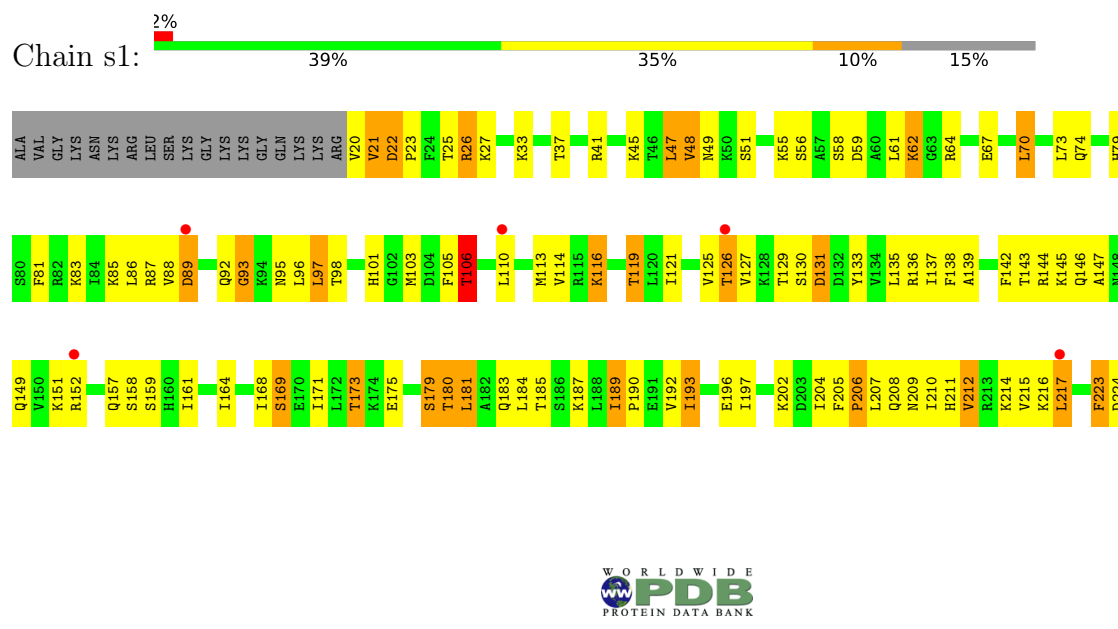
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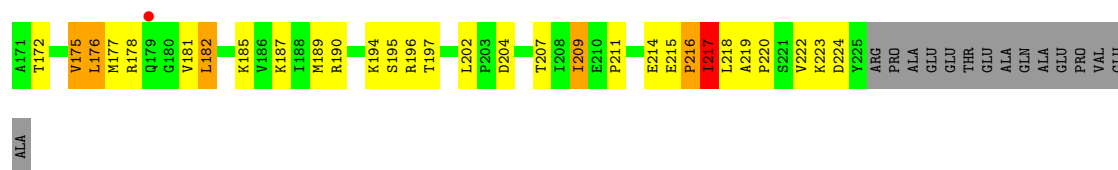
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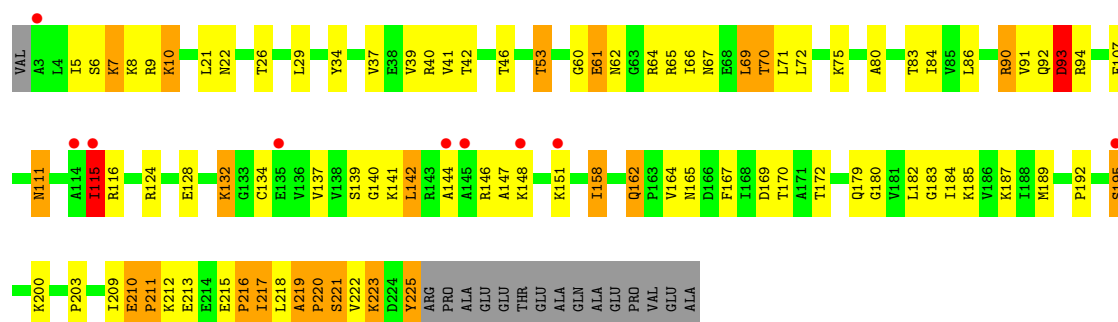
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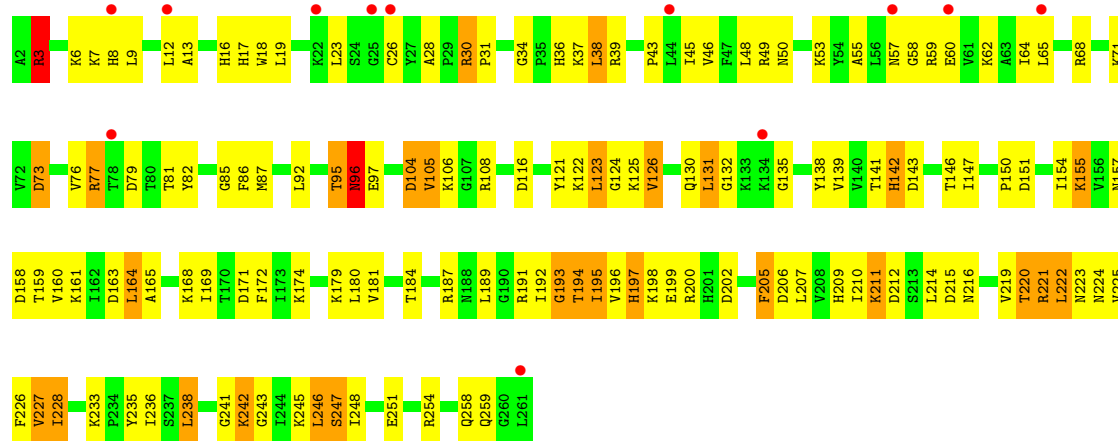




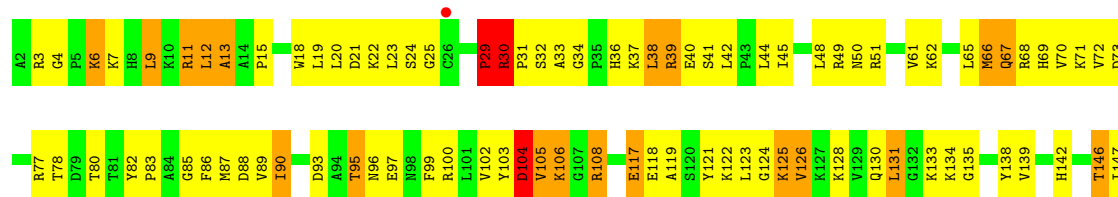
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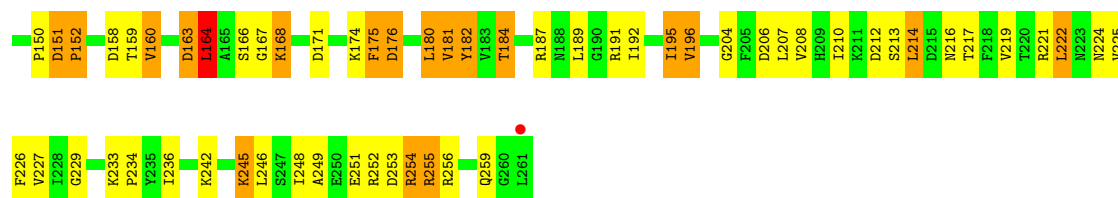


• Molecule 6: 40S ribosomal protein S4-A

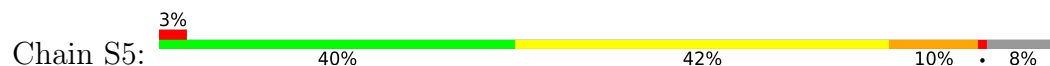


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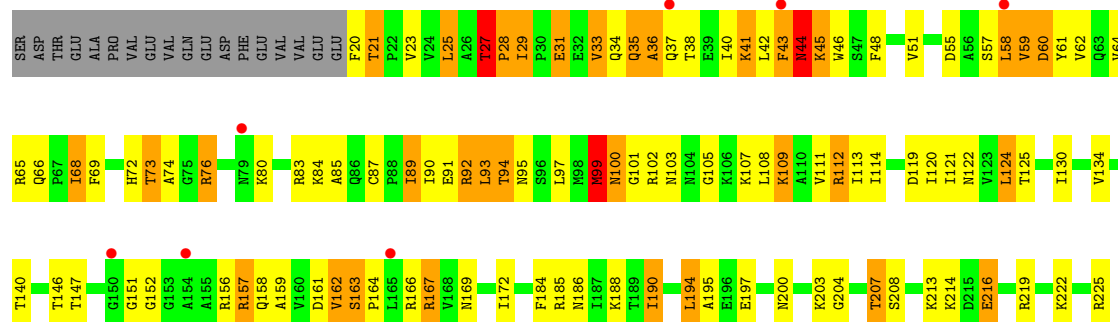




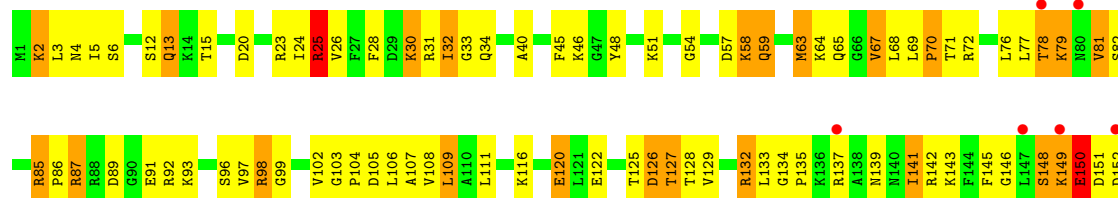
• Molecule 7: 40S ribosomal protein S5



• Molecule 7: 40S ribosomal protein S5

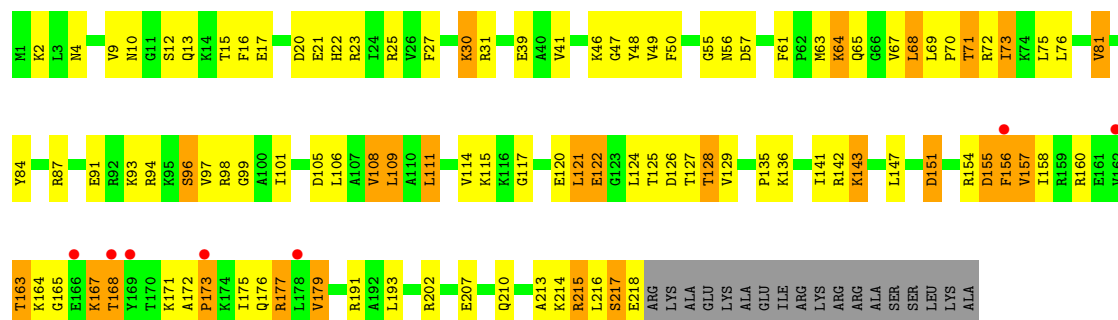


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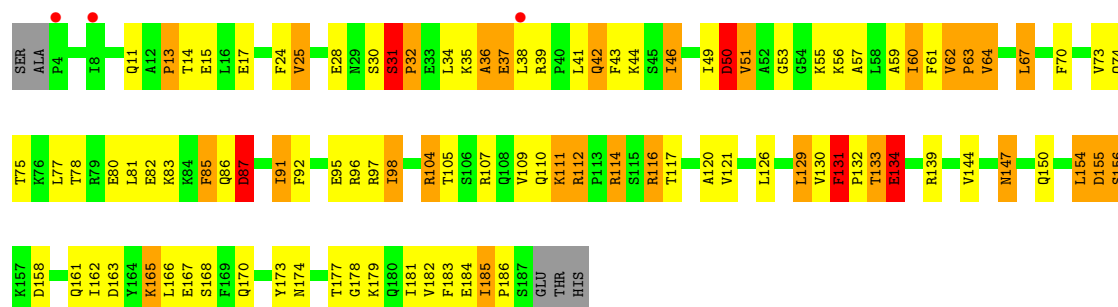
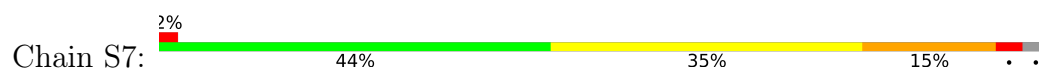




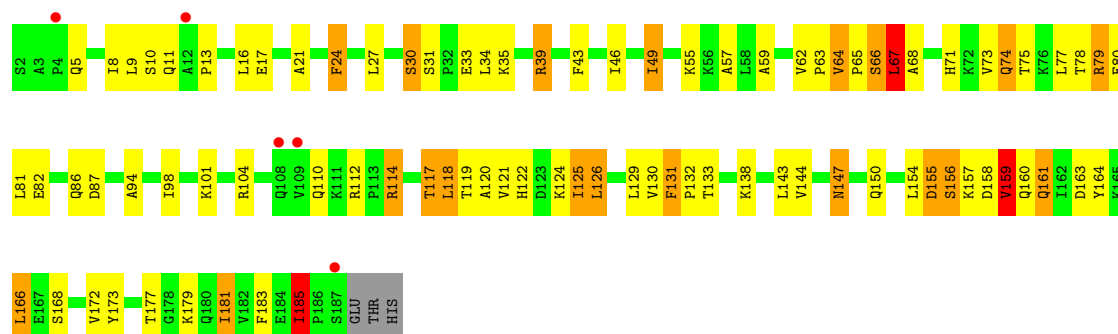
• Molecule 8: 40S ribosomal protein S6-A



• Molecule 9: 40S ribosomal protein S7-A

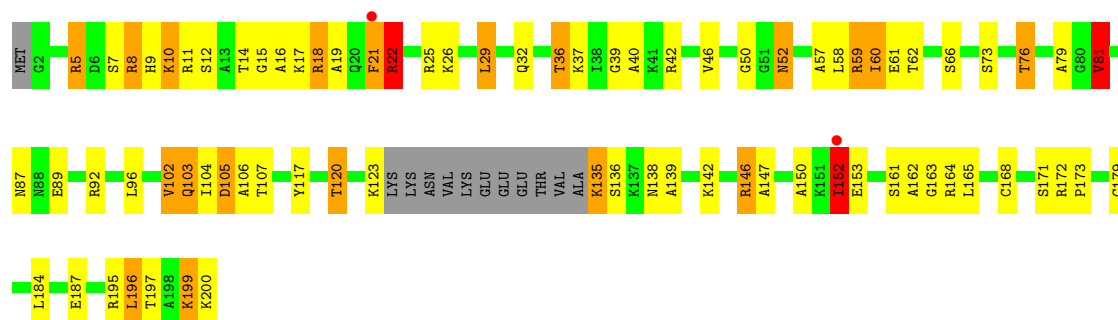


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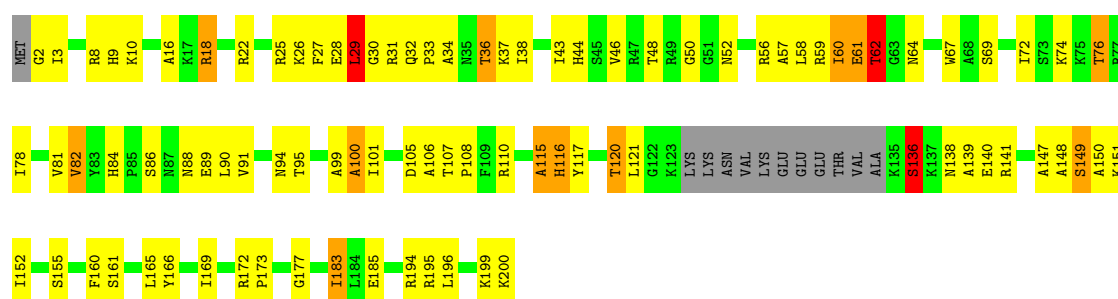
• Molecule 10: 40S ribosomal protein S8-A





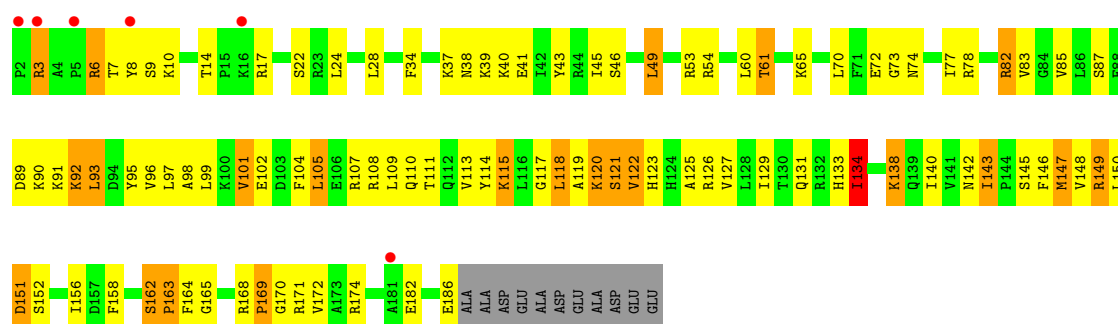
• Molecule 10: 40S ribosomal protein S8-A

Chain s8: 48% 38% 6% • 6%



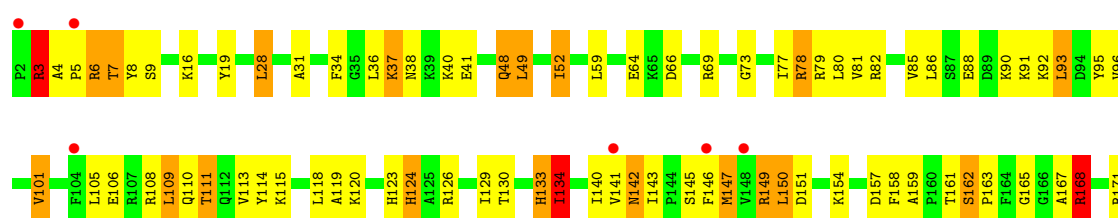
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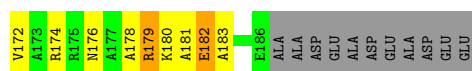
Chain S9: 3% 44% 38% 11% • 6%



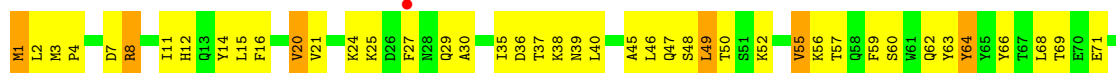
• Molecule 11: 40S ribosomal protein S9-A

Chain s9: 3% 48% 34% 11% • 6%

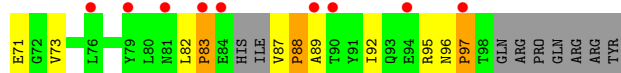
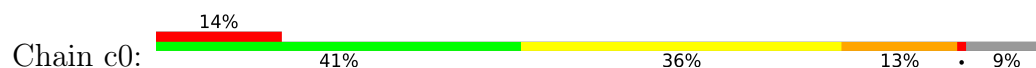




• Molecule 12: 40S ribosomal protein S10-B



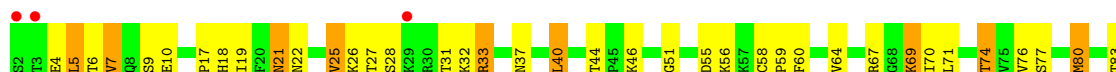
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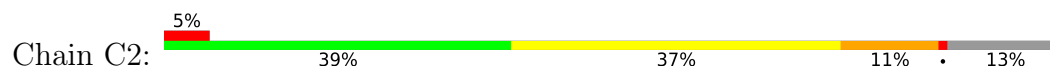
• Molecule 13: 40S ribosomal protein S11-A



• Molecule 13: 40S ribosomal protein S11-A



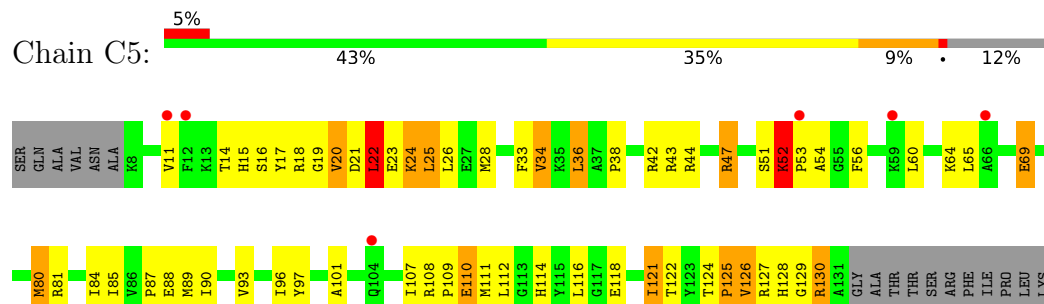
• Molecule 14: 40S ribosomal protein S12



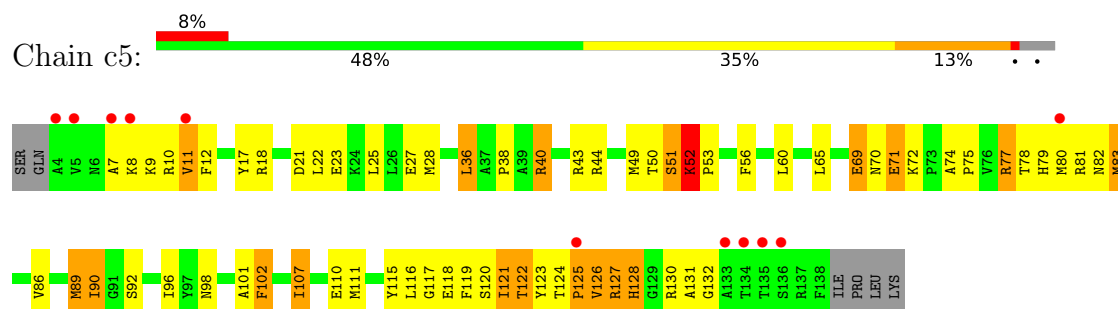
- Molecule 16: 40S ribosomal protein S14-A



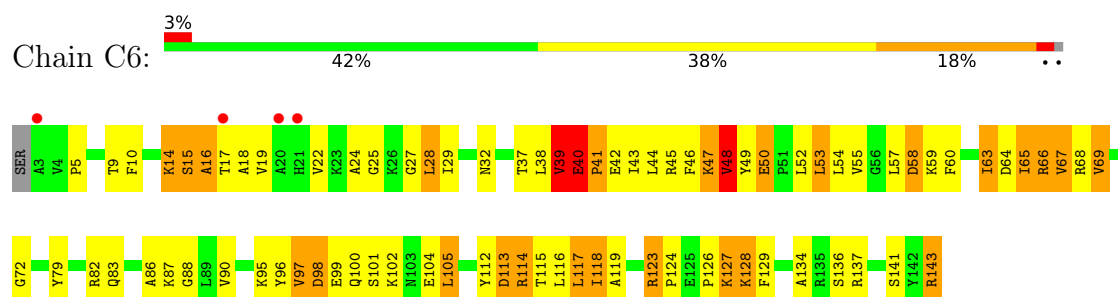
- Molecule 17: 40S ribosomal protein S15



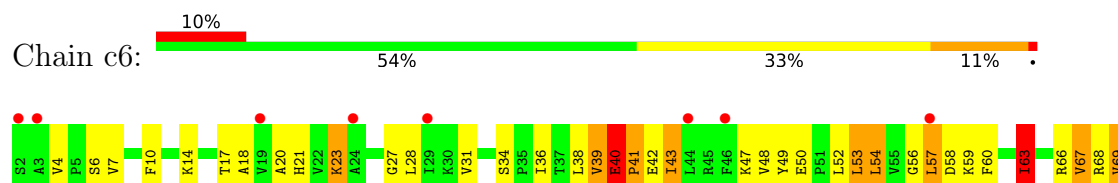
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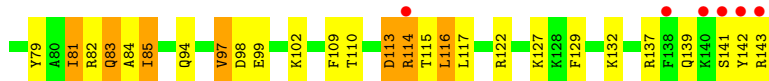


- Molecule 18: 40S ribosomal protein S16-A



- Molecule 18: 40S ribosomal protein S16-A

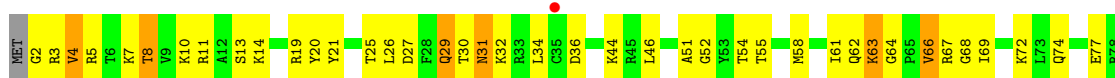
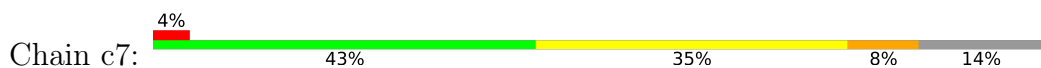




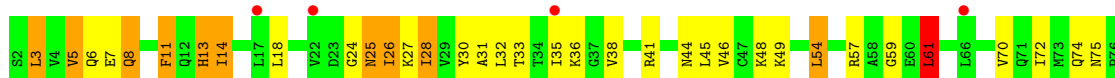
• Molecule 19: 40S ribosomal protein S17-A



• Molecule 19: 40S ribosomal protein S17-A



• Molecule 20: 40S ribosomal protein S18-A

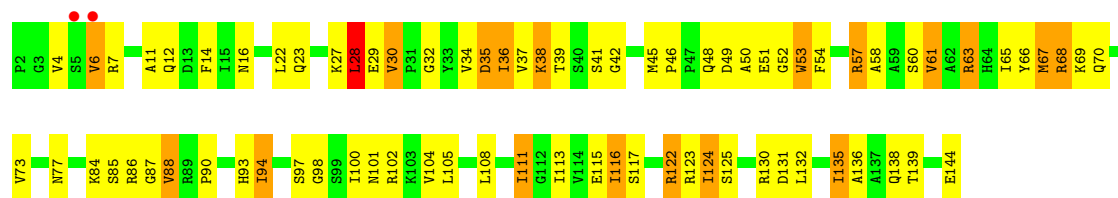


• Molecule 20: 40S ribosomal protein S18-A

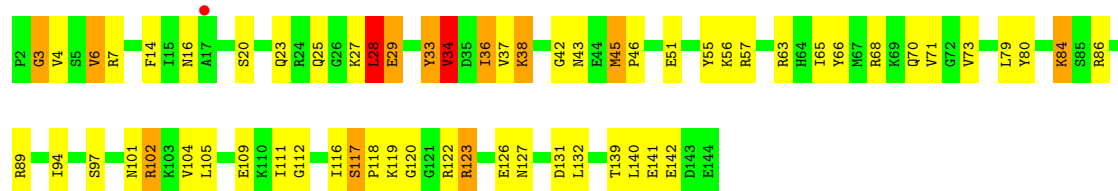


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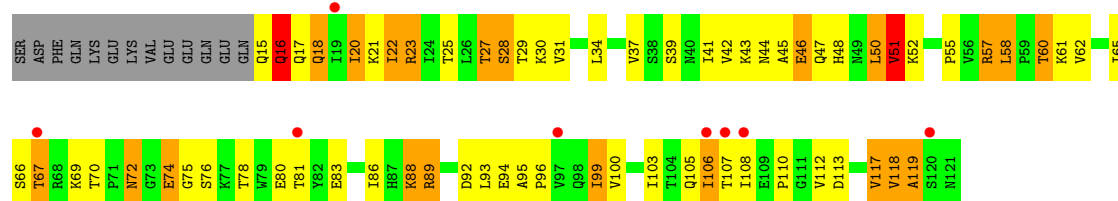




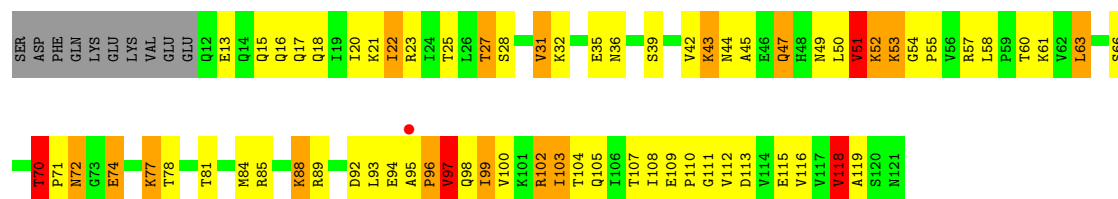
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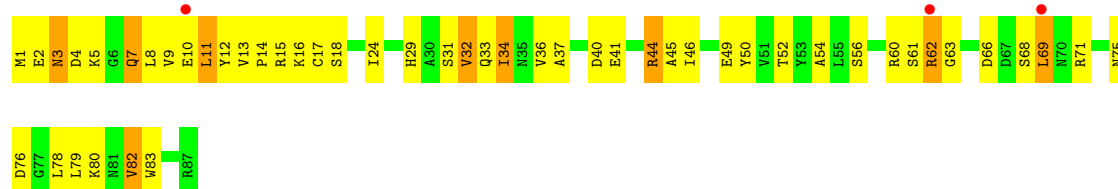
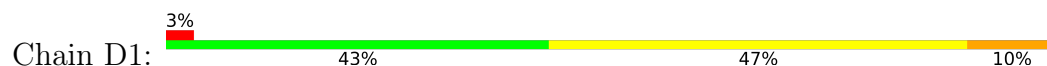
- Molecule 22: 40S ribosomal protein S20



- Molecule 22: 40S ribosomal protein S20



- Molecule 23: 40S ribosomal protein S21-A



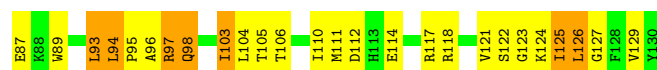
- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 



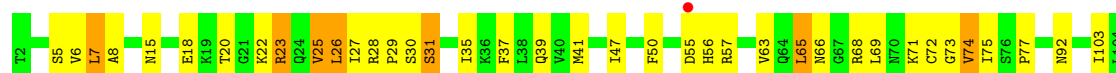
• Molecule 24: 40S ribosomal protein S22-A

Chain D2: 



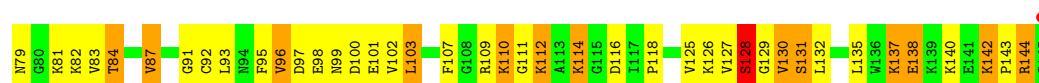
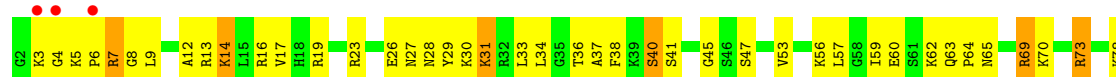
• Molecule 24: 40S ribosomal protein S22-A

Chain d2: 



• Molecule 25: 40S ribosomal protein S23-A

Chain D3: 

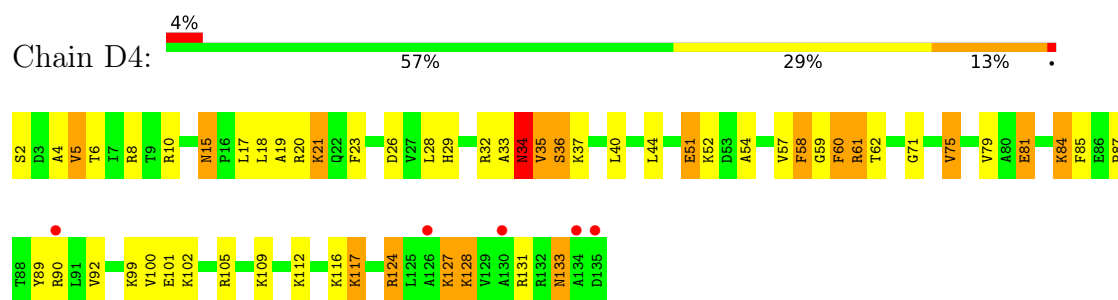


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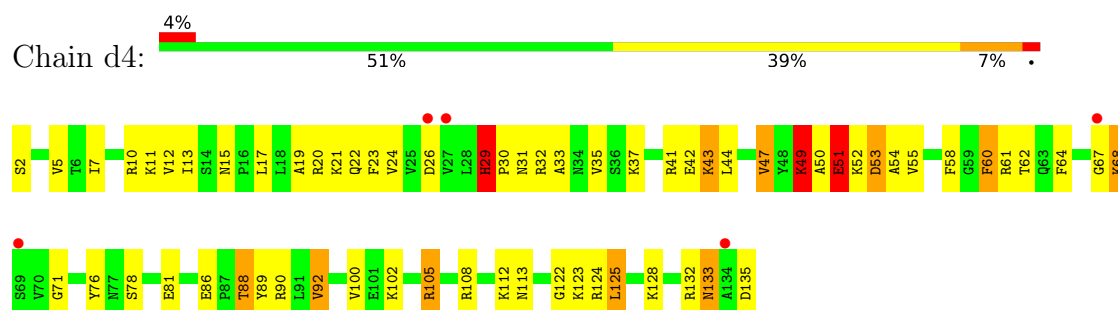
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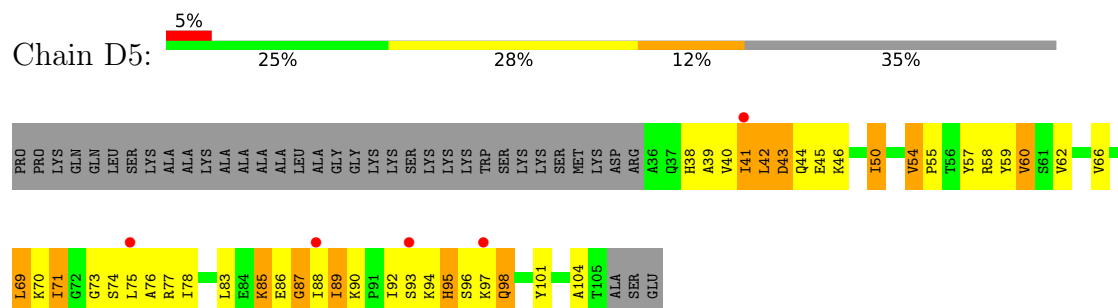
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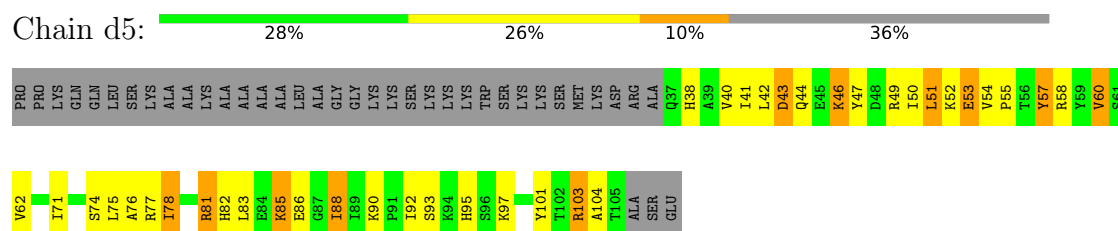
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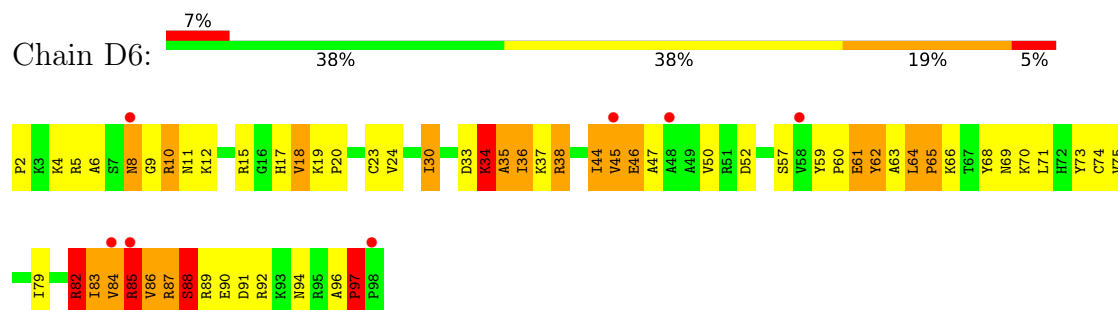
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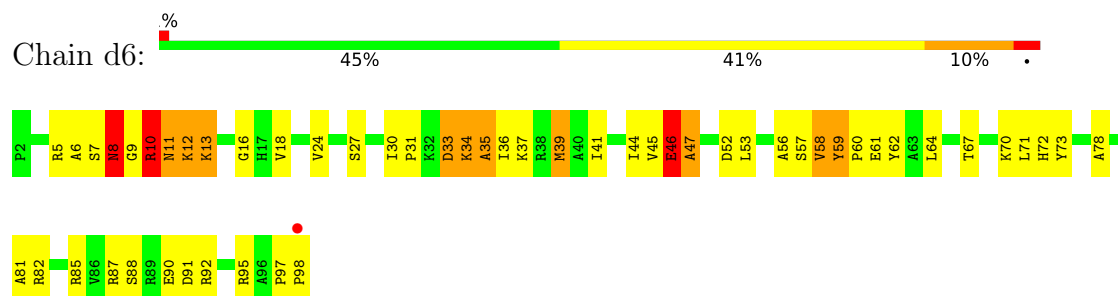
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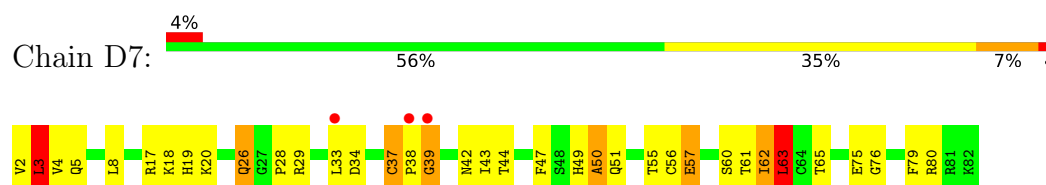
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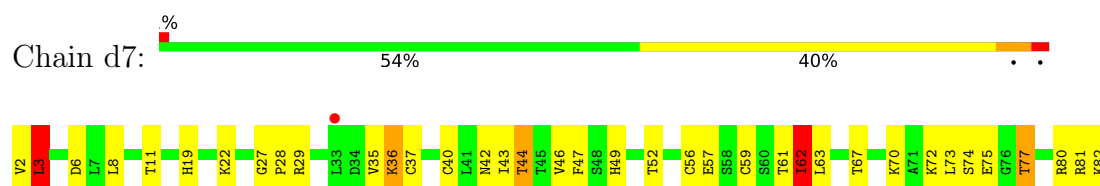
• Molecule 28: 40S ribosomal protein S26-B



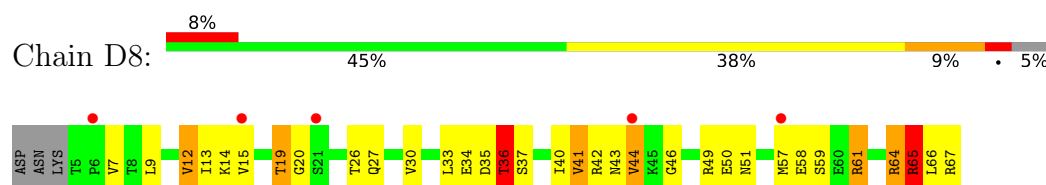
• Molecule 29: 40S ribosomal protein S27-A



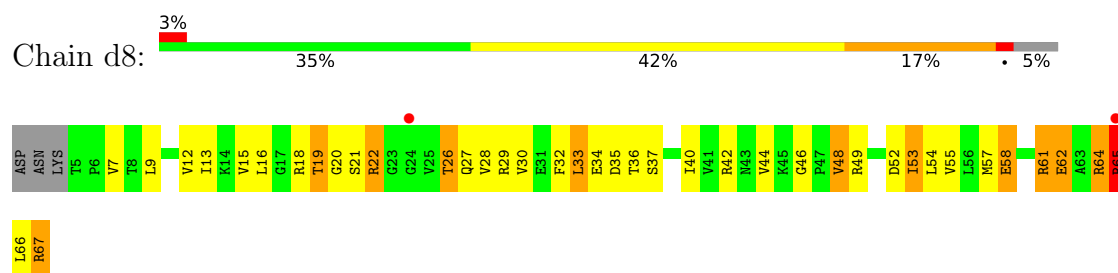
• Molecule 29: 40S ribosomal protein S27-A



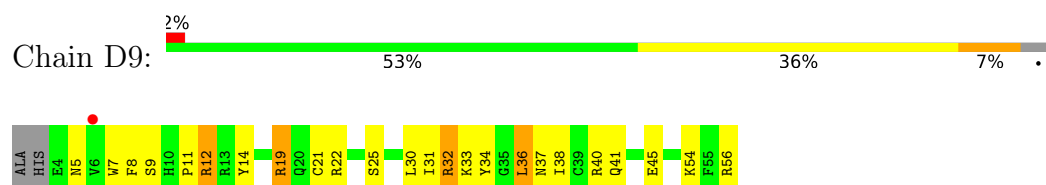
• Molecule 30: 40S ribosomal protein S28-A



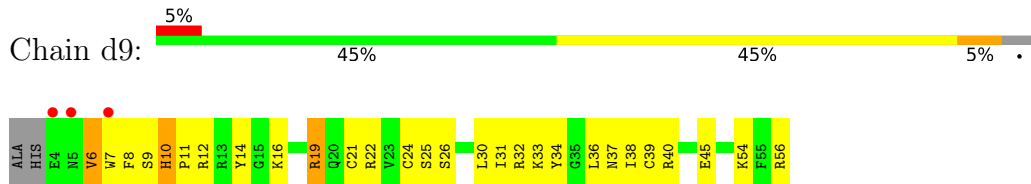
• Molecule 30: 40S ribosomal protein S28-A



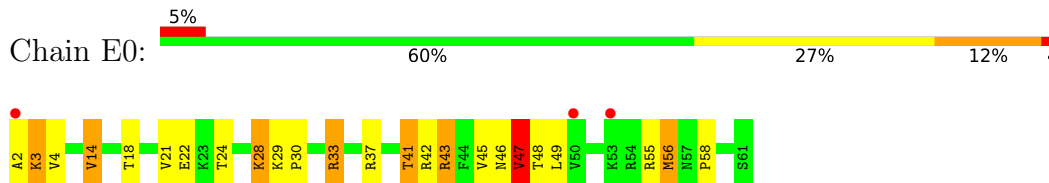
• Molecule 31: 40S ribosomal protein S29-A



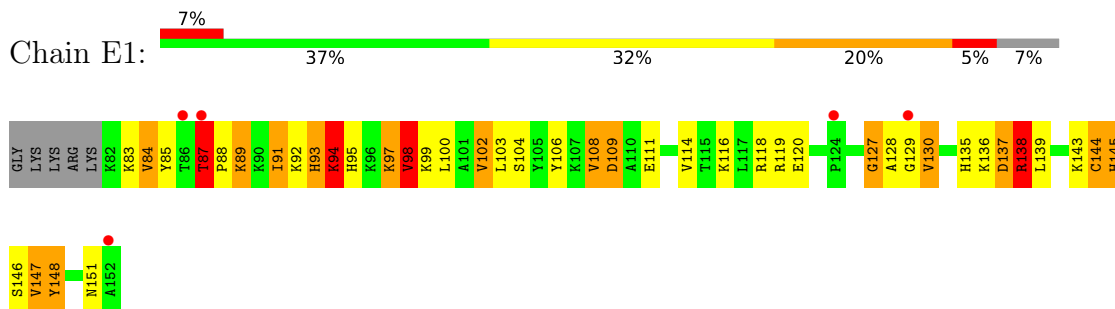
- Molecule 31: 40S ribosomal protein S29-A



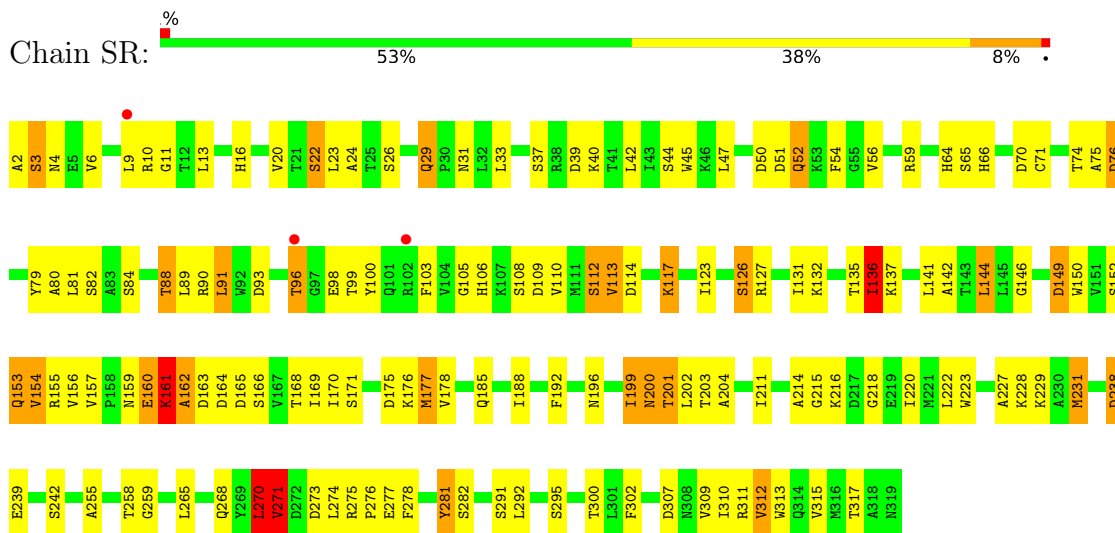
- Molecule 32: 40S ribosomal protein S30-A



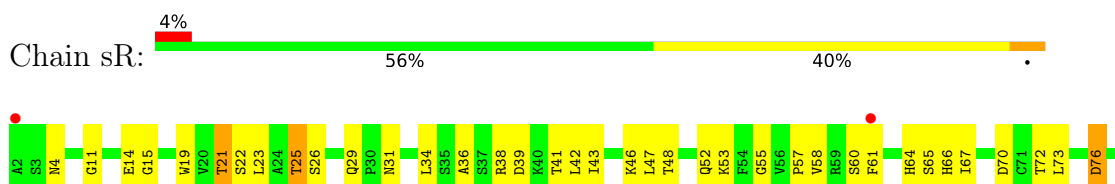
- Molecule 33: Ubiquitin-40S ribosomal protein S31

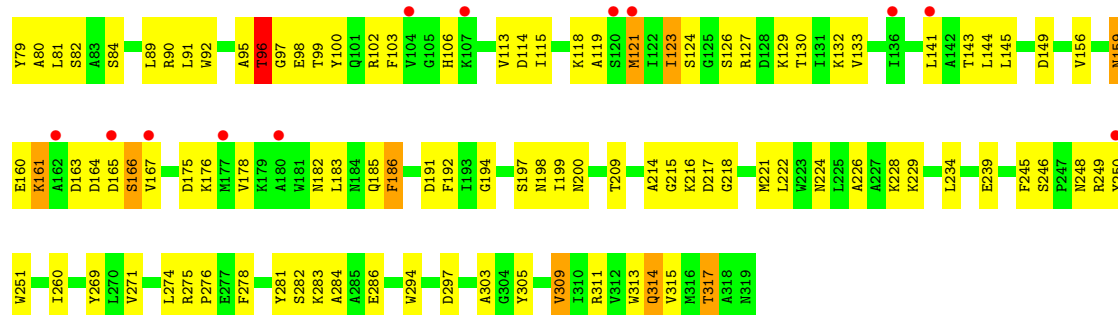


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

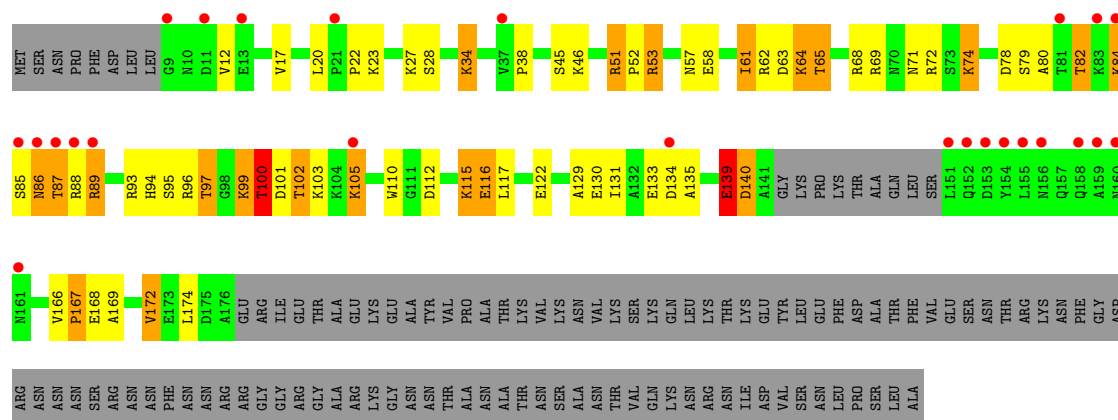
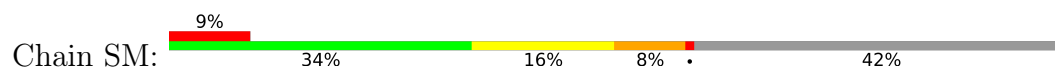


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein.

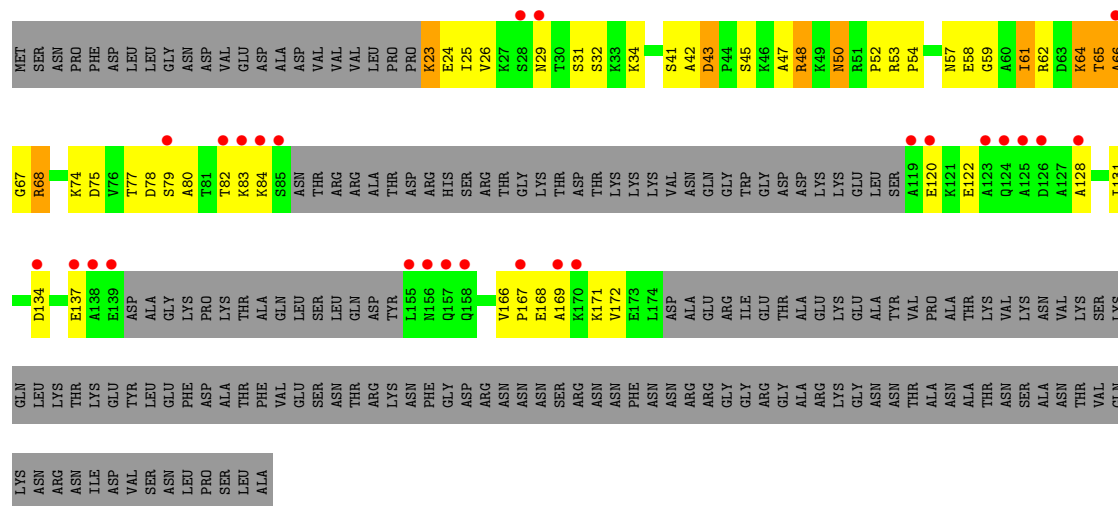




• Molecule 35: Suppressor protein STM1



• Molecule 35: Suppressor protein STM1

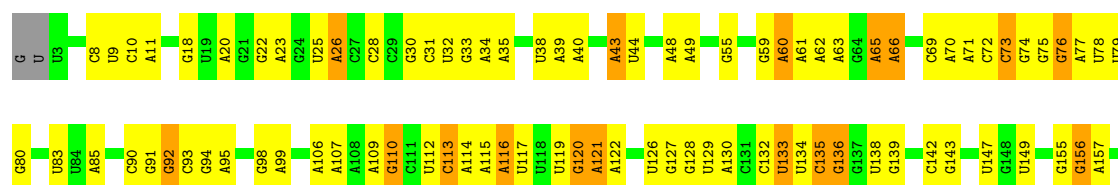
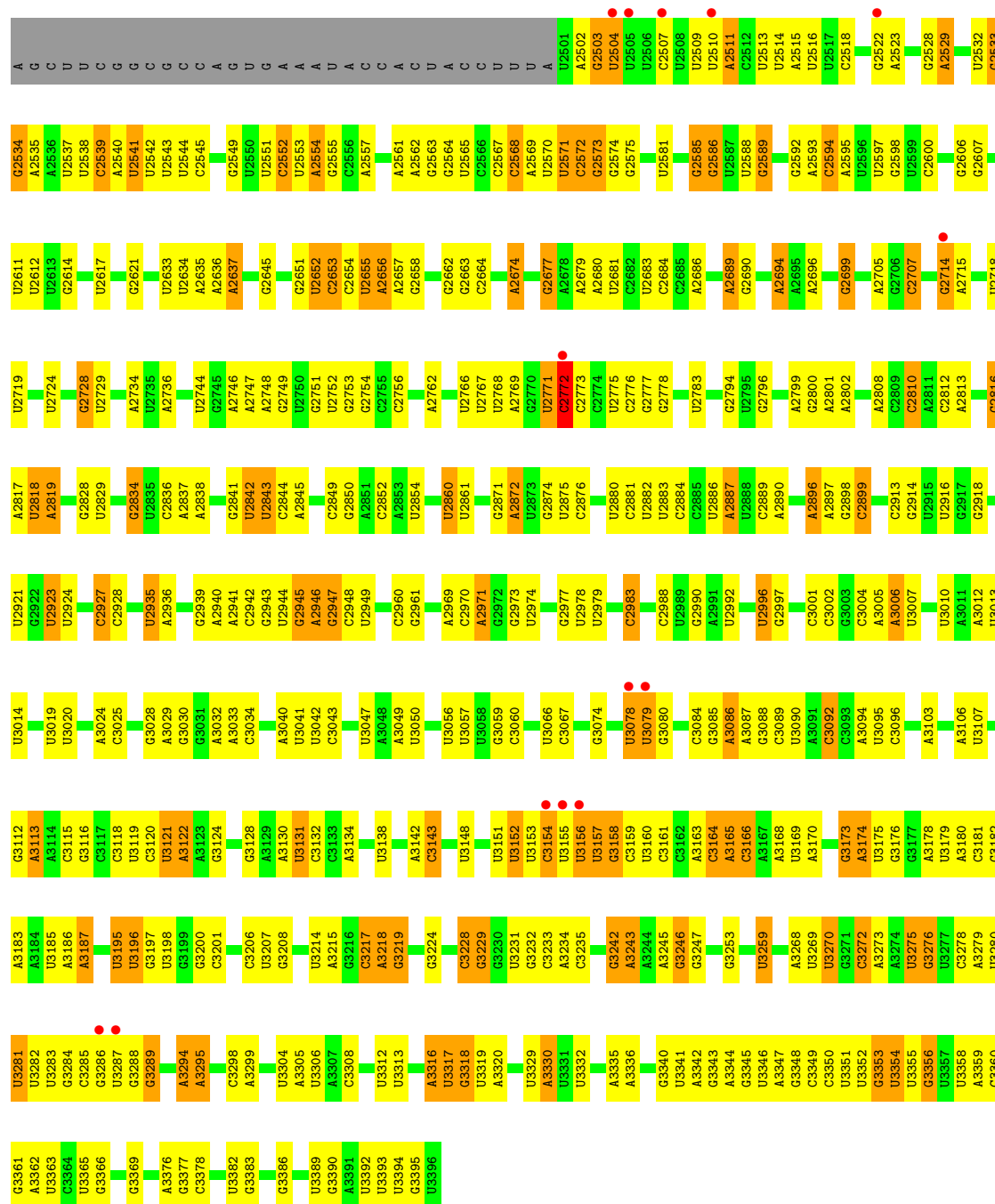


• Molecule 36: 25s rRNA



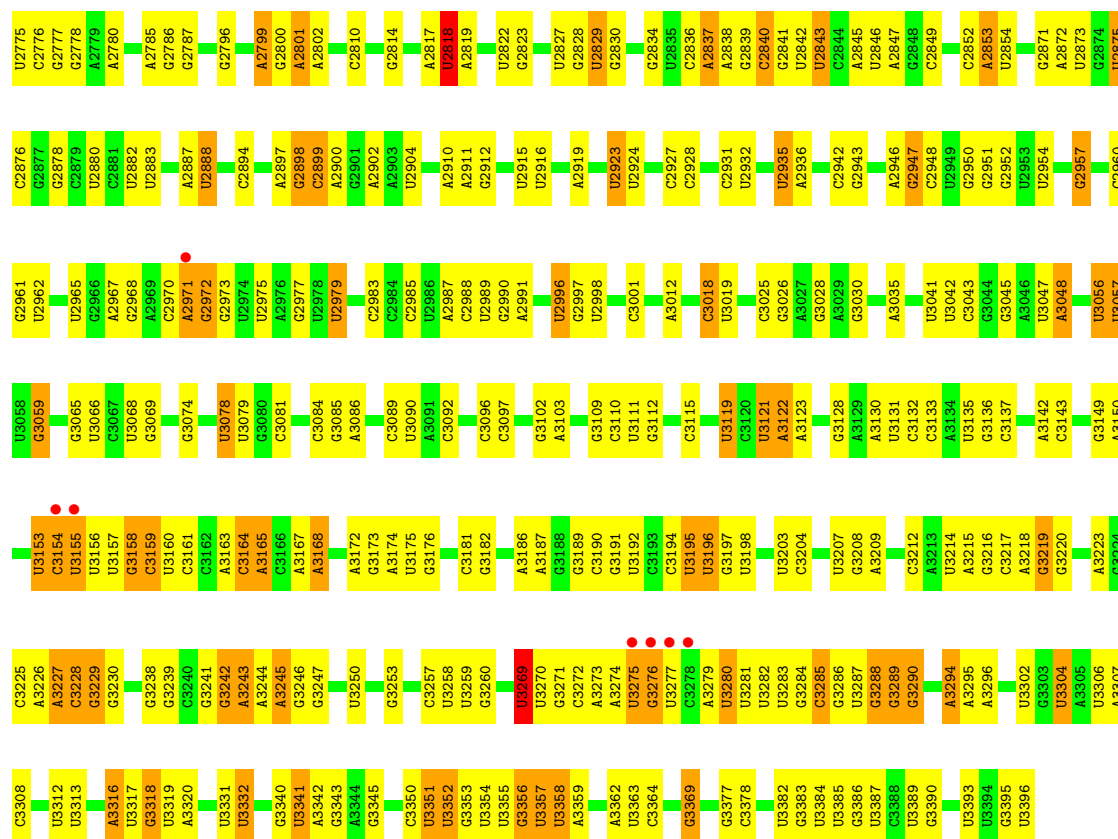
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G1207	A1101	G1022	U850	G678	C593	A516	G	G267	U182	C93	U3	
U1208	G1102	A1025	U852	U679	G594	G517	U	U270	U184	A95	C7	
U1209	A1103	A1026	G853	U681	G595	U520	U	C271	A187	A99	C8	
U1210	G1104	U1027	G860	G684	A598	A521	U	A272			A12	
A1211	U1109	U1028	C861	G685	U601	A522	G	A273	U190	C102	A13	
A1212	U1110	A1030	U862	G686	A602	A523	U	G274	G103	G103	A16	
G1213	U1111	C1031	G864	U687	A603	C525	C	U275	C192	U112	G17	
U1214	A1112	C1032		U776	G604	U528	C	U278	A199	A107	U19	
U1215	U1113	U1033	G870	U777	A691	A529	U	U279	C200	A108	U19	
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A1217	G1115	A1035	U872	G779	G609	G530	C	G281		G110	A20	
A1221	G1116	U1036	U873	G780	G610	G531	C	A374	U207	C111	G22	
G1222	G1117	C1037	U874	G781	A611	U534	G	A375	U208	U112		
A1223	U1118	C1038	U875	G782	G612	G535	U	G376	C208	G113		
C1227	G1119	U1039	U876	G783	G613	U536	U	U381	A209	A114		
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G1233	G1145	G964	U889	U790	G627	G542	G	A395	G216	A122		
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G1242	U1167	C977	U898	G805	A720	U549	G	U401	U230	U134		
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G1268	A1193	U1094	C927	C840	U662	G582	U	C439	U261	C174		
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A1270	A1195	G1097	A929	U846	U664	A585	U	U	U263	G178		
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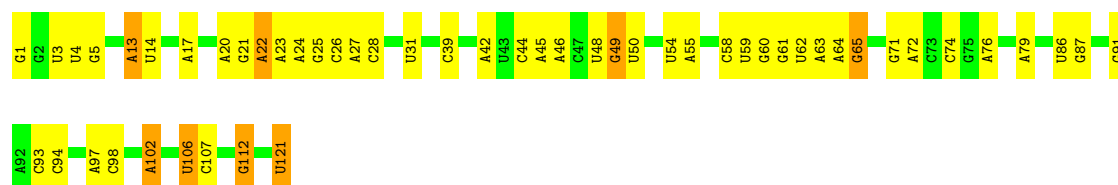
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A1435	G1245	G1245	A1150	A1066	C982	A896	C758	U662	A579	U492	U428	C350	U251	U169
U1436	A1350	G1246	U1151	G1066	A983	U937	U759	U662	G579	U493	U429	A351	U252	G170
C1437	U1351	G1249	G1152	C1069	G984	G900	G760	C670	A585	G495	U430	A357	A253	G171
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U1439	U1353	A1251	U1154	U986	U987	A906	C766	A677	U587	C497	G437	G353	A255	G173
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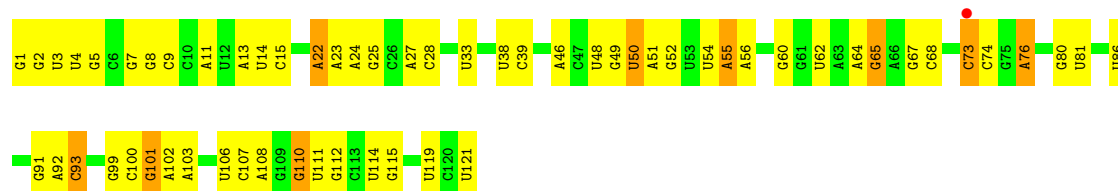
• Molecule 37: 5.8s rRNA

