wwPDB X-ray Structure Validation Summary Report (i)

Mar 6, 2026 – 07:45 PM UTC

PDB ID	:	4U4R / pdb_00004u4r
Title	:	Crystal structure of Lactimidomycin bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-24
Resolution	:	2.80 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 (i) symbol.

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

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

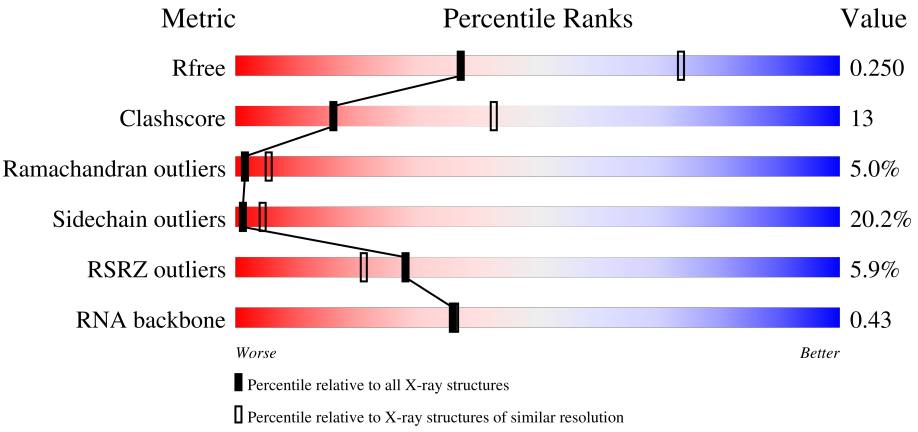
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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

Mol	Chain	Length	Quality of chain
1	2	1800	5% 45% 38% 14% ·
1	6	1800	5% 48% 38% 14%
2	S0	251	15% 29% 39% 13% · 18%
2	s0	251	8% 39% 32% 10% · 18%

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Mol	Chain	Length	Quality of chain
3	S1	254	19% 33% 37% 13% 16%
3	s1	254	3% 43% 31% 11% 15%
4	S2	253	6% 42% 34% 8% 14%
4	s2	253	3% 45% 29% 12% 14%
5	S3	239	9% 55% 31% 7% 7%
5	s3	239	5% 54% 27% 11% 7%
6	S4	260	3% 54% 35% 9%
6	s4	260	2% 49% 39% 12%
7	S5	224	10% 45% 38% 9% 8%
7	s5	224	10% 45% 33% 12% 8%
8	S6	236	17% 56% 32% 7%
8	s6	236	8% 57% 24% 11% 8%
9	S7	189	14% 47% 34% 14%
9	s7	189	15% 52% 34% 10%
10	S8	200	8% 56% 28% 9% 6%
10	s8	200	6% 60% 26% 8% 6%
11	S9	196	8% 48% 35% 9% 6%
11	s9	196	2% 53% 29% 10% 6%
12	C0	105	10% 43% 35% 11% 9%
12	c0	105	17% 45% 32% 13% 9%
13	C1	155	11% 64% 28% 7%
13	c1	155	8% 58% 27% 9% 6%
14	C2	142	15% 38% 34% 14% 13%
14	c2	142	20% 42% 32% 11% 13%
15	C3	150	3% 51% 37% 12%

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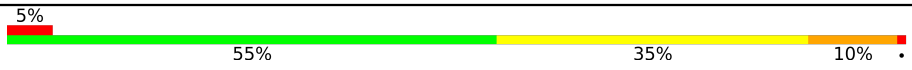
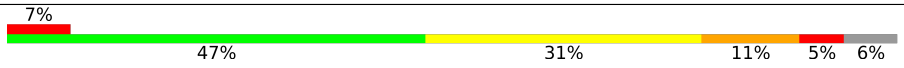
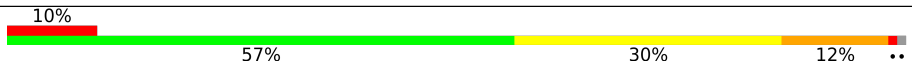
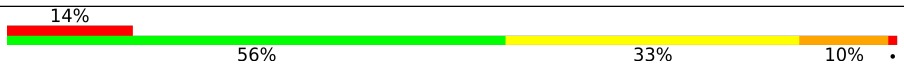
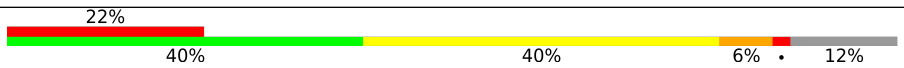
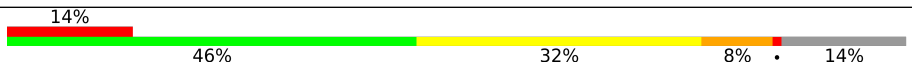
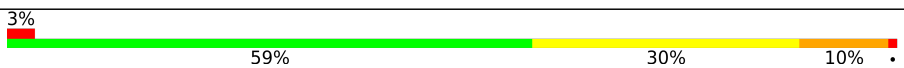
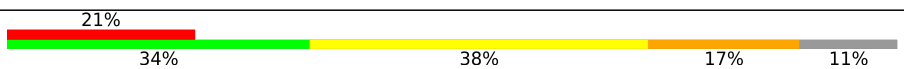
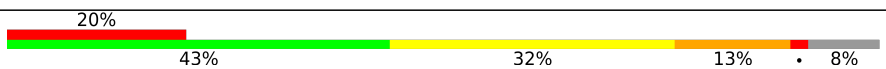
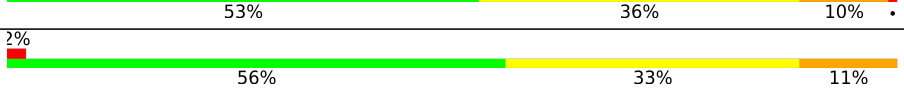
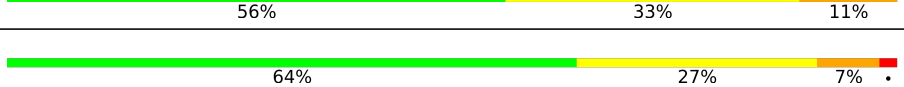
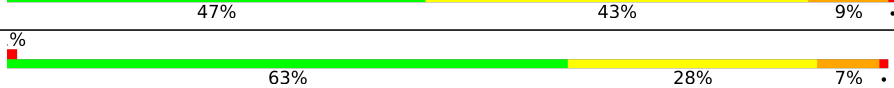
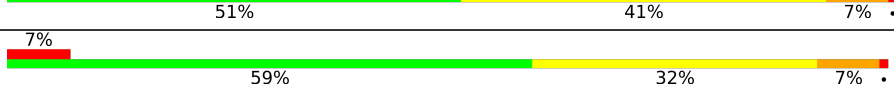
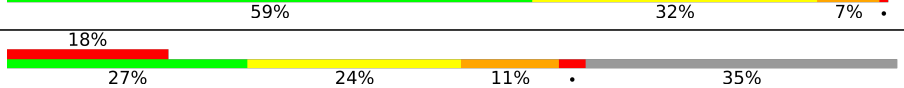
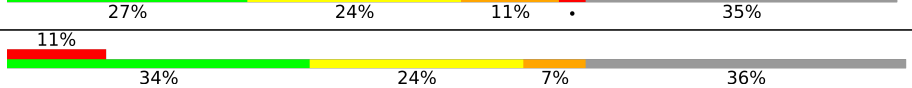
Mol	Chain	Length	Quality of chain
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	

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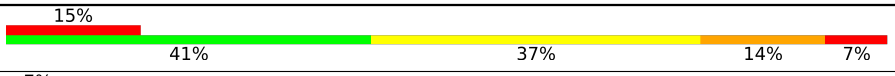
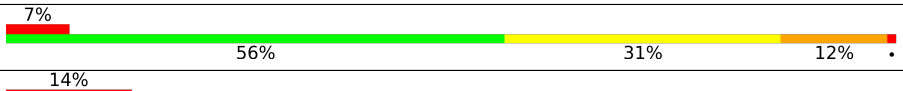
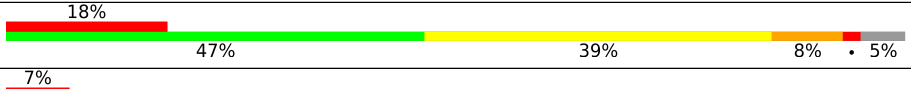
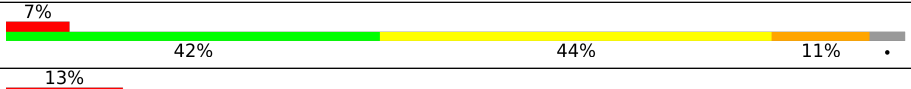
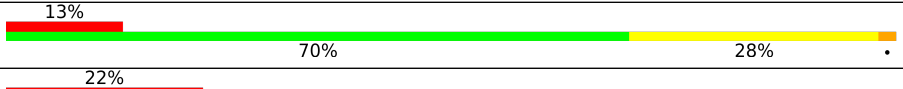
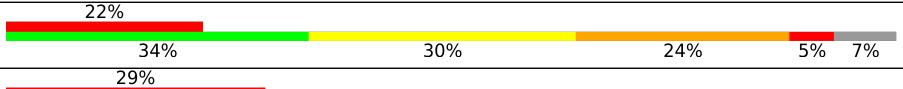
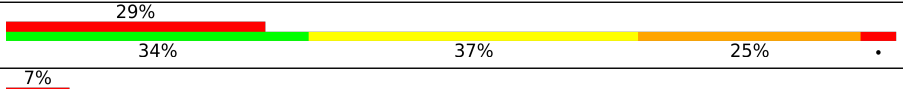
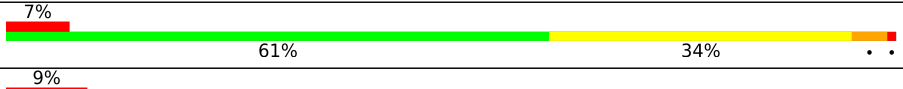
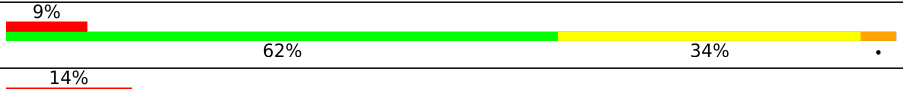
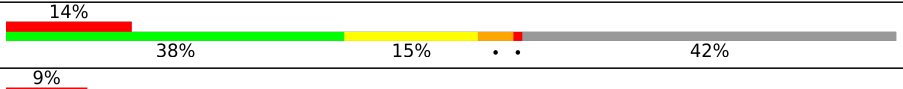
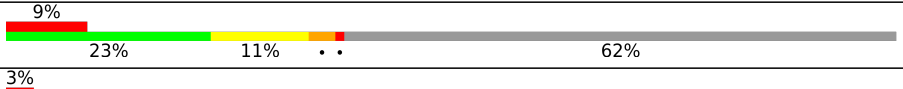
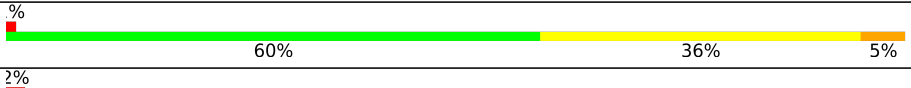
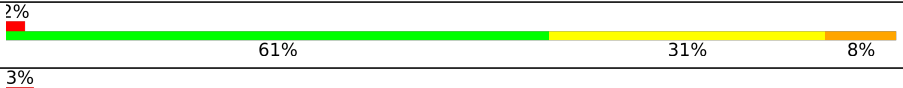
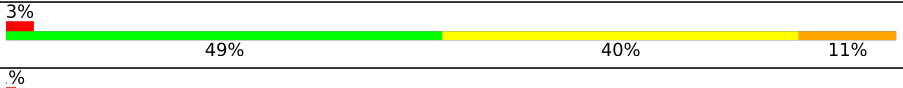
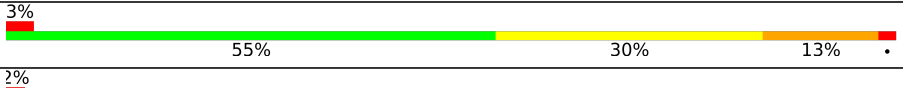
Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	

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Mol	Chain	Length	Quality of chain
41	L4	361	3% 56% 30% 12%
41	l4	361	4% 55% 33% 10%
42	L5	296	3% 54% 34% 11%
42	l5	296	3% 57% 31% 9%
43	L6	175	2% 61% 22% 5% 11%
43	l6	175	3% 53% 27% 9% 10%
44	L7	243	2% 62% 22% 5% 9%
44	l7	243	2% 63% 22% 6% 8%
45	L8	255	6% 53% 29% 10% 9%
45	l8	255	6% 51% 29% 9% 9%
46	L9	191	% 52% 35% 12%
46	l9	191	3% 54% 35% 10%
47	M0	220	3% 56% 30% 9%
47	m0	220	5% 53% 33% 11%
48	M1	173	2% 49% 35% 12%
48	m1	173	2% 53% 33% 10%
49	M3	198	2% 58% 30% 6%
49	m3	198	4% 59% 30% 9%
50	M4	137	3% 60% 31% 7%
50	m4	137	4% 63% 30% 7%
51	M5	203	60% 28% 11%
51	m5	203	58% 32% 9%
52	M6	198	3% 61% 29% 8%
52	m6	198	3% 64% 23% 11%
53	M7	183	9% 56% 34% 9%

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Mol	Chain	Length	Quality of chain
53	m7	183	49% 31% 15%
54	M8	185	60% 30% 9%
54	m8	185	60% 30% 9%
55	M9	188	10% 66% 26% 7%
55	m9	188	6% 69% 25% 5%
56	N0	172	59% 30% 8%
56	n0	172	3% 59% 33% 8%
57	N1	159	56% 33% 11%
57	n1	159	64% 23% 12%
58	N2	120	8% 52% 28% 17%
58	n2	120	6% 49% 26% 7% 18%
59	N3	136	4% 60% 32% 9%
59	n3	136	65% 29% 5%
60	N4	155	23% 43% 18% 37%
60	n4	155	24% 59% 25% 13%
61	N5	141	46% 28% 12% 14%
61	n5	141	48% 29% 6% 15%
62	N6	126	66% 25% 8%
62	n6	126	55% 36% 8%
63	N7	135	47% 41% 11%
63	n7	135	4% 48% 40% 11%
64	N8	148	54% 32% 10%
64	n8	148	55% 31% 9% 5%
65	N9	58	9% 59% 31% 10%
65	n9	58	7% 52% 24% 17% 7%

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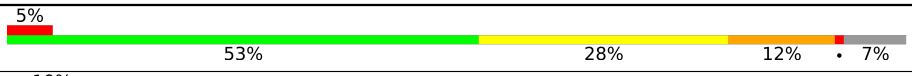
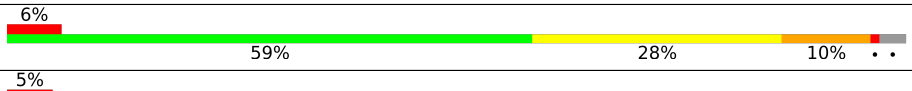
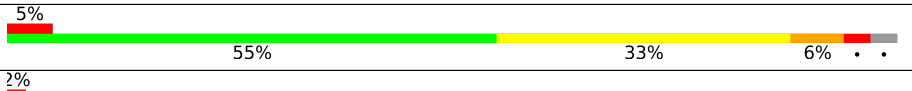
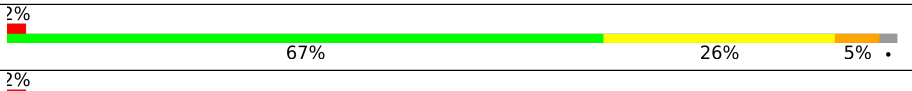
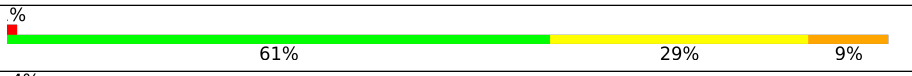
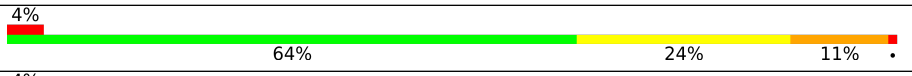
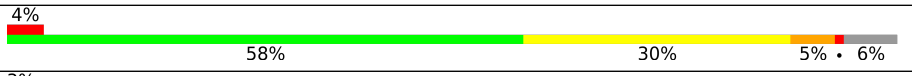
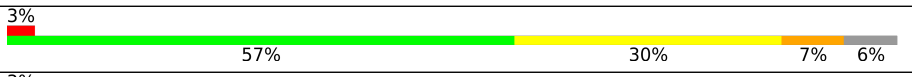
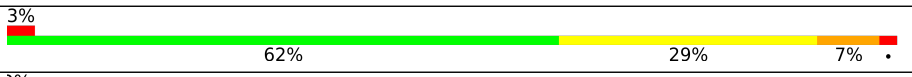
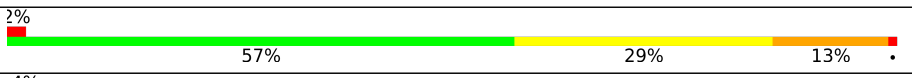
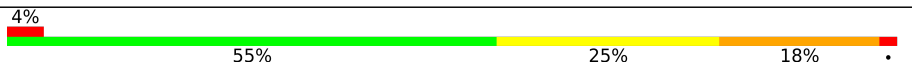
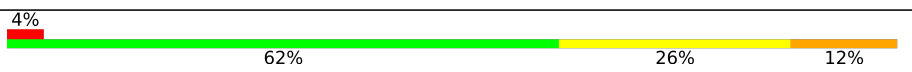
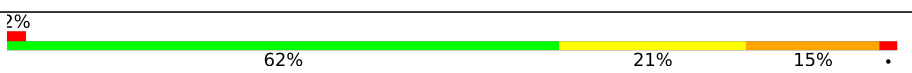
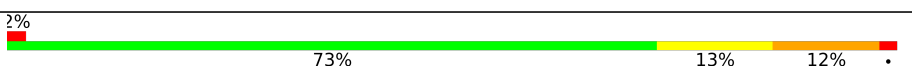
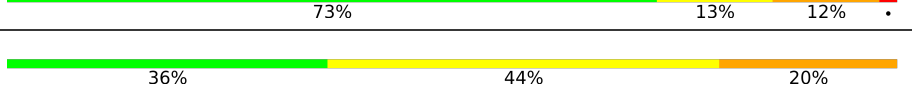
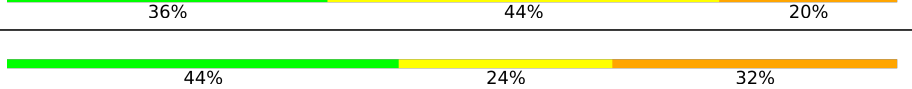
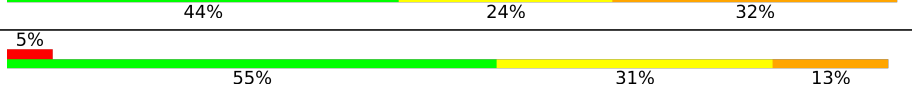
Mol	Chain	Length	Quality of chain
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	

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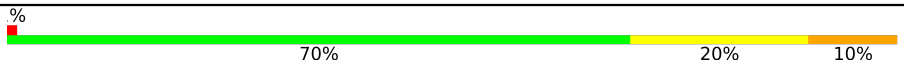
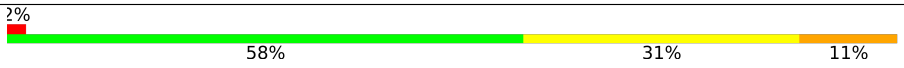
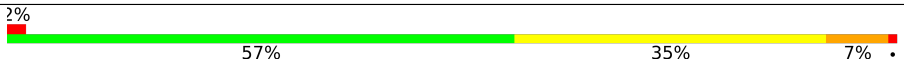
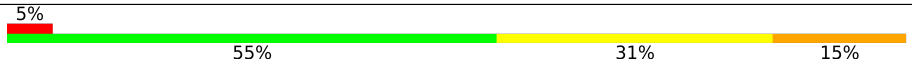
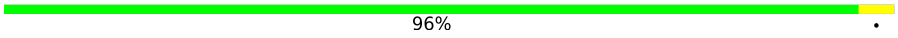
Mol	Chain	Length	Quality of chain
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	
81	m2	160	
82	p0	311	
83	p1	47	
84	p2	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	1	3405	-	-	-	X
85	MG	1	3652	-	-	-	X
85	MG	1	3677	-	-	-	X
85	MG	1	3809	-	-	-	X
85	MG	1	3820	-	-	-	X
85	MG	1	3865	-	-	-	X
85	MG	2	1915	-	-	-	X
85	MG	2	1928	-	-	-	X
85	MG	2	1951	-	-	-	X
85	MG	2	1954	-	-	-	X
85	MG	2	1960	-	-	-	X
85	MG	2	1968	-	-	-	X
85	MG	2	1975	-	-	-	X
85	MG	2	1991	-	-	-	X
85	MG	2	2018	-	-	-	X
85	MG	2	2020	-	-	-	X
85	MG	5	3466	-	-	-	X
85	MG	5	3661	-	-	-	X
85	MG	5	3707	-	-	-	X
85	MG	5	3881	-	-	-	X
85	MG	5	3886	-	-	-	X
85	MG	6	1924	-	-	-	X
85	MG	6	2035	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	6	2039	-	-	-	X
85	MG	6	2040	-	-	-	X
85	MG	M3	203	-	-	-	X
86	OHX	1	3943	-	-	X	-
86	OHX	1	3962	-	-	X	-
86	OHX	1	3964	-	-	X	-
86	OHX	1	3976	-	-	X	-
86	OHX	1	3980	-	-	X	-
86	OHX	1	4007	-	-	X	-
86	OHX	1	4023	-	-	X	-
86	OHX	1	4032	-	-	X	-
86	OHX	1	4036	-	-	X	-
86	OHX	1	4047	-	-	X	-
86	OHX	1	4048	-	-	X	-
86	OHX	1	4056	-	-	X	-
86	OHX	1	4059	-	-	X	-
86	OHX	1	4060	-	-	X	-
86	OHX	1	4061	-	-	X	-
86	OHX	1	4065	-	-	X	-
86	OHX	1	4071	-	-	X	-
86	OHX	1	4084	-	-	X	-
86	OHX	1	4088	-	-	X	-
86	OHX	1	4089	-	-	X	-
86	OHX	1	4118	-	-	X	-
86	OHX	1	4143	-	-	X	-
86	OHX	1	4149	-	-	X	-
86	OHX	1	4153	-	-	X	-
86	OHX	1	4157	-	-	X	-
86	OHX	1	4158	-	-	X	-
86	OHX	1	4159	-	-	X	-
86	OHX	1	4163	-	-	X	-
86	OHX	1	4166	-	-	X	-
86	OHX	1	4175	-	-	X	-
86	OHX	1	4177	-	-	X	-
86	OHX	1	4200	-	-	X	-
86	OHX	2	2032	-	-	X	-
86	OHX	2	2045	-	-	X	-
86	OHX	2	2076	-	-	X	-
86	OHX	2	2084	-	-	X	-
86	OHX	2	2086	-	-	X	-
86	OHX	2	2090	-	-	X	-
86	OHX	2	2091	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	2	2096	-	-	X	-
86	OHX	2	2099	-	-	X	-
86	OHX	2	2109	-	-	X	-
86	OHX	2	2116	-	-	X	-
86	OHX	2	2132	-	-	X	-
86	OHX	2	2147	-	-	X	-
86	OHX	2	2155	-	-	X	-
86	OHX	2	2163	-	-	X	-
86	OHX	5	3962	-	-	X	-
86	OHX	5	3973	-	-	X	-
86	OHX	5	3978	-	-	X	-
86	OHX	5	4000	-	-	X	-
86	OHX	5	4001	-	-	X	-
86	OHX	5	4011	-	-	X	-
86	OHX	5	4020	-	-	X	-
86	OHX	5	4033	-	-	X	-
86	OHX	5	4034	-	-	X	-
86	OHX	5	4055	-	-	X	-
86	OHX	5	4065	-	-	X	-
86	OHX	5	4066	-	-	X	-
86	OHX	5	4074	-	-	X	-
86	OHX	5	4076	-	-	X	-
86	OHX	5	4081	-	-	X	-
86	OHX	5	4090	-	-	X	-
86	OHX	5	4093	-	-	X	-
86	OHX	5	4094	-	-	X	-
86	OHX	5	4141	-	-	X	-
86	OHX	5	4187	-	-	X	-
86	OHX	5	4189	-	-	X	-
86	OHX	5	4190	-	-	X	-
86	OHX	5	4196	-	-	X	-
86	OHX	5	4197	-	-	X	-
86	OHX	5	4198	-	-	X	-
86	OHX	5	4201	-	-	X	-
86	OHX	5	4212	-	-	X	-
86	OHX	5	4215	-	-	X	-
86	OHX	5	4222	-	-	X	-
86	OHX	5	4234	-	-	X	-
86	OHX	5	4241	-	-	X	-
86	OHX	6	2060	-	-	X	-
86	OHX	6	2121	-	-	X	-
86	OHX	6	2147	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	6	2150	-	-	X	-
86	OHX	6	2171	-	-	X	-
86	OHX	7	218	-	-	X	-
86	OHX	7	219	-	-	X	-
86	OHX	7	224	-	-	X	-
86	OHX	7	226	-	-	X	-
86	OHX	8	215	-	-	X	-
86	OHX	8	223	-	-	X	-
86	OHX	8	224	-	-	X	-
86	OHX	C1	201	-	-	X	-
86	OHX	O7	103	-	-	X	-
86	OHX	O9	101	-	-	X	-
86	OHX	c1	202	-	-	X	-
86	OHX	o4	203	-	-	X	-
87	ZN	Q2	501	-	-	X	-

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 411226 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total 890	C 560	N 156	O 172	S 2	0	0	0
14	c2	124	Total 890	C 560	N 156	O 172	S 2	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total 926	C 577	N 177	O 170	S 2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			
35	sM	104	Total	C	N	O	0	0	0
			680	403	140	137			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O	0	0	0
			1521	935	326	260			
55	m9	188	Total	C	N	O	0	0	0
			1521	935	326	260			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 Unknown protein m2.

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

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

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

- Molecule 83 is a protein called Unknown protein p1.

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

- Molecule 84 is a protein called Unknown protein p2.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	2	126	Total Mg 126 126	0	0
85	S8	1	Total Mg 1 1	0	0
85	C3	1	Total Mg 1 1	0	0
85	SM	1	Total Mg 1 1	0	0
85	1	475	Total Mg 475 475	0	0
85	3	14	Total Mg 14 14	0	0
85	4	21	Total Mg 21 21	0	0
85	L2	1	Total Mg 1 1	0	0
85	L3	2	Total Mg 2 2	0	0
85	L4	3	Total Mg 3 3	0	0
85	L5	1	Total Mg 1 1	0	0
85	L6	1	Total Mg 1 1	0	0
85	L7	2	Total Mg 2 2	0	0
85	L8	1	Total Mg 1 1	0	0
85	M0	2	Total Mg 2 2	0	0
85	M1	1	Total Mg 1 1	0	0
85	M3	4	Total Mg 4 4	0	0
85	M5	2	Total Mg 2 2	0	0
85	M6	1	Total Mg 1 1	0	0
85	M7	6	Total Mg 6 6	0	0
85	M9	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	N0	1	Total Mg 1 1	0	0
85	N3	3	Total Mg 3 3	0	0
85	N5	1	Total Mg 1 1	0	0
85	N8	2	Total Mg 2 2	0	0
85	O3	1	Total Mg 1 1	0	0
85	O4	1	Total Mg 1 1	0	0
85	O7	1	Total Mg 1 1	0	0
85	Q2	1	Total Mg 1 1	0	0
85	6	147	Total Mg 147 147	0	0
85	s1	1	Total Mg 1 1	0	0
85	s6	1	Total Mg 1 1	0	0
85	s8	2	Total Mg 2 2	0	0
85	c1	1	Total Mg 1 1	0	0
85	c7	1	Total Mg 1 1	0	0
85	c8	2	Total Mg 2 2	0	0
85	d2	1	Total Mg 1 1	0	0
85	d3	1	Total Mg 1 1	0	0
85	d6	1	Total Mg 1 1	0	0
85	sM	2	Total Mg 2 2	0	0
85	5	504	Total Mg 504 504	0	0
85	7	15	Total Mg 15 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	8	13	Total Mg 13 13	0	0
85	l2	2	Total Mg 2 2	0	0
85	l3	1	Total Mg 1 1	0	0
85	l4	1	Total Mg 1 1	0	0
85	l5	3	Total Mg 3 3	0	0
85	l7	1	Total Mg 1 1	0	0
85	m1	2	Total Mg 2 2	0	0
85	m4	1	Total Mg 1 1	0	0
85	m5	1	Total Mg 1 1	0	0
85	m6	1	Total Mg 1 1	0	0
85	m7	5	Total Mg 5 5	0	0
85	n0	2	Total Mg 2 2	0	0
85	n3	2	Total Mg 2 2	0	0
85	n6	2	Total Mg 2 2	0	0
85	n8	4	Total Mg 4 4	0	0
85	n9	2	Total Mg 2 2	0	0
85	o1	1	Total Mg 1 1	0	0
85	o3	2	Total Mg 2 2	0	0
85	o4	2	Total Mg 2 2	0	0
85	q0	1	Total Mg 1 1	0	0
85	q1	1	Total Mg 1 1	0	0

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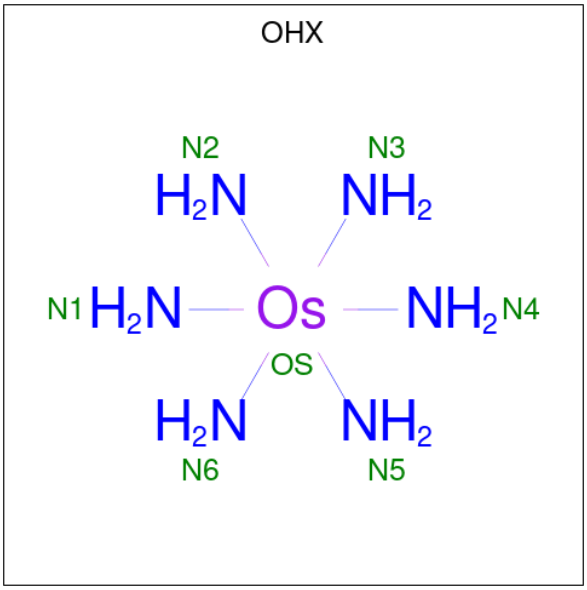
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	q3	1	Total Mg 1 1	0	0

- Molecule 86 is osmium (III) hexammine (CCD ID: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 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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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	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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86	C1	1	Total N Os 7 6 1	0	0
86	C3	1	Total N Os 7 6 1	0	0
86	C5	1	Total N Os 7 6 1	0	0
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86	D9	1	Total N Os 7 6 1	0	0
86	SR	1	Total N Os 7 6 1	0	0
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86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
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86	1	1	Total N Os 7 6 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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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0
86	L3	1	Total N Os 7 6 1	0	0
86	L3	1	Total N Os 7 6 1	0	0
86	L4	1	Total N Os 7 6 1	0	0
86	L6	1	Total N Os 7 6 1	0	0
86	M0	1	Total N Os 7 6 1	0	0
86	M5	1	Total N Os 7 6 1	0	0
86	M5	1	Total N Os 7 6 1	0	0
86	M6	1	Total N Os 7 6 1	0	0
86	M7	1	Total N Os 7 6 1	0	0
86	M7	1	Total N Os 7 6 1	0	0
86	M9	1	Total N Os 7 6 1	0	0
86	N9	1	Total N Os 7 6 1	0	0
86	O2	1	Total N Os 7 6 1	0	0
86	O3	1	Total N Os 7 6 1	0	0
86	O7	1	Total N Os 7 6 1	0	0
86	O7	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	O9	1	Total	N	Os	0	0
			7	6	1		
86	Q2	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	m6	1	Total N Os 7 6 1	0	0
86	m7	1	Total N Os 7 6 1	0	0
86	m8	1	Total N Os 7 6 1	0	0
86	n3	1	Total N Os 7 6 1	0	0
86	n9	1	Total N Os 7 6 1	0	0
86	o2	1	Total N Os 7 6 1	0	0
86	o3	1	Total N Os 7 6 1	0	0
86	o4	1	Total N Os 7 6 1	0	0
86	o7	1	Total N Os 7 6 1	0	0
86	q2	1	Total N Os 7 6 1	0	0

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

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

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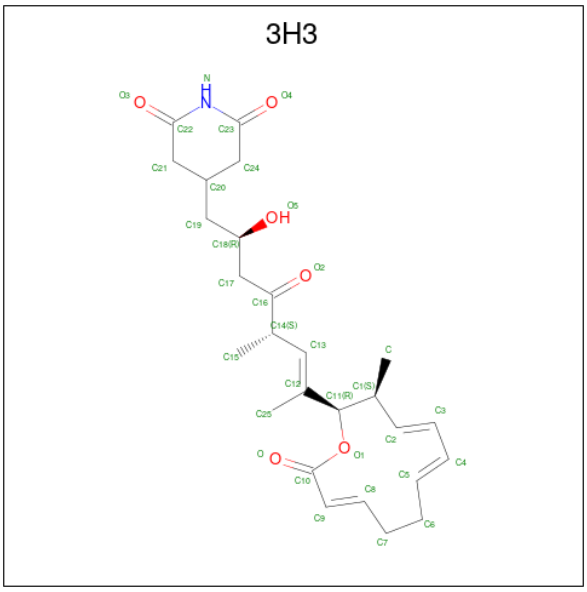
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	d7	1	Total Zn 1 1	0	0
87	d9	1	Total Zn 1 1	0	0
87	e1	1	Total Zn 1 1	0	0
87	o7	1	Total Zn 1 1	0	0
87	q0	1	Total Zn 1 1	0	0
87	q2	1	Total Zn 1 1	0	0
87	q3	1	Total Zn 1 1	0	0

- Molecule 88 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxo oxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (CCD ID: 3H3) (formula: $C_{26}H_{35}NO_6$).



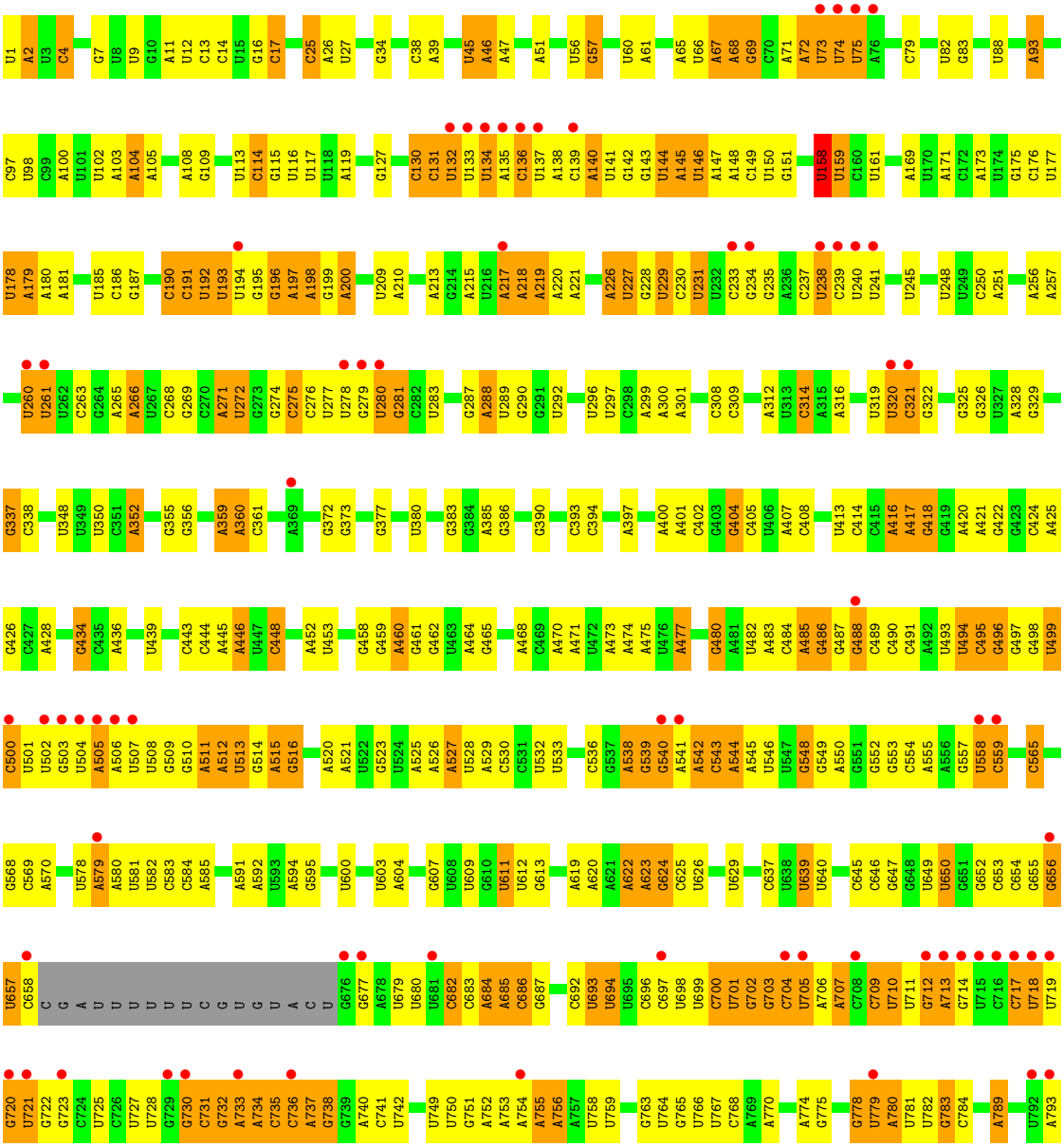
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	1	1	Total C N O 33 26 1 6	0	0
88	5	1	Total C N O 33 26 1 6	0	0

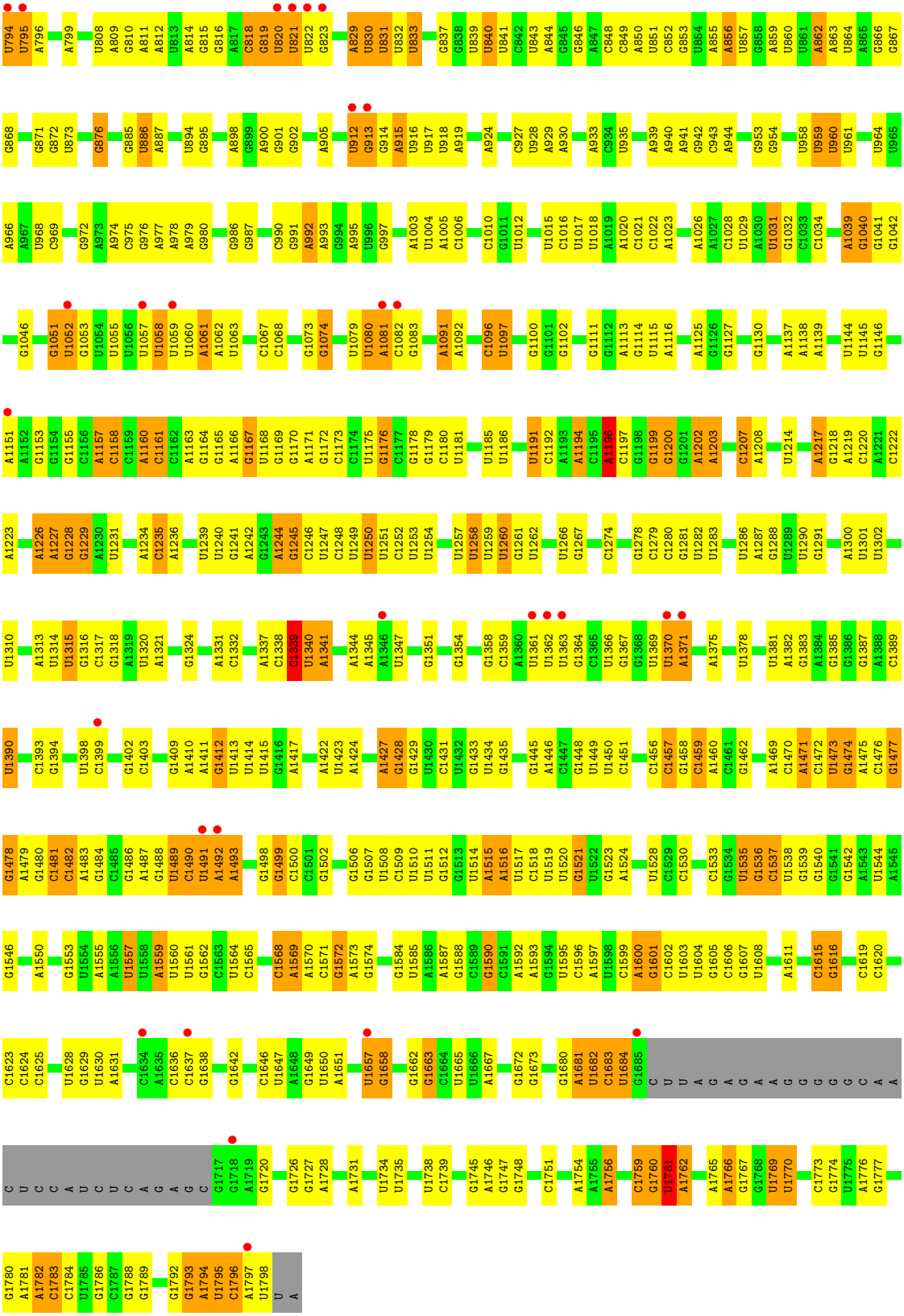
3 Residue-property plots (i)

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

- Molecule 1: 18S ribosomal RNA

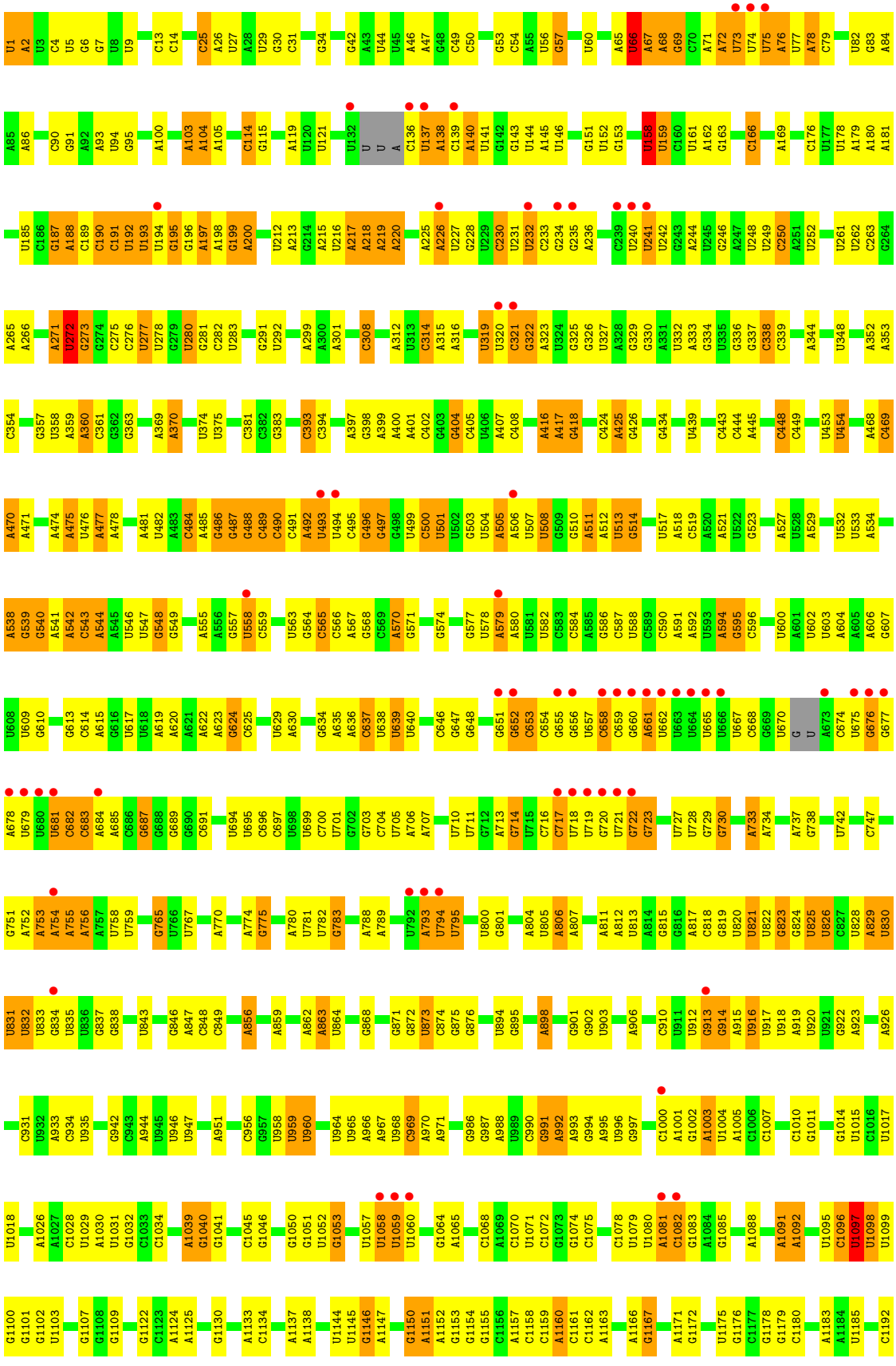
Chain 2:





• Molecule 1: 18S ribosomal RNA

Chain 6: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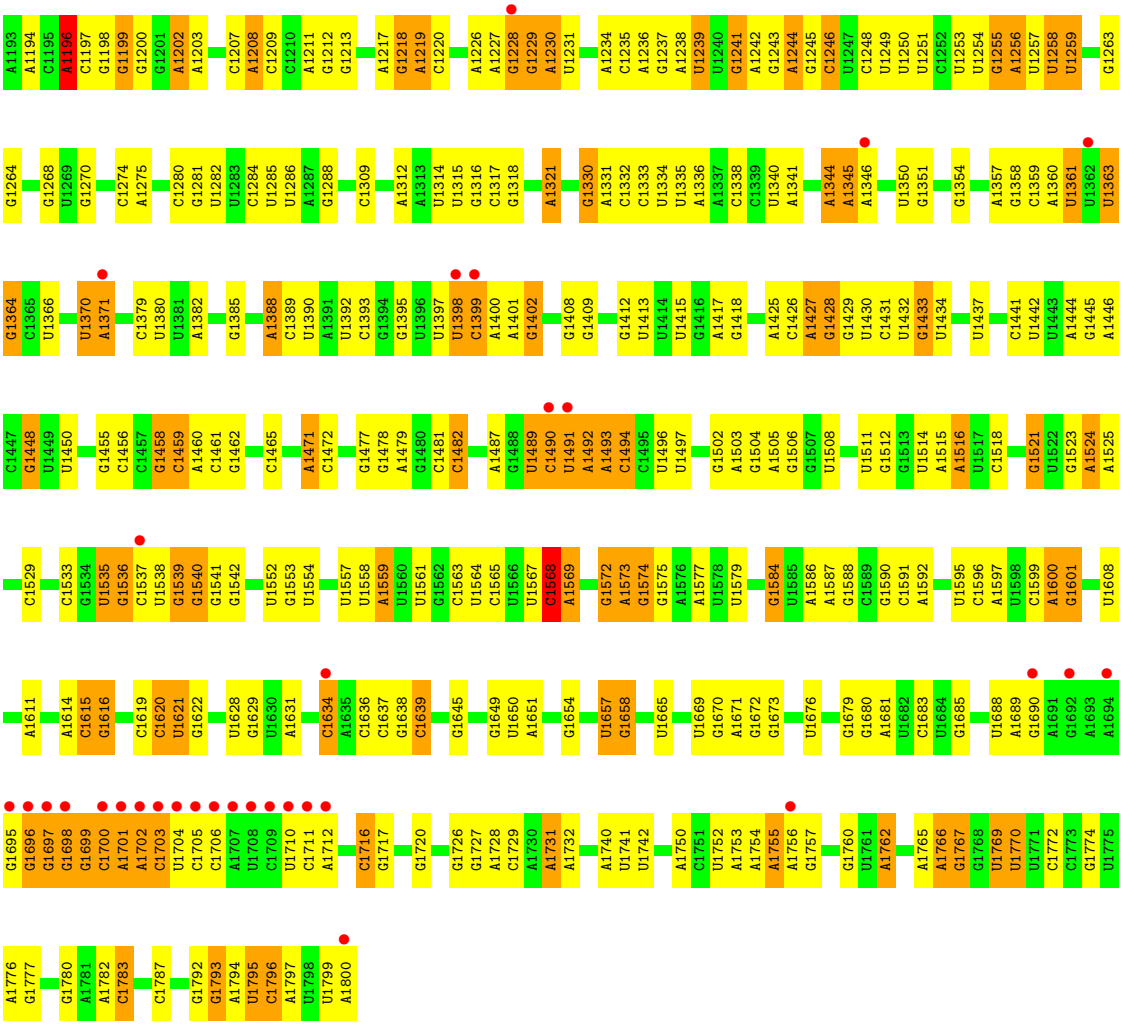
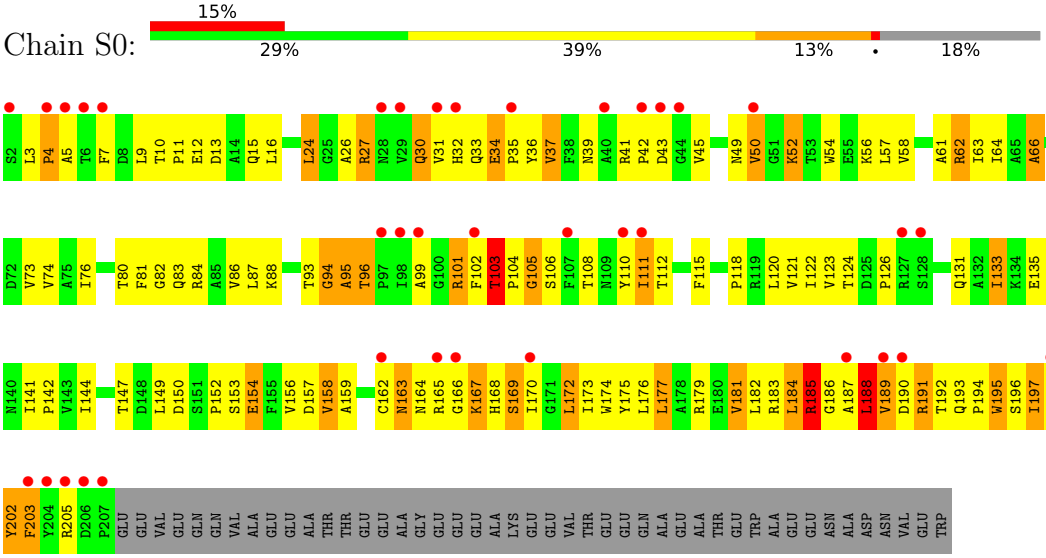
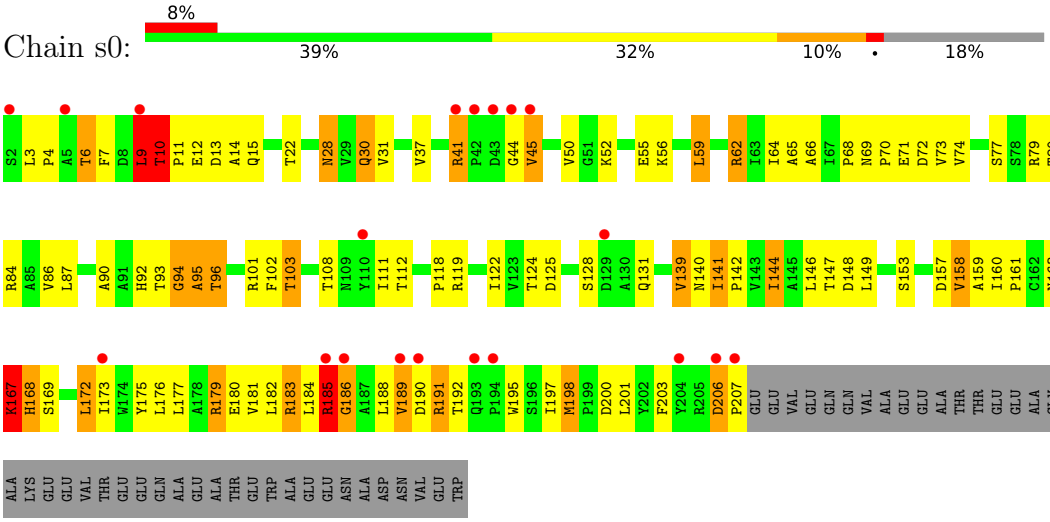


• Molecule 2: 40S ribosomal protein S0-A



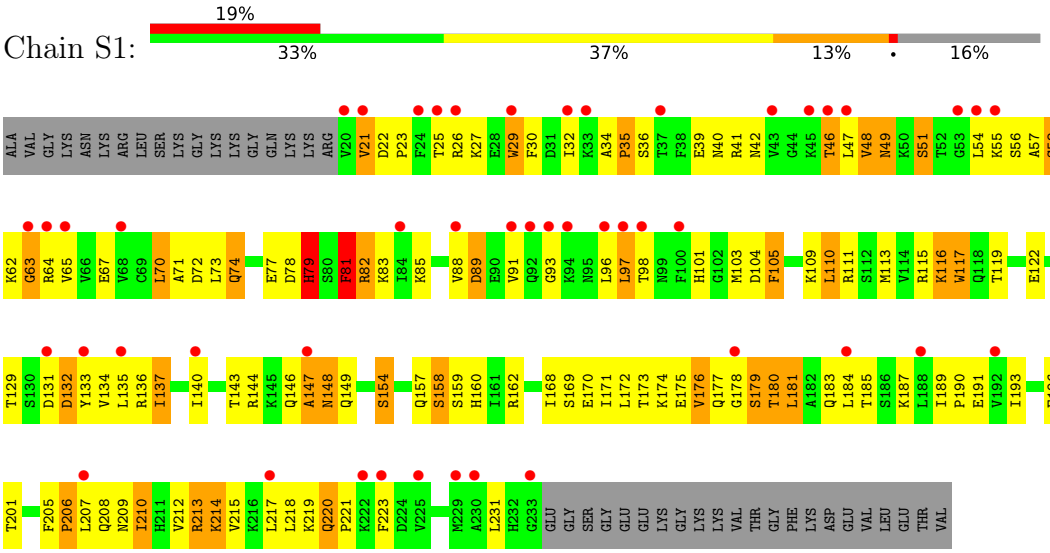
• Molecule 2: 40S ribosomal protein S0-A

Chain s0:



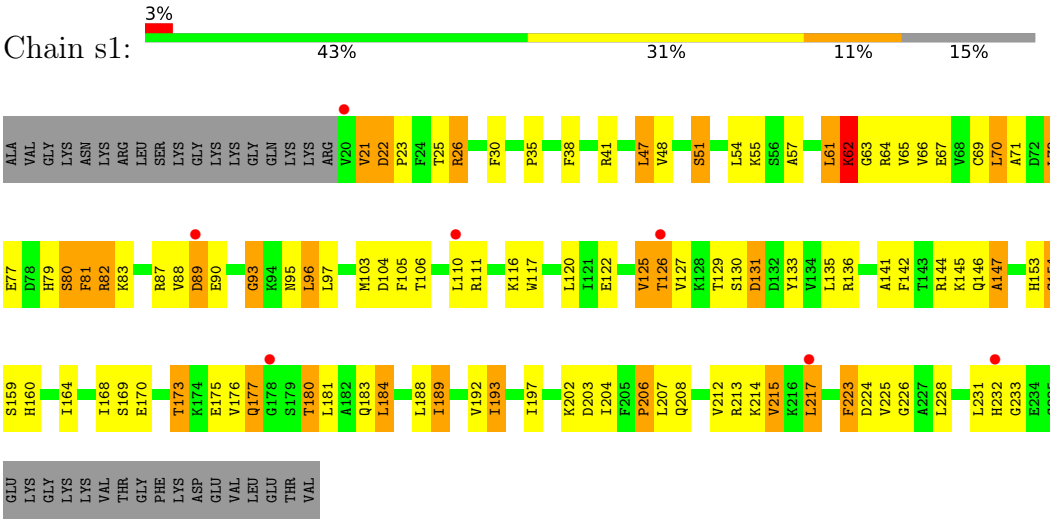
• Molecule 3: 40S ribosomal protein S1-A

Chain S1:



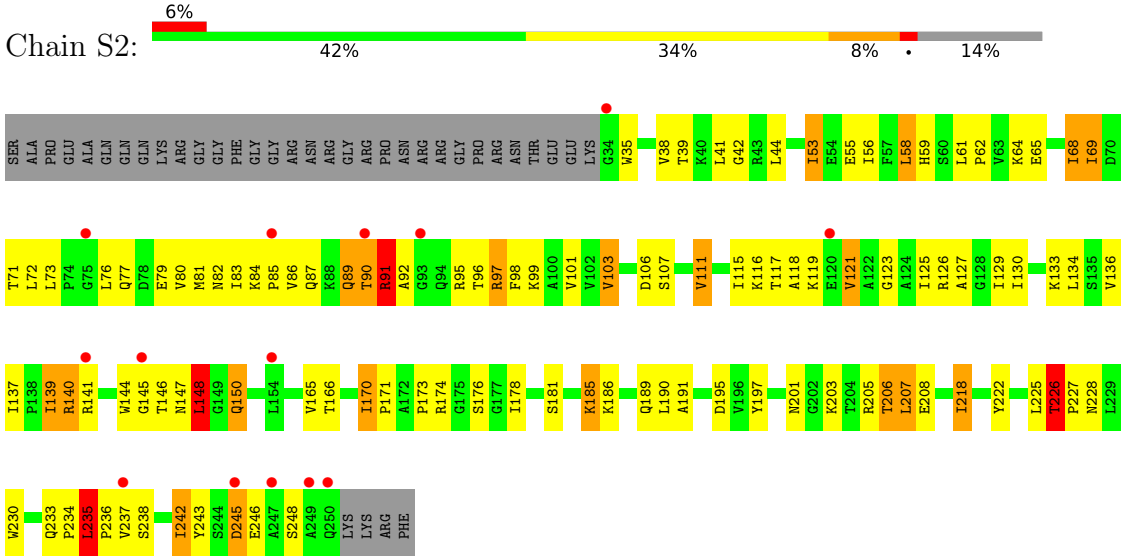
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



• Molecule 4: 40S ribosomal protein S2

Chain S2:



• Molecule 4: 40S ribosomal protein S2

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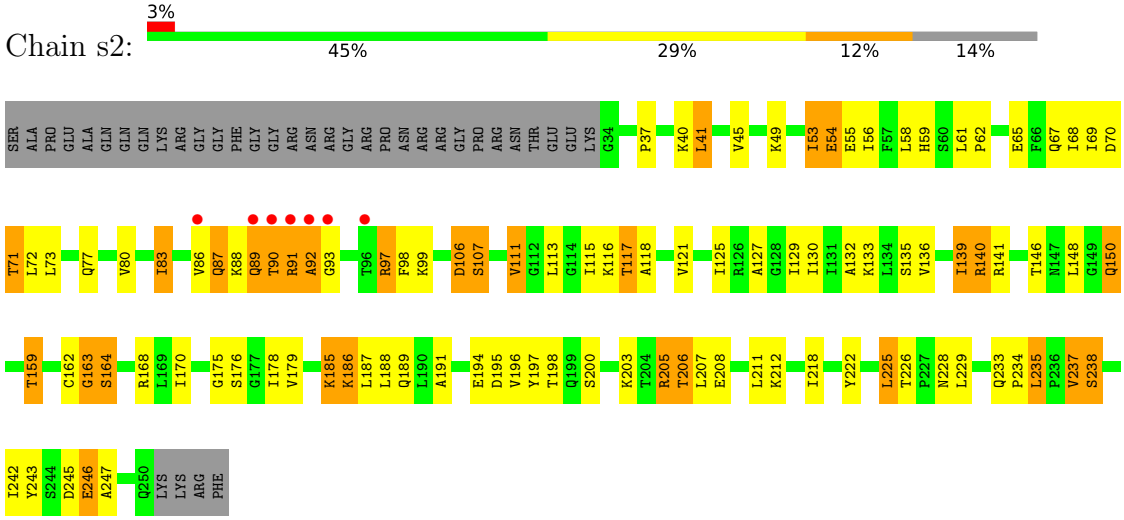
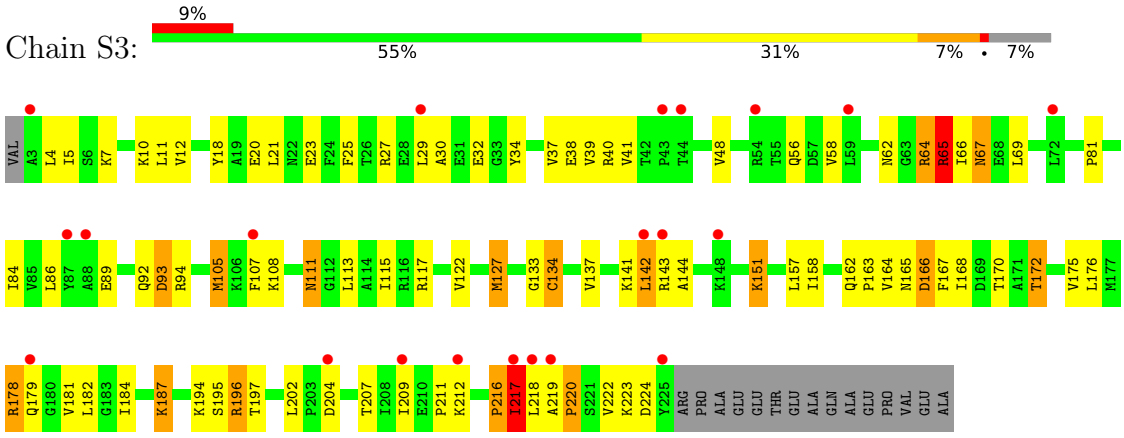


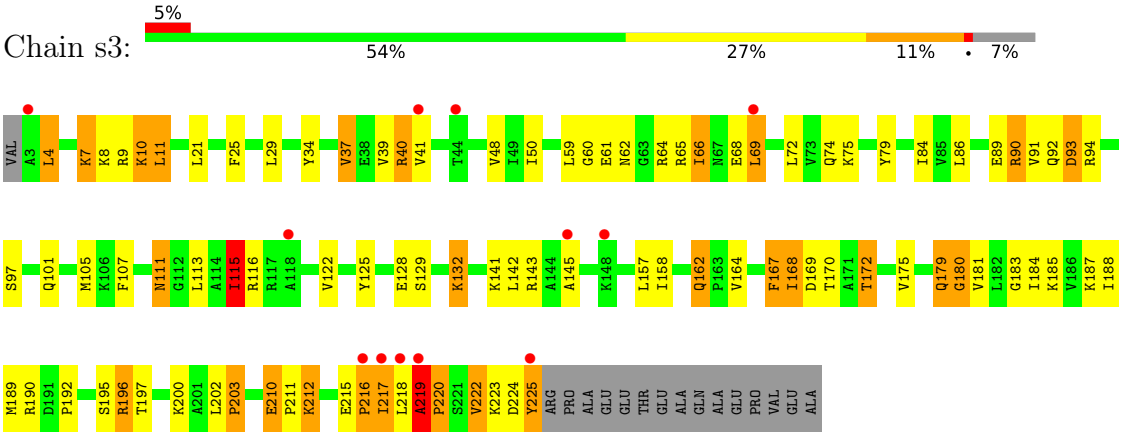
• Molecule 5: 40S ribosomal protein S3

Chain S3:



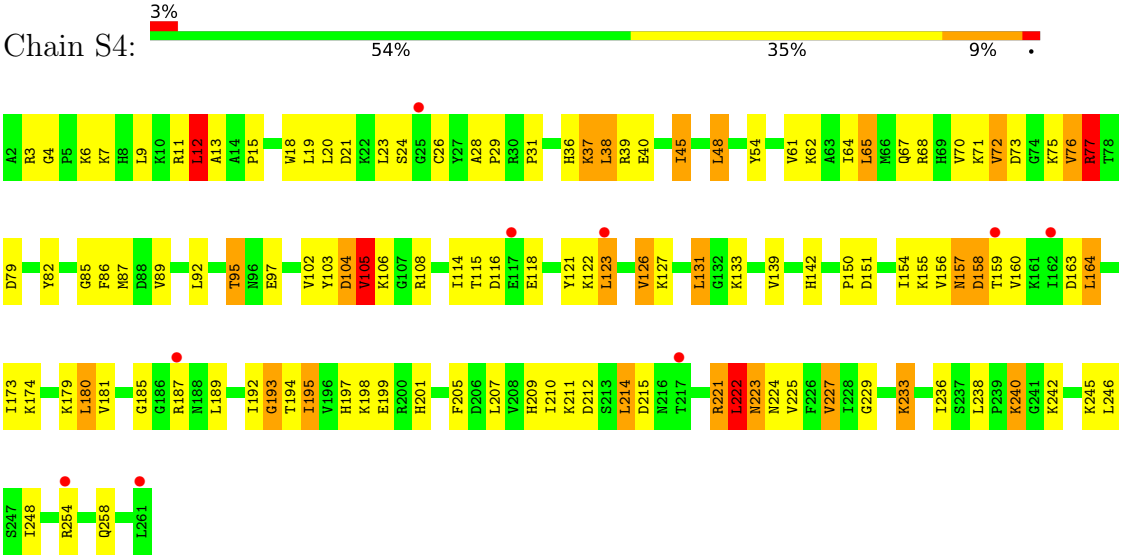
• Molecule 5: 40S ribosomal protein S3

Chain s3:



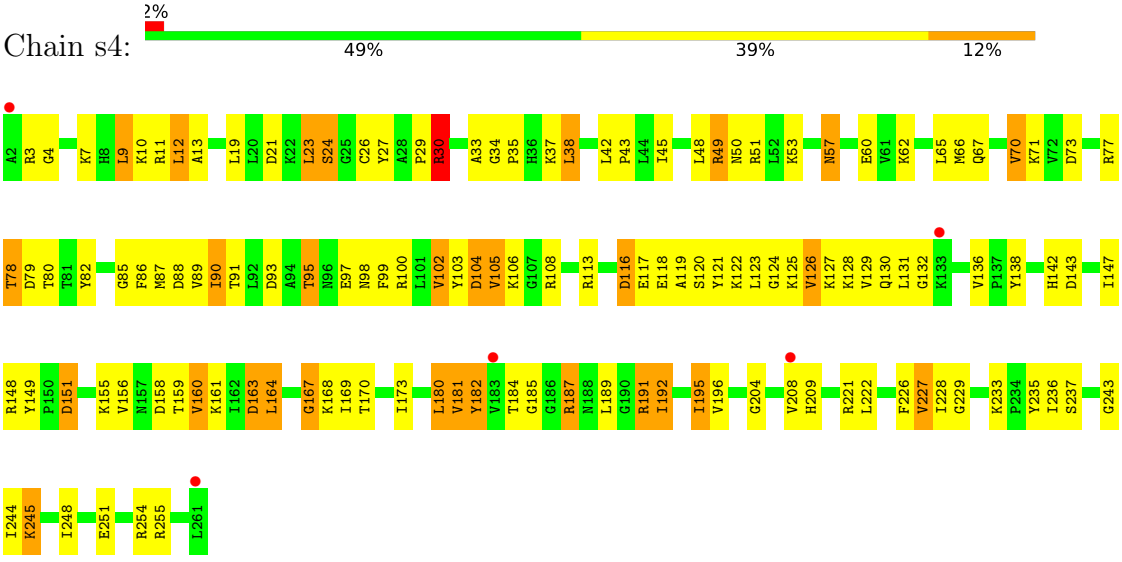
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



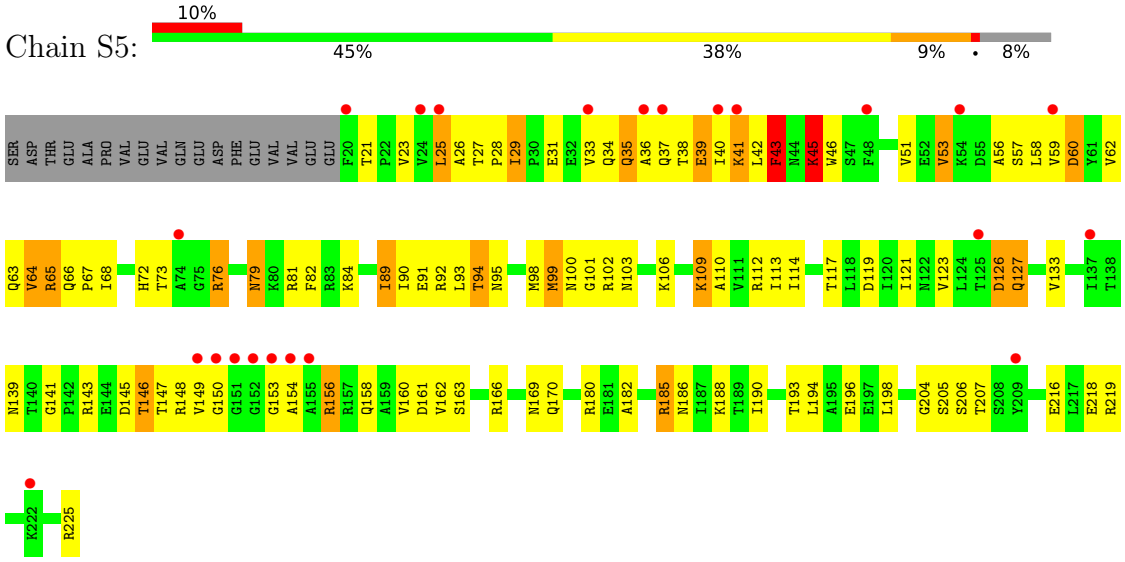
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



• Molecule 7: 40S ribosomal protein S5

Chain S5:



• Molecule 7: 40S ribosomal protein S5

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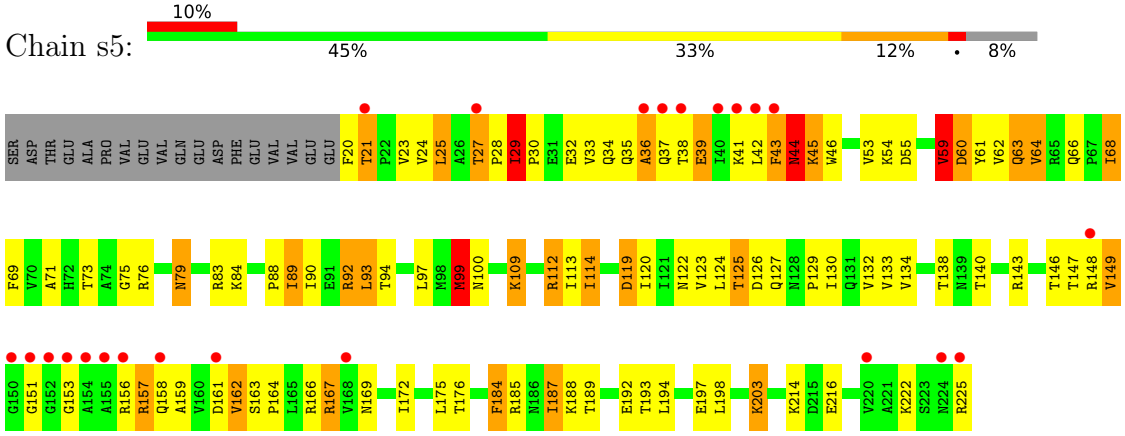
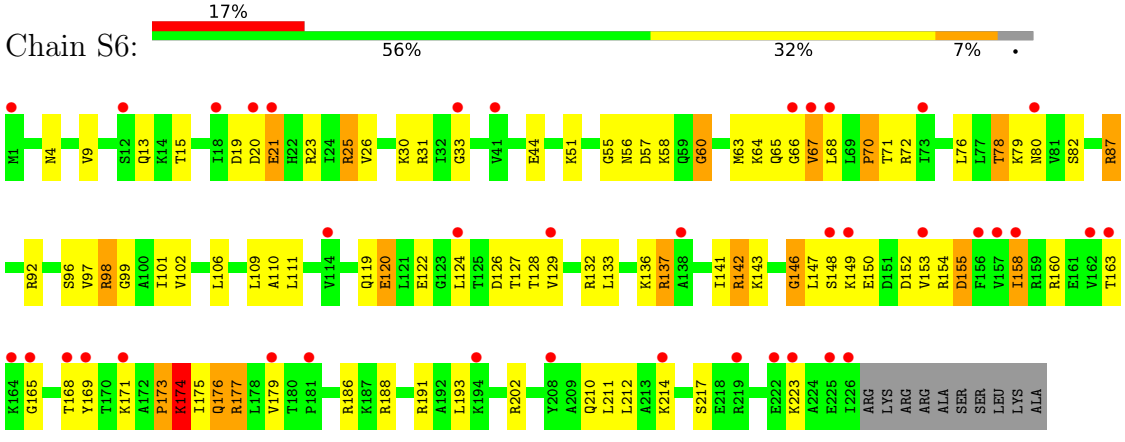


• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



• Molecule 8: 40S ribosomal protein S6-A

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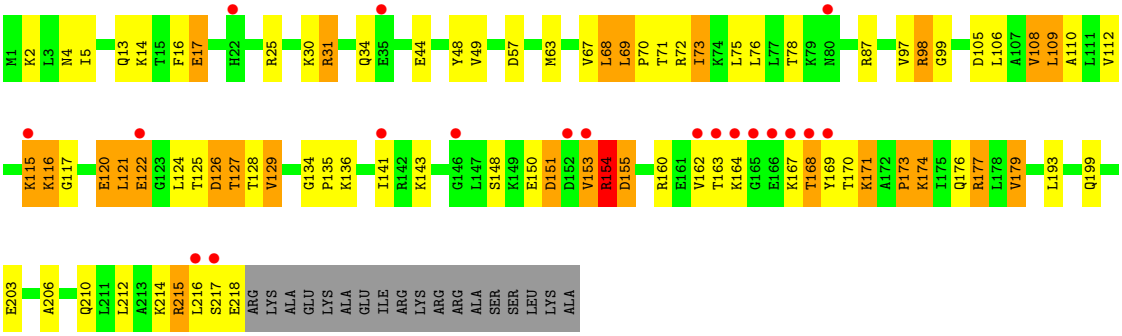
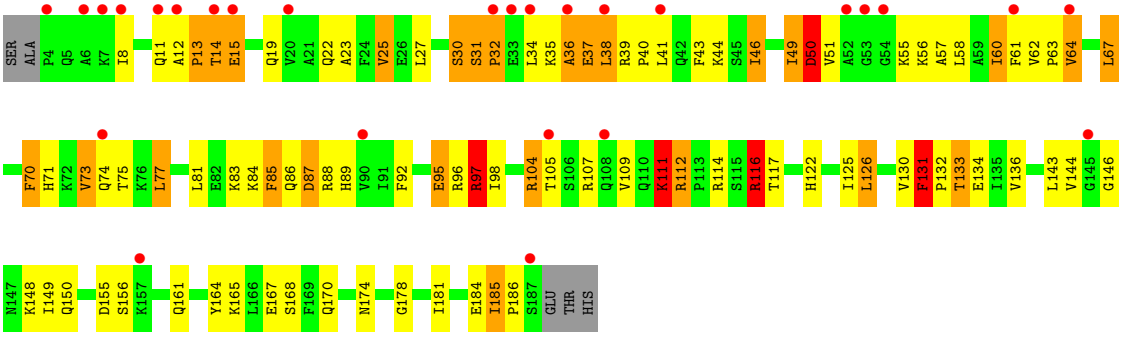


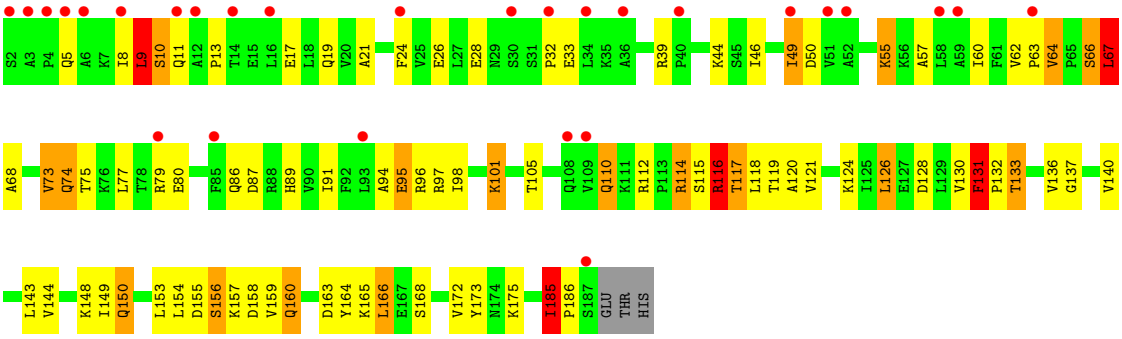
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



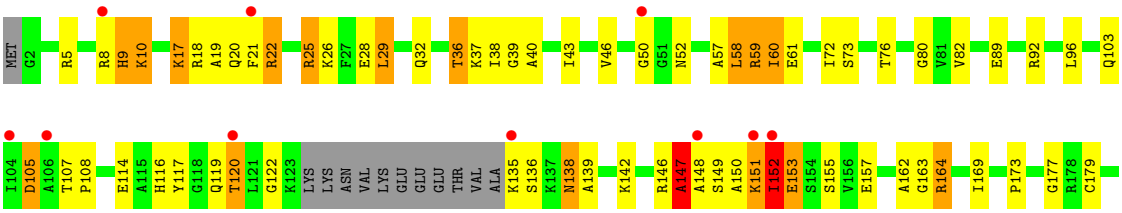
• Molecule 9: 40S ribosomal protein S7-A

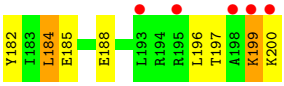
Chain s7:



• Molecule 10: 40S ribosomal protein S8-A

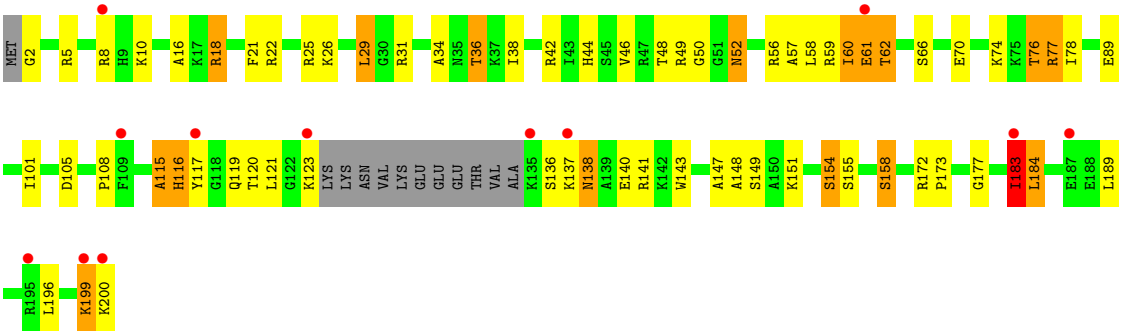
Chain S8:





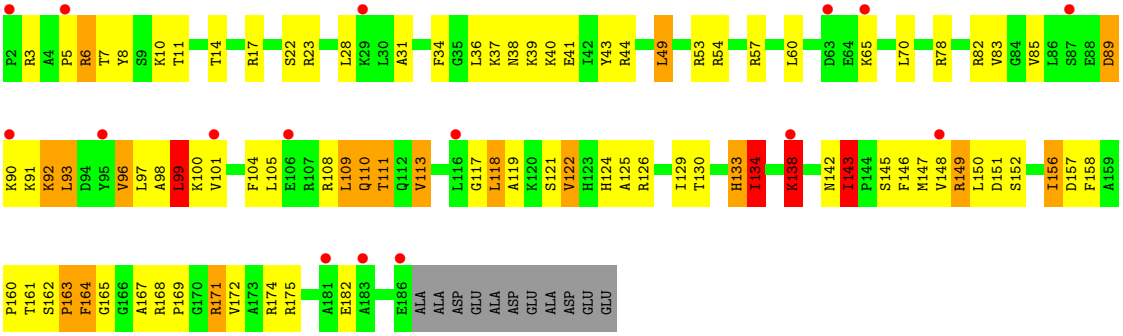
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



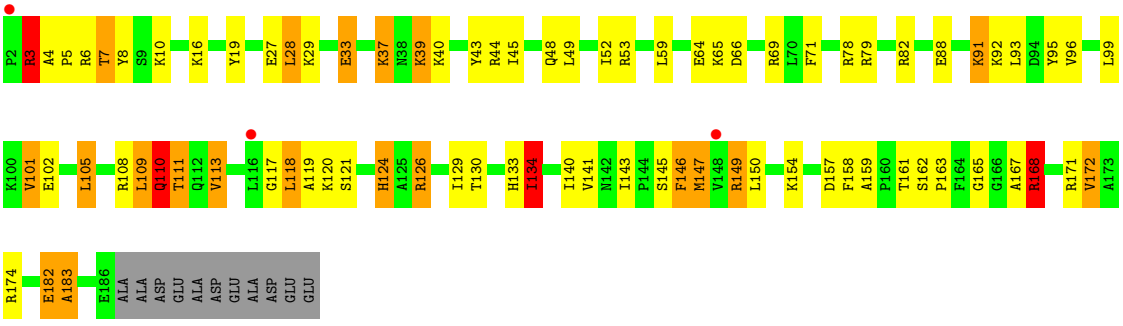
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



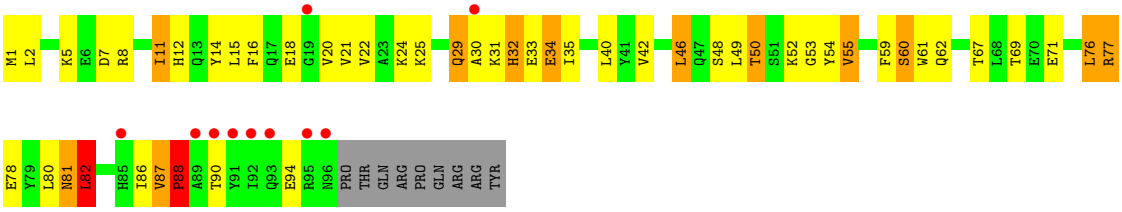
• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



• Molecule 12: 40S ribosomal protein S10-A

Chain C0:



• Molecule 12: 40S ribosomal protein S10-A

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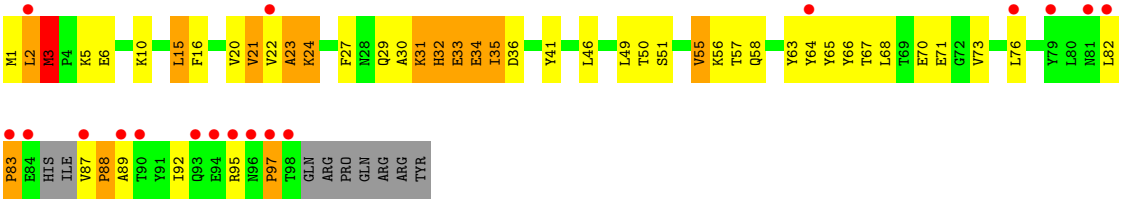
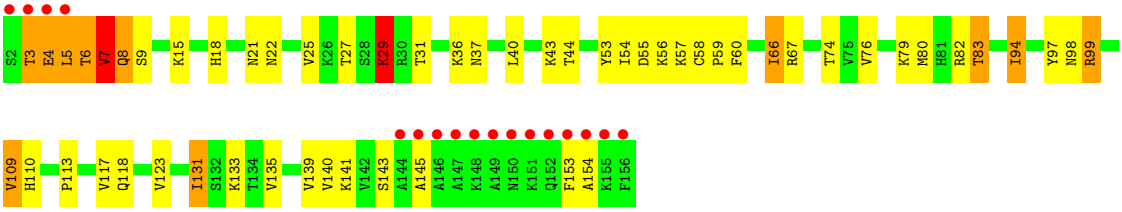


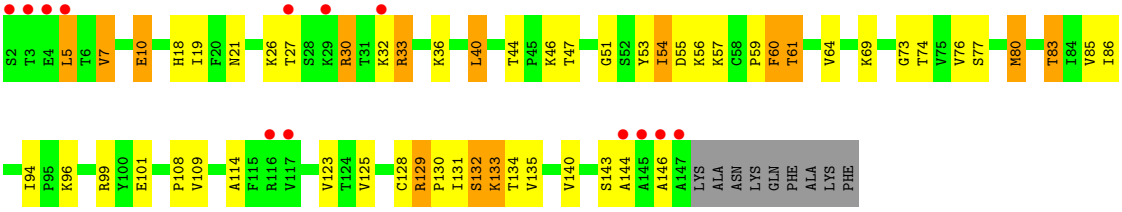
• Molecule 13: 40S ribosomal protein S11-A

Chain C1:



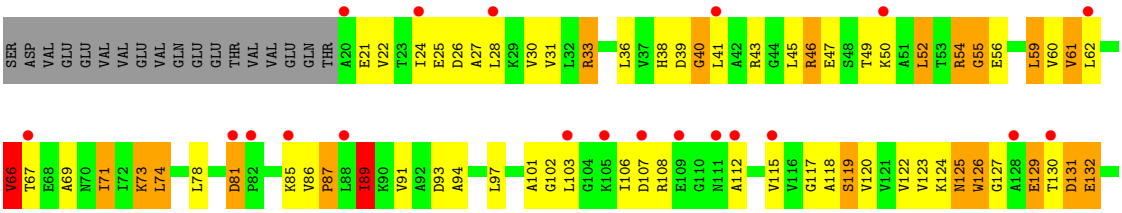
• Molecule 13: 40S ribosomal protein S11-A

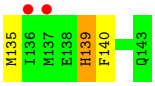
Chain c1:



• Molecule 14: 40S ribosomal protein S12

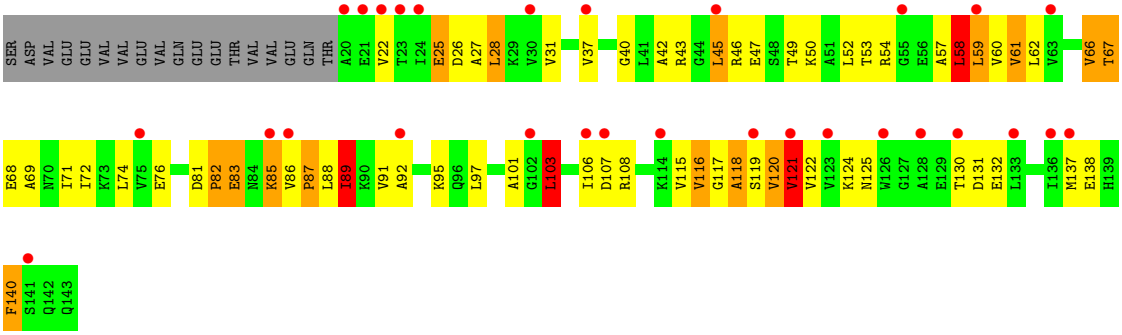
Chain C2:





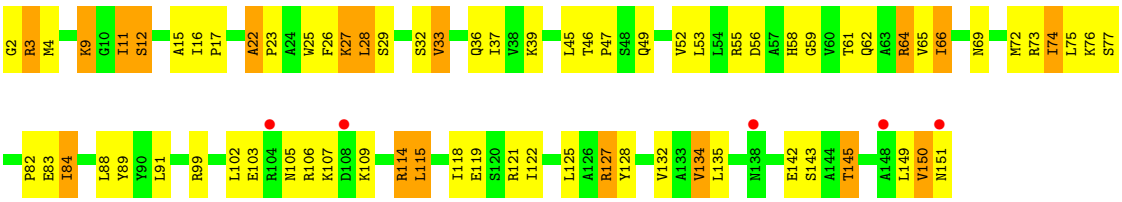
• Molecule 14: 40S ribosomal protein S12

Chain c2:



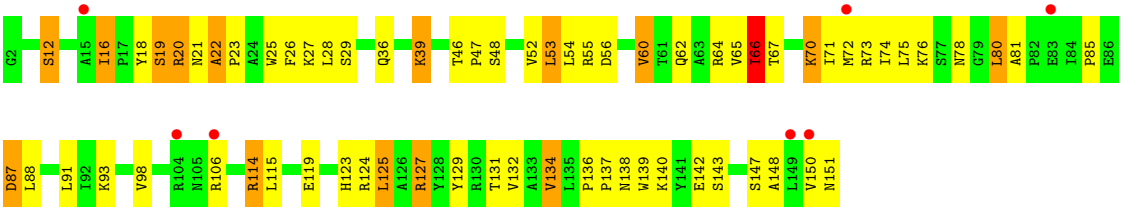
• Molecule 15: 40S ribosomal protein S13

Chain C3:



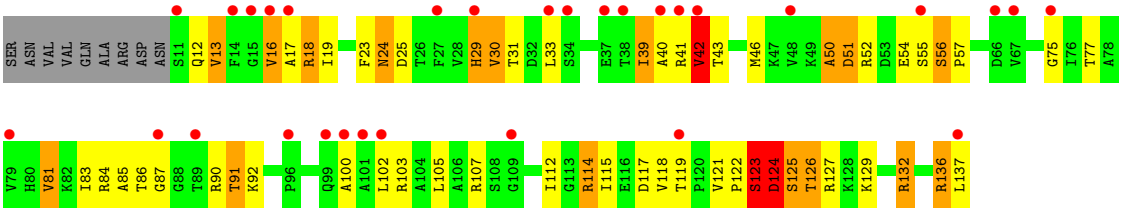
• Molecule 15: 40S ribosomal protein S13

Chain c3:



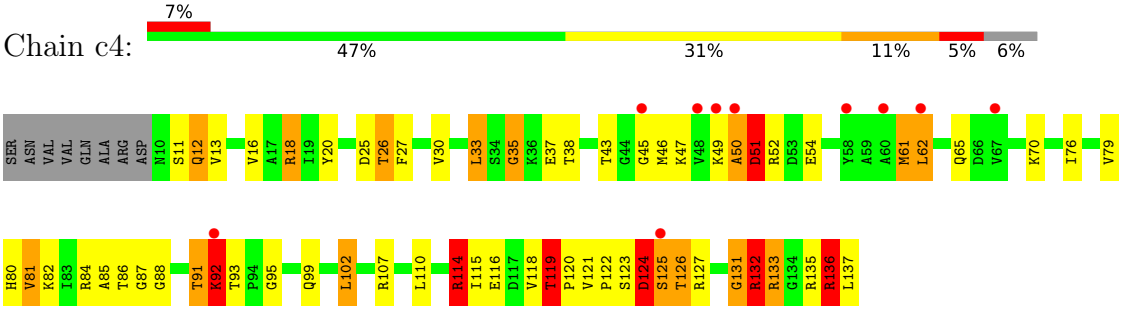
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



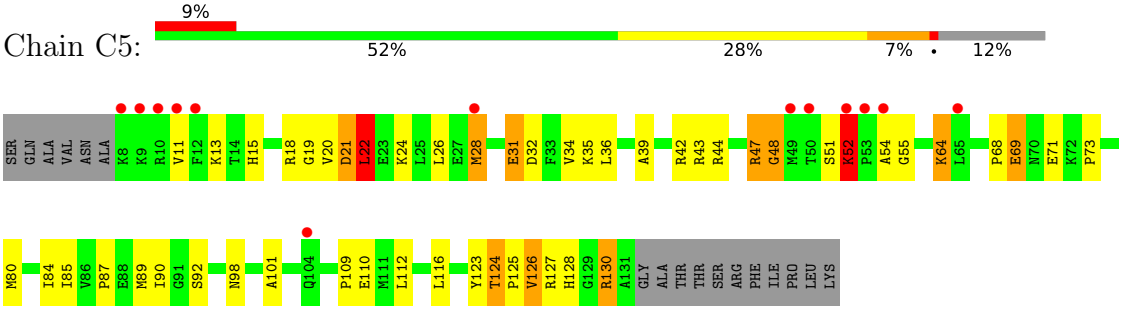
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



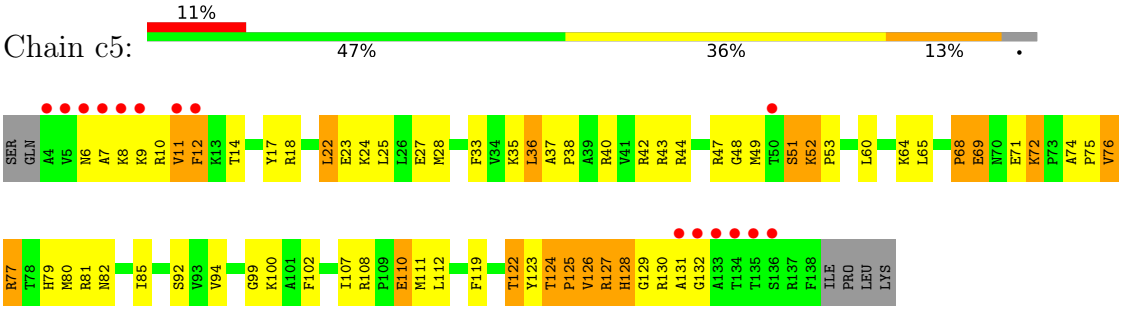
• Molecule 17: 40S ribosomal protein S15

Chain C5:



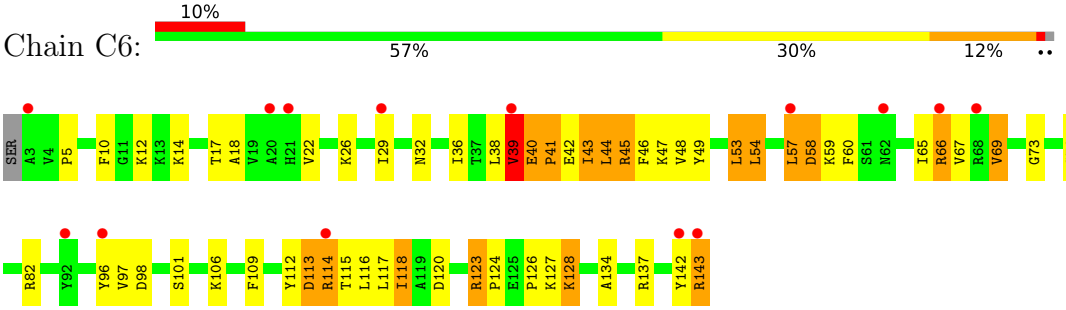
• Molecule 17: 40S ribosomal protein S15

Chain c5:



• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



• Molecule 18: 40S ribosomal protein S16-A

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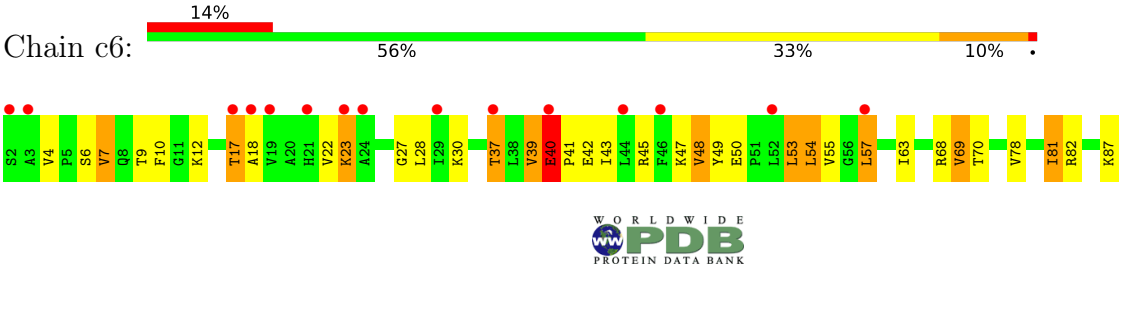
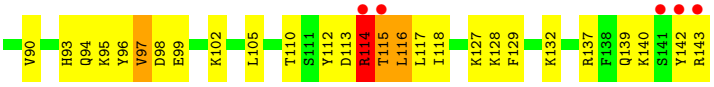
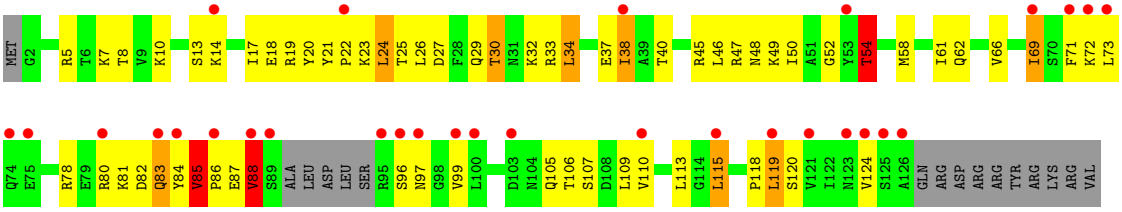




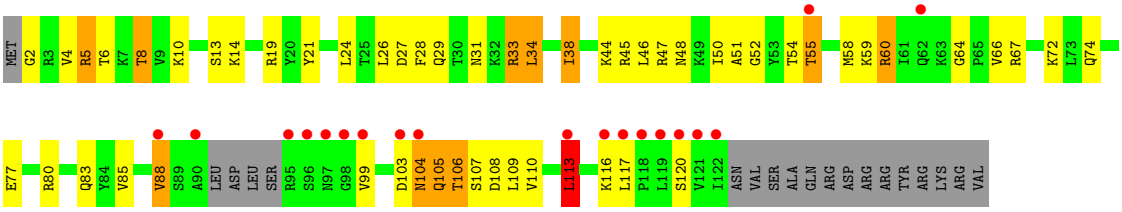
• Molecule 19: 40S ribosomal protein S17-A

Chain C7:



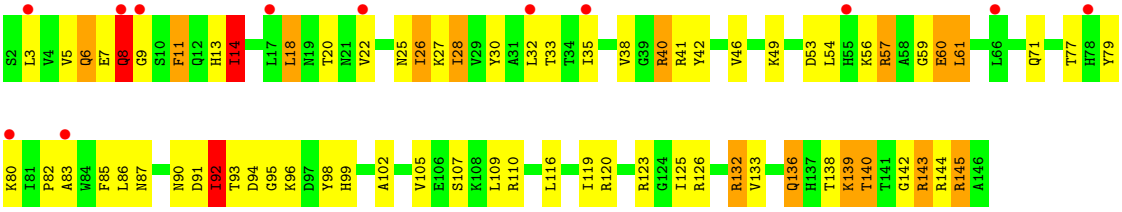
• Molecule 19: 40S ribosomal protein S17-A

Chain c7:



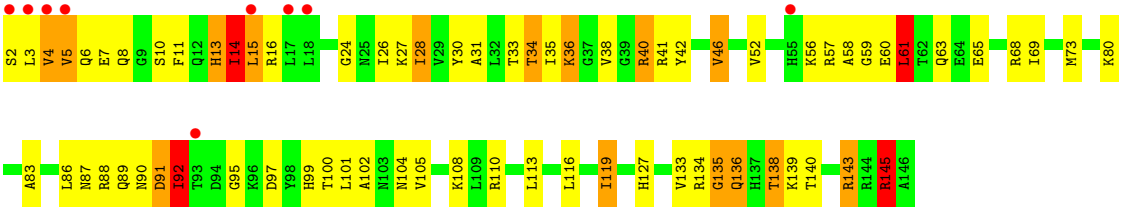
• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



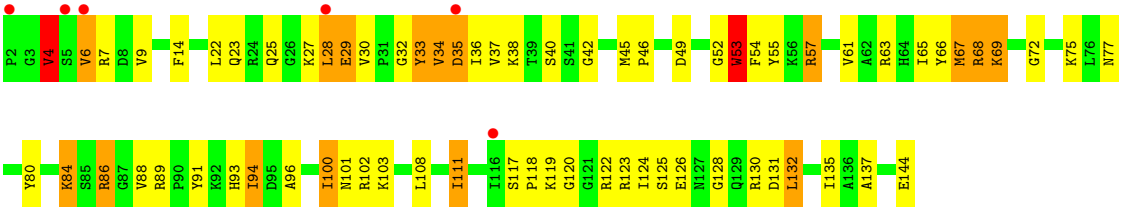
• Molecule 20: 40S ribosomal protein S18-A

Chain c8:

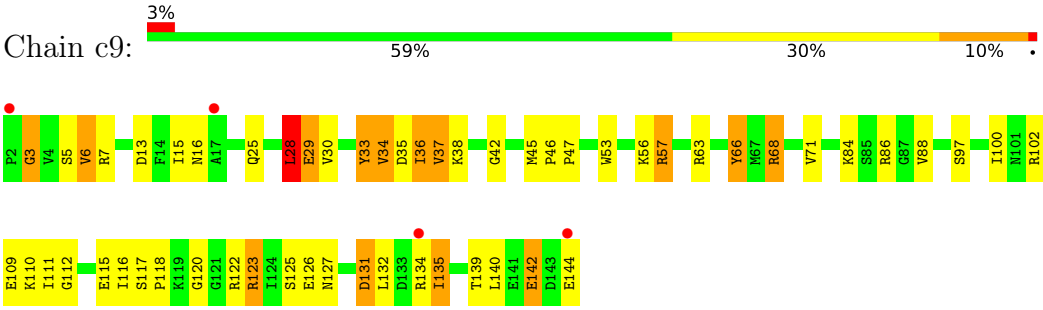


• Molecule 21: 40S ribosomal protein S19-A

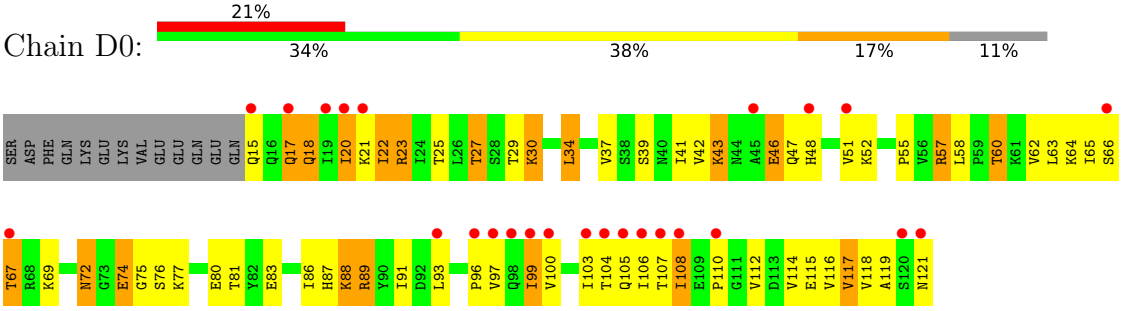
Chain C9:



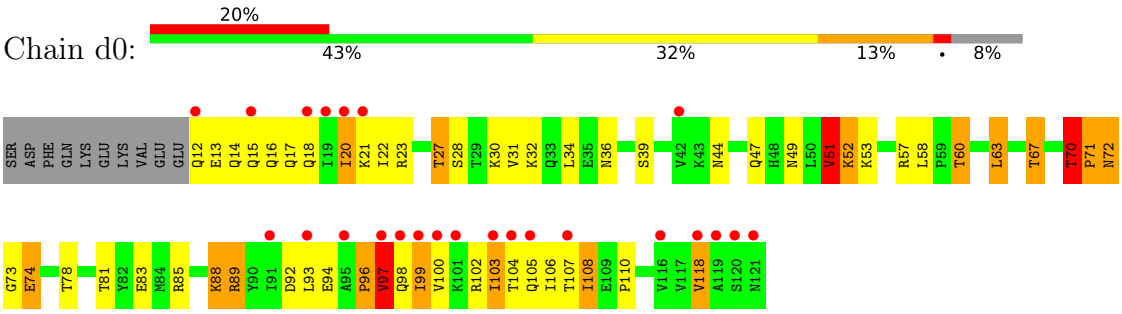
• Molecule 21: 40S ribosomal protein S19-A



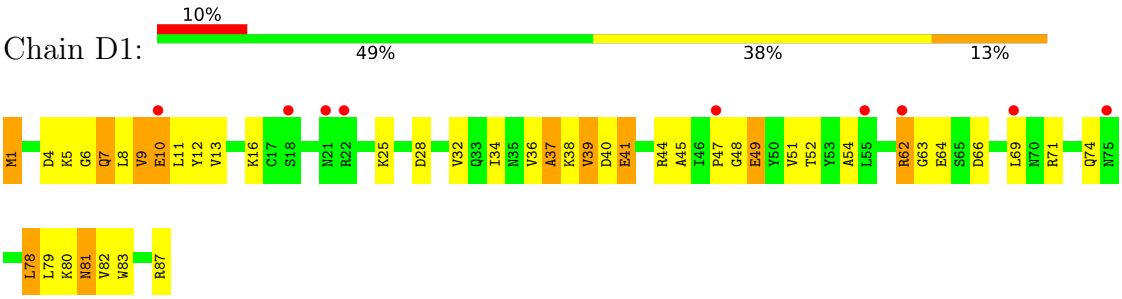
• Molecule 22: 40S ribosomal protein S20



• Molecule 22: 40S ribosomal protein S20

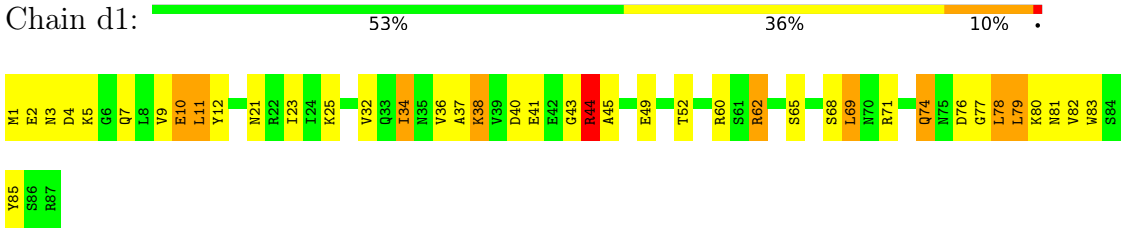


• Molecule 23: 40S ribosomal protein S21-A



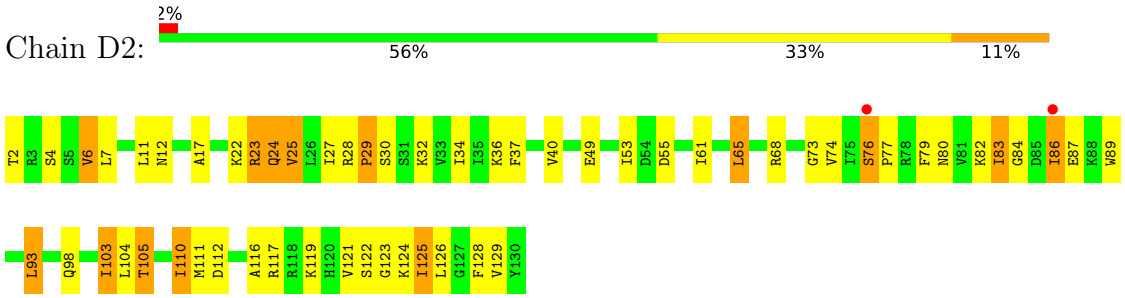
• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



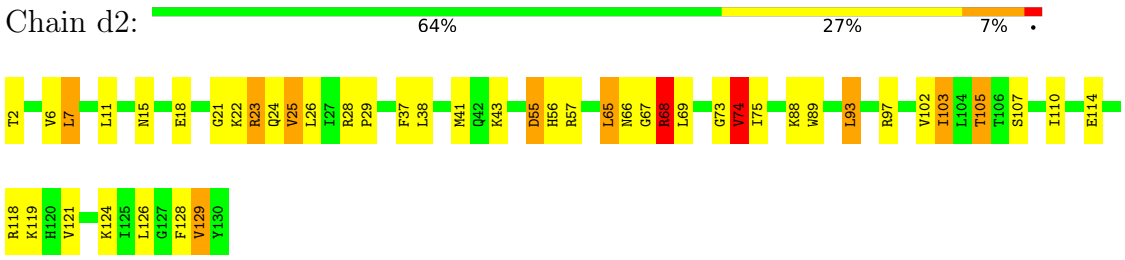
• Molecule 24: 40S ribosomal protein S22-A

Chain D2:



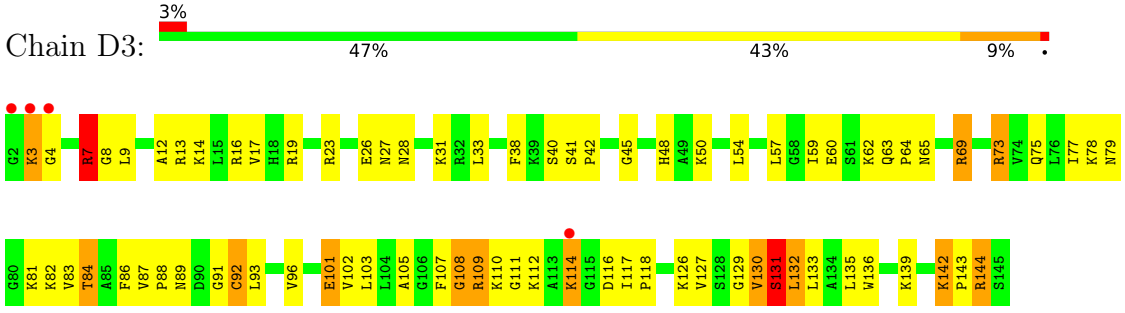
• Molecule 24: 40S ribosomal protein S22-A

Chain d2:



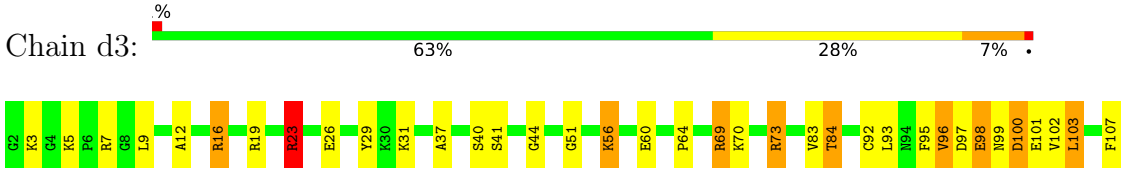
• Molecule 25: 40S ribosomal protein S23-A

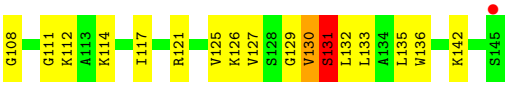
Chain D3:



• Molecule 25: 40S ribosomal protein S23-A

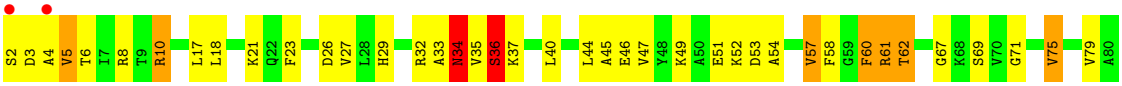
Chain d3:

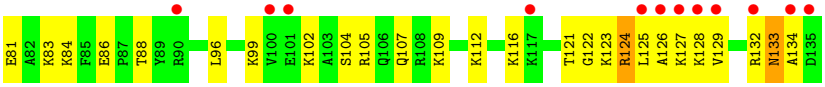




• Molecule 26: 40S ribosomal protein S24-A

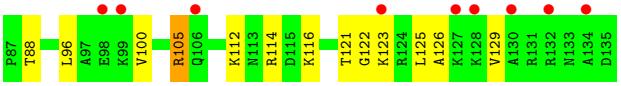
Chain D4:





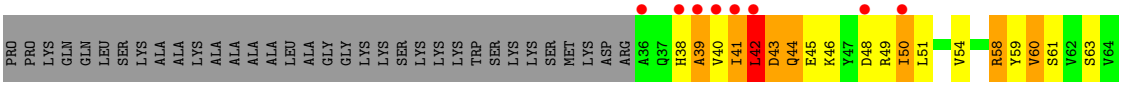
• Molecule 26: 40S ribosomal protein S24-A

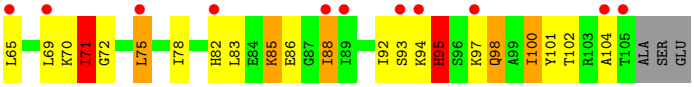
Chain d4:



• Molecule 27: 40S ribosomal protein S25-A

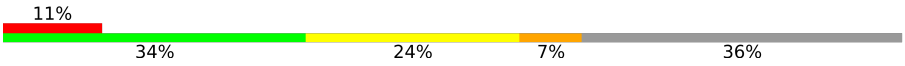
Chain D5:

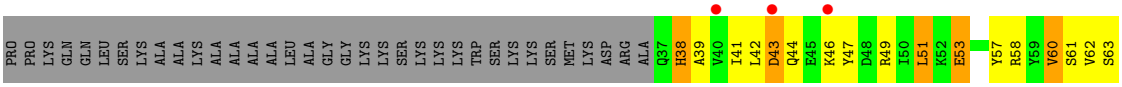


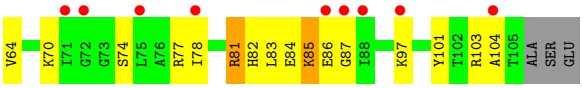


• Molecule 27: 40S ribosomal protein S25-A

Chain d5:

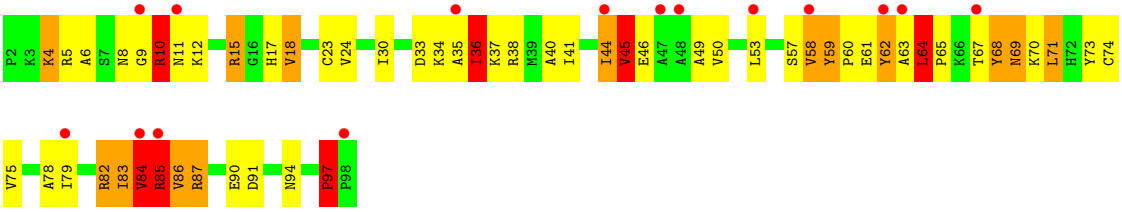




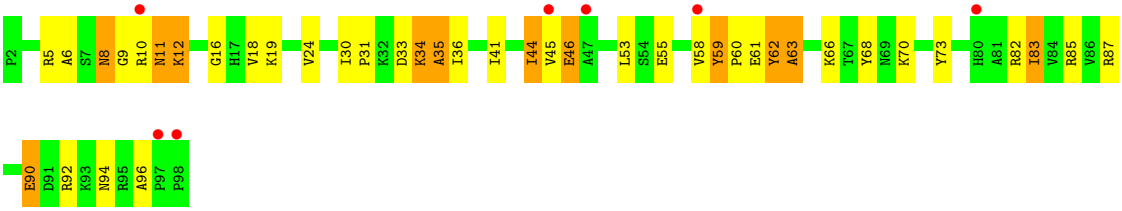


• Molecule 28: 40S ribosomal protein S26-B

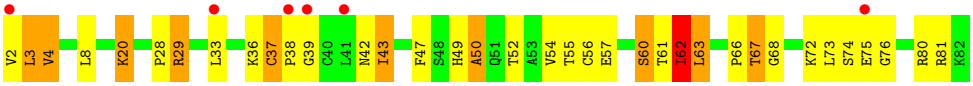
Chain D6:



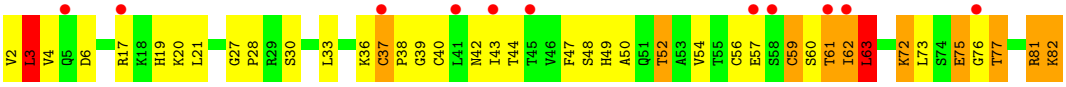
• Molecule 28: 40S ribosomal protein S26-B



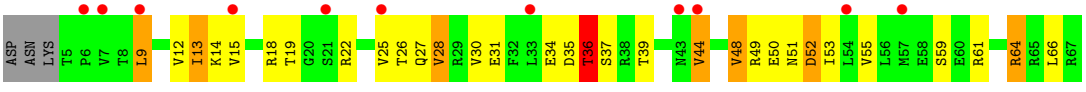
• Molecule 29: 40S ribosomal protein S27-A



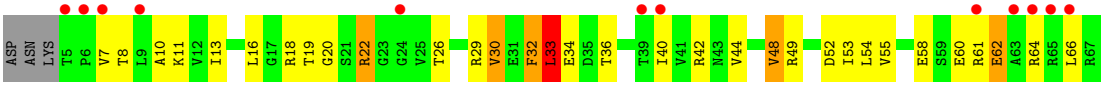
• Molecule 29: 40S ribosomal protein S27-A



• Molecule 30: 40S ribosomal protein S28-A

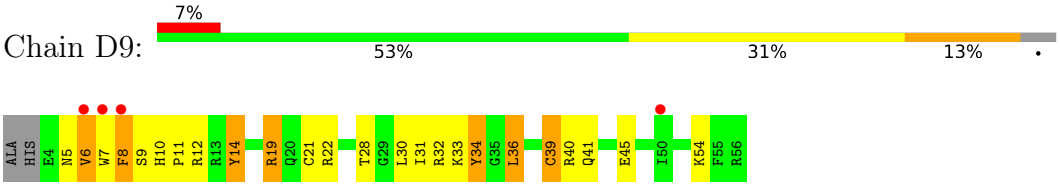


• Molecule 30: 40S ribosomal protein S28-A



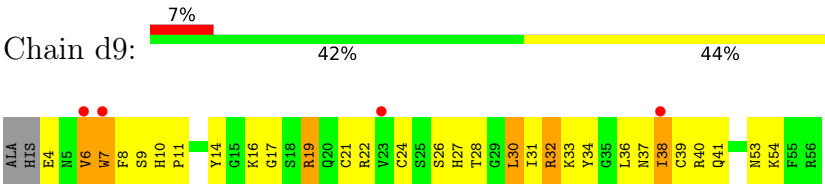
• Molecule 31: 40S ribosomal protein S29-A

Chain D9:



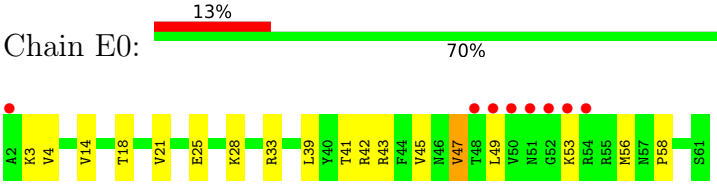
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



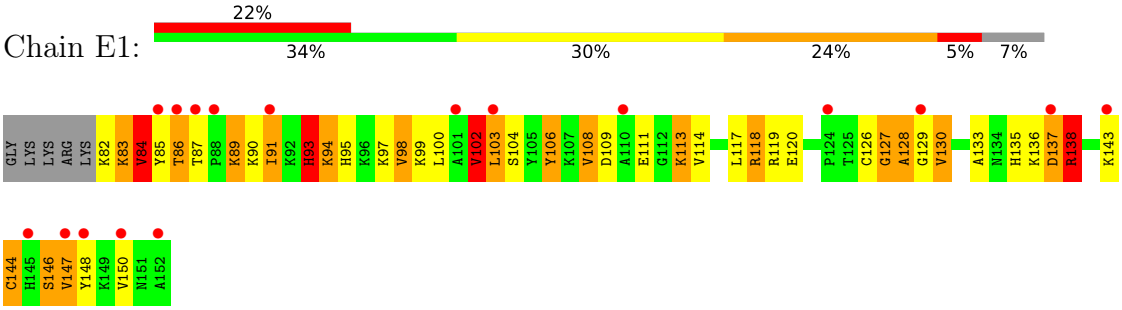
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



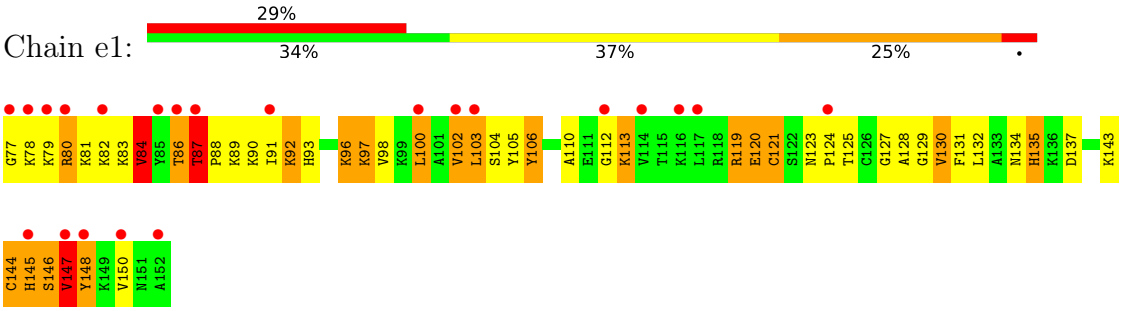
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



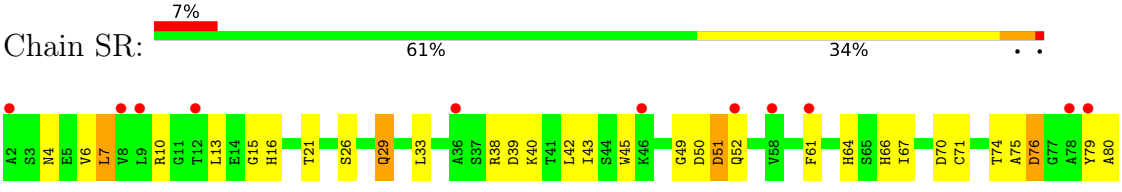
• Molecule 33: Ubiquitin-40S ribosomal protein S31

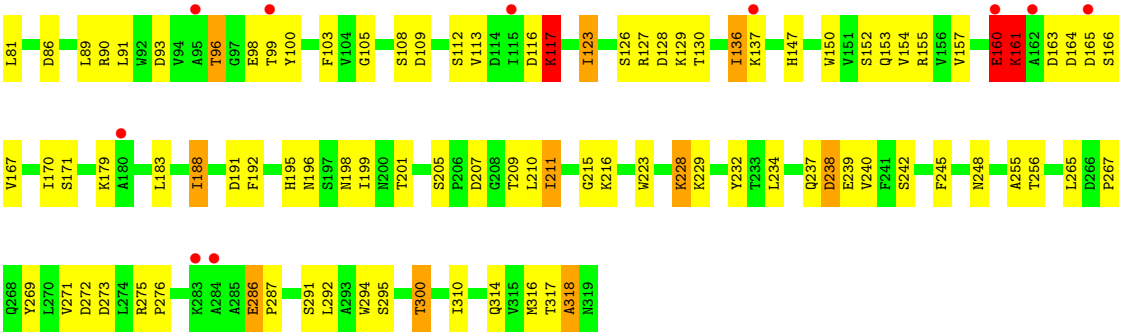
Chain e1:



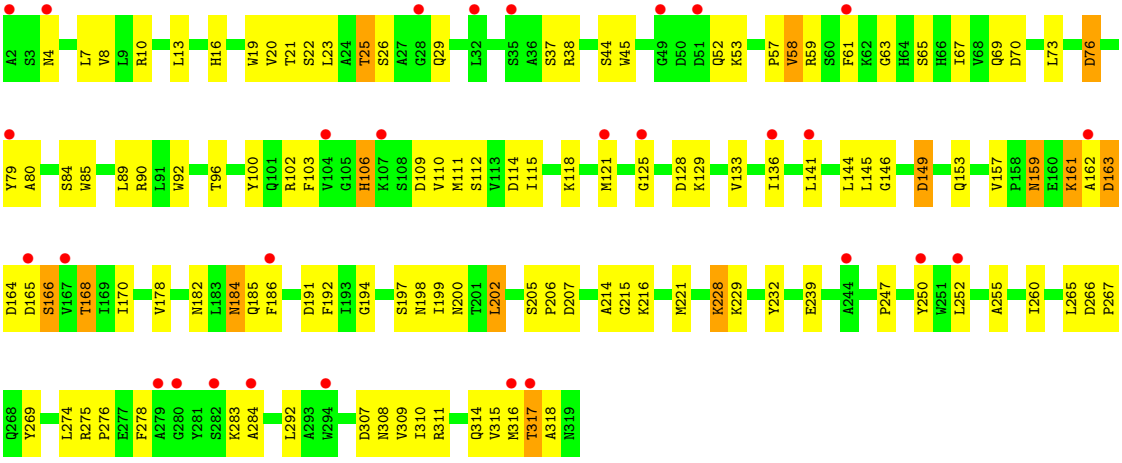
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:

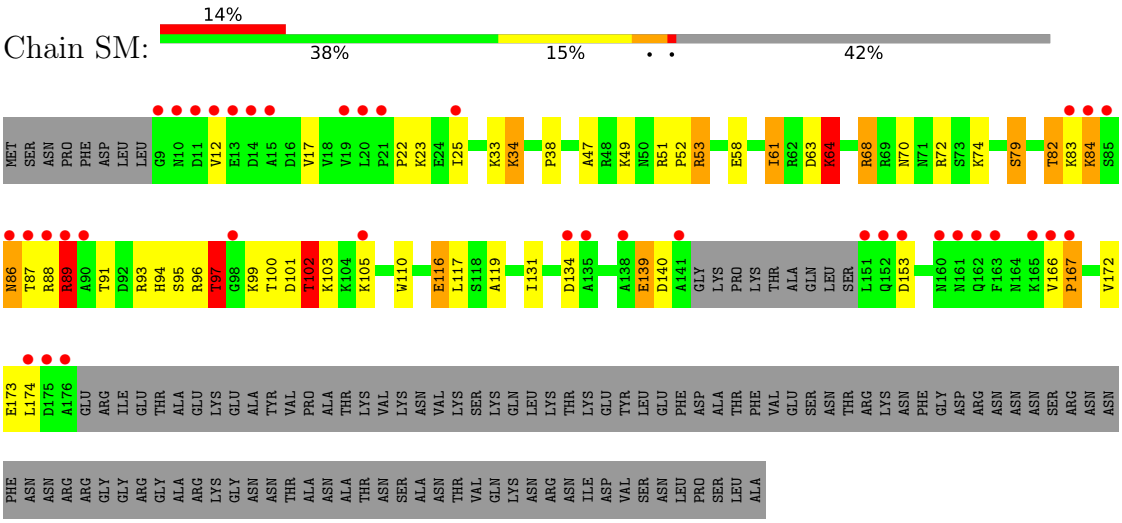




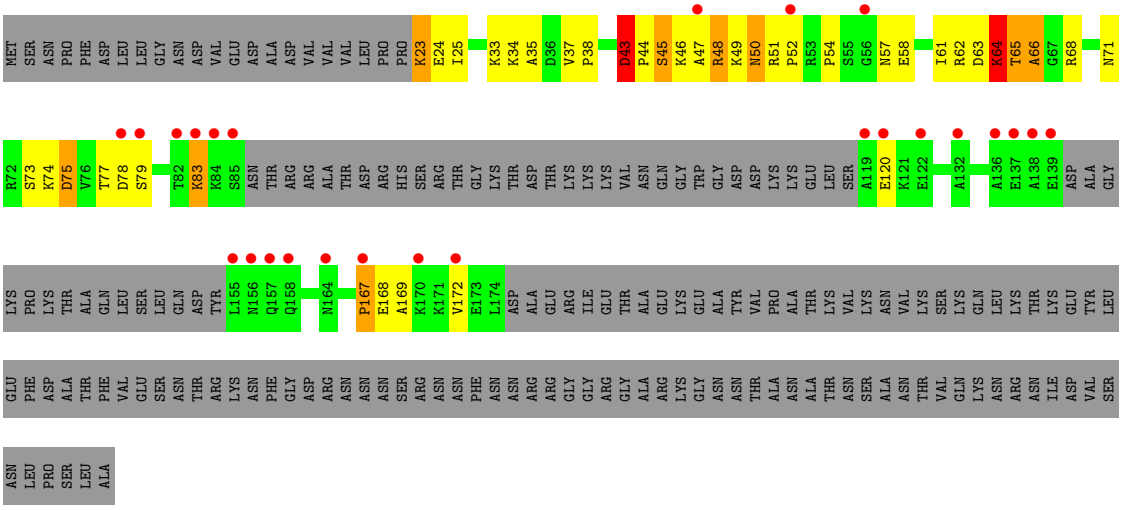
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 35: Suppressor protein STM1