Chain 3: 57% 36% 7%



• Molecule 37: 5.8s rRNA

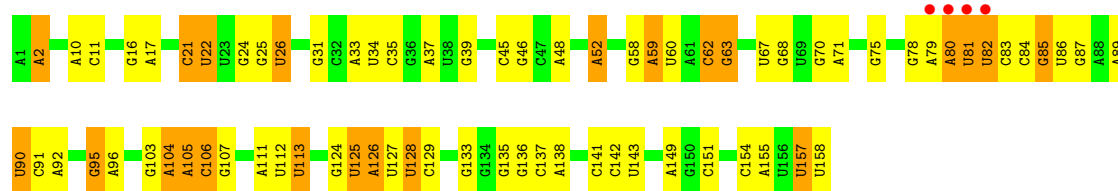
Chain 7: 50% 42% 7%



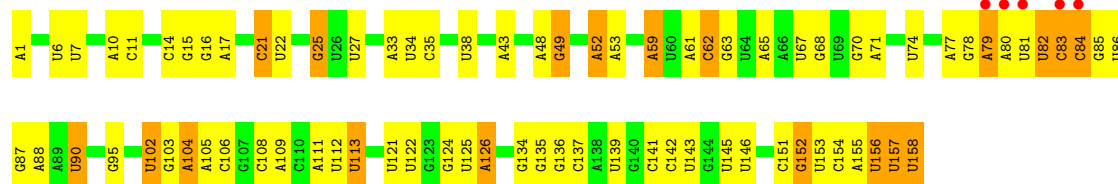
• Molecule 38: 5.8s rRNA

Chain 4: 3% 53% 33% 14%

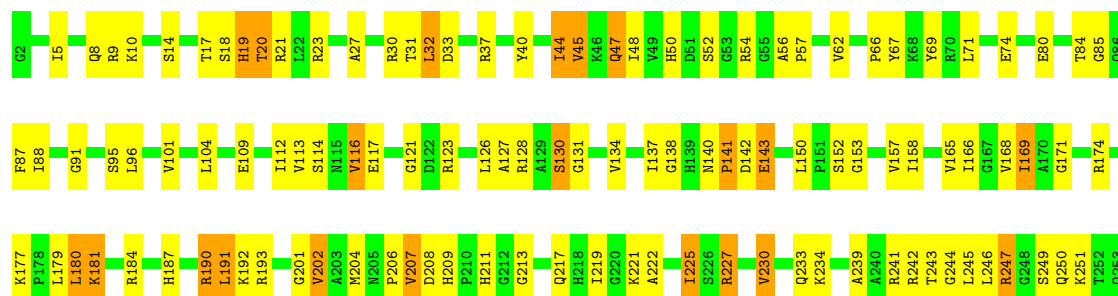




• Molecule 38: 5.8s rRNA

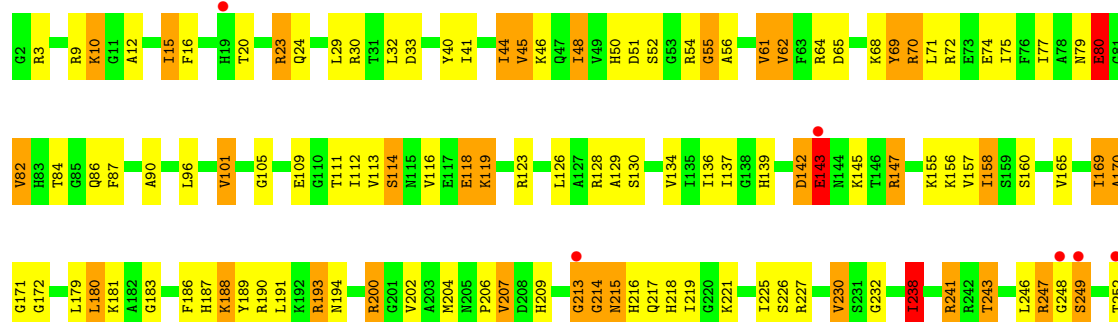


• Molecule 39: 60S ribosomal protein L2-A



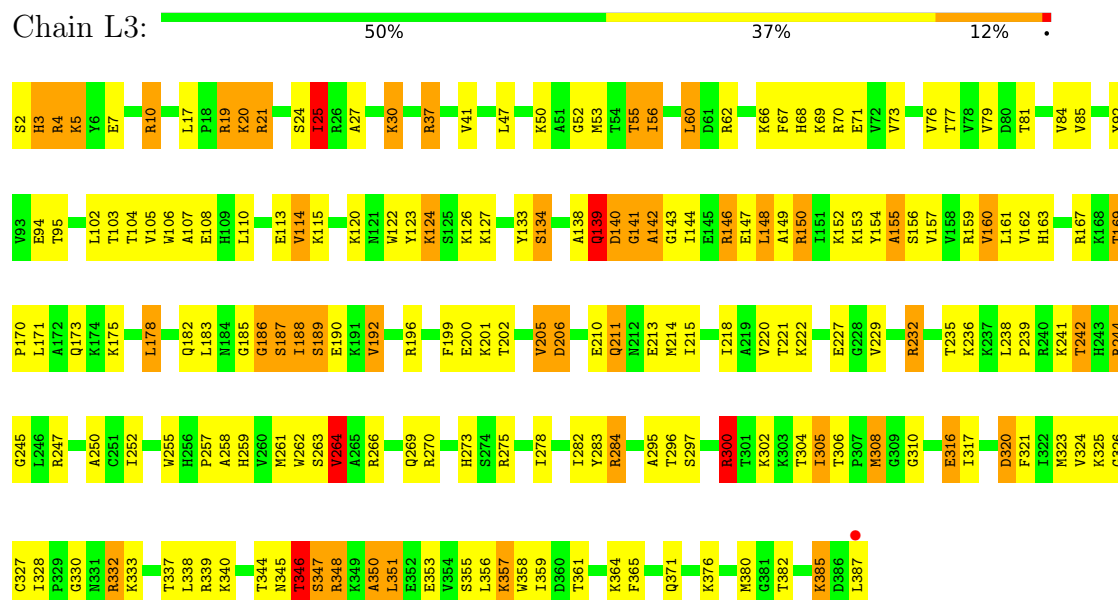
ASP

• Molecule 39: 60S ribosomal protein L2-A

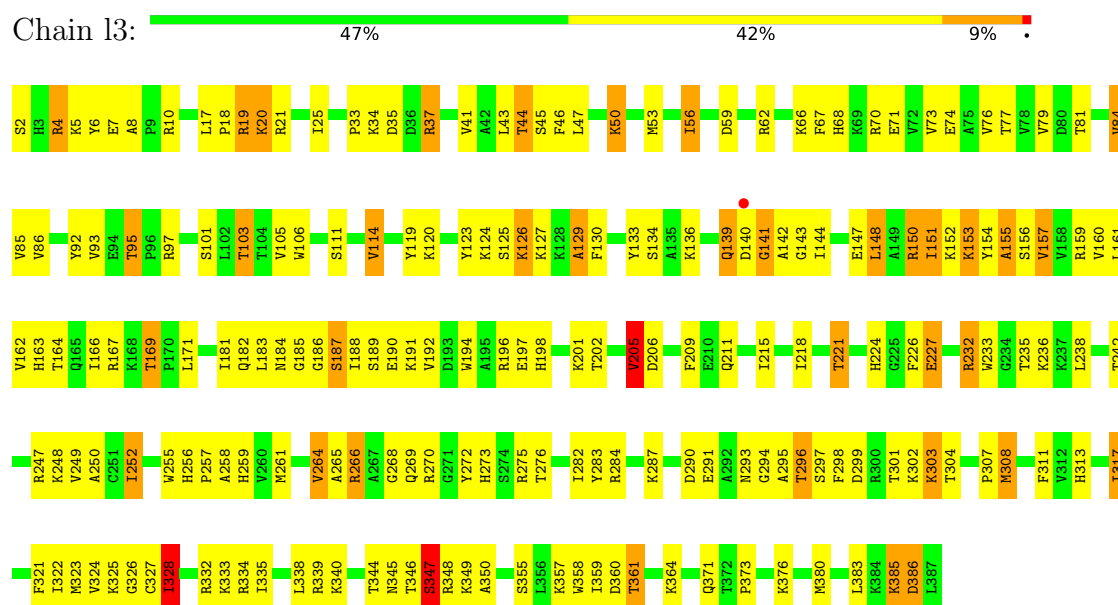


Q253
ASP

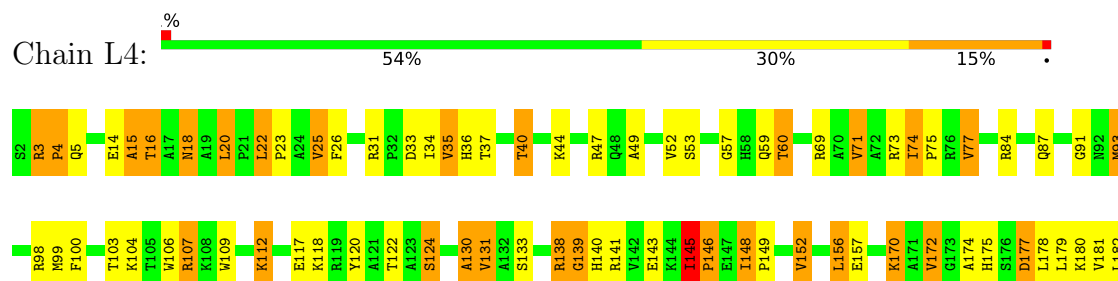
• Molecule 40: 60S ribosomal protein L3

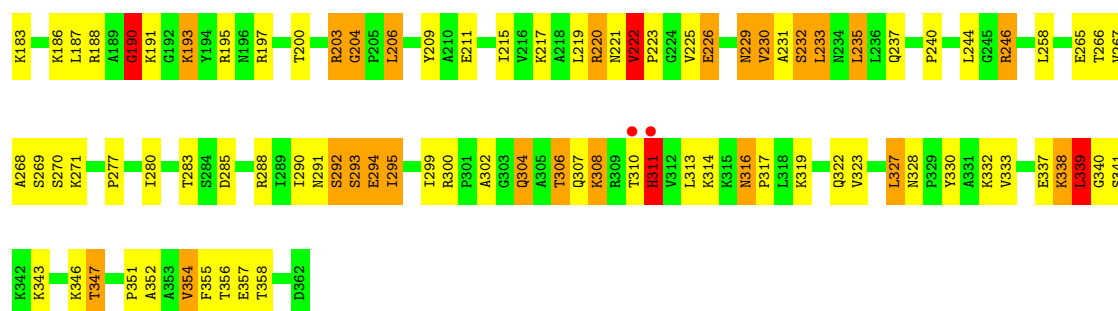


• Molecule 40: 60S ribosomal protein L3

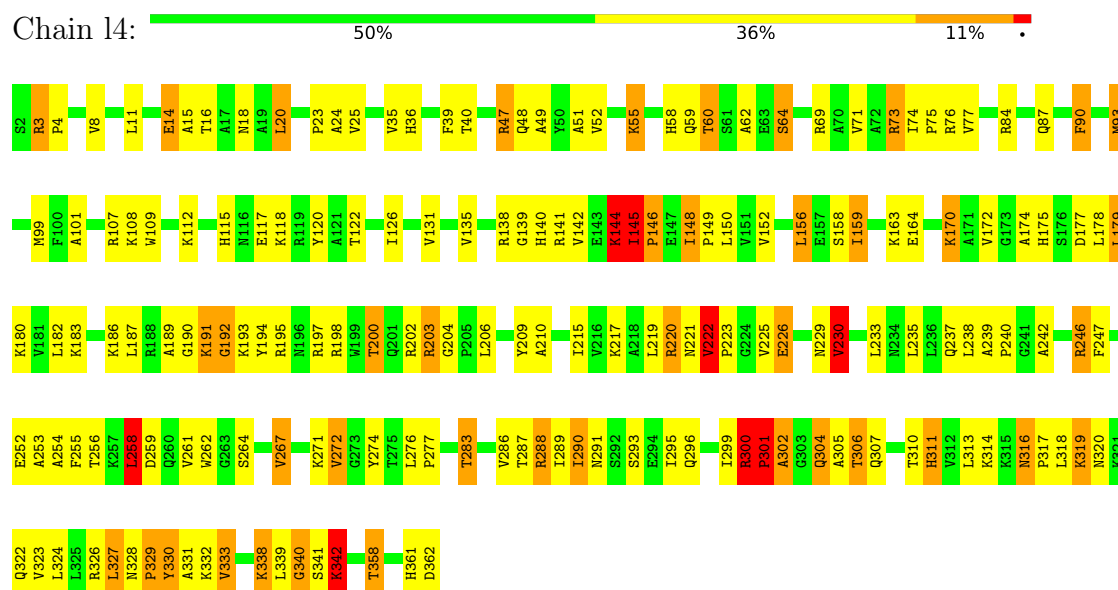


• Molecule 41: 60S ribosomal protein L4-A

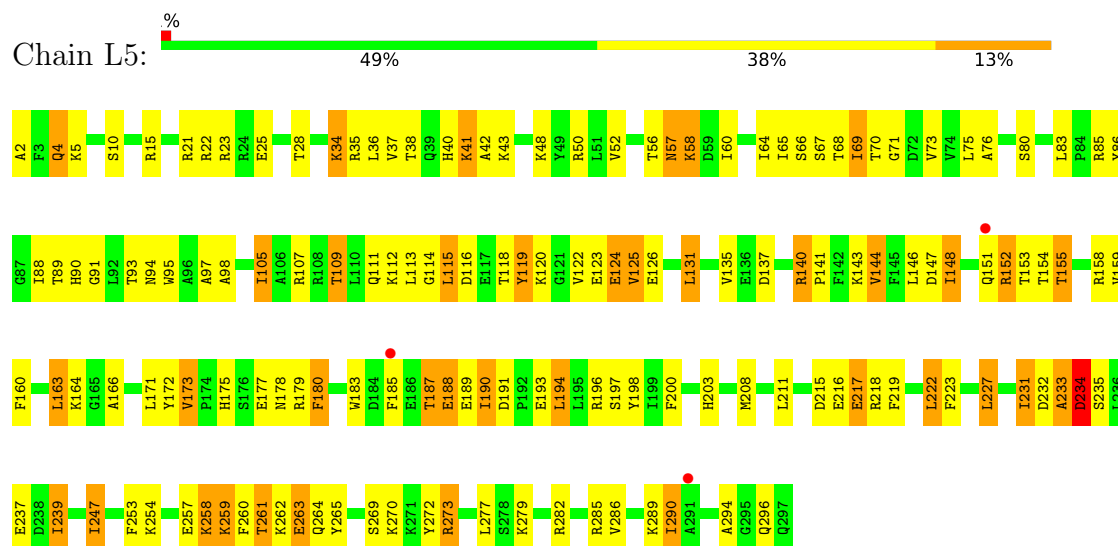




- Molecule 41: 60S ribosomal protein L4-A

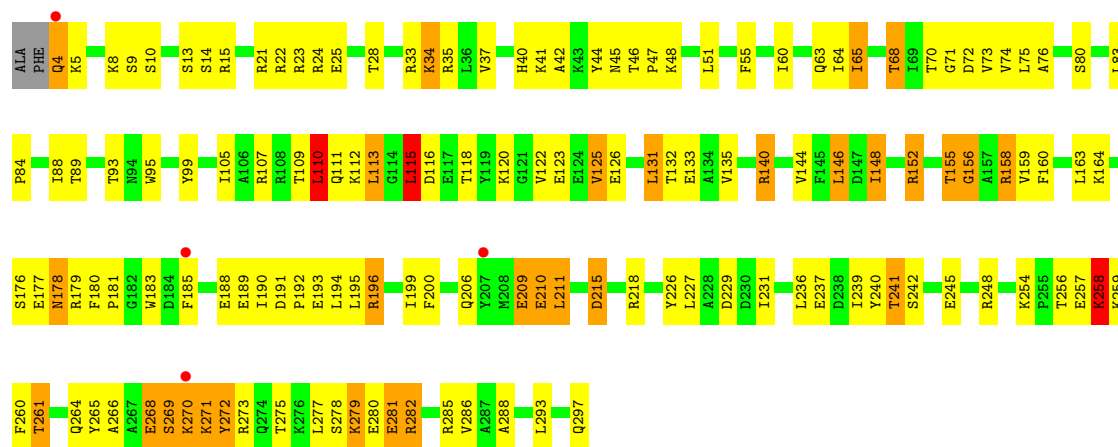


- Molecule 42: 60S ribosomal protein L5

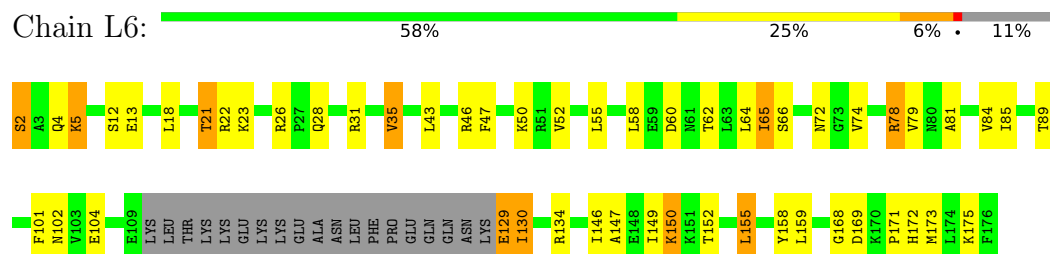


- Molecule 42: 60S ribosomal protein L5

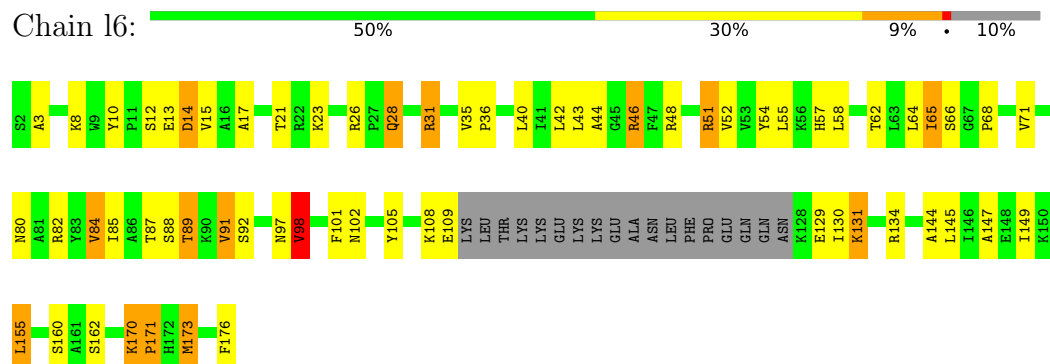




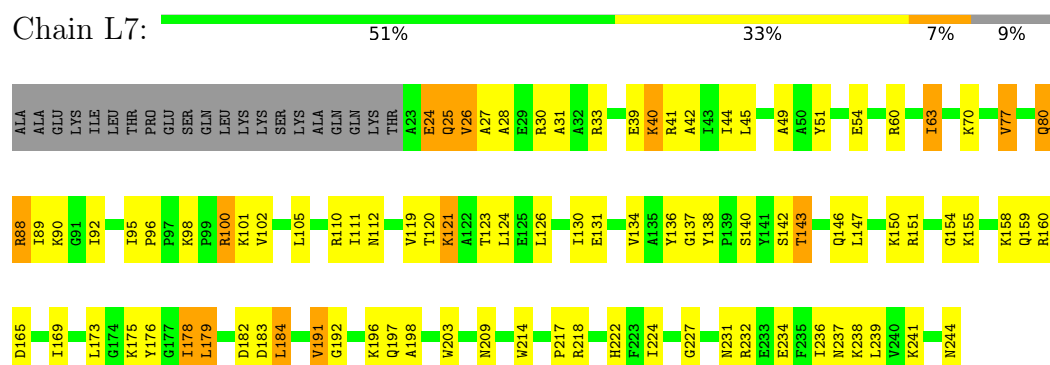
• Molecule 43: 60S ribosomal protein L6-A



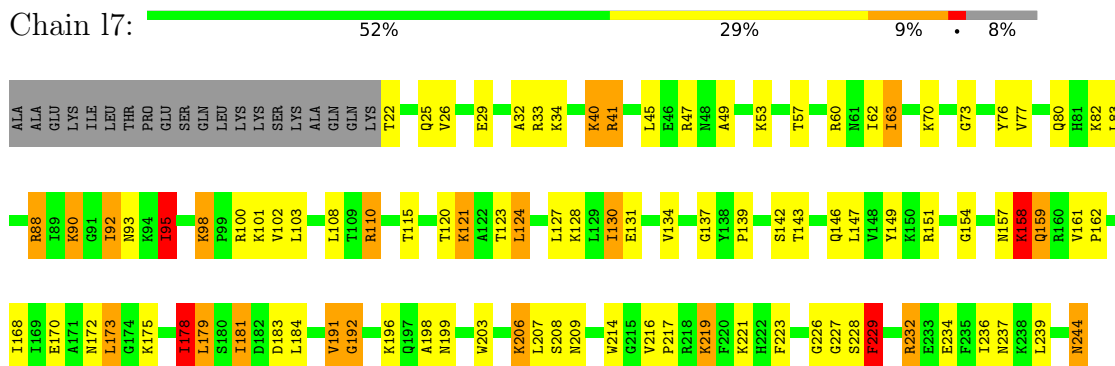
• Molecule 43: 60S ribosomal protein L6-A



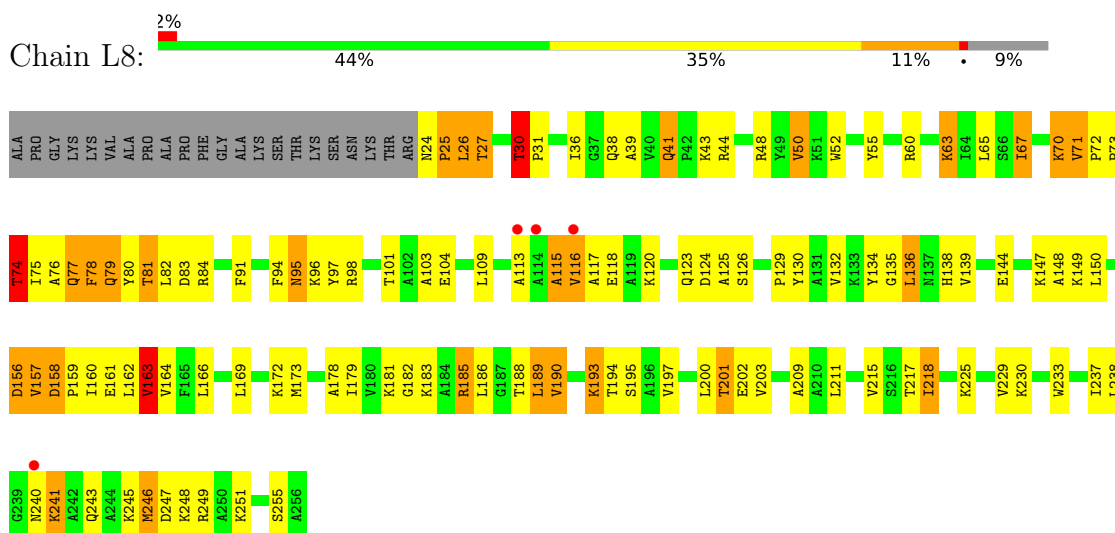
• Molecule 44: 60S ribosomal protein L7-A



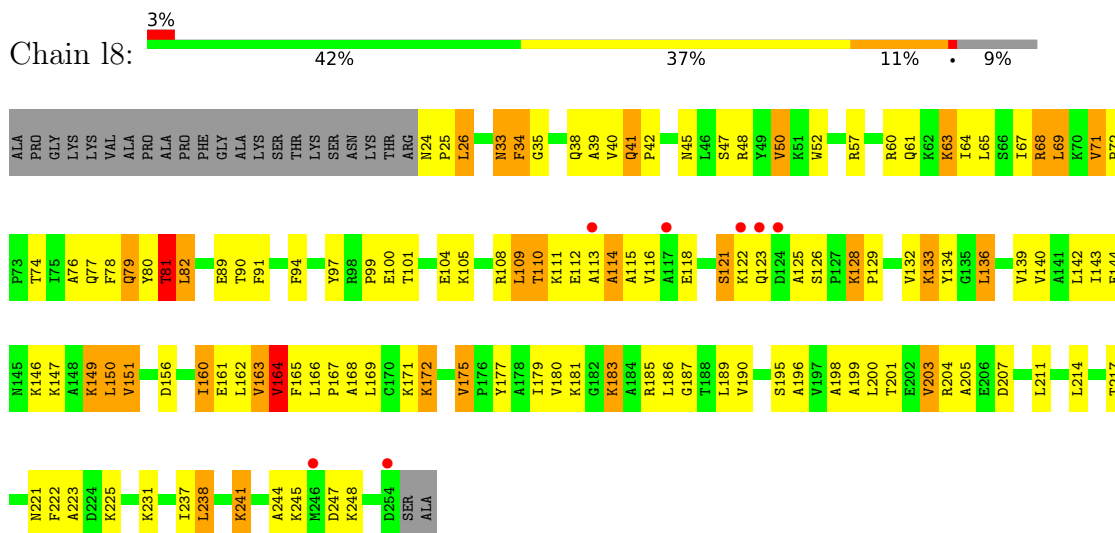
- Molecule 44: 60S ribosomal protein L7-A



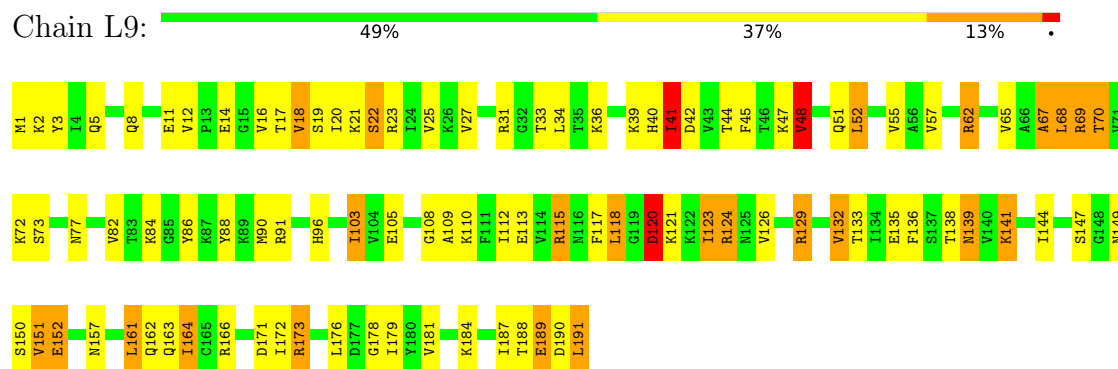
- Molecule 45: 60S ribosomal protein L8-A



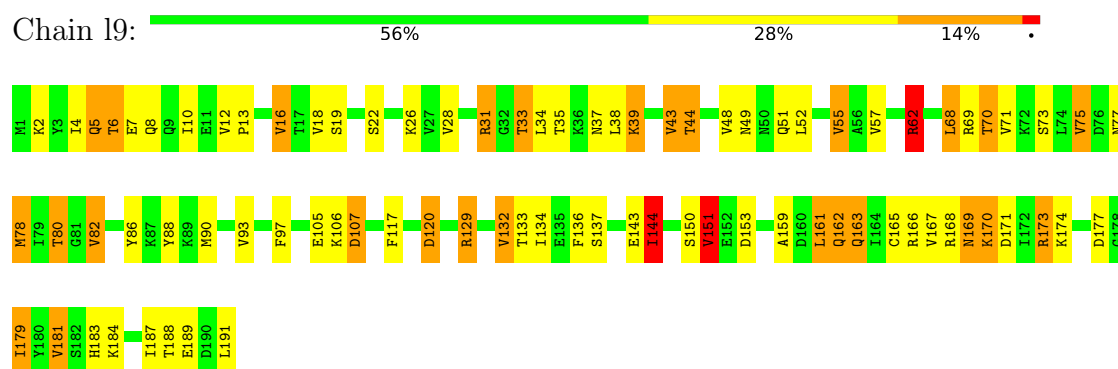
- Molecule 45: 60S ribosomal protein L8-A



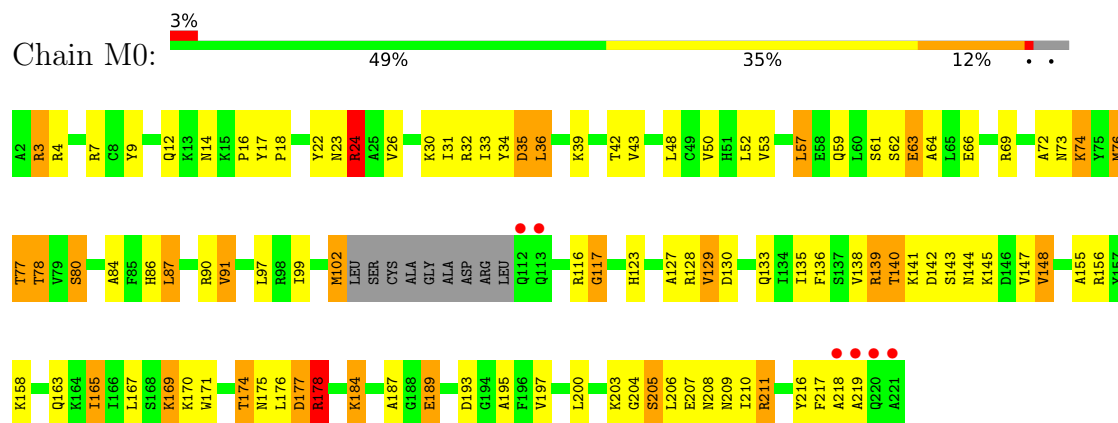
- Molecule 46: 60S ribosomal protein L9-A



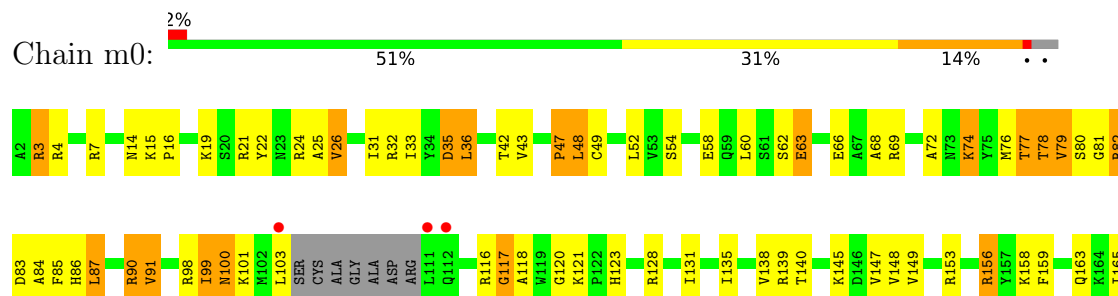
• Molecule 46: 60S ribosomal protein L9-A

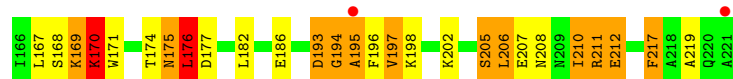


• Molecule 47: 60S ribosomal protein L10

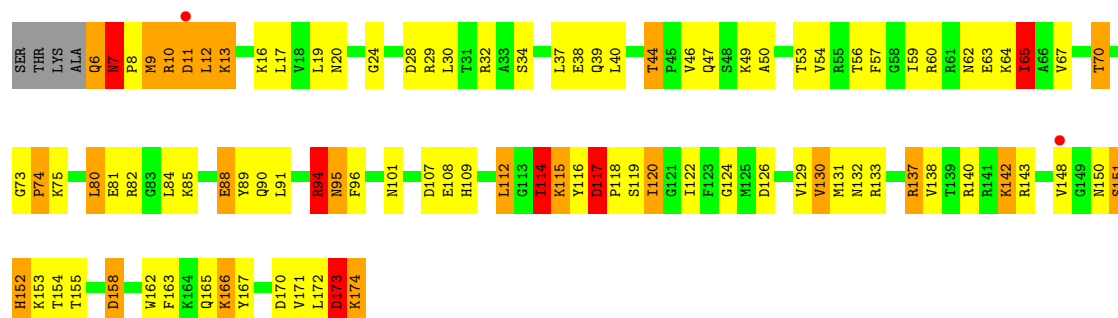
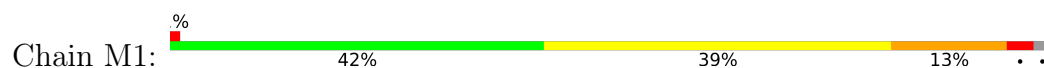


• Molecule 47: 60S ribosomal protein L10

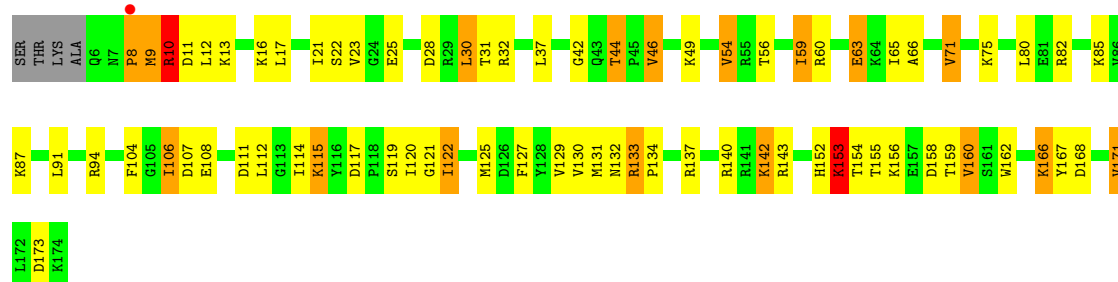




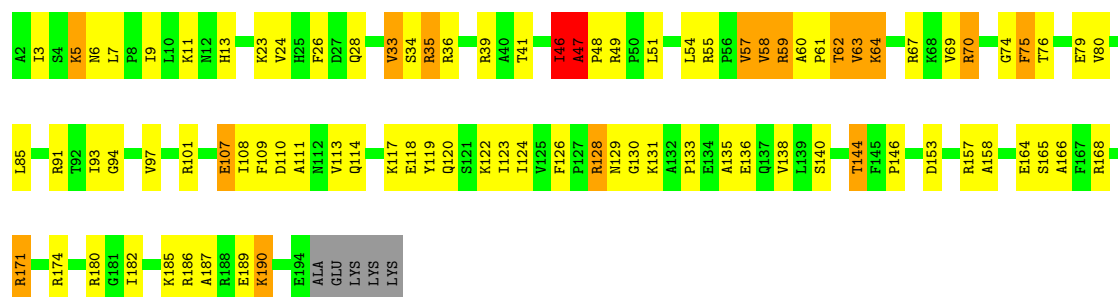
- Molecule 48: 60S ribosomal protein L11-B



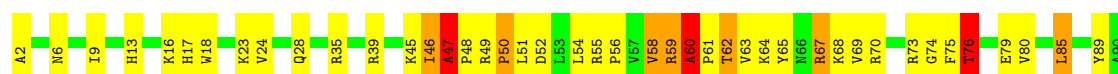
- Molecule 48: 60S ribosomal protein L11-B

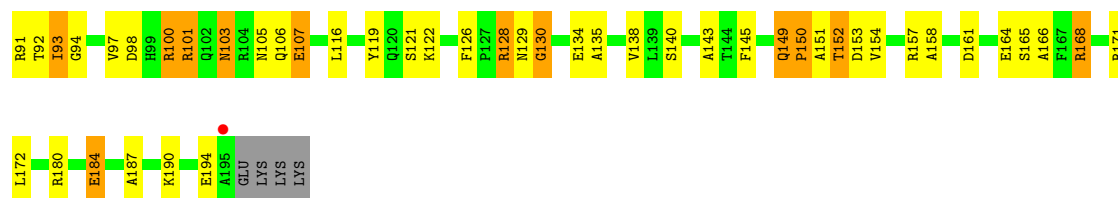


- Molecule 49: 60S ribosomal protein L13-A

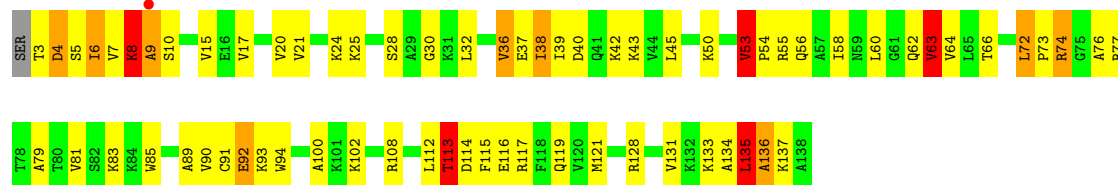


- Molecule 49: 60S ribosomal protein L13-A

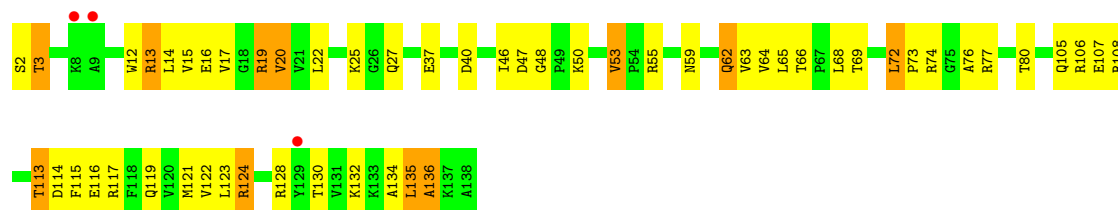




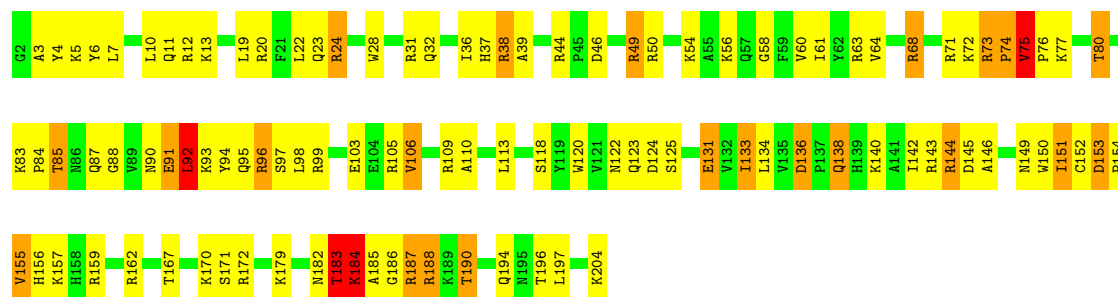
- Molecule 50: 60S ribosomal protein L14-A



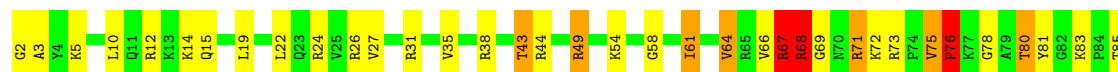
- Molecule 50: 60S ribosomal protein L14-A



- Molecule 51: 60S ribosomal protein L15-A

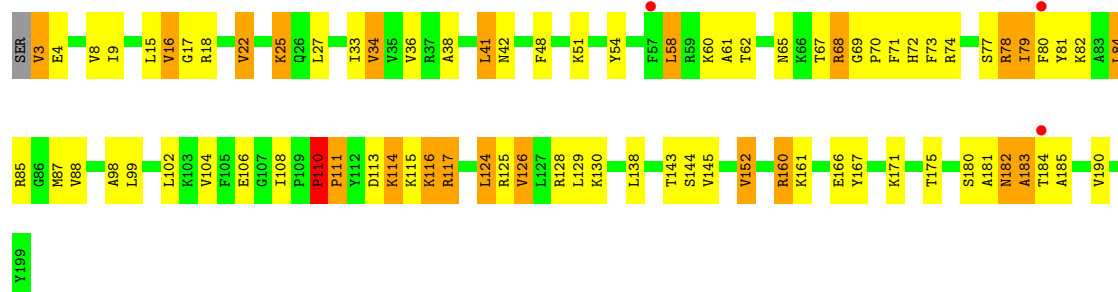


- Molecule 51: 60S ribosomal protein L15-A

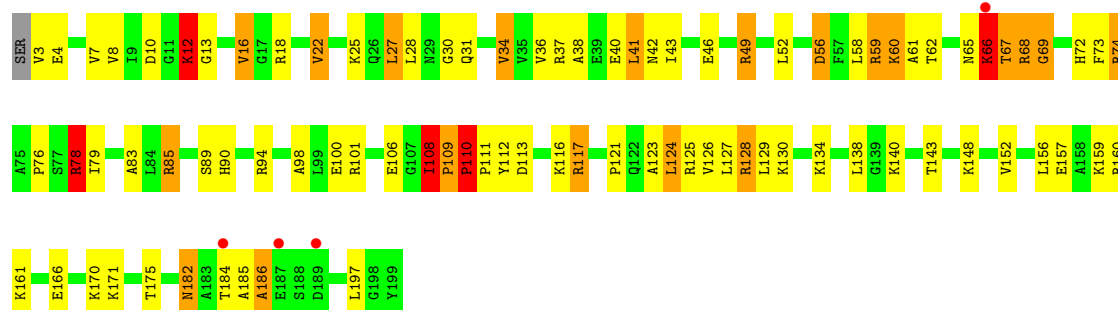




• Molecule 52: 60S ribosomal protein L16-A



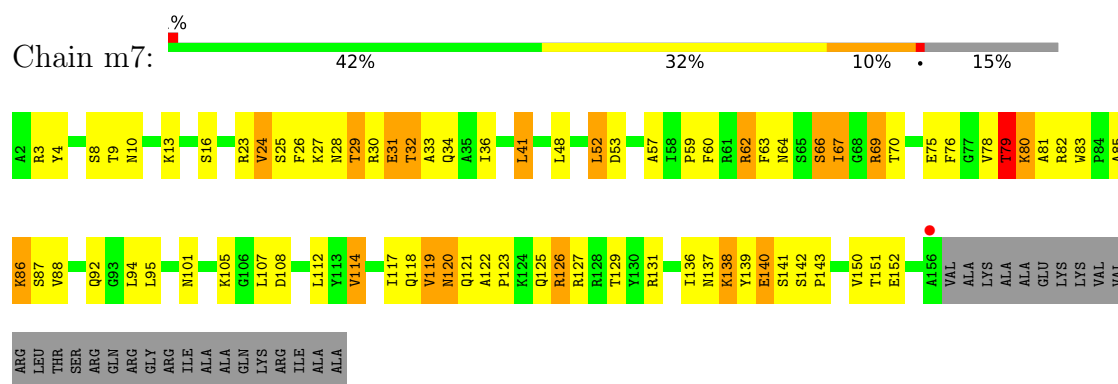
• Molecule 52: 60S ribosomal protein L16-A



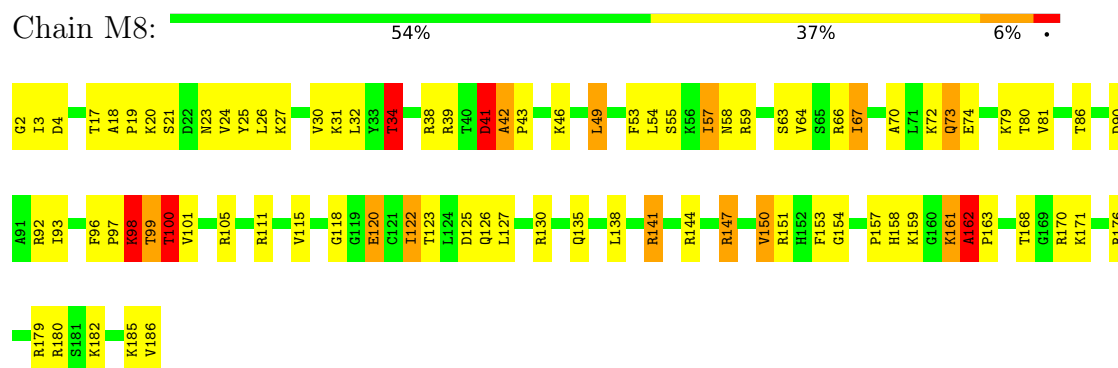
• Molecule 53: 60S ribosomal protein L17-A



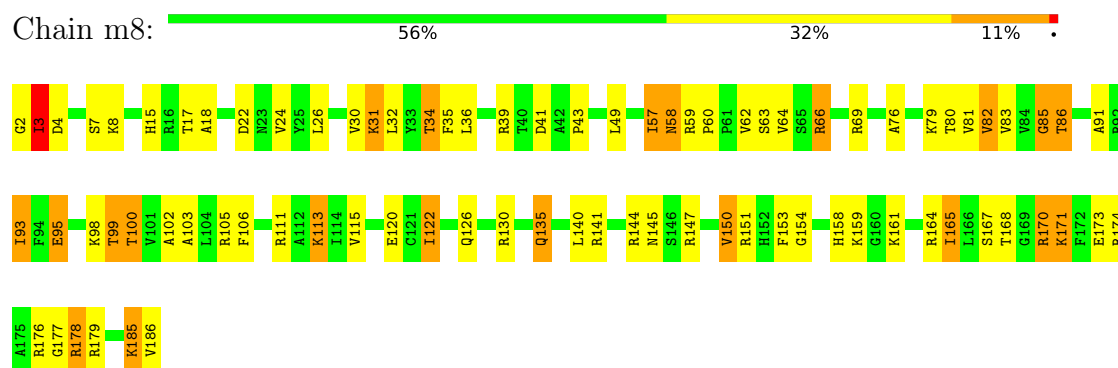
• Molecule 53: 60S ribosomal protein L17-A



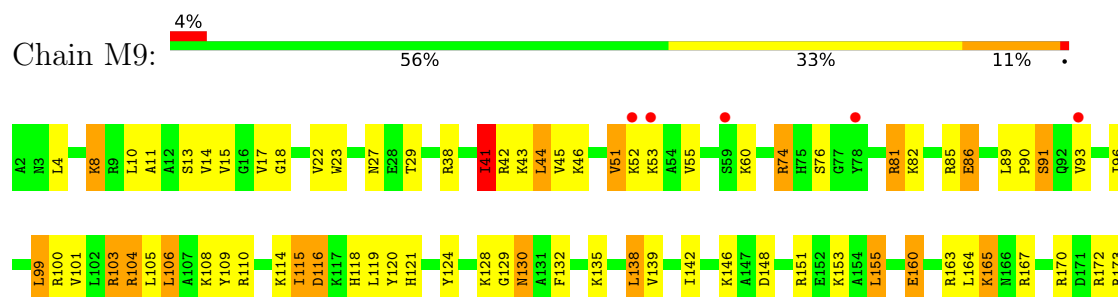
• Molecule 54: 60S ribosomal protein L18-A



• Molecule 54: 60S ribosomal protein L18-A

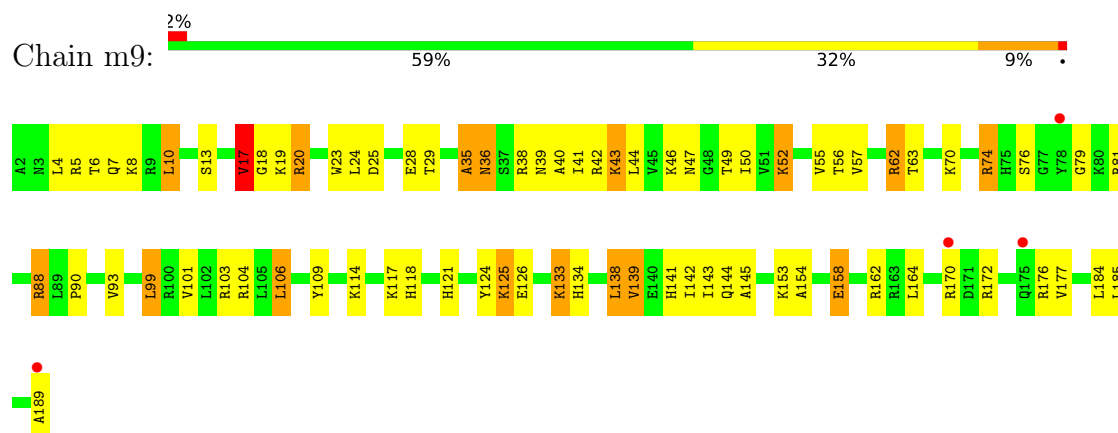


• Molecule 55: 60S ribosomal protein L19-A

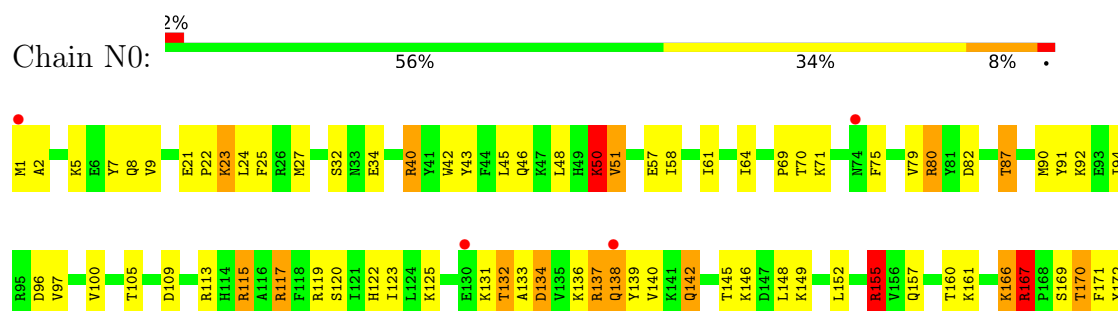




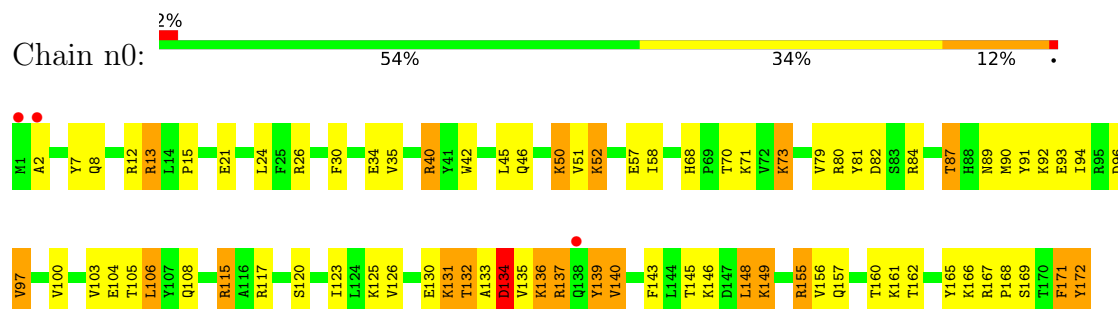
- Molecule 55: 60S ribosomal protein L19-A



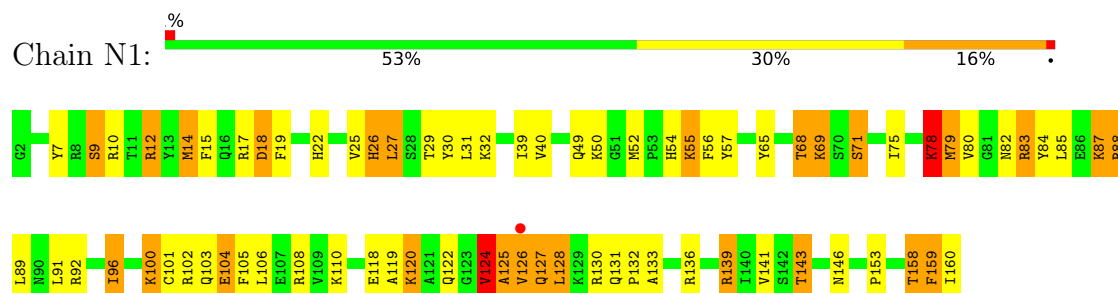
- Molecule 56: 60S ribosomal protein L20-A



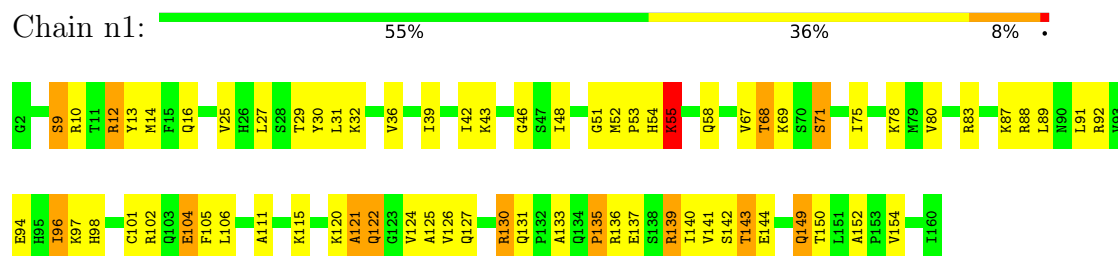
- Molecule 56: 60S ribosomal protein L20-A



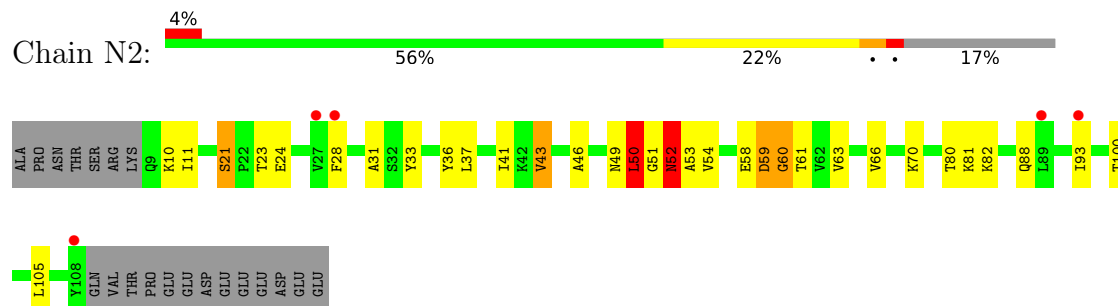
- Molecule 57: 60S ribosomal protein L21-A



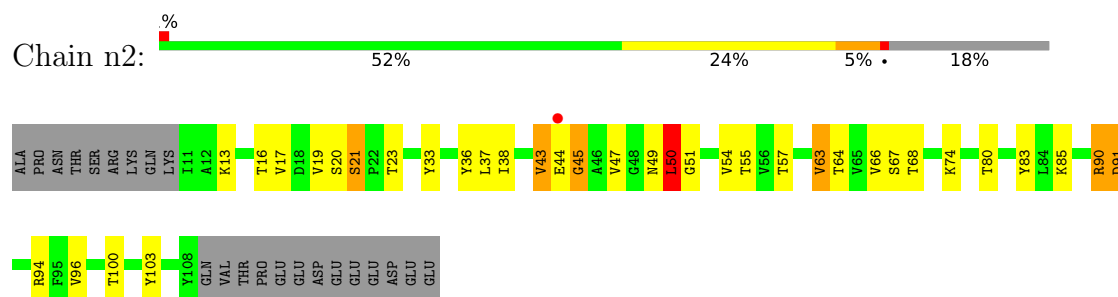
- Molecule 57: 60S ribosomal protein L21-A



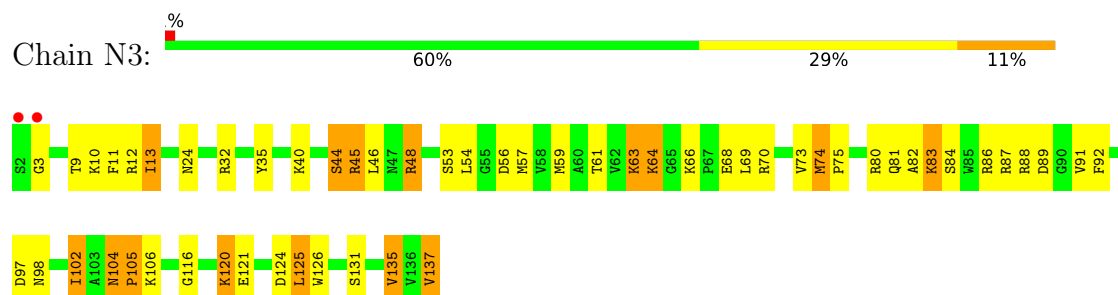
- Molecule 58: 60S ribosomal protein L22-A



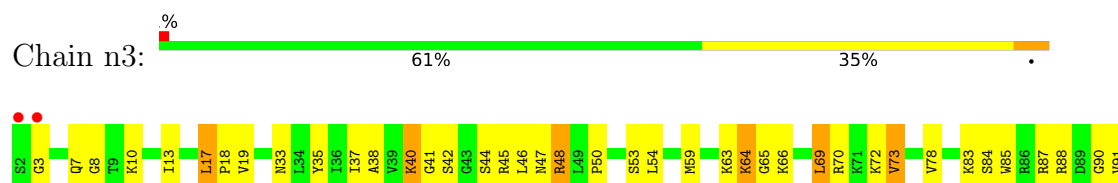
- Molecule 58: 60S ribosomal protein L22-A

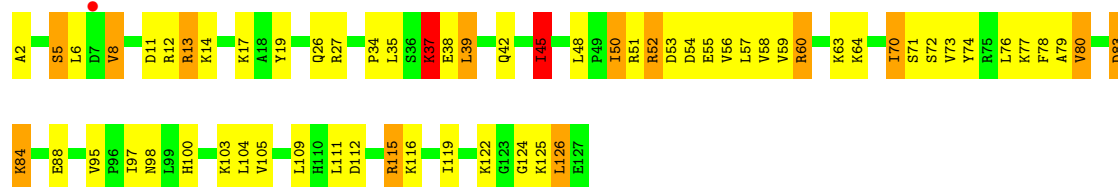


- Molecule 59: 60S ribosomal protein L23-A

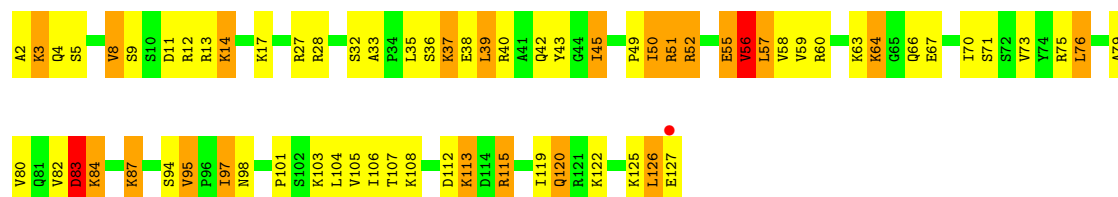


- Molecule 59: 60S ribosomal protein L23-A

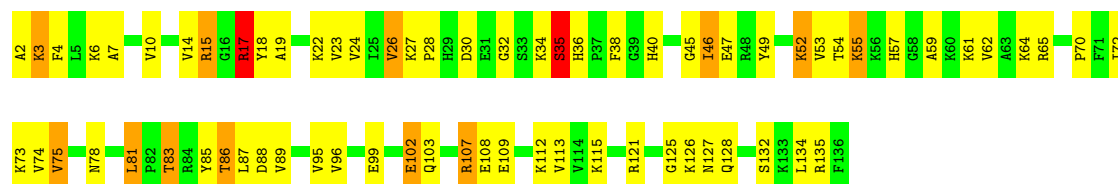




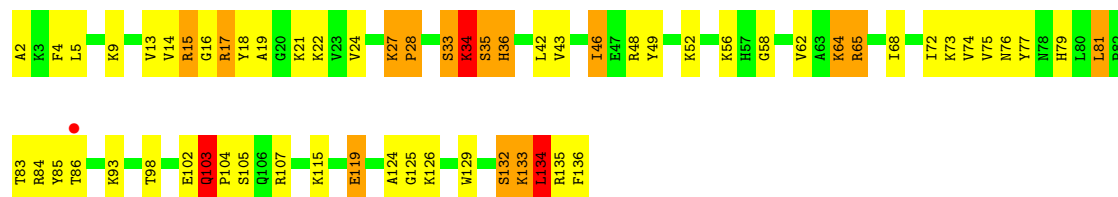
• Molecule 62: 60S ribosomal protein L26-A



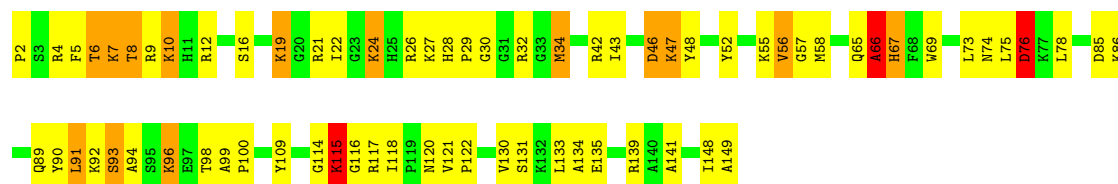
• Molecule 63: 60S ribosomal protein L27-A



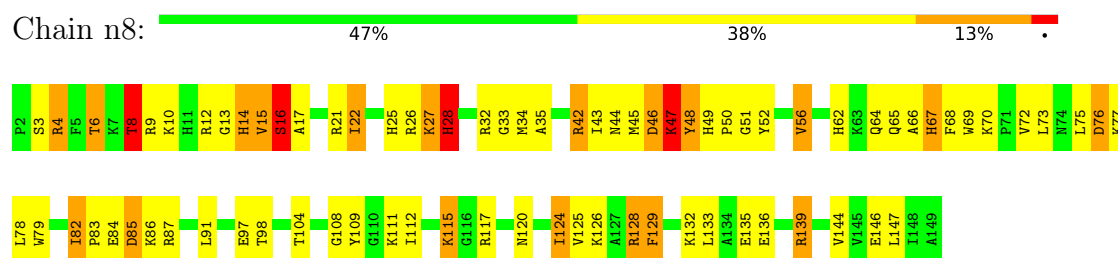
• Molecule 63: 60S ribosomal protein L27-A



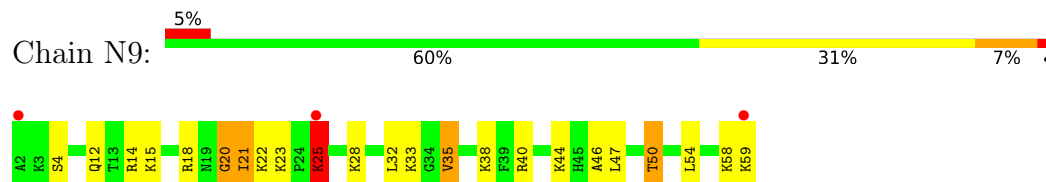
• Molecule 64: 60S ribosomal protein L28



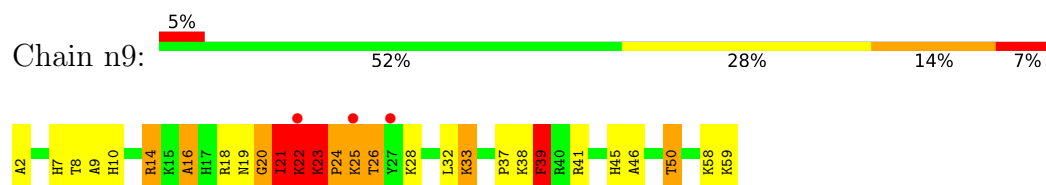
- Molecule 64: 60S ribosomal protein L28



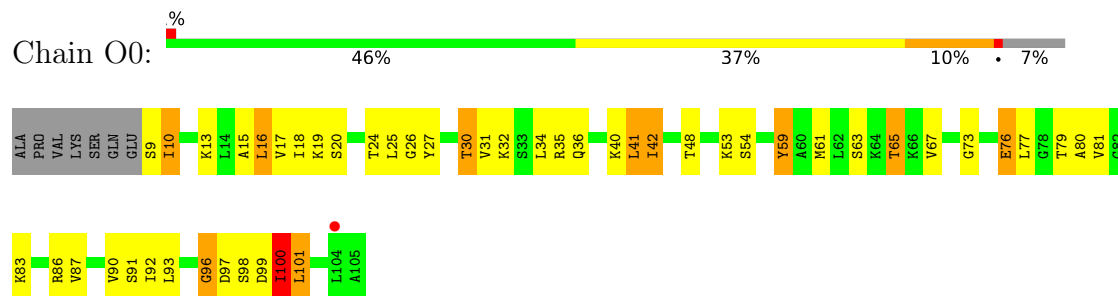
- Molecule 65: 60S ribosomal protein L29



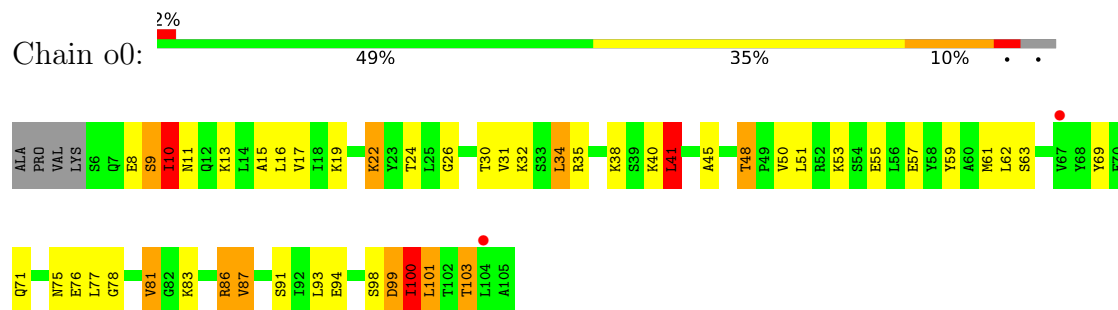
- Molecule 65: 60S ribosomal protein L29



- Molecule 66: 60S ribosomal protein L30

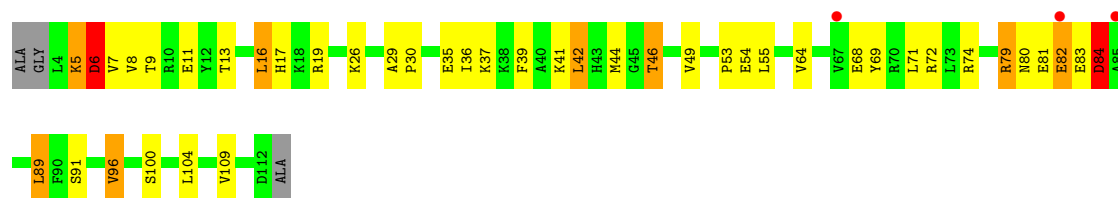


- Molecule 66: 60S ribosomal protein L30

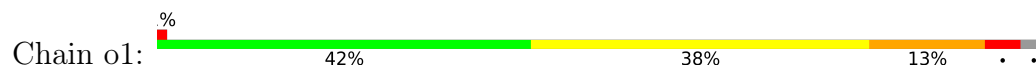


- Molecule 67: 60S ribosomal protein L31-A

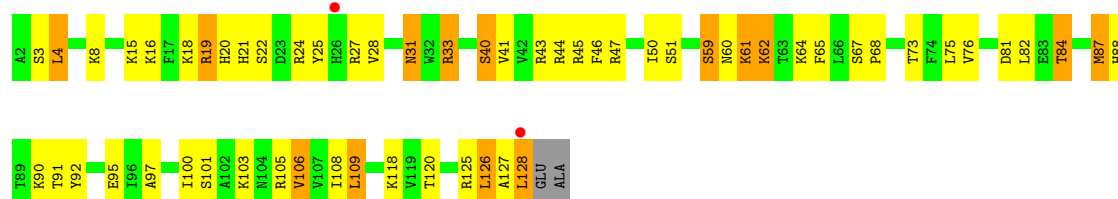




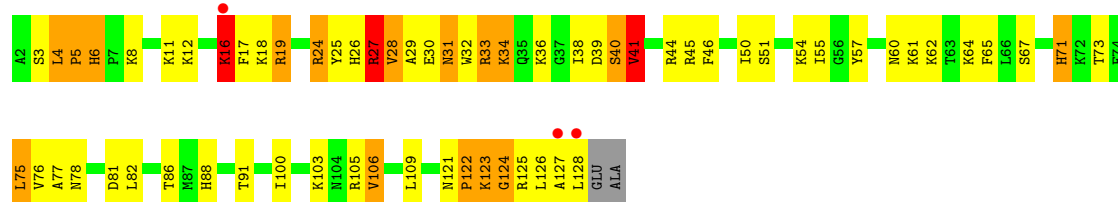
- Molecule 67: 60S ribosomal protein L31-A



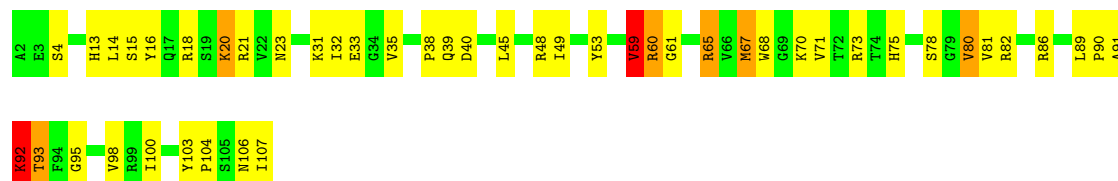
- Molecule 68: 60S ribosomal protein L32



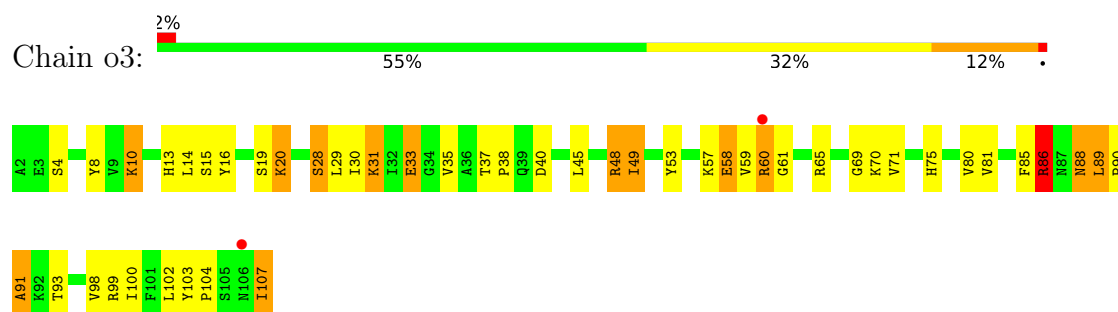
- Molecule 68: 60S ribosomal protein L32



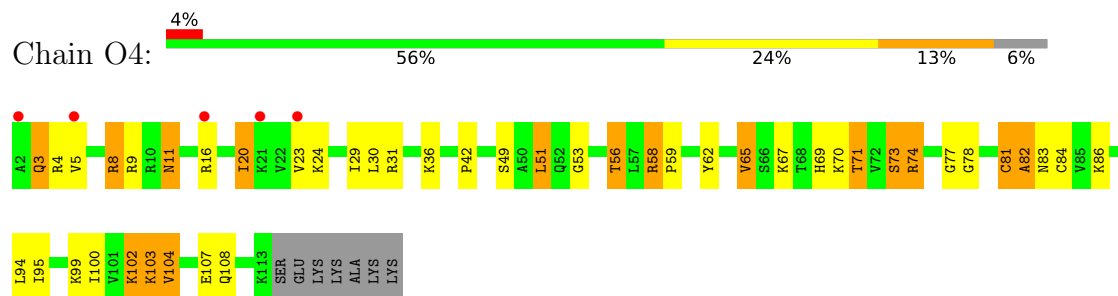
- Molecule 69: 60S ribosomal protein L33-A



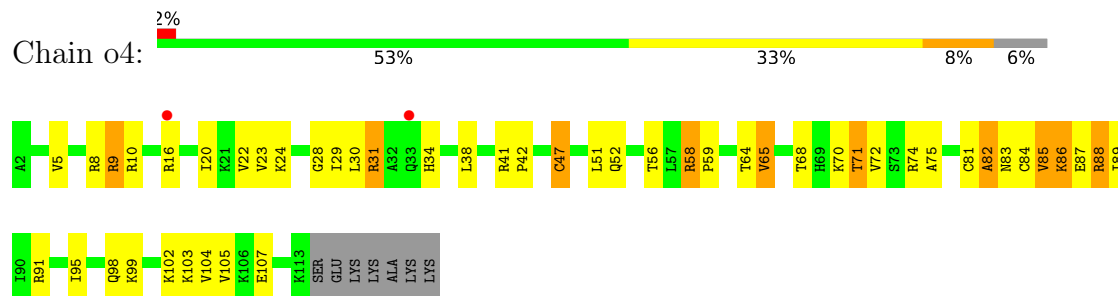
- Molecule 69: 60S ribosomal protein L33-A



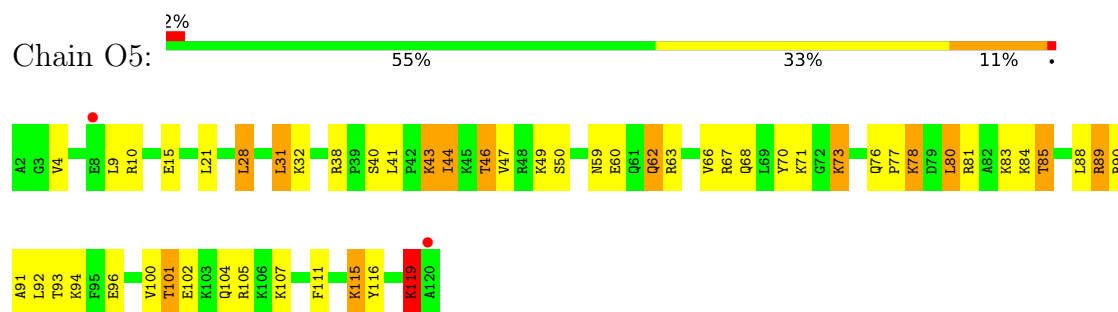
- Molecule 70: 60S ribosomal protein L34-A



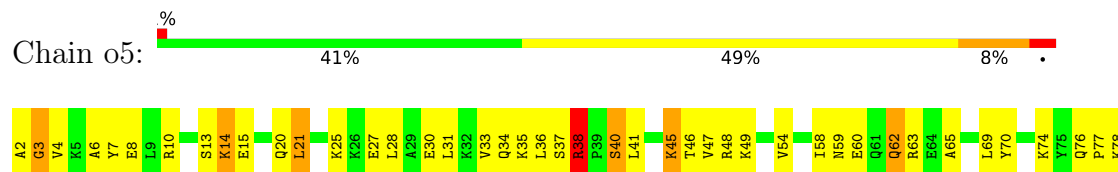
- Molecule 70: 60S ribosomal protein L34-A

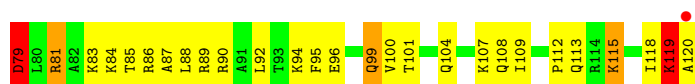


- Molecule 71: 60S ribosomal protein L35-A

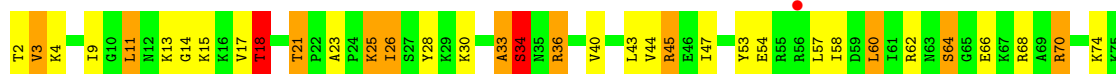


- Molecule 71: 60S ribosomal protein L35-A

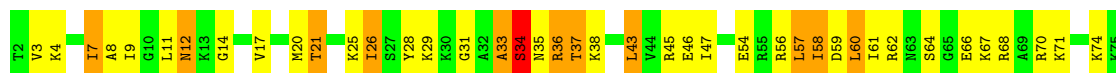




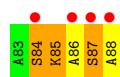
- Molecule 72: 60S ribosomal protein L36-A



- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A

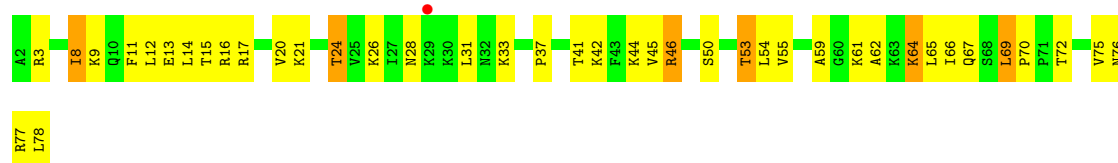


- Molecule 73: 60S ribosomal protein L37-A



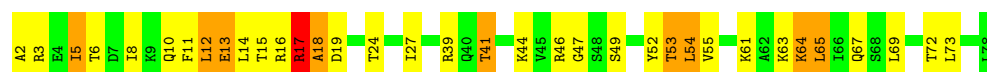
- Molecule 74: 60S ribosomal protein L38





- Molecule 74: 60S ribosomal protein L38

Chain o8: 55% 32% 12%



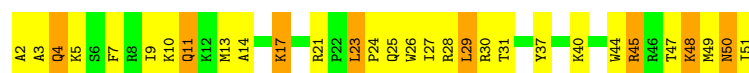
- Molecule 75: 60S ribosomal protein L39

Chain O9: 46% 36% 18%



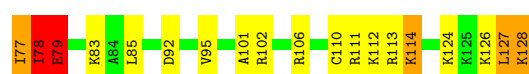
- Molecule 75: 60S ribosomal protein L39

Chain o9: 40% 44% 16%



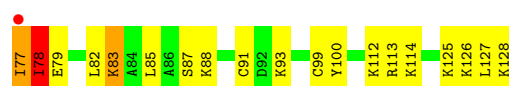
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 63% 25% 8%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0: 63% 31% 2%

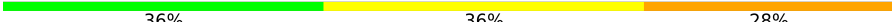


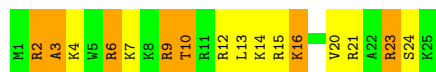
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1: 4% 16% 60% 24%



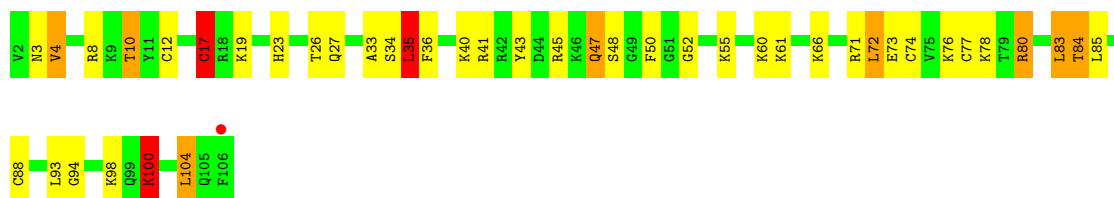
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  36% 36% 28%



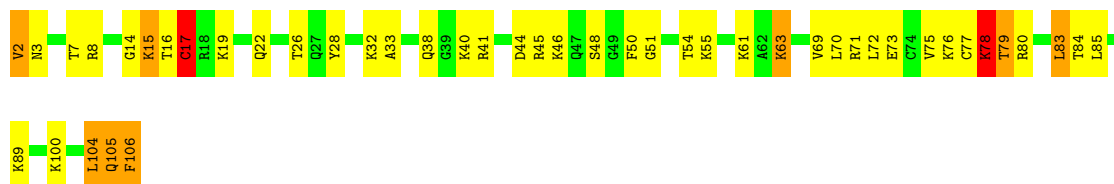
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  59% 30% 8%

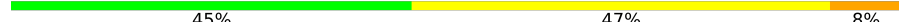


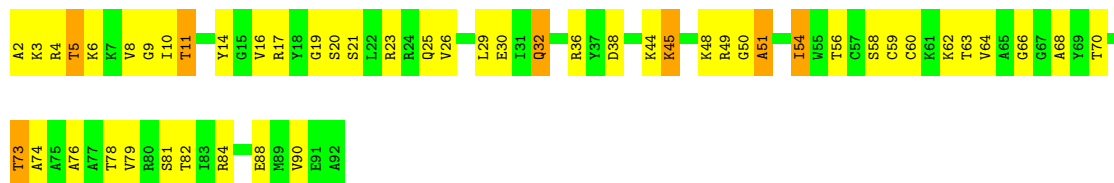
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  56% 34% 8%



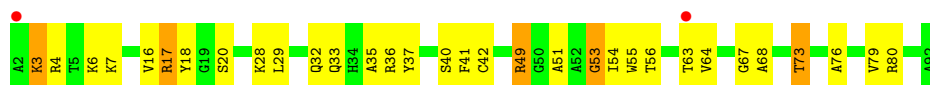
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  45% 47% 8%



- Molecule 79: 60S ribosomal protein L43-A

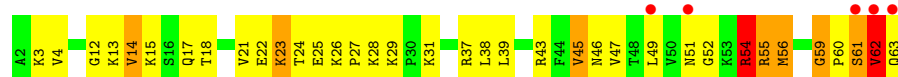
Chain q3:  65% 30% 5%



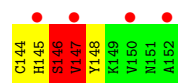
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  42% 44% 11%

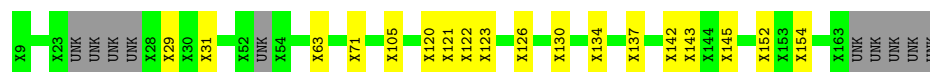
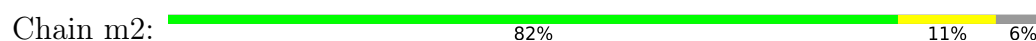




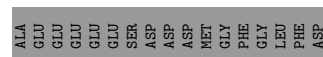
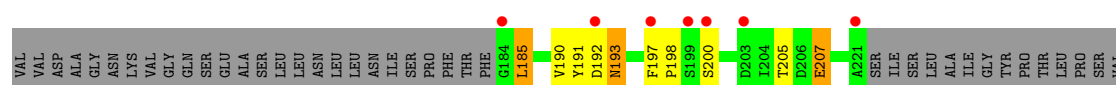
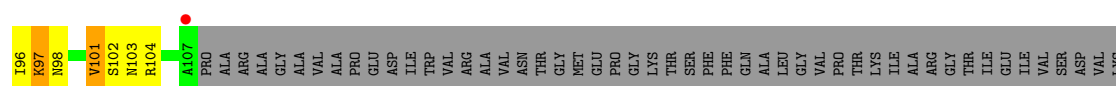
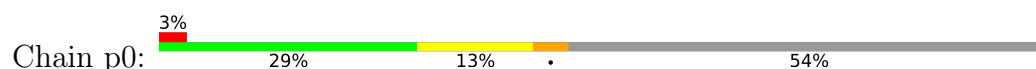
- Molecule 81: Ubiquitin-40S ribosomal protein S31



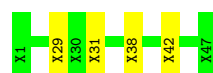
- Molecule 82: UNKNOWN PROTEIN m2



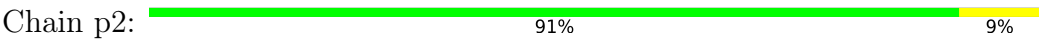
- Molecule 83: 60S acidic ribosomal protein P0



- Molecule 84: UNKNOWN PROTEIN p1



- Molecule 85: UNKNOWN PROTEIN p2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.68Å 287.99Å 304.76Å 90.00° 99.01° 90.00°	Depositor
Resolution (Å)	99.80 – 3.00 99.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.80-3.00) 99.9 (99.80-3.00)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.199 , 0.245 (Not available) , 0.220	Depositor DCC
R_{free} test set	29589 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	411204	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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, OHX, ANM, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.43	0/41698	0.63	5/64972 (0.0%)
1	6	0.50	0/42765	0.67	8/66634 (0.0%)
2	S0	0.64	0/1617	1.08	9/2215 (0.4%)
2	s0	0.67	0/1623	1.12	7/2222 (0.3%)
3	S1	0.52	0/1735	0.94	4/2335 (0.2%)
3	s1	0.67	0/1748	1.08	9/2352 (0.4%)
4	S2	0.67	0/1665	1.15	9/2263 (0.4%)
4	s2	0.81	0/1665	1.11	4/2263 (0.2%)
5	S3	0.65	0/1759	1.01	4/2368 (0.2%)
5	s3	0.60	0/1759	0.99	8/2368 (0.3%)
6	S4	0.64	0/2109	1.10	12/2839 (0.4%)
6	s4	0.73	0/2109	1.14	12/2839 (0.4%)
7	S5	0.57	0/1629	1.01	3/2202 (0.1%)
7	s5	0.63	0/1629	1.05	7/2202 (0.3%)
8	S6	0.61	0/1823	1.01	6/2439 (0.2%)
8	s6	0.72	0/1779	1.07	4/2379 (0.2%)
9	S7	0.57	0/1506	1.02	5/2028 (0.2%)
9	s7	0.65	1/1516 (0.1%)	1.08	9/2043 (0.4%)
10	S8	0.76	0/1514	1.10	4/2021 (0.2%)
10	s8	0.84	0/1514	1.11	4/2021 (0.2%)
11	S9	0.66	0/1519	1.01	3/2035 (0.1%)
11	s9	0.73	0/1519	1.17	12/2035 (0.6%)
12	C0	0.57	0/790	1.09	4/1069 (0.4%)
12	c0	0.50	0/777	0.98	3/1049 (0.3%)
13	C1	0.79	0/1240	1.10	5/1675 (0.3%)
13	c1	0.82	0/1194	1.15	4/1610 (0.2%)
14	C2	0.54	0/900	0.97	3/1224 (0.2%)
14	c2	0.46	0/900	0.89	0/1224
15	C3	0.68	0/1215	1.07	8/1638 (0.5%)
15	c3	0.77	0/1215	1.15	3/1638 (0.2%)
16	C4	0.58	0/901	1.05	3/1217 (0.2%)
16	c4	0.73	0/960	1.20	6/1290 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.66	0/998	1.06	2/1341 (0.1%)
17	c5	0.67	1/1060 (0.1%)	1.19	7/1426 (0.5%)
18	C6	0.61	0/1125	1.00	3/1510 (0.2%)
18	c6	0.70	0/1131	1.12	7/1518 (0.5%)
19	C7	0.63	0/935	1.04	3/1254 (0.2%)
19	c7	0.70	0/914	1.21	6/1224 (0.5%)
20	C8	0.60	0/1211	0.99	3/1628 (0.2%)
20	c8	0.64	0/1211	1.02	2/1628 (0.1%)
21	C9	0.63	0/1130	0.97	3/1517 (0.2%)
21	c9	0.65	0/1130	1.08	6/1517 (0.4%)
22	D0	0.65	0/865	0.98	3/1169 (0.3%)
22	d0	0.67	0/892	1.07	6/1205 (0.5%)
23	D1	0.63	0/693	0.96	0/935
23	d1	0.70	0/693	1.06	0/935
24	D2	0.69	0/1038	1.05	5/1395 (0.4%)
24	d2	0.84	0/1038	1.15	4/1395 (0.3%)
25	D3	0.83	0/1139	1.16	7/1518 (0.5%)
25	d3	0.95	0/1139	1.20	3/1518 (0.2%)
26	D4	0.60	0/1087	0.97	2/1449 (0.1%)
26	d4	0.70	0/1087	1.05	2/1449 (0.1%)
27	D5	0.56	0/571	1.08	6/768 (0.8%)
27	d5	0.59	0/566	1.05	3/761 (0.4%)
28	D6	0.65	0/782	1.07	3/1047 (0.3%)
28	d6	0.71	0/782	1.06	3/1047 (0.3%)
29	D7	0.62	0/620	1.01	4/838 (0.5%)
29	d7	0.62	0/620	1.05	3/838 (0.4%)
30	D8	0.47	0/499	0.87	0/670
30	d8	0.58	0/499	1.13	4/670 (0.6%)
31	D9	0.67	0/452	1.05	1/600 (0.2%)
31	d9	0.68	0/452	1.02	3/600 (0.5%)
32	E0	0.64	0/483	1.07	0/643
33	E1	0.67	0/577	1.15	3/770 (0.4%)
34	SR	0.56	1/2494 (0.0%)	0.95	9/3393 (0.3%)
34	sR	0.54	0/2495	0.86	1/3395 (0.0%)
35	SM	0.72	0/1113	1.14	6/1502 (0.4%)
35	sM	0.74	0/683	1.13	2/923 (0.2%)
36	1	0.65	0/75394	0.79	23/117545 (0.0%)
36	5	0.68	0/75414	0.80	18/117575 (0.0%)
37	3	0.55	0/2883	0.69	0/4491
37	7	0.67	0/2883	0.80	0/4491
38	4	0.64	0/3746	0.76	0/5832
38	8	0.59	0/3746	0.71	0/5832
39	L2	0.94	1/1948 (0.1%)	1.26	8/2617 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	l2	1.04	2/1946 (0.1%)	1.27	13/2614 (0.5%)
40	L3	0.95	2/3146 (0.1%)	1.21	13/4228 (0.3%)
40	l3	1.10	1/3146 (0.0%)	1.27	10/4228 (0.2%)
41	L4	1.07	1/2800 (0.0%)	1.36	21/3790 (0.6%)
41	l4	1.02	1/2800 (0.0%)	1.31	18/3790 (0.5%)
42	L5	0.70	0/2425	1.05	8/3271 (0.2%)
42	l5	0.92	0/2408	1.19	8/3248 (0.2%)
43	L6	1.01	0/1260	1.18	3/1694 (0.2%)
43	l6	0.97	0/1269	1.19	5/1705 (0.3%)
44	L7	1.04	1/1821 (0.1%)	1.27	11/2451 (0.4%)
44	l7	1.06	2/1828 (0.1%)	1.32	21/2461 (0.9%)
45	L8	0.73	0/1836	1.15	16/2481 (0.6%)
45	l8	0.70	0/1795	1.05	7/2429 (0.3%)
46	L9	0.85	0/1539	1.13	6/2073 (0.3%)
46	l9	1.04	0/1539	1.27	12/2073 (0.6%)
47	M0	0.97	2/1741 (0.1%)	1.24	13/2335 (0.6%)
47	m0	0.95	0/1758	1.17	8/2358 (0.3%)
48	M1	0.69	0/1374	1.10	9/1842 (0.5%)
48	m1	0.89	0/1374	1.21	8/1842 (0.4%)
49	M3	1.02	1/1568 (0.1%)	1.23	8/2106 (0.4%)
49	m3	0.96	1/1573 (0.1%)	1.22	10/2113 (0.5%)
50	M4	0.99	0/1068	1.18	8/1438 (0.6%)
50	m4	1.06	0/1074	1.21	2/1446 (0.1%)
51	M5	1.01	2/1757 (0.1%)	1.24	12/2354 (0.5%)
51	m5	0.89	0/1757	1.19	15/2354 (0.6%)
52	M6	1.05	0/1585	1.29	5/2128 (0.2%)
52	m6	1.27	3/1585 (0.2%)	1.40	7/2128 (0.3%)
53	M7	1.05	1/1443 (0.1%)	1.27	12/1944 (0.6%)
53	m7	1.17	3/1250 (0.2%)	1.29	8/1683 (0.5%)
54	M8	1.07	0/1465	1.32	10/1965 (0.5%)
54	m8	1.00	0/1465	1.32	10/1965 (0.5%)
55	M9	0.77	0/1538	1.09	7/2050 (0.3%)
55	m9	0.82	0/1538	1.05	1/2050 (0.0%)
56	N0	1.01	0/1481	1.21	8/1990 (0.4%)
56	n0	1.10	2/1481 (0.1%)	1.29	7/1990 (0.4%)
57	N1	0.95	0/1300	1.19	5/1743 (0.3%)
57	n1	1.02	0/1300	1.25	9/1743 (0.5%)
58	N2	0.54	0/812	0.97	3/1099 (0.3%)
58	n2	0.62	0/794	1.04	4/1076 (0.4%)
59	N3	0.95	0/1018	1.23	3/1369 (0.2%)
59	n3	1.12	1/1018 (0.1%)	1.34	10/1369 (0.7%)
60	N4	0.78	0/712	1.37	4/958 (0.4%)
60	n4	0.93	1/1052 (0.1%)	1.20	7/1398 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	N5	0.79	0/979	1.13	3/1321 (0.2%)
61	n5	0.86	0/974	1.14	5/1314 (0.4%)
62	N6	0.94	0/1004	1.25	5/1341 (0.4%)
62	n6	0.88	0/1004	1.22	3/1341 (0.2%)
63	N7	0.65	0/1118	1.07	4/1497 (0.3%)
63	n7	0.61	0/1118	1.10	4/1497 (0.3%)
64	N8	1.06	1/1204 (0.1%)	1.26	10/1612 (0.6%)
64	n8	1.06	1/1204 (0.1%)	1.36	12/1612 (0.7%)
65	N9	1.01	0/473	1.12	1/629 (0.2%)
65	n9	1.11	2/473 (0.4%)	1.34	6/629 (1.0%)
66	O0	0.64	0/751	0.99	1/1008 (0.1%)
66	o0	0.66	0/775	0.98	0/1040
67	O1	0.83	0/890	1.12	0/1196
67	o1	0.99	0/897	1.29	5/1205 (0.4%)
68	O2	1.16	2/1041 (0.2%)	1.28	4/1394 (0.3%)
68	o2	1.16	2/1041 (0.2%)	1.30	10/1394 (0.7%)
69	O3	1.13	0/868	1.27	4/1168 (0.3%)
69	o3	1.15	0/868	1.24	3/1168 (0.3%)
70	O4	0.86	0/890	1.14	4/1189 (0.3%)
70	o4	0.80	0/890	1.19	2/1189 (0.2%)
71	O5	0.93	1/978 (0.1%)	1.16	4/1301 (0.3%)
71	o5	0.75	0/974	1.05	5/1297 (0.4%)
72	O6	0.89	1/778 (0.1%)	1.22	5/1034 (0.5%)
72	o6	0.77	0/777	1.07	2/1033 (0.2%)
73	O7	1.11	1/696 (0.1%)	1.31	6/923 (0.7%)
73	o7	0.93	0/696	1.27	3/923 (0.3%)
74	O8	0.64	0/618	1.08	5/826 (0.6%)
74	o8	0.59	0/614	1.00	1/822 (0.1%)
75	O9	1.04	0/443	1.23	1/588 (0.2%)
75	o9	0.90	0/443	1.26	2/588 (0.3%)
76	Q0	0.93	0/423	1.13	2/562 (0.4%)
76	q0	1.15	0/423	1.24	1/562 (0.2%)
77	Q1	0.81	0/234	1.02	1/300 (0.3%)
77	q1	1.03	1/234 (0.4%)	1.15	0/300
78	Q2	1.02	1/860 (0.1%)	1.20	4/1136 (0.4%)
78	q2	0.94	1/860 (0.1%)	1.17	2/1136 (0.2%)
79	Q3	0.94	0/701	1.16	1/934 (0.1%)
79	q3	0.90	0/701	1.23	4/934 (0.4%)
80	e0	0.73	0/499	1.24	5/665 (0.8%)
81	e1	0.59	0/619	1.05	5/822 (0.6%)
83	p0	0.56	0/1092	1.00	2/1474 (0.1%)
All	All	0.71	45/430074 (0.0%)	0.92	893/631364 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	2
9	S7	0	1
9	s7	0	1
16	C4	0	1
16	c4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	2
22	d0	0	1
26	d4	0	1
27	D5	0	1
28	D6	0	2
33	E1	0	1
39	L2	0	1
39	l2	0	1
40	L3	0	1
41	L4	0	1
43	l6	0	1
44	l7	0	3
45	L8	0	2
48	m1	0	1
49	M3	0	1
50	M4	0	1
52	M6	0	2
52	m6	0	1
53	m7	0	1
59	n3	0	1
60	n4	0	1
64	N8	0	1
64	n8	0	1
65	N9	0	1
65	n9	0	1
67	O1	0	1
75	o9	0	1
79	q3	0	1
81	e1	0	1
All	All	0	43

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	M5	75	VAL	CA-CB	7.79	1.64	1.54
39	l2	213	GLY	C-O	7.78	1.34	1.23
49	m3	24	VAL	CA-CB	-7.62	1.45	1.54
78	Q2	17	CYS	CB-SG	7.52	2.06	1.81
41	L4	71	VAL	CA-CB	-7.43	1.47	1.55

The worst 5 of 893 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	N4	80	ARG	CA-C-N	18.37	142.81	119.84
60	N4	80	ARG	C-N-CA	18.37	142.81	119.84
41	L4	3	ARG	CA-C-N	13.02	136.11	119.84
41	L4	3	ARG	C-N-CA	13.02	136.11	119.84
15	c3	136	PRO	CA-C-N	12.42	135.37	119.84

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	124	ASP	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
9	S7	131	PHE	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	18757	854	0
1	6	38238	0	19240	811	0
2	S0	1577	0	1567	85	0
2	s0	1583	0	1578	85	0
3	S1	1709	0	1784	109	0
3	s1	1722	0	1793	64	0
4	S2	1635	0	1723	82	0
4	s2	1635	0	1723	62	0
5	S3	1734	0	1817	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	s3	1734	0	1817	61	0
6	S4	2068	0	2154	78	0
6	s4	2068	0	2154	103	0
7	S5	1609	0	1675	85	0
7	s5	1609	0	1675	89	0
8	S6	1799	0	1879	86	0
8	s6	1755	0	1845	70	0
9	S7	1481	0	1572	70	0
9	s7	1491	0	1578	49	0
10	S8	1489	0	1525	61	0
10	s8	1489	0	1525	64	0
11	S9	1494	0	1573	72	0
11	s9	1494	0	1573	69	0
12	C0	773	0	729	35	0
12	c0	762	0	699	24	0
13	C1	1214	0	1259	43	0
13	c1	1168	0	1231	40	0
14	C2	892	0	891	36	0
14	c2	892	0	891	30	0
15	C3	1192	0	1255	47	0
15	c3	1192	0	1255	55	0
16	C4	891	0	883	56	0
16	c4	949	0	985	55	0
17	C5	977	0	1002	52	0
17	c5	1039	0	1050	46	0
18	C6	1105	0	1166	66	0
18	c6	1111	0	1171	43	0
19	C7	926	0	930	45	0
19	c7	906	0	909	33	0
20	C8	1192	0	1222	63	0
20	c8	1192	0	1222	58	0
21	C9	1112	0	1124	50	0
21	c9	1112	0	1124	36	0
22	D0	855	0	917	54	0
22	d0	882	0	939	39	0
23	D1	684	0	672	30	0
23	d1	684	0	672	32	0
24	D2	1021	0	1060	47	0
24	d2	1021	0	1060	34	0
25	D3	1121	0	1196	54	0
25	d3	1121	0	1196	36	0
26	D4	1073	0	1132	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	d4	1073	0	1132	39	0
27	D5	563	0	603	20	0
27	d5	558	0	598	30	0
28	D6	769	0	814	58	0
28	d6	769	0	814	46	0
29	D7	610	0	631	15	0
29	d7	610	0	632	25	0
30	D8	497	0	535	17	0
30	d8	497	0	535	28	0
31	D9	442	0	428	18	0
31	d9	442	0	428	15	0
32	E0	475	0	525	20	0
33	E1	566	0	602	33	0
34	SR	2441	0	2397	104	0
34	sR	2442	0	2392	85	1
35	SM	1104	0	996	54	0
35	sM	680	0	607	39	0
36	1	67355	0	33846	1139	1
36	5	67376	0	33854	1162	0
37	3	2579	0	1304	49	0
37	7	2579	0	1303	47	0
38	4	3353	0	1695	67	0
38	8	3353	0	1695	68	0
39	L2	1914	0	1981	71	0
39	l2	1912	0	1976	76	0
40	L3	3075	0	3142	122	0
40	l3	3075	0	3142	140	0
41	L4	2748	0	2859	112	0
41	l4	2748	0	2859	116	0
42	L5	2375	0	2325	112	0
42	l5	2359	0	2311	98	0
43	L6	1239	0	1326	37	0
43	l6	1248	0	1339	41	0
44	L7	1784	0	1862	64	0
44	l7	1791	0	1869	58	0
45	L8	1804	0	1875	79	0
45	l8	1763	0	1817	85	0
46	L9	1518	0	1587	65	0
46	l9	1518	0	1587	51	0
47	M0	1705	0	1736	71	0
47	m0	1722	0	1755	73	0
48	M1	1353	0	1383	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	m1	1353	0	1383	40	0
49	M3	1543	0	1608	55	0
49	m3	1548	0	1613	75	0
50	M4	1053	0	1149	47	0
50	m4	1059	0	1154	38	0
51	M5	1720	0	1779	80	0
51	m5	1720	0	1779	67	0
52	M6	1555	0	1659	50	0
52	m6	1555	0	1659	61	0
53	M7	1420	0	1437	62	0
53	m7	1227	0	1236	54	0
54	M8	1441	0	1543	57	0
54	m8	1441	0	1543	57	0
55	M9	1521	0	1617	63	0
55	m9	1521	0	1617	52	0
56	N0	1445	0	1487	50	0
56	n0	1445	0	1487	47	0
57	N1	1276	0	1323	60	0
57	n1	1276	0	1323	48	0
58	N2	796	0	812	14	0
58	n2	778	0	791	15	0
59	N3	1003	0	1048	42	0
59	n3	1003	0	1048	30	0
60	N4	699	0	640	19	0
60	n4	1038	0	1071	32	0
61	N5	964	0	1025	31	0
61	n5	959	0	1023	44	0
62	N6	993	0	1081	35	0
62	n6	993	0	1081	46	0
63	N7	1092	0	1155	42	0
63	n7	1092	0	1155	39	0
64	N8	1173	0	1215	41	0
64	n8	1173	0	1215	61	0
65	N9	462	0	491	13	0
65	n9	462	0	491	24	0
66	O0	743	0	797	32	0
66	o0	767	0	816	30	0
67	O1	876	0	912	22	0
67	o1	883	0	918	36	0
68	O2	1020	0	1090	39	0
68	o2	1020	0	1090	41	0
69	O3	850	0	880	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	o3	850	0	880	29	0
70	O4	880	0	945	34	0
70	o4	880	0	945	30	0
71	O5	969	0	1078	33	0
71	o5	965	0	1067	47	0
72	O6	771	0	849	31	0
72	o6	770	0	846	33	0
73	O7	681	0	683	26	0
73	o7	681	0	683	24	0
74	O8	612	0	682	22	0
74	o8	608	0	671	22	0
75	O9	436	0	475	26	0
75	o9	436	0	475	25	0
76	Q0	417	0	455	11	0
76	q0	417	0	455	7	0
77	Q1	233	0	284	17	0
77	q1	233	0	284	12	0
78	Q2	847	0	916	31	0
78	q2	847	0	915	35	0
79	Q3	694	0	734	35	0
79	q3	694	0	734	20	0
80	e0	491	0	542	20	0
81	e1	608	0	655	28	0
82	m2	750	0	175	10	0
83	p0	1077	0	1041	29	0
84	p1	235	0	51	3	0
85	p2	230	0	54	2	0
86	1	474	0	0	0	0
86	2	124	0	0	0	0
86	3	14	0	0	0	0
86	4	23	0	0	0	0
86	5	507	0	0	0	0
86	6	145	0	0	0	0
86	7	15	0	0	0	0
86	8	12	0	0	0	0
86	D3	1	0	0	0	0
86	L2	1	0	0	0	0
86	L3	2	0	0	0	0
86	L4	1	0	0	0	0
86	L5	1	0	0	0	0
86	L7	2	0	0	0	0
86	L8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	M0	2	0	0	0	0
86	M1	1	0	0	0	0
86	M3	3	0	0	0	0
86	M5	2	0	0	0	0
86	M6	1	0	0	0	0
86	M7	5	0	0	0	0
86	M9	1	0	0	0	0
86	N0	1	0	0	0	0
86	N3	3	0	0	0	0
86	N5	1	0	0	0	0
86	N6	1	0	0	0	0
86	N8	4	0	0	0	0
86	O1	1	0	0	0	0
86	O4	1	0	0	0	0
86	O7	2	0	0	0	0
86	Q2	1	0	0	0	0
86	S2	2	0	0	0	0
86	S8	1	0	0	0	0
86	SM	1	0	0	0	0
86	c1	2	0	0	0	0
86	c7	2	0	0	0	0
86	c8	1	0	0	0	0
86	c9	1	0	0	0	0
86	d3	2	0	0	0	0
86	d4	1	0	0	0	0
86	d6	1	0	0	0	0
86	l2	2	0	0	0	0
86	l3	2	0	0	0	0
86	l4	1	0	0	0	0
86	l5	3	0	0	0	0
86	l7	1	0	0	0	0
86	m1	1	0	0	0	0
86	m5	4	0	0	0	0
86	m6	1	0	0	0	0
86	m7	5	0	0	0	0
86	n0	2	0	0	0	0
86	n3	2	0	0	0	0
86	n6	2	0	0	0	0
86	n8	4	0	0	0	0
86	n9	1	0	0	0	0
86	o1	2	0	0	0	0
86	o3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	o4	1	0	0	0	0
86	q0	1	0	0	0	0
86	q1	1	0	0	0	0
86	q3	1	0	0	0	0
86	s1	1	0	0	0	0
86	s8	2	0	0	0	0
86	sM	2	0	0	0	0
87	1	2450	0	0	243	0
87	2	1113	0	0	125	0
87	3	84	0	0	4	0
87	4	105	0	0	7	0
87	5	2499	0	0	244	0
87	6	1120	0	0	107	0
87	7	77	0	0	9	0
87	8	98	0	0	21	0
87	C3	7	0	0	0	0
87	C5	7	0	0	2	0
87	C8	7	0	0	0	0
87	D9	7	0	0	0	0
87	L3	14	0	0	1	0
87	L4	7	0	0	2	0
87	M0	7	0	0	0	0
87	M5	7	0	0	1	0
87	M6	7	0	0	0	0
87	M7	14	0	0	1	0
87	M8	7	0	0	0	0
87	M9	7	0	0	1	0
87	N9	7	0	0	0	0
87	O1	7	0	0	6	0
87	O2	7	0	0	0	0
87	O3	7	0	0	1	0
87	O7	7	0	0	6	0
87	Q2	7	0	0	1	0
87	S8	7	0	0	0	0
87	SR	7	0	0	0	0
87	c3	7	0	0	0	0
87	c5	7	0	0	1	0
87	c8	7	0	0	0	0
87	d4	7	0	0	1	0
87	d9	7	0	0	0	0
87	l3	14	0	0	0	0
87	l4	14	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	l5	21	0	0	1	0
87	l9	7	0	0	0	0
87	m0	14	0	0	1	0
87	m1	7	0	0	1	0
87	m4	7	0	0	0	0
87	m5	7	0	0	1	0
87	m6	7	0	0	0	0
87	m7	7	0	0	1	0
87	m8	7	0	0	0	0
87	n3	7	0	0	0	0
87	n9	7	0	0	0	0
87	o2	7	0	0	0	0
87	o3	7	0	0	0	0
87	o7	7	0	0	1	0
87	o9	7	0	0	1	0
87	q2	7	0	0	3	0
87	s1	14	0	0	1	0
87	s4	7	0	0	1	0
87	s8	7	0	0	1	0
87	sR	7	0	0	0	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	0	0
88	Q2	1	0	0	2	0
88	Q3	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
89	1	19	0	19	0	0
89	5	19	0	19	0	0
All	All	411204	0	297319	10160	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 15.

The worst 5 of 10160 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:SG	78:Q2:17:CYS:CB	2.06	1.44
78:Q2:17:CYS:CB	88:Q2:501:ZN:ZN	1.06	1.30
78:q2:17:CYS:SG	78:q2:77:CYS:HB3	1.80	1.21
78:Q2:17:CYS:SG	88:Q2:501:ZN:ZN	1.35	1.16
36:5:2273:G:O6	87:5:4206:OHX:N5	1.88	1.06

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)
36:1:3156:U:O4	34:sR:46:LYS:NZ[2_656]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	141 (69%)	40 (20%)	23 (11%)	0	1
2	s0	204/251 (81%)	156 (76%)	27 (13%)	21 (10%)	0	2
3	S1	212/254 (84%)	147 (69%)	38 (18%)	27 (13%)	0	1
3	s1	214/254 (84%)	179 (84%)	27 (13%)	8 (4%)	2	15
4	S2	215/253 (85%)	179 (83%)	22 (10%)	14 (6%)	1	5
4	s2	215/253 (85%)	178 (83%)	26 (12%)	11 (5%)	1	10
5	S3	221/239 (92%)	181 (82%)	32 (14%)	8 (4%)	2	16
5	s3	221/239 (92%)	185 (84%)	24 (11%)	12 (5%)	1	9
6	S4	258/260 (99%)	206 (80%)	33 (13%)	19 (7%)	1	4
6	s4	258/260 (99%)	209 (81%)	34 (13%)	15 (6%)	1	8
7	S5	204/224 (91%)	159 (78%)	27 (13%)	18 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	s5	204/224 (91%)	159 (78%)	32 (16%)	13 (6%)	1	6
8	S6	224/236 (95%)	198 (88%)	13 (6%)	13 (6%)	1	8
8	s6	216/236 (92%)	188 (87%)	21 (10%)	7 (3%)	3	18
9	S7	182/189 (96%)	134 (74%)	25 (14%)	23 (13%)	0	1
9	s7	184/189 (97%)	145 (79%)	27 (15%)	12 (6%)	1	5
10	S8	184/200 (92%)	149 (81%)	24 (13%)	11 (6%)	1	7
10	s8	184/200 (92%)	152 (83%)	22 (12%)	10 (5%)	1	9
11	S9	183/196 (93%)	152 (83%)	20 (11%)	11 (6%)	1	7
11	s9	183/196 (93%)	150 (82%)	27 (15%)	6 (3%)	3	17
12	C0	94/105 (90%)	74 (79%)	11 (12%)	9 (10%)	0	2
12	c0	92/105 (88%)	61 (66%)	12 (13%)	19 (21%)	0	0
13	C1	153/155 (99%)	120 (78%)	18 (12%)	15 (10%)	0	2
13	c1	144/155 (93%)	126 (88%)	14 (10%)	4 (3%)	4	21
14	C2	122/142 (86%)	69 (57%)	33 (27%)	20 (16%)	0	0
14	c2	122/142 (86%)	72 (59%)	35 (29%)	15 (12%)	0	1
15	C3	148/150 (99%)	123 (83%)	19 (13%)	6 (4%)	2	13
15	c3	148/150 (99%)	120 (81%)	17 (12%)	11 (7%)	1	4
16	C4	125/136 (92%)	96 (77%)	17 (14%)	12 (10%)	0	2
16	c4	126/136 (93%)	102 (81%)	17 (14%)	7 (6%)	1	8
17	C5	122/141 (86%)	96 (79%)	15 (12%)	11 (9%)	0	3
17	c5	133/141 (94%)	96 (72%)	20 (15%)	17 (13%)	0	1
18	C6	139/142 (98%)	115 (83%)	17 (12%)	7 (5%)	1	10
18	c6	140/142 (99%)	123 (88%)	9 (6%)	8 (6%)	1	8
19	C7	116/136 (85%)	88 (76%)	20 (17%)	8 (7%)	1	5
19	c7	113/136 (83%)	89 (79%)	19 (17%)	5 (4%)	2	12
20	C8	143/145 (99%)	114 (80%)	19 (13%)	10 (7%)	1	4
20	c8	143/145 (99%)	116 (81%)	18 (13%)	9 (6%)	1	6
21	C9	141/143 (99%)	114 (81%)	22 (16%)	5 (4%)	3	16
21	c9	141/143 (99%)	120 (85%)	16 (11%)	5 (4%)	3	16
22	D0	105/120 (88%)	83 (79%)	14 (13%)	8 (8%)	1	4
22	d0	108/120 (90%)	84 (78%)	13 (12%)	11 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	D1	85/87 (98%)	62 (73%)	18 (21%)	5 (6%)	1	7
23	d1	85/87 (98%)	71 (84%)	12 (14%)	2 (2%)	4	24
24	D2	127/129 (98%)	108 (85%)	17 (13%)	2 (2%)	7	34
24	d2	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	7	34
25	D3	142/144 (99%)	110 (78%)	17 (12%)	15 (11%)	0	2
25	d3	142/144 (99%)	120 (84%)	18 (13%)	4 (3%)	4	21
26	D4	132/134 (98%)	114 (86%)	8 (6%)	10 (8%)	1	4
26	d4	132/134 (98%)	104 (79%)	20 (15%)	8 (6%)	1	7
27	D5	68/107 (64%)	48 (71%)	13 (19%)	7 (10%)	0	2
27	d5	67/107 (63%)	46 (69%)	16 (24%)	5 (8%)	1	4
28	D6	95/97 (98%)	62 (65%)	14 (15%)	19 (20%)	0	0
28	d6	95/97 (98%)	73 (77%)	10 (10%)	12 (13%)	0	1
29	D7	79/81 (98%)	54 (68%)	17 (22%)	8 (10%)	0	2
29	d7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	2	15
30	D8	61/66 (92%)	49 (80%)	7 (12%)	5 (8%)	0	3
30	d8	61/66 (92%)	43 (70%)	12 (20%)	6 (10%)	0	2
31	D9	51/55 (93%)	42 (82%)	6 (12%)	3 (6%)	1	7
31	d9	51/55 (93%)	41 (80%)	6 (12%)	4 (8%)	1	4
32	E0	58/60 (97%)	46 (79%)	10 (17%)	2 (3%)	3	17
33	E1	69/76 (91%)	36 (52%)	14 (20%)	19 (28%)	0	0
34	SR	316/318 (99%)	248 (78%)	51 (16%)	17 (5%)	1	9
34	sR	316/318 (99%)	274 (87%)	30 (10%)	12 (4%)	2	15
35	SM	155/273 (57%)	111 (72%)	24 (16%)	20 (13%)	0	1
35	sM	98/273 (36%)	64 (65%)	20 (20%)	14 (14%)	0	1
39	L2	250/253 (99%)	224 (90%)	17 (7%)	9 (4%)	2	16
39	l2	250/253 (99%)	218 (87%)	21 (8%)	11 (4%)	2	12
40	L3	384/386 (100%)	346 (90%)	22 (6%)	16 (4%)	2	13
40	l3	384/386 (100%)	345 (90%)	30 (8%)	9 (2%)	5	25
41	L4	359/361 (99%)	312 (87%)	28 (8%)	19 (5%)	1	9
41	l4	359/361 (99%)	298 (83%)	44 (12%)	17 (5%)	2	11
42	L5	294/296 (99%)	252 (86%)	29 (10%)	13 (4%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	l5	292/296 (99%)	254 (87%)	26 (9%)	12 (4%)	2	13
43	L6	152/175 (87%)	132 (87%)	16 (10%)	4 (3%)	4	23
43	l6	153/175 (87%)	132 (86%)	16 (10%)	5 (3%)	3	17
44	L7	220/243 (90%)	196 (89%)	19 (9%)	5 (2%)	5	25
44	l7	221/243 (91%)	194 (88%)	22 (10%)	5 (2%)	5	25
45	L8	231/255 (91%)	188 (81%)	31 (13%)	12 (5%)	1	9
45	l8	229/255 (90%)	182 (80%)	31 (14%)	16 (7%)	1	4
46	L9	189/191 (99%)	162 (86%)	21 (11%)	6 (3%)	3	18
46	l9	189/191 (99%)	165 (87%)	19 (10%)	5 (3%)	4	23
47	M0	207/220 (94%)	179 (86%)	21 (10%)	7 (3%)	3	17
47	m0	209/220 (95%)	170 (81%)	22 (10%)	17 (8%)	1	3
48	M1	167/173 (96%)	133 (80%)	17 (10%)	17 (10%)	0	2
48	m1	167/173 (96%)	141 (84%)	17 (10%)	9 (5%)	1	9
49	M3	191/198 (96%)	160 (84%)	26 (14%)	5 (3%)	4	23
49	m3	192/198 (97%)	160 (83%)	20 (10%)	12 (6%)	1	6
50	M4	134/137 (98%)	113 (84%)	12 (9%)	9 (7%)	1	5
50	m4	135/137 (98%)	126 (93%)	6 (4%)	3 (2%)	5	26
51	M5	201/203 (99%)	183 (91%)	12 (6%)	6 (3%)	3	19
51	m5	201/203 (99%)	185 (92%)	10 (5%)	6 (3%)	3	19
52	M6	195/198 (98%)	175 (90%)	15 (8%)	5 (3%)	4	23
52	m6	195/198 (98%)	179 (92%)	9 (5%)	7 (4%)	2	16
53	M7	181/183 (99%)	156 (86%)	20 (11%)	5 (3%)	4	21
53	m7	153/183 (84%)	142 (93%)	10 (6%)	1 (1%)	18	53
54	M8	183/185 (99%)	161 (88%)	18 (10%)	4 (2%)	5	26
54	m8	183/185 (99%)	155 (85%)	21 (12%)	7 (4%)	2	15
55	M9	186/188 (99%)	166 (89%)	19 (10%)	1 (0%)	24	60
55	m9	186/188 (99%)	170 (91%)	13 (7%)	3 (2%)	7	34
56	N0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	10	40
56	n0	170/172 (99%)	158 (93%)	10 (6%)	2 (1%)	10	40
57	N1	157/159 (99%)	139 (88%)	11 (7%)	7 (4%)	2	12
57	n1	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	N2	98/120 (82%)	72 (74%)	19 (19%)	7 (7%)	1	4
58	n2	96/120 (80%)	81 (84%)	11 (12%)	4 (4%)	2	13
59	N3	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	8	35
59	n3	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
60	N4	96/155 (62%)	75 (78%)	12 (12%)	9 (9%)	0	2
60	n4	133/155 (86%)	105 (79%)	16 (12%)	12 (9%)	0	3
61	N5	119/141 (84%)	106 (89%)	12 (10%)	1 (1%)	16	50
61	n5	118/141 (84%)	101 (86%)	12 (10%)	5 (4%)	2	13
62	N6	124/126 (98%)	112 (90%)	6 (5%)	6 (5%)	2	11
62	n6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	2	14
63	N7	133/135 (98%)	112 (84%)	12 (9%)	9 (7%)	1	5
63	n7	133/135 (98%)	106 (80%)	19 (14%)	8 (6%)	1	7
64	N8	146/148 (99%)	119 (82%)	19 (13%)	8 (6%)	1	8
64	n8	146/148 (99%)	124 (85%)	15 (10%)	7 (5%)	2	11
65	N9	56/58 (97%)	48 (86%)	4 (7%)	4 (7%)	1	4
65	n9	56/58 (97%)	43 (77%)	6 (11%)	7 (12%)	0	1
66	O0	95/104 (91%)	86 (90%)	6 (6%)	3 (3%)	3	18
66	o0	98/104 (94%)	84 (86%)	11 (11%)	3 (3%)	3	19
67	O1	107/112 (96%)	96 (90%)	7 (6%)	4 (4%)	2	15
67	o1	107/112 (96%)	88 (82%)	7 (6%)	12 (11%)	0	1
68	O2	125/129 (97%)	110 (88%)	14 (11%)	1 (1%)	16	50
68	o2	125/129 (97%)	108 (86%)	12 (10%)	5 (4%)	2	14
69	O3	104/106 (98%)	96 (92%)	6 (6%)	2 (2%)	6	30
69	o3	104/106 (98%)	95 (91%)	7 (7%)	2 (2%)	6	30
70	O4	110/119 (92%)	95 (86%)	13 (12%)	2 (2%)	6	31
70	o4	110/119 (92%)	99 (90%)	10 (9%)	1 (1%)	14	48
71	O5	117/119 (98%)	106 (91%)	10 (8%)	1 (1%)	14	48
71	o5	117/119 (98%)	97 (83%)	11 (9%)	9 (8%)	1	4
72	O6	97/99 (98%)	80 (82%)	11 (11%)	6 (6%)	1	6
72	o6	97/99 (98%)	84 (87%)	9 (9%)	4 (4%)	2	13
73	O7	85/87 (98%)	73 (86%)	8 (9%)	4 (5%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	o7	85/87 (98%)	72 (85%)	12 (14%)	1 (1%)	10	40
74	O8	75/77 (97%)	66 (88%)	8 (11%)	1 (1%)	9	38
74	o8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	2	14
75	O9	48/50 (96%)	43 (90%)	4 (8%)	1 (2%)	5	27
75	o9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	5	27
76	Q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	2	14
76	q0	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	6	28
77	Q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	12
77	q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
78	Q2	103/105 (98%)	82 (80%)	18 (18%)	3 (3%)	3	20
78	q2	103/105 (98%)	93 (90%)	8 (8%)	2 (2%)	6	30
79	Q3	89/91 (98%)	77 (86%)	10 (11%)	2 (2%)	5	26
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	11	43
80	e0	60/62 (97%)	45 (75%)	8 (13%)	7 (12%)	0	1
81	e1	74/76 (97%)	36 (49%)	19 (26%)	19 (26%)	0	0
83	p0	139/311 (45%)	119 (86%)	16 (12%)	4 (3%)	3	20
All	All	22333/24141 (92%)	18606 (83%)	2512 (11%)	1215 (5%)	1	9

5 of 1215 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	66	ALA
2	S0	139	VAL
2	S0	140	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	134 (82%)	30 (18%)	2	9
2	s0	165/209 (79%)	129 (78%)	36 (22%)	1	6
3	S1	191/223 (86%)	156 (82%)	35 (18%)	2	9
3	s1	192/223 (86%)	147 (77%)	45 (23%)	1	4
4	S2	176/204 (86%)	136 (77%)	40 (23%)	1	5
4	s2	176/204 (86%)	121 (69%)	55 (31%)	0	1
5	S3	182/194 (94%)	136 (75%)	46 (25%)	0	3
5	s3	182/194 (94%)	150 (82%)	32 (18%)	2	10
6	S4	221/221 (100%)	180 (81%)	41 (19%)	1	9
6	s4	221/221 (100%)	174 (79%)	47 (21%)	1	6
7	S5	173/190 (91%)	146 (84%)	27 (16%)	2	13
7	s5	173/190 (91%)	131 (76%)	42 (24%)	1	4
8	S6	188/201 (94%)	150 (80%)	38 (20%)	1	7
8	s6	187/201 (93%)	147 (79%)	40 (21%)	1	6
9	S7	165/169 (98%)	132 (80%)	33 (20%)	1	7
9	s7	165/169 (98%)	138 (84%)	27 (16%)	2	12
10	S8	150/161 (93%)	125 (83%)	25 (17%)	2	12
10	s8	150/161 (93%)	128 (85%)	22 (15%)	3	15
11	S9	158/165 (96%)	124 (78%)	34 (22%)	1	6
11	s9	158/165 (96%)	124 (78%)	34 (22%)	1	6
12	C0	77/98 (79%)	65 (84%)	12 (16%)	2	13
12	c0	73/98 (74%)	62 (85%)	11 (15%)	3	14
13	C1	129/136 (95%)	102 (79%)	27 (21%)	1	7
13	c1	129/136 (95%)	107 (83%)	22 (17%)	2	11
14	C2	88/118 (75%)	66 (75%)	22 (25%)	0	3
14	c2	88/118 (75%)	64 (73%)	24 (27%)	0	2
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	7
15	c3	127/127 (100%)	101 (80%)	26 (20%)	1	7
16	C4	81/104 (78%)	53 (65%)	28 (35%)	0	1
16	c4	97/104 (93%)	79 (81%)	18 (19%)	1	9
17	C5	101/117 (86%)	84 (83%)	17 (17%)	2	11
17	c5	103/117 (88%)	83 (81%)	20 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C6	117/118 (99%)	84 (72%)	33 (28%)	0	2
18	c6	118/118 (100%)	93 (79%)	25 (21%)	1	6
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	7
19	c7	92/124 (74%)	67 (73%)	25 (27%)	0	2
20	C8	128/128 (100%)	101 (79%)	27 (21%)	1	6
20	c8	128/128 (100%)	100 (78%)	28 (22%)	1	5
21	C9	115/115 (100%)	87 (76%)	28 (24%)	1	4
21	c9	115/115 (100%)	93 (81%)	22 (19%)	1	8
22	D0	100/113 (88%)	69 (69%)	31 (31%)	0	1
22	d0	103/113 (91%)	76 (74%)	27 (26%)	0	3
23	D1	74/74 (100%)	51 (69%)	23 (31%)	0	1
23	d1	74/74 (100%)	57 (77%)	17 (23%)	1	5
24	D2	110/110 (100%)	83 (76%)	27 (24%)	1	4
24	d2	110/110 (100%)	99 (90%)	11 (10%)	7	29
25	D3	119/119 (100%)	93 (78%)	26 (22%)	1	6
25	d3	119/119 (100%)	96 (81%)	23 (19%)	1	8
26	D4	112/112 (100%)	91 (81%)	21 (19%)	1	9
26	d4	112/112 (100%)	90 (80%)	22 (20%)	1	8
27	D5	61/88 (69%)	44 (72%)	17 (28%)	0	2
27	d5	61/88 (69%)	47 (77%)	14 (23%)	1	5
28	D6	83/83 (100%)	68 (82%)	15 (18%)	2	9
28	d6	83/83 (100%)	70 (84%)	13 (16%)	2	13
29	D7	70/70 (100%)	57 (81%)	13 (19%)	1	9
29	d7	70/70 (100%)	58 (83%)	12 (17%)	2	11
30	D8	56/59 (95%)	40 (71%)	16 (29%)	0	2
30	d8	56/59 (95%)	41 (73%)	15 (27%)	0	2
31	D9	47/48 (98%)	40 (85%)	7 (15%)	3	15
31	d9	47/48 (98%)	39 (83%)	8 (17%)	2	11
32	E0	51/51 (100%)	39 (76%)	12 (24%)	1	4
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	4
34	SR	260/261 (100%)	227 (87%)	33 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	sR	260/261 (100%)	233 (90%)	27 (10%)	7	28
35	SM	97/228 (42%)	76 (78%)	21 (22%)	1	6
35	sM	54/228 (24%)	44 (82%)	10 (18%)	1	9
39	L2	193/195 (99%)	150 (78%)	43 (22%)	1	5
39	l2	192/195 (98%)	146 (76%)	46 (24%)	1	4
40	L3	321/322 (100%)	240 (75%)	81 (25%)	0	3
40	l3	320/322 (99%)	253 (79%)	67 (21%)	1	7
41	L4	288/288 (100%)	231 (80%)	57 (20%)	1	8
41	l4	288/288 (100%)	223 (77%)	65 (23%)	1	5
42	L5	244/244 (100%)	192 (79%)	52 (21%)	1	6
42	l5	243/244 (100%)	186 (76%)	57 (24%)	1	4
43	L6	134/152 (88%)	115 (86%)	19 (14%)	3	16
43	l6	135/152 (89%)	105 (78%)	30 (22%)	1	5
44	L7	186/204 (91%)	158 (85%)	28 (15%)	3	14
44	l7	187/204 (92%)	155 (83%)	32 (17%)	2	11
45	L8	187/207 (90%)	150 (80%)	37 (20%)	1	8
45	l8	177/207 (86%)	139 (78%)	38 (22%)	1	6
46	L9	171/171 (100%)	129 (75%)	42 (25%)	1	4
46	l9	171/171 (100%)	133 (78%)	38 (22%)	1	5
47	M0	177/186 (95%)	137 (77%)	40 (23%)	1	5
47	m0	179/186 (96%)	143 (80%)	36 (20%)	1	7
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1	6
48	m1	147/150 (98%)	112 (76%)	35 (24%)	1	4
49	M3	154/158 (98%)	121 (79%)	33 (21%)	1	6
49	m3	154/158 (98%)	132 (86%)	22 (14%)	3	16
50	M4	107/108 (99%)	84 (78%)	23 (22%)	1	6
50	m4	108/108 (100%)	88 (82%)	20 (18%)	1	9
51	M5	175/175 (100%)	141 (81%)	34 (19%)	1	8
51	m5	175/175 (100%)	144 (82%)	31 (18%)	2	10
52	M6	160/161 (99%)	129 (81%)	31 (19%)	1	8
52	m6	160/161 (99%)	121 (76%)	39 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	M7	140/145 (97%)	105 (75%)	35 (25%)	0	3
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	10
54	M8	150/150 (100%)	116 (77%)	34 (23%)	1	5
54	m8	150/150 (100%)	117 (78%)	33 (22%)	1	5
55	M9	153/153 (100%)	124 (81%)	29 (19%)	1	8
55	m9	153/153 (100%)	122 (80%)	31 (20%)	1	7
56	N0	156/156 (100%)	124 (80%)	32 (20%)	1	7
56	n0	156/156 (100%)	114 (73%)	42 (27%)	0	2
57	N1	136/136 (100%)	105 (77%)	31 (23%)	1	5
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	7
58	N2	87/106 (82%)	76 (87%)	11 (13%)	4	20
58	n2	85/106 (80%)	71 (84%)	14 (16%)	2	12
59	N3	104/104 (100%)	84 (81%)	20 (19%)	1	8
59	n3	104/104 (100%)	92 (88%)	12 (12%)	5	24
60	N4	57/129 (44%)	48 (84%)	9 (16%)	2	13
60	n4	100/129 (78%)	84 (84%)	16 (16%)	2	12
61	N5	104/117 (89%)	80 (77%)	24 (23%)	1	5
61	n5	104/117 (89%)	80 (77%)	24 (23%)	1	5
62	N6	109/109 (100%)	83 (76%)	26 (24%)	1	4
62	n6	109/109 (100%)	79 (72%)	30 (28%)	0	2
63	N7	115/115 (100%)	92 (80%)	23 (20%)	1	7
63	n7	115/115 (100%)	86 (75%)	29 (25%)	0	3
64	N8	118/118 (100%)	94 (80%)	24 (20%)	1	7
64	n8	118/118 (100%)	91 (77%)	27 (23%)	1	5
65	N9	46/46 (100%)	35 (76%)	11 (24%)	1	4
65	n9	46/46 (100%)	36 (78%)	10 (22%)	1	6
66	O0	81/87 (93%)	65 (80%)	16 (20%)	1	8
66	o0	84/87 (97%)	63 (75%)	21 (25%)	0	3
67	O1	92/96 (96%)	73 (79%)	19 (21%)	1	7
67	o1	94/96 (98%)	68 (72%)	26 (28%)	0	2
68	O2	109/110 (99%)	84 (77%)	25 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	o2	109/110 (99%)	84 (77%)	25 (23%)	1	5
69	O3	90/90 (100%)	74 (82%)	16 (18%)	2	10
69	o3	90/90 (100%)	73 (81%)	17 (19%)	1	9
70	O4	95/101 (94%)	74 (78%)	21 (22%)	1	5
70	o4	95/101 (94%)	72 (76%)	23 (24%)	1	4
71	O5	104/104 (100%)	77 (74%)	27 (26%)	0	3
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1	7
72	O6	81/81 (100%)	61 (75%)	20 (25%)	1	4
72	o6	80/81 (99%)	54 (68%)	26 (32%)	0	1
73	O7	70/70 (100%)	57 (81%)	13 (19%)	1	9
73	o7	70/70 (100%)	55 (79%)	15 (21%)	1	6
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	4
74	o8	67/68 (98%)	52 (78%)	15 (22%)	1	5
75	O9	45/45 (100%)	34 (76%)	11 (24%)	1	4
75	o9	45/45 (100%)	35 (78%)	10 (22%)	1	5
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1	6
76	q0	47/47 (100%)	35 (74%)	12 (26%)	0	3
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	q1	23/23 (100%)	12 (52%)	11 (48%)	0	0
78	Q2	90/90 (100%)	66 (73%)	24 (27%)	0	3
78	q2	90/90 (100%)	70 (78%)	20 (22%)	1	5
79	Q3	71/71 (100%)	52 (73%)	19 (27%)	0	2
79	q3	71/71 (100%)	60 (84%)	11 (16%)	2	13
80	e0	53/53 (100%)	36 (68%)	17 (32%)	0	1
81	e1	66/66 (100%)	50 (76%)	16 (24%)	1	4
83	p0	105/253 (42%)	85 (81%)	20 (19%)	1	8
All	All	18729/20239 (92%)	14778 (79%)	3951 (21%)	1	6