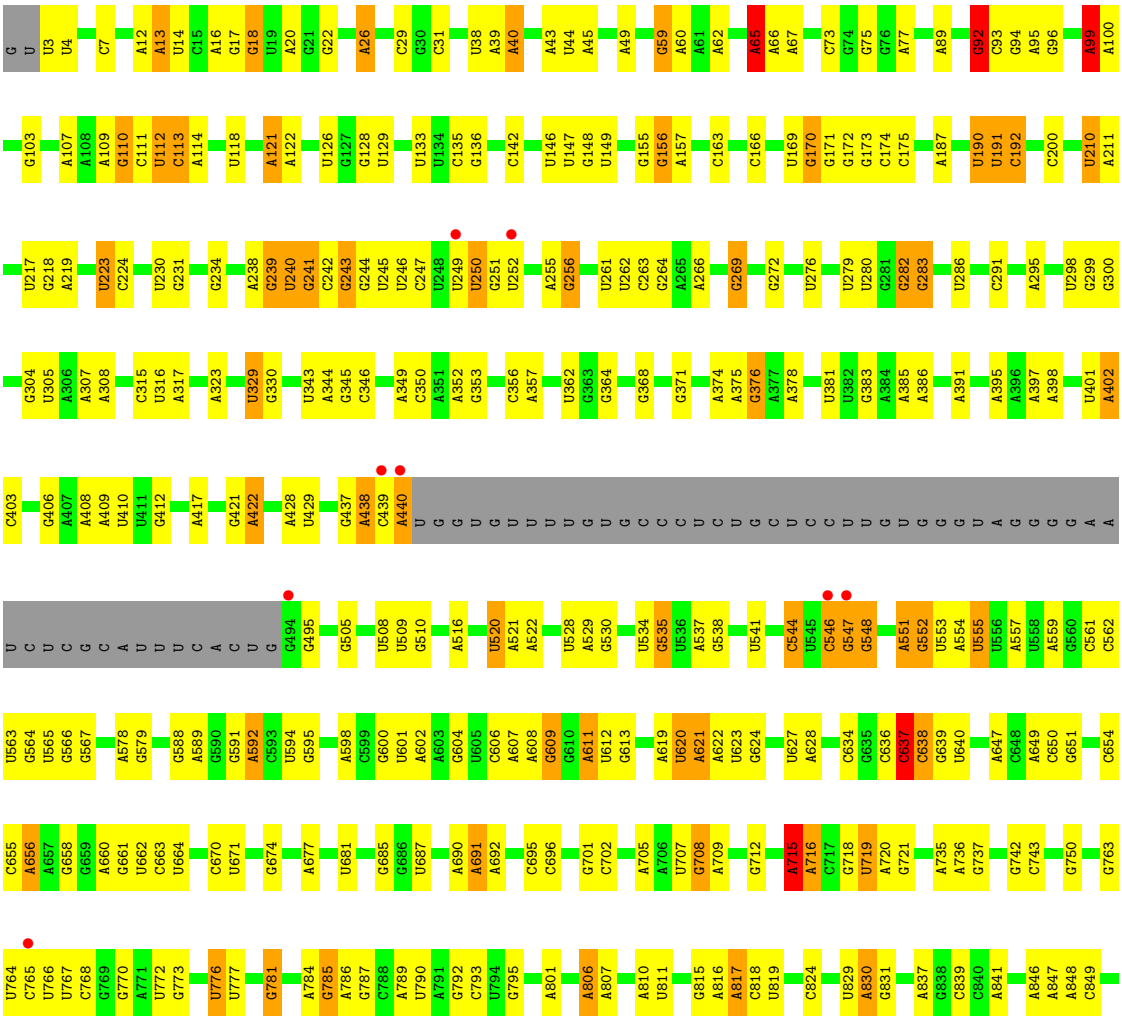


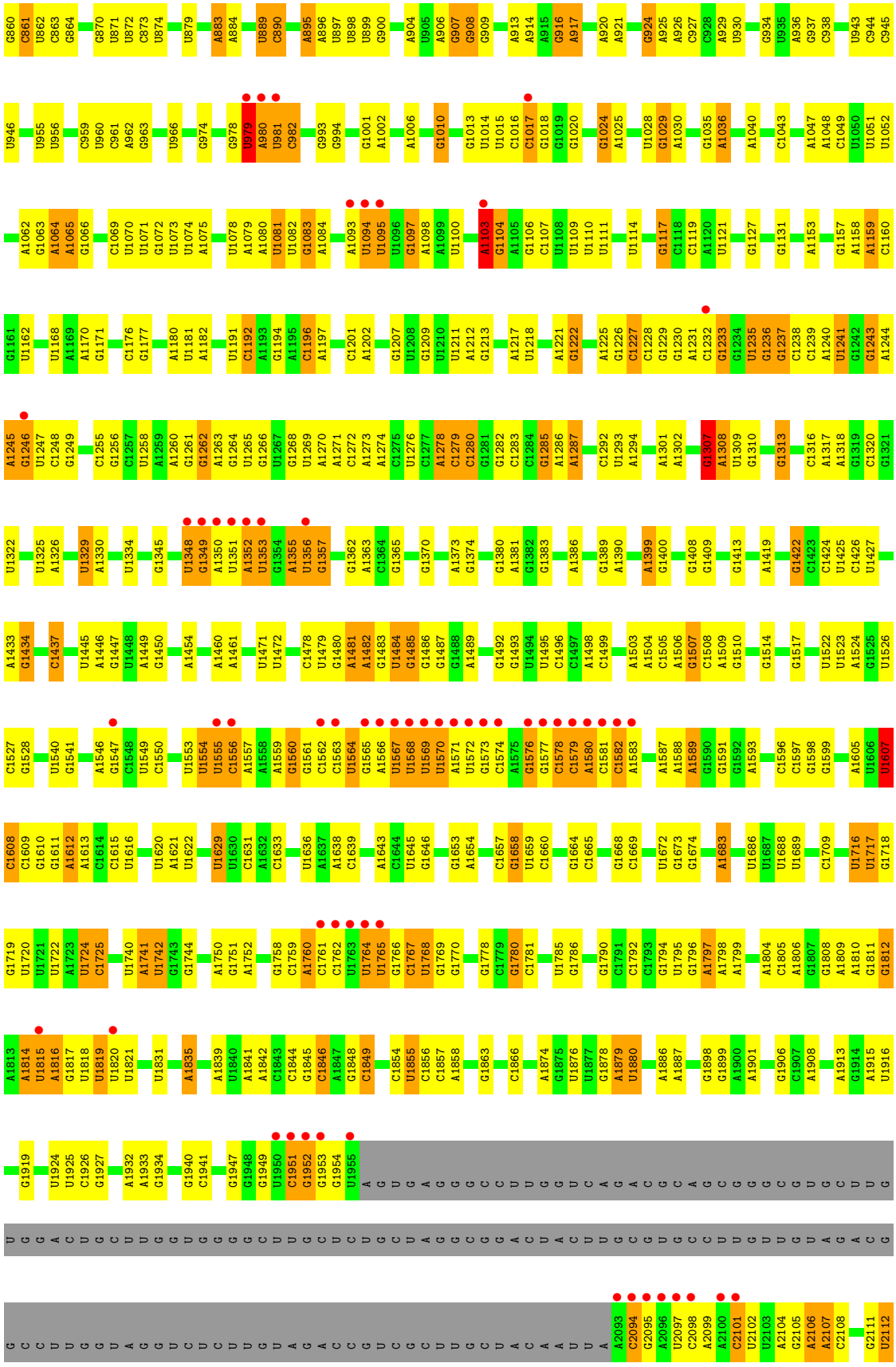
• Molecule 35: Suppressor protein STM1



• Molecule 36: 25S ribosomal RNA

Chain 1:




G860 C861 U862 C863 G864 G870 U871 U872 C873 U874 U879 A883 A884 U889 C890 A895 A896 U897 U898 U899 G900 A904 U905 A906 G907 G908 G909 A913 A914 A915 G916 A917 A920 A921 G924 A925 A926 C927 C928 A929 U930 G934 U935 A936 G937 C938 U943 C944 C945
U946 U955 U956 C959 U960 C961 A962 G963 U966 G974 G978 U979 A980 U981 C982 G993 G994 G1001 A1002 A1006 G1010 G1013 U1014 U1015 C1016 C1017 G1018 G1019 G1020 G1024 A1025 U1028 G1029 A1030 G1035 A1036 A1040 C1043 A1047 A1048 C1049 U1050 U1051 U1052
A1062 G1063 A1064 A1065 G1066 C1069 U1070 U1071 G1072 U1073 U1074 A1075 U1078 A1079 A1080 U1081 U1082 G1083 A1084 A1093 U1094 U1095 U1096 G1097 A1098 A1099 U1100 A1103 G1104 A1105 G1106 C1107 U1108 U1109 U1110 U1111 U1114 G1117 C1118 C1119 A1120 U1121 G1127 G1131 A1153 G1157 A1158 A1159 C1160
G1161 U1162 U1168 A1169 A1170 G1171 C1176 G1177 A1180 U1181 A1182 U1191 C1192 A1193 G1194 A1195 C1196 A1197 C1201 A1202 G1207 U1208 G1209 U1210 U1211 A1212 G1213 A1217 U1218 A1221 G1222 A1225 G1226 C1227 C1228 G1229 G1230 A1231 C1232 G1233 G1234 U1235 G1236 G1237 C1238 C1239 A1240 U1241 G1242 G1243 A1244
A1245 G1246 U1247 C1248 G1249 C1255 G1256 C1257 U1258 A1259 A1260 G1261 G1262 A1263 G1264 U1265 G1266 U1267 G1268 U1269 A1270 A1271 C1272 A1273 A1274 C1275 U1276 C1277 A1278 C1279 C1280 G1281 G1282 C1283 C1284 G1285 A1286 A1287 C1292 U1293 A1294 A1301 A1302 G1307 A1308 U1309 G1310 G1313 C1316 A1317 A1318 G1319 C1320 G1321
U1322 U1325 A1326 U1329 A1330 U1334 G1345 U1348 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 C1362 A1363 C1364 G1365 G1370 A1373 G1374 G1380 A1381 C1382 G1383 A1386 G1389 A1390 A1399 G1400 G1408 G1409 G1413 A1419 G1422 C1423 C1424 U1425 C1426 U1427
A1433 G1434 C1437 U1445 A1446 G1447 U1448 A1449 G1450 A1454 A1460 A1461 U1471 U1472 C1478 U1479 G1480 A1481 A1482 G1483 U1484 G1485 G1486 G1487 G1488 A1489 G1492 G1493 U1494 U1495 C1496 C1497 A1498 C1499 A1503 A1504 C1505 A1506 G1507 C1508 A1509 G1510 G1514 G1517 U1522 U1523 A1524 G1525 U1526
C1527 G1528 U1540 G1541 A1546 G1547 C1548 U1549 C1550 U1553 U1554 U1555 C1556 A1557 A1558 A1559 G1560 G1561 C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569 U1570 A1571 U1572 G1573 C1574 A1575 G1576 G1577 C1578 C1579 A1580 C1581 C1582 A1583 A1587 A1588 A1589 G1590 G1591 G1592 A1593 C1596 C1597 G1598 G1599 A1605 U1606 U1607
C1608 C1609 G1610 G1611 A1612 A1613 C1614 C1615 U1616 U1620 A1621 U1622 U1629 U1630 C1631 A1632 C1633 U1636 A1637 A1638 C1639 A1643 C1644 U1645 G1646 G1653 A1654 C1657 G1658 U1659 C1660 G1664 C1665 G1668 C1669 U1672 G1673 G1674 A1683 U1686 U1687 U1688 U1689 C1709 U1716 U1717 G1718
G1719 U1720 U1721 U1722 A1723 U1724 C1725 U1740 A1741 U1742 G1743 G1744 A1750 G1751 A1752 G1758 C1759 A1760 C1761 C1762 U1763 U1764 U1765 G1766 C1767 U1768 G1769 G1770 G1778 C1779 G1780 C1781 U1785 G1786 G1790 C1791 C1792 C1793 G1794 U1795 G1796 A1797 A1798 A1799 A1804 C1805 A1806 G1807 G1808 A1809 A1810 G1811 G1812
A1813 A1814 U1815 A1816 G1817 U1818 U1819 U1820 U1821 U1831 A1835 A1839 U1840 A1841 A1842 C1843 C1844 G1845 C1846 A1847 G1848 C1849 C1854 U1855 C1856 C1857 A1858 G1863 C1866 A1874 G1875 U1876 U1877 G1878 A1879 U1880 A1886 A1887 G1898 G1899 A1900 A1901 G1906 C1907 A1908 A1913 G1914 A1915 U1916
G1919 U1924 U1925 C1926 G1927 A1932 A1933 G1934 G1940 C1941 G1947 G1948 G1949 U1950 C1951 G1952 G1953 G1954 U1955 A G G U G C G A A G G G C C C U G U U U G U G U G U U U G G G C U U C G C U U G C A A A U C U U A
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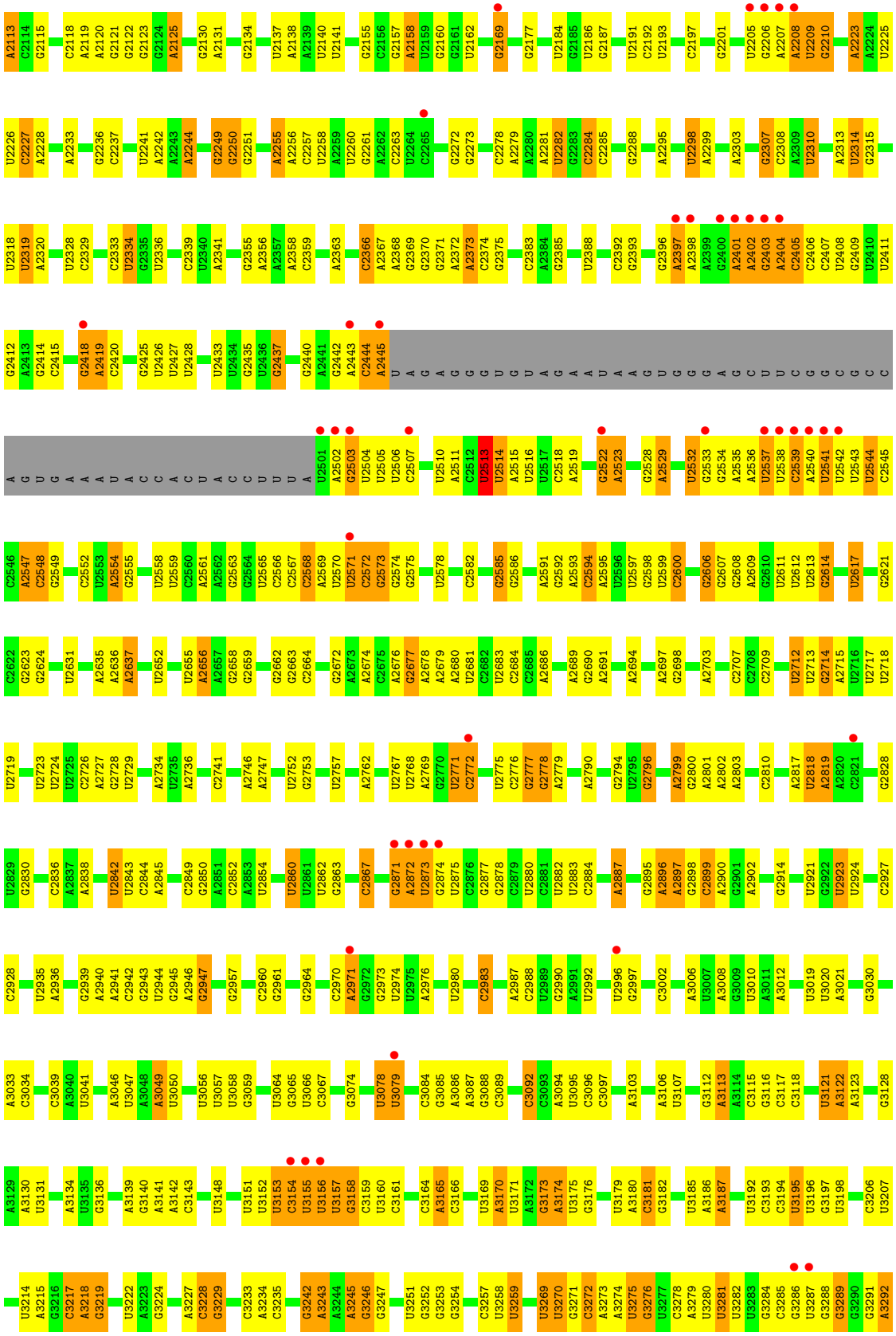
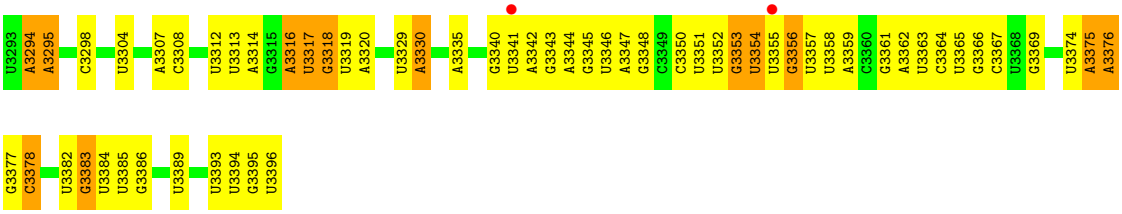
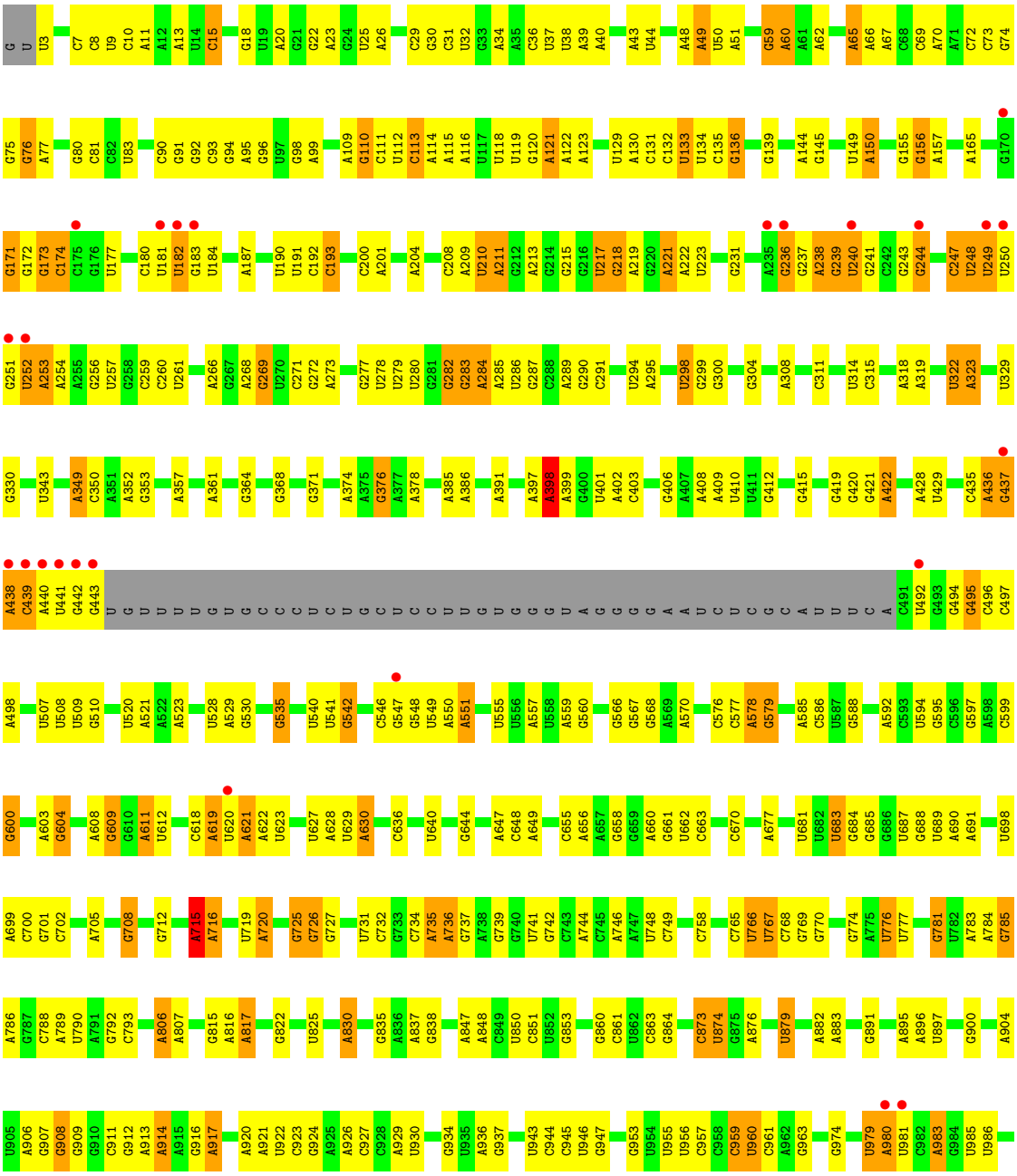
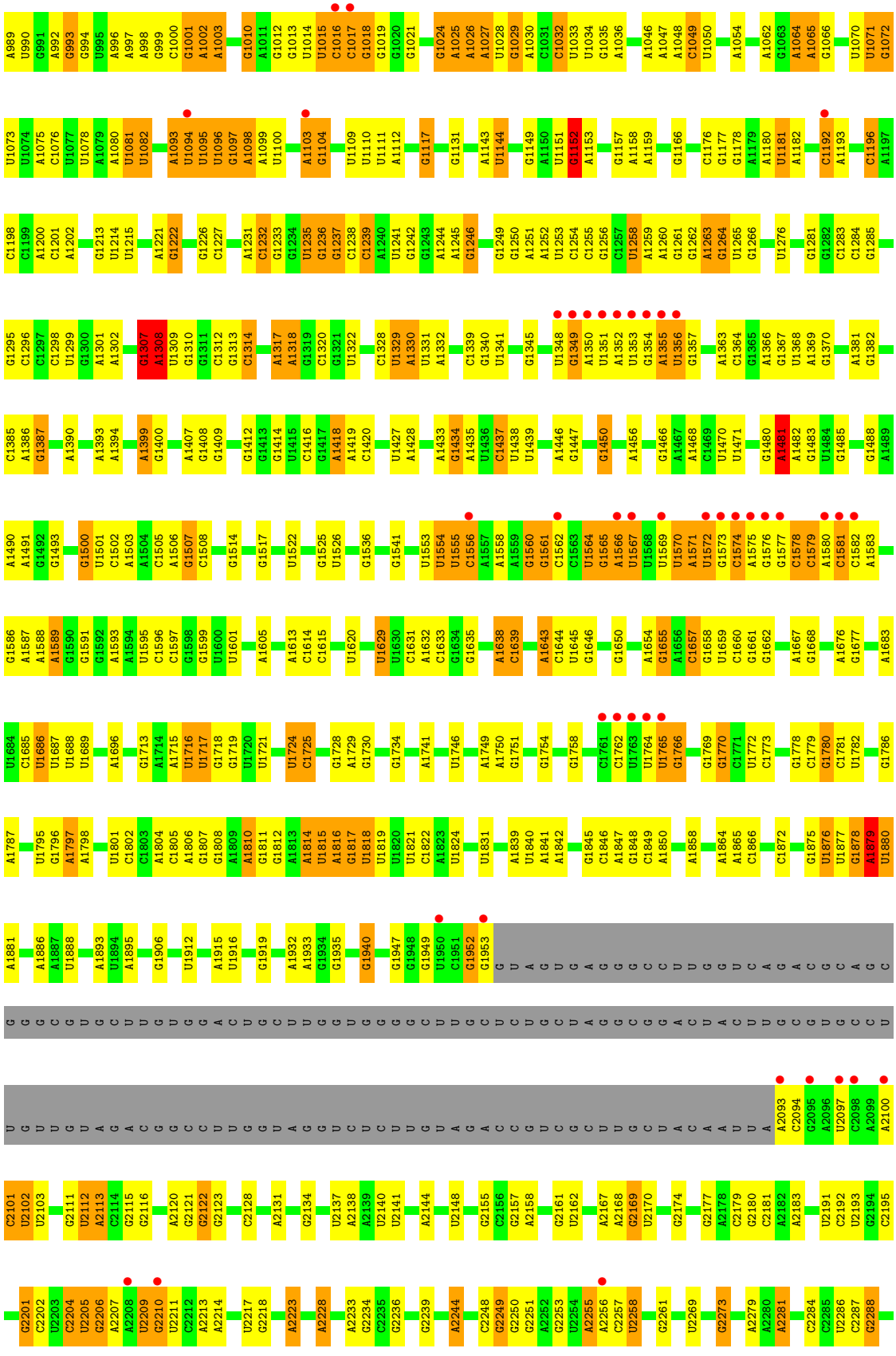


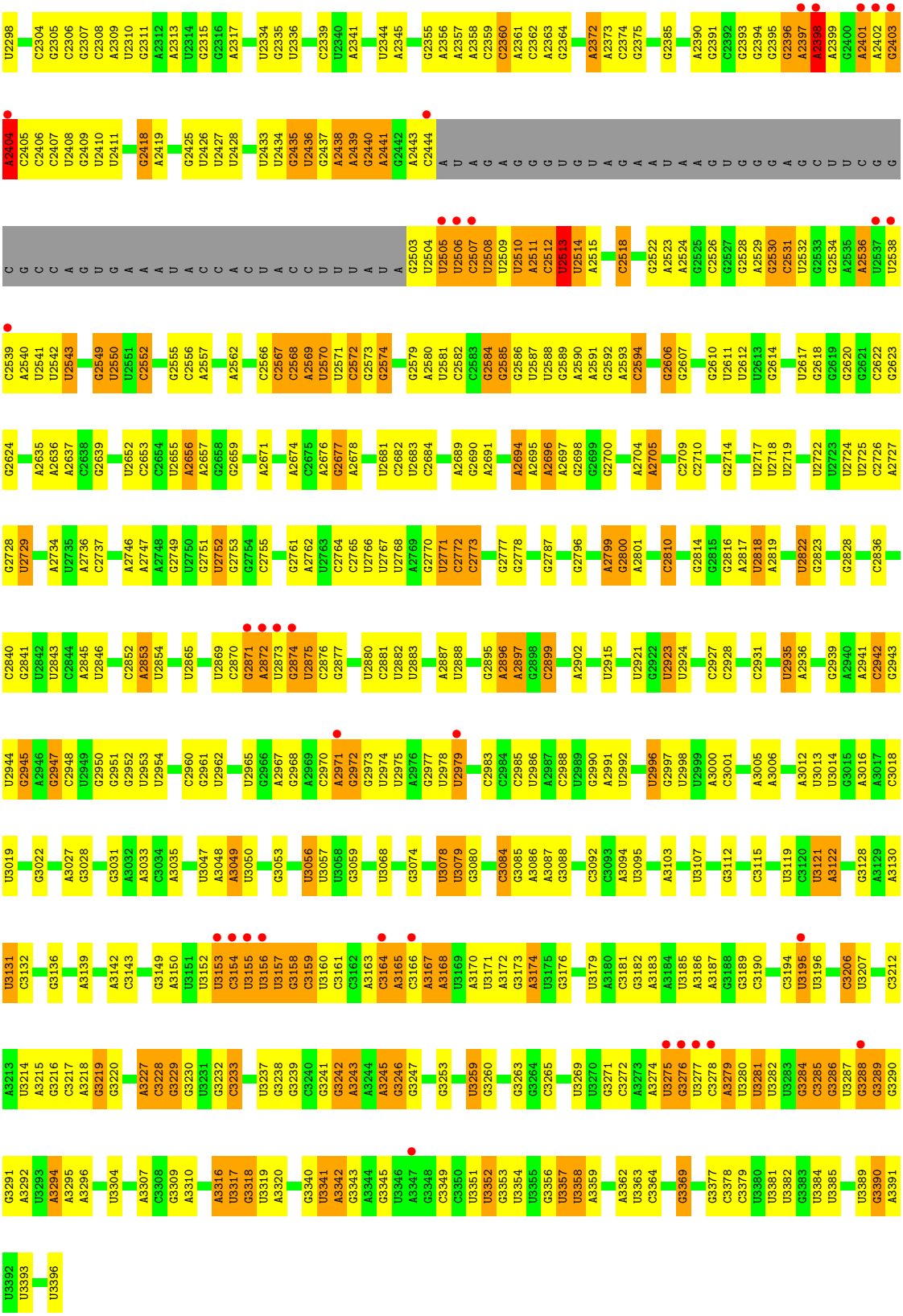


• Molecule 36: 25S ribosomal RNA

Chain 5:

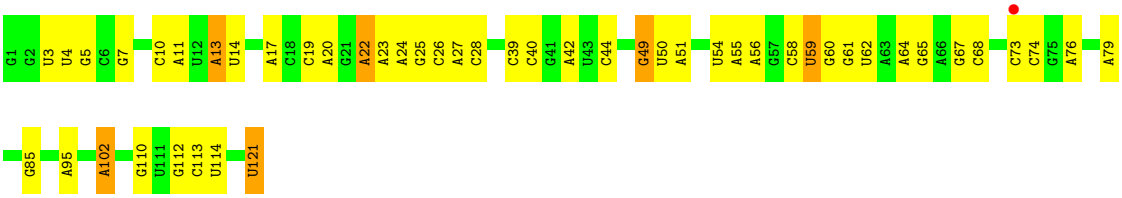






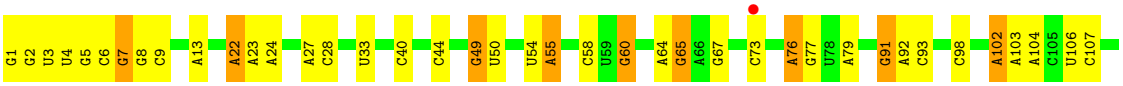
• Molecule 37: 5S ribosomal RNA

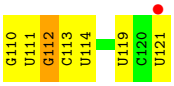
Chain 3:



• Molecule 37: 5S ribosomal RNA

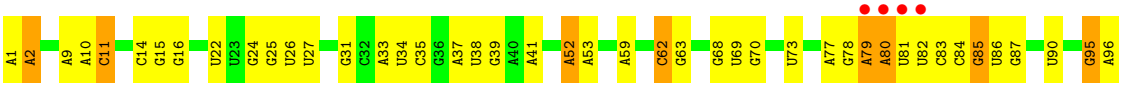
Chain 7:

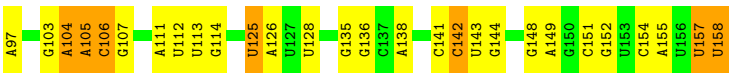




• Molecule 38: 5.8S ribosomal RNA

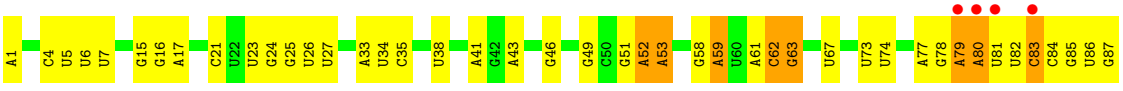
Chain 4:

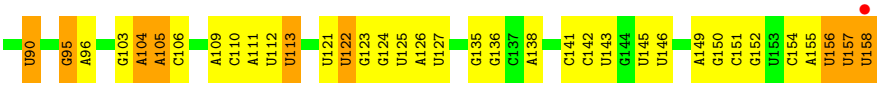




• Molecule 38: 5.8S ribosomal RNA

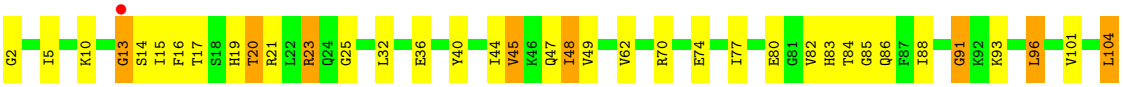
Chain 8:

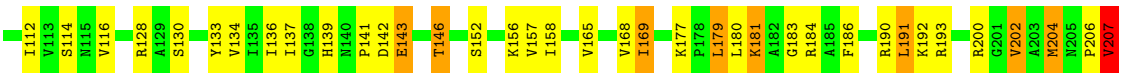


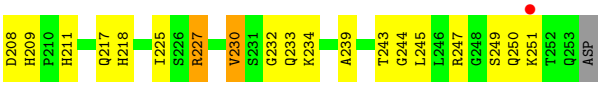


• Molecule 39: 60S ribosomal protein L2-A

Chain L2:

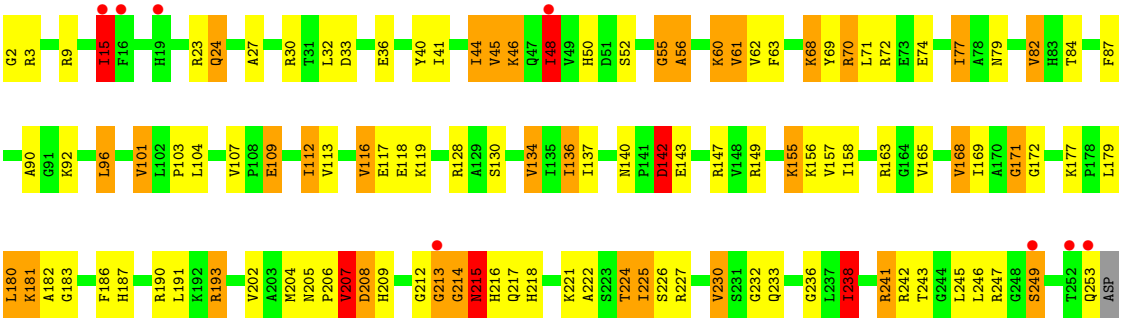






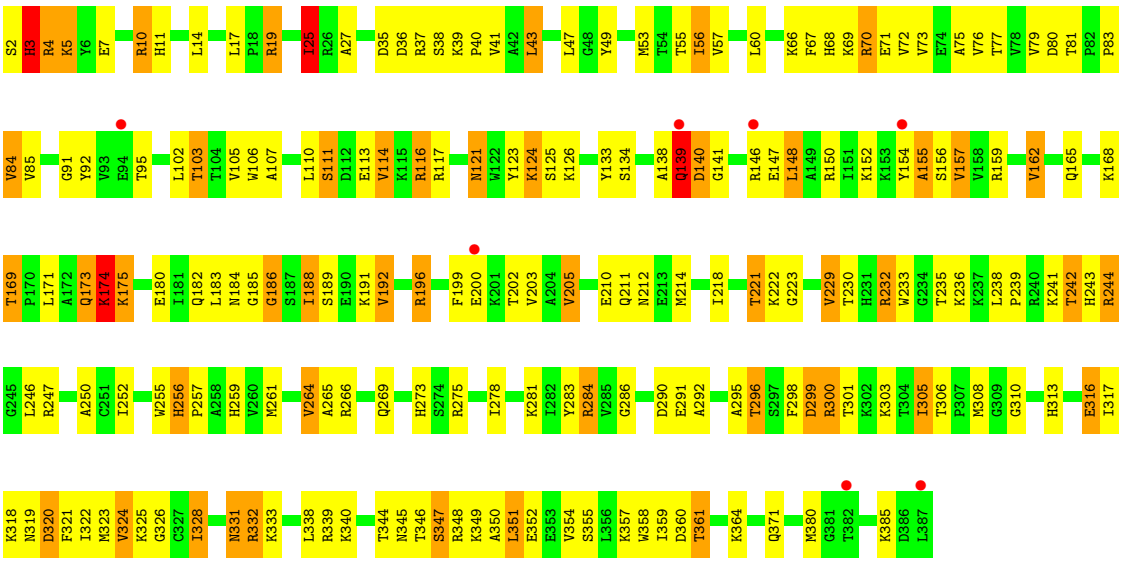
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:



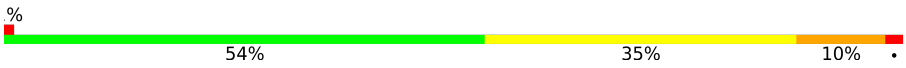
• Molecule 40: 60S ribosomal protein L3

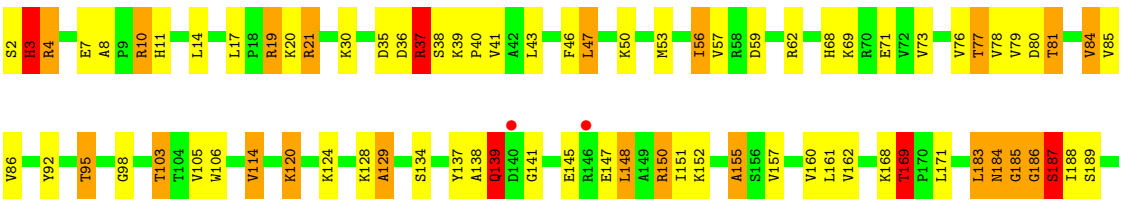
Chain L3:

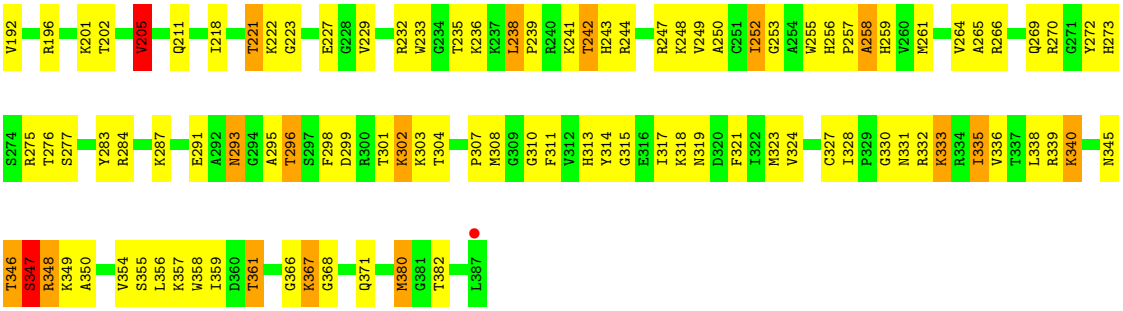


• Molecule 40: 60S ribosomal protein L3

Chain l3:

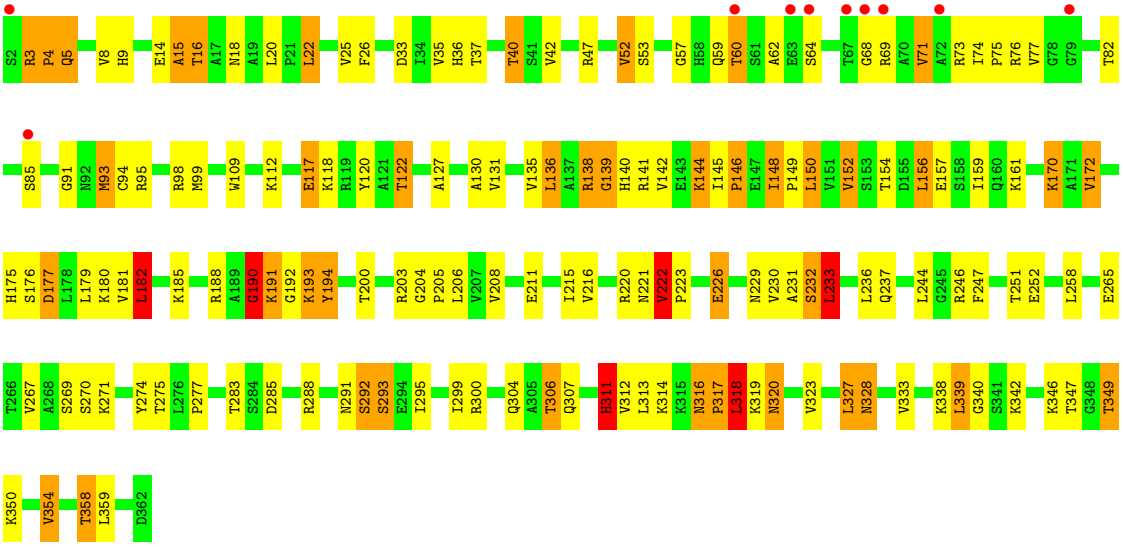






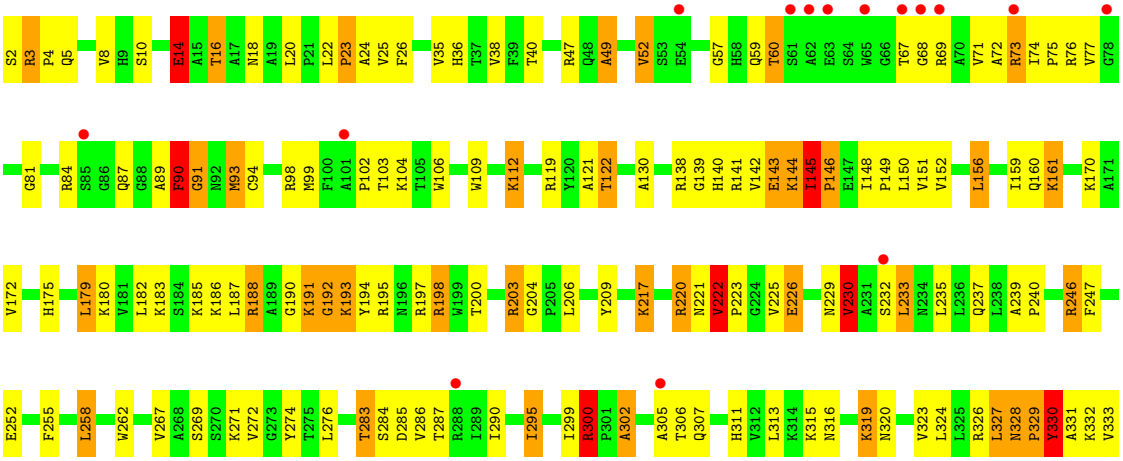
• Molecule 41: 60S ribosomal protein L4-A

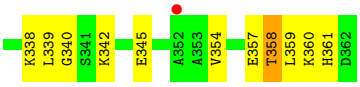
Chain L4:



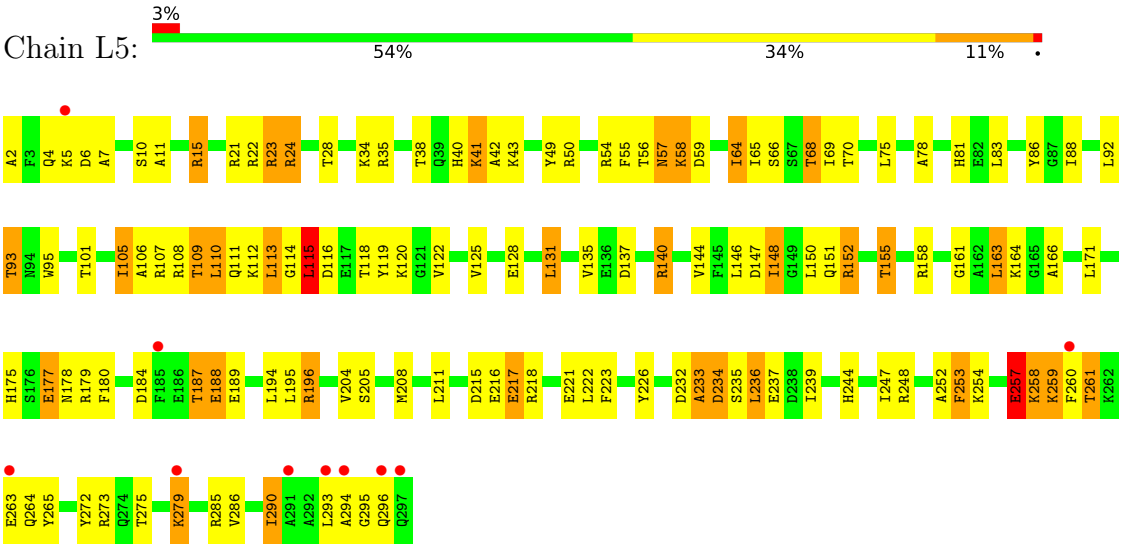
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:

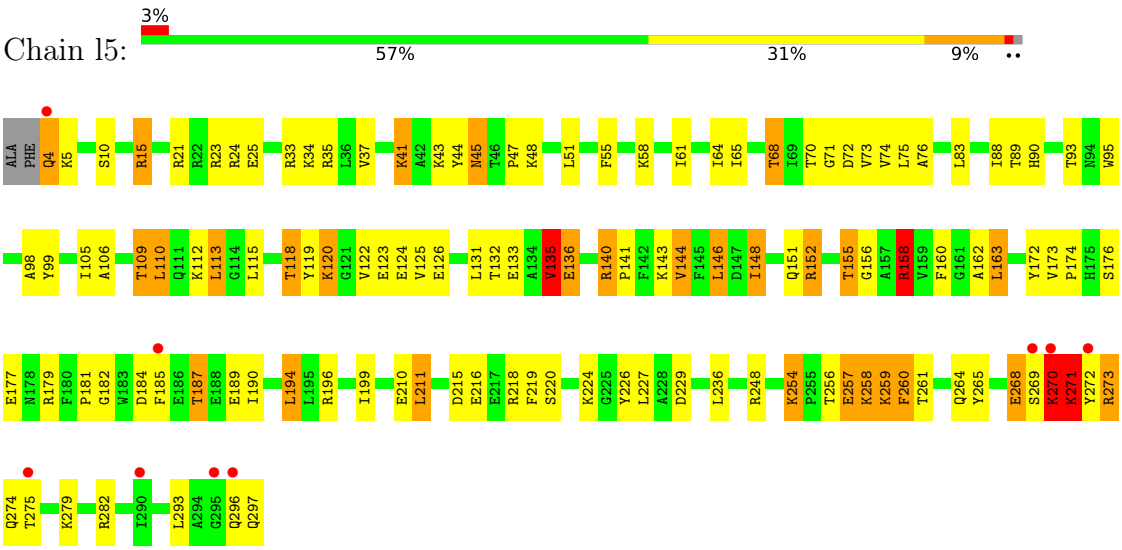




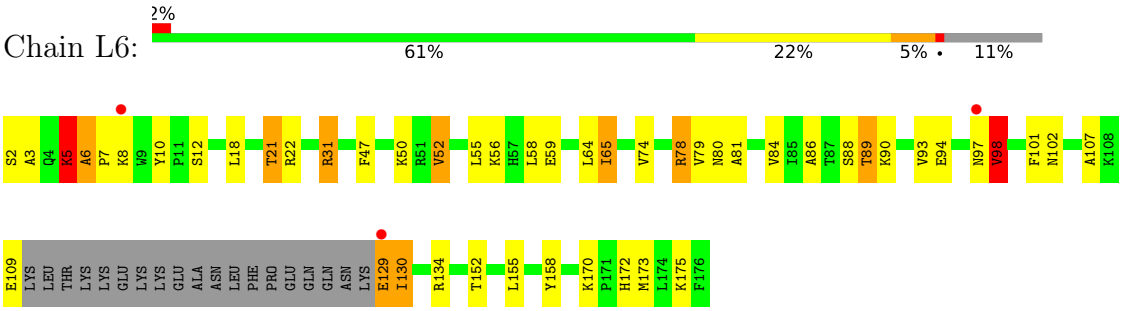
• Molecule 42: 60S ribosomal protein L5



• Molecule 42: 60S ribosomal protein L5

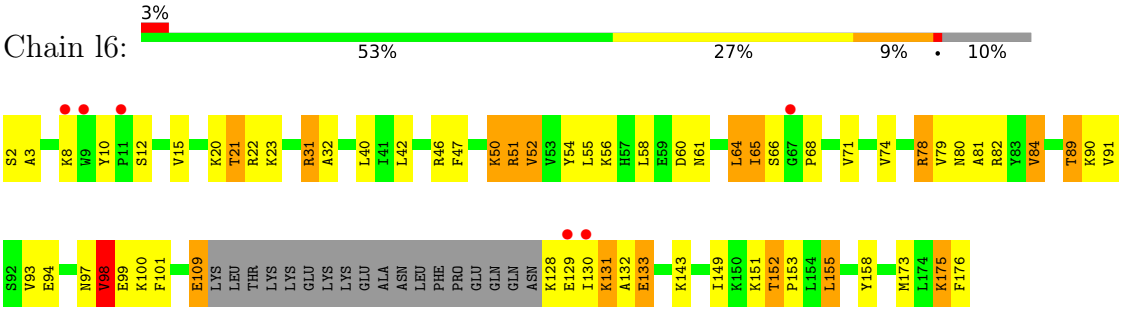


• Molecule 43: 60S ribosomal protein L6-A



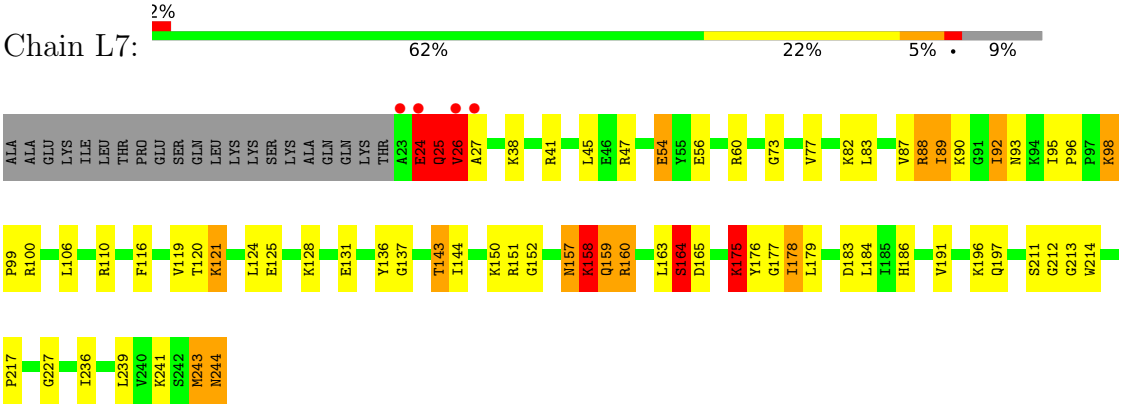
• Molecule 43: 60S ribosomal protein L6-A

Chain l6:



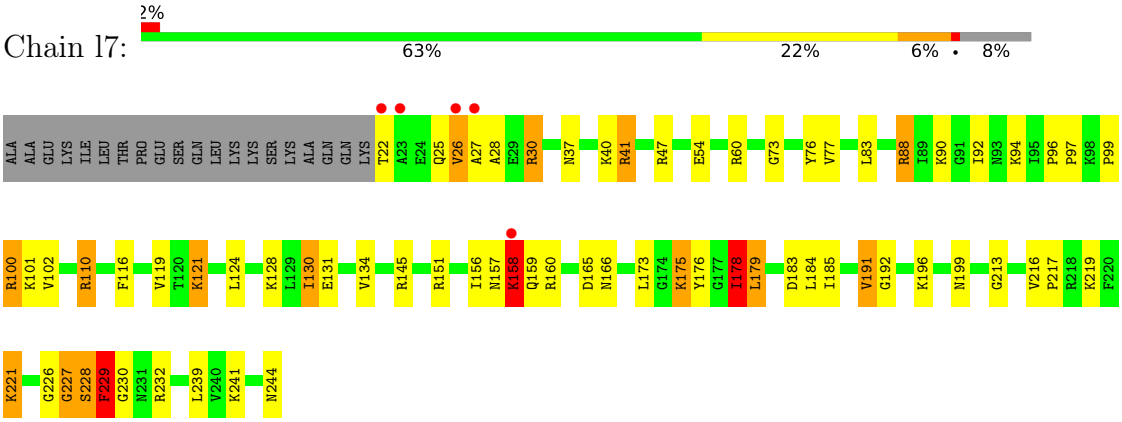
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:



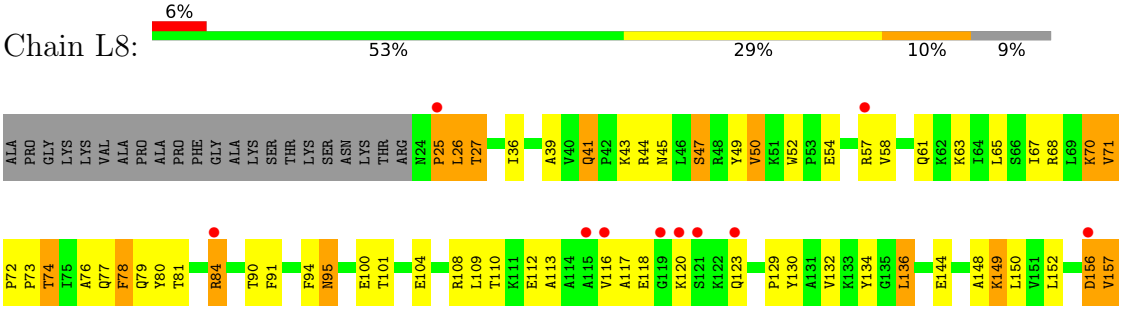
• Molecule 44: 60S ribosomal protein L7-A

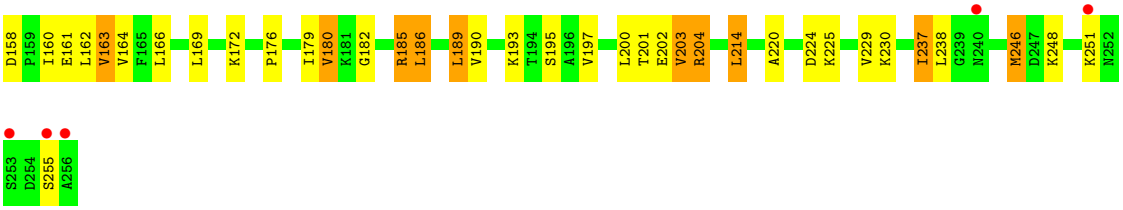
Chain l7:



• Molecule 45: 60S ribosomal protein L8-A

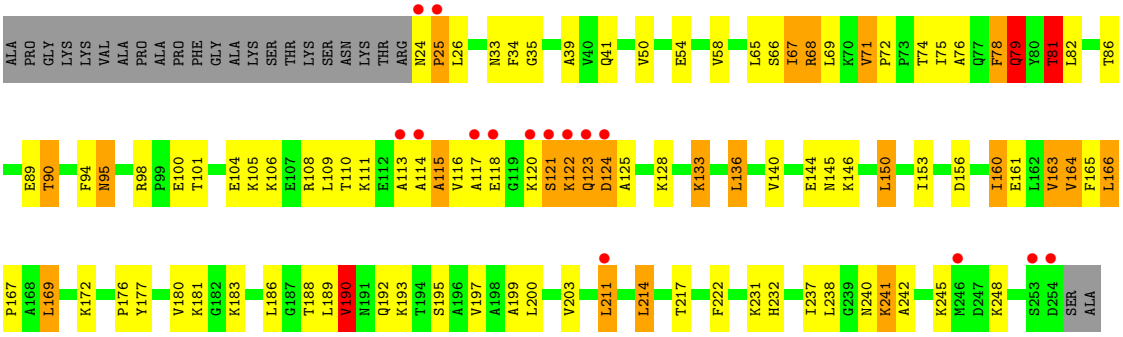
Chain L8:





• Molecule 45: 60S ribosomal protein L8-A

Chain l8:

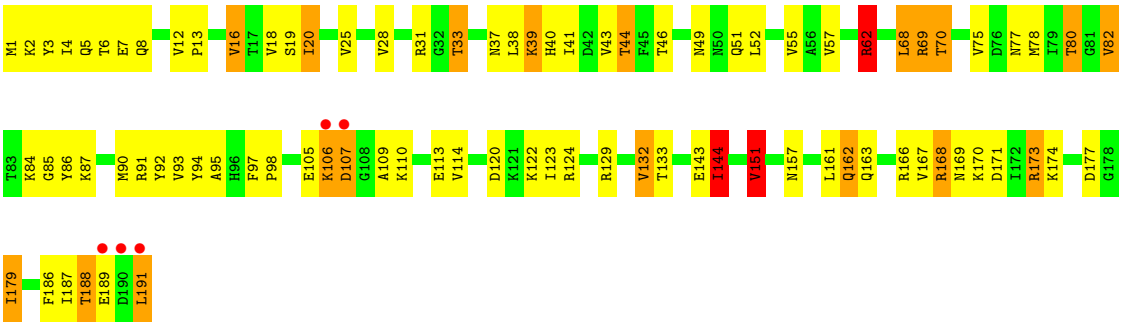


• Molecule 46: 60S ribosomal protein L9-A

Chain L9:

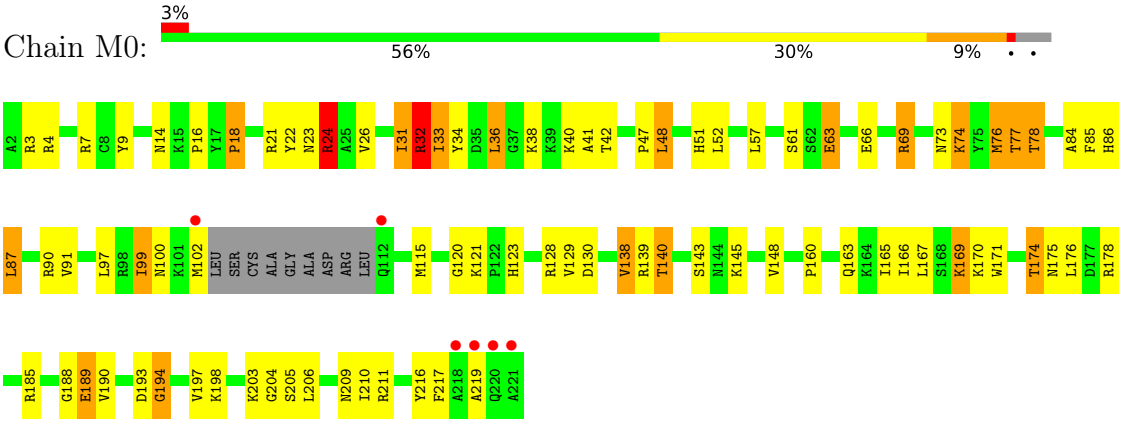
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



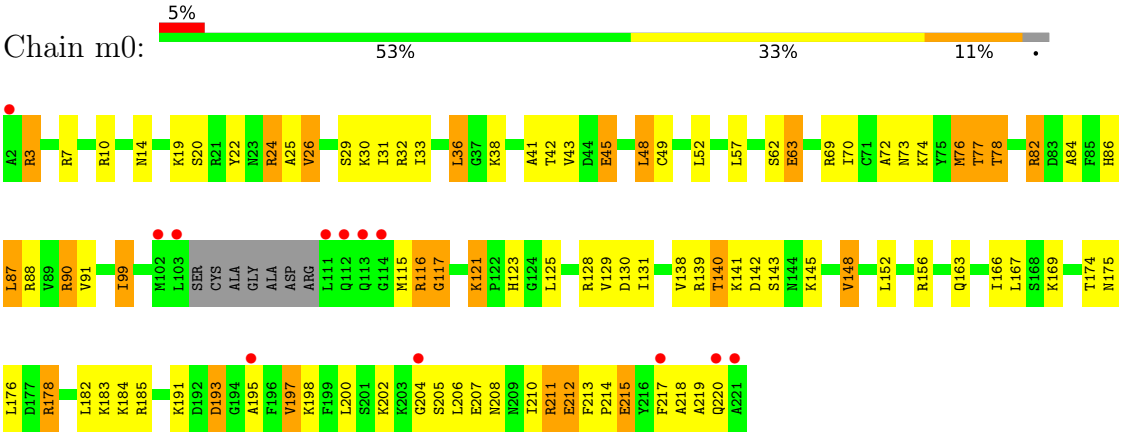
• Molecule 47: 60S ribosomal protein L10

Chain M0:



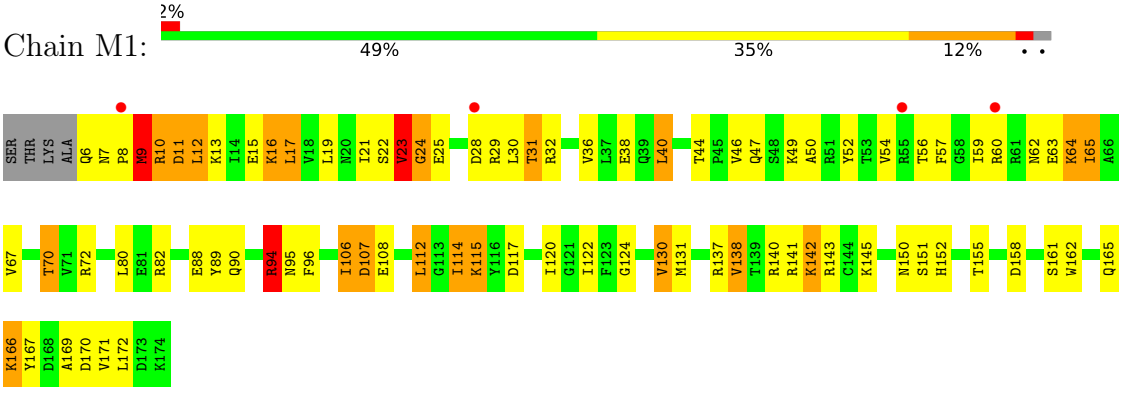
• Molecule 47: 60S ribosomal protein L10

Chain m0:



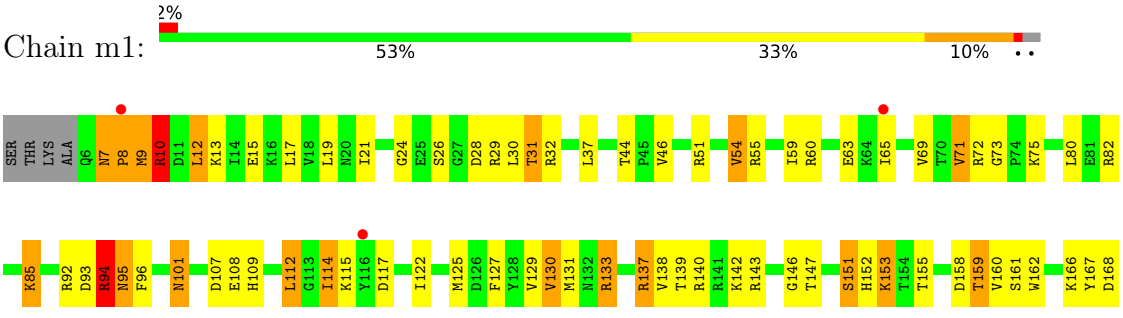
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



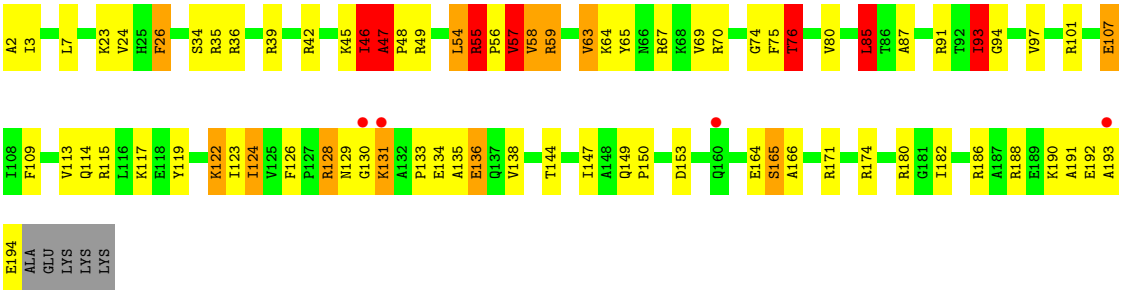
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



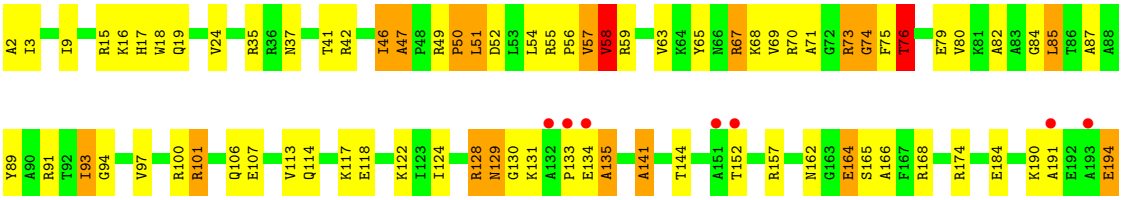
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



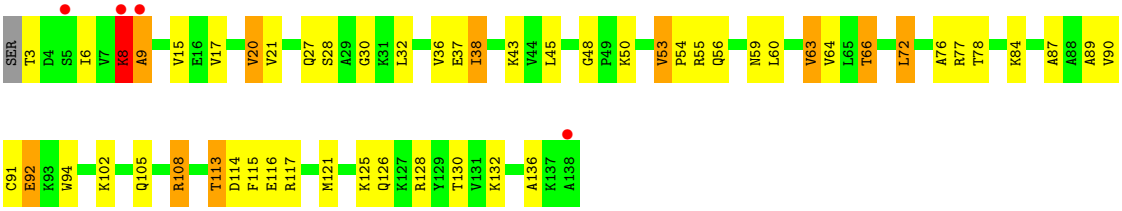
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



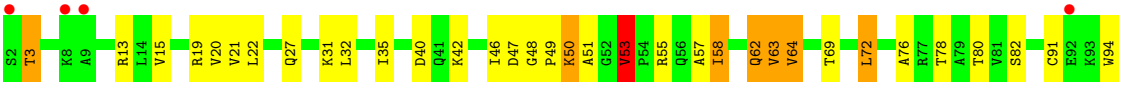
• Molecule 50: 60S ribosomal protein L14-A

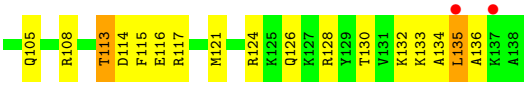
Chain M4:



• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



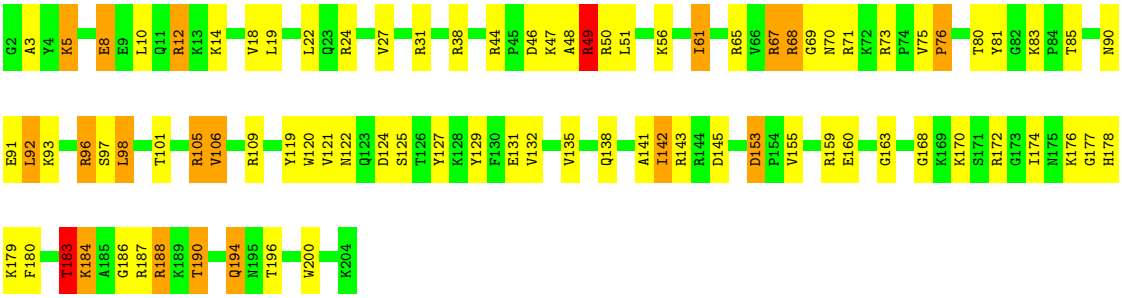


• Molecule 51: 60S ribosomal protein L15-A

Chain M5:

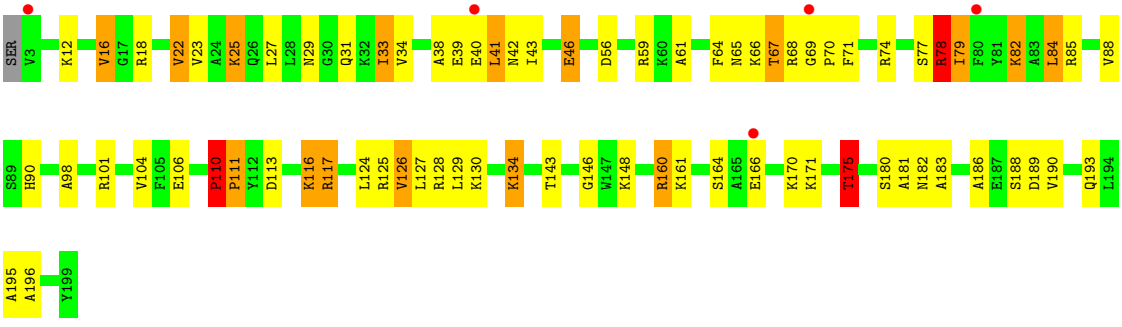
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



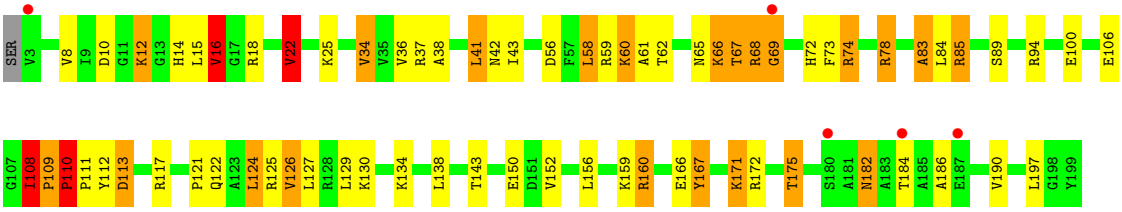
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



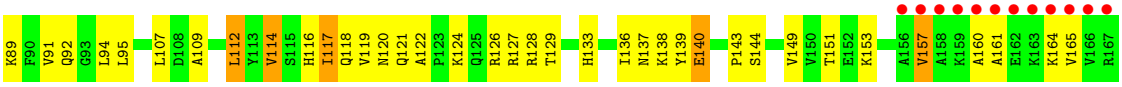
• Molecule 52: 60S ribosomal protein L16-A

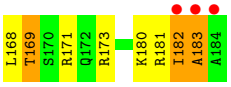
Chain m6:



• Molecule 53: 60S ribosomal protein L17-A

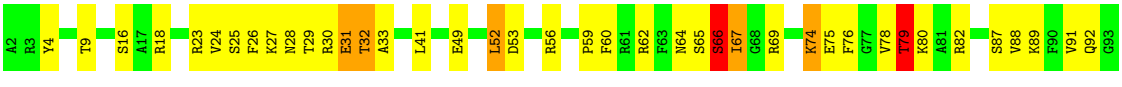
Chain M7:

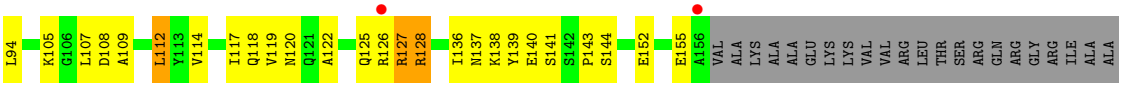




• Molecule 53: 60S ribosomal protein L17-A

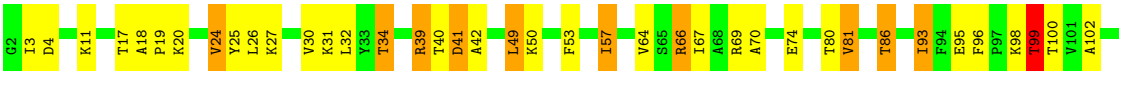
Chain m7:





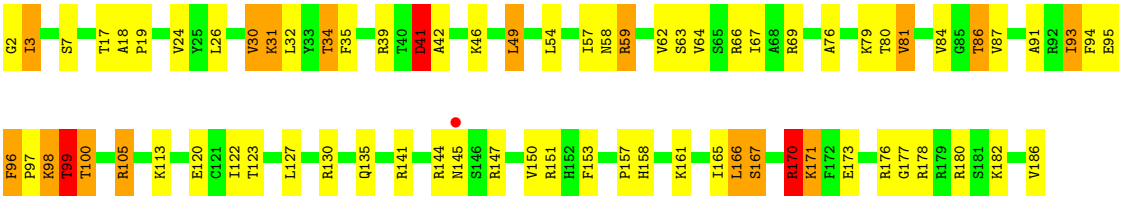
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



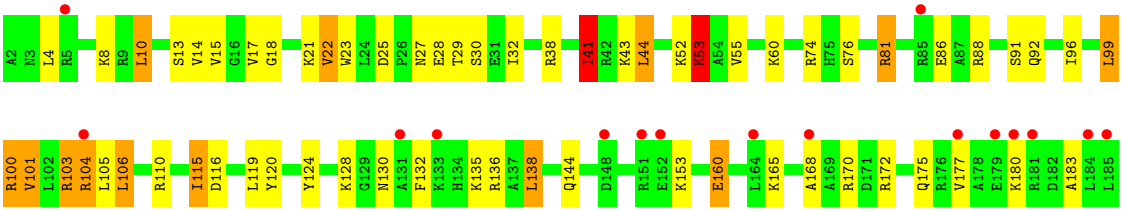
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



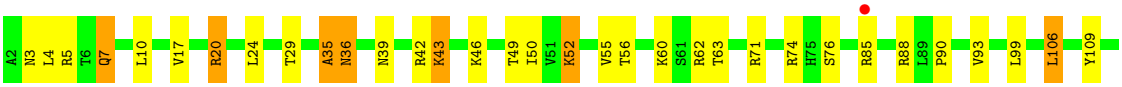
• Molecule 55: 60S ribosomal protein L19-A

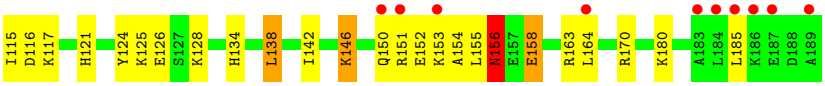
Chain M9:



• Molecule 55: 60S ribosomal protein L19-A

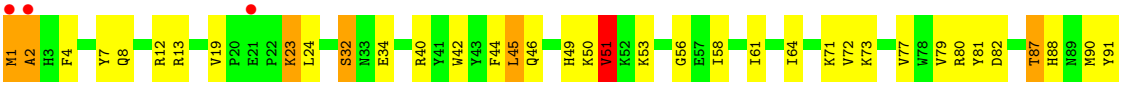
Chain m9:

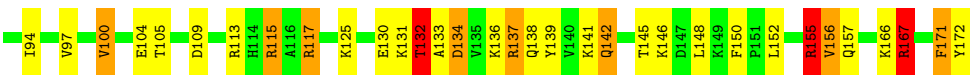




• Molecule 56: 60S ribosomal protein L20-A

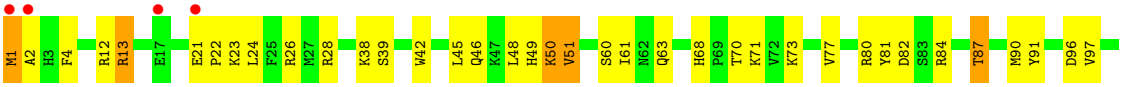
Chain N0:

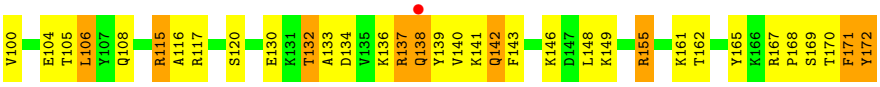




• Molecule 56: 60S ribosomal protein L20-A

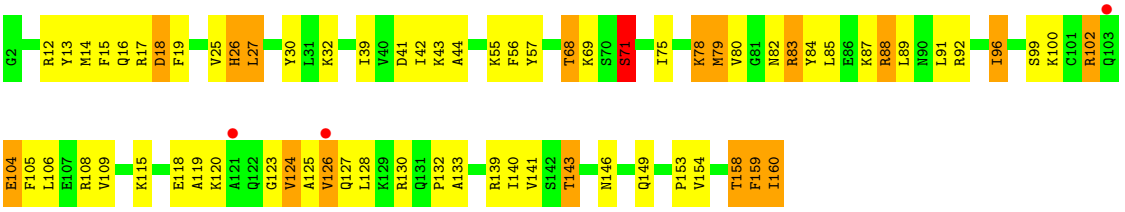
Chain n0:





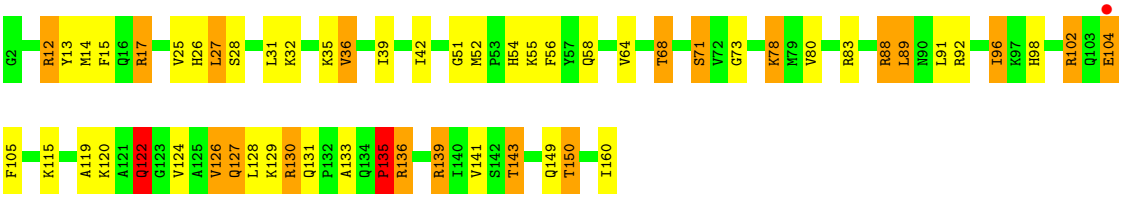
• Molecule 57: 60S ribosomal protein L21-A

Chain N1:



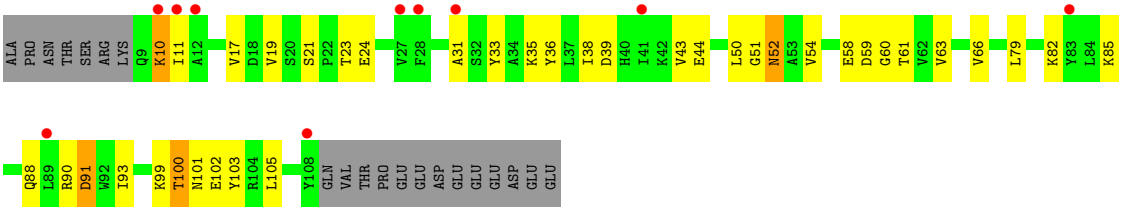
• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



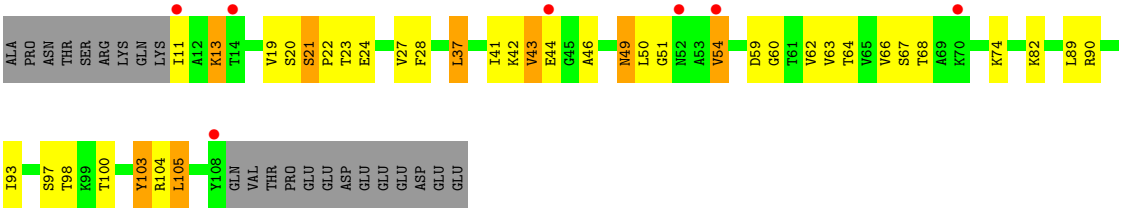
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



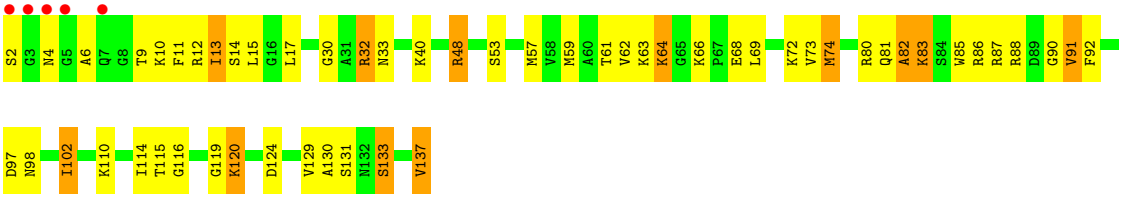
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



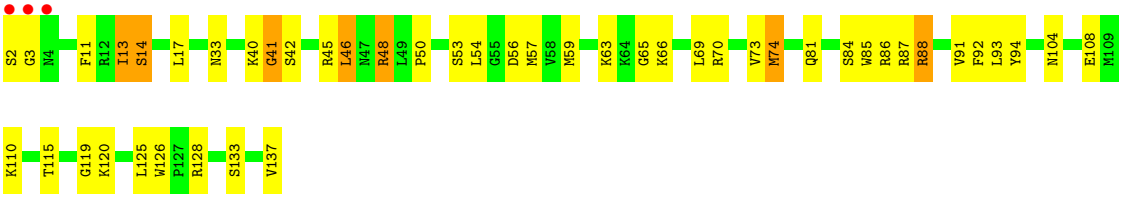
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



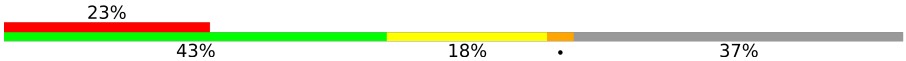
• Molecule 59: 60S ribosomal protein L23-A

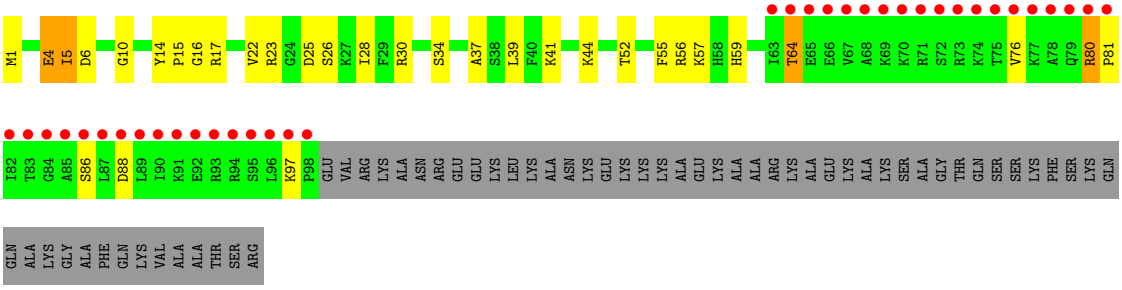
Chain n3:



• Molecule 60: 60S ribosomal protein L24-A

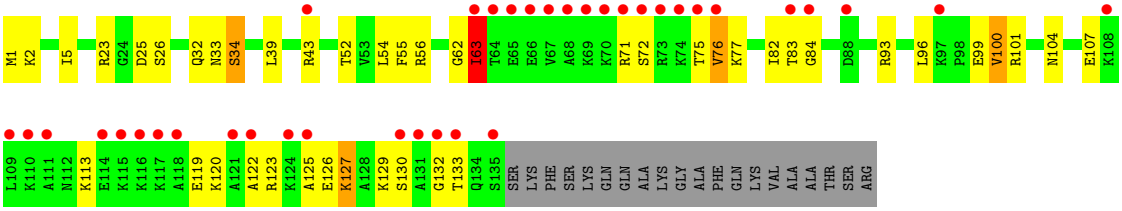
Chain N4:





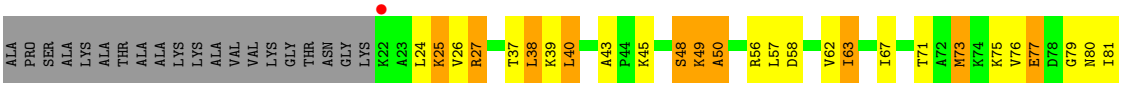
• Molecule 60: 60S ribosomal protein L24-A

Chain n4:



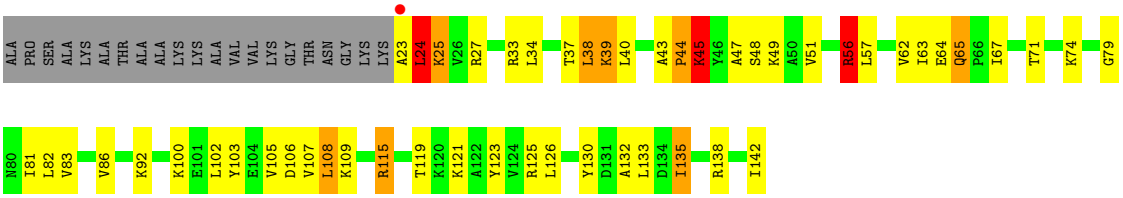
• Molecule 61: 60S ribosomal protein L25

Chain N5:



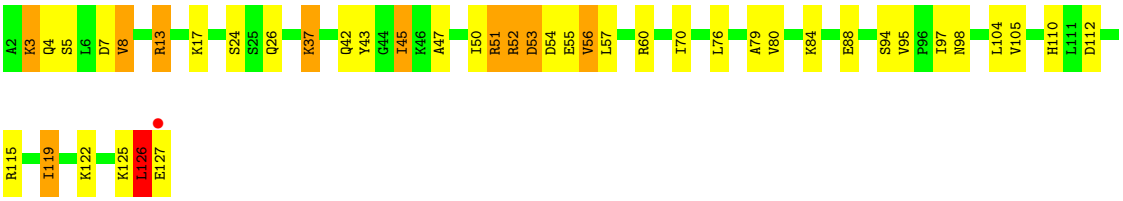
• Molecule 61: 60S ribosomal protein L25

Chain n5:



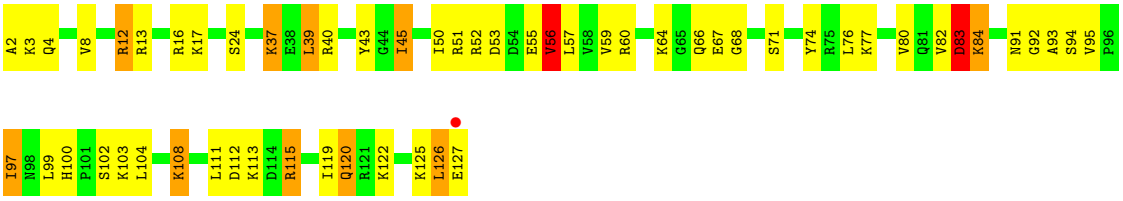
• Molecule 62: 60S ribosomal protein L26-A

Chain N6:



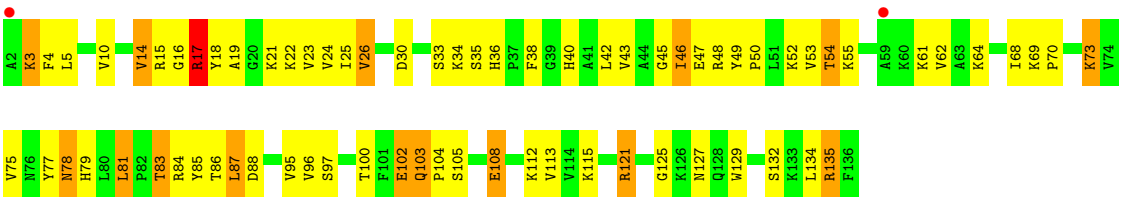
• Molecule 62: 60S ribosomal protein L26-A

Chain n6:



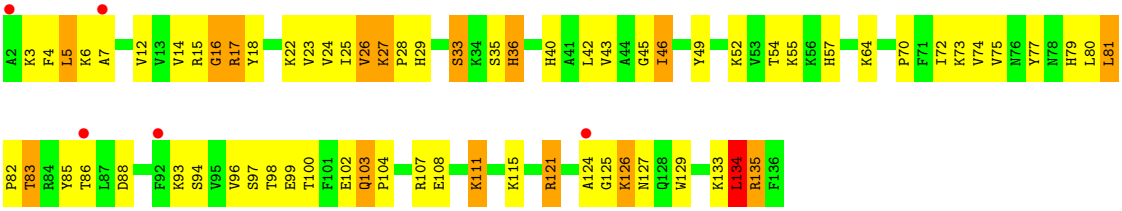
• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



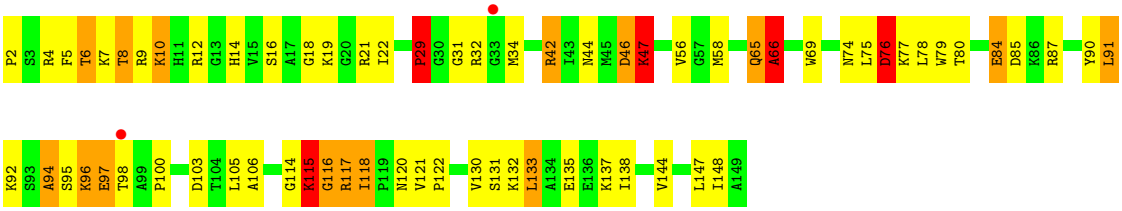
• Molecule 63: 60S ribosomal protein L27-A

Chain n7:



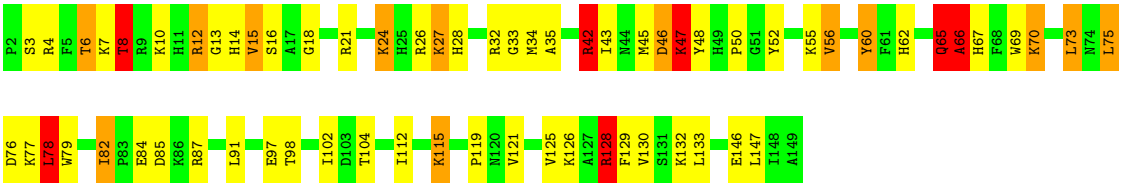
• Molecule 64: 60S ribosomal protein L28

Chain N8:



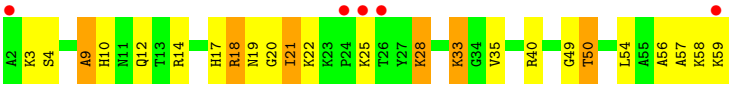
• Molecule 64: 60S ribosomal protein L28

Chain n8:



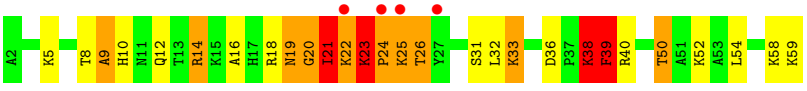
• Molecule 65: 60S ribosomal protein L29

Chain N9:



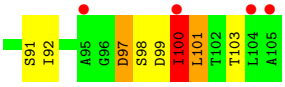
• Molecule 65: 60S ribosomal protein L29

Chain n9:



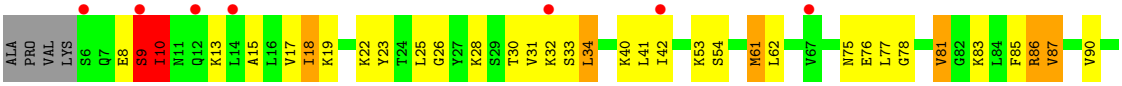
• Molecule 66: 60S ribosomal protein L30

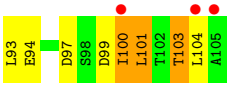
Chain O0:



• Molecule 66: 60S ribosomal protein L30

Chain o0:



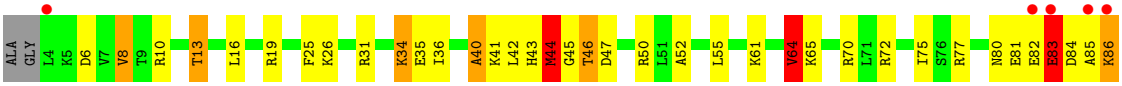


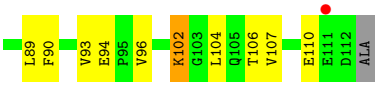
• Molecule 67: 60S ribosomal protein L31-A

Chain O1:

• Molecule 67: 60S ribosomal protein L31-A

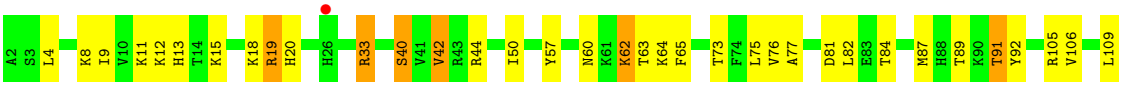
Chain o1:

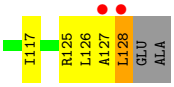




• Molecule 68: 60S ribosomal protein L32

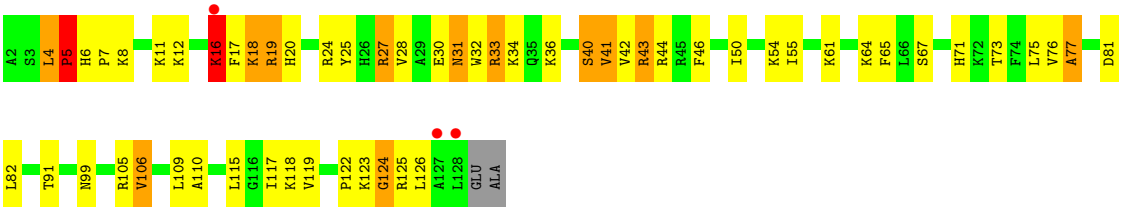
Chain O2:





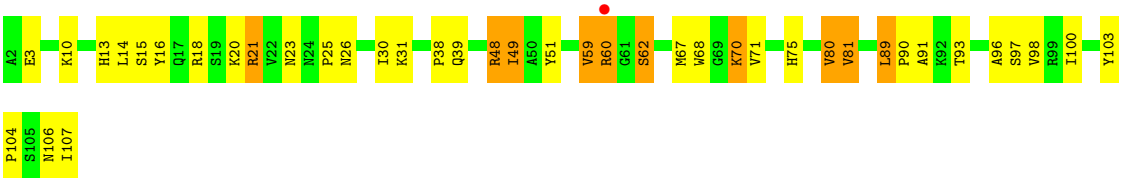
• Molecule 68: 60S ribosomal protein L32

Chain o2:



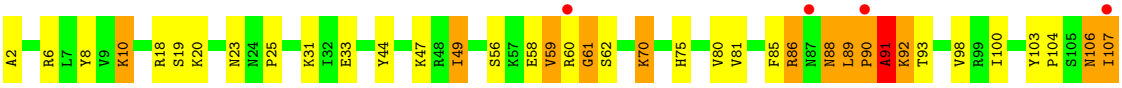
• Molecule 69: 60S ribosomal protein L33-A

Chain O3:



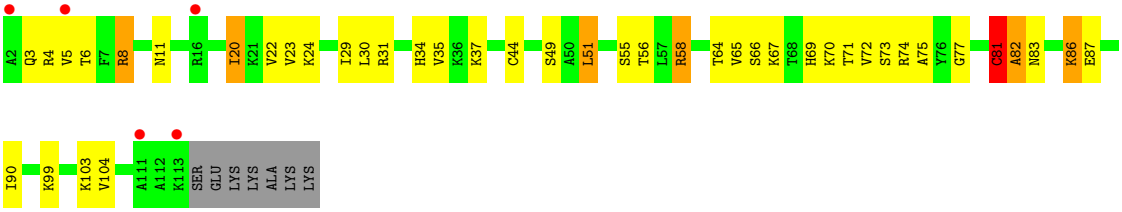
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



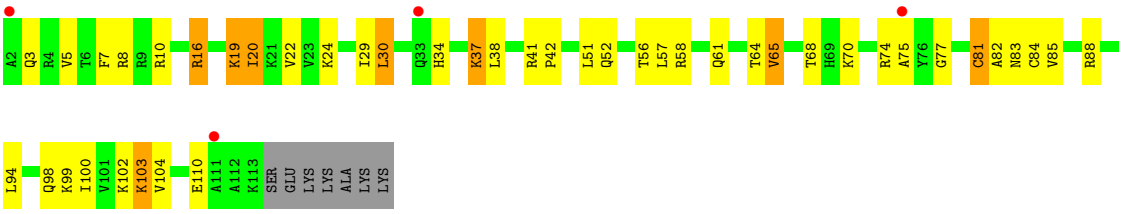
• Molecule 70: 60S ribosomal protein L34-A

Chain O4:



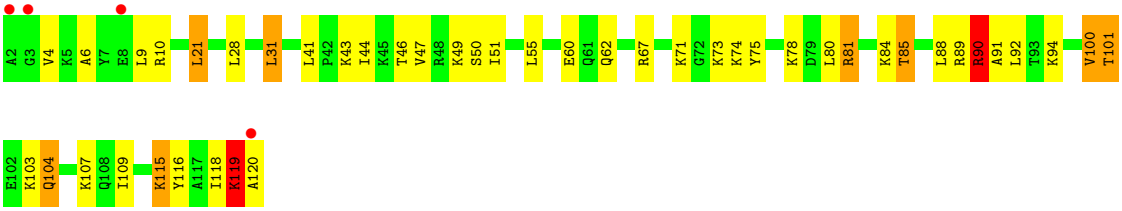
• Molecule 70: 60S ribosomal protein L34-A

Chain o4:



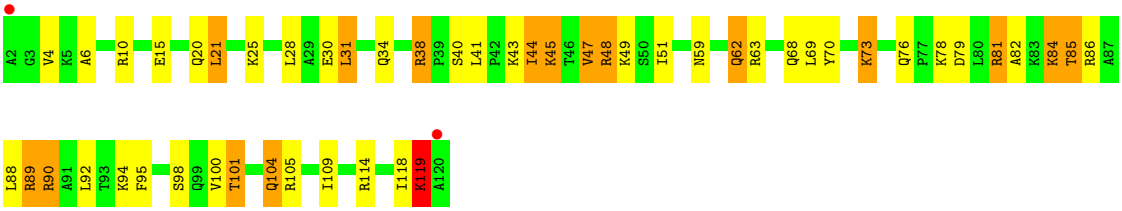
• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



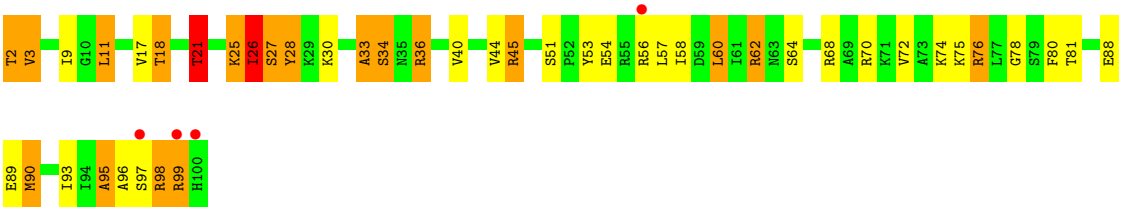
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



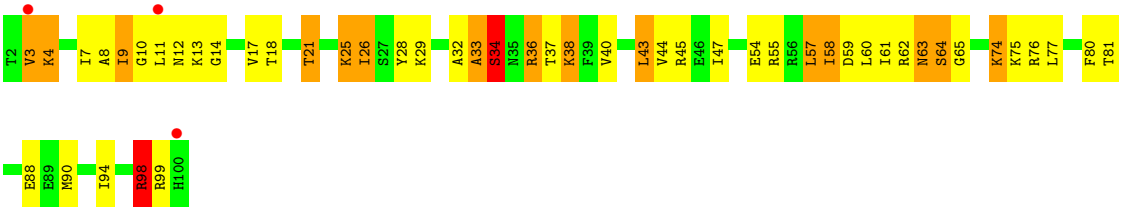
• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



• Molecule 72: 60S ribosomal protein L36-A

Chain o6:

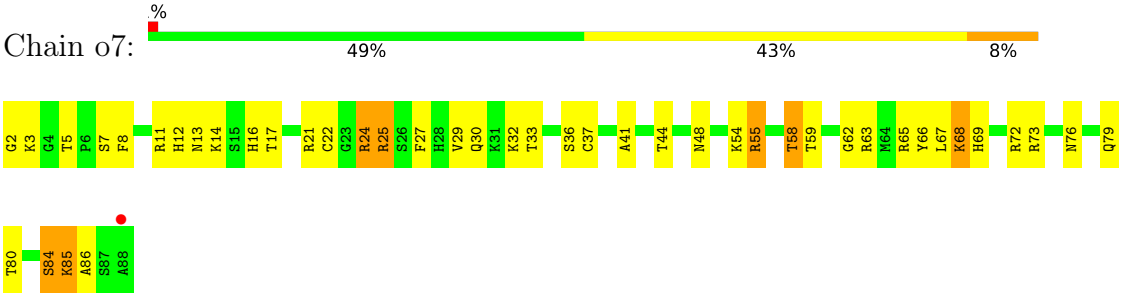


• Molecule 73: 60S ribosomal protein L37-A

Chain O7:

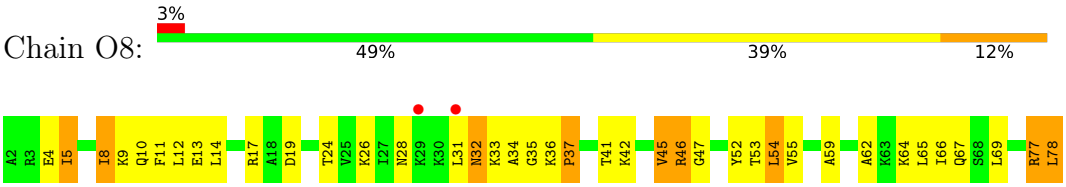
• Molecule 73: 60S ribosomal protein L37-A

Chain o7:



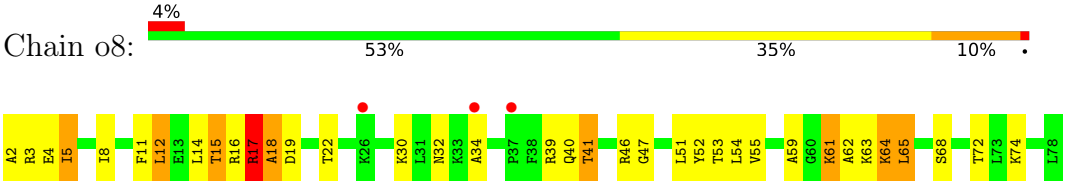
• Molecule 74: 60S ribosomal protein L38

Chain O8:



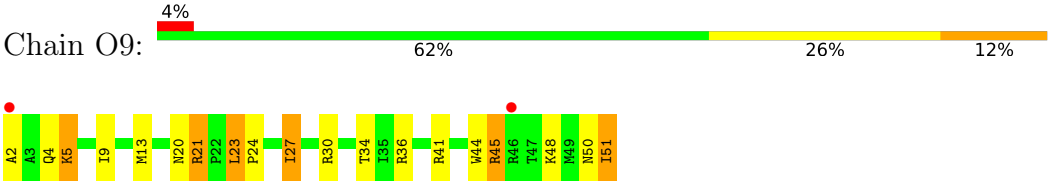
• Molecule 74: 60S ribosomal protein L38

Chain o8:



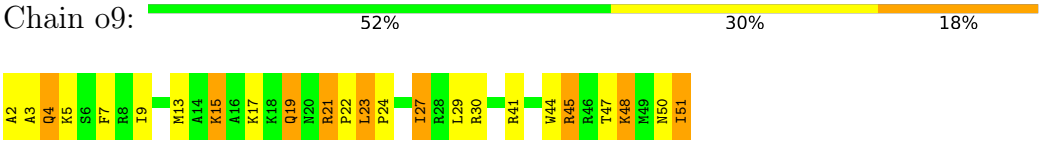
• Molecule 75: 60S ribosomal protein L39

Chain O9:



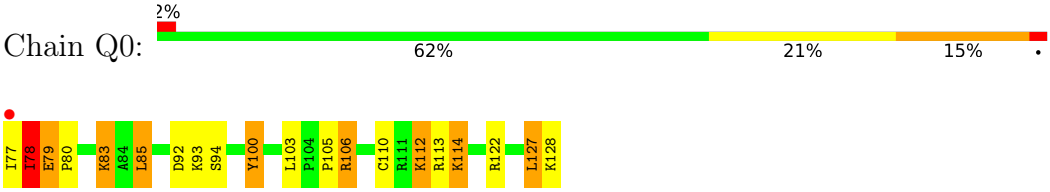
• Molecule 75: 60S ribosomal protein L39

Chain o9:



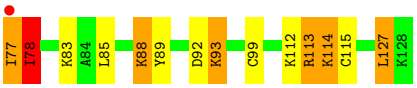
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



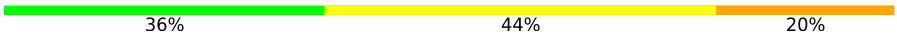
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



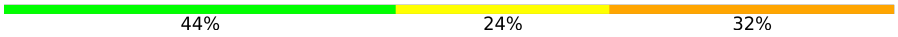
• Molecule 77: 60S ribosomal protein L41-A

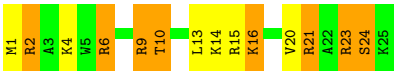
Chain Q1:



• Molecule 77: 60S ribosomal protein L41-A

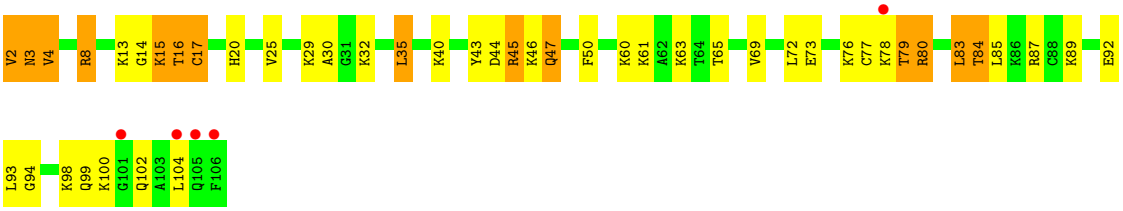
Chain q1:





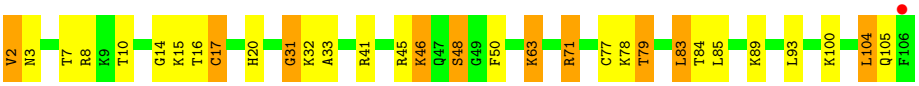
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



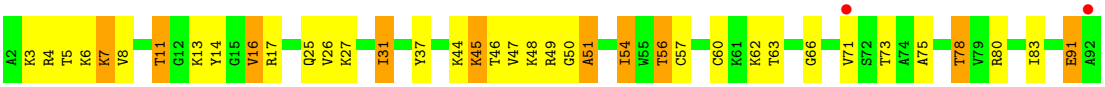
• Molecule 78: 60S ribosomal protein L42-A

Chain q2:



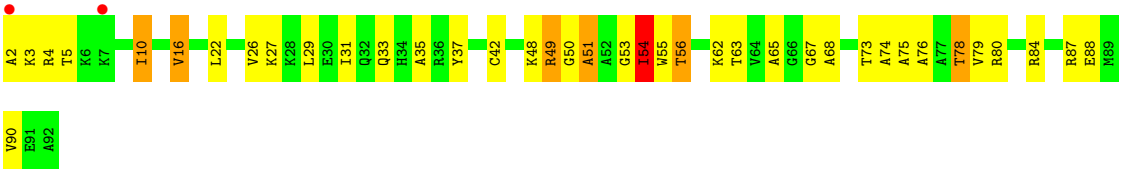
• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



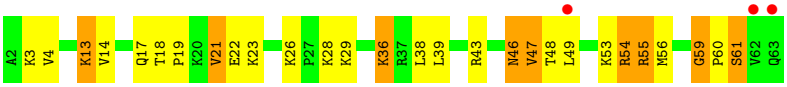
• Molecule 79: 60S ribosomal protein L43-A

Chain q3:



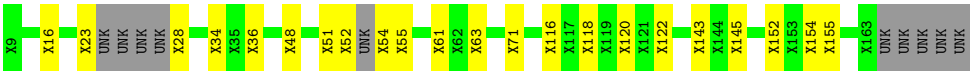
• Molecule 80: 40S ribosomal protein S30-A

Chain e0:



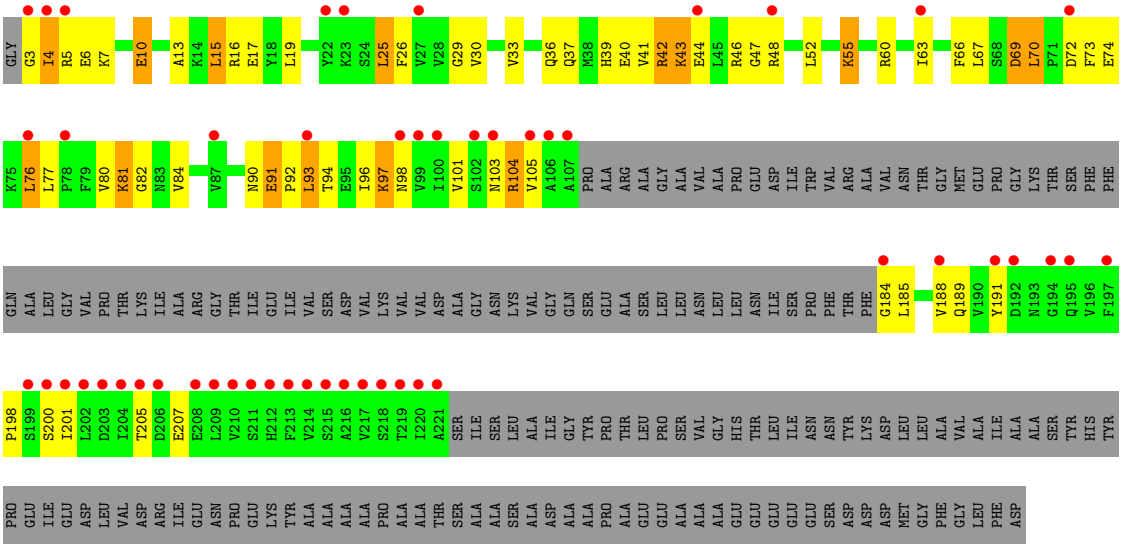
• Molecule 81: Unknown protein m2

Chain m2:



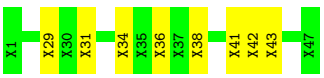
• Molecule 82: 60S acidic ribosomal protein P0

Chain p0:



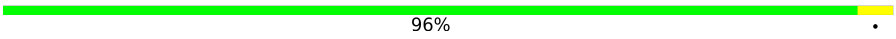
• Molecule 83: Unknown protein p1

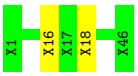
Chain p1:



• Molecule 84: Unknown protein p2

Chain p2:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	436.64Å 287.69Å 304.39Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	300.66 – 2.80 300.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (300.66-2.80) 99.5 (300.66-2.80)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.208 , 0.246 0.214 , 0.250	Depositor DCC
R_{free} test set	34000 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	411226	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OHX, MG, ZN, 3H3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.41	0/41698	0.62	7/64972 (0.0%)
1	6	0.48	0/42765	0.67	8/66634 (0.0%)
2	S0	0.59	0/1617	1.07	10/2215 (0.5%)
2	s0	0.69	0/1623	1.15	7/2222 (0.3%)
3	S1	0.50	0/1735	0.90	1/2335 (0.0%)
3	s1	0.65	0/1748	1.04	7/2352 (0.3%)
4	S2	0.66	0/1665	1.04	10/2263 (0.4%)
4	s2	0.80	0/1665	1.12	3/2263 (0.1%)
5	S3	0.62	0/1759	1.00	3/2368 (0.1%)
5	s3	0.60	0/1759	0.96	7/2368 (0.3%)
6	S4	0.64	0/2109	1.04	6/2839 (0.2%)
6	s4	0.71	0/2109	1.12	11/2839 (0.4%)
7	S5	0.56	0/1629	1.00	7/2202 (0.3%)
7	s5	0.59	0/1629	1.02	9/2202 (0.4%)
8	S6	0.60	0/1823	0.97	1/2439 (0.0%)
8	s6	0.70	0/1779	1.01	6/2379 (0.3%)
9	S7	0.57	0/1506	0.99	6/2028 (0.3%)
9	s7	0.69	0/1516	1.11	5/2043 (0.2%)
10	S8	0.72	0/1514	1.05	1/2021 (0.0%)
10	s8	0.79	1/1514 (0.1%)	1.05	0/2021
11	S9	0.63	0/1519	1.02	4/2035 (0.2%)
11	s9	0.71	0/1519	1.12	9/2035 (0.4%)
12	C0	0.58	0/790	1.01	6/1069 (0.6%)
12	c0	0.50	0/777	0.97	5/1049 (0.5%)
13	C1	0.73	0/1240	1.05	4/1675 (0.2%)
13	c1	0.83	0/1194	1.19	3/1610 (0.2%)
14	C2	0.51	0/898	0.93	3/1220 (0.2%)
14	c2	0.44	0/898	0.87	1/1220 (0.1%)
15	C3	0.65	0/1215	1.02	6/1638 (0.4%)
15	c3	0.77	0/1215	1.11	4/1638 (0.2%)
16	C4	0.54	0/901	0.99	3/1217 (0.2%)
16	c4	0.69	0/960	1.18	12/1290 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.64	0/998	1.00	4/1341 (0.3%)
17	c5	0.64	0/1060	1.04	2/1426 (0.1%)
18	C6	0.57	0/1125	1.05	4/1510 (0.3%)
18	c6	0.65	0/1131	1.06	5/1518 (0.3%)
19	C7	0.62	0/935	1.00	3/1254 (0.2%)
19	c7	0.65	0/914	1.14	5/1224 (0.4%)
20	C8	0.61	0/1211	1.02	4/1628 (0.2%)
20	c8	0.65	1/1211 (0.1%)	1.02	1/1628 (0.1%)
21	C9	0.62	0/1130	1.01	2/1517 (0.1%)
21	c9	0.62	0/1130	1.00	1/1517 (0.1%)
22	D0	0.61	0/865	0.98	1/1169 (0.1%)
22	d0	0.63	0/892	1.08	4/1205 (0.3%)
23	D1	0.59	0/693	1.00	3/935 (0.3%)
23	d1	0.70	0/693	1.06	0/935
24	D2	0.71	0/1038	1.10	3/1395 (0.2%)
24	d2	0.86	0/1038	1.09	7/1395 (0.5%)
25	D3	0.79	0/1139	1.21	11/1518 (0.7%)
25	d3	0.87	0/1139	1.20	9/1518 (0.6%)
26	D4	0.58	0/1087	0.95	2/1449 (0.1%)
26	d4	0.65	0/1087	1.02	1/1449 (0.1%)
27	D5	0.57	0/571	1.14	4/768 (0.5%)
27	d5	0.60	0/566	0.98	0/761
28	D6	0.63	0/782	1.04	5/1047 (0.5%)
28	d6	0.73	0/782	1.03	0/1047
29	D7	0.59	0/620	1.00	3/838 (0.4%)
29	d7	0.65	0/620	1.15	4/838 (0.5%)
30	D8	0.44	0/499	0.83	0/670
30	d8	0.60	0/499	1.08	2/670 (0.3%)
31	D9	0.68	0/452	1.01	3/600 (0.5%)
31	d9	0.68	0/452	1.04	1/600 (0.2%)
32	E0	0.60	0/483	0.97	0/643
33	E1	0.65	0/577	1.16	4/770 (0.5%)
33	e1	0.63	0/619	1.18	7/822 (0.9%)
34	SR	1.57	2/2494 (0.1%)	2.00	10/3393 (0.3%)
34	sR	0.52	0/2495	0.88	0/3395
35	SM	0.74	0/1113	1.09	3/1502 (0.2%)
35	sM	0.70	0/683	1.09	4/923 (0.4%)
36	1	0.63	0/75394	0.79	29/117545 (0.0%)
36	5	0.65	2/75414 (0.0%)	0.79	18/117575 (0.0%)
37	3	0.52	0/2883	0.67	0/4491
37	7	0.61	0/2883	0.76	0/4491
38	4	0.62	0/3746	0.74	0/5832
38	8	0.55	0/3746	0.70	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	L2	0.93	0/1948	1.21	8/2617 (0.3%)
39	l2	1.04	3/1946 (0.2%)	1.33	10/2614 (0.4%)
40	L3	0.95	3/3146 (0.1%)	1.20	13/4228 (0.3%)
40	l3	1.04	3/3146 (0.1%)	1.25	24/4228 (0.6%)
41	L4	1.05	2/2800 (0.1%)	1.38	22/3790 (0.6%)
41	l4	0.98	1/2800 (0.0%)	1.25	23/3790 (0.6%)
42	L5	0.70	0/2425	1.05	4/3271 (0.1%)
42	l5	0.88	0/2408	1.15	7/3248 (0.2%)
43	L6	0.95	1/1260 (0.1%)	1.15	4/1694 (0.2%)
43	l6	0.90	0/1269	1.17	5/1705 (0.3%)
44	L7	1.03	1/1821 (0.1%)	1.27	11/2451 (0.4%)
44	l7	1.03	0/1828	1.27	15/2461 (0.6%)
45	L8	0.71	0/1836	1.04	6/2481 (0.2%)
45	l8	0.71	0/1795	1.02	5/2429 (0.2%)
46	L9	0.81	0/1539	1.13	5/2073 (0.2%)
46	l9	0.98	0/1539	1.20	5/2073 (0.2%)
47	M0	0.92	0/1741	1.19	8/2335 (0.3%)
47	m0	0.97	0/1758	1.16	8/2358 (0.3%)
48	M1	0.68	0/1374	1.08	3/1842 (0.2%)
48	m1	0.86	1/1374 (0.1%)	1.21	7/1842 (0.4%)
49	M3	0.98	3/1568 (0.2%)	1.28	12/2106 (0.6%)
49	m3	0.97	1/1573 (0.1%)	1.23	11/2113 (0.5%)
50	M4	1.00	1/1068 (0.1%)	1.24	2/1438 (0.1%)
50	m4	1.01	1/1074 (0.1%)	1.22	4/1446 (0.3%)
51	M5	0.96	2/1757 (0.1%)	1.26	11/2354 (0.5%)
51	m5	0.88	0/1757	1.15	8/2354 (0.3%)
52	M6	1.04	1/1585 (0.1%)	1.22	7/2128 (0.3%)
52	m6	1.20	1/1585 (0.1%)	1.40	15/2128 (0.7%)
53	M7	0.99	0/1443	1.23	13/1944 (0.7%)
53	m7	1.11	1/1250 (0.1%)	1.23	3/1683 (0.2%)
54	M8	1.05	0/1465	1.37	8/1965 (0.4%)
54	m8	0.96	0/1465	1.32	11/1965 (0.6%)
55	M9	0.73	0/1538	0.99	2/2050 (0.1%)
55	m9	0.81	0/1538	1.03	2/2050 (0.1%)
56	N0	1.01	0/1481	1.18	8/1990 (0.4%)
56	n0	0.98	0/1481	1.23	7/1990 (0.4%)
57	N1	0.95	1/1300 (0.1%)	1.22	4/1743 (0.2%)
57	n1	0.99	0/1300	1.17	4/1743 (0.2%)
58	N2	0.52	0/812	0.93	1/1099 (0.1%)
58	n2	0.61	0/794	1.01	4/1076 (0.4%)
59	N3	0.95	0/1018	1.23	2/1369 (0.1%)
59	n3	1.08	0/1018	1.30	5/1369 (0.4%)
60	N4	0.74	0/712	1.30	2/958 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	n4	0.82	0/1052	1.04	3/1398 (0.2%)
61	N5	0.78	0/979	1.15	3/1321 (0.2%)
61	n5	0.82	0/974	1.24	9/1314 (0.7%)
62	N6	0.92	0/1004	1.12	3/1341 (0.2%)
62	n6	0.81	0/1004	1.12	4/1341 (0.3%)
63	N7	0.64	0/1118	1.07	2/1497 (0.1%)
63	n7	0.61	0/1118	1.03	2/1497 (0.1%)
64	N8	1.06	2/1204 (0.2%)	1.30	12/1612 (0.7%)
64	n8	1.03	2/1204 (0.2%)	1.31	14/1612 (0.9%)
65	N9	0.98	1/473 (0.2%)	1.06	2/629 (0.3%)
65	n9	1.12	2/473 (0.4%)	1.35	9/629 (1.4%)
66	O0	0.62	0/751	1.05	2/1008 (0.2%)
66	o0	0.63	0/775	1.01	2/1040 (0.2%)
67	O1	0.85	0/890	1.10	0/1196
67	o1	1.02	1/897 (0.1%)	1.26	8/1205 (0.7%)
68	O2	1.06	0/1041	1.19	2/1394 (0.1%)
68	o2	1.07	2/1041 (0.2%)	1.27	9/1394 (0.6%)
69	O3	1.05	0/868	1.19	3/1168 (0.3%)
69	o3	1.16	4/868 (0.5%)	1.26	3/1168 (0.3%)
70	O4	0.76	0/890	1.12	4/1189 (0.3%)
70	o4	0.81	0/890	1.06	1/1189 (0.1%)
71	O5	0.84	0/978	1.12	4/1301 (0.3%)
71	o5	0.75	1/974 (0.1%)	1.01	4/1297 (0.3%)
72	O6	0.89	0/778	1.20	4/1034 (0.4%)
72	o6	0.73	0/777	1.06	3/1033 (0.3%)
73	O7	1.05	0/696	1.28	6/923 (0.7%)
73	o7	0.90	0/696	1.11	3/923 (0.3%)
74	O8	0.60	0/618	0.97	0/826
74	o8	0.63	0/614	1.07	1/822 (0.1%)
75	O9	0.99	0/443	1.16	0/588
75	o9	0.97	0/443	1.22	0/588
76	Q0	0.88	0/423	1.16	3/562 (0.5%)
76	q0	1.08	0/423	1.18	0/562
77	Q1	0.82	0/234	1.05	0/300
77	q1	1.03	0/234	1.24	1/300 (0.3%)
78	Q2	1.00	1/860 (0.1%)	1.21	1/1136 (0.1%)
78	q2	0.94	0/860	1.09	0/1136
79	Q3	0.87	0/701	1.21	3/934 (0.3%)
79	q3	0.92	1/701 (0.1%)	1.21	3/934 (0.3%)
80	e0	0.69	0/499	1.22	2/665 (0.3%)
82	p0	0.54	0/1092	0.96	0/1474
All	All	0.70	50/430070 (0.0%)	0.92	818/631356 (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
2	S0	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	2
17	c5	0	1
19	C7	0	1
22	d0	0	1
25	D3	0	1
25	d3	0	1
26	d4	0	2
27	D5	0	1
28	D6	0	3
31	d9	0	1
33	E1	0	1
34	SR	0	2
39	L2	0	1
39	l2	0	2
40	l3	0	2
41	L4	0	2
41	l4	0	1
42	L5	0	1
42	l5	0	2
43	l6	0	1
44	L7	0	1
44	l7	0	2
51	M5	0	1
52	M6	0	2
52	m6	0	1
53	M7	0	1
53	m7	0	1
57	N1	0	1
59	n3	0	1
62	n6	0	1
63	N7	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
67	O1	0	1
67	o1	0	1
72	O6	0	1
All	All	0	57

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SR	160	GLU	C-N	-63.03	0.45	1.33
34	SR	161	LYS	C-N	-37.75	0.66	1.33
39	l2	213	GLY	C-O	11.31	1.39	1.23
53	m7	66	SER	C-O	9.96	1.36	1.24
78	Q2	17	CYS	CB-SG	8.56	2.09	1.81

The worst 5 of 818 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	SR	161	LYS	O-C-N	-58.54	44.74	122.59
34	SR	160	GLU	CA-C-N	-56.30	14.02	121.54
34	SR	160	GLU	C-N-CA	-56.30	14.02	121.54
34	SR	160	GLU	O-C-N	-24.85	89.54	122.59
60	N4	80	ARG	CA-C-N	17.64	141.89	119.84

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
2	S0	188	LEU	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	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	752	0
1	6	38238	0	19241	718	0
2	S0	1577	0	1567	83	0
2	s0	1583	0	1578	74	0
3	S1	1709	0	1784	89	0
3	s1	1722	0	1793	67	0
4	S2	1635	0	1723	64	0
4	s2	1635	0	1723	60	0
5	S3	1734	0	1817	54	0
5	s3	1734	0	1817	50	0
6	S4	2068	0	2154	72	0
6	s4	2068	0	2154	92	0
7	S5	1609	0	1675	65	0
7	s5	1609	0	1675	78	0
8	S6	1799	0	1879	62	0
8	s6	1755	0	1846	55	0
9	S7	1481	0	1572	62	0
9	s7	1491	0	1578	47	0
10	S8	1489	0	1525	56	0
10	s8	1489	0	1525	50	0
11	S9	1494	0	1573	63	0
11	s9	1494	0	1573	62	0
12	C0	773	0	729	37	0
12	c0	762	0	699	27	0
13	C1	1214	0	1259	29	0
13	c1	1168	0	1231	35	0
14	C2	890	0	887	37	0
14	c2	890	0	887	32	0
15	C3	1192	0	1255	46	0
15	c3	1192	0	1255	37	0
16	C4	891	0	883	53	0
16	c4	949	0	985	49	0
17	C5	977	0	1002	34	0
17	c5	1039	0	1050	46	0
18	C6	1105	0	1166	51	0
18	c6	1111	0	1171	45	0
19	C7	926	0	930	40	0
19	c7	906	0	909	41	0
20	C8	1192	0	1222	41	0
20	c8	1192	0	1222	57	0
21	C9	1112	0	1124	56	0
21	c9	1112	0	1124	35	0
22	D0	855	0	917	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	d0	882	0	939	36	0
23	D1	684	0	672	33	0
23	d1	684	0	672	26	0
24	D2	1021	0	1060	39	0
24	d2	1021	0	1060	33	0
25	D3	1121	0	1196	43	0
25	d3	1121	0	1196	37	0
26	D4	1073	0	1132	45	0
26	d4	1073	0	1132	28	0
27	D5	563	0	603	29	0
27	d5	558	0	598	25	0
28	D6	769	0	814	50	0
28	d6	769	0	814	36	0
29	D7	610	0	631	24	0
29	d7	610	0	631	28	0
30	D8	497	0	535	17	0
30	d8	497	0	535	20	0
31	D9	442	0	428	19	0
31	d9	442	0	428	18	0
32	E0	475	0	525	8	0
33	E1	566	0	602	39	0
33	e1	608	0	657	32	0
34	SR	2441	0	2395	74	0
34	sR	2442	0	2392	70	0
35	SM	1104	0	996	38	0
35	sM	680	0	607	33	0
36	1	67355	0	33840	1048	0
36	5	67376	0	33857	1050	0
37	3	2579	0	1304	39	0
37	7	2579	0	1304	42	0
38	4	3353	0	1695	51	0
38	8	3353	0	1695	59	0
39	L2	1914	0	1981	55	0
39	l2	1912	0	1976	88	0
40	L3	3075	0	3142	148	0
40	l3	3075	0	3142	114	0
41	L4	2748	0	2859	100	0
41	l4	2748	0	2859	105	0
42	L5	2375	0	2325	97	0
42	l5	2359	0	2311	89	0
43	L6	1239	0	1326	29	0
43	l6	1248	0	1339	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	L7	1784	0	1862	45	0
44	l7	1791	0	1869	41	0
45	L8	1804	0	1877	66	0
45	l8	1763	0	1819	60	0
46	L9	1518	0	1587	71	0
46	l9	1518	0	1587	49	0
47	M0	1705	0	1736	63	0
47	m0	1722	0	1755	59	0
48	M1	1353	0	1383	51	0
48	m1	1353	0	1383	48	0
49	M3	1543	0	1608	52	0
49	m3	1548	0	1613	48	0
50	M4	1053	0	1149	32	0
50	m4	1059	0	1154	30	0
51	M5	1720	0	1779	66	0
51	m5	1720	0	1779	66	0
52	M6	1555	0	1659	42	0
52	m6	1555	0	1659	50	0
53	M7	1420	0	1437	49	0
53	m7	1227	0	1236	43	0
54	M8	1441	0	1543	48	0
54	m8	1441	0	1543	48	0
55	M9	1521	0	1617	48	0
55	m9	1521	0	1617	30	0
56	N0	1445	0	1487	43	0
56	n0	1445	0	1487	41	0
57	N1	1276	0	1323	44	0
57	n1	1276	0	1323	46	0
58	N2	796	0	812	14	0
58	n2	778	0	791	17	0
59	N3	1003	0	1048	49	0
59	n3	1003	0	1048	29	0
60	N4	699	0	640	17	0
60	n4	1038	0	1071	18	0
61	N5	964	0	1025	41	0
61	n5	959	0	1023	31	0
62	N6	993	0	1081	24	0
62	n6	993	0	1081	37	0
63	N7	1092	0	1155	47	0
63	n7	1092	0	1155	39	0
64	N8	1173	0	1215	54	0
64	n8	1173	0	1215	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	N9	462	0	491	14	0
65	n9	462	0	491	21	0
66	O0	743	0	797	27	0
66	o0	767	0	816	28	0
67	O1	876	0	912	25	0
67	o1	883	0	918	21	0
68	O2	1020	0	1090	17	0
68	o2	1020	0	1090	38	0
69	O3	850	0	880	28	0
69	o3	850	0	880	28	0
70	O4	880	0	945	25	0
70	o4	880	0	945	35	0
71	O5	969	0	1078	31	0
71	o5	965	0	1067	37	0
72	O6	771	0	849	32	0
72	o6	770	0	846	29	0
73	O7	681	0	683	33	0
73	o7	681	0	683	31	0
74	O8	612	0	682	23	0
74	o8	608	0	671	27	0
75	O9	436	0	475	18	0
75	o9	436	0	475	19	0
76	Q0	417	0	455	14	0
76	q0	417	0	455	13	0
77	Q1	233	0	284	15	0
77	q1	233	0	284	13	0
78	Q2	847	0	916	35	0
78	q2	847	0	914	20	0
79	Q3	694	0	734	22	0
79	q3	694	0	734	26	0
80	e0	491	0	542	19	0
81	m2	750	0	175	13	0
82	p0	1077	0	1041	39	0
83	p1	235	0	51	4	0
84	p2	230	0	50	1	0
85	1	475	0	0	0	0
85	2	126	0	0	0	0
85	3	14	0	0	0	0
85	4	21	0	0	0	0
85	5	504	0	0	0	0
85	6	147	0	0	0	0
85	7	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	8	13	0	0	0	0
85	C3	1	0	0	0	0
85	L2	1	0	0	0	0
85	L3	2	0	0	0	0
85	L4	3	0	0	0	0
85	L5	1	0	0	0	0
85	L6	1	0	0	0	0
85	L7	2	0	0	0	0
85	L8	1	0	0	0	0
85	M0	2	0	0	0	0
85	M1	1	0	0	0	0
85	M3	4	0	0	0	0
85	M5	2	0	0	0	0
85	M6	1	0	0	0	0
85	M7	6	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	3	0	0	0	0
85	N5	1	0	0	0	0
85	N8	2	0	0	0	0
85	O3	1	0	0	0	0
85	O4	1	0	0	0	0
85	O7	1	0	0	0	0
85	Q2	1	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	2	0	0	0	0
85	d2	1	0	0	0	0
85	d3	1	0	0	0	0
85	d6	1	0	0	0	0
85	l2	2	0	0	0	0
85	l3	1	0	0	0	0
85	l4	1	0	0	0	0
85	l5	3	0	0	0	0
85	l7	1	0	0	0	0
85	m1	2	0	0	0	0
85	m4	1	0	0	0	0
85	m5	1	0	0	0	0
85	m6	1	0	0	0	0
85	m7	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	n0	2	0	0	0	0
85	n3	2	0	0	0	0
85	n6	2	0	0	0	0
85	n8	4	0	0	0	0
85	n9	2	0	0	0	0
85	o1	1	0	0	0	0
85	o3	2	0	0	0	0
85	o4	2	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	1	0	0	0	0
85	s1	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2436	0	0	247	0
86	2	1106	0	0	132	0
86	3	84	0	0	5	0
86	4	105	0	0	5	0
86	5	2471	0	0	236	0
86	6	1106	0	0	101	0
86	7	84	0	0	12	0
86	8	112	0	0	21	0
86	C1	7	0	0	7	0
86	C3	7	0	0	1	0
86	C5	7	0	0	2	0
86	C8	7	0	0	1	0
86	D9	7	0	0	0	0
86	L3	14	0	0	1	0
86	L4	7	0	0	2	0
86	L6	7	0	0	0	0
86	M0	7	0	0	0	0
86	M5	14	0	0	2	0
86	M6	7	0	0	1	0
86	M7	14	0	0	1	0
86	M9	7	0	0	1	0
86	N9	7	0	0	1	0
86	O2	7	0	0	0	0
86	O3	7	0	0	0	0
86	O7	14	0	0	7	0
86	O9	7	0	0	4	0
86	Q2	7	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	S8	7	0	0	1	0
86	SR	7	0	0	0	0
86	c1	7	0	0	7	0
86	c3	7	0	0	3	0
86	c5	7	0	0	2	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	1	0
86	l3	21	0	0	0	0
86	l4	14	0	0	3	0
86	l5	21	0	0	1	0
86	l9	7	0	0	0	0
86	m0	14	0	0	2	0
86	m1	7	0	0	1	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	1	0
86	m8	7	0	0	0	0
86	n3	7	0	0	0	0
86	n9	7	0	0	0	0
86	o2	7	0	0	0	0
86	o3	7	0	0	0	0
86	o4	7	0	0	4	0
86	o7	7	0	0	1	0
86	q2	7	0	0	3	0
86	s1	14	0	0	1	0
86	s4	7	0	0	1	0
86	s8	7	0	0	1	0
86	s9	7	0	0	2	0
86	sR	7	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	3	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	0	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
88	1	33	0	35	1	0
88	5	33	0	35	1	0
All	All	411226	0	297341	9121	0

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 13.

The worst 5 of 9121 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)
52:m6:66:LYS:NZ	52:m6:66:LYS:CE	1.70	1.54
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	2.09	1.40
78:Q2:17:CYS:CB	87:Q2:501:ZN:ZN	1.31	1.09
40:l3:296:THR:HG22	40:l3:298:PHE:H	1.18	1.07
47:m0:76:MET:HE1	47:m0:148:VAL:HA	1.34	1.05

There are no symmetry-related clashes.