5 of 3951 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
72	O6	18	THR
60	n4	39	LEU

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Mol	Chain	Res	Type
9	s7	166	LEU
57	n1	135	PRO
70	o4	88	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 173 such sidechains are listed below:

Mol	Chain	Res	Type
81	e1	123	ASN
52	m6	26	GLN
35	sM	50	ASN
43	l6	28	GLN
57	n1	131	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	454 (25%)	52 (2%)
1	6	1792/1800 (99%)	448 (25%)	46 (2%)
36	1	3145/3396 (92%)	669 (21%)	86 (2%)
36	5	3145/3396 (92%)	645 (20%)	90 (2%)
37	3	120/121 (99%)	14 (11%)	2 (1%)
37	7	120/121 (99%)	23 (19%)	1 (0%)
38	4	157/158 (99%)	35 (22%)	5 (3%)
38	8	157/158 (99%)	35 (22%)	2 (1%)
All	All	10383/10950 (94%)	2323 (22%)	284 (2%)

5 of 2323 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	8	U
1	2	17	C
1	2	25	C

5 of 284 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	1560	G
36	5	1841	A

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Mol	Chain	Res	Type
36	5	2772	C
36	1	1841	A
36	1	1751	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2561 ligands modelled in this entry, 1426 are monoatomic - leaving 1135 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	$\# Z > 2$
87	OHX	1	4011	-	0,6,6	-	-	-		
87	OHX	1	3874	-	0,6,6	-	-	-		
87	OHX	5	4227	-	0,6,6	-	-	-		
87	OHX	5	4114	-	0,6,6	-	-	-		
87	OHX	1	3989	-	0,6,6	-	-	-		
87	OHX	5	4191	-	0,6,6	-	-	-		
87	OHX	1	4217	-	0,6,6	-	-	-		
87	OHX	2	2166	-	0,6,6	-	-	-		
87	OHX	5	3978	-	0,6,6	-	-	-		
87	OHX	5	4041	-	0,6,6	-	-	-		
87	OHX	5	4187	-	0,6,6	-	-	-		
87	OHX	6	2085	-	0,6,6	-	-	-		
87	OHX	6	2075	-	0,6,6	-	-	-		
87	OHX	6	2104	-	0,6,6	-	-	-		
87	OHX	1	4089	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	M8	201	-	0,6,6	-	-	-		
87	OHX	5	3953	-	0,6,6	-	-	-		
87	OHX	1	4034	-	0,6,6	-	-	-		
87	OHX	1	4096	-	0,6,6	-	-	-		
87	OHX	5	4049	-	0,6,6	-	-	-		
87	OHX	6	2096	-	0,6,6	-	-	-		
87	OHX	1	4008	-	0,6,6	-	-	-		
87	OHX	5	3993	-	0,6,6	-	-	-		
87	OHX	1	4006	-	0,6,6	-	-	-		
87	OHX	2	2115	-	0,6,6	-	-	-		
87	OHX	5	3960	-	0,6,6	-	-	-		
87	OHX	5	4018	-	0,6,6	-	-	-		
87	OHX	2	2106	-	0,6,6	-	-	-		
87	OHX	5	4203	-	0,6,6	-	-	-		
87	OHX	1	3919	-	0,6,6	-	-	-		
87	OHX	1	3947	-	0,6,6	-	-	-		
87	OHX	2	2158	-	0,6,6	-	-	-		
87	OHX	2	2133	-	0,6,6	-	-	-		
87	OHX	1	4086	-	0,6,6	-	-	-		
87	OHX	1	4148	-	0,6,6	-	-	-		
87	OHX	5	4152	-	0,6,6	-	-	-		
87	OHX	7	222	-	0,6,6	-	-	-		
87	OHX	1	3995	-	0,6,6	-	-	-		
87	OHX	2	2095	-	0,6,6	-	-	-		
87	OHX	6	2199	-	0,6,6	-	-	-		
87	OHX	1	3946	-	0,6,6	-	-	-		
87	OHX	5	3963	-	0,6,6	-	-	-		
87	OHX	2	2153	-	0,6,6	-	-	-		
87	OHX	2	2061	-	0,6,6	-	-	-		
87	OHX	2	2113	-	0,6,6	-	-	-		
87	OHX	1	4118	-	0,6,6	-	-	-		
87	OHX	5	4219	-	0,6,6	-	-	-		
87	OHX	1	4021	-	0,6,6	-	-	-		
87	OHX	c5	201	-	0,6,6	-	-	-		
87	OHX	1	4150	-	0,6,6	-	-	-		
87	OHX	5	3990	-	0,6,6	-	-	-		
87	OHX	5	4222	-	0,6,6	-	-	-		
87	OHX	5	4040	-	0,6,6	-	-	-		
87	OHX	15	305	-	0,6,6	-	-	-		
87	OHX	6	2155	-	0,6,6	-	-	-		
87	OHX	5	3944	-	0,6,6	-	-	-		
87	OHX	6	2135	-	0,6,6	-	-	-		
87	OHX	5	4170	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4200	-	0,6,6	-	-	-		
87	OHX	2	2088	-	0,6,6	-	-	-		
87	OHX	1	4080	-	0,6,6	-	-	-		
87	OHX	5	4091	-	0,6,6	-	-	-		
87	OHX	5	3989	-	0,6,6	-	-	-		
87	OHX	5	4028	-	0,6,6	-	-	-		
87	OHX	2	2108	-	0,6,6	-	-	-		
87	OHX	1	4003	-	0,6,6	-	-	-		
87	OHX	M5	303	-	0,6,6	-	-	-		
87	OHX	6	2060	-	0,6,6	-	-	-		
87	OHX	1	4068	-	0,6,6	-	-	-		
87	OHX	1	4162	-	0,6,6	-	-	-		
87	OHX	1	4126	-	0,6,6	-	-	-		
87	OHX	1	4155	-	0,6,6	-	-	-		
87	OHX	8	214	-	0,6,6	-	-	-		
87	OHX	1	4179	-	0,6,6	-	-	-		
87	OHX	5	4081	-	0,6,6	-	-	-		
87	OHX	2	2143	-	0,6,6	-	-	-		
87	OHX	6	2152	-	0,6,6	-	-	-		
87	OHX	1	4024	-	0,6,6	-	-	-		
87	OHX	L3	403	-	0,6,6	-	-	-		
87	OHX	1	4174	-	0,6,6	-	-	-		
87	OHX	2	2025	-	0,6,6	-	-	-		
87	OHX	6	2173	-	0,6,6	-	-	-		
87	OHX	1	3901	-	0,6,6	-	-	-		
87	OHX	5	4197	-	0,6,6	-	-	-		
87	OHX	2	2177	-	0,6,6	-	-	-		
87	OHX	5	3958	-	0,6,6	-	-	-		
87	OHX	5	4254	-	0,6,6	-	-	-		
87	OHX	8	222	-	0,6,6	-	-	-		
87	OHX	1	4170	-	0,6,6	-	-	-		
87	OHX	5	4086	-	0,6,6	-	-	-		
87	OHX	5	4046	-	0,6,6	-	-	-		
87	OHX	1	4193	-	0,6,6	-	-	-		
87	OHX	1	4028	-	0,6,6	-	-	-		
87	OHX	5	4016	-	0,6,6	-	-	-		
87	OHX	5	4259	-	0,6,6	-	-	-		
87	OHX	6	2168	-	0,6,6	-	-	-		
87	OHX	5	4090	-	0,6,6	-	-	-		
87	OHX	5	4163	-	0,6,6	-	-	-		
87	OHX	5	4093	-	0,6,6	-	-	-		
87	OHX	1	4119	-	0,6,6	-	-	-		
87	OHX	1	4164	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2129	-	0,6,6	-	-	-		
87	OHX	6	2121	-	0,6,6	-	-	-		
87	OHX	5	4063	-	0,6,6	-	-	-		
87	OHX	1	4026	-	0,6,6	-	-	-		
87	OHX	5	4079	-	0,6,6	-	-	-		
87	OHX	1	4196	-	0,6,6	-	-	-		
87	OHX	o3	202	-	0,6,6	-	-	-		
87	OHX	8	221	-	0,6,6	-	-	-		
87	OHX	5	4143	-	0,6,6	-	-	-		
87	OHX	5	4166	-	0,6,6	-	-	-		
87	OHX	5	3907	-	0,6,6	-	-	-		
87	OHX	6	2181	-	0,6,6	-	-	-		
87	OHX	1	4009	-	0,6,6	-	-	-		
87	OHX	1	3897	-	0,6,6	-	-	-		
87	OHX	6	2150	-	0,6,6	-	-	-		
87	OHX	1	4084	-	0,6,6	-	-	-		
87	OHX	1	4077	-	0,6,6	-	-	-		
87	OHX	5	4137	-	0,6,6	-	-	-		
87	OHX	1	4005	-	0,6,6	-	-	-		
87	OHX	1	4139	-	0,6,6	-	-	-		
87	OHX	5	4119	-	0,6,6	-	-	-		
87	OHX	1	4038	-	0,6,6	-	-	-		
87	OHX	2	2073	-	0,6,6	-	-	-		
87	OHX	7	225	-	0,6,6	-	-	-		
87	OHX	5	4059	-	0,6,6	-	-	-		
87	OHX	1	4123	-	0,6,6	-	-	-		
87	OHX	5	4146	-	0,6,6	-	-	-		
87	OHX	2	2135	-	0,6,6	-	-	-		
87	OHX	1	3903	-	0,6,6	-	-	-		
87	OHX	1	4085	-	0,6,6	-	-	-		
89	ANM	1	4218	-	20,20,20	0.90	0	24,27,27	1.47	4 (16%)
87	OHX	1	4007	-	0,6,6	-	-	-		
87	OHX	6	2141	-	0,6,6	-	-	-		
87	OHX	1	3916	-	0,6,6	-	-	-		
87	OHX	7	219	-	0,6,6	-	-	-		
87	OHX	1	4102	-	0,6,6	-	-	-		
87	OHX	2	2150	-	0,6,6	-	-	-		
87	OHX	5	4084	-	0,6,6	-	-	-		
87	OHX	2	2112	-	0,6,6	-	-	-		
87	OHX	1	4182	-	0,6,6	-	-	-		
87	OHX	m4	201	-	0,6,6	-	-	-		
87	OHX	1	4171	-	0,6,6	-	-	-		
87	OHX	2	2118	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4020	-	0,6,6	-	-	-		
87	OHX	5	3955	-	0,6,6	-	-	-		
87	OHX	1	4144	-	0,6,6	-	-	-		
87	OHX	5	3916	-	0,6,6	-	-	-		
87	OHX	2	2152	-	0,6,6	-	-	-		
87	OHX	1	3923	-	0,6,6	-	-	-		
87	OHX	6	2095	-	0,6,6	-	-	-		
87	OHX	6	2055	-	0,6,6	-	-	-		
87	OHX	5	4025	-	0,6,6	-	-	-		
87	OHX	1	3872	-	0,6,6	-	-	-		
87	OHX	5	3947	87	0,6,6	-	-	-		
87	OHX	4	227	-	0,6,6	-	-	-		
87	OHX	1	3996	-	0,6,6	-	-	-		
87	OHX	5	4156	-	0,6,6	-	-	-		
87	OHX	1	4146	-	0,6,6	-	-	-		
87	OHX	1	3956	-	0,6,6	-	-	-		
87	OHX	1	4201	-	0,6,6	-	-	-		
87	OHX	1	4169	-	0,6,6	-	-	-		
87	OHX	4	235	-	0,6,6	-	-	-		
87	OHX	1	3896	-	0,6,6	-	-	-		
87	OHX	5	4026	-	0,6,6	-	-	-		
87	OHX	2	2083	-	0,6,6	-	-	-		
87	OHX	2	2089	-	0,6,6	-	-	-		
87	OHX	2	2104	-	0,6,6	-	-	-		
87	OHX	6	2142	-	0,6,6	-	-	-		
87	OHX	6	2188	-	0,6,6	-	-	-		
87	OHX	5	4094	-	0,6,6	-	-	-		
87	OHX	6	2049	-	0,6,6	-	-	-		
87	OHX	5	4066	-	0,6,6	-	-	-		
87	OHX	2	2142	-	0,6,6	-	-	-		
87	OHX	Q2	503	-	0,6,6	-	-	-		
87	OHX	1	3969	-	0,6,6	-	-	-		
87	OHX	5	4215	-	0,6,6	-	-	-		
87	OHX	5	4009	-	0,6,6	-	-	-		
87	OHX	5	4118	-	0,6,6	-	-	-		
87	OHX	5	4150	-	0,6,6	-	-	-		
87	OHX	8	223	-	0,6,6	-	-	-		
87	OHX	5	4250	-	0,6,6	-	-	-		
87	OHX	5	4139	-	0,6,6	-	-	-		
87	OHX	2	2167	-	0,6,6	-	-	-		
87	OHX	5	4058	-	0,6,6	-	-	-		
87	OHX	1	3928	-	0,6,6	-	-	-		
87	OHX	2	2175	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3970	-	0,6,6	-	-	-		
87	OHX	sR	401	-	0,6,6	-	-	-		
87	OHX	5	4209	-	0,6,6	-	-	-		
87	OHX	2	2078	-	0,6,6	-	-	-		
87	OHX	5	3924	-	0,6,6	-	-	-		
87	OHX	6	2094	-	0,6,6	-	-	-		
87	OHX	6	2097	-	0,6,6	-	-	-		
87	OHX	6	2099	-	0,6,6	-	-	-		
87	OHX	5	3930	-	0,6,6	-	-	-		
87	OHX	1	3922	-	0,6,6	-	-	-		
87	OHX	6	2180	-	0,6,6	-	-	-		
87	OHX	2	2130	-	0,6,6	-	-	-		
87	OHX	2	2053	-	0,6,6	-	-	-		
87	OHX	1	3887	-	0,6,6	-	-	-		
87	OHX	1	4064	-	0,6,6	-	-	-		
87	OHX	5	4023	-	0,6,6	-	-	-		
87	OHX	6	2193	-	0,6,6	-	-	-		
87	OHX	2	2180	-	0,6,6	-	-	-		
87	OHX	6	2120	-	0,6,6	-	-	-		
87	OHX	SR	401	-	0,6,6	-	-	-		
87	OHX	5	4196	-	0,6,6	-	-	-		
87	OHX	5	4003	-	0,6,6	-	-	-		
87	OHX	1	3951	-	0,6,6	-	-	-		
87	OHX	1	3929	-	0,6,6	-	-	-		
87	OHX	6	2187	-	0,6,6	-	-	-		
87	OHX	6	2192	-	0,6,6	-	-	-		
87	OHX	6	2138	-	0,6,6	-	-	-		
87	OHX	5	3998	-	0,6,6	-	-	-		
87	OHX	5	4179	-	0,6,6	-	-	-		
87	OHX	2	2051	-	0,6,6	-	-	-		
87	OHX	14	402	-	0,6,6	-	-	-		
87	OHX	5	4024	-	0,6,6	-	-	-		
87	OHX	5	4190	-	0,6,6	-	-	-		
87	OHX	7	218	-	0,6,6	-	-	-		
87	OHX	2	2163	-	0,6,6	-	-	-		
87	OHX	2	2120	-	0,6,6	-	-	-		
87	OHX	1	4058	-	0,6,6	-	-	-		
87	OHX	5	3923	-	0,6,6	-	-	-		
87	OHX	5	4205	-	0,6,6	-	-	-		
87	OHX	1	4209	-	0,6,6	-	-	-		
87	OHX	6	2136	-	0,6,6	-	-	-		
87	OHX	6	2090	-	0,6,6	-	-	-		
87	OHX	1	3924	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3942	-	0,6,6	-	-	-		
87	OHX	2	2060	-	0,6,6	-	-	-		
87	OHX	4	226	-	0,6,6	-	-	-		
87	OHX	1	4101	-	0,6,6	-	-	-		
87	OHX	6	2064	-	0,6,6	-	-	-		
87	OHX	3	220	-	0,6,6	-	-	-		
87	OHX	1	3985	-	0,6,6	-	-	-		
87	OHX	5	3956	-	0,6,6	-	-	-		
87	OHX	6	2153	-	0,6,6	-	-	-		
87	OHX	1	3945	-	0,6,6	-	-	-		
87	OHX	1	3991	-	0,6,6	-	-	-		
87	OHX	5	4233	-	0,6,6	-	-	-		
87	OHX	5	4164	-	0,6,6	-	-	-		
87	OHX	1	4167	-	0,6,6	-	-	-		
87	OHX	1	4120	-	0,6,6	-	-	-		
87	OHX	5	3969	-	0,6,6	-	-	-		
87	OHX	6	2147	-	0,6,6	-	-	-		
87	OHX	2	2040	-	0,6,6	-	-	-		
87	OHX	1	3870	-	0,6,6	-	-	-		
87	OHX	6	2114	-	0,6,6	-	-	-		
87	OHX	5	3906	-	0,6,6	-	-	-		
87	OHX	1	3972	-	0,6,6	-	-	-		
87	OHX	1	3881	-	0,6,6	-	-	-		
87	OHX	1	4062	-	0,6,6	-	-	-		
87	OHX	5	4245	-	0,6,6	-	-	-		
87	OHX	1	4050	-	0,6,6	-	-	-		
87	OHX	1	4165	-	0,6,6	-	-	-		
87	OHX	1	4191	-	0,6,6	-	-	-		
87	OHX	8	219	-	0,6,6	-	-	-		
87	OHX	15	304	-	0,6,6	-	-	-		
87	OHX	1	3890	-	0,6,6	-	-	-		
87	OHX	1	4205	-	0,6,6	-	-	-		
87	OHX	1	3871	-	0,6,6	-	-	-		
87	OHX	5	4075	-	0,6,6	-	-	-		
87	OHX	5	4038	-	0,6,6	-	-	-		
87	OHX	4	229	-	0,6,6	-	-	-		
87	OHX	6	2101	-	0,6,6	-	-	-		
87	OHX	s4	301	-	0,6,6	-	-	-		
87	OHX	o7	502	-	0,6,6	-	-	-		
87	OHX	5	3938	-	0,6,6	-	-	-		
87	OHX	5	4056	-	0,6,6	-	-	-		
87	OHX	5	4123	-	0,6,6	-	-	-		
87	OHX	5	3903	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4085	-	0,6,6	-	-	-		
87	OHX	5	4007	-	0,6,6	-	-	-		
87	OHX	6	2158	-	0,6,6	-	-	-		
87	OHX	1	4188	-	0,6,6	-	-	-		
87	OHX	5	4178	-	0,6,6	-	-	-		
87	OHX	6	2184	-	0,6,6	-	-	-		
87	OHX	5	4181	-	0,6,6	-	-	-		
87	OHX	1	3958	-	0,6,6	-	-	-		
87	OHX	5	4188	-	0,6,6	-	-	-		
87	OHX	6	2144	-	0,6,6	-	-	-		
87	OHX	O7	104	-	0,6,6	-	-	-		
87	OHX	1	4199	-	0,6,6	-	-	-		
87	OHX	6	2183	-	0,6,6	-	-	-		
87	OHX	6	2050	-	0,6,6	-	-	-		
87	OHX	6	2201	-	0,6,6	-	-	-		
87	OHX	1	3869	-	0,6,6	-	-	-		
87	OHX	6	2174	-	0,6,6	-	-	-		
87	OHX	5	4171	-	0,6,6	-	-	-		
87	OHX	6	2112	-	0,6,6	-	-	-		
87	OHX	6	2113	-	0,6,6	-	-	-		
87	OHX	5	4020	-	0,6,6	-	-	-		
87	OHX	1	4198	-	0,6,6	-	-	-		
87	OHX	1	4093	-	0,6,6	-	-	-		
87	OHX	1	4142	-	0,6,6	-	-	-		
87	OHX	5	4144	-	0,6,6	-	-	-		
87	OHX	5	4217	-	0,6,6	-	-	-		
87	OHX	15	306	-	0,6,6	-	-	-		
87	OHX	6	2110	-	0,6,6	-	-	-		
87	OHX	5	4121	-	0,6,6	-	-	-		
87	OHX	6	2109	-	0,6,6	-	-	-		
87	OHX	5	4070	-	0,6,6	-	-	-		
87	OHX	1	4140	-	0,6,6	-	-	-		
87	OHX	5	4101	-	0,6,6	-	-	-		
87	OHX	2	2048	-	0,6,6	-	-	-		
87	OHX	1	4046	-	0,6,6	-	-	-		
87	OHX	1	4014	-	0,6,6	-	-	-		
87	OHX	5	4185	-	0,6,6	-	-	-		
87	OHX	6	2102	-	0,6,6	-	-	-		
87	OHX	5	4161	-	0,6,6	-	-	-		
87	OHX	5	3996	-	0,6,6	-	-	-		
87	OHX	5	4244	-	0,6,6	-	-	-		
87	OHX	13	403	-	0,6,6	-	-	-		
87	OHX	5	3945	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2090	-	0,6,6	-	-	-		
87	OHX	5	4201	-	0,6,6	-	-	-		
87	OHX	6	2059	-	0,6,6	-	-	-		
87	OHX	1	4178	-	0,6,6	-	-	-		
87	OHX	5	3981	-	0,6,6	-	-	-		
87	OHX	5	4120	-	0,6,6	-	-	-		
87	OHX	1	3966	-	0,6,6	-	-	-		
87	OHX	1	3968	-	0,6,6	-	-	-		
87	OHX	1	4031	-	0,6,6	-	-	-		
87	OHX	5	4232	-	0,6,6	-	-	-		
87	OHX	c8	202	-	0,6,6	-	-	-		
87	OHX	o2	201	-	0,6,6	-	-	-		
87	OHX	2	2029	-	0,6,6	-	-	-		
87	OHX	2	2087	-	0,6,6	-	-	-		
87	OHX	1	3911	-	0,6,6	-	-	-		
87	OHX	5	3995	-	0,6,6	-	-	-		
87	OHX	S8	302	-	0,6,6	-	-	-		
87	OHX	1	4112	-	0,6,6	-	-	-		
87	OHX	6	2107	-	0,6,6	-	-	-		
87	OHX	1	3977	-	0,6,6	-	-	-		
87	OHX	2	2147	-	0,6,6	-	-	-		
87	OHX	1	4213	-	0,6,6	-	-	-		
87	OHX	2	2114	-	0,6,6	-	-	-		
87	OHX	2	2151	-	0,6,6	-	-	-		
87	OHX	5	3970	-	0,6,6	-	-	-		
87	OHX	2	2026	-	0,6,6	-	-	-		
87	OHX	m8	201	-	0,6,6	-	-	-		
87	OHX	1	4023	-	0,6,6	-	-	-		
87	OHX	1	4210	-	0,6,6	-	-	-		
87	OHX	5	4102	-	0,6,6	-	-	-		
87	OHX	6	2077	-	0,6,6	-	-	-		
87	OHX	6	2140	-	0,6,6	-	-	-		
87	OHX	1	3912	-	0,6,6	-	-	-		
87	OHX	1	3955	-	0,6,6	-	-	-		
87	OHX	1	4161	-	0,6,6	-	-	-		
87	OHX	5	4064	-	0,6,6	-	-	-		
87	OHX	5	4240	-	0,6,6	-	-	-		
87	OHX	5	4019	-	0,6,6	-	-	-		
87	OHX	5	4199	-	0,6,6	-	-	-		
87	OHX	1	3933	-	0,6,6	-	-	-		
87	OHX	5	3951	-	0,6,6	-	-	-		
87	OHX	5	3929	-	0,6,6	-	-	-		
87	OHX	5	4216	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4044	-	0,6,6	-	-	-		
87	OHX	5	3943	-	0,6,6	-	-	-		
87	OHX	1	4095	-	0,6,6	-	-	-		
87	OHX	1	4176	-	0,6,6	-	-	-		
87	OHX	2	2071	-	0,6,6	-	-	-		
87	OHX	1	3882	-	0,6,6	-	-	-		
87	OHX	1	4157	-	0,6,6	-	-	-		
87	OHX	1	3917	-	0,6,6	-	-	-		
87	OHX	6	2149	-	0,6,6	-	-	-		
87	OHX	5	4198	-	0,6,6	-	-	-		
87	OHX	1	4061	-	0,6,6	-	-	-		
87	OHX	6	2191	-	0,6,6	-	-	-		
87	OHX	6	2091	-	0,6,6	-	-	-		
87	OHX	5	4257	-	0,6,6	-	-	-		
87	OHX	2	2091	-	0,6,6	-	-	-		
87	OHX	5	4125	-	0,6,6	-	-	-		
87	OHX	2	2125	-	0,6,6	-	-	-		
87	OHX	5	3987	-	0,6,6	-	-	-		
87	OHX	6	2087	-	0,6,6	-	-	-		
87	OHX	5	4095	-	0,6,6	-	-	-		
87	OHX	2	2109	-	0,6,6	-	-	-		
87	OHX	1	3957	-	0,6,6	-	-	-		
87	OHX	1	3905	-	0,6,6	-	-	-		
87	OHX	5	4017	-	0,6,6	-	-	-		
87	OHX	5	4089	-	0,6,6	-	-	-		
87	OHX	6	2052	-	0,6,6	-	-	-		
87	OHX	5	3991	-	0,6,6	-	-	-		
87	OHX	m6	202	-	0,6,6	-	-	-		
87	OHX	1	3976	-	0,6,6	-	-	-		
87	OHX	1	4013	-	0,6,6	-	-	-		
87	OHX	6	2056	-	0,6,6	-	-	-		
87	OHX	6	2084	-	0,6,6	-	-	-		
87	OHX	1	4145	-	0,6,6	-	-	-		
87	OHX	5	4230	-	0,6,6	-	-	-		
87	OHX	1	3884	-	0,6,6	-	-	-		
87	OHX	1	3910	-	0,6,6	-	-	-		
87	OHX	5	4062	-	0,6,6	-	-	-		
87	OHX	5	4165	-	0,6,6	-	-	-		
87	OHX	5	4110	-	0,6,6	-	-	-		
87	OHX	O1	202	-	0,6,6	-	-	-		
87	OHX	6	2130	-	0,6,6	-	-	-		
87	OHX	c3	201	-	0,6,6	-	-	-		
87	OHX	1	4134	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	7	220	-	0,6,6	-	-	-		
87	OHX	1	4027	-	0,6,6	-	-	-		
87	OHX	1	4136	-	0,6,6	-	-	-		
87	OHX	6	2203	-	0,6,6	-	-	-		
87	OHX	2	2058	-	0,6,6	-	-	-		
87	OHX	1	3937	-	0,6,6	-	-	-		
87	OHX	6	2068	-	0,6,6	-	-	-		
87	OHX	6	2133	-	0,6,6	-	-	-		
87	OHX	1	4083	-	0,6,6	-	-	-		
87	OHX	1	4138	-	0,6,6	-	-	-		
87	OHX	2	2161	-	0,6,6	-	-	-		
87	OHX	5	4126	-	0,6,6	-	-	-		
87	OHX	5	4231	-	0,6,6	-	-	-		
87	OHX	6	2105	-	0,6,6	-	-	-		
87	OHX	6	2179	-	0,6,6	-	-	-		
87	OHX	5	4176	-	0,6,6	-	-	-		
87	OHX	5	4157	-	0,6,6	-	-	-		
87	OHX	6	2074	-	0,6,6	-	-	-		
87	OHX	1	4025	-	0,6,6	-	-	-		
87	OHX	C8	201	-	0,6,6	-	-	-		
87	OHX	2	2145	-	0,6,6	-	-	-		
87	OHX	1	4130	-	0,6,6	-	-	-		
87	OHX	m1	202	-	0,6,6	-	-	-		
87	OHX	5	3984	-	0,6,6	-	-	-		
87	OHX	6	2137	-	0,6,6	-	-	-		
87	OHX	8	215	-	0,6,6	-	-	-		
87	OHX	D9	102	-	0,6,6	-	-	-		
87	OHX	6	2098	-	0,6,6	-	-	-		
87	OHX	5	4142	-	0,6,6	-	-	-		
87	OHX	5	3946	-	0,6,6	-	-	-		
87	OHX	5	3940	-	0,6,6	-	-	-		
87	OHX	1	3873	-	0,6,6	-	-	-		
87	OHX	2	2137	-	0,6,6	-	-	-		
87	OHX	2	2099	-	0,6,6	-	-	-		
87	OHX	5	3918	-	0,6,6	-	-	-		
87	OHX	8	226	-	0,6,6	-	-	-		
87	OHX	n3	203	-	0,6,6	-	-	-		
87	OHX	6	2198	-	0,6,6	-	-	-		
87	OHX	5	4140	-	0,6,6	-	-	-		
87	OHX	1	3920	-	0,6,6	-	-	-		
87	OHX	1	4147	-	0,6,6	-	-	-		
87	OHX	5	4223	-	0,6,6	-	-	-		
87	OHX	5	4014	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2075	-	0,6,6	-	-	-		
87	OHX	6	2057	-	0,6,6	-	-	-		
87	OHX	8	218	-	0,6,6	-	-	-		
87	OHX	7	223	-	0,6,6	-	-	-		
87	OHX	6	2048	-	0,6,6	-	-	-		
87	OHX	7	217	-	0,6,6	-	-	-		
87	OHX	1	4075	-	0,6,6	-	-	-		
87	OHX	5	3966	-	0,6,6	-	-	-		
87	OHX	5	4204	-	0,6,6	-	-	-		
87	OHX	5	4031	-	0,6,6	-	-	-		
87	OHX	5	4154	-	0,6,6	-	-	-		
87	OHX	2	2067	-	0,6,6	-	-	-		
87	OHX	2	2070	-	0,6,6	-	-	-		
87	OHX	5	3920	-	0,6,6	-	-	-		
87	OHX	1	3936	-	0,6,6	-	-	-		
87	OHX	1	4133	-	0,6,6	-	-	-		
87	OHX	5	3911	-	0,6,6	-	-	-		
87	OHX	5	3931	-	0,6,6	-	-	-		
87	OHX	5	4112	-	0,6,6	-	-	-		
87	OHX	2	2033	-	0,6,6	-	-	-		
87	OHX	s1	302	-	0,6,6	-	-	-		
87	OHX	5	4184	-	0,6,6	-	-	-		
87	OHX	1	4039	-	0,6,6	-	-	-		
87	OHX	1	3921	-	0,6,6	-	-	-		
87	OHX	4	238	-	0,6,6	-	-	-		
87	OHX	5	4213	-	0,6,6	-	-	-		
87	OHX	L4	402	-	0,6,6	-	-	-		
87	OHX	6	2063	-	0,6,6	-	-	-		
87	OHX	1	3940	-	0,6,6	-	-	-		
87	OHX	6	2157	-	0,6,6	-	-	-		
87	OHX	1	3900	-	0,6,6	-	-	-		
87	OHX	2	2064	-	0,6,6	-	-	-		
87	OHX	6	2166	-	0,6,6	-	-	-		
87	OHX	6	2159	-	0,6,6	-	-	-		
87	OHX	5	4210	-	0,6,6	-	-	-		
87	OHX	2	2110	-	0,6,6	-	-	-		
87	OHX	1	3868	-	0,6,6	-	-	-		
87	OHX	1	3998	-	0,6,6	-	-	-		
87	OHX	1	3974	-	0,6,6	-	-	-		
87	OHX	1	4067	-	0,6,6	-	-	-		
87	OHX	5	3912	-	0,6,6	-	-	-		
87	OHX	6	2190	-	0,6,6	-	-	-		
87	OHX	1	4121	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2119	-	0,6,6	-	-	-		
87	OHX	5	4218	-	0,6,6	-	-	-		
87	OHX	5	3933	-	0,6,6	-	-	-		
87	OHX	1	3961	-	0,6,6	-	-	-		
87	OHX	1	3891	-	0,6,6	-	-	-		
87	OHX	5	3999	-	0,6,6	-	-	-		
87	OHX	5	4044	-	0,6,6	-	-	-		
87	OHX	4	237	-	0,6,6	-	-	-		
87	OHX	1	4185	-	0,6,6	-	-	-		
87	OHX	6	2178	-	0,6,6	-	-	-		
87	OHX	1	3942	-	0,6,6	-	-	-		
87	OHX	5	4214	-	0,6,6	-	-	-		
87	OHX	6	2081	-	0,6,6	-	-	-		
87	OHX	2	2156	-	0,6,6	-	-	-		
87	OHX	6	2197	-	0,6,6	-	-	-		
87	OHX	2	2134	-	0,6,6	-	-	-		
87	OHX	1	4088	-	0,6,6	-	-	-		
87	OHX	6	2092	-	0,6,6	-	-	-		
87	OHX	2	2081	-	0,6,6	-	-	-		
87	OHX	2	2105	-	0,6,6	-	-	-		
87	OHX	1	3926	-	0,6,6	-	-	-		
87	OHX	1	3979	-	0,6,6	-	-	-		
87	OHX	5	4061	-	0,6,6	-	-	-		
87	OHX	1	3877	-	0,6,6	-	-	-		
87	OHX	6	2146	-	0,6,6	-	-	-		
87	OHX	1	3889	-	0,6,6	-	-	-		
87	OHX	3	221	-	0,6,6	-	-	-		
87	OHX	5	4228	-	0,6,6	-	-	-		
87	OHX	1	3935	-	0,6,6	-	-	-		
87	OHX	6	2072	-	0,6,6	-	-	-		
87	OHX	1	3876	-	0,6,6	-	-	-		
87	OHX	6	2175	-	0,6,6	-	-	-		
87	OHX	3	216	-	0,6,6	-	-	-		
87	OHX	6	2143	-	0,6,6	-	-	-		
87	OHX	5	3957	-	0,6,6	-	-	-		
87	OHX	2	2032	-	0,6,6	-	-	-		
87	OHX	6	2202	-	0,6,6	-	-	-		
87	OHX	2	2085	-	0,6,6	-	-	-		
87	OHX	1	3973	-	0,6,6	-	-	-		
87	OHX	5	3977	-	0,6,6	-	-	-		
87	OHX	5	4180	-	0,6,6	-	-	-		
87	OHX	8	225	-	0,6,6	-	-	-		
87	OHX	2	2174	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3976	-	0,6,6	-	-	-		
87	OHX	6	2139	-	0,6,6	-	-	-		
87	OHX	1	3999	-	0,6,6	-	-	-		
87	OHX	5	3985	-	0,6,6	-	-	-		
87	OHX	4	225	-	0,6,6	-	-	-		
89	ANM	5	4260	-	20,20,20	1.44	3 (15%)	24,27,27	1.86	5 (20%)
87	OHX	5	4145	-	0,6,6	-	-	-		
87	OHX	1	4019	-	0,6,6	-	-	-		
87	OHX	1	4056	-	0,6,6	-	-	-		
87	OHX	1	3965	-	0,6,6	-	-	-		
87	OHX	5	3910	-	0,6,6	-	-	-		
87	OHX	1	4172	-	0,6,6	-	-	-		
87	OHX	1	4153	-	0,6,6	-	-	-		
87	OHX	1	4181	-	0,6,6	-	-	-		
87	OHX	2	2168	-	0,6,6	-	-	-		
87	OHX	1	3927	-	0,6,6	-	-	-		
87	OHX	1	3943	-	0,6,6	-	-	-		
87	OHX	2	2102	-	0,6,6	-	-	-		
87	OHX	5	4134	-	0,6,6	-	-	-		
87	OHX	5	3974	-	0,6,6	-	-	-		
87	OHX	1	4001	-	0,6,6	-	-	-		
87	OHX	7	224	-	0,6,6	-	-	-		
87	OHX	5	4027	-	0,6,6	-	-	-		
87	OHX	5	4136	-	0,6,6	-	-	-		
87	OHX	5	3937	-	0,6,6	-	-	-		
87	OHX	1	3982	-	0,6,6	-	-	-		
87	OHX	1	4004	-	0,6,6	-	-	-		
87	OHX	5	4211	-	0,6,6	-	-	-		
87	OHX	1	3934	-	0,6,6	-	-	-		
87	OHX	2	2059	-	0,6,6	-	-	-		
87	OHX	1	4195	-	0,6,6	-	-	-		
87	OHX	2	2027	-	0,6,6	-	-	-		
87	OHX	2	2159	-	0,6,6	-	-	-		
87	OHX	1	4108	-	0,6,6	-	-	-		
87	OHX	5	4247	-	0,6,6	-	-	-		
87	OHX	1	4105	-	0,6,6	-	-	-		
87	OHX	5	4083	-	0,6,6	-	-	-		
87	OHX	5	4138	-	0,6,6	-	-	-		
87	OHX	2	2028	-	0,6,6	-	-	-		
87	OHX	1	4070	-	0,6,6	-	-	-		
87	OHX	1	4116	-	0,6,6	-	-	-		
87	OHX	5	4237	-	0,6,6	-	-	-		
87	OHX	2	2148	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3967	-	0,6,6	-	-	-		
87	OHX	1	4035	-	0,6,6	-	-	-		
87	OHX	1	4069	-	0,6,6	-	-	-		
87	OHX	1	3894	-	0,6,6	-	-	-		
87	OHX	5	4175	-	0,6,6	-	-	-		
87	OHX	M7	206	-	0,6,6	-	-	-		
87	OHX	6	2154	-	0,6,6	-	-	-		
87	OHX	1	4131	-	0,6,6	-	-	-		
87	OHX	6	2160	-	0,6,6	-	-	-		
87	OHX	6	2172	-	0,6,6	-	-	-		
87	OHX	5	4071	-	0,6,6	-	-	-		
87	OHX	1	4000	-	0,6,6	-	-	-		
87	OHX	2	2077	-	0,6,6	-	-	-		
87	OHX	2	2140	-	0,6,6	-	-	-		
87	OHX	5	4141	-	0,6,6	-	-	-		
87	OHX	8	216	-	0,6,6	-	-	-		
87	OHX	1	4159	-	0,6,6	-	-	-		
87	OHX	6	2047	-	0,6,6	-	-	-		
87	OHX	2	2138	-	0,6,6	-	-	-		
87	OHX	1	4030	-	0,6,6	-	-	-		
87	OHX	6	2122	-	0,6,6	-	-	-		
87	OHX	5	4147	-	0,6,6	-	-	-		
87	OHX	5	4220	-	0,6,6	-	-	-		
87	OHX	6	2069	-	0,6,6	-	-	-		
87	OHX	5	3967	-	0,6,6	-	-	-		
87	OHX	5	4234	-	0,6,6	-	-	-		
87	OHX	5	4013	-	0,6,6	-	-	-		
87	OHX	2	2093	-	0,6,6	-	-	-		
87	OHX	2	2179	-	0,6,6	-	-	-		
87	OHX	5	4103	-	0,6,6	-	-	-		
87	OHX	N9	101	-	0,6,6	-	-	-		
87	OHX	1	3962	-	0,6,6	-	-	-		
87	OHX	1	3939	-	0,6,6	-	-	-		
87	OHX	1	4036	-	0,6,6	-	-	-		
87	OHX	1	4132	-	0,6,6	-	-	-		
87	OHX	8	217	-	0,6,6	-	-	-		
87	OHX	6	2185	-	0,6,6	-	-	-		
87	OHX	5	4131	-	0,6,6	-	-	-		
87	OHX	l3	404	-	0,6,6	-	-	-		
87	OHX	1	4051	-	0,6,6	-	-	-		
87	OHX	1	3883	-	0,6,6	-	-	-		
87	OHX	6	2046	-	0,6,6	-	-	-		
87	OHX	1	3915	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4055	-	0,6,6	-	-	-		
87	OHX	2	2055	-	0,6,6	-	-	-		
87	OHX	5	4246	-	0,6,6	-	-	-		
87	OHX	5	4073	-	0,6,6	-	-	-		
87	OHX	s8	303	-	0,6,6	-	-	-		
87	OHX	5	4133	-	0,6,6	-	-	-		
87	OHX	1	4048	-	0,6,6	-	-	-		
87	OHX	1	3952	-	0,6,6	-	-	-		
87	OHX	5	3968	-	0,6,6	-	-	-		
87	OHX	5	4039	-	0,6,6	-	-	-		
87	OHX	5	3921	-	0,6,6	-	-	-		
87	OHX	1	4010	-	0,6,6	-	-	-		
87	OHX	1	4216	-	0,6,6	-	-	-		
87	OHX	5	4229	-	0,6,6	-	-	-		
87	OHX	1	3879	-	0,6,6	-	-	-		
87	OHX	2	2049	-	0,6,6	-	-	-		
87	OHX	5	4099	-	0,6,6	-	-	-		
87	OHX	3	222	-	0,6,6	-	-	-		
87	OHX	6	2118	-	0,6,6	-	-	-		
87	OHX	5	3972	-	0,6,6	-	-	-		
87	OHX	1	4078	-	0,6,6	-	-	-		
87	OHX	2	2052	-	0,6,6	-	-	-		
87	OHX	2	2072	-	0,6,6	-	-	-		
87	OHX	1	4186	-	0,6,6	-	-	-		
87	OHX	5	4067	-	0,6,6	-	-	-		
87	OHX	6	2115	-	0,6,6	-	-	-		
87	OHX	1	4151	-	0,6,6	-	-	-		
87	OHX	1	3918	-	0,6,6	-	-	-		
87	OHX	1	4103	-	0,6,6	-	-	-		
87	OHX	5	4104	-	0,6,6	-	-	-		
87	OHX	1	3909	-	0,6,6	-	-	-		
87	OHX	5	4249	-	0,6,6	-	-	-		
87	OHX	1	3997	-	0,6,6	-	-	-		
87	OHX	5	4258	-	0,6,6	-	-	-		
87	OHX	5	4115	-	0,6,6	-	-	-		
87	OHX	m5	305	-	0,6,6	-	-	-		
87	OHX	5	3961	-	0,6,6	-	-	-		
87	OHX	5	4241	87	0,6,6	-	-	-		
87	OHX	1	4125	-	0,6,6	-	-	-		
87	OHX	s1	303	-	0,6,6	-	-	-		
87	OHX	2	2097	-	0,6,6	-	-	-		
87	OHX	5	4069	-	0,6,6	-	-	-		
87	OHX	6	2169	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4098	-	0,6,6	-	-	-		
87	OHX	1	4177	-	0,6,6	-	-	-		
87	OHX	5	4088	-	0,6,6	-	-	-		
87	OHX	1	4017	-	0,6,6	-	-	-		
87	OHX	1	4206	-	0,6,6	-	-	-		
87	OHX	1	3913	-	0,6,6	-	-	-		
87	OHX	1	3994	-	0,6,6	-	-	-		
87	OHX	6	2132	-	0,6,6	-	-	-		
87	OHX	5	3926	-	0,6,6	-	-	-		
87	OHX	1	3898	-	0,6,6	-	-	-		
87	OHX	1	4204	-	0,6,6	-	-	-		
87	OHX	2	2132	-	0,6,6	-	-	-		
87	OHX	6	2089	-	0,6,6	-	-	-		
87	OHX	1	4160	-	0,6,6	-	-	-		
87	OHX	1	4042	-	0,6,6	-	-	-		
87	OHX	5	4226	-	0,6,6	-	-	-		
87	OHX	2	2173	-	0,6,6	-	-	-		
87	OHX	5	3917	-	0,6,6	-	-	-		
87	OHX	5	3935	-	0,6,6	-	-	-		
87	OHX	2	2160	-	0,6,6	-	-	-		
87	OHX	1	3980	-	0,6,6	-	-	-		
87	OHX	1	4099	-	0,6,6	-	-	-		
87	OHX	4	228	-	0,6,6	-	-	-		
87	OHX	2	2047	-	0,6,6	-	-	-		
87	OHX	1	3888	-	0,6,6	-	-	-		
87	OHX	1	4047	-	0,6,6	-	-	-		
87	OHX	5	3904	-	0,6,6	-	-	-		
87	OHX	1	4173	-	0,6,6	-	-	-		
87	OHX	5	3939	-	0,6,6	-	-	-		
87	OHX	1	4104	-	0,6,6	-	-	-		
87	OHX	5	3936	-	0,6,6	-	-	-		
87	OHX	1	4110	-	0,6,6	-	-	-		
87	OHX	19	600	-	0,6,6	-	-	-		
87	OHX	6	2165	-	0,6,6	-	-	-		
87	OHX	5	3973	-	0,6,6	-	-	-		
87	OHX	1	4154	-	0,6,6	-	-	-		
87	OHX	5	4072	-	0,6,6	-	-	-		
87	OHX	6	2103	-	0,6,6	-	-	-		
87	OHX	2	2074	-	0,6,6	-	-	-		
87	OHX	6	2117	-	0,6,6	-	-	-		
87	OHX	6	2127	-	0,6,6	-	-	-		
87	OHX	8	224	-	0,6,6	-	-	-		
87	OHX	2	2136	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3875	-	0,6,6	-	-	-		
87	OHX	5	3905	-	0,6,6	-	-	-		
87	OHX	1	3931	-	0,6,6	-	-	-		
87	OHX	6	2065	-	0,6,6	-	-	-		
87	OHX	5	3941	-	0,6,6	-	-	-		
87	OHX	5	4048	-	0,6,6	-	-	-		
87	OHX	2	2046	-	0,6,6	-	-	-		
87	OHX	1	4065	-	0,6,6	-	-	-		
87	OHX	4	232	-	0,6,6	-	-	-		
87	OHX	5	3965	-	0,6,6	-	-	-		
87	OHX	5	4010	-	0,6,6	-	-	-		
87	OHX	5	4172	-	0,6,6	-	-	-		
87	OHX	1	3895	-	0,6,6	-	-	-		
87	OHX	5	4153	-	0,6,6	-	-	-		
87	OHX	1	3914	-	0,6,6	-	-	-		
87	OHX	o9	101	-	0,6,6	-	-	-		
87	OHX	5	4001	-	0,6,6	-	-	-		
87	OHX	5	3992	-	0,6,6	-	-	-		
87	OHX	5	3982	-	0,6,6	-	-	-		
87	OHX	5	4004	-	0,6,6	-	-	-		
87	OHX	5	3934	-	0,6,6	-	-	-		
87	OHX	6	2177	-	0,6,6	-	-	-		
87	OHX	5	3909	-	0,6,6	-	-	-		
87	OHX	6	2062	-	0,6,6	-	-	-		
87	OHX	1	3954	-	0,6,6	-	-	-		
87	OHX	1	3984	-	0,6,6	-	-	-		
87	OHX	1	4076	-	0,6,6	-	-	-		
87	OHX	2	2068	-	0,6,6	-	-	-		
87	OHX	1	4107	-	0,6,6	-	-	-		
87	OHX	5	4108	-	0,6,6	-	-	-		
87	OHX	5	4195	-	0,6,6	-	-	-		
87	OHX	2	2036	-	0,6,6	-	-	-		
87	OHX	M7	207	-	0,6,6	-	-	-		
87	OHX	4	234	-	0,6,6	-	-	-		
87	OHX	M6	202	-	0,6,6	-	-	-		
87	OHX	1	4072	-	0,6,6	-	-	-		
87	OHX	6	2086	-	0,6,6	-	-	-		
87	OHX	5	4080	-	0,6,6	-	-	-		
87	OHX	5	4239	-	0,6,6	-	-	-		
87	OHX	5	4116	-	0,6,6	-	-	-		
87	OHX	5	3948	-	0,6,6	-	-	-		
87	OHX	5	3914	-	0,6,6	-	-	-		
87	OHX	3	224	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4053	-	0,6,6	-	-	-		
87	OHX	m7	206	-	0,6,6	-	-	-		
87	OHX	C5	201	-	0,6,6	-	-	-		
87	OHX	1	4045	-	0,6,6	-	-	-		
87	OHX	5	4035	-	0,6,6	-	-	-		
87	OHX	1	4180	-	0,6,6	-	-	-		
87	OHX	2	2092	-	0,6,6	-	-	-		
87	OHX	3	223	-	0,6,6	-	-	-		
87	OHX	2	2030	-	0,6,6	-	-	-		
87	OHX	1	4124	-	0,6,6	-	-	-		
87	OHX	2	2169	-	0,6,6	-	-	-		
87	OHX	1	4100	-	0,6,6	-	-	-		
87	OHX	1	4043	-	0,6,6	-	-	-		
87	OHX	4	231	-	0,6,6	-	-	-		
87	OHX	M9	202	-	0,6,6	-	-	-		
87	OHX	1	4149	-	0,6,6	-	-	-		
87	OHX	5	4183	-	0,6,6	-	-	-		
87	OHX	5	4159	-	0,6,6	-	-	-		
87	OHX	3	225	-	0,6,6	-	-	-		
87	OHX	5	4030	-	0,6,6	-	-	-		
87	OHX	2	2050	-	0,6,6	-	-	-		
87	OHX	2	2042	-	0,6,6	-	-	-		
87	OHX	6	2170	-	0,6,6	-	-	-		
87	OHX	6	2124	-	0,6,6	-	-	-		
87	OHX	5	4012	-	0,6,6	-	-	-		
87	OHX	6	2131	-	0,6,6	-	-	-		
87	OHX	5	4224	-	0,6,6	-	-	-		
87	OHX	1	3992	-	0,6,6	-	-	-		
87	OHX	5	4135	-	0,6,6	-	-	-		
87	OHX	2	2124	-	0,6,6	-	-	-		
87	OHX	1	4184	-	0,6,6	-	-	-		
87	OHX	1	3932	-	0,6,6	-	-	-		
87	OHX	1	4189	-	0,6,6	-	-	-		
87	OHX	6	2164	-	0,6,6	-	-	-		
87	OHX	6	2073	-	0,6,6	-	-	-		
87	OHX	6	2176	-	0,6,6	-	-	-		
87	OHX	6	2196	-	0,6,6	-	-	-		
87	OHX	5	3962	-	0,6,6	-	-	-		
87	OHX	5	4092	-	0,6,6	-	-	-		
87	OHX	5	4036	-	0,6,6	-	-	-		
87	OHX	2	2079	-	0,6,6	-	-	-		
87	OHX	5	4132	-	0,6,6	-	-	-		
87	OHX	2	2178	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2088	-	0,6,6	-	-	-		
87	OHX	5	4256	-	0,6,6	-	-	-		
87	OHX	5	3915	-	0,6,6	-	-	-		
87	OHX	2	2128	-	0,6,6	-	-	-		
87	OHX	4	236	-	0,6,6	-	-	-		
87	OHX	1	4211	-	0,6,6	-	-	-		
87	OHX	1	3948	-	0,6,6	-	-	-		
87	OHX	2	2024	-	0,6,6	-	-	-		
87	OHX	6	2080	-	0,6,6	-	-	-		
87	OHX	1	3899	-	0,6,6	-	-	-		
87	OHX	1	4114	-	0,6,6	-	-	-		
87	OHX	1	4032	-	0,6,6	-	-	-		
87	OHX	2	2127	-	0,6,6	-	-	-		
87	OHX	6	2100	-	0,6,6	-	-	-		
87	OHX	6	2161	-	0,6,6	-	-	-		
87	OHX	6	2053	-	0,6,6	-	-	-		
87	OHX	5	3952	-	0,6,6	-	-	-		
87	OHX	2	2065	-	0,6,6	-	-	-		
87	OHX	1	3959	-	0,6,6	-	-	-		
87	OHX	1	4074	-	0,6,6	-	-	-		
87	OHX	4	233	-	0,6,6	-	-	-		
87	OHX	6	2145	-	0,6,6	-	-	-		
87	OHX	1	4187	-	0,6,6	-	-	-		
87	OHX	6	2163	-	0,6,6	-	-	-		
87	OHX	1	4175	-	0,6,6	-	-	-		
87	OHX	1	4214	-	0,6,6	-	-	-		
87	OHX	6	2045	-	0,6,6	-	-	-		
87	OHX	2	2116	-	0,6,6	-	-	-		
87	OHX	6	2051	-	0,6,6	-	-	-		
87	OHX	5	4078	-	0,6,6	-	-	-		
87	OHX	5	4107	-	0,6,6	-	-	-		
87	OHX	5	4186	-	0,6,6	-	-	-		
87	OHX	5	4252	-	0,6,6	-	-	-		
87	OHX	2	2107	-	0,6,6	-	-	-		
87	OHX	5	4151	-	0,6,6	-	-	-		
87	OHX	5	3997	-	0,6,6	-	-	-		
87	OHX	1	3993	-	0,6,6	-	-	-		
87	OHX	1	4194	-	0,6,6	-	-	-		
87	OHX	1	4033	-	0,6,6	-	-	-		
87	OHX	1	4158	-	0,6,6	-	-	-		
87	OHX	d9	102	-	0,6,6	-	-	-		
87	OHX	5	4097	-	0,6,6	-	-	-		
87	OHX	2	2062	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2165	-	0,6,6	-	-	-		
87	OHX	2	2103	-	0,6,6	-	-	-		
87	OHX	6	2111	-	0,6,6	-	-	-		
87	OHX	5	4087	-	0,6,6	-	-	-		
87	OHX	1	3964	-	0,6,6	-	-	-		
87	OHX	2	2111	-	0,6,6	-	-	-		
87	OHX	6	2082	-	0,6,6	-	-	-		
87	OHX	6	2083	-	0,6,6	-	-	-		
87	OHX	1	4212	-	0,6,6	-	-	-		
87	OHX	5	3950	-	0,6,6	-	-	-		
87	OHX	5	4177	-	0,6,6	-	-	-		
87	OHX	2	2123	-	0,6,6	-	-	-		
87	OHX	2	2101	-	0,6,6	-	-	-		
87	OHX	1	4057	-	0,6,6	-	-	-		
87	OHX	5	3913	-	0,6,6	-	-	-		
87	OHX	6	2071	-	0,6,6	-	-	-		
87	OHX	5	3994	-	0,6,6	-	-	-		
87	OHX	6	2079	-	0,6,6	-	-	-		
87	OHX	5	4235	-	0,6,6	-	-	-		
87	OHX	3	219	-	0,6,6	-	-	-		
87	OHX	1	4168	-	0,6,6	-	-	-		
87	OHX	5	4160	-	0,6,6	-	-	-		
87	OHX	5	4033	-	0,6,6	-	-	-		
87	OHX	1	4073	-	0,6,6	-	-	-		
87	OHX	1	3902	-	0,6,6	-	-	-		
87	OHX	1	3990	-	0,6,6	-	-	-		
87	OHX	1	3878	-	0,6,6	-	-	-		
87	OHX	5	3932	-	0,6,6	-	-	-		
87	OHX	5	3980	-	0,6,6	-	-	-		
87	OHX	6	2076	-	0,6,6	-	-	-		
87	OHX	1	4066	-	0,6,6	-	-	-		
87	OHX	2	2149	-	0,6,6	-	-	-		
87	OHX	6	2078	-	0,6,6	-	-	-		
87	OHX	5	4096	-	0,6,6	-	-	-		
87	OHX	5	4130	-	0,6,6	-	-	-		
87	OHX	5	4047	-	0,6,6	-	-	-		
87	OHX	5	4173	-	0,6,6	-	-	-		
87	OHX	5	4158	-	0,6,6	-	-	-		
87	OHX	1	4207	-	0,6,6	-	-	-		
87	OHX	6	2171	-	0,6,6	-	-	-		
87	OHX	5	3919	-	0,6,6	-	-	-		
87	OHX	5	4148	-	0,6,6	-	-	-		
87	OHX	5	3925	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3886	-	0,6,6	-	-	-		
87	OHX	1	4097	-	0,6,6	-	-	-		
87	OHX	6	2186	-	0,6,6	-	-	-		
87	OHX	2	2035	-	0,6,6	-	-	-		
87	OHX	1	4087	-	0,6,6	-	-	-		
87	OHX	1	4091	-	0,6,6	-	-	-		
87	OHX	6	2119	-	0,6,6	-	-	-		
87	OHX	2	2154	-	0,6,6	-	-	-		
87	OHX	1	4111	-	0,6,6	-	-	-		
87	OHX	5	4065	-	0,6,6	-	-	-		
87	OHX	3	218	-	0,6,6	-	-	-		
87	OHX	1	4060	-	0,6,6	-	-	-		
87	OHX	1	4052	-	0,6,6	-	-	-		
87	OHX	5	4192	-	0,6,6	-	-	-		
87	OHX	5	4221	-	0,6,6	-	-	-		
87	OHX	2	2038	-	0,6,6	-	-	-		
87	OHX	1	3986	-	0,6,6	-	-	-		
87	OHX	5	4253	-	0,6,6	-	-	-		
87	OHX	5	4251	-	0,6,6	-	-	-		
87	OHX	2	2080	-	0,6,6	-	-	-		
87	OHX	1	4122	-	0,6,6	-	-	-		
87	OHX	2	2121	-	0,6,6	-	-	-		
87	OHX	1	3971	-	0,6,6	-	-	-		
87	OHX	5	4037	-	0,6,6	-	-	-		
87	OHX	1	4106	-	0,6,6	-	-	-		
87	OHX	1	4098	-	0,6,6	-	-	-		
87	OHX	6	2106	-	0,6,6	-	-	-		
87	OHX	6	2195	-	0,6,6	-	-	-		
87	OHX	5	4236	-	0,6,6	-	-	-		
87	OHX	2	2084	-	0,6,6	-	-	-		
87	OHX	3	215	-	0,6,6	-	-	-		
87	OHX	1	3893	-	0,6,6	-	-	-		
87	OHX	2	2131	-	0,6,6	-	-	-		
87	OHX	2	2034	-	0,6,6	-	-	-		
87	OHX	1	4127	-	0,6,6	-	-	-		
87	OHX	5	3954	-	0,6,6	-	-	-		
87	OHX	2	2063	-	0,6,6	-	-	-		
87	OHX	5	4076	-	0,6,6	-	-	-		
87	OHX	1	3988	-	0,6,6	-	-	-		
87	OHX	1	4071	-	0,6,6	-	-	-		
87	OHX	1	4141	-	0,6,6	-	-	-		
87	OHX	3	226	-	0,6,6	-	-	-		
87	OHX	2	2171	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2093	-	0,6,6	-	-	-		
87	OHX	2	2031	-	0,6,6	-	-	-		
87	OHX	1	4113	-	0,6,6	-	-	-		
87	OHX	1	4156	-	0,6,6	-	-	-		
87	OHX	5	4109	-	0,6,6	-	-	-		
87	OHX	5	4206	-	0,6,6	-	-	-		
87	OHX	2	2043	-	0,6,6	-	-	-		
87	OHX	1	3949	-	0,6,6	-	-	-		
87	OHX	m0	302	-	0,6,6	-	-	-		
87	OHX	5	4011	-	0,6,6	-	-	-		
87	OHX	6	2134	-	0,6,6	-	-	-		
87	OHX	5	4106	-	0,6,6	-	-	-		
87	OHX	2	2041	-	0,6,6	-	-	-		
87	OHX	1	3983	-	0,6,6	-	-	-		
87	OHX	1	4094	-	0,6,6	-	-	-		
87	OHX	5	4068	-	0,6,6	-	-	-		
87	OHX	5	4045	-	0,6,6	-	-	-		
87	OHX	5	4105	-	0,6,6	-	-	-		
87	OHX	5	4155	-	0,6,6	-	-	-		
87	OHX	1	4054	-	0,6,6	-	-	-		
87	OHX	5	4124	-	0,6,6	-	-	-		
87	OHX	7	221	-	0,6,6	-	-	-		
87	OHX	2	2096	-	0,6,6	-	-	-		
87	OHX	1	4022	-	0,6,6	-	-	-		
87	OHX	5	4043	-	0,6,6	-	-	-		
87	OHX	5	4149	-	0,6,6	-	-	-		
87	OHX	5	4238	-	0,6,6	-	-	-		
87	OHX	5	4113	-	0,6,6	-	-	-		
87	OHX	1	4002	-	0,6,6	-	-	-		
87	OHX	5	4242	-	0,6,6	-	-	-		
87	OHX	1	4049	-	0,6,6	-	-	-		
87	OHX	5	4225	-	0,6,6	-	-	-		
87	OHX	1	4015	-	0,6,6	-	-	-		
87	OHX	5	3979	-	0,6,6	-	-	-		
87	OHX	5	4000	-	0,6,6	-	-	-		
87	OHX	1	3906	-	0,6,6	-	-	-		
87	OHX	5	4189	-	0,6,6	-	-	-		
87	OHX	5	4029	-	0,6,6	-	-	-		
87	OHX	5	4008	-	0,6,6	-	-	-		
87	OHX	5	4006	-	0,6,6	-	-	-		
87	OHX	2	2076	-	0,6,6	-	-	-		
87	OHX	5	4193	-	0,6,6	-	-	-		
87	OHX	8	220	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	q2	502	-	0,6,6	-	-	-		
87	OHX	5	4002	-	0,6,6	-	-	-		
87	OHX	1	3963	-	0,6,6	-	-	-		
87	OHX	6	2126	-	0,6,6	-	-	-		
87	OHX	2	2086	-	0,6,6	-	-	-		
87	OHX	5	4015	-	0,6,6	-	-	-		
87	OHX	2	2170	-	0,6,6	-	-	-		
87	OHX	5	4122	-	0,6,6	-	-	-		
87	OHX	2	2057	-	0,6,6	-	-	-		
87	OHX	5	4051	-	0,6,6	-	-	-		
87	OHX	5	3971	-	0,6,6	-	-	-		
87	OHX	6	2189	-	0,6,6	-	-	-		
87	OHX	6	2148	-	0,6,6	-	-	-		
87	OHX	5	4074	-	0,6,6	-	-	-		
87	OHX	5	3959	-	0,6,6	-	-	-		
87	OHX	1	4115	-	0,6,6	-	-	-		
87	OHX	1	4053	-	0,6,6	-	-	-		
87	OHX	2	2157	-	0,6,6	-	-	-		
87	OHX	5	4021	-	0,6,6	-	-	-		
87	OHX	2	2146	-	0,6,6	-	-	-		
87	OHX	5	4005	-	0,6,6	-	-	-		
87	OHX	2	2056	-	0,6,6	-	-	-		
87	OHX	2	2082	-	0,6,6	-	-	-		
87	OHX	5	3988	-	0,6,6	-	-	-		
87	OHX	2	2117	-	0,6,6	-	-	-		
87	OHX	1	3978	-	0,6,6	-	-	-		
87	OHX	1	4041	-	0,6,6	-	-	-		
87	OHX	1	4029	-	0,6,6	-	-	-		
87	OHX	6	2044	-	0,6,6	-	-	-		
87	OHX	6	2129	-	0,6,6	-	-	-		
87	OHX	5	3927	-	0,6,6	-	-	-		
87	OHX	6	2066	-	0,6,6	-	-	-		
87	OHX	5	4194	-	0,6,6	-	-	-		
87	OHX	2	2164	-	0,6,6	-	-	-		
87	OHX	1	4012	-	0,6,6	-	-	-		
87	OHX	C3	201	-	0,6,6	-	-	-		
87	OHX	6	2182	-	0,6,6	-	-	-		
87	OHX	2	2066	-	0,6,6	-	-	-		
87	OHX	1	4082	-	0,6,6	-	-	-		
87	OHX	5	3975	-	0,6,6	-	-	-		
87	OHX	1	4135	-	0,6,6	-	-	-		
87	OHX	1	4092	-	0,6,6	-	-	-		
87	OHX	1	3885	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3964	-	0,6,6	-	-	-		
87	OHX	5	4212	-	0,6,6	-	-	-		
87	OHX	1	3904	-	0,6,6	-	-	-		
87	OHX	5	4182	-	0,6,6	-	-	-		
87	OHX	5	4057	-	0,6,6	-	-	-		
87	OHX	1	3960	-	0,6,6	-	-	-		
87	OHX	1	3880	-	0,6,6	-	-	-		
87	OHX	1	4018	-	0,6,6	-	-	-		
87	OHX	2	2045	-	0,6,6	-	-	-		
87	OHX	1	4203	-	0,6,6	-	-	-		
87	OHX	5	4162	-	0,6,6	-	-	-		
87	OHX	2	2039	-	0,6,6	-	-	-		
87	OHX	5	4168	-	0,6,6	-	-	-		
87	OHX	O2	201	-	0,6,6	-	-	-		
87	OHX	1	4059	-	0,6,6	-	-	-		
87	OHX	1	4152	-	0,6,6	-	-	-		
87	OHX	6	2123	-	0,6,6	-	-	-		
87	OHX	1	4215	-	0,6,6	-	-	-		
87	OHX	L3	404	-	0,6,6	-	-	-		
87	OHX	1	4197	-	0,6,6	-	-	-		
87	OHX	2	2162	-	0,6,6	-	-	-		
87	OHX	6	2067	-	0,6,6	-	-	-		
87	OHX	1	3941	-	0,6,6	-	-	-		
87	OHX	6	2070	-	0,6,6	-	-	-		
87	OHX	6	2151	-	0,6,6	-	-	-		
87	OHX	5	4117	-	0,6,6	-	-	-		
87	OHX	5	4174	-	0,6,6	-	-	-		
87	OHX	6	2058	-	0,6,6	-	-	-		
87	OHX	2	2176	-	0,6,6	-	-	-		
87	OHX	6	2128	-	0,6,6	-	-	-		
87	OHX	5	4032	-	0,6,6	-	-	-		
87	OHX	5	4207	-	0,6,6	-	-	-		
87	OHX	5	4129	-	0,6,6	-	-	-		
87	OHX	2	2098	-	0,6,6	-	-	-		
87	OHX	1	3930	-	0,6,6	-	-	-		
87	OHX	1	4040	-	0,6,6	-	-	-		
87	OHX	1	4128	-	0,6,6	-	-	-		
87	OHX	5	4243	-	0,6,6	-	-	-		
87	OHX	1	3944	-	0,6,6	-	-	-		
87	OHX	1	3975	-	0,6,6	-	-	-		
87	OHX	5	4169	-	0,6,6	-	-	-		
87	OHX	1	4079	-	0,6,6	-	-	-		
87	OHX	2	2181	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4111	-	0,6,6	-	-	-		
87	OHX	5	4077	-	0,6,6	-	-	-		
87	OHX	5	4060	-	0,6,6	-	-	-		
87	OHX	5	4052	-	0,6,6	-	-	-		
87	OHX	O3	201	-	0,6,6	-	-	-		
87	OHX	5	3986	-	0,6,6	-	-	-		
87	OHX	1	3907	-	0,6,6	-	-	-		
87	OHX	2	2126	-	0,6,6	-	-	-		
87	OHX	5	4055	-	0,6,6	-	-	-		
87	OHX	2	2139	-	0,6,6	-	-	-		
87	OHX	1	3908	-	0,6,6	-	-	-		
87	OHX	4	224	-	0,6,6	-	-	-		
87	OHX	1	3950	-	0,6,6	-	-	-		
87	OHX	5	4128	-	0,6,6	-	-	-		
87	OHX	5	3928	-	0,6,6	-	-	-		
87	OHX	6	2061	-	0,6,6	-	-	-		
87	OHX	6	2156	-	0,6,6	-	-	-		
87	OHX	14	403	-	0,6,6	-	-	-		
87	OHX	5	4202	-	0,6,6	-	-	-		
87	OHX	1	4117	-	0,6,6	-	-	-		
87	OHX	4	230	-	0,6,6	-	-	-		
87	OHX	2	2155	-	0,6,6	-	-	-		
87	OHX	2	2037	-	0,6,6	-	-	-		
87	OHX	1	4081	-	0,6,6	-	-	-		
87	OHX	5	3922	-	0,6,6	-	-	-		
87	OHX	5	4082	-	0,6,6	-	-	-		
87	OHX	1	4129	-	0,6,6	-	-	-		
87	OHX	1	4183	-	0,6,6	-	-	-		
87	OHX	5	4255	-	0,6,6	-	-	-		
87	OHX	5	3949	-	0,6,6	-	-	-		
87	OHX	m0	301	-	0,6,6	-	-	-		
87	OHX	2	2100	-	0,6,6	-	-	-		
87	OHX	6	2054	-	0,6,6	-	-	-		
87	OHX	2	2044	-	0,6,6	-	-	-		
87	OHX	6	2162	-	0,6,6	-	-	-		
87	OHX	2	2023	-	0,6,6	-	-	-		
87	OHX	2	2094	-	0,6,6	-	-	-		
87	OHX	5	3908	-	0,6,6	-	-	-		
87	OHX	5	3983	-	0,6,6	-	-	-		
87	OHX	1	3953	-	0,6,6	-	-	-		
87	OHX	1	3892	-	0,6,6	-	-	-		
87	OHX	1	4190	-	0,6,6	-	-	-		
87	OHX	1	4208	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	3	217	-	0,6,6	-	-	-		
87	OHX	6	2167	-	0,6,6	-	-	-		
87	OHX	1	3987	-	0,6,6	-	-	-		
87	OHX	6	2194	-	0,6,6	-	-	-		
87	OHX	8	213	-	0,6,6	-	-	-		
87	OHX	1	3925	-	0,6,6	-	-	-		
87	OHX	5	4054	-	0,6,6	-	-	-		
87	OHX	2	2144	-	0,6,6	-	-	-		
87	OHX	5	4022	-	0,6,6	-	-	-		
87	OHX	5	4042	-	0,6,6	-	-	-		
87	OHX	2	2172	-	0,6,6	-	-	-		
87	OHX	d4	202	-	0,6,6	-	-	-		
87	OHX	6	2200	-	0,6,6	-	-	-		
87	OHX	1	4016	-	0,6,6	-	-	-		
87	OHX	1	4090	-	0,6,6	-	-	-		
87	OHX	1	4163	-	0,6,6	-	-	-		
87	OHX	1	4192	-	0,6,6	-	-	-		
87	OHX	5	4248	-	0,6,6	-	-	-		
87	OHX	1	3981	-	0,6,6	-	-	-		
87	OHX	5	4100	-	0,6,6	-	-	-		
87	OHX	2	2054	-	0,6,6	-	-	-		
87	OHX	1	4063	-	0,6,6	-	-	-		
87	OHX	1	4202	-	0,6,6	-	-	-		
87	OHX	1	4037	-	0,6,6	-	-	-		
87	OHX	M0	303	-	0,6,6	-	-	-		
87	OHX	6	2116	-	0,6,6	-	-	-		
87	OHX	5	4208	-	0,6,6	-	-	-		
87	OHX	7	216	-	0,6,6	-	-	-		
87	OHX	n9	102	-	0,6,6	-	-	-		
87	OHX	1	4143	-	0,6,6	-	-	-		
87	OHX	1	4166	-	0,6,6	-	-	-		
87	OHX	5	4050	-	0,6,6	-	-	-		
87	OHX	2	2122	-	0,6,6	-	-	-		
87	OHX	1	3938	-	0,6,6	-	-	-		
87	OHX	5	4034	-	0,6,6	-	-	-		
87	OHX	7	215	-	0,6,6	-	-	-		
87	OHX	1	4137	-	0,6,6	-	-	-		
87	OHX	6	2125	-	0,6,6	-	-	-		
87	OHX	2	2069	-	0,6,6	-	-	-		
87	OHX	5	4167	-	0,6,6	-	-	-		
87	OHX	6	2108	-	0,6,6	-	-	-		
87	OHX	1	4109	-	0,6,6	-	-	-		
87	OHX	5	4127	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2141	-	0,6,6	-	-	-		
87	OHX	1	4200	-	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
89	ANM	5	4260	-	-	0/10/23/23	0/2/2/2
89	ANM	1	4218	-	-	0/10/23/23	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4260	ANM	C11-C10	3.11	1.43	1.38
89	5	4260	ANM	C13-C1	3.08	1.43	1.38
89	5	4260	ANM	O1-C9	2.62	1.42	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	5	4260	ANM	O2-C2-C16	-4.39	102.23	110.50
89	5	4260	ANM	C10-C9-C1	4.01	126.01	120.16
89	5	4260	ANM	O2-C2-C3	-3.41	101.21	109.49
89	1	4218	ANM	O2-C2-C3	-3.38	101.28	109.49
89	5	4260	ANM	C13-C1-C9	-3.36	115.89	119.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

489 monomers are involved in 786 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4114	OHX	1	0
87	1	3989	OHX	1	0
87	2	2166	OHX	1	0
87	5	3978	OHX	6	0
87	5	4041	OHX	5	0
87	5	4187	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2104	OHX	1	0
87	1	4089	OHX	2	0
87	5	3953	OHX	1	0
87	1	4034	OHX	2	0
87	1	4006	OHX	2	0
87	2	2115	OHX	2	0
87	5	4018	OHX	2	0
87	2	2106	OHX	1	0
87	5	4203	OHX	2	0
87	1	3919	OHX	2	0
87	2	2158	OHX	2	0
87	2	2133	OHX	1	0
87	1	4086	OHX	1	0
87	1	4148	OHX	2	0
87	2	2095	OHX	6	0
87	2	2153	OHX	1	0
87	1	4021	OHX	1	0
87	c5	201	OHX	1	0
87	5	4040	OHX	1	0
87	6	2155	OHX	1	0
87	5	3944	OHX	1	0
87	6	2135	OHX	2	0
87	5	4170	OHX	1	0
87	5	4200	OHX	6	0
87	1	4080	OHX	1	0
87	2	2108	OHX	1	0
87	M5	303	OHX	1	0
87	1	4126	OHX	1	0
87	1	4155	OHX	3	0
87	8	214	OHX	6	0
87	1	4179	OHX	2	0
87	6	2152	OHX	2	0
87	L3	403	OHX	1	0
87	1	4174	OHX	2	0
87	6	2173	OHX	1	0
87	5	4197	OHX	3	0
87	5	3958	OHX	2	0
87	8	222	OHX	6	0
87	1	4170	OHX	1	0
87	5	4086	OHX	1	0
87	5	4016	OHX	6	0
87	6	2168	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2121	OHX	2	0
87	8	221	OHX	7	0
87	5	4166	OHX	2	0
87	6	2181	OHX	1	0
87	1	3897	OHX	1	0
87	1	4084	OHX	4	0
87	5	4137	OHX	1	0
87	1	4005	OHX	2	0
87	1	4139	OHX	1	0
87	1	4038	OHX	1	0
87	2	2073	OHX	1	0
87	5	4059	OHX	1	0
87	1	4123	OHX	1	0
87	1	3903	OHX	1	0
87	1	4007	OHX	7	0
87	6	2141	OHX	1	0
87	1	3916	OHX	1	0
87	1	4102	OHX	1	0
87	2	2150	OHX	1	0
87	1	4144	OHX	5	0
87	6	2055	OHX	1	0
87	5	4025	OHX	1	0
87	5	3947	OHX	7	0
87	5	4156	OHX	1	0
87	1	4146	OHX	1	0
87	1	4201	OHX	1	0
87	1	4169	OHX	2	0
87	1	3896	OHX	1	0
87	5	4026	OHX	7	0
87	2	2083	OHX	2	0
87	2	2089	OHX	4	0
87	2	2104	OHX	1	0
87	6	2142	OHX	1	0
87	6	2188	OHX	2	0
87	5	4094	OHX	1	0
87	2	2142	OHX	1	0
87	Q2	503	OHX	1	0
87	1	3969	OHX	1	0
87	5	4118	OHX	1	0
87	5	4150	OHX	6	0
87	8	223	OHX	2	0
87	5	4250	OHX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2167	OHX	2	0
87	5	4058	OHX	1	0
87	5	4209	OHX	1	0
87	2	2078	OHX	1	0
87	5	3924	OHX	1	0
87	6	2094	OHX	2	0
87	2	2130	OHX	2	0
87	2	2053	OHX	1	0
87	1	3887	OHX	2	0
87	1	4064	OHX	1	0
87	1	3951	OHX	1	0
87	6	2187	OHX	2	0
87	14	402	OHX	2	0
87	5	4024	OHX	2	0
87	7	218	OHX	3	0
87	2	2163	OHX	6	0
87	5	4205	OHX	1	0
87	6	2136	OHX	1	0
87	6	2090	OHX	1	0
87	1	3924	OHX	1	0
87	4	226	OHX	1	0
87	1	3985	OHX	1	0
87	6	2153	OHX	1	0
87	1	3945	OHX	1	0
87	5	4233	OHX	1	0
87	5	3969	OHX	1	0
87	6	2147	OHX	1	0
87	1	3972	OHX	1	0
87	5	4245	OHX	5	0
87	1	4165	OHX	1	0
87	15	304	OHX	1	0
87	1	3890	OHX	2	0
87	6	2101	OHX	1	0
87	s4	301	OHX	1	0
87	o7	502	OHX	1	0
87	5	4056	OHX	1	0
87	5	4007	OHX	2	0
87	1	4188	OHX	1	0
87	5	4181	OHX	1	0
87	5	4188	OHX	1	0
87	6	2144	OHX	1	0
87	O7	104	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2201	OHX	1	0
87	6	2112	OHX	2	0
87	1	4198	OHX	1	0
87	1	4142	OHX	2	0
87	5	4144	OHX	1	0
87	6	2110	OHX	1	0
87	5	4121	OHX	1	0
87	6	2109	OHX	1	0
87	5	4101	OHX	6	0
87	2	2048	OHX	1	0
87	1	4046	OHX	1	0
87	5	4161	OHX	1	0
87	5	3996	OHX	3	0
87	5	4244	OHX	1	0
87	2	2090	OHX	6	0
87	5	4201	OHX	1	0
87	6	2059	OHX	1	0
87	5	3981	OHX	1	0
87	1	4031	OHX	2	0
87	1	3911	OHX	1	0
87	6	2107	OHX	1	0
87	2	2147	OHX	7	0
87	1	4213	OHX	1	0
87	2	2026	OHX	1	0
87	1	4023	OHX	5	0
87	6	2077	OHX	1	0
87	6	2140	OHX	1	0
87	1	4161	OHX	7	0
87	5	4019	OHX	1	0
87	5	4199	OHX	3	0
87	5	3929	OHX	1	0
87	5	4216	OHX	1	0
87	1	4044	OHX	1	0
87	5	3943	OHX	1	0
87	2	2071	OHX	1	0
87	1	3882	OHX	1	0
87	6	2149	OHX	1	0
87	1	4061	OHX	5	0
87	6	2091	OHX	1	0
87	5	4095	OHX	1	0
87	2	2109	OHX	8	0
87	1	3957	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3905	OHX	2	0
87	6	2052	OHX	1	0
87	5	3991	OHX	1	0
87	1	3976	OHX	1	0
87	1	4145	OHX	2	0
87	5	4230	OHX	1	0
87	1	3884	OHX	1	0
87	1	3910	OHX	1	0
87	5	4062	OHX	1	0
87	O1	202	OHX	6	0
87	1	4136	OHX	2	0
87	1	3937	OHX	3	0
87	6	2068	OHX	1	0
87	2	2161	OHX	2	0
87	5	4126	OHX	1	0
87	5	4231	OHX	4	0
87	6	2105	OHX	2	0
87	6	2074	OHX	1	0
87	2	2145	OHX	1	0
87	m1	202	OHX	1	0
87	8	215	OHX	1	0
87	6	2098	OHX	3	0
87	5	3946	OHX	1	0
87	1	3873	OHX	1	0
87	2	2137	OHX	2	0
87	2	2099	OHX	7	0
87	5	4140	OHX	1	0
87	1	3920	OHX	1	0
87	1	4147	OHX	1	0
87	2	2075	OHX	6	0
87	6	2057	OHX	6	0
87	8	218	OHX	2	0
87	7	217	OHX	6	0
87	5	4154	OHX	1	0
87	5	3920	OHX	1	0
87	5	3911	OHX	2	0
87	5	4112	OHX	2	0
87	2	2033	OHX	1	0
87	s1	302	OHX	1	0
87	1	4039	OHX	1	0
87	4	238	OHX	1	0
87	L4	402	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2063	OHX	1	0
87	6	2157	OHX	3	0
87	2	2064	OHX	1	0
87	6	2159	OHX	1	0
87	2	2110	OHX	1	0
87	1	3868	OHX	1	0
87	1	4067	OHX	1	0
87	2	2119	OHX	1	0
87	1	3961	OHX	6	0
87	1	4185	OHX	1	0
87	6	2081	OHX	2	0
87	2	2156	OHX	1	0
87	1	4088	OHX	6	0
87	2	2105	OHX	1	0
87	1	3979	OHX	1	0
87	5	4061	OHX	6	0
87	3	221	OHX	1	0
87	5	4228	OHX	1	0
87	1	3935	OHX	2	0
87	6	2072	OHX	1	0
87	1	3876	OHX	1	0
87	2	2085	OHX	2	0
87	5	3977	OHX	2	0
87	8	225	OHX	1	0
87	5	4145	OHX	1	0
87	1	4019	OHX	1	0
87	1	4056	OHX	2	0
87	1	4172	OHX	3	0
87	2	2168	OHX	1	0
87	5	3974	OHX	1	0
87	7	224	OHX	6	0
87	5	3937	OHX	1	0
87	5	4211	OHX	5	0
87	5	4247	OHX	2	0
87	5	4138	OHX	2	0
87	1	4070	OHX	1	0
87	1	3967	OHX	2	0
87	5	4175	OHX	1	0
87	M7	206	OHX	1	0
87	6	2160	OHX	1	0
87	5	4071	OHX	2	0
87	1	4000	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4159	OHX	4	0
87	6	2047	OHX	2	0
87	6	2122	OHX	1	0
87	6	2069	OHX	1	0
87	5	3967	OHX	4	0
87	5	4234	OHX	1	0
87	2	2093	OHX	1	0
87	5	4103	OHX	1	0
87	1	3962	OHX	1	0
87	1	4036	OHX	6	0
87	1	4132	OHX	1	0
87	8	217	OHX	1	0
87	1	4051	OHX	2	0
87	s8	303	OHX	1	0
87	1	4048	OHX	7	0
87	5	4039	OHX	1	0
87	5	3921	OHX	2	0
87	1	4010	OHX	2	0
87	5	4099	OHX	2	0
87	6	2118	OHX	8	0
87	2	2072	OHX	1	0
87	1	4186	OHX	4	0
87	1	4151	OHX	6	0
87	5	4104	OHX	1	0
87	m5	305	OHX	1	0
87	5	3961	OHX	1	0
87	5	4241	OHX	6	0
87	2	2097	OHX	2	0
87	6	2169	OHX	8	0
87	5	4098	OHX	1	0
87	1	4177	OHX	9	0
87	1	4017	OHX	1	0
87	1	4206	OHX	1	0
87	1	3994	OHX	1	0
87	1	4204	OHX	1	0
87	2	2132	OHX	8	0
87	1	4160	OHX	2	0
87	1	4042	OHX	2	0
87	5	3917	OHX	1	0
87	5	3935	OHX	1	0
87	1	3980	OHX	1	0
87	1	4099	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2047	OHX	2	0
87	1	3888	OHX	2	0
87	1	4047	OHX	4	0
87	1	4173	OHX	2	0
87	5	4072	OHX	7	0
87	6	2103	OHX	1	0
87	6	2117	OHX	2	0
87	1	3875	OHX	1	0
87	1	3931	OHX	2	0
87	5	3941	OHX	1	0
87	1	4065	OHX	3	0
87	o9	101	OHX	1	0
87	5	3992	OHX	1	0
87	5	4004	OHX	1	0
87	6	2177	OHX	1	0
87	5	3909	OHX	2	0
87	1	3954	OHX	2	0
87	1	3984	OHX	1	0
87	1	4076	OHX	1	0
87	2	2036	OHX	3	0
87	4	234	OHX	3	0
87	6	2086	OHX	1	0
87	5	4080	OHX	2	0
87	5	4239	OHX	1	0
87	m7	206	OHX	1	0
87	C5	201	OHX	2	0
87	5	4035	OHX	1	0
87	2	2092	OHX	1	0
87	1	4043	OHX	1	0
87	M9	202	OHX	1	0
87	1	4149	OHX	1	0
87	5	4030	OHX	1	0
87	6	2124	OHX	3	0
87	5	4012	OHX	2	0
87	5	4224	OHX	8	0
87	1	3992	OHX	1	0
87	1	4184	OHX	1	0
87	1	4189	OHX	1	0
87	6	2073	OHX	1	0
87	6	2176	OHX	2	0
87	5	3962	OHX	3	0
87	5	4036	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4256	OHX	1	0
87	2	2128	OHX	1	0
87	1	4211	OHX	1	0
87	1	4032	OHX	5	0
87	2	2127	OHX	1	0
87	6	2100	OHX	2	0
87	6	2145	OHX	7	0
87	2	2116	OHX	4	0
87	5	4078	OHX	1	0
87	5	4151	OHX	1	0
87	2	2062	OHX	1	0
87	5	4087	OHX	1	0
87	2	2111	OHX	2	0
87	5	4177	OHX	1	0
87	2	2123	OHX	1	0
87	6	2071	OHX	2	0
87	5	4235	OHX	1	0
87	1	4168	OHX	6	0
87	5	4160	OHX	1	0
87	1	3878	OHX	1	0
87	1	4066	OHX	1	0
87	2	2149	OHX	1	0
87	5	4096	OHX	7	0
87	5	4173	OHX	1	0
87	1	3886	OHX	1	0
87	2	2035	OHX	1	0
87	1	4091	OHX	1	0
87	6	2119	OHX	1	0
87	1	4111	OHX	1	0
87	5	4065	OHX	1	0
87	3	218	OHX	2	0
87	1	4060	OHX	4	0
87	1	4052	OHX	1	0
87	5	4192	OHX	1	0
87	5	4221	OHX	4	0
87	2	2038	OHX	1	0
87	1	3986	OHX	1	0
87	5	4251	OHX	1	0
87	1	4122	OHX	1	0
87	2	2121	OHX	3	0
87	5	4037	OHX	1	0
87	1	4098	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2106	OHX	1	0
87	5	4236	OHX	1	0
87	2	2084	OHX	1	0
87	1	3893	OHX	1	0
87	2	2131	OHX	1	0
87	2	2034	OHX	1	0
87	5	3954	OHX	1	0
87	3	226	OHX	1	0
87	6	2093	OHX	1	0
87	2	2031	OHX	7	0
87	1	4113	OHX	1	0
87	5	4109	OHX	1	0
87	5	4206	OHX	11	0
87	m0	302	OHX	1	0
87	5	4106	OHX	1	0
87	1	4094	OHX	1	0
87	5	4045	OHX	1	0
87	1	4054	OHX	1	0
87	5	4124	OHX	1	0
87	2	2096	OHX	4	0
87	5	4149	OHX	1	0
87	5	4113	OHX	1	0
87	1	4049	OHX	1	0
87	5	3979	OHX	1	0
87	5	4000	OHX	1	0
87	5	4029	OHX	3	0
87	5	4008	OHX	1	0
87	5	4006	OHX	7	0
87	2	2076	OHX	1	0
87	5	4193	OHX	1	0
87	q2	502	OHX	3	0
87	1	3963	OHX	6	0
87	6	2126	OHX	1	0
87	2	2086	OHX	1	0
87	2	2170	OHX	1	0
87	2	2057	OHX	1	0
87	5	3971	OHX	1	0
87	6	2189	OHX	2	0
87	6	2148	OHX	3	0
87	5	4074	OHX	1	0
87	5	3959	OHX	1	0
87	2	2146	OHX	2	0

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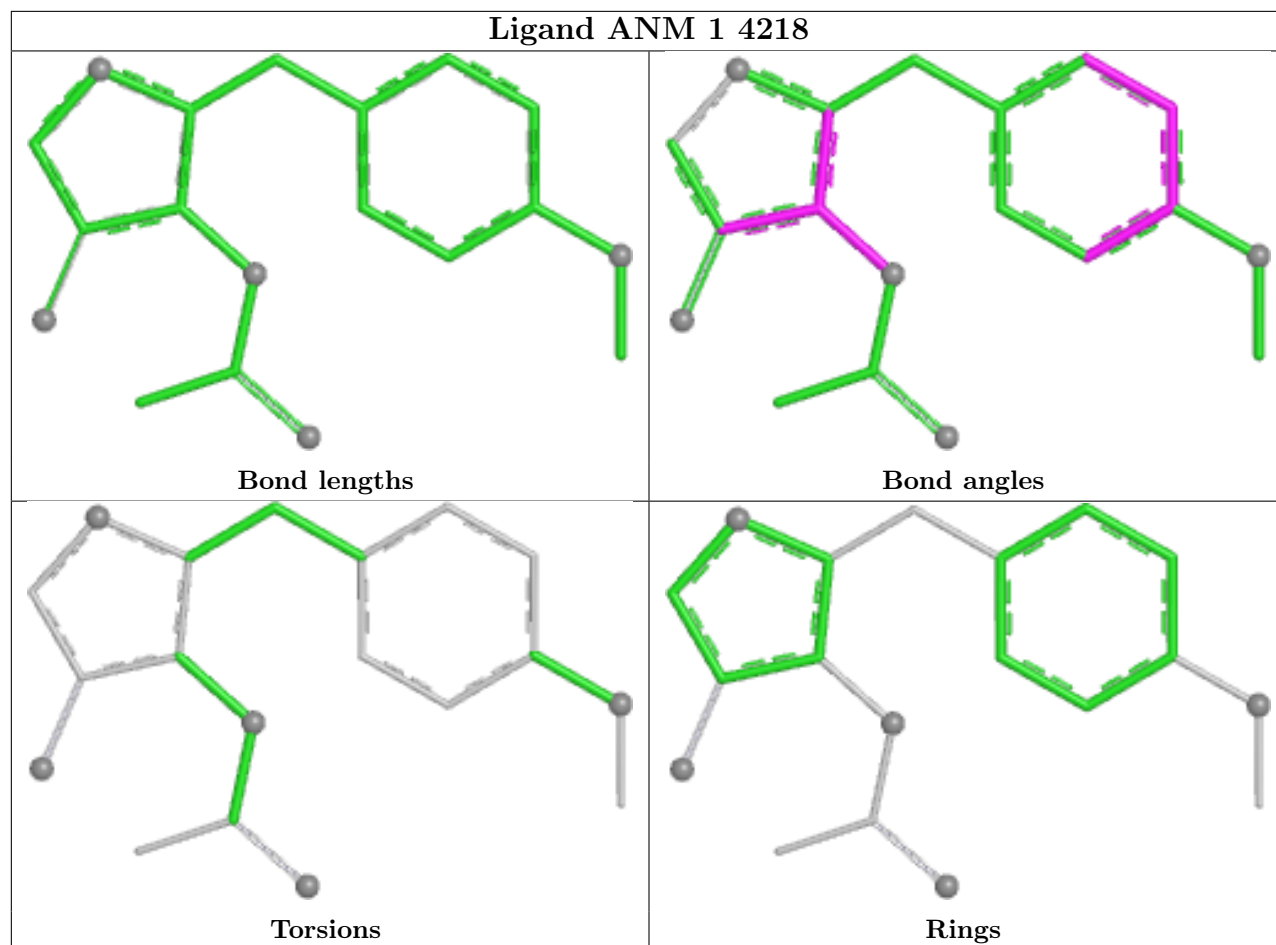
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4005	OHX	6	0
87	2	2082	OHX	1	0
87	5	3988	OHX	1	0
87	2	2117	OHX	1	0
87	1	3978	OHX	1	0
87	1	4041	OHX	3	0
87	5	3927	OHX	1	0
87	6	2066	OHX	1	0
87	1	4012	OHX	1	0
87	6	2182	OHX	1	0
87	1	4082	OHX	1	0
87	1	4135	OHX	1	0
87	1	4092	OHX	1	0
87	1	3885	OHX	1	0
87	1	3904	OHX	1	0
87	5	4057	OHX	1	0
87	1	3960	OHX	2	0
87	1	3880	OHX	1	0
87	2	2045	OHX	1	0
87	1	4203	OHX	7	0
87	2	2039	OHX	2	0
87	1	4059	OHX	6	0
87	1	4152	OHX	1	0
87	6	2123	OHX	5	0
87	1	3941	OHX	1	0
87	5	4117	OHX	1	0
87	6	2058	OHX	1	0
87	6	2128	OHX	1	0
87	5	4207	OHX	7	0
87	5	4243	OHX	7	0
87	1	3975	OHX	6	0
87	5	4169	OHX	2	0
87	1	4079	OHX	1	0
87	5	4052	OHX	1	0
87	O3	201	OHX	1	0
87	2	2126	OHX	1	0
87	5	4055	OHX	1	0
87	2	2139	OHX	1	0
87	4	224	OHX	1	0
87	5	4202	OHX	1	0
87	4	230	OHX	1	0
87	2	2155	OHX	2	0

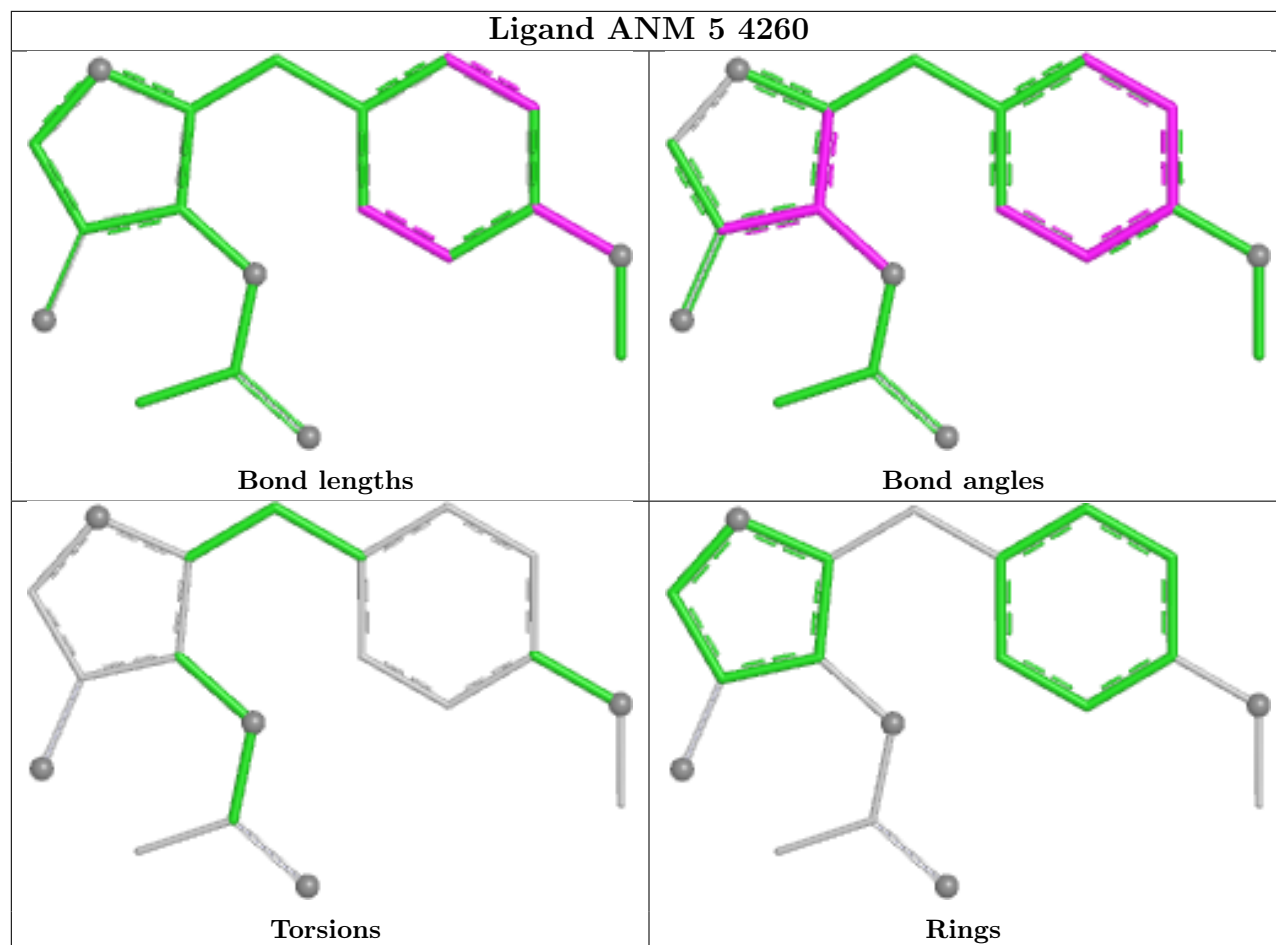
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	3922	OHX	2	0
87	2	2044	OHX	7	0
87	2	2023	OHX	1	0
87	5	3983	OHX	9	0
87	1	3892	OHX	1	0
87	1	4208	OHX	2	0
87	1	3987	OHX	1	0
87	6	2194	OHX	1	0
87	8	213	OHX	1	0
87	1	3925	OHX	1	0
87	d4	202	OHX	1	0
87	5	4100	OHX	3	0
87	2	2054	OHX	1	0
87	1	4037	OHX	2	0
87	5	4208	OHX	7	0
87	1	4143	OHX	3	0
87	1	3938	OHX	1	0
87	5	4034	OHX	1	0
87	1	4137	OHX	1	0
87	2	2141	OHX	1	0
87	1	4200	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%)	-0.01	23 (1%) 75 53	49, 84, 160, 254	0
1	6	1795/1800 (99%)	-0.15	27 (1%) 72 49	38, 71, 169, 252	0
2	S0	206/251 (82%)	0.48	11 (5%) 32 16	87, 103, 117, 148	0
2	s0	206/251 (82%)	0.14	5 (2%) 59 36	69, 87, 103, 110	0
3	S1	214/254 (84%)	0.69	12 (5%) 30 15	90, 120, 148, 161	0
3	s1	216/254 (85%)	0.16	6 (2%) 55 32	62, 77, 102, 114	0
4	S2	217/253 (85%)	0.36	8 (3%) 45 25	66, 82, 98, 117	0
4	s2	217/253 (85%)	0.24	8 (3%) 45 25	52, 69, 88, 104	0
5	S3	223/239 (93%)	0.32	5 (2%) 62 39	72, 84, 112, 134	0
5	s3	223/239 (93%)	0.61	9 (4%) 42 23	66, 93, 117, 123	0
6	S4	260/260 (100%)	0.42	12 (4%) 37 20	61, 83, 95, 128	0
6	s4	260/260 (100%)	-0.08	2 (0%) 82 64	48, 72, 86, 117	0
7	S5	206/224 (91%)	0.61	7 (3%) 48 27	88, 109, 128, 142	0
7	s5	206/224 (91%)	0.33	7 (3%) 48 27	65, 89, 116, 131	0
8	S6	226/236 (95%)	0.55	17 (7%) 20 10	60, 96, 117, 139	0
8	s6	218/236 (92%)	0.30	7 (3%) 50 29	49, 77, 104, 127	0
9	S7	184/189 (97%)	0.43	3 (1%) 70 47	81, 112, 138, 146	0
9	s7	186/189 (98%)	0.36	5 (2%) 56 33	65, 97, 132, 145	0
10	S8	188/200 (94%)	0.18	2 (1%) 78 57	52, 69, 106, 127	0
10	s8	188/200 (94%)	0.10	0 100 100	42, 63, 110, 128	0
11	S9	185/196 (94%)	0.40	6 (3%) 50 29	76, 91, 127, 160	0
11	s9	185/196 (94%)	0.25	6 (3%) 50 29	60, 75, 110, 145	0
12	C0	96/105 (91%)	0.60	8 (8%) 17 9	76, 97, 131, 144	0
12	c0	96/105 (91%)	0.99	15 (15%) 5 3	86, 117, 141, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	0.45	11 (7%) 22 11	55, 68, 118, 135	0
13	c1	146/155 (94%)	0.25	7 (4%) 35 19	46, 60, 97, 112	0
14	C2	124/142 (87%)	0.73	7 (5%) 30 15	118, 135, 160, 182	0
14	c2	124/142 (87%)	0.84	6 (4%) 35 19	157, 177, 196, 203	0
15	C3	150/150 (100%)	0.30	4 (2%) 56 33	64, 82, 99, 105	0
15	c3	150/150 (100%)	0.19	2 (1%) 75 53	53, 69, 87, 102	0
16	C4	127/136 (93%)	0.66	5 (3%) 43 24	63, 119, 138, 141	0
16	c4	128/136 (94%)	0.17	0 100 100	53, 78, 88, 92	0
17	C5	124/141 (87%)	0.47	7 (5%) 30 15	72, 88, 128, 161	0
17	c5	135/141 (95%)	0.51	11 (8%) 18 9	70, 91, 118, 151	0
18	C6	141/142 (99%)	0.51	4 (2%) 55 32	78, 101, 109, 113	0
18	c6	142/142 (100%)	0.59	14 (9%) 13 7	61, 82, 99, 121	0
19	C7	120/136 (88%)	0.58	8 (6%) 24 12	85, 101, 128, 130	0
19	c7	117/136 (86%)	0.28	5 (4%) 40 21	70, 85, 115, 122	0
20	C8	145/145 (100%)	0.39	6 (4%) 41 23	72, 97, 124, 132	0
20	c8	145/145 (100%)	0.19	3 (2%) 63 40	67, 81, 109, 127	0
21	C9	143/143 (100%)	0.36	2 (1%) 73 51	82, 98, 117, 128	0
21	c9	143/143 (100%)	-0.00	1 (0%) 84 66	61, 74, 96, 114	0
22	D0	107/120 (89%)	0.74	8 (7%) 20 10	70, 104, 139, 145	0
22	d0	110/120 (91%)	0.41	1 (0%) 81 61	61, 97, 137, 154	0
23	D1	87/87 (100%)	0.15	3 (3%) 48 27	83, 90, 110, 126	0
23	d1	87/87 (100%)	-0.08	0 100 100	65, 73, 98, 113	0
24	D2	129/129 (100%)	0.12	1 (0%) 82 64	65, 76, 84, 94	0
24	d2	129/129 (100%)	-0.09	1 (0%) 82 64	50, 61, 68, 78	0
25	D3	144/144 (100%)	0.31	4 (2%) 55 32	54, 60, 73, 85	0
25	d3	144/144 (100%)	0.06	3 (2%) 63 40	44, 48, 63, 80	0
26	D4	134/134 (100%)	0.34	5 (3%) 45 25	70, 97, 114, 124	0
26	d4	134/134 (100%)	0.18	5 (3%) 45 25	55, 79, 94, 124	0
27	D5	70/107 (65%)	0.62	5 (7%) 22 11	104, 121, 134, 142	0
27	d5	69/107 (64%)	0.25	0 100 100	80, 104, 121, 125	0
28	D6	97/97 (100%)	0.78	7 (7%) 21 11	68, 83, 141, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.32	1 (1%) 79 59	50, 61, 93, 104	0
29	D7	81/81 (100%)	0.43	3 (3%) 45 25	79, 93, 128, 136	0
29	d7	81/81 (100%)	0.10	1 (1%) 76 55	63, 79, 124, 126	0
30	D8	63/66 (95%)	0.78	5 (7%) 18 10	102, 120, 136, 162	0
30	d8	63/66 (95%)	0.49	2 (3%) 50 29	82, 100, 119, 127	0
31	D9	53/55 (96%)	0.36	1 (1%) 66 43	70, 74, 95, 106	0
31	d9	53/55 (96%)	0.50	3 (5%) 29 15	65, 72, 111, 123	0
32	E0	60/60 (100%)	0.45	3 (5%) 34 18	59, 90, 128, 133	0
33	E1	71/76 (93%)	0.67	5 (7%) 22 12	94, 115, 132, 136	0
34	SR	318/318 (100%)	0.25	3 (0%) 81 61	64, 106, 128, 148	0
34	sR	318/318 (100%)	0.51	14 (4%) 39 21	86, 106, 125, 144	0
35	SM	159/273 (58%)	0.82	25 (15%) 5 3	62, 85, 134, 137	0
35	sM	104/273 (38%)	1.10	26 (25%) 2 1	56, 93, 172, 177	0
36	1	3149/3396 (92%)	-0.39	47 (1%) 72 49	26, 48, 130, 253	0
36	5	3150/3396 (92%)	-0.45	41 (1%) 75 53	27, 47, 120, 255	0
37	3	121/121 (100%)	-0.59	0 100 100	39, 67, 82, 88	0
37	7	121/121 (100%)	-0.69	1 (0%) 82 64	31, 49, 63, 71	0
38	4	158/158 (100%)	-0.34	4 (2%) 58 35	32, 50, 90, 129	0
38	8	158/158 (100%)	-0.26	5 (3%) 50 29	38, 57, 95, 123	0
39	L2	252/253 (99%)	-0.19	0 100 100	31, 46, 64, 74	0
39	l2	252/253 (99%)	-0.05	7 (2%) 55 32	31, 49, 68, 80	0
40	L3	386/386 (100%)	-0.21	1 (0%) 90 79	33, 52, 67, 96	0
40	l3	386/386 (100%)	-0.31	1 (0%) 90 79	26, 39, 52, 84	0
41	L4	361/361 (100%)	-0.34	2 (0%) 85 69	27, 42, 61, 75	0
41	l4	361/361 (100%)	-0.28	0 100 100	30, 47, 66, 83	0
42	L5	296/296 (100%)	0.05	3 (1%) 79 59	50, 74, 94, 118	0
42	l5	294/296 (99%)	-0.17	4 (1%) 73 51	38, 54, 83, 127	0
43	L6	156/175 (89%)	-0.36	0 100 100	38, 45, 66, 86	0
43	l6	157/175 (89%)	-0.28	0 100 100	39, 47, 69, 82	0
44	L7	222/243 (91%)	-0.35	0 100 100	31, 39, 68, 115	0
44	l7	223/243 (91%)	-0.41	0 100 100	29, 36, 78, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	L8	233/255 (91%)	0.09	4 (1%) 69 45	53, 68, 105, 116	0
45	l8	231/255 (90%)	0.30	7 (3%) 52 30	65, 78, 105, 114	0
46	L9	191/191 (100%)	-0.09	0 100 100	47, 60, 74, 96	0
46	l9	191/191 (100%)	-0.25	0 100 100	34, 44, 66, 97	0
47	M0	211/220 (95%)	-0.11	6 (2%) 55 32	34, 51, 90, 103	0
47	m0	213/220 (96%)	-0.06	5 (2%) 61 38	34, 57, 80, 99	0
48	M1	169/173 (97%)	0.07	2 (1%) 76 55	56, 77, 91, 105	0
48	m1	169/173 (97%)	-0.20	1 (0%) 85 69	40, 59, 72, 84	0
49	M3	193/198 (97%)	-0.22	0 100 100	30, 51, 92, 117	0
49	m3	194/198 (97%)	-0.07	1 (0%) 87 72	39, 61, 97, 121	0
50	M4	136/137 (99%)	-0.22	1 (0%) 84 66	40, 49, 63, 72	0
50	m4	137/137 (100%)	-0.19	3 (2%) 62 39	36, 42, 62, 76	0
51	M5	203/203 (100%)	-0.18	0 100 100	30, 45, 55, 61	0
51	m5	203/203 (100%)	-0.02	0 100 100	36, 53, 64, 70	0
52	M6	197/198 (99%)	-0.13	3 (1%) 72 49	31, 40, 59, 63	0
52	m6	197/198 (99%)	-0.12	4 (2%) 65 41	26, 31, 57, 64	0
53	M7	183/183 (100%)	0.09	9 (4%) 35 18	34, 42, 105, 127	0
53	m7	155/183 (84%)	-0.34	1 (0%) 85 69	28, 38, 51, 81	0
54	M8	185/185 (100%)	-0.24	0 100 100	32, 42, 54, 65	0
54	m8	185/185 (100%)	-0.27	0 100 100	35, 45, 54, 62	0
55	M9	188/188 (100%)	0.34	8 (4%) 40 21	47, 63, 154, 163	0
55	m9	188/188 (100%)	0.20	4 (2%) 63 40	45, 56, 131, 144	0
56	N0	172/172 (100%)	-0.11	4 (2%) 61 38	39, 47, 62, 70	0
56	n0	172/172 (100%)	-0.27	3 (1%) 69 45	32, 39, 50, 60	0
57	N1	159/159 (100%)	-0.05	1 (0%) 85 69	36, 47, 89, 97	0
57	n1	159/159 (100%)	-0.27	0 100 100	33, 40, 77, 86	0
58	N2	100/120 (83%)	0.51	5 (5%) 34 18	78, 95, 113, 123	0
58	n2	98/120 (81%)	0.26	1 (1%) 79 59	69, 84, 97, 101	0
59	N3	136/136 (100%)	-0.20	2 (1%) 72 49	36, 47, 61, 72	0
59	n3	136/136 (100%)	-0.31	2 (1%) 72 49	27, 38, 55, 58	0
60	N4	98/155 (63%)	0.80	18 (18%) 3 2	47, 60, 151, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	n4	135/155 (87%)	0.41	10 (7%) 20 10	37, 85, 116, 135	0
61	N5	121/141 (85%)	-0.08	1 (0%) 82 64	43, 57, 74, 108	0
61	n5	120/141 (85%)	0.21	6 (5%) 34 18	46, 62, 81, 89	0
62	N6	126/126 (100%)	-0.35	1 (0%) 82 64	35, 52, 65, 75	0
62	n6	126/126 (100%)	-0.04	1 (0%) 82 64	42, 56, 74, 81	0
63	N7	135/135 (100%)	-0.06	0 100 100	65, 81, 95, 106	0
63	n7	135/135 (100%)	0.28	1 (0%) 84 66	71, 87, 108, 120	0
64	N8	148/148 (100%)	-0.26	0 100 100	26, 44, 68, 80	0
64	n8	148/148 (100%)	-0.27	0 100 100	30, 48, 69, 73	0
65	N9	58/58 (100%)	0.24	3 (5%) 33 17	34, 51, 102, 120	0
65	n9	58/58 (100%)	0.12	3 (5%) 33 17	31, 49, 78, 92	0
66	O0	97/104 (93%)	-0.09	1 (1%) 79 59	63, 72, 97, 105	0
66	o0	100/104 (96%)	0.15	2 (2%) 65 41	64, 75, 103, 114	0
67	O1	109/112 (97%)	0.19	3 (2%) 55 32	44, 57, 94, 110	0
67	o1	109/112 (97%)	-0.23	1 (0%) 81 61	37, 49, 87, 107	0
68	O2	127/129 (98%)	-0.32	2 (1%) 70 47	24, 39, 50, 71	0
68	o2	127/129 (98%)	-0.24	3 (2%) 59 36	25, 44, 57, 74	0
69	O3	106/106 (100%)	-0.31	0 100 100	32, 38, 57, 67	0
69	o3	106/106 (100%)	-0.32	2 (1%) 66 43	29, 36, 61, 74	0
70	O4	112/119 (94%)	0.27	5 (4%) 38 20	44, 62, 104, 116	0
70	o4	112/119 (94%)	0.44	2 (1%) 67 44	44, 64, 107, 117	0
71	O5	119/119 (100%)	-0.04	2 (1%) 69 45	41, 60, 68, 70	0
71	o5	119/119 (100%)	0.13	1 (0%) 82 64	50, 66, 76, 81	0
72	O6	99/99 (100%)	-0.07	1 (1%) 79 59	49, 60, 92, 109	0
72	o6	99/99 (100%)	-0.05	0 100 100	55, 68, 91, 115	0
73	O7	87/87 (100%)	0.08	4 (4%) 37 20	32, 38, 68, 97	0
73	o7	87/87 (100%)	0.11	4 (4%) 37 20	37, 41, 74, 110	0
74	O8	77/77 (100%)	0.11	1 (1%) 75 53	68, 82, 106, 117	0
74	o8	77/77 (100%)	0.22	0 100 100	70, 86, 107, 112	0
75	O9	50/50 (100%)	0.11	0 100 100	41, 45, 53, 58	0
75	o9	50/50 (100%)	0.09	0 100 100	43, 49, 60, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	Q0	52/52 (100%)	-0.22	0 100 100	45, 50, 74, 84	0
76	q0	52/52 (100%)	-0.49	1 (1%) 66 43	30, 37, 49, 58	0
77	Q1	25/25 (100%)	0.29	1 (4%) 42 23	49, 53, 62, 64	0
77	q1	25/25 (100%)	-0.10	0 100 100	39, 45, 56, 64	0
78	Q2	105/105 (100%)	-0.12	1 (0%) 79 59	33, 51, 75, 112	0
78	q2	105/105 (100%)	-0.27	0 100 100	37, 48, 66, 100	0
79	Q3	91/91 (100%)	-0.07	0 100 100	38, 49, 67, 83	0
79	q3	91/91 (100%)	0.03	2 (2%) 62 39	37, 49, 65, 76	0
80	e0	62/62 (100%)	0.37	5 (8%) 18 9	52, 76, 115, 124	0
81	e1	76/76 (100%)	1.34	16 (21%) 2 1	133, 145, 162, 169	0
82	m2	0/160	-	-	-	-
83	p0	143/311 (45%)	0.65	9 (6%) 26 13	84, 102, 169, 178	0
84	p1	0/47	-	-	-	-
85	p2	0/46	-	-	-	-
All	All	33063/35344 (93%)	-0.01	755 (2%) 61 38	24, 64, 126, 255	0

The worst 5 of 755 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	S5	37	GLN	8.1
35	SM	85	SER	7.5
81	e1	77	ALA	7.2
73	o7	88	ALA	7.0
60	N4	86	SER	6.4