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%)	154 (76%)	27 (13%)	23 (11%)	0 1
2	s0	204/251 (81%)	161 (79%)	27 (13%)	16 (8%)	1 2
3	S1	212/254 (84%)	152 (72%)	31 (15%)	29 (14%)	0 0
3	s1	214/254 (84%)	179 (84%)	23 (11%)	12 (6%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	S2	215/253 (85%)	181 (84%)	25 (12%)	9 (4%)	2 7
4	s2	215/253 (85%)	187 (87%)	16 (7%)	12 (6%)	1 4
5	S3	221/239 (92%)	198 (90%)	14 (6%)	9 (4%)	2 8
5	s3	221/239 (92%)	193 (87%)	15 (7%)	13 (6%)	1 3
6	S4	258/260 (99%)	219 (85%)	27 (10%)	12 (5%)	2 6
6	s4	258/260 (99%)	223 (86%)	23 (9%)	12 (5%)	2 6
7	S5	204/224 (91%)	162 (79%)	21 (10%)	21 (10%)	0 1
7	s5	204/224 (91%)	164 (80%)	23 (11%)	17 (8%)	0 1
8	S6	224/236 (95%)	195 (87%)	21 (9%)	8 (4%)	2 10
8	s6	216/236 (92%)	194 (90%)	14 (6%)	8 (4%)	2 9
9	S7	182/189 (96%)	143 (79%)	21 (12%)	18 (10%)	0 1
9	s7	184/189 (97%)	148 (80%)	22 (12%)	14 (8%)	1 2
10	S8	184/200 (92%)	159 (86%)	12 (6%)	13 (7%)	1 2
10	s8	184/200 (92%)	164 (89%)	11 (6%)	9 (5%)	1 6
11	S9	183/196 (93%)	159 (87%)	15 (8%)	9 (5%)	1 6
11	s9	183/196 (93%)	148 (81%)	23 (13%)	12 (7%)	1 3
12	C0	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	1 3
12	c0	92/105 (88%)	63 (68%)	16 (17%)	13 (14%)	0 0
13	C1	153/155 (99%)	125 (82%)	18 (12%)	10 (6%)	1 3
13	c1	144/155 (93%)	117 (81%)	18 (12%)	9 (6%)	1 3
14	C2	122/142 (86%)	70 (57%)	26 (21%)	26 (21%)	0 0
14	c2	122/142 (86%)	71 (58%)	29 (24%)	22 (18%)	0 0
15	C3	148/150 (99%)	132 (89%)	13 (9%)	3 (2%)	6 21
15	c3	148/150 (99%)	123 (83%)	16 (11%)	9 (6%)	1 3
16	C4	125/136 (92%)	97 (78%)	16 (13%)	12 (10%)	0 1
16	c4	126/136 (93%)	101 (80%)	15 (12%)	10 (8%)	1 1
17	C5	122/141 (86%)	95 (78%)	16 (13%)	11 (9%)	0 1
17	c5	133/141 (94%)	97 (73%)	16 (12%)	20 (15%)	0 0
18	C6	139/142 (98%)	121 (87%)	13 (9%)	5 (4%)	2 10
18	c6	140/142 (99%)	121 (86%)	11 (8%)	8 (6%)	1 4
19	C7	116/136 (85%)	87 (75%)	22 (19%)	7 (6%)	1 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	c7	113/136 (83%)	96 (85%)	11 (10%)	6 (5%)	1	5
20	C8	143/145 (99%)	121 (85%)	11 (8%)	11 (8%)	1	2
20	c8	143/145 (99%)	115 (80%)	21 (15%)	7 (5%)	1	6
21	C9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	3	10
21	c9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	3	10
22	D0	105/120 (88%)	88 (84%)	15 (14%)	2 (2%)	6	22
22	d0	108/120 (90%)	85 (79%)	15 (14%)	8 (7%)	1	2
23	D1	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	1	2
23	d1	85/87 (98%)	75 (88%)	5 (6%)	5 (6%)	1	3
24	D2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	16	44
24	d2	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	16	44
25	D3	142/144 (99%)	117 (82%)	14 (10%)	11 (8%)	1	2
25	d3	142/144 (99%)	131 (92%)	10 (7%)	1 (1%)	18	47
26	D4	132/134 (98%)	110 (83%)	14 (11%)	8 (6%)	1	3
26	d4	132/134 (98%)	106 (80%)	15 (11%)	11 (8%)	0	1
27	D5	68/107 (64%)	51 (75%)	9 (13%)	8 (12%)	0	1
27	d5	67/107 (63%)	48 (72%)	13 (19%)	6 (9%)	0	1
28	D6	95/97 (98%)	69 (73%)	12 (13%)	14 (15%)	0	0
28	d6	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	0	1
29	D7	79/81 (98%)	62 (78%)	12 (15%)	5 (6%)	1	3
29	d7	79/81 (98%)	60 (76%)	10 (13%)	9 (11%)	0	1
30	D8	61/66 (92%)	51 (84%)	7 (12%)	3 (5%)	1	6
30	d8	61/66 (92%)	46 (75%)	10 (16%)	5 (8%)	0	1
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	1	3
31	d9	51/55 (93%)	42 (82%)	5 (10%)	4 (8%)	1	2
32	E0	58/60 (97%)	45 (78%)	12 (21%)	1 (2%)	7	25
33	E1	69/76 (91%)	36 (52%)	14 (20%)	19 (28%)	0	0
33	e1	74/76 (97%)	38 (51%)	16 (22%)	20 (27%)	0	0
34	SR	316/318 (99%)	274 (87%)	29 (9%)	13 (4%)	2	8
34	sR	316/318 (99%)	268 (85%)	40 (13%)	8 (2%)	4	16
35	SM	155/273 (57%)	109 (70%)	26 (17%)	20 (13%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	sM	98/273 (36%)	61 (62%)	24 (24%)	13 (13%)	0 0
39	L2	250/253 (99%)	226 (90%)	20 (8%)	4 (2%)	7 27
39	l2	250/253 (99%)	214 (86%)	27 (11%)	9 (4%)	2 10
40	L3	384/386 (100%)	340 (88%)	31 (8%)	13 (3%)	3 11
40	l3	384/386 (100%)	350 (91%)	25 (6%)	9 (2%)	5 18
41	L4	359/361 (99%)	315 (88%)	23 (6%)	21 (6%)	1 4
41	l4	359/361 (99%)	308 (86%)	38 (11%)	13 (4%)	2 10
42	L5	294/296 (99%)	253 (86%)	23 (8%)	18 (6%)	1 3
42	l5	292/296 (99%)	262 (90%)	21 (7%)	9 (3%)	3 12
43	L6	152/175 (87%)	141 (93%)	8 (5%)	3 (2%)	6 21
43	l6	153/175 (87%)	132 (86%)	17 (11%)	4 (3%)	4 15
44	L7	220/243 (90%)	205 (93%)	6 (3%)	9 (4%)	2 8
44	l7	221/243 (91%)	203 (92%)	15 (7%)	3 (1%)	9 30
45	L8	231/255 (91%)	193 (84%)	30 (13%)	8 (4%)	3 10
45	l8	229/255 (90%)	184 (80%)	25 (11%)	20 (9%)	0 1
46	L9	189/191 (99%)	170 (90%)	14 (7%)	5 (3%)	4 15
46	l9	189/191 (99%)	173 (92%)	10 (5%)	6 (3%)	3 11
47	M0	207/220 (94%)	185 (89%)	17 (8%)	5 (2%)	4 17
47	m0	209/220 (95%)	181 (87%)	20 (10%)	8 (4%)	2 9
48	M1	167/173 (96%)	133 (80%)	20 (12%)	14 (8%)	0 1
48	m1	167/173 (96%)	146 (87%)	11 (7%)	10 (6%)	1 3
49	M3	191/198 (96%)	164 (86%)	19 (10%)	8 (4%)	2 7
49	m3	192/198 (97%)	164 (85%)	17 (9%)	11 (6%)	1 4
50	M4	134/137 (98%)	118 (88%)	11 (8%)	5 (4%)	2 9
50	m4	135/137 (98%)	127 (94%)	6 (4%)	2 (2%)	8 28
51	M5	201/203 (99%)	188 (94%)	7 (4%)	6 (3%)	3 12
51	m5	201/203 (99%)	180 (90%)	14 (7%)	7 (4%)	3 10
52	M6	195/198 (98%)	185 (95%)	6 (3%)	4 (2%)	5 20
52	m6	195/198 (98%)	185 (95%)	8 (4%)	2 (1%)	12 38
53	M7	181/183 (99%)	159 (88%)	16 (9%)	6 (3%)	3 11
53	m7	153/183 (84%)	140 (92%)	10 (6%)	3 (2%)	6 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
54	M8	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	5 19
54	m8	183/185 (99%)	165 (90%)	11 (6%)	7 (4%)	2 9
55	M9	186/188 (99%)	173 (93%)	12 (6%)	1 (0%)	24 55
55	m9	186/188 (99%)	175 (94%)	8 (4%)	3 (2%)	7 27
56	N0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	10 34
56	n0	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	6 23
57	N1	157/159 (99%)	138 (88%)	14 (9%)	5 (3%)	3 11
57	n1	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	4 16
58	N2	98/120 (82%)	79 (81%)	15 (15%)	4 (4%)	2 8
58	n2	96/120 (80%)	84 (88%)	9 (9%)	3 (3%)	3 12
59	N3	134/136 (98%)	126 (94%)	7 (5%)	1 (1%)	18 47
59	n3	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	18 47
60	N4	96/155 (62%)	77 (80%)	14 (15%)	5 (5%)	1 5
60	n4	133/155 (86%)	113 (85%)	12 (9%)	8 (6%)	1 3
61	N5	119/141 (84%)	110 (92%)	8 (7%)	1 (1%)	16 44
61	n5	118/141 (84%)	100 (85%)	13 (11%)	5 (4%)	2 7
62	N6	124/126 (98%)	114 (92%)	6 (5%)	4 (3%)	3 11
62	n6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	2 8
63	N7	133/135 (98%)	111 (84%)	12 (9%)	10 (8%)	1 2
63	n7	133/135 (98%)	111 (84%)	14 (10%)	8 (6%)	1 3
64	N8	146/148 (99%)	122 (84%)	16 (11%)	8 (6%)	1 4
64	n8	146/148 (99%)	126 (86%)	16 (11%)	4 (3%)	4 15
65	N9	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	2 10
65	n9	56/58 (97%)	43 (77%)	9 (16%)	4 (7%)	1 2
66	O0	95/104 (91%)	87 (92%)	6 (6%)	2 (2%)	5 20
66	o0	98/104 (94%)	89 (91%)	7 (7%)	2 (2%)	6 21
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2 6
67	o1	107/112 (96%)	98 (92%)	5 (5%)	4 (4%)	2 9
68	O2	125/129 (97%)	116 (93%)	8 (6%)	1 (1%)	16 44
68	o2	125/129 (97%)	111 (89%)	11 (9%)	3 (2%)	4 17
69	O3	104/106 (98%)	101 (97%)	2 (2%)	1 (1%)	12 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
69	o3	104/106 (98%)	92 (88%)	7 (7%)	5 (5%)	2 6
70	O4	110/119 (92%)	103 (94%)	4 (4%)	3 (3%)	4 15
70	o4	110/119 (92%)	100 (91%)	8 (7%)	2 (2%)	6 23
71	O5	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	3 11
71	o5	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	7 25
72	O6	97/99 (98%)	78 (80%)	11 (11%)	8 (8%)	0 1
72	o6	97/99 (98%)	81 (84%)	9 (9%)	7 (7%)	1 2
73	O7	85/87 (98%)	76 (89%)	6 (7%)	3 (4%)	3 10
73	o7	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	3 10
74	O8	75/77 (97%)	62 (83%)	10 (13%)	3 (4%)	2 8
74	o8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	2 8
75	O9	48/50 (96%)	44 (92%)	4 (8%)	0	100 100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	5 20
76	Q0	50/52 (96%)	48 (96%)	0	2 (4%)	2 8
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	6 21
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100 100
77	q1	23/25 (92%)	23 (100%)	0	0	100 100
78	Q2	103/105 (98%)	90 (87%)	10 (10%)	3 (3%)	3 13
78	q2	103/105 (98%)	92 (89%)	8 (8%)	3 (3%)	3 13
79	Q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	5 19
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	11 36
80	e0	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1 3
82	p0	139/311 (45%)	117 (84%)	19 (14%)	3 (2%)	5 19
All	All	22333/24141 (92%)	19119 (86%)	2092 (9%)	1122 (5%)	1 5

5 of 1122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	39	ASN
2	S0	66	ALA
2	S0	103	THR
2	S0	158	VAL
2	S0	163	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	131 (80%)	33 (20%)	1	4
2	s0	165/209 (79%)	129 (78%)	36 (22%)	1	3
3	S1	191/223 (86%)	161 (84%)	30 (16%)	2	9
3	s1	192/223 (86%)	155 (81%)	37 (19%)	1	5
4	S2	176/204 (86%)	130 (74%)	46 (26%)	0	2
4	s2	176/204 (86%)	136 (77%)	40 (23%)	1	3
5	S3	182/194 (94%)	145 (80%)	37 (20%)	1	4
5	s3	182/194 (94%)	145 (80%)	37 (20%)	1	4
6	S4	221/221 (100%)	175 (79%)	46 (21%)	1	4
6	s4	221/221 (100%)	181 (82%)	40 (18%)	2	6
7	S5	173/190 (91%)	144 (83%)	29 (17%)	2	8
7	s5	173/190 (91%)	134 (78%)	39 (22%)	1	3
8	S6	188/201 (94%)	149 (79%)	39 (21%)	1	4
8	s6	187/201 (93%)	150 (80%)	37 (20%)	1	5
9	S7	165/169 (98%)	132 (80%)	33 (20%)	1	4
9	s7	165/169 (98%)	127 (77%)	38 (23%)	1	3
10	S8	150/161 (93%)	127 (85%)	23 (15%)	3	10
10	s8	150/161 (93%)	127 (85%)	23 (15%)	3	10
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	3
11	s9	158/165 (96%)	127 (80%)	31 (20%)	1	5
12	C0	77/98 (79%)	59 (77%)	18 (23%)	1	3
12	c0	73/98 (74%)	59 (81%)	14 (19%)	1	5
13	C1	129/136 (95%)	102 (79%)	27 (21%)	1	4
13	c1	129/136 (95%)	105 (81%)	24 (19%)	1	5
14	C2	88/118 (75%)	66 (75%)	22 (25%)	0	2
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1 4
15	c3	127/127 (100%)	102 (80%)	25 (20%)	1 5
16	C4	81/104 (78%)	61 (75%)	20 (25%)	1 2
16	c4	97/104 (93%)	77 (79%)	20 (21%)	1 4
17	C5	101/117 (86%)	84 (83%)	17 (17%)	2 8
17	c5	103/117 (88%)	82 (80%)	21 (20%)	1 4
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1 5
18	c6	118/118 (100%)	96 (81%)	22 (19%)	1 5
19	C7	94/124 (76%)	72 (77%)	22 (23%)	1 3
19	c7	92/124 (74%)	74 (80%)	18 (20%)	1 5
20	C8	128/128 (100%)	99 (77%)	29 (23%)	1 3
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1 3
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1 4
21	c9	115/115 (100%)	91 (79%)	24 (21%)	1 4
22	D0	100/113 (88%)	68 (68%)	32 (32%)	0 1
22	d0	103/113 (91%)	77 (75%)	26 (25%)	0 2
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1 4
23	d1	74/74 (100%)	53 (72%)	21 (28%)	0 1
24	D2	110/110 (100%)	89 (81%)	21 (19%)	1 5
24	d2	110/110 (100%)	95 (86%)	15 (14%)	3 13
25	D3	119/119 (100%)	94 (79%)	25 (21%)	1 4
25	d3	119/119 (100%)	98 (82%)	21 (18%)	2 7
26	D4	112/112 (100%)	91 (81%)	21 (19%)	1 5
26	d4	112/112 (100%)	91 (81%)	21 (19%)	1 5
27	D5	61/88 (69%)	43 (70%)	18 (30%)	0 1
27	d5	61/88 (69%)	53 (87%)	8 (13%)	4 14
28	D6	83/83 (100%)	60 (72%)	23 (28%)	0 1
28	d6	83/83 (100%)	72 (87%)	11 (13%)	4 14
29	D7	70/70 (100%)	57 (81%)	13 (19%)	1 5
29	d7	70/70 (100%)	59 (84%)	11 (16%)	2 9
30	D8	56/59 (95%)	41 (73%)	15 (27%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	d8	56/59 (95%)	46 (82%)	10 (18%)	2 6
31	D9	47/48 (98%)	40 (85%)	7 (15%)	3 10
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1 4
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1 5
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1 2
33	e1	66/66 (100%)	47 (71%)	19 (29%)	0 1
34	SR	260/261 (100%)	234 (90%)	26 (10%)	7 24
34	sR	260/261 (100%)	234 (90%)	26 (10%)	7 24
35	SM	97/228 (42%)	77 (79%)	20 (21%)	1 4
35	sM	54/228 (24%)	46 (85%)	8 (15%)	3 10
39	L2	193/195 (99%)	153 (79%)	40 (21%)	1 4
39	l2	192/195 (98%)	146 (76%)	46 (24%)	1 2
40	L3	321/322 (100%)	249 (78%)	72 (22%)	1 3
40	l3	320/322 (99%)	246 (77%)	74 (23%)	1 3
41	L4	288/288 (100%)	229 (80%)	59 (20%)	1 4
41	l4	288/288 (100%)	228 (79%)	60 (21%)	1 4
42	L5	244/244 (100%)	194 (80%)	50 (20%)	1 4
42	l5	243/244 (100%)	183 (75%)	60 (25%)	1 2
43	L6	134/152 (88%)	112 (84%)	22 (16%)	2 8
43	l6	135/152 (89%)	108 (80%)	27 (20%)	1 4
44	L7	186/204 (91%)	159 (86%)	27 (14%)	3 11
44	l7	187/204 (92%)	160 (86%)	27 (14%)	3 11
45	L8	187/207 (90%)	154 (82%)	33 (18%)	2 7
45	l8	177/207 (86%)	143 (81%)	34 (19%)	1 5
46	L9	171/171 (100%)	139 (81%)	32 (19%)	1 5
46	l9	171/171 (100%)	135 (79%)	36 (21%)	1 4
47	M0	177/186 (95%)	142 (80%)	35 (20%)	1 5
47	m0	179/186 (96%)	136 (76%)	43 (24%)	1 2
48	M1	147/150 (98%)	118 (80%)	29 (20%)	1 5
48	m1	147/150 (98%)	117 (80%)	30 (20%)	1 4
49	M3	154/158 (98%)	126 (82%)	28 (18%)	2 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	m3	154/158 (98%)	129 (84%)	25 (16%)	2 8
50	M4	107/108 (99%)	85 (79%)	22 (21%)	1 4
50	m4	108/108 (100%)	85 (79%)	23 (21%)	1 4
51	M5	175/175 (100%)	144 (82%)	31 (18%)	2 6
51	m5	175/175 (100%)	146 (83%)	29 (17%)	2 8
52	M6	160/161 (99%)	130 (81%)	30 (19%)	1 5
52	m6	160/161 (99%)	125 (78%)	35 (22%)	1 3
53	M7	140/145 (97%)	105 (75%)	35 (25%)	0 2
53	m7	125/145 (86%)	104 (83%)	21 (17%)	2 8
54	M8	150/150 (100%)	118 (79%)	32 (21%)	1 4
54	m8	150/150 (100%)	119 (79%)	31 (21%)	1 4
55	M9	153/153 (100%)	129 (84%)	24 (16%)	2 9
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1 3
56	N0	156/156 (100%)	124 (80%)	32 (20%)	1 4
56	n0	156/156 (100%)	124 (80%)	32 (20%)	1 4
57	N1	136/136 (100%)	105 (77%)	31 (23%)	1 3
57	n1	136/136 (100%)	110 (81%)	26 (19%)	1 5
58	N2	87/106 (82%)	74 (85%)	13 (15%)	3 10
58	n2	85/106 (80%)	70 (82%)	15 (18%)	2 7
59	N3	104/104 (100%)	87 (84%)	17 (16%)	2 8
59	n3	104/104 (100%)	95 (91%)	9 (9%)	9 30
60	N4	57/129 (44%)	51 (90%)	6 (10%)	6 22
60	n4	100/129 (78%)	85 (85%)	15 (15%)	3 10
61	N5	104/117 (89%)	78 (75%)	26 (25%)	0 2
61	n5	104/117 (89%)	77 (74%)	27 (26%)	0 2
62	N6	109/109 (100%)	84 (77%)	25 (23%)	1 3
62	n6	109/109 (100%)	83 (76%)	26 (24%)	1 3
63	N7	115/115 (100%)	89 (77%)	26 (23%)	1 3
63	n7	115/115 (100%)	88 (76%)	27 (24%)	1 3
64	N8	118/118 (100%)	95 (80%)	23 (20%)	1 5
64	n8	118/118 (100%)	93 (79%)	25 (21%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1 5
65	n9	46/46 (100%)	34 (74%)	12 (26%)	0 2
66	O0	81/87 (93%)	65 (80%)	16 (20%)	1 5
66	o0	84/87 (97%)	68 (81%)	16 (19%)	1 5
67	O1	92/96 (96%)	70 (76%)	22 (24%)	1 3
67	o1	94/96 (98%)	71 (76%)	23 (24%)	1 2
68	O2	109/110 (99%)	91 (84%)	18 (16%)	2 8
68	o2	109/110 (99%)	90 (83%)	19 (17%)	2 7
69	O3	90/90 (100%)	76 (84%)	14 (16%)	2 9
69	o3	90/90 (100%)	82 (91%)	8 (9%)	9 29
70	O4	95/101 (94%)	74 (78%)	21 (22%)	1 3
70	o4	95/101 (94%)	78 (82%)	17 (18%)	2 6
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1 4
71	o5	103/104 (99%)	75 (73%)	28 (27%)	0 1
72	O6	81/81 (100%)	58 (72%)	23 (28%)	0 1
72	o6	80/81 (99%)	53 (66%)	27 (34%)	0 0
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1 4
73	o7	70/70 (100%)	59 (84%)	11 (16%)	2 9
74	O8	68/68 (100%)	54 (79%)	14 (21%)	1 4
74	o8	67/68 (98%)	57 (85%)	10 (15%)	3 10
75	O9	45/45 (100%)	35 (78%)	10 (22%)	1 3
75	o9	45/45 (100%)	32 (71%)	13 (29%)	0 1
76	Q0	47/47 (100%)	38 (81%)	9 (19%)	1 5
76	q0	47/47 (100%)	38 (81%)	9 (19%)	1 5
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0 0
77	q1	23/23 (100%)	13 (56%)	10 (44%)	0 0
78	Q2	90/90 (100%)	71 (79%)	19 (21%)	1 4
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1 4
79	Q3	71/71 (100%)	55 (78%)	16 (22%)	1 3
79	q3	71/71 (100%)	57 (80%)	14 (20%)	1 5
80	e0	53/53 (100%)	40 (76%)	13 (24%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
82	p0	105/253 (42%)	81 (77%)	24 (23%)	1 3
All	All	18729/20239 (92%)	14953 (80%)	3776 (20%)	1 4

5 of 3776 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
78	Q2	60	LYS
67	o1	13	THR
14	c2	116	VAL
64	n8	97	GLU
52	m6	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 190 such sidechains are listed below:

Mol	Chain	Res	Type
10	s8	138	ASN
34	sR	101	GLN
12	c0	58	GLN
22	d0	49	ASN
40	l3	224	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	453 (25%)	63 (3%)
1	6	1794/1800 (99%)	436 (24%)	59 (3%)
36	1	3145/3396 (92%)	624 (19%)	99 (3%)
36	5	3145/3396 (92%)	632 (20%)	101 (3%)
37	3	120/121 (99%)	17 (14%)	2 (1%)
37	7	120/121 (99%)	15 (12%)	1 (0%)
38	4	157/158 (99%)	36 (22%)	3 (1%)
38	8	157/158 (99%)	37 (23%)	2 (1%)
All	All	10385/10950 (94%)	2250 (21%)	330 (3%)

5 of 2250 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C

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Mol	Chain	Res	Type
1	2	17	C
1	2	25	C
1	2	26	A

5 of 330 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	217	U
36	5	2255	A
36	5	647	A
36	5	1307	G
36	5	2585	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 2559 ligands modelled in this entry, 1424 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	$\#\|Z\| > 2$
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	l4	403	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	M6	202	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	m1	203	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	l3	402	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	O2	201	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	6	2204	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	1	4215	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	1	4211	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	O7	103	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	4250	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
88	3H3	5	4251	-	34,34,34	1.04	2 (5%)	36,45,45	1.45	4 (11%)
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	m5	302	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	O9	101	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	2	2179	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	m4	202	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	5	4248	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	3	225	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	2	2147	86	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	l9	600	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
88	3H3	1	4216	-	34,34,34	1.09	3 (8%)	36,45,45	2.02	8 (22%)
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	5	3899	-	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	1	4212	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	O3	202	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	2	2180	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4195	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	n3	203	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	M5	304	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	2	2181	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	5	4246	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	5	3898	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	7	227	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	2	2032	86	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	o2	201	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	o4	203	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	l5	305	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	5	3942	86	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	m6	202	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	M7	208	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	o3	203	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	l5	306	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4204	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	l4	402	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	7	216	-	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	3	226	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	6	2190	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	m7	206	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	5	4232	86	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	C3	202	-	0,6,6	-	-	-		
86	OHX	5	4233	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	Q2	503	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	L6	202	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	M7	207	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	L4	404	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	C1	201	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	5	4249	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	2	2178	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	1	4213	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	l3	403	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	1	4214	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	c1	202	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	n9	3803	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	O7	104	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	l5	304	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	3H3	1	4216	-	-	8/39/51/51	0/1/2/2
88	3H3	5	4251	-	-	8/39/51/51	0/1/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4216	3H3	C3-C2	3.85	1.47	1.33
88	5	4251	3H3	C14-C16	3.70	1.56	1.53
88	5	4251	3H3	C15-C14	-3.01	1.50	1.54
88	1	4216	3H3	C15-C14	-3.01	1.50	1.54
88	1	4216	3H3	C14-C13	2.33	1.54	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	1	4216	3H3	C-C1-C11	6.38	119.56	110.78
88	1	4216	3H3	C1-C11-C12	5.18	122.64	113.19
88	5	4251	3H3	C15-C14-C16	4.98	116.50	109.31
88	1	4216	3H3	C15-C14-C16	4.94	116.44	109.31
88	5	4251	3H3	C1-C11-C12	4.10	120.67	113.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	1	4216	3H3	C2-C1-C11-O1
88	1	4216	3H3	C2-C1-C11-C12
88	1	4216	3H3	C-C1-C11-O1
88	1	4216	3H3	C-C1-C11-C12
88	5	4251	3H3	C12-C11-O1-C10

There are no ring outliers.

481 monomers are involved in 810 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	C5	201	OHX	2	0
86	2	2170	OHX	1	0
86	6	2171	OHX	8	0
86	5	4003	OHX	1	0
86	6	2138	OHX	1	0
86	1	3937	OHX	1	0
86	2	2163	OHX	6	0
86	M6	202	OHX	1	0
86	5	4182	OHX	1	0
86	5	4076	OHX	4	0
86	6	2136	OHX	1	0
86	5	4001	OHX	7	0
86	5	4193	OHX	1	0
86	6	2157	OHX	1	0
86	m1	203	OHX	1	0
86	6	2103	OHX	2	0
86	1	4054	OHX	1	0
86	1	4182	OHX	1	0
86	1	4012	OHX	1	0
86	5	4089	OHX	1	0
86	1	3935	OHX	2	0
86	1	4158	OHX	4	0
86	6	2062	OHX	1	0
86	1	4138	OHX	3	0
86	5	4205	OHX	1	0
86	1	4208	OHX	1	0
86	1	4034	OHX	2	0
86	1	4171	OHX	1	0
86	2	2043	OHX	1	0
86	s9	201	OHX	2	0
86	5	4191	OHX	1	0
86	2	2150	OHX	1	0
86	1	4167	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3943	OHX	6	0
86	2	2037	OHX	3	0
86	5	4066	OHX	7	0
86	1	3970	OHX	1	0
86	2	2072	OHX	1	0
86	1	3883	OHX	1	0
86	2	2049	OHX	1	0
86	5	3972	OHX	1	0
86	6	2073	OHX	1	0
86	1	4068	OHX	1	0
86	7	224	OHX	4	0
86	2	2086	OHX	4	0
86	6	2149	OHX	1	0
86	2	2133	OHX	1	0
86	6	2060	OHX	6	0
86	1	4005	OHX	1	0
86	1	4047	OHX	4	0
86	2	2167	OHX	2	0
86	5	4013	OHX	2	0
86	2	2073	OHX	1	0
86	2	2160	OHX	2	0
86	m0	301	OHX	1	0
86	6	2163	OHX	1	0
86	7	219	OHX	4	0
86	1	3971	OHX	1	0
86	2	2065	OHX	1	0
86	5	4185	OHX	1	0
86	2	2074	OHX	1	0
86	5	4118	OHX	1	0
86	2	2121	OHX	2	0
86	1	3888	OHX	1	0
86	1	4102	OHX	1	0
86	1	4147	OHX	1	0
86	5	4224	OHX	2	0
86	1	4041	OHX	3	0
86	6	2066	OHX	1	0
86	1	4066	OHX	1	0
86	5	4128	OHX	1	0
86	8	219	OHX	2	0
86	1	4095	OHX	1	0
86	6	2175	OHX	1	0
86	1	3967	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3987	OHX	2	0
86	5	3924	OHX	3	0
86	2	2130	OHX	2	0
86	2	2117	OHX	1	0
86	6	2154	OHX	2	0
86	1	4023	OHX	7	0
86	5	4145	OHX	1	0
86	1	4203	OHX	1	0
86	2	2071	OHX	1	0
86	6	2074	OHX	2	0
86	6	2150	OHX	5	0
86	6	2143	OHX	1	0
86	5	4196	OHX	9	0
86	5	4051	OHX	1	0
86	1	4049	OHX	1	0
86	1	4153	OHX	7	0
86	5	4072	OHX	1	0
86	5	4039	OHX	1	0
86	5	3904	OHX	1	0
86	N9	101	OHX	1	0
86	1	4094	OHX	1	0
86	5	4183	OHX	1	0
86	1	4064	OHX	1	0
86	O7	103	OHX	7	0
86	1	3976	OHX	7	0
86	1	4187	OHX	1	0
86	1	3979	OHX	1	0
86	2	2109	OHX	7	0
86	6	2188	OHX	1	0
86	5	3948	OHX	1	0
86	5	4144	OHX	1	0
86	1	4166	OHX	6	0
86	5	4026	OHX	1	0
86	5	3912	OHX	1	0
86	2	2155	OHX	4	0
86	5	4238	OHX	2	0
86	3	218	OHX	3	0
86	2	2172	OHX	2	0
86	6	2096	OHX	1	0
86	5	4002	OHX	2	0
86	2	2142	OHX	1	0
86	1	4048	OHX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2077	OHX	1	0
86	5	4161	OHX	1	0
86	1	4134	OHX	1	0
86	5	4109	OHX	1	0
86	1	3968	OHX	3	0
86	1	4038	OHX	1	0
86	6	2192	OHX	1	0
86	5	4176	OHX	1	0
86	6	2094	OHX	1	0
86	7	226	OHX	6	0
86	2	2157	OHX	1	0
86	1	4032	OHX	6	0
86	8	215	OHX	6	0
86	6	2115	OHX	2	0
86	6	2155	OHX	1	0
86	5	4024	OHX	2	0
86	1	4043	OHX	2	0
86	5	4108	OHX	3	0
86	s8	303	OHX	1	0
86	1	4014	OHX	1	0
86	2	2119	OHX	1	0
86	5	4141	OHX	6	0
86	6	2142	OHX	1	0
86	7	221	OHX	1	0
86	1	4183	OHX	1	0
86	6	2097	OHX	1	0
86	6	2113	OHX	1	0
86	5	4131	OHX	1	0
86	5	4241	OHX	7	0
88	5	4251	3H3	1	0
86	2	2105	OHX	1	0
86	1	3952	OHX	1	0
86	6	2055	OHX	1	0
86	5	4127	OHX	1	0
86	5	4215	OHX	8	0
86	1	3948	OHX	1	0
86	6	2160	OHX	1	0
86	5	4102	OHX	2	0
86	5	4226	OHX	1	0
86	5	4242	OHX	1	0
86	1	4056	OHX	6	0
86	1	4151	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3987	OHX	1	0
86	5	4177	OHX	2	0
86	6	2093	OHX	1	0
86	6	2089	OHX	1	0
86	O9	101	OHX	4	0
86	1	4210	OHX	1	0
86	6	2196	OHX	1	0
86	8	218	OHX	1	0
86	1	4122	OHX	2	0
86	1	4113	OHX	1	0
86	2	2158	OHX	3	0
86	6	2061	OHX	1	0
86	5	3973	OHX	6	0
86	5	4132	OHX	1	0
86	5	4187	OHX	7	0
86	5	4181	OHX	1	0
86	5	4212	OHX	6	0
86	5	4179	OHX	1	0
86	1	3897	OHX	1	0
86	5	4097	OHX	1	0
86	2	2090	OHX	6	0
86	1	4021	OHX	1	0
86	5	4235	OHX	1	0
86	8	224	OHX	6	0
86	5	4130	OHX	1	0
86	1	4061	OHX	5	0
86	1	4083	OHX	1	0
86	5	4033	OHX	4	0
86	2	2147	OHX	7	0
86	1	4177	OHX	6	0
88	1	4216	3H3	1	0
86	1	3903	OHX	1	0
86	5	4094	OHX	6	0
86	d9	102	OHX	1	0
86	5	4200	OHX	1	0
86	5	4206	OHX	1	0
86	1	3875	OHX	1	0
86	2	2127	OHX	1	0
86	5	4157	OHX	2	0
86	2	2168	OHX	1	0
86	1	4059	OHX	7	0
86	5	4020	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4071	OHX	6	0
86	5	3941	OHX	1	0
86	2	2166	OHX	1	0
86	1	4135	OHX	3	0
86	2	2116	OHX	7	0
86	5	4096	OHX	1	0
86	1	4046	OHX	2	0
86	6	2144	OHX	1	0
86	1	4201	OHX	1	0
86	5	4160	OHX	2	0
86	5	4227	OHX	1	0
86	2	2173	OHX	2	0
86	6	2075	OHX	2	0
86	6	2183	OHX	1	0
86	8	225	OHX	1	0
86	1	3990	OHX	1	0
86	5	3953	OHX	1	0
86	6	2168	OHX	1	0
86	5	3966	OHX	1	0
86	6	2067	OHX	1	0
86	1	4099	OHX	1	0
86	C8	201	OHX	1	0
86	1	3898	OHX	1	0
86	5	4225	OHX	1	0
86	2	2096	OHX	6	0
86	3	216	OHX	1	0
86	q2	502	OHX	3	0
86	5	3921	OHX	1	0
86	1	3887	OHX	1	0
86	5	3969	OHX	1	0
86	1	4168	OHX	1	0
86	5	4088	OHX	1	0
86	6	2147	OHX	7	0
86	2	2094	OHX	1	0
86	1	4200	OHX	6	0
86	2	2110	OHX	1	0
86	5	3957	OHX	1	0
86	5	4106	OHX	1	0
86	1	4157	OHX	5	0
86	5	3991	OHX	2	0
86	1	3980	OHX	5	0
86	1	4079	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3983	OHX	1	0
86	2	2097	OHX	1	0
86	5	4129	OHX	1	0
86	1	4042	OHX	1	0
86	5	3949	OHX	1	0
86	5	4207	OHX	2	0
86	2	2027	OHX	2	0
86	2	2174	OHX	1	0
86	5	4138	OHX	1	0
86	1	4017	OHX	1	0
86	5	3978	OHX	8	0
86	1	4070	OHX	1	0
86	1	4118	OHX	6	0
86	M5	304	OHX	1	0
86	6	2102	OHX	1	0
86	5	4110	OHX	1	0
86	2	2137	OHX	1	0
86	8	222	OHX	2	0
86	2	2045	OHX	6	0
86	2	2131	OHX	1	0
86	5	4017	OHX	1	0
86	1	4179	OHX	1	0
86	1	4010	OHX	1	0
86	5	4166	OHX	1	0
86	5	4222	OHX	6	0
86	1	3931	OHX	1	0
86	1	3911	OHX	1	0
86	1	4123	OHX	1	0
86	6	2108	OHX	1	0
86	1	3973	OHX	1	0
86	1	4016	OHX	1	0
86	5	4221	OHX	1	0
86	6	2135	OHX	1	0
86	6	2180	OHX	1	0
86	6	2202	OHX	2	0
86	1	4044	OHX	2	0
86	1	3962	OHX	5	0
86	5	4007	OHX	1	0
86	5	4198	OHX	7	0
86	5	4117	OHX	3	0
86	1	4088	OHX	7	0
86	1	4186	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2085	OHX	1	0
86	6	2123	OHX	1	0
86	5	3955	OHX	2	0
86	5	4090	OHX	7	0
86	5	4189	OHX	7	0
86	4	227	OHX	1	0
86	1	4136	OHX	3	0
86	5	4204	OHX	1	0
86	1	3873	OHX	1	0
86	2	2039	OHX	1	0
86	4	224	OHX	1	0
86	5	4093	OHX	4	0
86	2	2145	OHX	1	0
86	5	4074	OHX	5	0
86	8	216	OHX	1	0
86	2	2032	OHX	7	0
86	2	2162	OHX	1	0
86	1	4170	OHX	2	0
86	5	4054	OHX	3	0
86	2	2115	OHX	2	0
86	1	4149	OHX	6	0
86	2	2161	OHX	2	0
86	4	232	OHX	2	0
86	5	4068	OHX	1	0
86	2	2169	OHX	1	0
86	1	3961	OHX	1	0
86	6	2124	OHX	1	0
86	1	4084	OHX	8	0
86	1	3993	OHX	1	0
86	2	2128	OHX	1	0
86	5	4046	OHX	1	0
86	o4	203	OHX	4	0
86	6	2101	OHX	3	0
86	1	4051	OHX	2	0
86	l5	305	OHX	1	0
86	5	3942	OHX	3	0
86	5	4030	OHX	1	0
86	2	2075	OHX	1	0
86	2	2040	OHX	2	0
86	6	2178	OHX	1	0
86	1	4092	OHX	1	0
86	5	4119	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	s4	301	OHX	1	0
86	2	2144	OHX	1	0
86	1	3876	OHX	1	0
86	5	4034	OHX	4	0
86	S8	302	OHX	1	0
86	1	4159	OHX	6	0
86	5	4146	OHX	1	0
86	M5	303	OHX	1	0
86	5	4151	OHX	1	0
86	1	4146	OHX	2	0
86	o7	502	OHX	1	0
86	1	4175	OHX	8	0
86	5	4065	OHX	5	0
86	5	4140	OHX	2	0
86	1	3886	OHX	1	0
86	6	2120	OHX	2	0
86	1	3985	OHX	1	0
86	5	4247	OHX	2	0
86	6	2162	OHX	1	0
86	2	2052	OHX	1	0
86	8	214	OHX	2	0
86	1	4077	OHX	1	0
86	6	2170	OHX	1	0
86	l4	402	OHX	3	0
86	1	4076	OHX	3	0
86	6	2118	OHX	1	0
86	1	4209	OHX	1	0
86	2	2076	OHX	6	0
86	1	4100	OHX	1	0
86	6	2107	OHX	1	0
86	6	2130	OHX	1	0
86	7	217	OHX	1	0
86	1	4036	OHX	6	0
86	2	2083	OHX	1	0
86	5	3962	OHX	4	0
86	2	2091	OHX	6	0
86	3	226	OHX	1	0
86	6	2112	OHX	1	0
86	6	2190	OHX	2	0
86	5	3959	OHX	1	0
86	m7	206	OHX	1	0
86	5	4170	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4163	OHX	5	0
86	2	2059	OHX	1	0
86	5	4011	OHX	6	0
86	5	4232	OHX	2	0
86	2	2111	OHX	2	0
86	1	4060	OHX	4	0
86	2	2058	OHX	1	0
86	5	4079	OHX	1	0
86	2	2132	OHX	8	0
86	5	4234	OHX	6	0
86	3	223	OHX	2	0
86	5	4203	OHX	1	0
86	5	4136	OHX	2	0
86	1	4007	OHX	8	0
86	1	4011	OHX	1	0
86	6	2159	OHX	3	0
86	5	4197	OHX	7	0
86	1	4205	OHX	2	0
86	2	2156	OHX	1	0
86	2	2139	OHX	1	0
86	2	2084	OHX	4	0
86	5	4000	OHX	5	0
86	6	2126	OHX	3	0
86	5	4091	OHX	1	0
86	1	4111	OHX	1	0
86	6	2189	OHX	2	0
86	5	4201	OHX	5	0
86	1	3945	OHX	1	0
86	C3	202	OHX	1	0
86	1	4103	OHX	1	0
86	5	3906	OHX	2	0
86	5	4125	OHX	1	0
86	5	4214	OHX	1	0
86	1	3924	OHX	1	0
86	Q2	503	OHX	2	0
86	1	4198	OHX	1	0
86	1	4184	OHX	3	0
86	c3	201	OHX	3	0
86	5	3999	OHX	1	0
86	6	2121	OHX	8	0
86	1	4006	OHX	1	0
86	1	4196	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2087	OHX	1	0
86	7	218	OHX	6	0
86	M7	207	OHX	1	0
86	m0	302	OHX	1	0
86	2	2079	OHX	1	0
86	6	2182	OHX	1	0
86	8	223	OHX	6	0
86	1	4143	OHX	6	0
86	1	3958	OHX	1	0
86	L4	404	OHX	2	0
86	5	4055	OHX	6	0
86	C1	201	OHX	7	0
86	6	2195	OHX	1	0
86	6	2071	OHX	1	0
86	6	2151	OHX	1	0
86	5	4249	OHX	1	0
86	s1	302	OHX	1	0
86	5	4081	OHX	4	0
86	1	4178	OHX	1	0
86	L3	403	OHX	1	0
86	5	4178	OHX	2	0
86	1	4037	OHX	1	0
86	1	4065	OHX	8	0
86	2	2099	OHX	7	0
86	5	4190	OHX	6	0
86	1	4125	OHX	1	0
86	6	2128	OHX	2	0
86	2	2146	OHX	2	0
86	5	4152	OHX	1	0
86	1	4144	OHX	1	0
86	6	2156	OHX	2	0
86	2	2048	OHX	1	0
86	1	4172	OHX	1	0
86	5	4230	OHX	2	0
86	M9	202	OHX	1	0
86	1	3986	OHX	2	0
86	5	4023	OHX	3	0
86	1	4194	OHX	1	0
86	2	2063	OHX	1	0
86	5	4052	OHX	1	0
86	5	4099	OHX	1	0
86	1	4031	OHX	2	0

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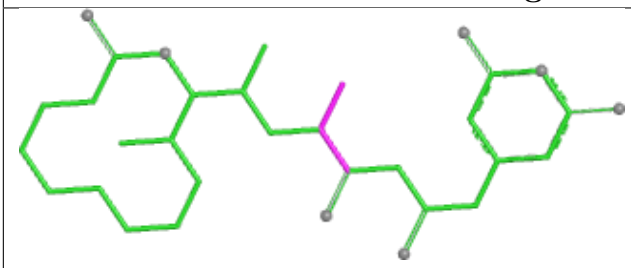
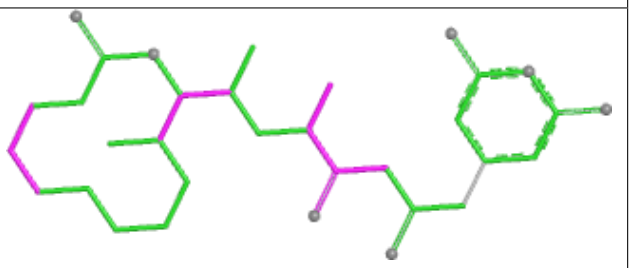
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4219	OHX	1	0
86	1	3938	OHX	1	0
86	5	4049	OHX	1	0
86	1	3915	OHX	1	0
86	2	2054	OHX	1	0
86	6	2146	OHX	1	0
86	5	4059	OHX	1	0
86	1	3995	OHX	1	0
86	5	4199	OHX	3	0
86	2	2093	OHX	2	0
86	5	4092	OHX	1	0
86	2	2095	OHX	1	0
86	1	3955	OHX	3	0
86	4	223	OHX	1	0
86	2	2046	OHX	1	0
86	6	2122	OHX	1	0
86	c1	202	OHX	7	0
86	5	4061	OHX	1	0
86	1	4002	OHX	2	0
86	1	3896	OHX	1	0
86	1	4128	OHX	1	0
86	1	4098	OHX	1	0
86	1	4142	OHX	3	0
86	1	3964	OHX	7	0
86	1	4089	OHX	4	0
86	c5	201	OHX	2	0
86	6	2125	OHX	1	0
86	6	2165	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