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

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

6.3 Carbohydrates ⓘ

There are no 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
86	MG	6	1924	1/1	0.06	0.43	104,104,104,104	0
86	MG	1	3809	1/1	0.08	0.31	199,199,199,199	0
86	MG	5	3777	1/1	0.28	0.33	99,99,99,99	0
86	MG	2	1953	1/1	0.29	0.42	105,105,105,105	0
86	MG	1	3819	1/1	0.34	0.45	105,105,105,105	0
86	MG	4	222	1/1	0.38	0.43	89,89,89,89	0
86	MG	2	1968	1/1	0.41	0.52	112,112,112,112	0
86	MG	1	3856	1/1	0.44	0.30	93,93,93,93	0
86	MG	2	1990	1/1	0.45	0.41	110,110,110,110	0
86	MG	6	1909	1/1	0.45	0.37	99,99,99,99	0
86	MG	6	2012	1/1	0.47	0.28	137,137,137,137	0
86	MG	5	3790	1/1	0.47	0.43	89,89,89,89	0
86	MG	5	3887	1/1	0.48	0.44	91,91,91,91	0
86	MG	2	2002	1/1	0.50	0.39	102,102,102,102	0
86	MG	5	3466	1/1	0.52	0.38	98,98,98,98	0
86	MG	2	2017	1/1	0.53	0.24	75,75,75,75	0
86	MG	6	2036	1/1	0.54	0.46	97,97,97,97	0
86	MG	5	3901	1/1	0.54	0.26	148,148,148,148	0
86	MG	1	3594	1/1	0.55	0.39	67,67,67,67	0
86	MG	6	1966	1/1	0.56	0.37	82,82,82,82	0
86	MG	2	1959	1/1	0.58	0.43	97,97,97,97	0
86	MG	2	1954	1/1	0.58	0.26	96,96,96,96	0
86	MG	5	3784	1/1	0.59	0.38	82,82,82,82	0
86	MG	1	3405	1/1	0.60	0.39	97,97,97,97	0
86	MG	2	1975	1/1	0.61	0.49	81,81,81,81	0
86	MG	5	3800	1/1	0.61	0.33	75,75,75,75	0
86	MG	6	2018	1/1	0.63	0.27	111,111,111,111	0
86	MG	3	212	1/1	0.63	0.17	76,76,76,76	0
86	MG	2	1951	1/1	0.63	0.39	90,90,90,90	0
86	MG	2	1915	1/1	0.64	0.42	66,66,66,66	0
86	MG	2	2016	1/1	0.64	0.36	70,70,70,70	0
86	MG	1	3734	1/1	0.64	0.30	82,82,82,82	0
86	MG	5	3711	1/1	0.64	0.30	85,85,85,85	0
86	MG	2	1972	1/1	0.64	0.38	81,81,81,81	0
86	MG	1	3652	1/1	0.65	0.45	91,91,91,91	0
86	MG	5	3785	1/1	0.65	0.39	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	2	1963	1/1	0.65	0.20	135,135,135,135	0
86	MG	2	1969	1/1	0.66	0.36	93,93,93,93	0
86	MG	2	1986	1/1	0.66	0.30	102,102,102,102	0
86	MG	2	1978	1/1	0.67	0.32	91,91,91,91	0
86	MG	6	2042	1/1	0.67	0.47	90,90,90,90	0
86	MG	5	3447	1/1	0.67	0.23	56,56,56,56	0
86	MG	N5	201	1/1	0.67	0.28	73,73,73,73	0
86	MG	6	1907	1/1	0.67	0.35	64,64,64,64	0
86	MG	2	2019	1/1	0.67	0.43	71,71,71,71	0
86	MG	2	1952	1/1	0.68	0.33	92,92,92,92	0
86	MG	5	3479	1/1	0.68	0.39	63,63,63,63	0
86	MG	2	2022	1/1	0.68	0.28	108,108,108,108	0
86	MG	5	3419	1/1	0.68	0.32	72,72,72,72	0
86	MG	6	1904	1/1	0.68	0.35	69,69,69,69	0
86	MG	6	2037	1/1	0.69	0.45	92,92,92,92	0
87	OHX	5	4236	7/7	0.69	0.31	121,121,121,121	0
87	OHX	1	4191	7/7	0.70	0.19	179,179,179,179	0
87	OHX	1	4194	7/7	0.70	0.28	135,135,135,135	0
86	MG	6	1963	1/1	0.70	0.30	87,87,87,87	0
86	MG	2	1982	1/1	0.71	0.24	78,78,78,78	0
86	MG	Q2	502	1/1	0.72	0.17	58,58,58,58	0
86	MG	2	1976	1/1	0.72	0.31	57,57,57,57	0
86	MG	1	3676	1/1	0.72	0.42	69,69,69,69	0
86	MG	3	201	1/1	0.72	0.29	69,69,69,69	0
86	MG	3	209	1/1	0.72	0.26	60,60,60,60	0
86	MG	2	1928	1/1	0.72	0.41	78,78,78,78	0
86	MG	5	3448	1/1	0.72	0.27	64,64,64,64	0
86	MG	1	3757	1/1	0.72	0.28	100,100,100,100	0
86	MG	6	1998	1/1	0.72	0.29	98,98,98,98	0
86	MG	1	3629	1/1	0.72	0.25	71,71,71,71	0
86	MG	5	3811	1/1	0.73	0.28	95,95,95,95	0
86	MG	6	2033	1/1	0.73	0.23	71,71,71,71	0
86	MG	6	2205	1/1	0.73	0.24	67,67,67,67	0
86	MG	2	2009	1/1	0.73	0.32	72,72,72,72	0
86	MG	5	3679	1/1	0.73	0.21	93,93,93,93	0
86	MG	2	2001	1/1	0.73	0.34	107,107,107,107	0
86	MG	2	2018	1/1	0.74	0.36	79,79,79,79	0
86	MG	6	2026	1/1	0.74	0.45	87,87,87,87	0
86	MG	5	3797	1/1	0.74	0.27	86,86,86,86	0
86	MG	1	3672	1/1	0.74	0.43	61,61,61,61	0
86	MG	5	3651	1/1	0.74	0.21	88,88,88,88	0
86	MG	1	3503	1/1	0.75	0.30	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	MG	1	3651	1/1	0.75	0.24	66,66,66,66	0
87	OHX	1	4176	7/7	0.75	0.27	133,133,133,133	0
86	MG	1	3525	1/1	0.75	0.19	42,42,42,42	0
86	MG	5	3469	1/1	0.75	0.18	109,109,109,109	0
86	MG	S8	301	1/1	0.75	0.24	60,60,60,60	0
86	MG	2	1966	1/1	0.76	0.32	82,82,82,82	0
86	MG	6	1934	1/1	0.76	0.29	73,73,73,73	0
86	MG	5	3654	1/1	0.76	0.38	44,44,44,44	0
86	MG	1	3638	1/1	0.76	0.17	50,50,50,50	0
86	MG	5	3818	1/1	0.76	0.16	80,80,80,80	0
86	MG	5	3820	1/1	0.76	0.24	56,56,56,56	0
86	MG	5	3864	1/1	0.76	0.28	82,82,82,82	0
86	MG	5	3683	1/1	0.76	0.36	84,84,84,84	0
86	MG	1	3508	1/1	0.76	0.35	30,30,30,30	0
86	MG	5	3731	1/1	0.76	0.23	97,97,97,97	0
86	MG	5	3464	1/1	0.76	0.11	36,36,36,36	0
86	MG	2	2011	1/1	0.76	0.39	71,71,71,71	0
87	OHX	5	4215	7/7	0.76	0.23	143,143,143,143	0
86	MG	2	1949	1/1	0.76	0.30	57,57,57,57	0
86	MG	1	3738	1/1	0.77	0.20	35,35,35,35	0
86	MG	5	3695	1/1	0.77	0.18	51,51,51,51	0
86	MG	6	1920	1/1	0.77	0.39	63,63,63,63	0
86	MG	2	1948	1/1	0.77	0.23	85,85,85,85	0
86	MG	2	1960	1/1	0.77	0.24	61,61,61,61	0
86	MG	1	3494	1/1	0.77	0.32	78,78,78,78	0
86	MG	7	213	1/1	0.77	0.21	47,47,47,47	0
87	OHX	2	2165	7/7	0.77	0.24	134,134,134,134	0
86	MG	1	3714	1/1	0.77	0.36	78,78,78,78	0
86	MG	1	3531	1/1	0.77	0.35	62,62,62,62	0
86	MG	c7	201	1/1	0.77	0.28	71,71,71,71	0
87	OHX	6	2189	7/7	0.77	0.21	133,133,133,133	0
86	MG	3	208	1/1	0.77	0.26	79,79,79,79	0
86	MG	5	3807	1/1	0.77	0.21	56,56,56,56	0
87	OHX	5	4243	7/7	0.77	0.22	133,133,133,133	0
87	OHX	5	4245	7/7	0.77	0.20	151,151,151,151	0
88	ZN	D7	101	1/1	0.77	0.24	147,147,147,147	0
87	OHX	1	4131	7/7	0.78	0.18	149,149,149,149	0
86	MG	5	3555	1/1	0.78	0.33	34,34,34,34	0
86	MG	1	3475	1/1	0.78	0.32	74,74,74,74	0
86	MG	2	1946	1/1	0.78	0.27	80,80,80,80	0
87	OHX	1	4200	7/7	0.78	0.19	129,129,129,129	0
86	MG	1	3529	1/1	0.78	0.31	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	4172	7/7	0.78	0.17	165,165,165,165	0
86	MG	6	1933	1/1	0.78	0.44	65,65,65,65	0
86	MG	5	3894	1/1	0.78	0.21	38,38,38,38	0
87	OHX	5	4242	7/7	0.78	0.19	151,151,151,151	0
86	MG	5	3687	1/1	0.78	0.28	60,60,60,60	0
86	MG	2	1989	1/1	0.78	0.34	58,58,58,58	0
87	OHX	5	4247	7/7	0.78	0.20	141,141,141,141	0
86	MG	1	3723	1/1	0.78	0.43	42,42,42,42	0
86	MG	1	3649	1/1	0.79	0.24	46,46,46,46	0
87	OHX	1	4146	7/7	0.79	0.27	110,110,110,110	0
86	MG	4	204	1/1	0.79	0.35	70,70,70,70	0
87	OHX	1	4180	7/7	0.79	0.19	146,146,146,146	0
86	MG	1	3751	1/1	0.79	0.15	45,45,45,45	0
86	MG	5	3420	1/1	0.79	0.26	94,94,94,94	0
87	OHX	1	4199	7/7	0.79	0.19	138,138,138,138	0
86	MG	5	3698	1/1	0.79	0.15	44,44,44,44	0
87	OHX	6	2146	7/7	0.79	0.20	132,132,132,132	0
87	OHX	6	2183	7/7	0.79	0.21	132,132,132,132	0
87	OHX	6	2187	7/7	0.79	0.19	145,145,145,145	0
86	MG	5	3492	1/1	0.79	0.39	59,59,59,59	0
86	MG	2	1964	1/1	0.79	0.24	89,89,89,89	0
86	MG	5	3773	1/1	0.79	0.14	101,101,101,101	0
86	MG	5	3774	1/1	0.79	0.25	68,68,68,68	0
86	MG	5	3591	1/1	0.79	0.33	35,35,35,35	0
86	MG	5	3781	1/1	0.79	0.19	58,58,58,58	0
86	MG	6	1958	1/1	0.79	0.36	52,52,52,52	0
87	OHX	2	2164	7/7	0.79	0.15	165,165,165,165	0
87	OHX	5	4255	7/7	0.79	0.19	148,148,148,148	0
87	OHX	14	402	7/7	0.79	0.18	142,142,142,142	0
87	OHX	14	403	7/7	0.79	0.21	135,135,135,135	0
86	MG	5	3455	1/1	0.79	0.25	86,86,86,86	0
88	ZN	d7	101	1/1	0.79	0.23	142,142,142,142	0
86	MG	1	3795	1/1	0.80	0.16	70,70,70,70	0
86	MG	6	1911	1/1	0.80	0.30	77,77,77,77	0
87	OHX	1	4145	7/7	0.80	0.23	134,134,134,134	0
86	MG	5	3721	1/1	0.80	0.30	62,62,62,62	0
86	MG	5	3725	1/1	0.80	0.23	51,51,51,51	0
86	MG	2	1934	1/1	0.80	0.35	74,74,74,74	0
86	MG	2	1958	1/1	0.80	0.41	79,79,79,79	0
87	OHX	1	4192	7/7	0.80	0.20	139,139,139,139	0
86	MG	2	1938	1/1	0.80	0.38	62,62,62,62	0
86	MG	1	3864	1/1	0.80	0.14	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	2	1926	1/1	0.80	0.38	86,86,86,86	0
86	MG	S2	301	1/1	0.80	0.47	65,65,65,65	0
86	MG	1	3705	1/1	0.80	0.32	66,66,66,66	0
86	MG	2	1971	1/1	0.80	0.32	71,71,71,71	0
86	MG	5	3489	1/1	0.80	0.14	30,30,30,30	0
86	MG	2	1929	1/1	0.80	0.36	63,63,63,63	0
87	OHX	5	4180	7/7	0.80	0.30	111,111,111,111	0
87	OHX	5	4196	7/7	0.80	0.17	146,146,146,146	0
86	MG	5	3528	1/1	0.80	0.32	52,52,52,52	0
87	OHX	5	4233	7/7	0.80	0.18	141,141,141,141	0
86	MG	1	3419	1/1	0.80	0.26	82,82,82,82	0
86	MG	M3	202	1/1	0.80	0.34	88,88,88,88	0
86	MG	6	2032	1/1	0.80	0.34	81,81,81,81	0
86	MG	5	3652	1/1	0.80	0.41	71,71,71,71	0
86	MG	M3	203	1/1	0.80	0.17	39,39,39,39	0
87	OHX	5	4248	7/7	0.80	0.17	180,180,180,180	0
87	OHX	5	4249	7/7	0.80	0.13	223,223,223,223	0
86	MG	5	3891	1/1	0.80	0.41	82,82,82,82	0
86	MG	1	3618	1/1	0.80	0.15	60,60,60,60	0
86	MG	1	3420	1/1	0.80	0.37	67,67,67,67	0
86	MG	1	3442	1/1	0.80	0.28	25,25,25,25	0
86	MG	1	3770	1/1	0.80	0.32	60,60,60,60	0
87	OHX	1	4182	7/7	0.81	0.18	148,148,148,148	0
87	OHX	1	4190	7/7	0.81	0.20	137,137,137,137	0
86	MG	1	3671	1/1	0.81	0.14	52,52,52,52	0
86	MG	6	1935	1/1	0.81	0.22	52,52,52,52	0
86	MG	1	3753	1/1	0.81	0.22	52,52,52,52	0
86	MG	5	3809	1/1	0.81	0.12	152,152,152,152	0
86	MG	5	3433	1/1	0.81	0.27	75,75,75,75	0
86	MG	2	1979	1/1	0.81	0.32	56,56,56,56	0
86	MG	2	1996	1/1	0.81	0.28	93,93,93,93	0
86	MG	6	1968	1/1	0.81	0.32	68,68,68,68	0
86	MG	1	3687	1/1	0.81	0.23	84,84,84,84	0
87	OHX	5	4161	7/7	0.81	0.25	118,118,118,118	0
86	MG	1	3699	1/1	0.81	0.34	74,74,74,74	0
86	MG	2	1965	1/1	0.81	0.29	62,62,62,62	0
86	MG	1	3836	1/1	0.81	0.28	52,52,52,52	0
86	MG	5	3751	1/1	0.81	0.32	37,37,37,37	0
87	OHX	5	4228	7/7	0.81	0.20	137,137,137,137	0
87	OHX	5	4229	7/7	0.81	0.18	151,151,151,151	0
86	MG	7	214	1/1	0.81	0.23	55,55,55,55	0
86	MG	8	209	1/1	0.81	0.31	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	4239	7/7	0.81	0.23	118,118,118,118	0
86	MG	15	303	1/1	0.81	0.23	63,63,63,63	0
87	OHX	2	2160	7/7	0.81	0.19	148,148,148,148	0
87	OHX	2	2161	7/7	0.81	0.21	132,132,132,132	0
86	MG	1	3842	1/1	0.81	0.32	50,50,50,50	0
86	MG	1	3712	1/1	0.81	0.27	60,60,60,60	0
87	OHX	2	2179	7/7	0.81	0.15	167,167,167,167	0
86	MG	2	1943	1/1	0.81	0.26	67,67,67,67	0
86	MG	2	1988	1/1	0.81	0.19	66,66,66,66	0
86	MG	2	1961	1/1	0.81	0.28	55,55,55,55	0
87	OHX	m4	201	7/7	0.81	0.12	202,202,202,202	0
86	MG	5	3636	1/1	0.81	0.20	50,50,50,50	0
86	MG	1	3555	1/1	0.81	0.28	34,34,34,34	0
87	OHX	1	4197	7/7	0.82	0.16	142,142,142,142	0
86	MG	1	3483	1/1	0.82	0.28	51,51,51,51	0
86	MG	1	3547	1/1	0.82	0.18	61,61,61,61	0
87	OHX	M9	202	7/7	0.82	0.15	156,156,156,156	0
86	MG	5	3503	1/1	0.82	0.25	42,42,42,42	0
87	OHX	6	2168	7/7	0.82	0.17	143,143,143,143	0
86	MG	7	204	1/1	0.82	0.32	63,63,63,63	0
86	MG	6	1936	1/1	0.82	0.30	77,77,77,77	0
86	MG	6	2043	1/1	0.82	0.31	71,71,71,71	0
87	OHX	6	2190	7/7	0.82	0.18	152,152,152,152	0
87	OHX	5	4149	7/7	0.82	0.19	123,123,123,123	0
86	MG	8	202	1/1	0.82	0.35	60,60,60,60	0
87	OHX	5	4167	7/7	0.82	0.22	126,126,126,126	0
86	MG	2	1947	1/1	0.82	0.24	61,61,61,61	0
86	MG	1	3667	1/1	0.82	0.38	75,75,75,75	0
86	MG	o1	202	1/1	0.82	0.09	73,73,73,73	0
86	MG	6	1902	1/1	0.82	0.24	49,49,49,49	0
86	MG	2	1999	1/1	0.82	0.32	69,69,69,69	0
86	MG	1	3470	1/1	0.82	0.26	51,51,51,51	0
86	MG	5	3664	1/1	0.82	0.49	58,58,58,58	0
87	OHX	2	2178	7/7	0.82	0.15	172,172,172,172	0
87	OHX	5	4238	7/7	0.82	0.18	146,146,146,146	0
86	MG	1	3620	1/1	0.82	0.25	60,60,60,60	0
86	MG	1	3626	1/1	0.82	0.42	88,88,88,88	0
86	MG	6	2022	1/1	0.82	0.17	66,66,66,66	0
86	MG	2	1924	1/1	0.82	0.52	79,79,79,79	0
87	OHX	1	4164	7/7	0.82	0.16	148,148,148,148	0
86	MG	6	2028	1/1	0.82	0.24	75,75,75,75	0
86	MG	5	3710	1/1	0.82	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	5	3822	1/1	0.82	0.19	43,43,43,43	0
87	OHX	8	223	7/7	0.82	0.19	124,124,124,124	0
87	OHX	1	4185	7/7	0.82	0.21	131,131,131,131	0
86	MG	5	3854	1/1	0.82	0.27	56,56,56,56	0
87	OHX	l5	306	7/7	0.82	0.20	136,136,136,136	0
87	OHX	m1	202	7/7	0.82	0.17	140,140,140,140	0
86	MG	5	3862	1/1	0.82	0.33	81,81,81,81	0
86	MG	1	3700	1/1	0.82	0.28	42,42,42,42	0
86	MG	1	3478	1/1	0.82	0.16	42,42,42,42	0
86	MG	1	3849	1/1	0.83	0.38	52,52,52,52	0
87	OHX	6	2185	7/7	0.83	0.19	137,137,137,137	0
87	OHX	2	2176	7/7	0.83	0.18	152,152,152,152	0
86	MG	5	3640	1/1	0.83	0.26	39,39,39,39	0
86	MG	5	3736	1/1	0.83	0.28	65,65,65,65	0
87	OHX	6	2203	7/7	0.83	0.18	140,140,140,140	0
87	OHX	5	4116	7/7	0.83	0.23	118,118,118,118	0
86	MG	5	3860	1/1	0.83	0.17	62,62,62,62	0
86	MG	5	3749	1/1	0.83	0.24	57,57,57,57	0
86	MG	2	1980	1/1	0.83	0.35	67,67,67,67	0
86	MG	c7	202	1/1	0.83	0.31	72,72,72,72	0
87	OHX	1	4171	7/7	0.83	0.25	113,113,113,113	0
87	OHX	1	4174	7/7	0.83	0.17	149,149,149,149	0
86	MG	6	1967	1/1	0.83	0.22	72,72,72,72	0
86	MG	5	3657	1/1	0.83	0.13	42,42,42,42	0
86	MG	1	3480	1/1	0.83	0.26	71,71,71,71	0
86	MG	5	3675	1/1	0.83	0.22	66,66,66,66	0
87	OHX	1	4187	7/7	0.83	0.18	134,134,134,134	0
87	OHX	1	4189	7/7	0.83	0.23	124,124,124,124	0
86	MG	7	208	1/1	0.83	0.20	48,48,48,48	0
86	MG	5	3421	1/1	0.83	0.30	38,38,38,38	0
86	MG	6	1906	1/1	0.83	0.30	52,52,52,52	0
87	OHX	1	4193	7/7	0.83	0.20	121,121,121,121	0
86	MG	5	3794	1/1	0.83	0.15	55,55,55,55	0
86	MG	1	3612	1/1	0.83	0.12	43,43,43,43	0
86	MG	1	3769	1/1	0.83	0.26	56,56,56,56	0
87	OHX	5	4253	7/7	0.83	0.20	147,147,147,147	0
86	MG	1	3670	1/1	0.83	0.31	75,75,75,75	0
87	OHX	5	4256	7/7	0.83	0.20	123,123,123,123	0
87	OHX	7	225	7/7	0.83	0.16	138,138,138,138	0
87	OHX	1	4202	7/7	0.83	0.21	125,125,125,125	0
87	OHX	1	4207	7/7	0.83	0.21	133,133,133,133	0
87	OHX	4	238	7/7	0.83	0.22	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	M7	206	7/7	0.83	0.29	103,103,103,103	0
86	MG	5	3595	1/1	0.83	0.26	40,40,40,40	0
87	OHX	6	2134	7/7	0.83	0.19	128,128,128,128	0
86	MG	5	3607	1/1	0.83	0.23	53,53,53,53	0
86	MG	5	3615	1/1	0.83	0.22	47,47,47,47	0
87	OHX	1	4205	7/7	0.84	0.19	132,132,132,132	0
86	MG	2	1955	1/1	0.84	0.23	62,62,62,62	0
87	OHX	4	235	7/7	0.84	0.16	142,142,142,142	0
86	MG	2	1932	1/1	0.84	0.42	55,55,55,55	0
86	MG	5	3900	1/1	0.84	0.24	59,59,59,59	0
87	OHX	M7	207	7/7	0.84	0.20	132,132,132,132	0
86	MG	1	3863	1/1	0.84	0.10	54,54,54,54	0
86	MG	2	1991	1/1	0.84	0.17	94,94,94,94	0
86	MG	5	3430	1/1	0.84	0.32	76,76,76,76	0
86	MG	2	1993	1/1	0.84	0.17	68,68,68,68	0
87	OHX	6	2176	7/7	0.84	0.20	122,122,122,122	0
87	OHX	6	2182	7/7	0.84	0.17	137,137,137,137	0
86	MG	6	1939	1/1	0.84	0.38	59,59,59,59	0
87	OHX	6	2184	7/7	0.84	0.13	162,162,162,162	0
86	MG	6	1940	1/1	0.84	0.38	82,82,82,82	0
86	MG	6	1950	1/1	0.84	0.32	42,42,42,42	0
86	MG	1	3635	1/1	0.84	0.16	56,56,56,56	0
86	MG	5	3735	1/1	0.84	0.12	47,47,47,47	0
87	OHX	6	2192	7/7	0.84	0.14	169,169,169,169	0
87	OHX	2	2138	7/7	0.84	0.14	157,157,157,157	0
87	OHX	s1	303	7/7	0.84	0.16	155,155,155,155	0
86	MG	1	3636	1/1	0.84	0.39	65,65,65,65	0
86	MG	5	3738	1/1	0.84	0.26	66,66,66,66	0
87	OHX	2	2163	7/7	0.84	0.16	163,163,163,163	0
86	MG	5	3742	1/1	0.84	0.33	69,69,69,69	0
86	MG	1	3439	1/1	0.84	0.31	40,40,40,40	0
87	OHX	2	2166	7/7	0.84	0.14	167,167,167,167	0
86	MG	4	202	1/1	0.84	0.39	56,56,56,56	0
87	OHX	5	4203	7/7	0.84	0.22	126,126,126,126	0
87	OHX	5	4204	7/7	0.84	0.17	134,134,134,134	0
87	OHX	5	4212	7/7	0.84	0.18	138,138,138,138	0
86	MG	1	3640	1/1	0.84	0.26	59,59,59,59	0
86	MG	6	1984	1/1	0.84	0.30	73,73,73,73	0
87	OHX	1	4066	7/7	0.84	0.20	123,123,123,123	0
87	OHX	5	4231	7/7	0.84	0.23	124,124,124,124	0
87	OHX	5	4232	7/7	0.84	0.18	137,137,137,137	0
86	MG	4	218	1/1	0.84	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	2	1921	1/1	0.84	0.39	47,47,47,47	0
86	MG	5	3538	1/1	0.84	0.30	38,38,38,38	0
87	OHX	1	4149	7/7	0.84	0.17	144,144,144,144	0
86	MG	5	3542	1/1	0.84	0.30	34,34,34,34	0
86	MG	5	3789	1/1	0.84	0.14	37,37,37,37	0
86	MG	1	3443	1/1	0.84	0.20	80,80,80,80	0
86	MG	5	3571	1/1	0.84	0.39	29,29,29,29	0
86	MG	1	3449	1/1	0.84	0.18	40,40,40,40	0
86	MG	1	3758	1/1	0.84	0.15	48,48,48,48	0
86	MG	6	2027	1/1	0.84	0.20	105,105,105,105	0
86	MG	1	3457	1/1	0.84	0.26	27,27,27,27	0
86	MG	5	3635	1/1	0.84	0.38	85,85,85,85	0
86	MG	1	3554	1/1	0.84	0.23	49,49,49,49	0
86	MG	2	1923	1/1	0.84	0.36	59,59,59,59	0
86	MG	2	1907	1/1	0.84	0.43	56,56,56,56	0
86	MG	1	3818	1/1	0.84	0.15	51,51,51,51	0
86	MG	1	3610	1/1	0.84	0.37	57,57,57,57	0
86	MG	2	1977	1/1	0.84	0.25	86,86,86,86	0
86	MG	6	1917	1/1	0.84	0.28	53,53,53,53	0
86	MG	5	3881	1/1	0.84	0.31	36,36,36,36	0
86	MG	1	3693	1/1	0.84	0.34	44,44,44,44	0
86	MG	6	2006	1/1	0.85	0.16	58,58,58,58	0
86	MG	1	3806	1/1	0.85	0.23	57,57,57,57	0
86	MG	1	3688	1/1	0.85	0.21	50,50,50,50	0
86	MG	5	3766	1/1	0.85	0.13	44,44,44,44	0
86	MG	2	1910	1/1	0.85	0.41	56,56,56,56	0
86	MG	5	3544	1/1	0.85	0.26	66,66,66,66	0
86	MG	6	2024	1/1	0.85	0.21	76,76,76,76	0
86	MG	2	1904	1/1	0.85	0.38	70,70,70,70	0
86	MG	1	3543	1/1	0.85	0.33	35,35,35,35	0
86	MG	1	3839	1/1	0.85	0.36	47,47,47,47	0
87	OHX	6	2199	7/7	0.85	0.17	145,145,145,145	0
87	OHX	6	2202	7/7	0.85	0.20	141,141,141,141	0
87	OHX	2	2181	7/7	0.85	0.18	156,156,156,156	0
86	MG	2	1942	1/1	0.85	0.31	73,73,73,73	0
86	MG	2	1901	1/1	0.85	0.37	75,75,75,75	0
86	MG	5	3622	1/1	0.85	0.20	41,41,41,41	0
86	MG	1	3491	1/1	0.85	0.12	44,44,44,44	0
86	MG	1	3557	1/1	0.85	0.36	37,37,37,37	0
87	OHX	1	4151	7/7	0.85	0.19	130,130,130,130	0
86	MG	6	2041	1/1	0.85	0.30	52,52,52,52	0
87	OHX	1	4169	7/7	0.85	0.19	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	1	3586	1/1	0.85	0.33	50,50,50,50	0
86	MG	1	3737	1/1	0.85	0.21	50,50,50,50	0
87	OHX	1	4175	7/7	0.85	0.16	158,158,158,158	0
87	OHX	5	4214	7/7	0.85	0.19	138,138,138,138	0
86	MG	3	206	1/1	0.85	0.36	36,36,36,36	0
87	OHX	5	4221	7/7	0.85	0.23	119,119,119,119	0
87	OHX	5	4226	7/7	0.85	0.19	130,130,130,130	0
86	MG	5	3656	1/1	0.85	0.19	53,53,53,53	0
86	MG	1	3593	1/1	0.85	0.34	50,50,50,50	0
86	MG	5	3658	1/1	0.85	0.18	53,53,53,53	0
86	MG	5	3662	1/1	0.85	0.25	29,29,29,29	0
86	MG	1	3656	1/1	0.85	0.30	45,45,45,45	0
87	OHX	5	4235	7/7	0.85	0.15	153,153,153,153	0
86	MG	1	3456	1/1	0.85	0.42	59,59,59,59	0
86	MG	5	3873	1/1	0.85	0.27	25,25,25,25	0
86	MG	1	3609	1/1	0.85	0.35	72,72,72,72	0
86	MG	6	1951	1/1	0.85	0.39	63,63,63,63	0
86	MG	6	1952	1/1	0.85	0.30	61,61,61,61	0
86	MG	1	3499	1/1	0.85	0.26	33,33,33,33	0
86	MG	5	3896	1/1	0.85	0.09	73,73,73,73	0
86	MG	4	211	1/1	0.85	0.22	53,53,53,53	0
87	OHX	1	4201	7/7	0.85	0.14	157,157,157,157	0
86	MG	5	3705	1/1	0.85	0.27	67,67,67,67	0
86	MG	2	1962	1/1	0.85	0.46	72,72,72,72	0
86	MG	1	3468	1/1	0.85	0.23	46,46,46,46	0
86	MG	1	3784	1/1	0.85	0.13	55,55,55,55	0
86	MG	6	1977	1/1	0.85	0.28	46,46,46,46	0
87	OHX	L4	402	7/7	0.85	0.17	127,127,127,127	0
86	MG	6	1980	1/1	0.85	0.34	65,65,65,65	0
86	MG	1	3793	1/1	0.85	0.21	85,85,85,85	0
86	MG	2	1950	1/1	0.85	0.42	80,80,80,80	0
86	MG	6	1999	1/1	0.85	0.10	53,53,53,53	0
87	OHX	2	2135	7/7	0.85	0.18	131,131,131,131	0
87	OHX	6	2154	7/7	0.85	0.15	160,160,160,160	0
87	OHX	1	4209	7/7	0.86	0.19	133,133,133,133	0
87	OHX	1	4212	7/7	0.86	0.22	119,119,119,119	0
87	OHX	1	4216	7/7	0.86	0.20	128,128,128,128	0
86	MG	5	3487	1/1	0.86	0.30	50,50,50,50	0
86	MG	1	3659	1/1	0.86	0.29	28,28,28,28	0
86	MG	1	3502	1/1	0.86	0.36	29,29,29,29	0
86	MG	2	1936	1/1	0.86	0.40	49,49,49,49	0
86	MG	1	3402	1/1	0.86	0.42	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	1	3516	1/1	0.86	0.35	37,37,37,37	0
87	OHX	6	2104	7/7	0.86	0.18	124,124,124,124	0
87	OHX	6	2124	7/7	0.86	0.27	107,107,107,107	0
87	OHX	2	2140	7/7	0.86	0.17	156,156,156,156	0
87	OHX	2	2146	7/7	0.86	0.17	134,134,134,134	0
87	OHX	2	2150	7/7	0.86	0.13	159,159,159,159	0
86	MG	1	3522	1/1	0.86	0.26	76,76,76,76	0
86	MG	2	1994	1/1	0.86	0.38	83,83,83,83	0
87	OHX	6	2179	7/7	0.86	0.21	128,128,128,128	0
87	OHX	2	2162	7/7	0.86	0.15	149,149,149,149	0
86	MG	1	3623	1/1	0.86	0.12	40,40,40,40	0
86	MG	5	3557	1/1	0.86	0.31	47,47,47,47	0
86	MG	2	1922	1/1	0.86	0.34	67,67,67,67	0
86	MG	5	3575	1/1	0.86	0.40	39,39,39,39	0
87	OHX	6	2188	7/7	0.86	0.17	135,135,135,135	0
86	MG	5	3589	1/1	0.86	0.27	66,66,66,66	0
86	MG	1	3627	1/1	0.86	0.20	33,33,33,33	0
86	MG	2	1941	1/1	0.86	0.23	65,65,65,65	0
87	OHX	6	2195	7/7	0.86	0.13	167,167,167,167	0
86	MG	1	3429	1/1	0.86	0.45	42,42,42,42	0
86	MG	6	1923	1/1	0.86	0.28	69,69,69,69	0
87	OHX	1	4076	7/7	0.86	0.28	103,103,103,103	0
87	OHX	1	4084	7/7	0.86	0.20	113,113,113,113	0
87	OHX	c3	201	7/7	0.86	0.15	148,148,148,148	0
87	OHX	d4	202	7/7	0.86	0.13	151,151,151,151	0
87	OHX	1	4099	7/7	0.86	0.14	136,136,136,136	0
87	OHX	1	4104	7/7	0.86	0.14	153,153,153,153	0
87	OHX	1	4129	7/7	0.86	0.23	117,117,117,117	0
87	OHX	5	4163	7/7	0.86	0.16	135,135,135,135	0
86	MG	2	1917	1/1	0.86	0.37	56,56,56,56	0
87	OHX	1	4133	7/7	0.86	0.15	151,151,151,151	0
87	OHX	1	4136	7/7	0.86	0.20	115,115,115,115	0
87	OHX	5	4187	7/7	0.86	0.18	129,129,129,129	0
87	OHX	5	4195	7/7	0.86	0.23	112,112,112,112	0
87	OHX	1	4143	7/7	0.86	0.25	109,109,109,109	0
86	MG	1	3853	1/1	0.86	0.26	53,53,53,53	0
86	MG	2	1992	1/1	0.86	0.15	56,56,56,56	0
86	MG	1	3639	1/1	0.86	0.22	53,53,53,53	0
87	OHX	5	4213	7/7	0.86	0.18	131,131,131,131	0
86	MG	1	3490	1/1	0.86	0.26	33,33,33,33	0
87	OHX	1	4152	7/7	0.86	0.17	137,137,137,137	0
87	OHX	5	4218	7/7	0.86	0.22	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	1	3641	1/1	0.86	0.13	64,64,64,64	0
87	OHX	1	4165	7/7	0.86	0.15	149,149,149,149	0
86	MG	1	3645	1/1	0.86	0.21	46,46,46,46	0
87	OHX	1	4170	7/7	0.86	0.10	204,204,204,204	0
86	MG	6	1941	1/1	0.86	0.30	49,49,49,49	0
87	OHX	1	4173	7/7	0.86	0.23	110,110,110,110	0
86	MG	5	3828	1/1	0.86	0.18	91,91,91,91	0
86	MG	5	3853	1/1	0.86	0.34	53,53,53,53	0
86	MG	sM	401	1/1	0.86	0.15	42,42,42,42	0
86	MG	5	3411	1/1	0.86	0.27	38,38,38,38	0
87	OHX	1	4181	7/7	0.86	0.24	119,119,119,119	0
86	MG	6	1946	1/1	0.86	0.38	62,62,62,62	0
87	OHX	1	4184	7/7	0.86	0.19	130,130,130,130	0
87	OHX	5	4244	7/7	0.86	0.22	129,129,129,129	0
86	MG	1	3739	1/1	0.86	0.23	61,61,61,61	0
86	MG	5	3869	1/1	0.86	0.32	54,54,54,54	0
86	MG	1	3750	1/1	0.86	0.14	52,52,52,52	0
86	MG	2	2006	1/1	0.86	0.47	71,71,71,71	0
86	MG	1	3577	1/1	0.86	0.26	25,25,25,25	0
86	MG	5	3889	1/1	0.86	0.30	56,56,56,56	0
86	MG	5	3684	1/1	0.86	0.10	31,31,31,31	0
87	OHX	5	4257	7/7	0.86	0.16	148,148,148,148	0
86	MG	4	203	1/1	0.86	0.40	54,54,54,54	0
86	MG	6	1964	1/1	0.86	0.21	56,56,56,56	0
86	MG	2	2007	1/1	0.86	0.38	50,50,50,50	0
86	MG	1	3455	1/1	0.86	0.25	52,52,52,52	0
86	MG	4	216	1/1	0.86	0.22	45,45,45,45	0
86	MG	1	3764	1/1	0.86	0.16	49,49,49,49	0
86	MG	1	3768	1/1	0.86	0.14	54,54,54,54	0
86	MG	5	3481	1/1	0.86	0.27	40,40,40,40	0
87	OHX	1	4208	7/7	0.86	0.19	127,127,127,127	0
86	MG	n8	203	1/1	0.87	0.09	36,36,36,36	0
87	OHX	4	237	7/7	0.87	0.18	127,127,127,127	0
86	MG	5	3692	1/1	0.87	0.24	43,43,43,43	0
87	OHX	2	2093	7/7	0.87	0.15	141,141,141,141	0
87	OHX	2	2100	7/7	0.87	0.17	142,142,142,142	0
87	OHX	2	2120	7/7	0.87	0.17	132,132,132,132	0
86	MG	L5	301	1/1	0.87	0.29	62,62,62,62	0
87	OHX	2	2137	7/7	0.87	0.19	125,125,125,125	0
86	MG	1	3426	1/1	0.87	0.15	54,54,54,54	0
86	MG	5	3704	1/1	0.87	0.15	59,59,59,59	0
86	MG	5	3453	1/1	0.87	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	5	3708	1/1	0.87	0.24	50,50,50,50	0
87	OHX	6	2165	7/7	0.87	0.12	172,172,172,172	0
86	MG	2	1939	1/1	0.87	0.37	69,69,69,69	0
87	OHX	6	2171	7/7	0.87	0.17	143,143,143,143	0
87	OHX	6	2172	7/7	0.87	0.22	123,123,123,123	0
87	OHX	6	2173	7/7	0.87	0.15	149,149,149,149	0
86	MG	5	3459	1/1	0.87	0.23	30,30,30,30	0
87	OHX	6	2177	7/7	0.87	0.16	133,133,133,133	0
87	OHX	6	2178	7/7	0.87	0.15	148,148,148,148	0
86	MG	M7	204	1/1	0.87	0.15	35,35,35,35	0
86	MG	6	1971	1/1	0.87	0.28	67,67,67,67	0
86	MG	6	1975	1/1	0.87	0.21	62,62,62,62	0
86	MG	2	2183	1/1	0.87	0.20	84,84,84,84	0
86	MG	N8	201	1/1	0.87	0.12	27,27,27,27	0
87	OHX	2	2173	7/7	0.87	0.18	146,146,146,146	0
87	OHX	2	2175	7/7	0.87	0.15	151,151,151,151	0
86	MG	5	3484	1/1	0.87	0.22	66,66,66,66	0
86	MG	2	1919	1/1	0.87	0.44	70,70,70,70	0
86	MG	1	3485	1/1	0.87	0.29	43,43,43,43	0
87	OHX	6	2194	7/7	0.87	0.14	156,156,156,156	0
86	MG	1	3658	1/1	0.87	0.21	39,39,39,39	0
87	OHX	6	2198	7/7	0.87	0.17	134,134,134,134	0
86	MG	5	3765	1/1	0.87	0.23	75,75,75,75	0
86	MG	5	3500	1/1	0.87	0.26	38,38,38,38	0
86	MG	6	2003	1/1	0.87	0.19	96,96,96,96	0
86	MG	5	3505	1/1	0.87	0.26	49,49,49,49	0
86	MG	6	2005	1/1	0.87	0.23	54,54,54,54	0
86	MG	1	3616	1/1	0.87	0.17	39,39,39,39	0
86	MG	1	3859	1/1	0.87	0.16	41,41,41,41	0
86	MG	6	2017	1/1	0.87	0.13	51,51,51,51	0
86	MG	5	3550	1/1	0.87	0.39	41,41,41,41	0
87	OHX	1	4142	7/7	0.87	0.18	131,131,131,131	0
86	MG	1	3537	1/1	0.87	0.41	48,48,48,48	0
86	MG	2	1914	1/1	0.87	0.36	67,67,67,67	0
87	OHX	5	4179	7/7	0.87	0.15	159,159,159,159	0
86	MG	5	3570	1/1	0.87	0.30	33,33,33,33	0
87	OHX	1	4147	7/7	0.87	0.14	132,132,132,132	0
87	OHX	5	4191	7/7	0.87	0.17	128,128,128,128	0
87	OHX	5	4192	7/7	0.87	0.18	118,118,118,118	0
86	MG	1	3865	1/1	0.87	0.23	42,42,42,42	0
87	OHX	1	4150	7/7	0.87	0.16	141,141,141,141	0
86	MG	5	3573	1/1	0.87	0.29	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	1	3544	1/1	0.87	0.30	37,37,37,37	0
87	OHX	5	4210	7/7	0.87	0.15	136,136,136,136	0
87	OHX	5	4211	7/7	0.87	0.22	123,123,123,123	0
87	OHX	1	4157	7/7	0.87	0.17	136,136,136,136	0
86	MG	6	1922	1/1	0.87	0.34	53,53,53,53	0
86	MG	1	3401	1/1	0.87	0.25	45,45,45,45	0
86	MG	6	2031	1/1	0.87	0.31	65,65,65,65	0
86	MG	2	1909	1/1	0.87	0.34	70,70,70,70	0
86	MG	6	1929	1/1	0.87	0.34	54,54,54,54	0
87	OHX	1	4172	7/7	0.87	0.19	113,113,113,113	0
87	OHX	5	4227	7/7	0.87	0.12	165,165,165,165	0
86	MG	5	3619	1/1	0.87	0.20	43,43,43,43	0
86	MG	2	1944	1/1	0.87	0.26	62,62,62,62	0
86	MG	5	3625	1/1	0.87	0.26	37,37,37,37	0
86	MG	1	3556	1/1	0.87	0.36	31,31,31,31	0
86	MG	3	214	1/1	0.87	0.25	55,55,55,55	0
86	MG	5	3637	1/1	0.87	0.29	48,48,48,48	0
86	MG	5	3871	1/1	0.87	0.13	48,48,48,48	0
87	OHX	5	4237	7/7	0.87	0.12	173,173,173,173	0
86	MG	5	3638	1/1	0.87	0.19	53,53,53,53	0
86	MG	4	201	1/1	0.87	0.36	50,50,50,50	0
86	MG	1	3407	1/1	0.87	0.23	40,40,40,40	0
86	MG	1	3785	1/1	0.87	0.20	45,45,45,45	0
86	MG	1	3637	1/1	0.87	0.26	63,63,63,63	0
86	MG	5	3655	1/1	0.87	0.25	66,66,66,66	0
86	MG	1	3558	1/1	0.87	0.10	51,51,51,51	0
86	MG	5	3898	1/1	0.87	0.20	111,111,111,111	0
86	MG	4	214	1/1	0.87	0.19	62,62,62,62	0
87	OHX	5	4252	7/7	0.87	0.18	133,133,133,133	0
86	MG	1	3564	1/1	0.87	0.28	46,46,46,46	0
86	MG	5	4264	1/1	0.87	0.40	34,34,34,34	0
86	MG	4	217	1/1	0.87	0.26	67,67,67,67	0
86	MG	2	2004	1/1	0.87	0.21	61,61,61,61	0
87	OHX	7	223	7/7	0.87	0.16	141,141,141,141	0
86	MG	6	1959	1/1	0.87	0.37	59,59,59,59	0
86	MG	6	1960	1/1	0.87	0.33	42,42,42,42	0
87	OHX	1	4206	7/7	0.87	0.18	131,131,131,131	0
86	MG	5	3431	1/1	0.87	0.11	34,34,34,34	0
86	MG	5	3432	1/1	0.87	0.26	41,41,41,41	0
86	MG	2	1908	1/1	0.87	0.27	70,70,70,70	0
86	MG	n3	201	1/1	0.87	0.30	26,26,26,26	0
87	OHX	m7	206	7/7	0.87	0.20	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	1	4213	7/7	0.87	0.22	121,121,121,121	0
86	MG	n6	201	1/1	0.87	0.23	59,59,59,59	0
87	OHX	6	2163	7/7	0.88	0.16	137,137,137,137	0
86	MG	5	3852	1/1	0.88	0.09	50,50,50,50	0
87	OHX	6	2167	7/7	0.88	0.15	146,146,146,146	0
87	OHX	2	2180	7/7	0.88	0.19	140,140,140,140	0
86	MG	5	3666	1/1	0.88	0.24	43,43,43,43	0
86	MG	5	3668	1/1	0.88	0.19	30,30,30,30	0
86	MG	5	3491	1/1	0.88	0.11	49,49,49,49	0
86	MG	6	2035	1/1	0.88	0.33	56,56,56,56	0
87	OHX	1	4096	7/7	0.88	0.14	145,145,145,145	0
86	MG	N0	201	1/1	0.88	0.29	50,50,50,50	0
86	MG	N3	202	1/1	0.88	0.24	60,60,60,60	0
87	OHX	1	4115	7/7	0.88	0.17	131,131,131,131	0
87	OHX	1	4116	7/7	0.88	0.23	110,110,110,110	0
87	OHX	1	4119	7/7	0.88	0.17	124,124,124,124	0
87	OHX	1	4124	7/7	0.88	0.18	129,129,129,129	0
87	OHX	1	4125	7/7	0.88	0.17	138,138,138,138	0
86	MG	6	2039	1/1	0.88	0.38	70,70,70,70	0
86	MG	5	3526	1/1	0.88	0.20	52,52,52,52	0
86	MG	5	3875	1/1	0.88	0.35	37,37,37,37	0
87	OHX	1	4135	7/7	0.88	0.16	149,149,149,149	0
86	MG	1	3614	1/1	0.88	0.31	51,51,51,51	0
87	OHX	1	4137	7/7	0.88	0.18	131,131,131,131	0
86	MG	3	203	1/1	0.88	0.17	88,88,88,88	0
86	MG	1	3799	1/1	0.88	0.07	30,30,30,30	0
86	MG	1	3653	1/1	0.88	0.24	66,66,66,66	0
86	MG	5	3892	1/1	0.88	0.31	59,59,59,59	0
86	MG	5	3546	1/1	0.88	0.48	49,49,49,49	0
87	OHX	s8	303	7/7	0.88	0.14	150,150,150,150	0
86	MG	c1	201	1/1	0.88	0.23	51,51,51,51	0
86	MG	1	3691	1/1	0.88	0.14	36,36,36,36	0
86	MG	5	3716	1/1	0.88	0.10	48,48,48,48	0
86	MG	1	3498	1/1	0.88	0.26	43,43,43,43	0
87	OHX	5	4154	7/7	0.88	0.19	107,107,107,107	0
87	OHX	5	4158	7/7	0.88	0.21	118,118,118,118	0
87	OHX	1	4154	7/7	0.88	0.14	141,141,141,141	0
86	MG	5	3569	1/1	0.88	0.28	28,28,28,28	0
86	MG	5	3728	1/1	0.88	0.25	36,36,36,36	0
87	OHX	5	4171	7/7	0.88	0.17	140,140,140,140	0
86	MG	1	3579	1/1	0.88	0.29	27,27,27,27	0
86	MG	7	211	1/1	0.88	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	5	3403	1/1	0.88	0.34	52,52,52,52	0
87	OHX	5	4184	7/7	0.88	0.17	131,131,131,131	0
86	MG	1	3831	1/1	0.88	0.25	49,49,49,49	0
87	OHX	5	4189	7/7	0.88	0.16	134,134,134,134	0
87	OHX	5	4190	7/7	0.88	0.15	139,139,139,139	0
86	MG	8	201	1/1	0.88	0.27	39,39,39,39	0
86	MG	1	3832	1/1	0.88	0.31	24,24,24,24	0
86	MG	6	1914	1/1	0.88	0.31	71,71,71,71	0
86	MG	12	302	1/1	0.88	0.17	37,37,37,37	0
87	OHX	5	4200	7/7	0.88	0.20	120,120,120,120	0
86	MG	6	1915	1/1	0.88	0.34	53,53,53,53	0
87	OHX	1	4178	7/7	0.88	0.12	167,167,167,167	0
86	MG	5	3423	1/1	0.88	0.25	59,59,59,59	0
86	MG	2	1997	1/1	0.88	0.12	77,77,77,77	0
86	MG	1	3838	1/1	0.88	0.28	45,45,45,45	0
86	MG	1	3664	1/1	0.88	0.08	51,51,51,51	0
86	MG	q1	101	1/1	0.88	0.31	44,44,44,44	0
86	MG	4	212	1/1	0.88	0.29	55,55,55,55	0
87	OHX	5	4217	7/7	0.88	0.16	140,140,140,140	0
86	MG	1	3761	1/1	0.88	0.10	35,35,35,35	0
87	OHX	5	4220	7/7	0.88	0.16	147,147,147,147	0
87	OHX	2	2116	7/7	0.88	0.16	133,133,133,133	0
86	MG	5	3632	1/1	0.88	0.40	75,75,75,75	0
86	MG	4	215	1/1	0.88	0.10	53,53,53,53	0
87	OHX	2	2136	7/7	0.88	0.18	129,129,129,129	0
86	MG	1	3709	1/1	0.88	0.11	49,49,49,49	0
87	OHX	5	4230	7/7	0.88	0.15	137,137,137,137	0
87	OHX	1	4195	7/7	0.88	0.17	131,131,131,131	0
86	MG	1	3541	1/1	0.88	0.25	61,61,61,61	0
86	MG	1	3500	1/1	0.88	0.41	73,73,73,73	0
87	OHX	2	2144	7/7	0.88	0.20	124,124,124,124	0
86	MG	4	219	1/1	0.88	0.17	49,49,49,49	0
87	OHX	2	2148	7/7	0.88	0.12	167,167,167,167	0
87	OHX	2	2149	7/7	0.88	0.20	115,115,115,115	0
86	MG	6	1938	1/1	0.88	0.24	40,40,40,40	0
87	OHX	2	2151	7/7	0.88	0.13	159,159,159,159	0
87	OHX	2	2152	7/7	0.88	0.12	180,180,180,180	0
87	OHX	2	2157	7/7	0.88	0.10	221,221,221,221	0
87	OHX	2	2158	7/7	0.88	0.20	114,114,114,114	0
87	OHX	5	4246	7/7	0.88	0.14	138,138,138,138	0
87	OHX	2	2159	7/7	0.88	0.09	276,276,276,276	0
86	MG	1	3404	1/1	0.88	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	3	224	7/7	0.88	0.13	154,154,154,154	0
87	OHX	4	234	7/7	0.88	0.19	113,113,113,113	0
86	MG	5	3801	1/1	0.88	0.17	54,54,54,54	0
87	OHX	5	4254	7/7	0.88	0.19	138,138,138,138	0
87	OHX	4	236	7/7	0.88	0.19	134,134,134,134	0
86	MG	5	3472	1/1	0.88	0.11	34,34,34,34	0
86	MG	1	3862	1/1	0.88	0.16	58,58,58,58	0
86	MG	5	3480	1/1	0.88	0.26	64,64,64,64	0
86	MG	5	3814	1/1	0.88	0.12	72,72,72,72	0
86	MG	M1	201	1/1	0.88	0.29	73,73,73,73	0
87	OHX	2	2172	7/7	0.88	0.18	145,145,145,145	0
86	MG	1	3725	1/1	0.88	0.11	53,53,53,53	0
87	OHX	6	2114	7/7	0.88	0.16	130,130,130,130	0
87	OHX	2	2174	7/7	0.88	0.16	138,138,138,138	0
86	MG	1	3410	1/1	0.88	0.23	46,46,46,46	0
87	OHX	6	2142	7/7	0.88	0.18	126,126,126,126	0
87	OHX	m8	201	7/7	0.88	0.18	129,129,129,129	0
86	MG	1	3572	1/1	0.88	0.37	42,42,42,42	0
86	MG	5	3847	1/1	0.88	0.11	51,51,51,51	0
87	OHX	2	2154	7/7	0.89	0.13	162,162,162,162	0
87	OHX	2	2155	7/7	0.89	0.13	145,145,145,145	0
87	OHX	2	2156	7/7	0.89	0.16	141,141,141,141	0
86	MG	5	3498	1/1	0.89	0.21	43,43,43,43	0
86	MG	2	1983	1/1	0.89	0.18	66,66,66,66	0
86	MG	5	3758	1/1	0.89	0.08	47,47,47,47	0
86	MG	5	3502	1/1	0.89	0.14	43,43,43,43	0
86	MG	1	3860	1/1	0.89	0.14	91,91,91,91	0
86	MG	6	2000	1/1	0.89	0.12	94,94,94,94	0
86	MG	5	3515	1/1	0.89	0.22	35,35,35,35	0
86	MG	2	1945	1/1	0.89	0.23	60,60,60,60	0
86	MG	1	3634	1/1	0.89	0.15	61,61,61,61	0
86	MG	5	3534	1/1	0.89	0.20	50,50,50,50	0
86	MG	1	3686	1/1	0.89	0.15	41,41,41,41	0
86	MG	5	3786	1/1	0.89	0.15	78,78,78,78	0
87	OHX	6	2170	7/7	0.89	0.15	139,139,139,139	0
86	MG	5	3788	1/1	0.89	0.28	31,31,31,31	0
86	MG	2	1987	1/1	0.89	0.26	70,70,70,70	0
86	MG	6	2014	1/1	0.89	0.19	67,67,67,67	0
86	MG	6	2016	1/1	0.89	0.35	49,49,49,49	0
86	MG	1	3867	1/1	0.89	0.26	63,63,63,63	0
86	MG	5	3551	1/1	0.89	0.34	51,51,51,51	0
86	MG	1	3565	1/1	0.89	0.27	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	6	2180	7/7	0.89	0.20	132,132,132,132	0
87	OHX	S8	302	7/7	0.89	0.12	154,154,154,154	0
87	OHX	1	4031	7/7	0.89	0.18	108,108,108,108	0
87	OHX	1	4039	7/7	0.89	0.17	119,119,119,119	0
87	OHX	1	4065	7/7	0.89	0.14	140,140,140,140	0
86	MG	1	3427	1/1	0.89	0.22	42,42,42,42	0
87	OHX	1	4073	7/7	0.89	0.19	114,114,114,114	0
86	MG	5	3562	1/1	0.89	0.37	34,34,34,34	0
86	MG	6	1916	1/1	0.89	0.33	62,62,62,62	0
87	OHX	1	4093	7/7	0.89	0.15	129,129,129,129	0
87	OHX	6	2193	7/7	0.89	0.13	173,173,173,173	0
86	MG	1	3774	1/1	0.89	0.11	52,52,52,52	0
86	MG	6	1918	1/1	0.89	0.34	67,67,67,67	0
86	MG	3	207	1/1	0.89	0.31	66,66,66,66	0
87	OHX	1	4113	7/7	0.89	0.15	126,126,126,126	0
86	MG	5	3574	1/1	0.89	0.29	31,31,31,31	0
86	MG	1	3775	1/1	0.89	0.15	52,52,52,52	0
86	MG	5	3581	1/1	0.89	0.25	38,38,38,38	0
86	MG	5	3849	1/1	0.89	0.18	51,51,51,51	0
86	MG	5	3583	1/1	0.89	0.30	36,36,36,36	0
86	MG	1	3779	1/1	0.89	0.21	70,70,70,70	0
87	OHX	d9	102	7/7	0.89	0.14	153,153,153,153	0
87	OHX	5	4103	7/7	0.89	0.14	142,142,142,142	0
87	OHX	5	4106	7/7	0.89	0.19	114,114,114,114	0
86	MG	3	211	1/1	0.89	0.12	75,75,75,75	0
87	OHX	5	4125	7/7	0.89	0.17	119,119,119,119	0
87	OHX	5	4135	7/7	0.89	0.17	121,121,121,121	0
87	OHX	5	4146	7/7	0.89	0.22	121,121,121,121	0
87	OHX	5	4147	7/7	0.89	0.14	135,135,135,135	0
87	OHX	5	4148	7/7	0.89	0.19	122,122,122,122	0
86	MG	6	1926	1/1	0.89	0.27	51,51,51,51	0
87	OHX	1	4134	7/7	0.89	0.15	144,144,144,144	0
87	OHX	5	4156	7/7	0.89	0.17	124,124,124,124	0
86	MG	5	3602	1/1	0.89	0.09	42,42,42,42	0
86	MG	1	3783	1/1	0.89	0.14	44,44,44,44	0
86	MG	6	1930	1/1	0.89	0.19	55,55,55,55	0
87	OHX	5	4165	7/7	0.89	0.16	131,131,131,131	0
87	OHX	5	4166	7/7	0.89	0.19	105,105,105,105	0
87	OHX	1	4141	7/7	0.89	0.19	122,122,122,122	0
87	OHX	5	4168	7/7	0.89	0.17	118,118,118,118	0
86	MG	6	1932	1/1	0.89	0.21	47,47,47,47	0
86	MG	2	1905	1/1	0.89	0.38	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	4176	7/7	0.89	0.17	127,127,127,127	0
86	MG	1	3697	1/1	0.89	0.15	47,47,47,47	0
86	MG	1	3788	1/1	0.89	0.18	48,48,48,48	0
86	MG	1	3437	1/1	0.89	0.24	33,33,33,33	0
87	OHX	5	4186	7/7	0.89	0.21	108,108,108,108	0
86	MG	2	2013	1/1	0.89	0.33	69,69,69,69	0
86	MG	4	209	1/1	0.89	0.33	49,49,49,49	0
86	MG	1	3701	1/1	0.89	0.15	42,42,42,42	0
86	MG	1	3532	1/1	0.89	0.26	26,26,26,26	0
87	OHX	1	4153	7/7	0.89	0.15	135,135,135,135	0
86	MG	2	2014	1/1	0.89	0.38	66,66,66,66	0
86	MG	5	3409	1/1	0.89	0.28	43,43,43,43	0
87	OHX	1	4162	7/7	0.89	0.15	133,133,133,133	0
87	OHX	5	4201	7/7	0.89	0.19	113,113,113,113	0
86	MG	1	3539	1/1	0.89	0.14	40,40,40,40	0
86	MG	5	3412	1/1	0.89	0.12	36,36,36,36	0
87	OHX	5	4205	7/7	0.89	0.20	116,116,116,116	0
87	OHX	1	4167	7/7	0.89	0.14	147,147,147,147	0
87	OHX	1	4168	7/7	0.89	0.13	150,150,150,150	0
86	MG	2	1912	1/1	0.89	0.27	63,63,63,63	0
86	MG	1	3826	1/1	0.89	0.19	66,66,66,66	0
86	MG	7	207	1/1	0.89	0.16	51,51,51,51	0
86	MG	6	1955	1/1	0.89	0.34	41,41,41,41	0
86	MG	7	209	1/1	0.89	0.25	44,44,44,44	0
86	MG	2	1930	1/1	0.89	0.20	61,61,61,61	0
87	OHX	5	4219	7/7	0.89	0.17	126,126,126,126	0
86	MG	5	3426	1/1	0.89	0.24	38,38,38,38	0
86	MG	1	3495	1/1	0.89	0.20	41,41,41,41	0
87	OHX	5	4223	7/7	0.89	0.18	133,133,133,133	0
87	OHX	5	4225	7/7	0.89	0.16	131,131,131,131	0
86	MG	1	3835	1/1	0.89	0.27	23,23,23,23	0
86	MG	6	1961	1/1	0.89	0.32	73,73,73,73	0
86	MG	8	204	1/1	0.89	0.32	47,47,47,47	0
86	MG	8	205	1/1	0.89	0.19	68,68,68,68	0
86	MG	8	206	1/1	0.89	0.22	51,51,51,51	0
86	MG	1	3545	1/1	0.89	0.15	35,35,35,35	0
87	OHX	1	4186	7/7	0.89	0.20	105,105,105,105	0
86	MG	5	3440	1/1	0.89	0.28	31,31,31,31	0
87	OHX	1	4188	7/7	0.89	0.15	140,140,140,140	0
86	MG	1	3617	1/1	0.89	0.16	35,35,35,35	0
86	MG	m5	304	1/1	0.89	0.20	93,93,93,93	0
86	MG	5	3685	1/1	0.89	0.13	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	6	1965	1/1	0.89	0.20	65,65,65,65	0
87	OHX	5	4240	7/7	0.89	0.12	159,159,159,159	0
86	MG	2	1974	1/1	0.89	0.29	65,65,65,65	0
86	MG	5	3454	1/1	0.89	0.17	44,44,44,44	0
86	MG	1	3841	1/1	0.89	0.27	36,36,36,36	0
86	MG	2	1913	1/1	0.89	0.31	65,65,65,65	0
86	MG	5	3463	1/1	0.89	0.22	49,49,49,49	0
86	MG	6	1970	1/1	0.89	0.23	60,60,60,60	0
86	MG	1	3666	1/1	0.89	0.19	44,44,44,44	0
87	OHX	2	2129	7/7	0.89	0.14	148,148,148,148	0
87	OHX	1	4204	7/7	0.89	0.19	120,120,120,120	0
87	OHX	2	2134	7/7	0.89	0.13	145,145,145,145	0
86	MG	1	3850	1/1	0.89	0.21	43,43,43,43	0
86	MG	N3	203	1/1	0.89	0.30	53,53,53,53	0
86	MG	6	1978	1/1	0.89	0.17	71,71,71,71	0
86	MG	1	3413	1/1	0.89	0.44	59,59,59,59	0
87	OHX	5	4258	7/7	0.89	0.16	131,131,131,131	0
87	OHX	5	4259	7/7	0.89	0.13	153,153,153,153	0
86	MG	5	3726	1/1	0.89	0.21	44,44,44,44	0
86	MG	6	1983	1/1	0.89	0.15	78,78,78,78	0
87	OHX	8	222	7/7	0.89	0.17	133,133,133,133	0
87	OHX	1	4215	7/7	0.89	0.13	155,155,155,155	0
87	OHX	2	2145	7/7	0.89	0.12	159,159,159,159	0
87	OHX	1	4217	7/7	0.89	0.18	147,147,147,147	0
86	MG	1	3458	1/1	0.89	0.19	40,40,40,40	0
87	OHX	19	600	7/7	0.89	0.17	119,119,119,119	0
86	MG	6	1986	1/1	0.89	0.12	65,65,65,65	0
86	MG	6	1990	1/1	0.89	0.32	70,70,70,70	0
86	MG	6	1993	1/1	0.89	0.31	55,55,55,55	0
86	MG	6	1994	1/1	0.89	0.07	43,43,43,43	0
86	MG	5	3748	1/1	0.89	0.24	41,41,41,41	0
87	OHX	L3	404	7/7	0.89	0.14	154,154,154,154	0
87	OHX	6	2175	7/7	0.90	0.20	113,113,113,113	0
87	OHX	1	4098	7/7	0.90	0.17	122,122,122,122	0
86	MG	5	3882	1/1	0.90	0.36	57,57,57,57	0
87	OHX	1	4103	7/7	0.90	0.17	115,115,115,115	0
86	MG	1	3601	1/1	0.90	0.19	36,36,36,36	0
86	MG	2	1973	1/1	0.90	0.27	75,75,75,75	0
86	MG	1	3717	1/1	0.90	0.19	46,46,46,46	0
86	MG	5	3475	1/1	0.90	0.23	76,76,76,76	0
86	MG	1	3718	1/1	0.90	0.28	68,68,68,68	0
87	OHX	1	4122	7/7	0.90	0.16	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	2	2020	1/1	0.90	0.37	59,59,59,59	0
86	MG	5	3897	1/1	0.90	0.28	61,61,61,61	0
87	OHX	1	4127	7/7	0.90	0.16	132,132,132,132	0
86	MG	6	2019	1/1	0.90	0.18	88,88,88,88	0
87	OHX	6	2191	7/7	0.90	0.14	151,151,151,151	0
86	MG	5	3670	1/1	0.90	0.15	38,38,38,38	0
86	MG	2	2015	1/1	0.90	0.39	61,61,61,61	0
86	MG	5	4261	1/1	0.90	0.20	35,35,35,35	0
86	MG	1	3821	1/1	0.90	0.12	44,44,44,44	0
87	OHX	6	2197	7/7	0.90	0.18	132,132,132,132	0
86	MG	4	213	1/1	0.90	0.17	35,35,35,35	0
86	MG	1	3727	1/1	0.90	0.16	44,44,44,44	0
87	OHX	6	2200	7/7	0.90	0.15	139,139,139,139	0
87	OHX	1	4138	7/7	0.90	0.18	109,109,109,109	0
86	MG	1	3517	1/1	0.90	0.34	37,37,37,37	0
86	MG	5	3495	1/1	0.90	0.21	28,28,28,28	0
86	MG	1	3735	1/1	0.90	0.16	64,64,64,64	0
87	OHX	1	4144	7/7	0.90	0.17	126,126,126,126	0
86	MG	1	3518	1/1	0.90	0.29	32,32,32,32	0
86	MG	5	3697	1/1	0.90	0.26	72,72,72,72	0
87	OHX	5	4095	7/7	0.90	0.22	106,106,106,106	0
86	MG	2	1970	1/1	0.90	0.22	72,72,72,72	0
86	MG	1	3523	1/1	0.90	0.24	55,55,55,55	0
87	OHX	5	4108	7/7	0.90	0.14	139,139,139,139	0
86	MG	2	2005	1/1	0.90	0.09	59,59,59,59	0
87	OHX	5	4118	7/7	0.90	0.15	127,127,127,127	0
86	MG	1	3560	1/1	0.90	0.27	26,26,26,26	0
86	MG	5	3517	1/1	0.90	0.27	36,36,36,36	0
87	OHX	5	4145	7/7	0.90	0.15	121,121,121,121	0
86	MG	5	3520	1/1	0.90	0.28	35,35,35,35	0
86	MG	8	210	1/1	0.90	0.33	53,53,53,53	0
86	MG	5	3521	1/1	0.90	0.32	40,40,40,40	0
87	OHX	1	4158	7/7	0.90	0.19	128,128,128,128	0
86	MG	l5	302	1/1	0.90	0.24	63,63,63,63	0
87	OHX	5	4155	7/7	0.90	0.18	120,120,120,120	0
86	MG	5	3525	1/1	0.90	0.29	30,30,30,30	0
86	MG	1	3752	1/1	0.90	0.29	60,60,60,60	0
87	OHX	5	4159	7/7	0.90	0.14	137,137,137,137	0
86	MG	m7	201	1/1	0.90	0.27	32,32,32,32	0
86	MG	1	3845	1/1	0.90	0.25	49,49,49,49	0
87	OHX	5	4164	7/7	0.90	0.14	129,129,129,129	0
86	MG	5	3727	1/1	0.90	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	5	3529	1/1	0.90	0.17	29,29,29,29	0
86	MG	1	3848	1/1	0.90	0.44	61,61,61,61	0
86	MG	o4	201	1/1	0.90	0.24	64,64,64,64	0
87	OHX	5	4169	7/7	0.90	0.19	111,111,111,111	0
86	MG	5	3537	1/1	0.90	0.35	45,45,45,45	0
87	OHX	2	2091	7/7	0.90	0.15	132,132,132,132	0
86	MG	M7	201	1/1	0.90	0.36	62,62,62,62	0
86	MG	6	2204	1/1	0.90	0.19	57,57,57,57	0
87	OHX	2	2112	7/7	0.90	0.12	149,149,149,149	0
87	OHX	1	4179	7/7	0.90	0.14	139,139,139,139	0
86	MG	5	3741	1/1	0.90	0.17	42,42,42,42	0
86	MG	5	3543	1/1	0.90	0.27	30,30,30,30	0
87	OHX	2	2128	7/7	0.90	0.15	127,127,127,127	0
86	MG	1	3624	1/1	0.90	0.18	49,49,49,49	0
86	MG	1	3561	1/1	0.90	0.25	40,40,40,40	0
86	MG	1	3851	1/1	0.90	0.34	50,50,50,50	0
87	OHX	5	4193	7/7	0.90	0.17	117,117,117,117	0
87	OHX	5	4194	7/7	0.90	0.19	121,121,121,121	0
86	MG	1	3492	1/1	0.90	0.22	28,28,28,28	0
86	MG	5	3552	1/1	0.90	0.30	32,32,32,32	0
86	MG	S2	302	1/1	0.90	0.46	69,69,69,69	0
86	MG	sM	402	1/1	0.90	0.11	45,45,45,45	0
87	OHX	2	2141	7/7	0.90	0.14	154,154,154,154	0
86	MG	5	3559	1/1	0.90	0.18	48,48,48,48	0
86	MG	1	3465	1/1	0.90	0.17	45,45,45,45	0
86	MG	5	3565	1/1	0.90	0.32	29,29,29,29	0
86	MG	5	3782	1/1	0.90	0.09	62,62,62,62	0
86	MG	5	3568	1/1	0.90	0.28	28,28,28,28	0
86	MG	5	3404	1/1	0.90	0.14	46,46,46,46	0
86	MG	1	3575	1/1	0.90	0.28	40,40,40,40	0
86	MG	6	1901	1/1	0.90	0.24	47,47,47,47	0
86	MG	1	3535	1/1	0.90	0.39	29,29,29,29	0
86	MG	5	3414	1/1	0.90	0.17	50,50,50,50	0
86	MG	5	3417	1/1	0.90	0.30	24,24,24,24	0
86	MG	1	3438	1/1	0.90	0.24	48,48,48,48	0
86	MG	1	3771	1/1	0.90	0.11	86,86,86,86	0
86	MG	5	3584	1/1	0.90	0.28	44,44,44,44	0
86	MG	1	3772	1/1	0.90	0.23	31,31,31,31	0
87	OHX	1	4210	7/7	0.90	0.20	115,115,115,115	0
87	OHX	1	4211	7/7	0.90	0.17	126,126,126,126	0
86	MG	5	3590	1/1	0.90	0.31	27,27,27,27	0
86	MG	5	3810	1/1	0.90	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	2	1981	1/1	0.90	0.34	60,60,60,60	0
86	MG	5	3813	1/1	0.90	0.11	36,36,36,36	0
86	MG	5	3425	1/1	0.90	0.14	42,42,42,42	0
86	MG	6	1910	1/1	0.90	0.25	49,49,49,49	0
87	OHX	5	4234	7/7	0.90	0.18	125,125,125,125	0
87	OHX	3	225	7/7	0.90	0.18	124,124,124,124	0
87	OHX	2	2170	7/7	0.90	0.15	143,143,143,143	0
86	MG	1	3694	1/1	0.90	0.09	45,45,45,45	0
86	MG	6	1913	1/1	0.90	0.29	36,36,36,36	0
86	MG	6	1987	1/1	0.90	0.10	45,45,45,45	0
86	MG	5	3829	1/1	0.90	0.19	60,60,60,60	0
86	MG	5	3834	1/1	0.90	0.22	28,28,28,28	0
87	OHX	2	2177	7/7	0.90	0.16	134,134,134,134	0
86	MG	6	1989	1/1	0.90	0.26	66,66,66,66	0
86	MG	5	3436	1/1	0.90	0.22	46,46,46,46	0
87	OHX	M8	201	7/7	0.90	0.17	126,126,126,126	0
86	MG	1	3777	1/1	0.90	0.12	62,62,62,62	0
87	OHX	6	2102	7/7	0.90	0.17	114,114,114,114	0
86	MG	1	3440	1/1	0.90	0.29	39,39,39,39	0
87	OHX	5	4250	7/7	0.90	0.20	99,99,99,99	0
87	OHX	5	4251	7/7	0.90	0.13	154,154,154,154	0
86	MG	1	3782	1/1	0.90	0.24	65,65,65,65	0
86	MG	1	3417	1/1	0.90	0.21	43,43,43,43	0
86	MG	1	3597	1/1	0.90	0.32	21,21,21,21	0
87	OHX	6	2138	7/7	0.90	0.17	122,122,122,122	0
86	MG	1	3644	1/1	0.90	0.24	45,45,45,45	0
86	MG	5	3867	1/1	0.90	0.10	42,42,42,42	0
87	OHX	6	2148	7/7	0.90	0.14	135,135,135,135	0
87	OHX	6	2150	7/7	0.90	0.15	150,150,150,150	0
87	OHX	1	4067	7/7	0.90	0.18	118,118,118,118	0
87	OHX	6	2155	7/7	0.90	0.19	133,133,133,133	0
87	OHX	6	2158	7/7	0.90	0.19	125,125,125,125	0
87	OHX	6	2162	7/7	0.90	0.11	182,182,182,182	0
87	OHX	8	225	7/7	0.90	0.18	118,118,118,118	0
87	OHX	8	226	7/7	0.90	0.18	130,130,130,130	0
86	MG	5	3644	1/1	0.90	0.35	58,58,58,58	0
87	OHX	1	4074	7/7	0.90	0.14	128,128,128,128	0
87	OHX	6	2166	7/7	0.90	0.21	113,113,113,113	0
86	MG	5	3458	1/1	0.90	0.08	67,67,67,67	0
87	OHX	m0	302	7/7	0.90	0.19	112,112,112,112	0
87	OHX	1	4081	7/7	0.90	0.20	118,118,118,118	0
86	MG	1	3599	1/1	0.90	0.31	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	1	4091	7/7	0.90	0.18	120,120,120,120	0
86	MG	3	213	1/1	0.90	0.33	57,57,57,57	0
87	OHX	o9	101	7/7	0.90	0.22	107,107,107,107	0
86	MG	1	3646	1/1	0.90	0.21	67,67,67,67	0
87	OHX	6	2174	7/7	0.90	0.20	103,103,103,103	0
86	MG	5	3629	1/1	0.91	0.18	61,61,61,61	0
87	OHX	6	2196	7/7	0.91	0.17	134,134,134,134	0
86	MG	1	3524	1/1	0.91	0.27	29,29,29,29	0
86	MG	5	3482	1/1	0.91	0.34	61,61,61,61	0
87	OHX	2	2122	7/7	0.91	0.14	137,137,137,137	0
87	OHX	2	2123	7/7	0.91	0.14	132,132,132,132	0
86	MG	6	1942	1/1	0.91	0.22	34,34,34,34	0
86	MG	L7	302	1/1	0.91	0.17	48,48,48,48	0
86	MG	M0	302	1/1	0.91	0.09	49,49,49,49	0
87	OHX	1	4163	7/7	0.91	0.15	125,125,125,125	0
86	MG	1	3605	1/1	0.91	0.20	37,37,37,37	0
86	MG	1	3704	1/1	0.91	0.27	49,49,49,49	0
87	OHX	1	4166	7/7	0.91	0.17	134,134,134,134	0
87	OHX	5	4022	7/7	0.91	0.14	144,144,144,144	0
86	MG	6	2038	1/1	0.91	0.35	66,66,66,66	0
87	OHX	5	4099	7/7	0.91	0.17	112,112,112,112	0
86	MG	1	3496	1/1	0.91	0.18	46,46,46,46	0
86	MG	M5	302	1/1	0.91	0.34	54,54,54,54	0
86	MG	5	3501	1/1	0.91	0.25	27,27,27,27	0
87	OHX	5	4115	7/7	0.91	0.16	123,123,123,123	0
87	OHX	2	2143	7/7	0.91	0.15	132,132,132,132	0
86	MG	1	3526	1/1	0.91	0.23	27,27,27,27	0
86	MG	2	1957	1/1	0.91	0.30	72,72,72,72	0
86	MG	M9	201	1/1	0.91	0.39	66,66,66,66	0
86	MG	1	3861	1/1	0.91	0.27	55,55,55,55	0
86	MG	s8	301	1/1	0.91	0.17	51,51,51,51	0
86	MG	5	3840	1/1	0.91	0.11	39,39,39,39	0
86	MG	1	3559	1/1	0.91	0.36	52,52,52,52	0
86	MG	1	3479	1/1	0.91	0.21	74,74,74,74	0
87	OHX	5	4152	7/7	0.91	0.18	130,130,130,130	0
86	MG	5	3851	1/1	0.91	0.11	32,32,32,32	0
86	MG	5	3669	1/1	0.91	0.09	30,30,30,30	0
87	OHX	1	4183	7/7	0.91	0.08	229,229,229,229	0
87	OHX	5	4157	7/7	0.91	0.14	140,140,140,140	0
86	MG	2	1937	1/1	0.91	0.28	55,55,55,55	0
86	MG	1	3722	1/1	0.91	0.26	52,52,52,52	0
86	MG	1	3866	1/1	0.91	0.38	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	5	3861	1/1	0.91	0.14	45,45,45,45	0
86	MG	1	3563	1/1	0.91	0.33	27,27,27,27	0
86	MG	2	2010	1/1	0.91	0.50	76,76,76,76	0
86	MG	5	3865	1/1	0.91	0.16	57,57,57,57	0
86	MG	5	3407	1/1	0.91	0.19	39,39,39,39	0
86	MG	1	3621	1/1	0.91	0.24	68,68,68,68	0
86	MG	3	205	1/1	0.91	0.22	36,36,36,36	0
86	MG	2	1984	1/1	0.91	0.21	56,56,56,56	0
87	OHX	2	2167	7/7	0.91	0.14	155,155,155,155	0
87	OHX	5	4174	7/7	0.91	0.16	123,123,123,123	0
87	OHX	5	4175	7/7	0.91	0.11	150,150,150,150	0
87	OHX	1	4196	7/7	0.91	0.13	140,140,140,140	0
87	OHX	5	4177	7/7	0.91	0.18	124,124,124,124	0
86	MG	1	3805	1/1	0.91	0.18	59,59,59,59	0
87	OHX	2	2171	7/7	0.91	0.14	133,133,133,133	0
87	OHX	5	4183	7/7	0.91	0.17	134,134,134,134	0
86	MG	1	3463	1/1	0.91	0.28	31,31,31,31	0
87	OHX	5	4185	7/7	0.91	0.17	124,124,124,124	0
86	MG	5	3701	1/1	0.91	0.13	37,37,37,37	0
86	MG	5	3418	1/1	0.91	0.18	33,33,33,33	0
86	MG	1	3514	1/1	0.91	0.31	23,23,23,23	0
86	MG	1	3542	1/1	0.91	0.21	30,30,30,30	0
86	MG	5	3553	1/1	0.91	0.18	44,44,44,44	0
86	MG	1	3422	1/1	0.91	0.19	31,31,31,31	0
86	MG	5	3895	1/1	0.91	0.23	22,22,22,22	0
86	MG	1	3749	1/1	0.91	0.12	55,55,55,55	0
86	MG	1	3823	1/1	0.91	0.12	44,44,44,44	0
86	MG	1	3824	1/1	0.91	0.13	58,58,58,58	0
87	OHX	5	4197	7/7	0.91	0.16	118,118,118,118	0
87	OHX	5	4198	7/7	0.91	0.14	132,132,132,132	0
87	OHX	5	4199	7/7	0.91	0.15	117,117,117,117	0
87	OHX	C3	201	7/7	0.91	0.13	154,154,154,154	0
87	OHX	D9	102	7/7	0.91	0.15	136,136,136,136	0
87	OHX	5	4202	7/7	0.91	0.12	163,163,163,163	0
87	OHX	1	4214	7/7	0.91	0.20	122,122,122,122	0
87	OHX	1	3956	7/7	0.91	0.16	98,98,98,98	0
87	OHX	1	4024	7/7	0.91	0.17	113,113,113,113	0
86	MG	5	3899	1/1	0.91	0.29	51,51,51,51	0
86	MG	1	3673	1/1	0.91	0.35	57,57,57,57	0
86	MG	6	1919	1/1	0.91	0.30	44,44,44,44	0
86	MG	1	3631	1/1	0.91	0.12	39,39,39,39	0
86	MG	5	4262	1/1	0.91	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	1	4070	7/7	0.91	0.19	106,106,106,106	0
87	OHX	5	4216	7/7	0.91	0.13	141,141,141,141	0
87	OHX	1	4071	7/7	0.91	0.17	122,122,122,122	0
86	MG	1	3585	1/1	0.91	0.26	40,40,40,40	0
86	MG	7	202	1/1	0.91	0.20	28,28,28,28	0
86	MG	7	203	1/1	0.91	0.29	52,52,52,52	0
86	MG	5	3733	1/1	0.91	0.37	72,72,72,72	0
87	OHX	1	4083	7/7	0.91	0.17	121,121,121,121	0
86	MG	6	2002	1/1	0.91	0.12	71,71,71,71	0
87	OHX	1	4085	7/7	0.91	0.14	128,128,128,128	0
86	MG	1	3424	1/1	0.91	0.23	45,45,45,45	0
86	MG	6	2004	1/1	0.91	0.39	69,69,69,69	0
86	MG	5	3739	1/1	0.91	0.11	40,40,40,40	0
86	MG	1	3493	1/1	0.91	0.32	71,71,71,71	0
87	OHX	6	2125	7/7	0.91	0.17	113,113,113,113	0
87	OHX	6	2132	7/7	0.91	0.15	119,119,119,119	0
86	MG	6	1925	1/1	0.91	0.41	40,40,40,40	0
87	OHX	1	4101	7/7	0.91	0.13	143,143,143,143	0
86	MG	5	3746	1/1	0.91	0.29	32,32,32,32	0
86	MG	1	3837	1/1	0.91	0.23	31,31,31,31	0
87	OHX	1	4105	7/7	0.91	0.16	126,126,126,126	0
87	OHX	1	4106	7/7	0.91	0.15	136,136,136,136	0
87	OHX	6	2151	7/7	0.91	0.13	139,139,139,139	0
87	OHX	6	2152	7/7	0.91	0.13	131,131,131,131	0
87	OHX	1	4108	7/7	0.91	0.18	117,117,117,117	0
87	OHX	1	4111	7/7	0.91	0.15	127,127,127,127	0
87	OHX	1	4112	7/7	0.91	0.15	117,117,117,117	0
87	OHX	6	2159	7/7	0.91	0.16	120,120,120,120	0
87	OHX	6	2160	7/7	0.91	0.18	114,114,114,114	0
86	MG	1	3689	1/1	0.91	0.13	34,34,34,34	0
87	OHX	1	4114	7/7	0.91	0.20	105,105,105,105	0
86	MG	1	3759	1/1	0.91	0.14	33,33,33,33	0
86	MG	2	2012	1/1	0.91	0.34	65,65,65,65	0
87	OHX	1	4117	7/7	0.91	0.11	167,167,167,167	0
86	MG	5	3760	1/1	0.91	0.13	41,41,41,41	0
86	MG	5	3764	1/1	0.91	0.17	48,48,48,48	0
86	MG	1	3595	1/1	0.91	0.29	30,30,30,30	0
86	MG	1	3596	1/1	0.91	0.33	28,28,28,28	0
86	MG	6	2020	1/1	0.91	0.22	50,50,50,50	0
86	MG	m1	201	1/1	0.91	0.19	57,57,57,57	0
86	MG	5	3603	1/1	0.91	0.08	61,61,61,61	0
87	OHX	1	4132	7/7	0.91	0.17	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	5	3775	1/1	0.91	0.19	67,67,67,67	0
86	MG	1	3846	1/1	0.91	0.25	50,50,50,50	0
86	MG	5	3778	1/1	0.91	0.10	41,41,41,41	0
86	MG	n8	202	1/1	0.91	0.17	41,41,41,41	0
87	OHX	6	2181	7/7	0.91	0.17	126,126,126,126	0
86	MG	5	3614	1/1	0.91	0.15	34,34,34,34	0
86	MG	1	3553	1/1	0.91	0.37	37,37,37,37	0
87	OHX	1	4139	7/7	0.91	0.17	111,111,111,111	0
87	OHX	l5	305	7/7	0.91	0.15	135,135,135,135	0
87	OHX	1	4140	7/7	0.91	0.15	108,108,108,108	0
87	OHX	6	2186	7/7	0.91	0.12	161,161,161,161	0
86	MG	o3	201	1/1	0.91	0.13	34,34,34,34	0
86	MG	5	3618	1/1	0.91	0.24	47,47,47,47	0
86	MG	2	1911	1/1	0.91	0.36	57,57,57,57	0
86	MG	4	223	1/1	0.91	0.14	67,67,67,67	0
86	MG	5	3624	1/1	0.91	0.28	38,38,38,38	0
86	MG	L3	402	1/1	0.91	0.11	41,41,41,41	0
87	OHX	2	2103	7/7	0.91	0.14	142,142,142,142	0
87	OHX	2	2108	7/7	0.91	0.15	125,125,125,125	0
86	MG	n0	201	1/1	0.92	0.12	44,44,44,44	0
86	MG	L8	301	1/1	0.92	0.26	55,55,55,55	0
86	MG	1	3742	1/1	0.92	0.25	60,60,60,60	0
86	MG	n8	201	1/1	0.92	0.09	32,32,32,32	0
86	MG	5	3560	1/1	0.92	0.27	30,30,30,30	0
86	MG	5	3754	1/1	0.92	0.21	43,43,43,43	0
86	MG	o1	201	1/1	0.92	0.08	42,42,42,42	0
86	MG	5	3755	1/1	0.92	0.25	49,49,49,49	0
86	MG	1	3436	1/1	0.92	0.17	40,40,40,40	0
86	MG	M3	201	1/1	0.92	0.12	55,55,55,55	0
87	OHX	1	4148	7/7	0.92	0.18	111,111,111,111	0
86	MG	2	1931	1/1	0.92	0.31	69,69,69,69	0
87	OHX	s4	301	7/7	0.92	0.14	140,140,140,140	0
86	MG	q3	502	1/1	0.92	0.14	61,61,61,61	0
87	OHX	2	2068	7/7	0.92	0.12	146,146,146,146	0
86	MG	1	3473	1/1	0.92	0.27	28,28,28,28	0
86	MG	1	3668	1/1	0.92	0.09	51,51,51,51	0
86	MG	5	3771	1/1	0.92	0.10	40,40,40,40	0
87	OHX	5	4033	7/7	0.92	0.15	103,103,103,103	0
87	OHX	5	4077	7/7	0.92	0.17	123,123,123,123	0
87	OHX	5	4094	7/7	0.92	0.16	108,108,108,108	0
86	MG	6	1969	1/1	0.92	0.27	58,58,58,58	0
86	MG	1	3414	1/1	0.92	0.26	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	2	1940	1/1	0.92	0.21	62,62,62,62	0
86	MG	6	1972	1/1	0.92	0.21	52,52,52,52	0
87	OHX	2	2118	7/7	0.92	0.12	151,151,151,151	0
87	OHX	5	4109	7/7	0.92	0.17	102,102,102,102	0
87	OHX	5	4110	7/7	0.92	0.11	146,146,146,146	0
87	OHX	2	2119	7/7	0.92	0.13	132,132,132,132	0
86	MG	5	3577	1/1	0.92	0.22	45,45,45,45	0
86	MG	M7	205	1/1	0.92	0.16	40,40,40,40	0
87	OHX	5	4123	7/7	0.92	0.11	138,138,138,138	0
86	MG	2	1985	1/1	0.92	0.16	59,59,59,59	0
87	OHX	5	4126	7/7	0.92	0.15	111,111,111,111	0
87	OHX	5	4127	7/7	0.92	0.15	117,117,117,117	0
87	OHX	5	4130	7/7	0.92	0.14	128,128,128,128	0
87	OHX	5	4131	7/7	0.92	0.13	137,137,137,137	0
87	OHX	2	2125	7/7	0.92	0.13	132,132,132,132	0
87	OHX	5	4139	7/7	0.92	0.11	173,173,173,173	0
87	OHX	5	4141	7/7	0.92	0.15	120,120,120,120	0
87	OHX	5	4144	7/7	0.92	0.18	123,123,123,123	0
86	MG	1	3441	1/1	0.92	0.20	41,41,41,41	0
86	MG	1	3482	1/1	0.92	0.20	30,30,30,30	0
87	OHX	2	2132	7/7	0.92	0.16	125,125,125,125	0
86	MG	1	3679	1/1	0.92	0.15	39,39,39,39	0
86	MG	1	3767	1/1	0.92	0.09	37,37,37,37	0
86	MG	2	1956	1/1	0.92	0.40	59,59,59,59	0
86	MG	5	3598	1/1	0.92	0.31	31,31,31,31	0
86	MG	5	3599	1/1	0.92	0.38	31,31,31,31	0
87	OHX	2	2139	7/7	0.92	0.13	134,134,134,134	0
86	MG	5	3796	1/1	0.92	0.14	40,40,40,40	0
86	MG	N8	203	1/1	0.92	0.14	47,47,47,47	0
86	MG	5	3799	1/1	0.92	0.09	46,46,46,46	0
86	MG	5	3437	1/1	0.92	0.36	60,60,60,60	0
86	MG	O7	102	1/1	0.92	0.38	57,57,57,57	0
86	MG	5	3805	1/1	0.92	0.13	41,41,41,41	0
86	MG	5	3611	1/1	0.92	0.20	34,34,34,34	0
86	MG	5	3443	1/1	0.92	0.11	31,31,31,31	0
86	MG	2	1998	1/1	0.92	0.12	102,102,102,102	0
86	MG	6	1991	1/1	0.92	0.08	50,50,50,50	0
86	MG	1	3527	1/1	0.92	0.24	30,30,30,30	0
87	OHX	5	4170	7/7	0.92	0.19	112,112,112,112	0
86	MG	1	3528	1/1	0.92	0.41	31,31,31,31	0
86	MG	5	3815	1/1	0.92	0.24	66,66,66,66	0
87	OHX	5	4173	7/7	0.92	0.16	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	MG	6	1997	1/1	0.92	0.27	58,58,58,58	0
86	MG	1	3568	1/1	0.92	0.29	31,31,31,31	0
86	MG	5	3628	1/1	0.92	0.20	51,51,51,51	0
86	MG	5	3824	1/1	0.92	0.07	65,65,65,65	0
86	MG	1	3445	1/1	0.92	0.22	45,45,45,45	0
86	MG	1	3423	1/1	0.92	0.21	45,45,45,45	0
87	OHX	5	4182	7/7	0.92	0.18	118,118,118,118	0
86	MG	5	3633	1/1	0.92	0.12	46,46,46,46	0
86	MG	5	3838	1/1	0.92	0.12	67,67,67,67	0
86	MG	5	3839	1/1	0.92	0.15	41,41,41,41	0
86	MG	5	3634	1/1	0.92	0.09	39,39,39,39	0
86	MG	1	3776	1/1	0.92	0.12	54,54,54,54	0
86	MG	1	3451	1/1	0.92	0.33	41,41,41,41	0
86	MG	1	3698	1/1	0.92	0.14	60,60,60,60	0
86	MG	5	3470	1/1	0.92	0.26	35,35,35,35	0
86	MG	5	3471	1/1	0.92	0.19	46,46,46,46	0
86	MG	5	3641	1/1	0.92	0.27	51,51,51,51	0
86	MG	1	3781	1/1	0.92	0.21	34,34,34,34	0
86	MG	1	3452	1/1	0.92	0.21	34,34,34,34	0
86	MG	6	2007	1/1	0.92	0.28	55,55,55,55	0
86	MG	6	2009	1/1	0.92	0.11	51,51,51,51	0
86	MG	1	3582	1/1	0.92	0.18	38,38,38,38	0
86	MG	1	3583	1/1	0.92	0.26	36,36,36,36	0
86	MG	1	3584	1/1	0.92	0.34	33,33,33,33	0
87	OHX	3	222	7/7	0.92	0.11	137,137,137,137	0
87	OHX	3	223	7/7	0.92	0.17	115,115,115,115	0
86	MG	5	3486	1/1	0.92	0.30	47,47,47,47	0
86	MG	2	2182	1/1	0.92	0.19	65,65,65,65	0
87	OHX	3	226	7/7	0.92	0.14	134,134,134,134	0
87	OHX	5	4207	7/7	0.92	0.15	109,109,109,109	0
86	MG	5	3663	1/1	0.92	0.33	50,50,50,50	0
86	MG	5	3488	1/1	0.92	0.33	31,31,31,31	0
86	MG	1	3790	1/1	0.92	0.13	35,35,35,35	0
87	OHX	1	4007	7/7	0.92	0.16	105,105,105,105	0
87	OHX	1	4020	7/7	0.92	0.09	145,145,145,145	0
86	MG	5	3883	1/1	0.92	0.27	26,26,26,26	0
86	MG	5	3490	1/1	0.92	0.32	51,51,51,51	0
86	MG	1	3708	1/1	0.92	0.06	55,55,55,55	0
86	MG	1	3406	1/1	0.92	0.24	37,37,37,37	0
86	MG	5	3672	1/1	0.92	0.10	33,33,33,33	0
86	MG	5	3893	1/1	0.92	0.30	46,46,46,46	0
86	MG	6	2021	1/1	0.92	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	1	3711	1/1	0.92	0.08	37,37,37,37	0
86	MG	1	3590	1/1	0.92	0.29	32,32,32,32	0
86	MG	1	3591	1/1	0.92	0.45	40,40,40,40	0
87	OHX	1	4075	7/7	0.92	0.14	137,137,137,137	0
87	OHX	6	2131	7/7	0.92	0.12	151,151,151,151	0
86	MG	1	3715	1/1	0.92	0.16	37,37,37,37	0
87	OHX	6	2133	7/7	0.92	0.13	128,128,128,128	0
87	OHX	1	4080	7/7	0.92	0.13	126,126,126,126	0
87	OHX	6	2136	7/7	0.92	0.14	118,118,118,118	0
86	MG	1	3814	1/1	0.92	0.08	38,38,38,38	0
87	OHX	6	2139	7/7	0.92	0.11	156,156,156,156	0
87	OHX	6	2141	7/7	0.92	0.13	134,134,134,134	0
86	MG	4	206	1/1	0.92	0.23	33,33,33,33	0
86	MG	5	3694	1/1	0.92	0.12	47,47,47,47	0
86	MG	5	3506	1/1	0.92	0.21	34,34,34,34	0
87	OHX	1	4087	7/7	0.92	0.12	136,136,136,136	0
86	MG	1	3815	1/1	0.92	0.18	48,48,48,48	0
86	MG	4	210	1/1	0.92	0.09	48,48,48,48	0
86	MG	5	4265	1/1	0.92	0.28	27,27,27,27	0
86	MG	5	3519	1/1	0.92	0.22	27,27,27,27	0
87	OHX	6	2156	7/7	0.92	0.14	131,131,131,131	0
87	OHX	6	2157	7/7	0.92	0.16	109,109,109,109	0
86	MG	6	2034	1/1	0.92	0.25	60,60,60,60	0
87	OHX	1	4100	7/7	0.92	0.11	147,147,147,147	0
86	MG	1	3592	1/1	0.92	0.27	39,39,39,39	0
86	MG	2	1927	1/1	0.92	0.35	49,49,49,49	0
86	MG	1	3820	1/1	0.92	0.06	37,37,37,37	0
86	MG	2	2000	1/1	0.92	0.21	81,81,81,81	0
86	MG	1	3650	1/1	0.92	0.16	46,46,46,46	0
86	MG	1	3459	1/1	0.92	0.36	66,66,66,66	0
86	MG	5	3723	1/1	0.92	0.12	44,44,44,44	0
87	OHX	6	2169	7/7	0.92	0.20	107,107,107,107	0
86	MG	1	3462	1/1	0.92	0.26	29,29,29,29	0
86	MG	1	3827	1/1	0.92	0.09	49,49,49,49	0
86	MG	5	3541	1/1	0.92	0.35	29,29,29,29	0
86	MG	1	3828	1/1	0.92	0.08	45,45,45,45	0
86	MG	6	1949	1/1	0.92	0.33	51,51,51,51	0
86	MG	8	207	1/1	0.92	0.16	58,58,58,58	0
87	OHX	1	4118	7/7	0.92	0.17	117,117,117,117	0
86	MG	1	3432	1/1	0.92	0.28	42,42,42,42	0
86	MG	5	3545	1/1	0.92	0.23	30,30,30,30	0
86	MG	8	211	1/1	0.92	0.46	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	l2	301	1/1	0.92	0.34	47,47,47,47	0
87	OHX	l5	304	7/7	0.92	0.11	133,133,133,133	0
87	OHX	1	4126	7/7	0.92	0.19	102,102,102,102	0
86	MG	1	3546	1/1	0.92	0.23	48,48,48,48	0
86	MG	L3	401	1/1	0.92	0.24	34,34,34,34	0
87	OHX	1	4130	7/7	0.92	0.14	134,134,134,134	0
86	MG	1	3435	1/1	0.92	0.18	43,43,43,43	0
86	MG	l7	301	1/1	0.92	0.23	42,42,42,42	0
86	MG	1	3552	1/1	0.92	0.33	32,32,32,32	0
86	MG	m5	301	1/1	0.92	0.23	49,49,49,49	0
86	MG	m5	303	1/1	0.92	0.08	52,52,52,52	0
86	MG	L7	301	1/1	0.92	0.10	42,42,42,42	0
86	MG	1	3661	1/1	0.92	0.22	35,35,35,35	0
86	MG	5	3793	1/1	0.93	0.21	24,24,24,24	0
87	OHX	2	2105	7/7	0.93	0.14	114,114,114,114	0
87	OHX	2	2106	7/7	0.93	0.14	125,125,125,125	0
86	MG	1	3847	1/1	0.93	0.30	34,34,34,34	0
86	MG	5	3795	1/1	0.93	0.13	52,52,52,52	0
87	OHX	2	2114	7/7	0.93	0.13	153,153,153,153	0
87	OHX	c5	201	7/7	0.93	0.10	147,147,147,147	0
86	MG	5	3621	1/1	0.93	0.24	41,41,41,41	0
87	OHX	2	2117	7/7	0.93	0.13	136,136,136,136	0
87	OHX	5	4000	7/7	0.93	0.14	107,107,107,107	0
87	OHX	5	4004	7/7	0.93	0.13	105,105,105,105	0
86	MG	1	3416	1/1	0.93	0.18	32,32,32,32	0
87	OHX	1	4155	7/7	0.93	0.14	109,109,109,109	0
87	OHX	5	4048	7/7	0.93	0.13	120,120,120,120	0
87	OHX	5	4049	7/7	0.93	0.16	111,111,111,111	0
87	OHX	5	4068	7/7	0.93	0.14	120,120,120,120	0
87	OHX	5	4069	7/7	0.93	0.12	120,120,120,120	0
86	MG	1	3797	1/1	0.93	0.14	27,27,27,27	0
86	MG	1	3643	1/1	0.93	0.13	38,38,38,38	0
86	MG	5	3627	1/1	0.93	0.13	60,60,60,60	0
87	OHX	5	4097	7/7	0.93	0.16	110,110,110,110	0
87	OHX	5	4098	7/7	0.93	0.17	109,109,109,109	0
86	MG	6	2040	1/1	0.93	0.26	48,48,48,48	0
86	MG	6	1974	1/1	0.93	0.21	59,59,59,59	0
87	OHX	5	4104	7/7	0.93	0.16	116,116,116,116	0
87	OHX	5	4105	7/7	0.93	0.13	128,128,128,128	0
87	OHX	2	2126	7/7	0.93	0.15	121,121,121,121	0
87	OHX	5	4107	7/7	0.93	0.15	119,119,119,119	0
86	MG	1	3800	1/1	0.93	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	1	3852	1/1	0.93	0.28	52,52,52,52	0
87	OHX	2	2130	7/7	0.93	0.10	181,181,181,181	0
87	OHX	5	4112	7/7	0.93	0.18	101,101,101,101	0
87	OHX	5	4113	7/7	0.93	0.18	107,107,107,107	0
86	MG	1	3464	1/1	0.93	0.12	36,36,36,36	0
86	MG	6	1979	1/1	0.93	0.31	65,65,65,65	0
86	MG	1	3504	1/1	0.93	0.26	27,27,27,27	0
87	OHX	5	4121	7/7	0.93	0.15	112,112,112,112	0
86	MG	s8	302	1/1	0.93	0.18	51,51,51,51	0
86	MG	1	3674	1/1	0.93	0.24	28,28,28,28	0
86	MG	5	3496	1/1	0.93	0.12	33,33,33,33	0
86	MG	5	3497	1/1	0.93	0.28	37,37,37,37	0
86	MG	5	3642	1/1	0.93	0.26	62,62,62,62	0
86	MG	c1	202	1/1	0.93	0.28	59,59,59,59	0
87	OHX	2	2142	7/7	0.93	0.11	155,155,155,155	0
87	OHX	5	4136	7/7	0.93	0.12	138,138,138,138	0
86	MG	5	3645	1/1	0.93	0.11	30,30,30,30	0
87	OHX	5	4140	7/7	0.93	0.16	112,112,112,112	0
86	MG	5	3833	1/1	0.93	0.15	39,39,39,39	0
86	MG	5	3499	1/1	0.93	0.21	30,30,30,30	0
86	MG	4	220	1/1	0.93	0.09	42,42,42,42	0
86	MG	6	1985	1/1	0.93	0.09	41,41,41,41	0
86	MG	c9	201	1/1	0.93	0.31	68,68,68,68	0
86	MG	d3	201	1/1	0.93	0.28	50,50,50,50	0
86	MG	5	3848	1/1	0.93	0.23	45,45,45,45	0
87	OHX	5	4151	7/7	0.93	0.17	112,112,112,112	0
86	MG	d4	201	1/1	0.93	0.18	53,53,53,53	0
87	OHX	2	2153	7/7	0.93	0.13	137,137,137,137	0
86	MG	1	3760	1/1	0.93	0.06	47,47,47,47	0
86	MG	5	3661	1/1	0.93	0.10	48,48,48,48	0
86	MG	5	3509	1/1	0.93	0.27	41,41,41,41	0
86	MG	2	1918	1/1	0.93	0.37	51,51,51,51	0
86	MG	5	3858	1/1	0.93	0.30	50,50,50,50	0
87	OHX	5	4160	7/7	0.93	0.18	102,102,102,102	0
86	MG	5	3859	1/1	0.93	0.12	69,69,69,69	0
86	MG	1	3817	1/1	0.93	0.21	48,48,48,48	0
86	MG	5	3518	1/1	0.93	0.35	26,26,26,26	0
86	MG	1	3551	1/1	0.93	0.27	38,38,38,38	0
86	MG	5	3405	1/1	0.93	0.21	29,29,29,29	0
86	MG	1	3681	1/1	0.93	0.23	61,61,61,61	0
86	MG	5	3522	1/1	0.93	0.27	33,33,33,33	0
87	OHX	1	4203	7/7	0.93	0.14	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	6	1992	1/1	0.93	0.15	51,51,51,51	0
86	MG	5	3677	1/1	0.93	0.12	41,41,41,41	0
86	MG	1	3685	1/1	0.93	0.28	51,51,51,51	0
86	MG	5	3874	1/1	0.93	0.28	28,28,28,28	0
86	MG	5	3681	1/1	0.93	0.19	46,46,46,46	0
86	MG	5	3878	1/1	0.93	0.22	43,43,43,43	0
86	MG	6	1927	1/1	0.93	0.27	50,50,50,50	0
86	MG	5	3413	1/1	0.93	0.28	29,29,29,29	0
87	OHX	5	4178	7/7	0.93	0.08	182,182,182,182	0
86	MG	6	1995	1/1	0.93	0.15	71,71,71,71	0
86	MG	5	3884	1/1	0.93	0.23	33,33,33,33	0
86	MG	5	3536	1/1	0.93	0.35	35,35,35,35	0
86	MG	5	3415	1/1	0.93	0.12	32,32,32,32	0
86	MG	5	3416	1/1	0.93	0.22	28,28,28,28	0
86	MG	1	3720	1/1	0.93	0.06	35,35,35,35	0
86	MG	1	3511	1/1	0.93	0.30	32,32,32,32	0
86	MG	1	4223	1/1	0.93	0.10	55,55,55,55	0
86	MG	5	3699	1/1	0.93	0.20	50,50,50,50	0
86	MG	1	4225	1/1	0.93	0.27	36,36,36,36	0
87	OHX	1	3966	7/7	0.93	0.14	97,97,97,97	0
87	OHX	1	3969	7/7	0.93	0.12	114,114,114,114	0
86	MG	5	3702	1/1	0.93	0.15	54,54,54,54	0
87	OHX	1	4015	7/7	0.93	0.13	121,121,121,121	0
86	MG	5	3703	1/1	0.93	0.10	40,40,40,40	0
86	MG	1	3512	1/1	0.93	0.37	41,41,41,41	0
86	MG	5	3422	1/1	0.93	0.16	41,41,41,41	0
87	OHX	1	4035	7/7	0.93	0.14	123,123,123,123	0
86	MG	5	3547	1/1	0.93	0.28	44,44,44,44	0
87	OHX	1	4045	7/7	0.93	0.14	117,117,117,117	0
87	OHX	1	4061	7/7	0.93	0.18	112,112,112,112	0
86	MG	5	3902	1/1	0.93	0.25	43,43,43,43	0
87	OHX	O3	201	7/7	0.93	0.19	109,109,109,109	0
87	OHX	6	2092	7/7	0.93	0.13	125,125,125,125	0
86	MG	5	3709	1/1	0.93	0.26	44,44,44,44	0
86	MG	3	202	1/1	0.93	0.22	56,56,56,56	0
87	OHX	5	4209	7/7	0.93	0.17	117,117,117,117	0
86	MG	5	4263	1/1	0.93	0.40	26,26,26,26	0
86	MG	1	3450	1/1	0.93	0.19	41,41,41,41	0
86	MG	5	3712	1/1	0.93	0.11	45,45,45,45	0
87	OHX	6	2129	7/7	0.93	0.11	141,141,141,141	0
87	OHX	6	2130	7/7	0.93	0.17	120,120,120,120	0
86	MG	1	3726	1/1	0.93	0.06	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	MG	5	3718	1/1	0.93	0.24	52,52,52,52	0
86	MG	M6	201	1/1	0.93	0.14	47,47,47,47	0
87	OHX	1	4079	7/7	0.93	0.14	119,119,119,119	0
86	MG	1	3403	1/1	0.93	0.29	34,34,34,34	0
86	MG	1	3654	1/1	0.93	0.09	45,45,45,45	0
86	MG	1	3633	1/1	0.93	0.11	31,31,31,31	0
87	OHX	5	4222	7/7	0.93	0.09	186,186,186,186	0
86	MG	6	1943	1/1	0.93	0.34	40,40,40,40	0
86	MG	5	3561	1/1	0.93	0.28	34,34,34,34	0
87	OHX	6	2144	7/7	0.93	0.13	125,125,125,125	0
87	OHX	1	4086	7/7	0.93	0.18	119,119,119,119	0
86	MG	6	2015	1/1	0.93	0.05	42,42,42,42	0
87	OHX	6	2149	7/7	0.93	0.18	111,111,111,111	0
87	OHX	1	4088	7/7	0.93	0.14	122,122,122,122	0
87	OHX	1	4090	7/7	0.93	0.14	123,123,123,123	0
86	MG	5	3438	1/1	0.93	0.21	32,32,32,32	0
86	MG	5	3439	1/1	0.93	0.33	38,38,38,38	0
86	MG	1	3833	1/1	0.93	0.30	28,28,28,28	0
86	MG	1	3834	1/1	0.93	0.22	33,33,33,33	0
86	MG	N3	201	1/1	0.93	0.23	33,33,33,33	0
86	MG	5	3740	1/1	0.93	0.16	49,49,49,49	0
86	MG	8	208	1/1	0.93	0.20	40,40,40,40	0
86	MG	1	3608	1/1	0.93	0.24	49,49,49,49	0
87	OHX	6	2161	7/7	0.93	0.14	124,124,124,124	0
86	MG	5	3449	1/1	0.93	0.23	31,31,31,31	0
86	MG	5	3450	1/1	0.93	0.15	35,35,35,35	0
86	MG	5	3452	1/1	0.93	0.42	44,44,44,44	0
87	OHX	1	4107	7/7	0.93	0.15	117,117,117,117	0
86	MG	1	3536	1/1	0.93	0.34	45,45,45,45	0
86	MG	l3	401	1/1	0.93	0.07	26,26,26,26	0
86	MG	1	3408	1/1	0.93	0.30	33,33,33,33	0
86	MG	5	3752	1/1	0.93	0.21	53,53,53,53	0
86	MG	5	3753	1/1	0.93	0.10	50,50,50,50	0
86	MG	1	3740	1/1	0.93	0.21	57,57,57,57	0
86	MG	1	3487	1/1	0.93	0.28	33,33,33,33	0
86	MG	1	3747	1/1	0.93	0.18	28,28,28,28	0
86	MG	1	3489	1/1	0.93	0.13	51,51,51,51	0
86	MG	4	205	1/1	0.93	0.33	44,44,44,44	0
87	OHX	1	4121	7/7	0.93	0.15	122,122,122,122	0
86	MG	m7	202	1/1	0.93	0.16	32,32,32,32	0
86	MG	5	3596	1/1	0.93	0.30	38,38,38,38	0
86	MG	5	3465	1/1	0.93	0.23	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	6	2030	1/1	0.93	0.12	54,54,54,54	0
86	MG	5	3600	1/1	0.93	0.16	40,40,40,40	0
87	OHX	1	4128	7/7	0.93	0.13	140,140,140,140	0
86	MG	1	3844	1/1	0.93	0.15	61,61,61,61	0
87	OHX	8	224	7/7	0.93	0.12	135,135,135,135	0
86	MG	6	1903	1/1	0.93	0.33	47,47,47,47	0
86	MG	n9	101	1/1	0.93	0.07	32,32,32,32	0
87	OHX	l3	404	7/7	0.93	0.13	132,132,132,132	0
86	MG	5	3604	1/1	0.93	0.17	46,46,46,46	0
86	MG	5	3605	1/1	0.93	0.15	43,43,43,43	0
86	MG	5	3606	1/1	0.93	0.12	40,40,40,40	0
86	MG	4	207	1/1	0.93	0.26	33,33,33,33	0
86	MG	5	3608	1/1	0.93	0.24	29,29,29,29	0
86	MG	1	3453	1/1	0.93	0.29	47,47,47,47	0
86	MG	1	3501	1/1	0.93	0.33	64,64,64,64	0
87	OHX	2	2081	7/7	0.93	0.14	126,126,126,126	0
87	OHX	2	2088	7/7	0.93	0.15	122,122,122,122	0
86	MG	5	3476	1/1	0.93	0.27	34,34,34,34	0
87	OHX	2	2092	7/7	0.93	0.22	114,114,114,114	0
86	MG	5	3616	1/1	0.93	0.08	41,41,41,41	0
86	MG	5	3477	1/1	0.93	0.22	26,26,26,26	0
87	OHX	2	2101	7/7	0.93	0.11	136,136,136,136	0
86	MG	1	3802	1/1	0.94	0.17	88,88,88,88	0
86	MG	1	3677	1/1	0.94	0.22	46,46,46,46	0
86	MG	5	3837	1/1	0.94	0.12	55,55,55,55	0
87	OHX	2	2124	7/7	0.94	0.13	136,136,136,136	0
86	MG	1	3678	1/1	0.94	0.18	46,46,46,46	0
87	OHX	5	3934	7/7	0.94	0.17	100,100,100,100	0
86	MG	6	1947	1/1	0.94	0.37	51,51,51,51	0
87	OHX	2	2127	7/7	0.94	0.12	133,133,133,133	0
87	OHX	5	4011	7/7	0.94	0.12	112,112,112,112	0
86	MG	5	3671	1/1	0.94	0.16	38,38,38,38	0
87	OHX	5	4029	7/7	0.94	0.13	104,104,104,104	0
87	OHX	5	4032	7/7	0.94	0.16	105,105,105,105	0
86	MG	1	3808	1/1	0.94	0.12	38,38,38,38	0
87	OHX	5	4036	7/7	0.94	0.15	113,113,113,113	0
87	OHX	5	4043	7/7	0.94	0.11	112,112,112,112	0
86	MG	5	3674	1/1	0.94	0.22	29,29,29,29	0
86	MG	5	3441	1/1	0.94	0.13	32,32,32,32	0
87	OHX	5	4057	7/7	0.94	0.14	104,104,104,104	0
87	OHX	2	2133	7/7	0.94	0.11	146,146,146,146	0
86	MG	5	3442	1/1	0.94	0.22	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	4075	7/7	0.94	0.10	138,138,138,138	0
87	OHX	5	4076	7/7	0.94	0.14	119,119,119,119	0
86	MG	M7	202	1/1	0.94	0.36	31,31,31,31	0
87	OHX	5	4079	7/7	0.94	0.13	111,111,111,111	0
87	OHX	5	4088	7/7	0.94	0.17	102,102,102,102	0
87	OHX	5	4090	7/7	0.94	0.10	134,134,134,134	0
87	OHX	5	4091	7/7	0.94	0.14	112,112,112,112	0
87	OHX	5	4092	7/7	0.94	0.14	116,116,116,116	0
87	OHX	1	4156	7/7	0.94	0.14	126,126,126,126	0
86	MG	5	3548	1/1	0.94	0.34	47,47,47,47	0
86	MG	1	3474	1/1	0.94	0.27	26,26,26,26	0
86	MG	1	3745	1/1	0.94	0.09	44,44,44,44	0
86	MG	6	1954	1/1	0.94	0.28	43,43,43,43	0
87	OHX	5	4102	7/7	0.94	0.12	117,117,117,117	0
86	MG	1	3430	1/1	0.94	0.30	44,44,44,44	0
86	MG	5	3688	1/1	0.94	0.22	72,72,72,72	0
86	MG	5	3689	1/1	0.94	0.11	44,44,44,44	0
86	MG	6	1957	1/1	0.94	0.36	54,54,54,54	0
86	MG	1	3431	1/1	0.94	0.24	48,48,48,48	0
86	MG	1	3460	1/1	0.94	0.31	31,31,31,31	0
86	MG	1	3461	1/1	0.94	0.27	26,26,26,26	0
86	MG	5	3870	1/1	0.94	0.32	68,68,68,68	0
86	MG	5	3456	1/1	0.94	0.25	26,26,26,26	0
86	MG	5	3457	1/1	0.94	0.26	33,33,33,33	0
87	OHX	5	4114	7/7	0.94	0.15	111,111,111,111	0
86	MG	1	3598	1/1	0.94	0.34	27,27,27,27	0
86	MG	5	3567	1/1	0.94	0.32	42,42,42,42	0
86	MG	5	3876	1/1	0.94	0.29	29,29,29,29	0
87	OHX	5	4120	7/7	0.94	0.19	101,101,101,101	0
86	MG	2	1916	1/1	0.94	0.31	51,51,51,51	0
87	OHX	5	4122	7/7	0.94	0.15	115,115,115,115	0
86	MG	5	3879	1/1	0.94	0.30	43,43,43,43	0
87	OHX	5	4124	7/7	0.94	0.17	99,99,99,99	0
86	MG	5	3460	1/1	0.94	0.11	32,32,32,32	0
86	MG	5	3461	1/1	0.94	0.27	42,42,42,42	0
86	MG	3	210	1/1	0.94	0.19	64,64,64,64	0
87	OHX	5	4129	7/7	0.94	0.12	132,132,132,132	0
86	MG	1	3434	1/1	0.94	0.09	44,44,44,44	0
86	MG	5	3885	1/1	0.94	0.21	38,38,38,38	0
87	OHX	5	4132	7/7	0.94	0.10	147,147,147,147	0
87	OHX	5	4134	7/7	0.94	0.13	124,124,124,124	0
86	MG	5	3886	1/1	0.94	0.31	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	N8	204	1/1	0.94	0.24	40,40,40,40	0
86	MG	O4	201	1/1	0.94	0.13	59,59,59,59	0
86	MG	5	3890	1/1	0.94	0.29	59,59,59,59	0
86	MG	5	3576	1/1	0.94	0.24	26,26,26,26	0
87	OHX	5	4142	7/7	0.94	0.15	114,114,114,114	0
86	MG	5	3714	1/1	0.94	0.17	40,40,40,40	0
86	MG	5	3467	1/1	0.94	0.10	33,33,33,33	0
87	OHX	2	2168	7/7	0.94	0.10	153,153,153,153	0
87	OHX	2	2169	7/7	0.94	0.17	117,117,117,117	0
86	MG	5	3578	1/1	0.94	0.26	36,36,36,36	0
86	MG	5	3719	1/1	0.94	0.20	63,63,63,63	0
87	OHX	5	4150	7/7	0.94	0.14	128,128,128,128	0
86	MG	5	3579	1/1	0.94	0.43	41,41,41,41	0
86	MG	5	3468	1/1	0.94	0.12	37,37,37,37	0
87	OHX	5	4153	7/7	0.94	0.17	112,112,112,112	0
86	MG	5	3724	1/1	0.94	0.13	37,37,37,37	0
86	MG	5	3582	1/1	0.94	0.29	33,33,33,33	0
86	MG	1	3484	1/1	0.94	0.08	47,47,47,47	0
86	MG	2	1906	1/1	0.94	0.26	49,49,49,49	0
86	MG	5	3587	1/1	0.94	0.34	23,23,23,23	0
86	MG	1	3534	1/1	0.94	0.13	34,34,34,34	0
86	MG	1	3506	1/1	0.94	0.20	35,35,35,35	0
86	MG	5	3473	1/1	0.94	0.28	61,61,61,61	0
86	MG	5	3592	1/1	0.94	0.27	41,41,41,41	0
86	MG	5	3737	1/1	0.94	0.09	39,39,39,39	0
87	OHX	C5	201	7/7	0.94	0.10	159,159,159,159	0
86	MG	5	3593	1/1	0.94	0.31	26,26,26,26	0
87	OHX	1	3955	7/7	0.94	0.12	103,103,103,103	0
86	MG	5	3474	1/1	0.94	0.32	48,48,48,48	0
86	MG	1	3611	1/1	0.94	0.15	41,41,41,41	0
86	MG	7	205	1/1	0.94	0.33	31,31,31,31	0
87	OHX	1	4000	7/7	0.94	0.12	159,159,159,159	0
87	OHX	1	4002	7/7	0.94	0.15	108,108,108,108	0
87	OHX	1	4004	7/7	0.94	0.15	108,108,108,108	0
87	OHX	1	4005	7/7	0.94	0.16	97,97,97,97	0
86	MG	6	1973	1/1	0.94	0.20	52,52,52,52	0
87	OHX	1	4010	7/7	0.94	0.16	101,101,101,101	0
87	OHX	1	4012	7/7	0.94	0.14	116,116,116,116	0
86	MG	1	3454	1/1	0.94	0.24	35,35,35,35	0
87	OHX	4	232	7/7	0.94	0.10	140,140,140,140	0
87	OHX	1	4019	7/7	0.94	0.14	109,109,109,109	0
86	MG	1	3567	1/1	0.94	0.33	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	1	4022	7/7	0.94	0.12	122,122,122,122	0
86	MG	7	210	1/1	0.94	0.15	63,63,63,63	0
87	OHX	1	4026	7/7	0.94	0.11	132,132,132,132	0
87	OHX	1	4027	7/7	0.94	0.11	132,132,132,132	0
86	MG	5	3601	1/1	0.94	0.17	40,40,40,40	0
87	OHX	1	4033	7/7	0.94	0.12	126,126,126,126	0
86	MG	7	212	1/1	0.94	0.09	42,42,42,42	0
86	MG	6	1976	1/1	0.94	0.14	44,44,44,44	0
87	OHX	1	4040	7/7	0.94	0.12	138,138,138,138	0
87	OHX	1	4041	7/7	0.94	0.15	112,112,112,112	0
87	OHX	6	2074	7/7	0.94	0.14	106,106,106,106	0
87	OHX	6	2082	7/7	0.94	0.11	126,126,126,126	0
86	MG	1	3615	1/1	0.94	0.25	42,42,42,42	0
87	OHX	6	2097	7/7	0.94	0.11	157,157,157,157	0
87	OHX	6	2100	7/7	0.94	0.15	110,110,110,110	0
87	OHX	1	4049	7/7	0.94	0.16	103,103,103,103	0
87	OHX	1	4053	7/7	0.94	0.15	106,106,106,106	0
87	OHX	1	4054	7/7	0.94	0.13	111,111,111,111	0
87	OHX	6	2122	7/7	0.94	0.14	125,125,125,125	0
87	OHX	6	2123	7/7	0.94	0.14	128,128,128,128	0
87	OHX	1	4060	7/7	0.94	0.18	97,97,97,97	0
86	MG	1	3509	1/1	0.94	0.33	25,25,25,25	0
87	OHX	6	2126	7/7	0.94	0.14	135,135,135,135	0
87	OHX	1	4064	7/7	0.94	0.09	140,140,140,140	0
86	MG	1	3655	1/1	0.94	0.10	33,33,33,33	0
86	MG	5	3485	1/1	0.94	0.12	46,46,46,46	0
86	MG	c8	201	1/1	0.94	0.38	71,71,71,71	0
86	MG	5	3757	1/1	0.94	0.15	51,51,51,51	0
86	MG	1	3510	1/1	0.94	0.22	41,41,41,41	0
86	MG	5	3759	1/1	0.94	0.20	59,59,59,59	0
87	OHX	6	2137	7/7	0.94	0.14	127,127,127,127	0
86	MG	6	1912	1/1	0.94	0.34	50,50,50,50	0
86	MG	1	3540	1/1	0.94	0.32	26,26,26,26	0
86	MG	1	3619	1/1	0.94	0.27	53,53,53,53	0
86	MG	1	3660	1/1	0.94	0.27	45,45,45,45	0
86	MG	5	3401	1/1	0.94	0.18	54,54,54,54	0
87	OHX	6	2145	7/7	0.94	0.17	107,107,107,107	0
86	MG	5	3494	1/1	0.94	0.10	34,34,34,34	0
87	OHX	1	4082	7/7	0.94	0.15	114,114,114,114	0
86	MG	14	401	1/1	0.94	0.13	35,35,35,35	0
86	MG	1	3488	1/1	0.94	0.16	35,35,35,35	0
86	MG	1	3466	1/1	0.94	0.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	1	3665	1/1	0.94	0.17	48,48,48,48	0
86	MG	2	1920	1/1	0.94	0.21	60,60,60,60	0
86	MG	1	3515	1/1	0.94	0.35	30,30,30,30	0
86	MG	6	1921	1/1	0.94	0.34	48,48,48,48	0
86	MG	1	3469	1/1	0.94	0.24	63,63,63,63	0
86	MG	5	3631	1/1	0.94	0.08	46,46,46,46	0
87	OHX	1	4094	7/7	0.94	0.10	146,146,146,146	0
86	MG	1	3669	1/1	0.94	0.09	43,43,43,43	0
86	MG	m7	204	1/1	0.94	0.13	32,32,32,32	0
86	MG	5	3787	1/1	0.94	0.20	56,56,56,56	0
86	MG	n0	202	1/1	0.94	0.14	48,48,48,48	0
87	OHX	6	2164	7/7	0.94	0.12	133,133,133,133	0
86	MG	1	3787	1/1	0.94	0.13	43,43,43,43	0
87	OHX	1	4102	7/7	0.94	0.18	107,107,107,107	0
86	MG	1	3444	1/1	0.94	0.30	58,58,58,58	0
86	MG	n6	202	1/1	0.94	0.18	47,47,47,47	0
86	MG	1	3628	1/1	0.94	0.33	43,43,43,43	0
86	MG	5	3792	1/1	0.94	0.21	48,48,48,48	0
86	MG	L2	301	1/1	0.94	0.08	36,36,36,36	0
86	MG	5	3510	1/1	0.94	0.35	31,31,31,31	0
87	OHX	1	4110	7/7	0.94	0.15	110,110,110,110	0
86	MG	5	3514	1/1	0.94	0.33	28,28,28,28	0
86	MG	5	3639	1/1	0.94	0.30	44,44,44,44	0
86	MG	1	3791	1/1	0.94	0.28	28,28,28,28	0
86	MG	1	3854	1/1	0.94	0.19	49,49,49,49	0
86	MG	1	3731	1/1	0.94	0.11	35,35,35,35	0
86	MG	1	3472	1/1	0.94	0.18	42,42,42,42	0
87	OHX	2	2040	7/7	0.94	0.15	98,98,98,98	0
86	MG	1	3796	1/1	0.94	0.23	41,41,41,41	0
87	OHX	2	2075	7/7	0.94	0.12	138,138,138,138	0
87	OHX	7	222	7/7	0.94	0.11	126,126,126,126	0
87	OHX	1	4120	7/7	0.94	0.12	125,125,125,125	0
87	OHX	7	224	7/7	0.94	0.16	105,105,105,105	0
87	OHX	2	2076	7/7	0.94	0.14	121,121,121,121	0
86	MG	5	3806	1/1	0.94	0.21	44,44,44,44	0
87	OHX	1	4123	7/7	0.94	0.16	105,105,105,105	0
86	MG	5	3646	1/1	0.94	0.12	52,52,52,52	0
86	MG	5	3648	1/1	0.94	0.39	55,55,55,55	0
86	MG	1	3548	1/1	0.94	0.21	43,43,43,43	0
86	MG	5	3424	1/1	0.94	0.19	42,42,42,42	0
87	OHX	2	2098	7/7	0.94	0.10	145,145,145,145	0
86	MG	M0	301	1/1	0.94	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	6	2011	1/1	0.94	0.21	62,62,62,62	0
86	MG	1	3798	1/1	0.94	0.15	49,49,49,49	0
87	OHX	2	2104	7/7	0.94	0.08	197,197,197,197	0
86	MG	5	3816	1/1	0.94	0.21	30,30,30,30	0
86	MG	1	3519	1/1	0.94	0.34	27,27,27,27	0
86	MG	5	3530	1/1	0.94	0.24	30,30,30,30	0
86	MG	5	3533	1/1	0.94	0.19	35,35,35,35	0
86	MG	1	3412	1/1	0.94	0.25	38,38,38,38	0
86	MG	5	3827	1/1	0.94	0.06	38,38,38,38	0
86	MG	1	3801	1/1	0.94	0.10	48,48,48,48	0
86	MG	5	3434	1/1	0.94	0.19	31,31,31,31	0
86	MG	5	3830	1/1	0.94	0.13	46,46,46,46	0
88	ZN	q2	501	1/1	0.94	0.16	70,70,70,70	0
87	OHX	5	4064	7/7	0.95	0.11	134,134,134,134	0
87	OHX	5	4067	7/7	0.95	0.15	98,98,98,98	0
87	OHX	1	3899	7/7	0.95	0.15	97,97,97,97	0
87	OHX	1	3914	7/7	0.95	0.18	88,88,88,88	0
87	OHX	5	4071	7/7	0.95	0.13	110,110,110,110	0
87	OHX	5	4073	7/7	0.95	0.11	123,123,123,123	0
87	OHX	5	4074	7/7	0.95	0.13	104,104,104,104	0
87	OHX	1	3924	7/7	0.95	0.12	110,110,110,110	0
87	OHX	1	3932	7/7	0.95	0.14	95,95,95,95	0
87	OHX	1	3950	7/7	0.95	0.12	85,85,85,85	0
87	OHX	5	4078	7/7	0.95	0.15	108,108,108,108	0
87	OHX	1	3953	7/7	0.95	0.13	115,115,115,115	0
87	OHX	5	4080	7/7	0.95	0.13	110,110,110,110	0
87	OHX	5	4081	7/7	0.95	0.16	113,113,113,113	0
87	OHX	5	4082	7/7	0.95	0.13	116,116,116,116	0
87	OHX	5	4083	7/7	0.95	0.09	157,157,157,157	0
87	OHX	5	4085	7/7	0.95	0.15	119,119,119,119	0
86	MG	5	3783	1/1	0.95	0.20	44,44,44,44	0
86	MG	1	3763	1/1	0.95	0.12	39,39,39,39	0
86	MG	1	3706	1/1	0.95	0.16	59,59,59,59	0
86	MG	1	3766	1/1	0.95	0.24	46,46,46,46	0
87	OHX	5	4093	7/7	0.95	0.13	116,116,116,116	0
87	OHX	1	3983	7/7	0.95	0.14	107,107,107,107	0
87	OHX	1	3986	7/7	0.95	0.12	100,100,100,100	0
87	OHX	1	3988	7/7	0.95	0.16	98,98,98,98	0
86	MG	O1	201	1/1	0.95	0.28	62,62,62,62	0
86	MG	5	3462	1/1	0.95	0.31	32,32,32,32	0
87	OHX	5	4101	7/7	0.95	0.12	121,121,121,121	0
86	MG	5	3554	1/1	0.95	0.45	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	1	3707	1/1	0.95	0.12	40,40,40,40	0
86	MG	5	3659	1/1	0.95	0.14	47,47,47,47	0
86	MG	5	3660	1/1	0.95	0.23	30,30,30,30	0
87	OHX	1	4198	7/7	0.95	0.10	166,166,166,166	0
86	MG	5	3556	1/1	0.95	0.29	47,47,47,47	0
87	OHX	1	4013	7/7	0.95	0.10	124,124,124,124	0
87	OHX	1	4014	7/7	0.95	0.13	119,119,119,119	0
86	MG	2	1935	1/1	0.95	0.34	53,53,53,53	0
87	OHX	5	4111	7/7	0.95	0.13	128,128,128,128	0
87	OHX	1	4016	7/7	0.95	0.10	130,130,130,130	0
86	MG	5	3558	1/1	0.95	0.28	26,26,26,26	0
86	MG	O7	103	1/1	0.95	0.26	36,36,36,36	0
87	OHX	1	4021	7/7	0.95	0.12	113,113,113,113	0
86	MG	5	3798	1/1	0.95	0.14	40,40,40,40	0
86	MG	1	3830	1/1	0.95	0.18	25,25,25,25	0
87	OHX	5	4119	7/7	0.95	0.14	117,117,117,117	0
86	MG	1	3433	1/1	0.95	0.22	37,37,37,37	0
86	MG	1	3566	1/1	0.95	0.26	35,35,35,35	0
86	MG	5	3802	1/1	0.95	0.09	39,39,39,39	0
87	OHX	1	4032	7/7	0.95	0.11	123,123,123,123	0
86	MG	s1	301	1/1	0.95	0.19	75,75,75,75	0
86	MG	1	3425	1/1	0.95	0.20	33,33,33,33	0
86	MG	n3	202	1/1	0.95	0.09	46,46,46,46	0
86	MG	1	3476	1/1	0.95	0.15	33,33,33,33	0
87	OHX	5	4128	7/7	0.95	0.09	140,140,140,140	0
86	MG	5	3673	1/1	0.95	0.28	51,51,51,51	0
87	OHX	3	221	7/7	0.95	0.12	122,122,122,122	0
86	MG	1	3477	1/1	0.95	0.22	46,46,46,46	0
87	OHX	1	4046	7/7	0.95	0.16	98,98,98,98	0
87	OHX	1	4047	7/7	0.95	0.13	107,107,107,107	0
87	OHX	1	4048	7/7	0.95	0.12	107,107,107,107	0
86	MG	1	3716	1/1	0.95	0.07	40,40,40,40	0
87	OHX	5	4138	7/7	0.95	0.12	110,110,110,110	0
87	OHX	4	231	7/7	0.95	0.10	114,114,114,114	0
87	OHX	1	4052	7/7	0.95	0.10	128,128,128,128	0
86	MG	5	3676	1/1	0.95	0.32	44,44,44,44	0
86	MG	6	1908	1/1	0.95	0.26	45,45,45,45	0
87	OHX	5	4143	7/7	0.95	0.11	131,131,131,131	0
87	OHX	1	4055	7/7	0.95	0.11	128,128,128,128	0
87	OHX	1	4058	7/7	0.95	0.18	100,100,100,100	0
86	MG	5	3572	1/1	0.95	0.33	27,27,27,27	0
87	OHX	L3	403	7/7	0.95	0.12	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	1	3573	1/1	0.95	0.22	31,31,31,31	0
87	OHX	1	4063	7/7	0.95	0.12	121,121,121,121	0
86	MG	5	3817	1/1	0.95	0.15	45,45,45,45	0
86	MG	4	208	1/1	0.95	0.31	41,41,41,41	0
86	MG	q0	202	1/1	0.95	0.09	43,43,43,43	0
86	MG	5	3819	1/1	0.95	0.09	53,53,53,53	0
86	MG	1	3602	1/1	0.95	0.23	27,27,27,27	0
87	OHX	6	2061	7/7	0.95	0.14	96,96,96,96	0
86	MG	1	3603	1/1	0.95	0.25	31,31,31,31	0
87	OHX	1	4072	7/7	0.95	0.15	119,119,119,119	0
86	MG	5	3686	1/1	0.95	0.11	50,50,50,50	0
86	MG	1	3840	1/1	0.95	0.27	33,33,33,33	0
86	MG	d6	102	1/1	0.95	0.13	50,50,50,50	0
87	OHX	2	2077	7/7	0.95	0.12	114,114,114,114	0
87	OHX	6	2103	7/7	0.95	0.14	109,109,109,109	0
87	OHX	1	4078	7/7	0.95	0.13	115,115,115,115	0
87	OHX	6	2105	7/7	0.95	0.14	107,107,107,107	0
87	OHX	6	2108	7/7	0.95	0.12	120,120,120,120	0
87	OHX	6	2113	7/7	0.95	0.12	120,120,120,120	0
87	OHX	2	2078	7/7	0.95	0.11	121,121,121,121	0
87	OHX	6	2116	7/7	0.95	0.11	130,130,130,130	0
87	OHX	6	2118	7/7	0.95	0.14	103,103,103,103	0
87	OHX	6	2119	7/7	0.95	0.10	135,135,135,135	0
87	OHX	6	2120	7/7	0.95	0.12	134,134,134,134	0
87	OHX	2	2080	7/7	0.95	0.10	153,153,153,153	0
86	MG	1	3409	1/1	0.95	0.19	31,31,31,31	0
87	OHX	2	2084	7/7	0.95	0.14	117,117,117,117	0
87	OHX	2	2085	7/7	0.95	0.11	135,135,135,135	0
86	MG	5	3690	1/1	0.95	0.13	40,40,40,40	0
87	OHX	2	2089	7/7	0.95	0.13	107,107,107,107	0
86	MG	5	3691	1/1	0.95	0.14	47,47,47,47	0
86	MG	1	3606	1/1	0.95	0.15	39,39,39,39	0
86	MG	5	3693	1/1	0.95	0.16	46,46,46,46	0
86	MG	D3	201	1/1	0.95	0.20	54,54,54,54	0
87	OHX	2	2099	7/7	0.95	0.13	114,114,114,114	0
86	MG	1	3578	1/1	0.95	0.18	27,27,27,27	0
86	MG	6	1988	1/1	0.95	0.14	76,76,76,76	0
87	OHX	1	4095	7/7	0.95	0.15	113,113,113,113	0
86	MG	5	3586	1/1	0.95	0.35	31,31,31,31	0
87	OHX	1	4097	7/7	0.95	0.10	134,134,134,134	0
86	MG	1	3533	1/1	0.95	0.23	36,36,36,36	0
87	OHX	6	2143	7/7	0.95	0.12	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	MG	1	3729	1/1	0.95	0.31	36,36,36,36	0
86	MG	5	3850	1/1	0.95	0.14	34,34,34,34	0
87	OHX	2	2107	7/7	0.95	0.13	112,112,112,112	0
86	MG	1	3680	1/1	0.95	0.22	63,63,63,63	0
86	MG	5	3410	1/1	0.95	0.28	52,52,52,52	0
87	OHX	2	2113	7/7	0.95	0.11	128,128,128,128	0
86	MG	1	3580	1/1	0.95	0.30	37,37,37,37	0
86	MG	5	3493	1/1	0.95	0.11	45,45,45,45	0
87	OHX	6	2153	7/7	0.95	0.13	109,109,109,109	0
86	MG	5	3855	1/1	0.95	0.20	48,48,48,48	0
86	MG	5	3706	1/1	0.95	0.06	47,47,47,47	0
87	OHX	1	4109	7/7	0.95	0.09	140,140,140,140	0
86	MG	5	3594	1/1	0.95	0.34	33,33,33,33	0
86	MG	1	3682	1/1	0.95	0.10	40,40,40,40	0
87	OHX	5	4208	7/7	0.95	0.12	114,114,114,114	0
87	OHX	2	2121	7/7	0.95	0.11	140,140,140,140	0
86	MG	4	221	1/1	0.95	0.35	54,54,54,54	0
86	MG	1	3581	1/1	0.95	0.27	38,38,38,38	0
86	MG	5	3863	1/1	0.95	0.12	46,46,46,46	0
86	MG	1	3794	1/1	0.95	0.06	55,55,55,55	0
86	MG	5	3713	1/1	0.95	0.17	86,86,86,86	0
86	MG	1	3613	1/1	0.95	0.14	45,45,45,45	0
86	MG	SM	301	1/1	0.95	0.10	52,52,52,52	0
86	MG	6	1928	1/1	0.95	0.34	67,67,67,67	0
86	MG	1	3467	1/1	0.95	0.15	44,44,44,44	0
86	MG	5	3872	1/1	0.95	0.20	35,35,35,35	0
86	MG	5	3720	1/1	0.95	0.14	40,40,40,40	0
86	MG	1	3857	1/1	0.95	0.21	22,22,22,22	0
86	MG	6	1931	1/1	0.95	0.42	58,58,58,58	0
86	MG	1	3858	1/1	0.95	0.30	71,71,71,71	0
87	OHX	5	4224	7/7	0.95	0.12	101,101,101,101	0
86	MG	5	3877	1/1	0.95	0.36	51,51,51,51	0
86	MG	1	3741	1/1	0.95	0.13	52,52,52,52	0
86	MG	1	3447	1/1	0.95	0.22	41,41,41,41	0
86	MG	5	3609	1/1	0.95	0.26	31,31,31,31	0
86	MG	5	3610	1/1	0.95	0.16	37,37,37,37	0
86	MG	1	3743	1/1	0.95	0.17	52,52,52,52	0
86	MG	5	3732	1/1	0.95	0.28	30,30,30,30	0
86	MG	5	3613	1/1	0.95	0.07	34,34,34,34	0
86	MG	5	3734	1/1	0.95	0.18	52,52,52,52	0
86	MG	5	3513	1/1	0.95	0.25	51,51,51,51	0
86	MG	1	3448	1/1	0.95	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	5	3428	1/1	0.95	0.21	28,28,28,28	0
86	MG	5	3516	1/1	0.95	0.18	32,32,32,32	0
86	MG	1	3746	1/1	0.95	0.15	53,53,53,53	0
86	MG	5	3620	1/1	0.95	0.13	42,42,42,42	0
86	MG	2	1967	1/1	0.95	0.37	61,61,61,61	0
87	OHX	5	4241	7/7	0.95	0.14	101,101,101,101	0
86	MG	1	3587	1/1	0.95	0.27	47,47,47,47	0
86	MG	5	3744	1/1	0.95	0.09	55,55,55,55	0
86	MG	5	3745	1/1	0.95	0.21	27,27,27,27	0
86	MG	1	3696	1/1	0.95	0.23	47,47,47,47	0
86	MG	5	3747	1/1	0.95	0.06	38,38,38,38	0
86	MG	M5	301	1/1	0.95	0.18	38,38,38,38	0
86	MG	5	3626	1/1	0.95	0.23	29,29,29,29	0
86	MG	5	3750	1/1	0.95	0.14	58,58,58,58	0
86	MG	1	3588	1/1	0.95	0.29	36,36,36,36	0
86	MG	1	4222	1/1	0.95	0.15	45,45,45,45	0
86	MG	1	3810	1/1	0.95	0.08	50,50,50,50	0
86	MG	1	4224	1/1	0.95	0.19	30,30,30,30	0
86	MG	M7	203	1/1	0.95	0.33	36,36,36,36	0
86	MG	6	2023	1/1	0.95	0.10	83,83,83,83	0
86	MG	1	3589	1/1	0.95	0.34	30,30,30,30	0
86	MG	6	2025	1/1	0.95	0.29	59,59,59,59	0
87	OHX	1	4159	7/7	0.95	0.15	121,121,121,121	0
86	MG	5	3535	1/1	0.95	0.26	37,37,37,37	0
87	OHX	c8	202	7/7	0.95	0.11	129,129,129,129	0
86	MG	5	3762	1/1	0.95	0.11	50,50,50,50	0
86	MG	1	3520	1/1	0.95	0.30	38,38,38,38	0
87	OHX	sR	401	7/7	0.95	0.10	153,153,153,153	0
87	OHX	8	218	7/7	0.95	0.15	110,110,110,110	0
87	OHX	8	221	7/7	0.95	0.13	116,116,116,116	0
86	MG	6	1953	1/1	0.95	0.46	58,58,58,58	0
86	MG	1	3486	1/1	0.95	0.23	39,39,39,39	0
86	MG	5	3769	1/1	0.95	0.06	59,59,59,59	0
86	MG	5	3770	1/1	0.95	0.19	41,41,41,41	0
86	MG	6	2029	1/1	0.95	0.28	62,62,62,62	0
87	OHX	5	4026	7/7	0.95	0.13	99,99,99,99	0
86	MG	1	3471	1/1	0.95	0.10	41,41,41,41	0
86	MG	7	226	1/1	0.95	0.17	36,36,36,36	0
86	MG	6	1956	1/1	0.95	0.36	46,46,46,46	0
86	MG	1	3702	1/1	0.95	0.07	45,45,45,45	0
87	OHX	5	4038	7/7	0.95	0.14	105,105,105,105	0
87	OHX	5	4042	7/7	0.95	0.10	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	m0	301	7/7	0.95	0.12	121,121,121,121	0
86	MG	1	3663	1/1	0.95	0.12	46,46,46,46	0
87	OHX	5	4047	7/7	0.95	0.11	144,144,144,144	0
86	MG	2	2003	1/1	0.95	0.15	79,79,79,79	0
86	MG	5	3647	1/1	0.95	0.19	33,33,33,33	0
87	OHX	5	4054	7/7	0.95	0.12	109,109,109,109	0
86	MG	1	3822	1/1	0.95	0.10	54,54,54,54	0
87	OHX	5	4058	7/7	0.95	0.13	100,100,100,100	0
87	OHX	5	4059	7/7	0.95	0.17	98,98,98,98	0
87	OHX	5	4060	7/7	0.95	0.14	101,101,101,101	0
89	ANM	5	4260	19/19	0.95	0.10	31,31,31,31	0
86	MG	1	3733	1/1	0.96	0.11	65,65,65,65	0
86	MG	2	1933	1/1	0.96	0.29	59,59,59,59	0
86	MG	m6	201	1/1	0.96	0.07	32,32,32,32	0
86	MG	1	3813	1/1	0.96	0.08	50,50,50,50	0
86	MG	1	3632	1/1	0.96	0.10	32,32,32,32	0
86	MG	5	3665	1/1	0.96	0.08	59,59,59,59	0
87	OHX	6	2109	7/7	0.96	0.12	117,117,117,117	0
87	OHX	6	2111	7/7	0.96	0.11	120,120,120,120	0
87	OHX	6	2112	7/7	0.96	0.10	115,115,115,115	0
86	MG	5	3523	1/1	0.96	0.38	45,45,45,45	0
86	MG	5	3667	1/1	0.96	0.19	46,46,46,46	0
86	MG	5	3857	1/1	0.96	0.18	58,58,58,58	0
86	MG	1	3736	1/1	0.96	0.14	40,40,40,40	0
86	MG	1	3816	1/1	0.96	0.19	54,54,54,54	0
86	MG	1	3549	1/1	0.96	0.29	44,44,44,44	0
87	OHX	6	2121	7/7	0.96	0.13	103,103,103,103	0
86	MG	2	1925	1/1	0.96	0.40	67,67,67,67	0
86	MG	1	3538	1/1	0.96	0.40	36,36,36,36	0
86	MG	1	3657	1/1	0.96	0.17	35,35,35,35	0
86	MG	1	3418	1/1	0.96	0.30	48,48,48,48	0
86	MG	N6	201	1/1	0.96	0.12	40,40,40,40	0
87	OHX	6	2127	7/7	0.96	0.09	130,130,130,130	0
86	MG	1	3780	1/1	0.96	0.21	56,56,56,56	0
86	MG	1	3600	1/1	0.96	0.35	24,24,24,24	0
86	MG	5	3678	1/1	0.96	0.11	37,37,37,37	0
86	MG	1	3710	1/1	0.96	0.24	35,35,35,35	0
86	MG	5	3539	1/1	0.96	0.42	37,37,37,37	0
86	MG	5	3682	1/1	0.96	0.07	36,36,36,36	0
87	OHX	5	4133	7/7	0.96	0.09	134,134,134,134	0
87	OHX	6	2135	7/7	0.96	0.14	117,117,117,117	0
86	MG	1	3825	1/1	0.96	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	2	2043	7/7	0.96	0.12	110,110,110,110	0
87	OHX	5	4137	7/7	0.96	0.09	134,134,134,134	0
87	OHX	2	2053	7/7	0.96	0.09	123,123,123,123	0
87	OHX	2	2054	7/7	0.96	0.10	126,126,126,126	0
87	OHX	SR	401	7/7	0.96	0.08	156,156,156,156	0
87	OHX	2	2057	7/7	0.96	0.10	129,129,129,129	0
87	OHX	2	2062	7/7	0.96	0.11	120,120,120,120	0
87	OHX	2	2063	7/7	0.96	0.09	124,124,124,124	0
87	OHX	2	2065	7/7	0.96	0.14	107,107,107,107	0
87	OHX	1	3939	7/7	0.96	0.12	97,97,97,97	0
87	OHX	6	2147	7/7	0.96	0.15	105,105,105,105	0
87	OHX	1	3943	7/7	0.96	0.11	98,98,98,98	0
87	OHX	1	3949	7/7	0.96	0.11	101,101,101,101	0
87	OHX	2	2066	7/7	0.96	0.10	130,130,130,130	0
87	OHX	1	3952	7/7	0.96	0.11	122,122,122,122	0
87	OHX	2	2067	7/7	0.96	0.09	134,134,134,134	0
86	MG	6	1937	1/1	0.96	0.32	42,42,42,42	0
87	OHX	2	2073	7/7	0.96	0.08	135,135,135,135	0
87	OHX	1	3965	7/7	0.96	0.09	118,118,118,118	0
86	MG	2	2008	1/1	0.96	0.43	55,55,55,55	0
86	MG	5	3478	1/1	0.96	0.27	64,64,64,64	0
87	OHX	1	3976	7/7	0.96	0.12	102,102,102,102	0
87	OHX	1	3980	7/7	0.96	0.17	85,85,85,85	0
86	MG	1	3428	1/1	0.96	0.16	48,48,48,48	0
86	MG	5	3776	1/1	0.96	0.14	30,30,30,30	0
87	OHX	2	2079	7/7	0.96	0.15	116,116,116,116	0
87	OHX	5	4162	7/7	0.96	0.13	111,111,111,111	0
87	OHX	1	3991	7/7	0.96	0.12	115,115,115,115	0
87	OHX	1	3993	7/7	0.96	0.12	105,105,105,105	0
87	OHX	1	3994	7/7	0.96	0.13	101,101,101,101	0
87	OHX	1	3995	7/7	0.96	0.12	111,111,111,111	0
87	OHX	1	3996	7/7	0.96	0.10	129,129,129,129	0
87	OHX	1	3999	7/7	0.96	0.23	94,94,94,94	0
86	MG	5	3880	1/1	0.96	0.35	43,43,43,43	0
86	MG	5	3612	1/1	0.96	0.27	49,49,49,49	0
87	OHX	2	2082	7/7	0.96	0.09	138,138,138,138	0
86	MG	1	3713	1/1	0.96	0.10	51,51,51,51	0
87	OHX	1	4006	7/7	0.96	0.10	120,120,120,120	0
87	OHX	1	4161	7/7	0.96	0.11	107,107,107,107	0
86	MG	5	3780	1/1	0.96	0.21	58,58,58,58	0
87	OHX	1	4008	7/7	0.96	0.12	113,113,113,113	0
87	OHX	1	4009	7/7	0.96	0.12	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	2	2086	7/7	0.96	0.13	109,109,109,109	0
87	OHX	1	4011	7/7	0.96	0.11	105,105,105,105	0
86	MG	1	4219	1/1	0.96	0.20	26,26,26,26	0
86	MG	2	2021	1/1	0.96	0.14	82,82,82,82	0
86	MG	5	3549	1/1	0.96	0.24	48,48,48,48	0
86	MG	5	3617	1/1	0.96	0.20	39,39,39,39	0
86	MG	5	3888	1/1	0.96	0.21	28,28,28,28	0
87	OHX	1	4017	7/7	0.96	0.12	113,113,113,113	0
87	OHX	1	4018	7/7	0.96	0.10	115,115,115,115	0
87	OHX	5	4188	7/7	0.96	0.08	149,149,149,149	0
87	OHX	2	2096	7/7	0.96	0.12	125,125,125,125	0
86	MG	5	3483	1/1	0.96	0.34	29,29,29,29	0
86	MG	5	3429	1/1	0.96	0.10	29,29,29,29	0
87	OHX	1	4177	7/7	0.96	0.11	103,103,103,103	0
86	MG	5	3696	1/1	0.96	0.08	48,48,48,48	0
86	MG	1	3505	1/1	0.96	0.31	36,36,36,36	0
87	OHX	1	4025	7/7	0.96	0.12	108,108,108,108	0
87	OHX	2	2102	7/7	0.96	0.09	131,131,131,131	0
86	MG	6	1944	1/1	0.96	0.38	62,62,62,62	0
87	OHX	1	4029	7/7	0.96	0.11	120,120,120,120	0
86	MG	1	3642	1/1	0.96	0.26	37,37,37,37	0
86	MG	5	3623	1/1	0.96	0.15	64,64,64,64	0
86	MG	1	3690	1/1	0.96	0.37	57,57,57,57	0
87	OHX	1	4034	7/7	0.96	0.12	101,101,101,101	0
86	MG	6	1905	1/1	0.96	0.32	62,62,62,62	0
87	OHX	1	4037	7/7	0.96	0.14	103,103,103,103	0
86	MG	5	3435	1/1	0.96	0.15	36,36,36,36	0
87	OHX	2	2109	7/7	0.96	0.09	145,145,145,145	0
86	MG	1	3622	1/1	0.96	0.15	41,41,41,41	0
87	OHX	1	4042	7/7	0.96	0.13	112,112,112,112	0
86	MG	1	3756	1/1	0.96	0.15	26,26,26,26	0
86	MG	1	3719	1/1	0.96	0.21	40,40,40,40	0
86	MG	3	204	1/1	0.96	0.33	47,47,47,47	0
86	MG	1	3576	1/1	0.96	0.27	21,21,21,21	0
86	MG	5	3564	1/1	0.96	0.42	36,36,36,36	0
87	OHX	1	4050	7/7	0.96	0.13	108,108,108,108	0
87	OHX	5	3965	7/7	0.96	0.11	72,72,72,72	0
87	OHX	5	3971	7/7	0.96	0.11	98,98,98,98	0
87	OHX	5	3979	7/7	0.96	0.11	103,103,103,103	0
87	OHX	5	3980	7/7	0.96	0.11	90,90,90,90	0
87	OHX	5	3982	7/7	0.96	0.13	93,93,93,93	0
86	MG	1	3607	1/1	0.96	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	5	3566	1/1	0.96	0.20	24,24,24,24	0
86	MG	1	3695	1/1	0.96	0.15	41,41,41,41	0
87	OHX	5	4017	7/7	0.96	0.12	101,101,101,101	0
86	MG	7	201	1/1	0.96	0.34	38,38,38,38	0
87	OHX	1	4057	7/7	0.96	0.12	128,128,128,128	0
87	OHX	5	4028	7/7	0.96	0.13	104,104,104,104	0
86	MG	1	3421	1/1	0.96	0.31	38,38,38,38	0
87	OHX	5	4031	7/7	0.96	0.12	107,107,107,107	0
87	OHX	1	4059	7/7	0.96	0.10	139,139,139,139	0
86	MG	5	3717	1/1	0.96	0.15	50,50,50,50	0
87	OHX	5	4035	7/7	0.96	0.20	95,95,95,95	0
86	MG	5	3444	1/1	0.96	0.30	41,41,41,41	0
87	OHX	5	4037	7/7	0.96	0.10	130,130,130,130	0
86	MG	5	3446	1/1	0.96	0.08	40,40,40,40	0
87	OHX	5	4039	7/7	0.96	0.14	104,104,104,104	0
87	OHX	5	4041	7/7	0.96	0.11	117,117,117,117	0
86	MG	7	206	1/1	0.96	0.09	43,43,43,43	0
86	MG	1	3762	1/1	0.96	0.17	48,48,48,48	0
87	OHX	5	4044	7/7	0.96	0.09	123,123,123,123	0
87	OHX	5	4046	7/7	0.96	0.11	119,119,119,119	0
86	MG	1	3647	1/1	0.96	0.18	37,37,37,37	0
86	MG	5	3722	1/1	0.96	0.15	51,51,51,51	0
87	OHX	2	2131	7/7	0.96	0.13	112,112,112,112	0
87	OHX	5	4051	7/7	0.96	0.11	115,115,115,115	0
87	OHX	5	4052	7/7	0.96	0.16	97,97,97,97	0
87	OHX	5	4053	7/7	0.96	0.11	117,117,117,117	0
86	MG	2	1902	1/1	0.96	0.28	40,40,40,40	0
87	OHX	5	4055	7/7	0.96	0.15	101,101,101,101	0
86	MG	5	3643	1/1	0.96	0.09	44,44,44,44	0
86	MG	6	2008	1/1	0.96	0.14	48,48,48,48	0
86	MG	5	3451	1/1	0.96	0.14	40,40,40,40	0
86	MG	5	3507	1/1	0.96	0.38	34,34,34,34	0
87	OHX	5	4062	7/7	0.96	0.14	102,102,102,102	0
87	OHX	5	4063	7/7	0.96	0.10	123,123,123,123	0
86	MG	1	3728	1/1	0.96	0.15	62,62,62,62	0
87	OHX	5	4066	7/7	0.96	0.09	133,133,133,133	0
87	OHX	1	4077	7/7	0.96	0.10	113,113,113,113	0
86	MG	d3	202	1/1	0.96	0.13	49,49,49,49	0
86	MG	5	3825	1/1	0.96	0.11	60,60,60,60	0
87	OHX	4	230	7/7	0.96	0.14	102,102,102,102	0
86	MG	5	3650	1/1	0.96	0.20	40,40,40,40	0
86	MG	5	3511	1/1	0.96	0.30	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	8	217	7/7	0.96	0.10	115,115,115,115	0
87	OHX	4	233	7/7	0.96	0.10	130,130,130,130	0
87	OHX	8	219	7/7	0.96	0.12	116,116,116,116	0
87	OHX	8	220	7/7	0.96	0.09	135,135,135,135	0
86	MG	5	3580	1/1	0.96	0.23	29,29,29,29	0
86	MG	5	3653	1/1	0.96	0.17	29,29,29,29	0
86	MG	5	3832	1/1	0.96	0.06	41,41,41,41	0
86	MG	6	2010	1/1	0.96	0.30	56,56,56,56	0
86	MG	6	1962	1/1	0.96	0.21	49,49,49,49	0
87	OHX	2	2147	7/7	0.96	0.10	120,120,120,120	0
86	MG	5	3835	1/1	0.96	0.18	46,46,46,46	0
87	OHX	1	4089	7/7	0.96	0.07	188,188,188,188	0
87	OHX	M0	303	7/7	0.96	0.12	101,101,101,101	0
87	OHX	5	4086	7/7	0.96	0.11	110,110,110,110	0
87	OHX	M5	303	7/7	0.96	0.11	107,107,107,107	0
87	OHX	5	4089	7/7	0.96	0.12	106,106,106,106	0
86	MG	1	3497	1/1	0.96	0.20	30,30,30,30	0
86	MG	6	2013	1/1	0.96	0.21	42,42,42,42	0
86	MG	5	3585	1/1	0.96	0.31	36,36,36,36	0
86	MG	1	3807	1/1	0.96	0.25	38,38,38,38	0
86	MG	5	3841	1/1	0.96	0.11	43,43,43,43	0
86	MG	5	3844	1/1	0.96	0.06	60,60,60,60	0
86	MG	5	3846	1/1	0.96	0.13	33,33,33,33	0
86	MG	1	3415	1/1	0.96	0.07	45,45,45,45	0
87	OHX	6	2083	7/7	0.96	0.12	101,101,101,101	0
88	ZN	Q2	501	1/1	0.96	0.16	77,77,77,77	0
87	OHX	6	2088	7/7	0.96	0.15	111,111,111,111	0
88	ZN	e1	501	1/1	0.96	0.05	150,150,150,150	0
86	MG	5	3743	1/1	0.96	0.19	38,38,38,38	0
89	ANM	1	4218	19/19	0.96	0.09	33,33,33,33	0
86	MG	m5	302	1/1	0.96	0.17	39,39,39,39	0
86	MG	1	3773	1/1	0.97	0.09	65,65,65,65	0
87	OHX	6	2201	7/7	0.97	0.07	185,185,185,185	0
86	MG	1	3754	1/1	0.97	0.09	57,57,57,57	0
87	OHX	1	4028	7/7	0.97	0.10	106,106,106,106	0
86	MG	6	1945	1/1	0.97	0.36	40,40,40,40	0
87	OHX	M6	202	7/7	0.97	0.10	103,103,103,103	0
87	OHX	1	4030	7/7	0.97	0.09	118,118,118,118	0
86	MG	1	3755	1/1	0.97	0.07	41,41,41,41	0
86	MG	5	3563	1/1	0.97	0.31	28,28,28,28	0
87	OHX	2	2087	7/7	0.97	0.11	121,121,121,121	0
87	OHX	O1	202	7/7	0.97	0.09	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	O2	201	7/7	0.97	0.20	93,93,93,93	0
86	MG	5	3649	1/1	0.97	0.18	44,44,44,44	0
87	OHX	5	3931	7/7	0.97	0.13	70,70,70,70	0
86	MG	1	3721	1/1	0.97	0.27	50,50,50,50	0
87	OHX	5	3954	7/7	0.97	0.10	97,97,97,97	0
87	OHX	5	3956	7/7	0.97	0.12	108,108,108,108	0
87	OHX	5	3960	7/7	0.97	0.11	92,92,92,92	0
87	OHX	5	3961	7/7	0.97	0.12	86,86,86,86	0
87	OHX	6	2063	7/7	0.97	0.14	109,109,109,109	0
87	OHX	5	3968	7/7	0.97	0.11	92,92,92,92	0
86	MG	5	3803	1/1	0.97	0.24	40,40,40,40	0
87	OHX	5	3978	7/7	0.97	0.14	94,94,94,94	0
87	OHX	6	2081	7/7	0.97	0.09	115,115,115,115	0
87	OHX	1	4038	7/7	0.97	0.07	139,139,139,139	0
86	MG	5	3804	1/1	0.97	0.16	69,69,69,69	0
87	OHX	5	3985	7/7	0.97	0.09	95,95,95,95	0
87	OHX	5	3995	7/7	0.97	0.10	99,99,99,99	0
87	OHX	5	3997	7/7	0.97	0.12	96,96,96,96	0
87	OHX	5	3998	7/7	0.97	0.24	90,90,90,90	0
87	OHX	5	3999	7/7	0.97	0.09	121,121,121,121	0
87	OHX	6	2085	7/7	0.97	0.09	114,114,114,114	0
87	OHX	5	4001	7/7	0.97	0.20	90,90,90,90	0
86	MG	6	1948	1/1	0.97	0.34	43,43,43,43	0
87	OHX	5	4007	7/7	0.97	0.20	75,75,75,75	0
87	OHX	5	4008	7/7	0.97	0.10	105,105,105,105	0
87	OHX	2	2095	7/7	0.97	0.08	142,142,142,142	0
87	OHX	5	4016	7/7	0.97	0.10	101,101,101,101	0
87	OHX	5	4181	7/7	0.97	0.25	89,89,89,89	0
87	OHX	6	2093	7/7	0.97	0.08	121,121,121,121	0
87	OHX	5	4018	7/7	0.97	0.08	139,139,139,139	0
87	OHX	5	4019	7/7	0.97	0.18	92,92,92,92	0
87	OHX	5	4021	7/7	0.97	0.09	101,101,101,101	0
87	OHX	6	2094	7/7	0.97	0.08	137,137,137,137	0
87	OHX	5	4025	7/7	0.97	0.12	106,106,106,106	0
87	OHX	6	2095	7/7	0.97	0.10	118,118,118,118	0
87	OHX	6	2096	7/7	0.97	0.08	150,150,150,150	0
86	MG	5	3524	1/1	0.97	0.26	33,33,33,33	0
87	OHX	6	2098	7/7	0.97	0.08	156,156,156,156	0
87	OHX	1	4043	7/7	0.97	0.12	105,105,105,105	0
87	OHX	2	2097	7/7	0.97	0.07	156,156,156,156	0
86	MG	1	3855	1/1	0.97	0.11	60,60,60,60	0
86	MG	5	3808	1/1	0.97	0.04	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	15	301	1/1	0.97	0.17	41,41,41,41	0
87	OHX	6	2106	7/7	0.97	0.09	113,113,113,113	0
87	OHX	6	2107	7/7	0.97	0.11	106,106,106,106	0
86	MG	1	3530	1/1	0.97	0.31	36,36,36,36	0
86	MG	5	3700	1/1	0.97	0.20	46,46,46,46	0
87	OHX	6	2110	7/7	0.97	0.11	101,101,101,101	0
87	OHX	1	4051	7/7	0.97	0.10	116,116,116,116	0
86	MG	1	3778	1/1	0.97	0.14	54,54,54,54	0
86	MG	5	3812	1/1	0.97	0.09	39,39,39,39	0
86	MG	1	3803	1/1	0.97	0.07	52,52,52,52	0
87	OHX	6	2115	7/7	0.97	0.12	105,105,105,105	0
86	MG	L4	401	1/1	0.97	0.11	33,33,33,33	0
87	OHX	6	2117	7/7	0.97	0.10	111,111,111,111	0
87	OHX	1	4056	7/7	0.97	0.07	135,135,135,135	0
86	MG	5	3532	1/1	0.97	0.27	47,47,47,47	0
86	MG	1	3684	1/1	0.97	0.22	55,55,55,55	0
87	OHX	5	4056	7/7	0.97	0.08	126,126,126,126	0
87	OHX	C8	201	7/7	0.97	0.10	107,107,107,107	0
86	MG	5	3756	1/1	0.97	0.21	40,40,40,40	0
87	OHX	2	2110	7/7	0.97	0.08	129,129,129,129	0
87	OHX	1	4062	7/7	0.97	0.07	163,163,163,163	0
87	OHX	2	2111	7/7	0.97	0.12	112,112,112,112	0
87	OHX	1	3900	7/7	0.97	0.13	76,76,76,76	0
86	MG	1	3648	1/1	0.97	0.16	32,32,32,32	0
87	OHX	5	4065	7/7	0.97	0.09	110,110,110,110	0
86	MG	5	3707	1/1	0.97	0.06	38,38,38,38	0
87	OHX	1	3927	7/7	0.97	0.11	87,87,87,87	0
87	OHX	1	4068	7/7	0.97	0.15	96,96,96,96	0
87	OHX	1	4069	7/7	0.97	0.08	138,138,138,138	0
87	OHX	5	4070	7/7	0.97	0.07	142,142,142,142	0
87	OHX	1	3930	7/7	0.97	0.12	106,106,106,106	0
86	MG	m7	203	1/1	0.97	0.15	50,50,50,50	0
87	OHX	2	2115	7/7	0.97	0.12	116,116,116,116	0
87	OHX	1	3941	7/7	0.97	0.12	89,89,89,89	0
87	OHX	1	3942	7/7	0.97	0.12	91,91,91,91	0
86	MG	1	3411	1/1	0.97	0.17	32,32,32,32	0
86	MG	m7	205	1/1	0.97	0.05	37,37,37,37	0
86	MG	5	3821	1/1	0.97	0.16	42,42,42,42	0
86	MG	1	3550	1/1	0.97	0.18	36,36,36,36	0
86	MG	5	3823	1/1	0.97	0.07	38,38,38,38	0
86	MG	5	3761	1/1	0.97	0.20	60,60,60,60	0
86	MG	1	3521	1/1	0.97	0.09	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	2	1903	1/1	0.97	0.30	46,46,46,46	0
86	MG	1	3811	1/1	0.97	0.12	37,37,37,37	0
86	MG	5	3540	1/1	0.97	0.23	21,21,21,21	0
87	OHX	1	3971	7/7	0.97	0.08	121,121,121,121	0
87	OHX	1	3972	7/7	0.97	0.11	98,98,98,98	0
87	OHX	1	3974	7/7	0.97	0.12	106,106,106,106	0
86	MG	5	3768	1/1	0.97	0.10	40,40,40,40	0
86	MG	1	3730	1/1	0.97	0.12	73,73,73,73	0
87	OHX	1	3981	7/7	0.97	0.26	87,87,87,87	0
87	OHX	1	3982	7/7	0.97	0.09	102,102,102,102	0
87	OHX	5	4096	7/7	0.97	0.20	96,96,96,96	0
86	MG	1	3786	1/1	0.97	0.27	33,33,33,33	0
86	MG	1	3765	1/1	0.97	0.26	49,49,49,49	0
86	MG	5	3772	1/1	0.97	0.10	45,45,45,45	0
87	OHX	5	4100	7/7	0.97	0.11	112,112,112,112	0
87	OHX	1	3989	7/7	0.97	0.09	114,114,114,114	0
87	OHX	1	3990	7/7	0.97	0.11	109,109,109,109	0
86	MG	5	3836	1/1	0.97	0.11	73,73,73,73	0
87	OHX	1	3992	7/7	0.97	0.14	95,95,95,95	0
86	MG	2	1995	1/1	0.97	0.27	45,45,45,45	0
86	MG	1	3843	1/1	0.97	0.27	31,31,31,31	0
87	OHX	7	216	7/7	0.97	0.12	84,84,84,84	0
87	OHX	7	221	7/7	0.97	0.10	103,103,103,103	0
86	MG	5	3504	1/1	0.97	0.37	33,33,33,33	0
87	OHX	2	2033	7/7	0.97	0.13	105,105,105,105	0
87	OHX	1	3997	7/7	0.97	0.10	114,114,114,114	0
87	OHX	1	3998	7/7	0.97	0.08	125,125,125,125	0
87	OHX	8	215	7/7	0.97	0.11	102,102,102,102	0
87	OHX	8	216	7/7	0.97	0.09	120,120,120,120	0
87	OHX	2	2037	7/7	0.97	0.11	116,116,116,116	0
86	MG	1	3748	1/1	0.97	0.09	37,37,37,37	0
86	MG	5	3630	1/1	0.97	0.21	35,35,35,35	0
86	MG	5	3588	1/1	0.97	0.23	28,28,28,28	0
86	MG	1	3732	1/1	0.97	0.28	24,24,24,24	0
87	OHX	2	2055	7/7	0.97	0.11	107,107,107,107	0
87	OHX	2	2056	7/7	0.97	0.08	125,125,125,125	0
86	MG	6	2001	1/1	0.97	0.09	54,54,54,54	0
86	MG	5	3508	1/1	0.97	0.28	26,26,26,26	0
87	OHX	3	216	7/7	0.97	0.12	106,106,106,106	0
87	OHX	3	217	7/7	0.97	0.11	101,101,101,101	0
87	OHX	3	218	7/7	0.97	0.11	99,99,99,99	0
87	OHX	3	219	7/7	0.97	0.09	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	3	220	7/7	0.97	0.09	119,119,119,119	0
86	MG	1	3792	1/1	0.97	0.09	69,69,69,69	0
86	MG	5	3680	1/1	0.97	0.12	41,41,41,41	0
86	MG	5	3729	1/1	0.97	0.04	54,54,54,54	0
86	MG	5	3730	1/1	0.97	0.20	45,45,45,45	0
86	MG	5	3406	1/1	0.97	0.14	36,36,36,36	0
87	OHX	2	2069	7/7	0.97	0.13	109,109,109,109	0
87	OHX	4	228	7/7	0.97	0.08	108,108,108,108	0
87	OHX	m5	305	7/7	0.97	0.11	114,114,114,114	0
87	OHX	2	2071	7/7	0.97	0.10	119,119,119,119	0
86	MG	1	3604	1/1	0.97	0.11	35,35,35,35	0
87	OHX	o3	202	7/7	0.97	0.12	103,103,103,103	0
87	OHX	2	2074	7/7	0.97	0.12	113,113,113,113	0
86	MG	5	3408	1/1	0.97	0.10	28,28,28,28	0
86	MG	1	3569	1/1	0.97	0.20	29,29,29,29	0
86	MG	5	3597	1/1	0.97	0.28	23,23,23,23	0
86	MG	1	3481	1/1	0.97	0.30	43,43,43,43	0
87	OHX	1	4023	7/7	0.97	0.11	108,108,108,108	0
86	MG	5	3445	1/1	0.97	0.12	43,43,43,43	0
86	MG	1	3625	1/1	0.97	0.26	53,53,53,53	0
86	MG	5	3866	1/1	0.98	0.07	57,57,57,57	0
87	OHX	6	2101	7/7	0.98	0.07	117,117,117,117	0
87	OHX	1	3973	7/7	0.98	0.08	105,105,105,105	0
87	OHX	5	3972	7/7	0.98	0.12	88,88,88,88	0
87	OHX	5	3973	7/7	0.98	0.08	84,84,84,84	0
87	OHX	5	3974	7/7	0.98	0.08	94,94,94,94	0
87	OHX	5	3977	7/7	0.98	0.10	79,79,79,79	0
86	MG	6	1996	1/1	0.98	0.08	50,50,50,50	0
87	OHX	1	3975	7/7	0.98	0.17	95,95,95,95	0
86	MG	5	3868	1/1	0.98	0.07	43,43,43,43	0
87	OHX	1	3977	7/7	0.98	0.07	118,118,118,118	0
87	OHX	5	3984	7/7	0.98	0.10	90,90,90,90	0
87	OHX	1	3978	7/7	0.98	0.10	102,102,102,102	0
87	OHX	5	3988	7/7	0.98	0.18	90,90,90,90	0
87	OHX	5	3989	7/7	0.98	0.12	87,87,87,87	0
87	OHX	5	3991	7/7	0.98	0.12	84,84,84,84	0
87	OHX	5	3992	7/7	0.98	0.08	93,93,93,93	0
87	OHX	5	3993	7/7	0.98	0.08	114,114,114,114	0
87	OHX	1	3979	7/7	0.98	0.10	101,101,101,101	0
87	OHX	2	2090	7/7	0.98	0.09	119,119,119,119	0
86	MG	8	212	1/1	0.98	0.27	35,35,35,35	0
86	MG	1	3570	1/1	0.98	0.29	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	N8	202	1/1	0.98	0.21	30,30,30,30	0
87	OHX	2	2094	7/7	0.98	0.06	142,142,142,142	0
87	OHX	5	4002	7/7	0.98	0.07	115,115,115,115	0
87	OHX	1	3987	7/7	0.98	0.14	92,92,92,92	0
87	OHX	5	4005	7/7	0.98	0.08	108,108,108,108	0
87	OHX	5	4006	7/7	0.98	0.16	92,92,92,92	0
87	OHX	2	2025	7/7	0.98	0.14	84,84,84,84	0
87	OHX	2	2028	7/7	0.98	0.10	93,93,93,93	0
87	OHX	5	4009	7/7	0.98	0.17	89,89,89,89	0
87	OHX	5	4010	7/7	0.98	0.11	100,100,100,100	0
87	OHX	2	2029	7/7	0.98	0.10	96,96,96,96	0
87	OHX	5	4012	7/7	0.98	0.06	118,118,118,118	0
87	OHX	2	2030	7/7	0.98	0.11	94,94,94,94	0
87	OHX	2	2031	7/7	0.98	0.07	109,109,109,109	0
86	MG	1	3789	1/1	0.98	0.05	42,42,42,42	0
87	OHX	2	2034	7/7	0.98	0.11	98,98,98,98	0
87	OHX	5	4020	7/7	0.98	0.10	99,99,99,99	0
87	OHX	2	2035	7/7	0.98	0.10	99,99,99,99	0
86	MG	13	402	1/1	0.98	0.36	25,25,25,25	0
87	OHX	5	4023	7/7	0.98	0.07	113,113,113,113	0
87	OHX	5	4024	7/7	0.98	0.10	99,99,99,99	0
87	OHX	2	2038	7/7	0.98	0.08	97,97,97,97	0
87	OHX	2	2039	7/7	0.98	0.08	93,93,93,93	0
87	OHX	5	4027	7/7	0.98	0.09	107,107,107,107	0
86	MG	5	3779	1/1	0.98	0.10	28,28,28,28	0
86	MG	1	3571	1/1	0.98	0.22	23,23,23,23	0
87	OHX	5	4030	7/7	0.98	0.07	111,111,111,111	0
87	OHX	6	2128	7/7	0.98	0.10	113,113,113,113	0
87	OHX	1	4001	7/7	0.98	0.07	138,138,138,138	0
87	OHX	2	2045	7/7	0.98	0.08	100,100,100,100	0
87	OHX	5	4034	7/7	0.98	0.11	86,86,86,86	0
87	OHX	2	2046	7/7	0.98	0.07	109,109,109,109	0
87	OHX	2	2048	7/7	0.98	0.07	110,110,110,110	0
87	OHX	2	2049	7/7	0.98	0.07	111,111,111,111	0
87	OHX	2	2050	7/7	0.98	0.09	112,112,112,112	0
87	OHX	2	2051	7/7	0.98	0.08	97,97,97,97	0
87	OHX	5	4040	7/7	0.98	0.09	102,102,102,102	0
87	OHX	2	2052	7/7	0.98	0.08	105,105,105,105	0
86	MG	6	1981	1/1	0.98	0.09	45,45,45,45	0
86	MG	5	3402	1/1	0.98	0.20	27,27,27,27	0
86	MG	5	3512	1/1	0.98	0.16	28,28,28,28	0
87	OHX	5	4045	7/7	0.98	0.24	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	4206	7/7	0.98	0.17	84,84,84,84	0
87	OHX	6	2140	7/7	0.98	0.09	118,118,118,118	0
86	MG	6	1982	1/1	0.98	0.13	49,49,49,49	0
86	MG	5	3845	1/1	0.98	0.07	66,66,66,66	0
87	OHX	2	2058	7/7	0.98	0.09	109,109,109,109	0
87	OHX	5	4050	7/7	0.98	0.19	93,93,93,93	0
87	OHX	2	2059	7/7	0.98	0.08	117,117,117,117	0
87	OHX	2	2061	7/7	0.98	0.07	122,122,122,122	0
86	MG	1	3724	1/1	0.98	0.07	56,56,56,56	0
86	MG	1	3562	1/1	0.98	0.31	38,38,38,38	0
87	OHX	2	2064	7/7	0.98	0.10	106,106,106,106	0
86	MG	5	3427	1/1	0.98	0.36	42,42,42,42	0
87	OHX	1	3894	7/7	0.98	0.13	76,76,76,76	0
87	OHX	3	215	7/7	0.98	0.09	95,95,95,95	0
86	MG	1	3507	1/1	0.98	0.41	40,40,40,40	0
86	MG	1	3662	1/1	0.98	0.11	32,32,32,32	0
87	OHX	5	4061	7/7	0.98	0.09	96,96,96,96	0
87	OHX	1	3901	7/7	0.98	0.10	77,77,77,77	0
87	OHX	1	3903	7/7	0.98	0.10	81,81,81,81	0
87	OHX	1	3904	7/7	0.98	0.09	82,82,82,82	0
87	OHX	1	3909	7/7	0.98	0.08	84,84,84,84	0
86	MG	1	3703	1/1	0.98	0.27	42,42,42,42	0
87	OHX	1	3915	7/7	0.98	0.10	91,91,91,91	0
87	OHX	1	3918	7/7	0.98	0.08	86,86,86,86	0
87	OHX	1	3920	7/7	0.98	0.10	86,86,86,86	0
87	OHX	1	3921	7/7	0.98	0.09	93,93,93,93	0
87	OHX	4	226	7/7	0.98	0.11	91,91,91,91	0
87	OHX	5	4072	7/7	0.98	0.08	111,111,111,111	0
86	MG	5	3791	1/1	0.98	0.06	42,42,42,42	0
87	OHX	4	229	7/7	0.98	0.10	116,116,116,116	0
87	OHX	1	3925	7/7	0.98	0.11	86,86,86,86	0
87	OHX	2	2070	7/7	0.98	0.07	122,122,122,122	0
87	OHX	1	3928	7/7	0.98	0.09	88,88,88,88	0
86	MG	1	4220	1/1	0.98	0.11	28,28,28,28	0
87	OHX	2	2072	7/7	0.98	0.08	111,111,111,111	0
87	OHX	1	3933	7/7	0.98	0.08	103,103,103,103	0
87	OHX	1	3936	7/7	0.98	0.09	95,95,95,95	0
87	OHX	1	3937	7/7	0.98	0.09	102,102,102,102	0
87	OHX	1	4044	7/7	0.98	0.08	126,126,126,126	0
86	MG	1	4221	1/1	0.98	0.07	66,66,66,66	0
87	OHX	1	3940	7/7	0.98	0.10	94,94,94,94	0
87	OHX	5	4087	7/7	0.98	0.11	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	5	3715	1/1	0.98	0.06	60,60,60,60	0
86	MG	5	3767	1/1	0.98	0.08	35,35,35,35	0
86	MG	1	3692	1/1	0.98	0.07	37,37,37,37	0
87	OHX	1	3944	7/7	0.98	0.09	95,95,95,95	0
87	OHX	1	3945	7/7	0.98	0.14	90,90,90,90	0
87	OHX	1	3947	7/7	0.98	0.08	104,104,104,104	0
86	MG	1	3630	1/1	0.98	0.18	65,65,65,65	0
86	MG	1	3683	1/1	0.98	0.14	49,49,49,49	0
87	OHX	1	3951	7/7	0.98	0.09	105,105,105,105	0
86	MG	8	203	1/1	0.98	0.37	45,45,45,45	0
86	MG	1	3574	1/1	0.98	0.30	34,34,34,34	0
87	OHX	O7	104	7/7	0.98	0.10	95,95,95,95	0
87	OHX	7	215	7/7	0.98	0.10	87,87,87,87	0
87	OHX	Q2	503	7/7	0.98	0.17	83,83,83,83	0
87	OHX	7	217	7/7	0.98	0.10	97,97,97,97	0
87	OHX	7	219	7/7	0.98	0.17	91,91,91,91	0
87	OHX	7	220	7/7	0.98	0.07	99,99,99,99	0
87	OHX	6	2048	7/7	0.98	0.11	73,73,73,73	0
87	OHX	6	2052	7/7	0.98	0.12	83,83,83,83	0
86	MG	1	3446	1/1	0.98	0.06	43,43,43,43	0
87	OHX	6	2062	7/7	0.98	0.08	97,97,97,97	0
86	MG	5	3527	1/1	0.98	0.34	34,34,34,34	0
87	OHX	8	214	7/7	0.98	0.07	106,106,106,106	0
87	OHX	6	2065	7/7	0.98	0.11	86,86,86,86	0
87	OHX	6	2068	7/7	0.98	0.07	106,106,106,106	0
87	OHX	6	2070	7/7	0.98	0.08	119,119,119,119	0
87	OHX	6	2071	7/7	0.98	0.08	126,126,126,126	0
87	OHX	1	3957	7/7	0.98	0.15	93,93,93,93	0
87	OHX	6	2080	7/7	0.98	0.07	112,112,112,112	0
87	OHX	1	3958	7/7	0.98	0.16	92,92,92,92	0
87	OHX	1	3960	7/7	0.98	0.13	87,87,87,87	0
87	OHX	1	4160	7/7	0.98	0.12	101,101,101,101	0
87	OHX	1	3962	7/7	0.98	0.07	103,103,103,103	0
87	OHX	6	2086	7/7	0.98	0.08	121,121,121,121	0
87	OHX	6	2087	7/7	0.98	0.09	104,104,104,104	0
87	OHX	l3	403	7/7	0.98	0.10	96,96,96,96	0
87	OHX	1	3963	7/7	0.98	0.07	105,105,105,105	0
87	OHX	6	2089	7/7	0.98	0.08	108,108,108,108	0
87	OHX	6	2090	7/7	0.98	0.08	100,100,100,100	0
87	OHX	6	2091	7/7	0.98	0.07	122,122,122,122	0
87	OHX	1	3964	7/7	0.98	0.10	96,96,96,96	0
87	OHX	2	2083	7/7	0.98	0.08	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	MG	n8	204	1/1	0.98	0.09	34,34,34,34	0
87	OHX	1	3968	7/7	0.98	0.08	97,97,97,97	0
87	OHX	5	3936	7/7	0.98	0.10	71,71,71,71	0
87	OHX	5	3944	7/7	0.98	0.10	89,89,89,89	0
87	OHX	5	3945	7/7	0.98	0.11	82,82,82,82	0
87	OHX	5	3946	7/7	0.98	0.09	80,80,80,80	0
87	OHX	m6	202	7/7	0.98	0.12	89,89,89,89	0
87	OHX	5	3948	7/7	0.98	0.09	77,77,77,77	0
87	OHX	5	3949	7/7	0.98	0.09	84,84,84,84	0
87	OHX	o2	201	7/7	0.98	0.18	93,93,93,93	0
87	OHX	5	3951	7/7	0.98	0.10	73,73,73,73	0
87	OHX	o7	502	7/7	0.98	0.10	96,96,96,96	0
87	OHX	5	3952	7/7	0.98	0.09	85,85,85,85	0
87	OHX	q2	502	7/7	0.98	0.14	82,82,82,82	0
86	MG	5	3831	1/1	0.98	0.11	38,38,38,38	0
88	ZN	E1	501	1/1	0.98	0.04	109,109,109,109	0
87	OHX	5	3955	7/7	0.98	0.08	79,79,79,79	0
87	OHX	1	3970	7/7	0.98	0.16	92,92,92,92	0
87	OHX	5	3957	7/7	0.98	0.08	98,98,98,98	0
86	MG	1	3513	1/1	0.98	0.30	25,25,25,25	0
87	OHX	6	2099	7/7	0.98	0.07	109,109,109,109	0
87	OHX	5	3963	7/7	0.98	0.10	83,83,83,83	0
87	OHX	6	2076	7/7	0.99	0.07	100,100,100,100	0
87	OHX	6	2077	7/7	0.99	0.07	97,97,97,97	0
87	OHX	6	2078	7/7	0.99	0.07	93,93,93,93	0
87	OHX	6	2079	7/7	0.99	0.06	101,101,101,101	0
87	OHX	2	2032	7/7	0.99	0.08	96,96,96,96	0
86	MG	1	3812	1/1	0.99	0.06	36,36,36,36	0
87	OHX	1	3938	7/7	0.99	0.10	77,77,77,77	0
87	OHX	1	4003	7/7	0.99	0.10	86,86,86,86	0
87	OHX	6	2084	7/7	0.99	0.07	106,106,106,106	0
86	MG	1	3829	1/1	0.99	0.06	57,57,57,57	0
87	OHX	1	3872	7/7	0.99	0.12	58,58,58,58	0
87	OHX	1	3873	7/7	0.99	0.11	54,54,54,54	0
87	OHX	1	3874	7/7	0.99	0.11	59,59,59,59	0
87	OHX	1	3877	7/7	0.99	0.09	59,59,59,59	0
87	OHX	1	3878	7/7	0.99	0.11	60,60,60,60	0
87	OHX	1	3882	7/7	0.99	0.10	64,64,64,64	0
87	OHX	1	3946	7/7	0.99	0.15	87,87,87,87	0
87	OHX	1	3883	7/7	0.99	0.09	63,63,63,63	0
87	OHX	1	3948	7/7	0.99	0.06	89,89,89,89	0
87	OHX	1	3884	7/7	0.99	0.06	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	1	3885	7/7	0.99	0.10	69,69,69,69	0
87	OHX	1	3886	7/7	0.99	0.10	64,64,64,64	0
87	OHX	1	3889	7/7	0.99	0.08	67,67,67,67	0
87	OHX	1	3891	7/7	0.99	0.09	78,78,78,78	0
87	OHX	1	3954	7/7	0.99	0.09	95,95,95,95	0
86	MG	5	3531	1/1	0.99	0.31	26,26,26,26	0
87	OHX	1	3895	7/7	0.99	0.06	67,67,67,67	0
87	OHX	1	3897	7/7	0.99	0.07	70,70,70,70	0
87	OHX	1	3898	7/7	0.99	0.07	72,72,72,72	0
87	OHX	1	3959	7/7	0.99	0.07	93,93,93,93	0
87	OHX	2	2036	7/7	0.99	0.06	91,91,91,91	0
87	OHX	1	4092	7/7	0.99	0.17	78,78,78,78	0
87	OHX	s1	302	7/7	0.99	0.10	81,81,81,81	0
87	OHX	1	3961	7/7	0.99	0.15	72,72,72,72	0
86	MG	1	3675	1/1	0.99	0.07	69,69,69,69	0
86	MG	1	3804	1/1	0.99	0.09	56,56,56,56	0
87	OHX	4	224	7/7	0.99	0.10	57,57,57,57	0
87	OHX	4	225	7/7	0.99	0.07	75,75,75,75	0
87	OHX	1	3902	7/7	0.99	0.08	71,71,71,71	0
87	OHX	4	227	7/7	0.99	0.10	93,93,93,93	0
87	OHX	2	2060	7/7	0.99	0.09	100,100,100,100	0
86	MG	1	3744	1/1	0.99	0.03	39,39,39,39	0
87	OHX	5	3903	7/7	0.99	0.11	48,48,48,48	0
87	OHX	5	3907	7/7	0.99	0.10	52,52,52,52	0
87	OHX	5	3911	7/7	0.99	0.14	63,63,63,63	0
87	OHX	5	3912	7/7	0.99	0.09	54,54,54,54	0
87	OHX	5	3914	7/7	0.99	0.12	64,64,64,64	0
87	OHX	5	3915	7/7	0.99	0.07	54,54,54,54	0
87	OHX	5	3917	7/7	0.99	0.10	59,59,59,59	0
87	OHX	5	3918	7/7	0.99	0.08	64,64,64,64	0
87	OHX	5	3919	7/7	0.99	0.11	63,63,63,63	0
87	OHX	5	3920	7/7	0.99	0.08	66,66,66,66	0
87	OHX	5	3922	7/7	0.99	0.06	60,60,60,60	0
87	OHX	5	3923	7/7	0.99	0.06	64,64,64,64	0
87	OHX	5	3925	7/7	0.99	0.07	63,63,63,63	0
87	OHX	5	3928	7/7	0.99	0.10	68,68,68,68	0
87	OHX	5	3929	7/7	0.99	0.06	64,64,64,64	0
87	OHX	1	3967	7/7	0.99	0.07	66,66,66,66	0
87	OHX	5	3932	7/7	0.99	0.06	72,72,72,72	0
87	OHX	5	3933	7/7	0.99	0.05	73,73,73,73	0
87	OHX	1	3905	7/7	0.99	0.07	66,66,66,66	0
87	OHX	1	3906	7/7	0.99	0.07	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	3937	7/7	0.99	0.12	88,88,88,88	0
87	OHX	5	3938	7/7	0.99	0.07	70,70,70,70	0
87	OHX	5	4084	7/7	0.99	0.13	93,93,93,93	0
87	OHX	5	3939	7/7	0.99	0.06	77,77,77,77	0
87	OHX	5	3940	7/7	0.99	0.05	74,74,74,74	0
87	OHX	5	3942	7/7	0.99	0.08	73,73,73,73	0
87	OHX	5	3943	7/7	0.99	0.07	78,78,78,78	0
87	OHX	1	3907	7/7	0.99	0.09	76,76,76,76	0
87	OHX	1	4036	7/7	0.99	0.07	98,98,98,98	0
87	OHX	1	3908	7/7	0.99	0.12	75,75,75,75	0
87	OHX	5	3947	7/7	0.99	0.08	87,87,87,87	0
87	OHX	2	2023	7/7	0.99	0.13	73,73,73,73	0
87	OHX	1	3910	7/7	0.99	0.08	86,86,86,86	0
87	OHX	5	3950	7/7	0.99	0.05	73,73,73,73	0
87	OHX	1	3911	7/7	0.99	0.06	80,80,80,80	0
87	OHX	1	3912	7/7	0.99	0.09	87,87,87,87	0
87	OHX	5	3953	7/7	0.99	0.10	95,95,95,95	0
87	OHX	2	2041	7/7	0.99	0.08	90,90,90,90	0
87	OHX	2	2042	7/7	0.99	0.06	94,94,94,94	0
87	OHX	1	3916	7/7	0.99	0.07	82,82,82,82	0
87	OHX	1	3917	7/7	0.99	0.07	82,82,82,82	0
87	OHX	5	3958	7/7	0.99	0.14	79,79,79,79	0
87	OHX	5	3959	7/7	0.99	0.06	89,89,89,89	0
87	OHX	2	2024	7/7	0.99	0.12	80,80,80,80	0
87	OHX	1	3919	7/7	0.99	0.07	94,94,94,94	0
87	OHX	5	3962	7/7	0.99	0.08	80,80,80,80	0
87	OHX	2	2044	7/7	0.99	0.06	97,97,97,97	0
87	OHX	5	3964	7/7	0.99	0.07	70,70,70,70	0
86	MG	5	3842	1/1	0.99	0.04	62,62,62,62	0
87	OHX	5	3966	7/7	0.99	0.06	88,88,88,88	0
87	OHX	5	3967	7/7	0.99	0.05	86,86,86,86	0
87	OHX	1	3984	7/7	0.99	0.12	81,81,81,81	0
87	OHX	5	3969	7/7	0.99	0.09	73,73,73,73	0
87	OHX	5	3970	7/7	0.99	0.08	94,94,94,94	0
87	OHX	N9	101	7/7	0.99	0.11	62,62,62,62	0
87	OHX	7	218	7/7	0.99	0.14	92,92,92,92	0
87	OHX	5	4117	7/7	0.99	0.13	81,81,81,81	0
87	OHX	1	3985	7/7	0.99	0.07	106,106,106,106	0
87	OHX	1	3922	7/7	0.99	0.09	93,93,93,93	0
87	OHX	1	3923	7/7	0.99	0.06	83,83,83,83	0
87	OHX	5	3975	7/7	0.99	0.06	93,93,93,93	0
87	OHX	5	3976	7/7	0.99	0.11	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	2	2026	7/7	0.99	0.09	82,82,82,82	0
87	OHX	2	2047	7/7	0.99	0.05	119,119,119,119	0
87	OHX	6	2045	7/7	0.99	0.12	69,69,69,69	0
87	OHX	6	2047	7/7	0.99	0.09	71,71,71,71	0
87	OHX	5	3981	7/7	0.99	0.05	99,99,99,99	0
87	OHX	1	3926	7/7	0.99	0.07	90,90,90,90	0
87	OHX	5	3983	7/7	0.99	0.12	77,77,77,77	0
87	OHX	6	2049	7/7	0.99	0.09	68,68,68,68	0
87	OHX	6	2050	7/7	0.99	0.09	73,73,73,73	0
87	OHX	5	3986	7/7	0.99	0.09	74,74,74,74	0
87	OHX	5	3987	7/7	0.99	0.09	77,77,77,77	0
87	OHX	6	2051	7/7	0.99	0.13	78,78,78,78	0
87	OHX	2	2027	7/7	0.99	0.08	73,73,73,73	0
87	OHX	5	3990	7/7	0.99	0.09	83,83,83,83	0
87	OHX	6	2053	7/7	0.99	0.09	68,68,68,68	0
87	OHX	6	2054	7/7	0.99	0.08	74,74,74,74	0
87	OHX	6	2055	7/7	0.99	0.06	82,82,82,82	0
87	OHX	5	3994	7/7	0.99	0.06	81,81,81,81	0
87	OHX	6	2056	7/7	0.99	0.10	94,94,94,94	0
87	OHX	5	3996	7/7	0.99	0.10	85,85,85,85	0
87	OHX	6	2057	7/7	0.99	0.05	81,81,81,81	0
87	OHX	6	2058	7/7	0.99	0.07	78,78,78,78	0
87	OHX	6	2059	7/7	0.99	0.06	85,85,85,85	0
87	OHX	6	2060	7/7	0.99	0.06	85,85,85,85	0
86	MG	5	3843	1/1	0.99	0.17	31,31,31,31	0
87	OHX	1	3929	7/7	0.99	0.08	72,72,72,72	0
87	OHX	5	4003	7/7	0.99	0.05	103,103,103,103	0
86	MG	5	3826	1/1	0.99	0.07	55,55,55,55	0
87	OHX	6	2064	7/7	0.99	0.14	92,92,92,92	0
87	OHX	1	3931	7/7	0.99	0.08	82,82,82,82	0
87	OHX	n3	203	7/7	0.99	0.05	84,84,84,84	0
87	OHX	n9	102	7/7	0.99	0.10	65,65,65,65	0
87	OHX	6	2066	7/7	0.99	0.07	94,94,94,94	0
87	OHX	6	2067	7/7	0.99	0.10	83,83,83,83	0
86	MG	5	3763	1/1	0.99	0.04	42,42,42,42	0
87	OHX	6	2069	7/7	0.99	0.13	84,84,84,84	0
86	MG	5	3856	1/1	0.99	0.10	45,45,45,45	0
87	OHX	1	3934	7/7	0.99	0.07	76,76,76,76	0
87	OHX	5	4013	7/7	0.99	0.07	63,63,63,63	0
87	OHX	5	4014	7/7	0.99	0.11	88,88,88,88	0
87	OHX	5	4015	7/7	0.99	0.07	100,100,100,100	0
87	OHX	6	2072	7/7	0.99	0.08	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	6	2073	7/7	0.99	0.07	100,100,100,100	0
87	OHX	1	3935	7/7	0.99	0.07	83,83,83,83	0
87	OHX	6	2075	7/7	0.99	0.10	89,89,89,89	0
87	OHX	1	3879	7/7	1.00	0.08	63,63,63,63	0
87	OHX	1	3892	7/7	1.00	0.05	71,71,71,71	0
87	OHX	1	3893	7/7	1.00	0.06	65,65,65,65	0
87	OHX	5	3921	7/7	1.00	0.05	60,60,60,60	0
87	OHX	6	2044	7/7	1.00	0.11	56,56,56,56	0
87	OHX	1	3880	7/7	1.00	0.07	57,57,57,57	0
87	OHX	5	3924	7/7	1.00	0.07	66,66,66,66	0
87	OHX	6	2046	7/7	1.00	0.10	62,62,62,62	0
87	OHX	5	3926	7/7	1.00	0.07	62,62,62,62	0
87	OHX	5	3927	7/7	1.00	0.07	64,64,64,64	0
87	OHX	1	3881	7/7	1.00	0.07	59,59,59,59	0
87	OHX	1	3896	7/7	1.00	0.04	63,63,63,63	0
87	OHX	5	3930	7/7	1.00	0.05	58,58,58,58	0
87	OHX	1	3869	7/7	1.00	0.11	50,50,50,50	0
87	OHX	1	3913	7/7	1.00	0.05	70,70,70,70	0
87	OHX	1	3870	7/7	1.00	0.10	47,47,47,47	0
87	OHX	1	3875	7/7	1.00	0.07	52,52,52,52	0
87	OHX	5	3935	7/7	1.00	0.05	60,60,60,60	0
87	OHX	5	3904	7/7	1.00	0.12	45,45,45,45	0
87	OHX	5	3905	7/7	1.00	0.11	45,45,45,45	0
87	OHX	5	3906	7/7	1.00	0.08	48,48,48,48	0
87	OHX	1	3876	7/7	1.00	0.10	62,62,62,62	0
87	OHX	5	3908	7/7	1.00	0.10	54,54,54,54	0
87	OHX	8	213	7/7	1.00	0.10	58,58,58,58	0
87	OHX	5	3941	7/7	1.00	0.04	65,65,65,65	0
87	OHX	5	3909	7/7	1.00	0.08	56,56,56,56	0
88	ZN	D6	500	1/1	1.00	0.01	76,76,76,76	0
87	OHX	5	3910	7/7	1.00	0.08	58,58,58,58	0
88	ZN	D9	101	1/1	1.00	0.04	74,74,74,74	0
87	OHX	1	3871	7/7	1.00	0.09	54,54,54,54	0
88	ZN	O7	101	1/1	1.00	0.01	36,36,36,36	0
88	ZN	Q0	500	1/1	1.00	0.02	48,48,48,48	0
87	OHX	1	3887	7/7	1.00	0.05	60,60,60,60	0
88	ZN	Q3	501	1/1	1.00	0.01	55,55,55,55	0
88	ZN	d6	101	1/1	1.00	0.03	55,55,55,55	0
87	OHX	5	3913	7/7	1.00	0.07	47,47,47,47	0
88	ZN	d9	101	1/1	1.00	0.03	72,72,72,72	0
87	OHX	1	3888	7/7	1.00	0.07	68,68,68,68	0
88	ZN	o7	501	1/1	1.00	0.02	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	ZN	q0	201	1/1	1.00	0.01	30,30,30,30	0
87	OHX	1	3868	7/7	1.00	0.11	45,45,45,45	0
88	ZN	q3	501	1/1	1.00	0.01	58,58,58,58	0
87	OHX	5	3916	7/7	1.00	0.07	55,55,55,55	0
87	OHX	1	3890	7/7	1.00	0.06	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.