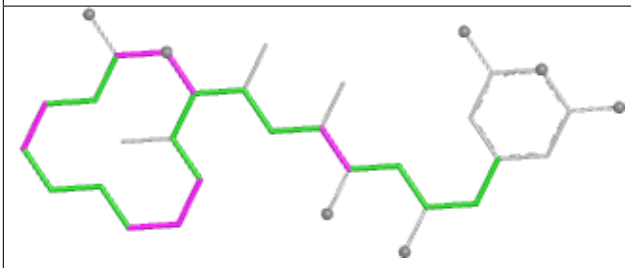
Ligand 3H3 5 4251



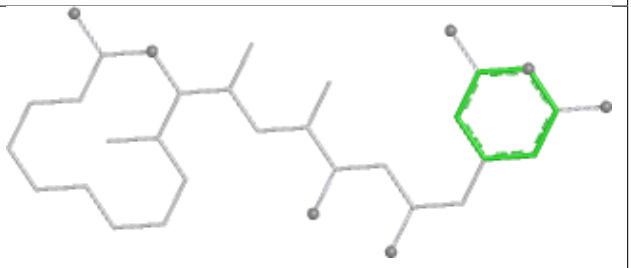
Bond lengths



Bond angles

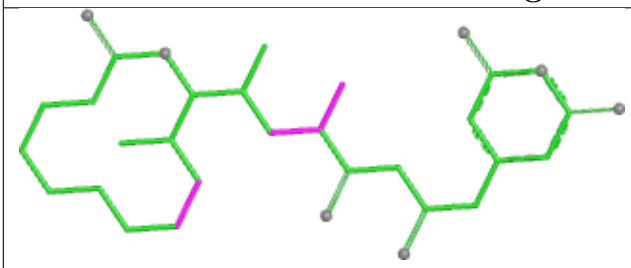


Torsions

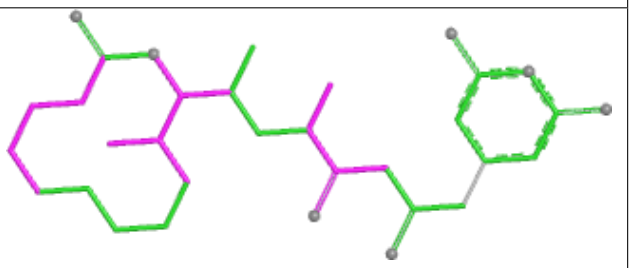


Rings

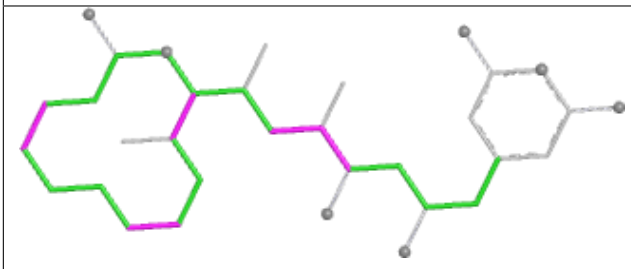
Ligand 3H3 1 4216



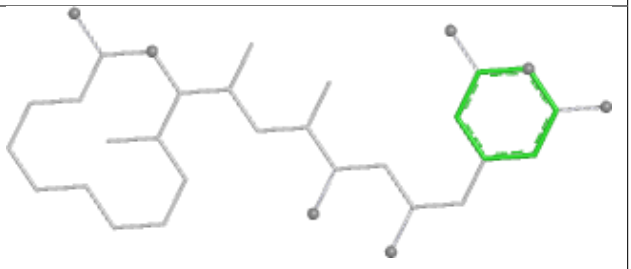
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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Mol	Chain	Number of breaks

Mol	Chain	Number of breaks
34	SR	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SR	161:LYS	C	162:ALA	N	0.66
1	SR	160:GLU	C	161:LYS	N	0.45

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	2	1750/1800 (97%)	0.30	97 (5%) 30 23	40, 69, 136, 230	0
1	6	1795/1800 (99%)	0.17	94 (5%) 33 25	30, 58, 149, 237	0
2	S0	206/251 (82%)	1.29	38 (18%) 3 2	73, 88, 101, 127	0
2	s0	206/251 (82%)	0.74	20 (9%) 13 10	54, 71, 86, 92	0
3	S1	214/254 (84%)	1.44	49 (22%) 2 1	79, 109, 140, 148	0
3	s1	216/254 (85%)	0.49	7 (3%) 50 40	53, 65, 88, 96	0
4	S2	217/253 (85%)	0.74	14 (6%) 25 18	54, 68, 83, 96	0
4	s2	217/253 (85%)	0.29	7 (3%) 50 40	42, 56, 69, 78	0
5	S3	223/239 (93%)	0.82	21 (9%) 14 10	59, 72, 92, 108	0
5	s3	223/239 (93%)	0.63	12 (5%) 31 24	55, 76, 98, 104	0
6	S4	260/260 (100%)	0.60	9 (3%) 47 38	47, 69, 80, 108	0
6	s4	260/260 (100%)	0.21	5 (1%) 66 57	37, 58, 69, 100	0
7	S5	206/224 (91%)	1.09	23 (11%) 10 7	73, 92, 107, 120	0
7	s5	206/224 (91%)	1.00	23 (11%) 10 7	56, 77, 101, 113	0
8	S6	226/236 (95%)	1.17	39 (17%) 4 3	49, 82, 98, 126	0
8	s6	218/236 (92%)	0.77	19 (8%) 16 11	38, 66, 87, 107	0
9	S7	184/189 (97%)	1.26	27 (14%) 6 4	65, 92, 123, 131	0
9	s7	186/189 (98%)	1.18	28 (15%) 5 4	49, 78, 112, 122	0
10	S8	188/200 (94%)	0.66	15 (7%) 18 13	40, 55, 89, 104	0
10	s8	188/200 (94%)	0.62	12 (6%) 25 18	33, 52, 95, 111	0
11	S9	185/196 (94%)	0.90	16 (8%) 16 12	64, 77, 113, 146	0
11	s9	185/196 (94%)	0.24	3 (1%) 70 61	49, 62, 99, 125	0
12	C0	96/105 (91%)	0.81	10 (10%) 11 8	63, 83, 110, 128	0
12	c0	96/105 (91%)	1.09	18 (18%) 3 2	69, 99, 122, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	C1	155/155 (100%)	0.78	17 (10%) 10 8	43, 53, 103, 117	0
13	c1	146/155 (94%)	0.72	13 (8%) 15 11	34, 48, 76, 96	0
14	C2	124/142 (87%)	1.18	22 (17%) 4 3	105, 118, 138, 151	0
14	c2	124/142 (87%)	1.60	29 (23%) 2 1	139, 159, 175, 184	0
15	C3	150/150 (100%)	0.62	5 (3%) 49 39	50, 67, 80, 86	0
15	c3	150/150 (100%)	0.50	7 (4%) 36 29	40, 55, 71, 85	0
16	C4	127/136 (93%)	1.46	30 (23%) 2 1	54, 113, 128, 131	0
16	c4	128/136 (94%)	0.78	10 (7%) 19 14	38, 71, 80, 83	0
17	C5	124/141 (87%)	0.74	13 (10%) 11 8	58, 72, 108, 128	0
17	c5	135/141 (95%)	0.93	15 (11%) 10 7	58, 74, 98, 120	0
18	C6	141/142 (99%)	0.82	14 (9%) 13 9	62, 82, 87, 89	0
18	c6	142/142 (100%)	0.94	20 (14%) 6 5	50, 71, 84, 105	0
19	C7	120/136 (88%)	1.36	30 (25%) 2 1	68, 85, 111, 113	0
19	c7	117/136 (86%)	0.97	19 (16%) 4 4	59, 72, 98, 109	0
20	C8	145/145 (100%)	0.78	12 (8%) 17 12	58, 80, 105, 114	0
20	c8	145/145 (100%)	0.52	9 (6%) 26 20	55, 65, 90, 103	0
21	C9	143/143 (100%)	0.68	6 (4%) 40 32	66, 80, 94, 105	0
21	c9	143/143 (100%)	0.54	4 (2%) 55 45	51, 64, 82, 98	0
22	D0	107/120 (89%)	1.23	25 (23%) 2 1	56, 87, 118, 128	0
22	d0	110/120 (91%)	1.25	24 (21%) 2 2	50, 82, 120, 132	0
23	D1	87/87 (100%)	0.95	9 (10%) 12 9	69, 75, 92, 99	0
23	d1	87/87 (100%)	0.20	0 100 100	53, 59, 77, 88	0
24	D2	129/129 (100%)	0.57	2 (1%) 70 61	52, 62, 68, 78	0
24	d2	129/129 (100%)	0.10	0 100 100	37, 47, 53, 61	0
25	D3	144/144 (100%)	0.28	4 (2%) 55 45	43, 49, 59, 73	0
25	d3	144/144 (100%)	-0.13	1 (0%) 84 77	33, 38, 52, 65	0
26	D4	134/134 (100%)	0.74	14 (10%) 11 8	59, 82, 97, 105	0
26	d4	134/134 (100%)	0.52	9 (6%) 24 17	46, 66, 81, 100	0
27	D5	70/107 (65%)	1.39	19 (27%) 1 1	87, 103, 115, 121	0
27	d5	69/107 (64%)	1.16	12 (17%) 4 3	66, 87, 99, 101	0
28	D6	97/97 (100%)	1.07	15 (15%) 5 4	59, 74, 129, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	d6	97/97 (100%)	0.64	7 (7%) 21 16	43, 55, 84, 93	0
29	D7	81/81 (100%)	0.88	6 (7%) 20 15	64, 79, 113, 123	0
29	d7	81/81 (100%)	0.94	11 (13%) 7 5	49, 66, 106, 109	0
30	D8	63/66 (95%)	1.42	11 (17%) 4 3	89, 104, 118, 130	0
30	d8	63/66 (95%)	1.41	12 (19%) 3 2	74, 89, 103, 112	0
31	D9	53/55 (96%)	0.37	4 (7%) 20 15	56, 60, 80, 89	0
31	d9	53/55 (96%)	0.52	4 (7%) 20 15	52, 58, 95, 109	0
32	E0	60/60 (100%)	0.70	8 (13%) 7 5	47, 79, 115, 121	0
33	E1	71/76 (93%)	1.37	17 (23%) 2 1	91, 102, 113, 115	0
33	e1	76/76 (100%)	1.67	22 (28%) 1 1	117, 130, 148, 153	0
34	SR	318/318 (100%)	0.71	21 (6%) 24 18	55, 87, 106, 129	0
34	sR	318/318 (100%)	0.93	29 (9%) 15 11	73, 91, 107, 124	0
35	SM	159/273 (58%)	1.29	38 (23%) 2 1	51, 73, 118, 120	0
35	sM	104/273 (38%)	1.16	25 (24%) 2 1	40, 75, 155, 158	0
36	1	3149/3396 (92%)	-0.19	113 (3%) 46 37	17, 37, 108, 219	0
36	5	3150/3396 (92%)	-0.23	100 (3%) 50 40	17, 36, 101, 220	0
37	3	121/121 (100%)	-0.40	1 (0%) 82 75	28, 53, 70, 75	0
37	7	121/121 (100%)	-0.48	2 (1%) 69 60	24, 40, 51, 59	0
38	4	158/158 (100%)	-0.50	4 (2%) 58 48	22, 40, 74, 105	0
38	8	158/158 (100%)	-0.30	5 (3%) 50 40	27, 46, 80, 102	0
39	L2	252/253 (99%)	-0.11	2 (0%) 82 75	20, 35, 50, 58	0
39	l2	252/253 (99%)	0.03	8 (3%) 50 40	21, 37, 55, 62	0
40	L3	386/386 (100%)	-0.13	7 (1%) 67 58	23, 41, 54, 87	0
40	l3	386/386 (100%)	-0.32	3 (0%) 82 75	17, 30, 42, 73	0
41	L4	361/361 (100%)	-0.03	10 (2%) 55 45	19, 33, 49, 57	0
41	l4	361/361 (100%)	0.23	16 (4%) 39 31	21, 38, 55, 62	0
42	L5	296/296 (100%)	0.25	10 (3%) 48 39	37, 59, 77, 103	0
42	l5	294/296 (99%)	0.01	9 (3%) 51 41	29, 43, 66, 101	0
43	L6	156/175 (89%)	0.00	3 (1%) 66 57	28, 35, 53, 69	0
43	l6	157/175 (89%)	0.18	6 (3%) 44 35	30, 38, 56, 68	0
44	L7	222/243 (91%)	-0.12	4 (1%) 67 58	21, 29, 54, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	l7	223/243 (91%)	-0.14	5 (2%) 62 52	20, 28, 65, 105	0
45	L8	233/255 (91%)	0.40	15 (6%) 25 18	42, 54, 88, 105	0
45	l8	231/255 (90%)	0.65	15 (6%) 25 18	51, 63, 88, 93	0
46	L9	191/191 (100%)	0.10	1 (0%) 87 82	37, 48, 60, 76	0
46	l9	191/191 (100%)	-0.01	5 (2%) 57 47	27, 35, 54, 75	0
47	M0	211/220 (95%)	0.02	6 (2%) 55 45	24, 38, 72, 91	0
47	m0	213/220 (96%)	0.21	12 (5%) 30 23	25, 41, 64, 83	0
48	M1	169/173 (97%)	0.40	4 (2%) 59 49	45, 63, 76, 84	0
48	m1	169/173 (97%)	0.12	4 (2%) 59 49	32, 48, 60, 71	0
49	M3	193/198 (97%)	-0.01	4 (2%) 63 54	21, 39, 73, 98	0
49	m3	194/198 (97%)	0.26	8 (4%) 41 33	27, 47, 80, 102	0
50	M4	136/137 (99%)	0.11	4 (2%) 53 43	31, 38, 51, 59	0
50	m4	137/137 (100%)	0.08	6 (4%) 39 31	28, 33, 51, 62	0
51	M5	203/203 (100%)	-0.27	0 100 100	20, 34, 42, 49	0
51	m5	203/203 (100%)	-0.16	0 100 100	25, 41, 51, 56	0
52	M6	197/198 (99%)	-0.08	5 (2%) 58 48	22, 29, 48, 54	0
52	m6	197/198 (99%)	-0.18	5 (2%) 58 48	18, 23, 47, 53	0
53	M7	183/183 (100%)	0.29	16 (8%) 16 11	25, 32, 82, 114	0
53	m7	155/183 (84%)	-0.25	2 (1%) 75 66	21, 28, 40, 64	0
54	M8	185/185 (100%)	-0.18	0 100 100	22, 31, 44, 56	0
54	m8	185/185 (100%)	-0.10	1 (0%) 87 82	26, 37, 46, 52	0
55	M9	188/188 (100%)	0.58	18 (9%) 13 10	38, 51, 127, 140	0
55	m9	188/188 (100%)	0.41	11 (5%) 28 21	34, 45, 105, 122	0
56	N0	172/172 (100%)	0.01	3 (1%) 69 60	29, 36, 48, 54	0
56	n0	172/172 (100%)	-0.01	5 (2%) 53 43	23, 30, 40, 48	0
57	N1	159/159 (100%)	0.03	3 (1%) 66 57	25, 35, 71, 78	0
57	n1	159/159 (100%)	-0.12	1 (0%) 85 80	25, 31, 64, 70	0
58	N2	100/120 (83%)	0.96	10 (10%) 12 9	67, 81, 92, 101	0
58	n2	98/120 (81%)	0.76	7 (7%) 22 16	58, 70, 80, 81	0
59	N3	136/136 (100%)	-0.04	5 (3%) 45 36	27, 37, 50, 57	0
59	n3	136/136 (100%)	-0.17	3 (2%) 62 52	19, 28, 42, 45	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
60	N4	98/155 (63%)	1.71	36 (36%) 1 0	37, 48, 127, 130	0
60	n4	135/155 (87%)	1.25	37 (27%) 1 1	28, 74, 108, 124	0
61	N5	121/141 (85%)	-0.04	1 (0%) 82 75	34, 46, 61, 83	0
61	n5	120/141 (85%)	0.20	1 (0%) 82 75	36, 49, 67, 72	0
62	N6	126/126 (100%)	-0.28	1 (0%) 82 75	27, 42, 53, 61	0
62	n6	126/126 (100%)	-0.05	1 (0%) 82 75	32, 45, 60, 65	0
63	N7	135/135 (100%)	0.35	2 (1%) 72 63	53, 66, 80, 88	0
63	n7	135/135 (100%)	0.68	5 (3%) 45 36	57, 72, 91, 99	0
64	N8	148/148 (100%)	-0.12	2 (1%) 73 64	18, 32, 54, 63	0
64	n8	148/148 (100%)	-0.02	0 100 100	19, 39, 56, 58	0
65	N9	58/58 (100%)	0.45	5 (8%) 16 12	19, 39, 79, 90	0
65	n9	58/58 (100%)	0.39	4 (6%) 23 16	19, 40, 59, 70	0
66	O0	97/104 (93%)	0.25	5 (5%) 33 25	51, 60, 81, 85	0
66	o0	100/104 (96%)	0.58	10 (10%) 12 9	54, 63, 88, 100	0
67	O1	109/112 (97%)	0.22	7 (6%) 25 18	35, 48, 77, 91	0
67	o1	109/112 (97%)	0.06	6 (5%) 30 23	28, 39, 72, 90	0
68	O2	127/129 (98%)	-0.12	3 (2%) 59 49	18, 30, 40, 56	0
68	o2	127/129 (98%)	-0.09	3 (2%) 59 49	19, 34, 46, 65	0
69	O3	106/106 (100%)	-0.21	1 (0%) 81 74	23, 28, 47, 56	0
69	o3	106/106 (100%)	-0.13	4 (3%) 44 35	20, 27, 51, 60	0
70	O4	112/119 (94%)	0.36	5 (4%) 38 30	34, 49, 87, 100	0
70	o4	112/119 (94%)	0.40	4 (3%) 46 37	34, 49, 85, 93	0
71	O5	119/119 (100%)	0.11	4 (3%) 48 39	32, 49, 55, 58	0
71	o5	119/119 (100%)	0.19	2 (1%) 69 60	40, 54, 62, 68	0
72	O6	99/99 (100%)	0.25	4 (4%) 42 33	36, 45, 72, 86	0
72	o6	99/99 (100%)	0.30	3 (3%) 52 42	45, 55, 74, 90	0
73	O7	87/87 (100%)	-0.11	2 (2%) 61 51	23, 28, 50, 71	0
73	o7	87/87 (100%)	-0.14	1 (1%) 78 70	24, 30, 60, 95	0
74	O8	77/77 (100%)	0.48	2 (2%) 57 47	57, 69, 90, 98	0
74	o8	77/77 (100%)	0.51	3 (3%) 43 34	57, 69, 87, 91	0
75	O9	50/50 (100%)	0.06	2 (4%) 42 33	32, 35, 44, 49	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
75	o9	50/50 (100%)	0.01	0 100 100	35, 38, 48, 52	0
76	Q0	52/52 (100%)	-0.15	1 (1%) 66 57	33, 38, 53, 64	0
76	q0	52/52 (100%)	-0.29	1 (1%) 66 57	23, 26, 38, 44	0
77	Q1	25/25 (100%)	0.16	0 100 100	41, 43, 47, 52	0
77	q1	25/25 (100%)	0.03	0 100 100	31, 35, 44, 50	0
78	Q2	105/105 (100%)	0.05	5 (4%) 35 28	22, 38, 56, 82	0
78	q2	105/105 (100%)	-0.08	1 (0%) 79 72	26, 38, 51, 78	0
79	Q3	91/91 (100%)	0.03	2 (2%) 62 52	28, 38, 53, 66	0
79	q3	91/91 (100%)	0.08	2 (2%) 62 52	26, 38, 51, 59	0
80	e0	62/62 (100%)	0.43	3 (4%) 35 28	46, 64, 97, 99	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	1.75	51 (35%) 1 0	72, 90, 159, 170	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35344 (93%)	0.27	1949 (5%) 28 21	17, 52, 109, 237	0

The worst 5 of 1949 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	5	2871	G	12.1
36	5	2873	U	11.2
13	c1	3	THR	11.1
60	N4	86	SER	10.7
36	5	2403	G	9.8

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3809	1/1	-0.57	0.52	162,162,162,162	0
85	MG	1	3405	1/1	0.30	0.51	95,95,95,95	0
85	MG	5	3803	1/1	0.31	0.24	132,132,132,132	0
85	MG	2	1960	1/1	0.32	0.50	87,87,87,87	0
85	MG	6	2015	1/1	0.34	0.33	104,104,104,104	0
85	MG	2	1954	1/1	0.34	0.56	87,87,87,87	0
85	MG	5	3770	1/1	0.40	0.36	70,70,70,70	0
85	MG	2	2003	1/1	0.44	0.39	96,96,96,96	0
85	MG	2	1991	1/1	0.44	0.48	102,102,102,102	0
85	MG	2	1968	1/1	0.45	0.54	97,97,97,97	0
85	MG	5	3794	1/1	0.50	0.30	64,64,64,64	0
85	MG	1	3652	1/1	0.51	0.48	84,84,84,84	0
85	MG	2	1955	1/1	0.51	0.31	79,79,79,79	0
85	MG	4	220	1/1	0.52	0.40	77,77,77,77	0
85	MG	1	3863	1/1	0.53	0.13	118,118,118,118	0
85	MG	1	3593	1/1	0.54	0.32	59,59,59,59	0
85	MG	6	1924	1/1	0.55	0.58	87,87,87,87	0
85	MG	5	3896	1/1	0.56	0.27	82,82,82,82	0
85	MG	5	3466	1/1	0.57	0.53	88,88,88,88	0
85	MG	5	3773	1/1	0.57	0.33	83,83,83,83	0
85	MG	5	3781	1/1	0.57	0.27	64,64,64,64	0
85	MG	5	3707	1/1	0.58	0.44	75,75,75,75	0
85	MG	5	3846	1/1	0.59	0.33	50,50,50,50	0
85	MG	3	212	1/1	0.59	0.17	63,63,63,63	0
85	MG	6	2040	1/1	0.60	0.52	82,82,82,82	0
85	MG	2	2023	1/1	0.61	0.38	101,101,101,101	0
85	MG	N5	201	1/1	0.61	0.26	61,61,61,61	0
85	MG	6	1909	1/1	0.62	0.38	79,79,79,79	0
85	MG	5	3661	1/1	0.63	0.49	59,59,59,59	0
85	MG	5	3881	1/1	0.63	0.51	81,81,81,81	0
85	MG	5	3791	1/1	0.63	0.27	74,74,74,74	0
85	MG	5	3649	1/1	0.65	0.38	59,59,59,59	0
85	MG	2	1975	1/1	0.65	0.50	71,71,71,71	0
85	MG	1	3756	1/1	0.65	0.31	91,91,91,91	0
85	MG	2	2010	1/1	0.66	0.40	62,62,62,62	0
85	MG	1	3833	1/1	0.67	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3820	1/1	0.67	0.47	84,84,84,84	0
86	OHX	5	4236	7/7	0.67	0.25	125,125,125,125	0
85	MG	5	3418	1/1	0.68	0.24	59,59,59,59	0
85	MG	5	3419	1/1	0.68	0.28	91,91,91,91	0
85	MG	1	3643	1/1	0.68	0.17	39,39,39,39	0
85	MG	2	1969	1/1	0.68	0.29	79,79,79,79	0
85	MG	6	2021	1/1	0.69	0.31	93,93,93,93	0
85	MG	2	1967	1/1	0.69	0.34	70,70,70,70	0
85	MG	1	3861	1/1	0.69	0.26	65,65,65,65	0
85	MG	2	1915	1/1	0.69	0.41	53,53,53,53	0
85	MG	3	209	1/1	0.69	0.34	50,50,50,50	0
85	MG	1	3704	1/1	0.69	0.32	53,53,53,53	0
85	MG	1	3443	1/1	0.70	0.29	65,65,65,65	0
85	MG	2	1972	1/1	0.70	0.35	66,66,66,66	0
85	MG	7	213	1/1	0.70	0.12	44,44,44,44	0
85	MG	n8	201	1/1	0.70	0.12	29,29,29,29	0
85	MG	1	3419	1/1	0.70	0.35	74,74,74,74	0
85	MG	5	3717	1/1	0.71	0.32	58,58,58,58	0
85	MG	5	3727	1/1	0.71	0.27	85,85,85,85	0
85	MG	s8	301	1/1	0.71	0.27	45,45,45,45	0
85	MG	5	3648	1/1	0.71	0.30	72,72,72,72	0
85	MG	1	3733	1/1	0.71	0.19	46,46,46,46	0
85	MG	2	2019	1/1	0.71	0.37	61,61,61,61	0
86	OHX	1	4174	7/7	0.71	0.30	112,112,112,112	0
85	MG	5	3448	1/1	0.71	0.23	54,54,54,54	0
85	MG	1	3651	1/1	0.72	0.23	51,51,51,51	0
85	MG	1	3711	1/1	0.72	0.23	52,52,52,52	0
86	OHX	2	2164	7/7	0.72	0.20	140,140,140,140	0
85	MG	6	2039	1/1	0.72	0.43	67,67,67,67	0
85	MG	1	3631	1/1	0.72	0.36	62,62,62,62	0
85	MG	6	1934	1/1	0.73	0.31	62,62,62,62	0
85	MG	6	2003	1/1	0.73	0.20	60,60,60,60	0
85	MG	M3	203	1/1	0.73	0.41	79,79,79,79	0
85	MG	2	1949	1/1	0.73	0.27	68,68,68,68	0
85	MG	2	1923	1/1	0.73	0.35	53,53,53,53	0
85	MG	5	3812	1/1	0.73	0.18	74,74,74,74	0
86	OHX	1	4189	7/7	0.73	0.22	145,145,145,145	0
85	MG	2	1964	1/1	0.73	0.16	117,117,117,117	0
85	MG	1	3564	1/1	0.74	0.20	35,35,35,35	0
85	MG	6	1912	1/1	0.74	0.28	60,60,60,60	0
85	MG	3	214	1/1	0.74	0.27	50,50,50,50	0
85	MG	2	1994	1/1	0.74	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4178	7/7	0.74	0.23	126,126,126,126	0
85	MG	2	2020	1/1	0.74	0.42	59,59,59,59	0
86	OHX	5	4229	7/7	0.74	0.22	131,131,131,131	0
86	OHX	5	4234	7/7	0.74	0.26	111,111,111,111	0
85	MG	2	2018	1/1	0.74	0.43	62,62,62,62	0
87	ZN	D7	101	1/1	0.74	0.19	133,133,133,133	0
85	MG	5	3683	1/1	0.75	0.31	51,51,51,51	0
85	MG	6	2035	1/1	0.75	0.42	74,74,74,74	0
85	MG	1	3402	1/1	0.75	0.36	51,51,51,51	0
85	MG	2	1983	1/1	0.75	0.31	62,62,62,62	0
85	MG	6	1936	1/1	0.75	0.30	57,57,57,57	0
85	MG	6	1966	1/1	0.75	0.33	73,73,73,73	0
85	MG	6	1978	1/1	0.75	0.23	67,67,67,67	0
85	MG	1	3530	1/1	0.75	0.26	52,52,52,52	0
85	MG	6	2005	1/1	0.75	0.29	81,81,81,81	0
85	MG	1	3865	1/1	0.75	0.42	67,67,67,67	0
85	MG	6	1923	1/1	0.75	0.27	56,56,56,56	0
85	MG	6	2030	1/1	0.75	0.25	83,83,83,83	0
85	MG	5	3679	1/1	0.76	0.08	28,28,28,28	0
85	MG	1	3844	1/1	0.76	0.18	40,40,40,40	0
85	MG	1	3854	1/1	0.76	0.34	52,52,52,52	0
85	MG	1	3767	1/1	0.76	0.14	50,50,50,50	0
85	MG	1	3456	1/1	0.76	0.37	50,50,50,50	0
86	OHX	1	4202	7/7	0.76	0.25	110,110,110,110	0
86	OHX	L6	202	7/7	0.76	0.26	112,112,112,112	0
86	OHX	5	4227	7/7	0.76	0.31	96,96,96,96	0
85	MG	2	1914	1/1	0.76	0.37	55,55,55,55	0
86	OHX	5	4230	7/7	0.76	0.28	99,99,99,99	0
85	MG	5	3886	1/1	0.76	0.47	80,80,80,80	0
85	MG	2	1997	1/1	0.76	0.31	80,80,80,80	0
86	OHX	5	4244	7/7	0.76	0.25	122,122,122,122	0
85	MG	1	3835	1/1	0.76	0.29	46,46,46,46	0
85	MG	s1	301	1/1	0.77	0.23	62,62,62,62	0
85	MG	5	3740	1/1	0.77	0.13	34,34,34,34	0
85	MG	3	202	1/1	0.77	0.18	39,39,39,39	0
86	OHX	1	4190	7/7	0.77	0.24	115,115,115,115	0
85	MG	1	3499	1/1	0.77	0.29	52,52,52,52	0
85	MG	1	3864	1/1	0.77	0.14	33,33,33,33	0
86	OHX	5	4205	7/7	0.77	0.26	113,113,113,113	0
85	MG	6	1907	1/1	0.77	0.32	53,53,53,53	0
85	MG	1	3677	1/1	0.77	0.42	60,60,60,60	0
86	OHX	2	2160	7/7	0.77	0.23	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4233	7/7	0.77	0.23	118,118,118,118	0
85	MG	5	3568	1/1	0.77	0.27	23,23,23,23	0
86	OHX	2	2165	7/7	0.77	0.24	125,125,125,125	0
86	OHX	2	2166	7/7	0.77	0.17	144,144,144,144	0
86	OHX	l4	403	7/7	0.77	0.26	111,111,111,111	0
86	OHX	2	2178	7/7	0.77	0.20	141,141,141,141	0
85	MG	4	221	1/1	0.78	0.39	45,45,45,45	0
85	MG	7	204	1/1	0.78	0.39	61,61,61,61	0
86	OHX	1	4197	7/7	0.78	0.21	117,117,117,117	0
85	MG	5	3786	1/1	0.78	0.33	70,70,70,70	0
85	MG	2	1951	1/1	0.78	0.46	68,68,68,68	0
86	OHX	M9	202	7/7	0.78	0.19	130,130,130,130	0
86	OHX	6	2184	7/7	0.78	0.23	108,108,108,108	0
86	OHX	6	2186	7/7	0.78	0.23	113,113,113,113	0
85	MG	2	1928	1/1	0.78	0.40	69,69,69,69	0
86	OHX	5	4220	7/7	0.78	0.21	133,133,133,133	0
85	MG	5	3732	1/1	0.78	0.34	65,65,65,65	0
85	MG	6	1999	1/1	0.78	0.28	87,87,87,87	0
85	MG	6	1904	1/1	0.78	0.38	56,56,56,56	0
85	MG	2	1907	1/1	0.78	0.37	46,46,46,46	0
86	OHX	2	2179	7/7	0.78	0.19	137,137,137,137	0
86	OHX	2	2181	7/7	0.78	0.22	130,130,130,130	0
86	OHX	5	4240	7/7	0.78	0.14	192,192,192,192	0
86	OHX	1	4144	7/7	0.78	0.26	112,112,112,112	0
85	MG	5	3780	1/1	0.78	0.35	70,70,70,70	0
85	MG	5	3895	1/1	0.78	0.25	51,51,51,51	0
86	OHX	1	4192	7/7	0.79	0.29	98,98,98,98	0
85	MG	2	1950	1/1	0.79	0.22	47,47,47,47	0
85	MG	1	3787	1/1	0.79	0.18	46,46,46,46	0
85	MG	1	3590	1/1	0.79	0.35	34,34,34,34	0
85	MG	1	3490	1/1	0.79	0.20	51,51,51,51	0
86	OHX	2	2161	7/7	0.79	0.24	109,109,109,109	0
85	MG	5	3602	1/1	0.79	0.18	40,40,40,40	0
86	OHX	6	2190	7/7	0.79	0.24	110,110,110,110	0
86	OHX	6	2193	7/7	0.79	0.18	142,142,142,142	0
86	OHX	6	2196	7/7	0.79	0.17	142,142,142,142	0
85	MG	1	3707	1/1	0.79	0.10	46,46,46,46	0
86	OHX	5	4212	7/7	0.79	0.28	98,98,98,98	0
85	MG	1	3495	1/1	0.79	0.21	36,36,36,36	0
85	MG	5	3654	1/1	0.79	0.08	35,35,35,35	0
85	MG	6	2031	1/1	0.79	0.28	59,59,59,59	0
85	MG	1	3840	1/1	0.79	0.28	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4142	7/7	0.79	0.31	89,89,89,89	0
85	MG	4	211	1/1	0.79	0.23	52,52,52,52	0
85	MG	1	3426	1/1	0.79	0.14	44,44,44,44	0
85	MG	1	3734	1/1	0.79	0.25	68,68,68,68	0
86	OHX	1	4188	7/7	0.79	0.23	115,115,115,115	0
86	OHX	7	227	7/7	0.79	0.19	127,127,127,127	0
85	MG	2	1976	1/1	0.79	0.28	43,43,43,43	0
86	OHX	m1	203	7/7	0.79	0.21	124,124,124,124	0
85	MG	6	1984	1/1	0.79	0.17	70,70,70,70	0
85	MG	1	3626	1/1	0.80	0.17	39,39,39,39	0
86	OHX	6	2185	7/7	0.80	0.16	143,143,143,143	0
85	MG	2	2002	1/1	0.80	0.22	87,87,87,87	0
85	MG	1	3636	1/1	0.80	0.15	43,43,43,43	0
85	MG	5	3667	1/1	0.80	0.12	31,31,31,31	0
85	MG	2	2183	1/1	0.80	0.34	73,73,73,73	0
86	OHX	5	4163	7/7	0.80	0.18	145,145,145,145	0
85	MG	1	3782	1/1	0.80	0.15	46,46,46,46	0
85	MG	5	3852	1/1	0.80	0.13	58,58,58,58	0
86	OHX	5	4219	7/7	0.80	0.24	111,111,111,111	0
85	MG	5	3875	1/1	0.80	0.29	30,30,30,30	0
86	OHX	5	4224	7/7	0.80	0.21	113,113,113,113	0
85	MG	S8	301	1/1	0.80	0.19	51,51,51,51	0
85	MG	2	1978	1/1	0.80	0.27	80,80,80,80	0
86	OHX	1	4180	7/7	0.80	0.21	120,120,120,120	0
86	OHX	1	4183	7/7	0.80	0.24	110,110,110,110	0
85	MG	6	2013	1/1	0.80	0.10	42,42,42,42	0
85	MG	2	1961	1/1	0.80	0.23	54,54,54,54	0
86	OHX	5	4238	7/7	0.80	0.23	117,117,117,117	0
86	OHX	5	4239	7/7	0.80	0.19	149,149,149,149	0
85	MG	5	3500	1/1	0.80	0.15	45,45,45,45	0
85	MG	2	1926	1/1	0.80	0.41	77,77,77,77	0
85	MG	5	3600	1/1	0.80	0.12	50,50,50,50	0
85	MG	o1	201	1/1	0.80	0.12	76,76,76,76	0
85	MG	2	1930	1/1	0.80	0.23	53,53,53,53	0
86	OHX	m4	202	7/7	0.80	0.14	190,190,190,190	0
85	MG	2	1946	1/1	0.80	0.36	64,64,64,64	0
85	MG	6	1939	1/1	0.81	0.33	51,51,51,51	0
85	MG	6	1963	1/1	0.81	0.25	67,67,67,67	0
86	OHX	M7	208	7/7	0.81	0.24	109,109,109,109	0
85	MG	1	3655	1/1	0.81	0.16	25,25,25,25	0
86	OHX	6	2181	7/7	0.81	0.24	113,113,113,113	0
85	MG	6	1968	1/1	0.81	0.34	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	8	209	1/1	0.81	0.24	56,56,56,56	0
85	MG	1	3624	1/1	0.81	0.43	69,69,69,69	0
86	OHX	6	2188	7/7	0.81	0.21	120,120,120,120	0
85	MG	2	1924	1/1	0.81	0.42	65,65,65,65	0
86	OHX	2	2159	7/7	0.81	0.12	260,260,260,260	0
85	MG	5	3756	1/1	0.81	0.14	36,36,36,36	0
86	OHX	6	2204	7/7	0.81	0.20	118,118,118,118	0
85	MG	N0	201	1/1	0.81	0.27	42,42,42,42	0
86	OHX	5	4186	7/7	0.81	0.21	120,120,120,120	0
86	OHX	5	4204	7/7	0.81	0.23	111,111,111,111	0
86	OHX	2	2163	7/7	0.81	0.18	138,138,138,138	0
85	MG	5	3469	1/1	0.81	0.24	101,101,101,101	0
85	MG	5	3477	1/1	0.81	0.32	59,59,59,59	0
85	MG	1	3808	1/1	0.81	0.17	30,30,30,30	0
85	MG	2	1905	1/1	0.81	0.35	51,51,51,51	0
85	MG	5	3789	1/1	0.81	0.19	36,36,36,36	0
85	MG	1	3819	1/1	0.81	0.08	42,42,42,42	0
85	MG	3	201	1/1	0.81	0.35	59,59,59,59	0
85	MG	5	3801	1/1	0.81	0.18	50,50,50,50	0
86	OHX	1	4167	7/7	0.81	0.24	103,103,103,103	0
86	OHX	1	4173	7/7	0.81	0.20	132,132,132,132	0
85	MG	5	3605	1/1	0.81	0.25	46,46,46,46	0
85	MG	1	3465	1/1	0.81	0.24	41,41,41,41	0
85	MG	5	3818	1/1	0.81	0.09	51,51,51,51	0
85	MG	6	2029	1/1	0.81	0.51	68,68,68,68	0
85	MG	1	3821	1/1	0.81	0.10	37,37,37,37	0
86	OHX	8	225	7/7	0.81	0.21	103,103,103,103	0
85	MG	1	3475	1/1	0.81	0.26	64,64,64,64	0
86	OHX	l5	306	7/7	0.81	0.21	114,114,114,114	0
85	MG	2	1931	1/1	0.81	0.33	60,60,60,60	0
85	MG	1	3493	1/1	0.81	0.34	69,69,69,69	0
86	OHX	m8	201	7/7	0.81	0.24	111,111,111,111	0
85	MG	5	3893	1/1	0.81	0.12	95,95,95,95	0
85	MG	8	206	1/1	0.82	0.17	44,44,44,44	0
85	MG	5	3767	1/1	0.82	0.10	29,29,29,29	0
86	OHX	O9	101	7/7	0.82	0.27	88,88,88,88	0
85	MG	5	3479	1/1	0.82	0.30	56,56,56,56	0
86	OHX	6	2183	7/7	0.82	0.20	118,118,118,118	0
85	MG	1	3687	1/1	0.82	0.33	69,69,69,69	0
85	MG	6	1952	1/1	0.82	0.34	53,53,53,53	0
85	MG	6	1958	1/1	0.82	0.36	46,46,46,46	0
85	MG	1	3828	1/1	0.82	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2189	7/7	0.82	0.22	115,115,115,115	0
85	MG	6	2034	1/1	0.82	0.23	50,50,50,50	0
85	MG	5	3636	1/1	0.82	0.10	40,40,40,40	0
85	MG	1	3616	1/1	0.82	0.14	32,32,32,32	0
85	MG	1	3479	1/1	0.82	0.32	70,70,70,70	0
85	MG	6	1970	1/1	0.82	0.13	49,49,49,49	0
85	MG	6	2045	1/1	0.82	0.41	63,63,63,63	0
85	MG	1	3470	1/1	0.82	0.19	37,37,37,37	0
85	MG	1	3731	1/1	0.82	0.11	40,40,40,40	0
85	MG	5	3401	1/1	0.82	0.26	36,36,36,36	0
86	OHX	5	4217	7/7	0.82	0.23	106,106,106,106	0
85	MG	5	3856	1/1	0.82	0.43	68,68,68,68	0
86	OHX	1	4169	7/7	0.82	0.28	90,90,90,90	0
85	MG	5	3865	1/1	0.82	0.17	38,38,38,38	0
86	OHX	5	4226	7/7	0.82	0.19	130,130,130,130	0
85	MG	5	3866	1/1	0.82	0.08	31,31,31,31	0
85	MG	1	3853	1/1	0.82	0.16	35,35,35,35	0
86	OHX	1	4179	7/7	0.82	0.28	101,101,101,101	0
85	MG	4	204	1/1	0.82	0.34	60,60,60,60	0
85	MG	2	1990	1/1	0.82	0.34	51,51,51,51	0
86	OHX	1	4185	7/7	0.82	0.22	111,111,111,111	0
85	MG	5	3887	1/1	0.82	0.40	53,53,53,53	0
85	MG	6	2007	1/1	0.82	0.14	50,50,50,50	0
85	MG	1	3611	1/1	0.82	0.09	36,36,36,36	0
86	OHX	1	4191	7/7	0.82	0.24	104,104,104,104	0
86	OHX	5	4246	7/7	0.82	0.20	122,122,122,122	0
86	OHX	7	225	7/7	0.82	0.21	118,118,118,118	0
85	MG	1	3752	1/1	0.82	0.24	48,48,48,48	0
85	MG	5	3762	1/1	0.82	0.19	34,34,34,34	0
86	OHX	1	4199	7/7	0.82	0.25	107,107,107,107	0
86	OHX	1	4200	7/7	0.82	0.22	112,112,112,112	0
85	MG	5	3765	1/1	0.82	0.12	46,46,46,46	0
86	OHX	1	4205	7/7	0.82	0.22	108,108,108,108	0
86	OHX	4	236	7/7	0.82	0.26	105,105,105,105	0
85	MG	7	215	1/1	0.82	0.31	48,48,48,48	0
86	OHX	6	2170	7/7	0.83	0.20	117,117,117,117	0
86	OHX	6	2178	7/7	0.83	0.20	114,114,114,114	0
85	MG	1	3407	1/1	0.83	0.17	34,34,34,34	0
86	OHX	2	2173	7/7	0.83	0.21	121,121,121,121	0
85	MG	1	3411	1/1	0.83	0.18	33,33,33,33	0
85	MG	6	1967	1/1	0.83	0.20	59,59,59,59	0
85	MG	1	3824	1/1	0.83	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4130	7/7	0.83	0.19	120,120,120,120	0
85	MG	2	1934	1/1	0.83	0.32	58,58,58,58	0
85	MG	1	3713	1/1	0.83	0.51	73,73,73,73	0
86	OHX	1	4162	7/7	0.83	0.19	121,121,121,121	0
86	OHX	6	2195	7/7	0.83	0.19	127,127,127,127	0
85	MG	1	3721	1/1	0.83	0.31	44,44,44,44	0
86	OHX	6	2203	7/7	0.83	0.21	117,117,117,117	0
85	MG	5	3884	1/1	0.83	0.39	55,55,55,55	0
86	OHX	c3	201	7/7	0.83	0.19	122,122,122,122	0
86	OHX	1	4172	7/7	0.83	0.18	123,123,123,123	0
85	MG	5	3429	1/1	0.83	0.34	59,59,59,59	0
86	OHX	5	4190	7/7	0.83	0.25	98,98,98,98	0
86	OHX	5	4193	7/7	0.83	0.25	107,107,107,107	0
86	OHX	5	4203	7/7	0.83	0.22	110,110,110,110	0
85	MG	6	1987	1/1	0.83	0.17	54,54,54,54	0
85	MG	1	3639	1/1	0.83	0.12	56,56,56,56	0
85	MG	5	3894	1/1	0.83	0.31	45,45,45,45	0
85	MG	2	1939	1/1	0.83	0.28	57,57,57,57	0
86	OHX	5	4218	7/7	0.83	0.16	141,141,141,141	0
85	MG	1	3607	1/1	0.83	0.27	45,45,45,45	0
85	MG	1	3738	1/1	0.83	0.16	24,24,24,24	0
86	OHX	5	4223	7/7	0.83	0.21	117,117,117,117	0
86	OHX	1	4187	7/7	0.83	0.25	105,105,105,105	0
85	MG	5	3484	1/1	0.83	0.27	42,42,42,42	0
85	MG	2	1904	1/1	0.83	0.46	62,62,62,62	0
85	MG	5	3550	1/1	0.83	0.17	36,36,36,36	0
85	MG	1	3615	1/1	0.83	0.20	31,31,31,31	0
85	MG	1	3659	1/1	0.83	0.16	49,49,49,49	0
86	OHX	1	4195	7/7	0.83	0.19	116,116,116,116	0
85	MG	1	3663	1/1	0.83	0.11	31,31,31,31	0
86	OHX	1	4198	7/7	0.83	0.18	125,125,125,125	0
85	MG	o4	202	1/1	0.83	0.31	50,50,50,50	0
86	OHX	2	2125	7/7	0.83	0.19	120,120,120,120	0
86	OHX	2	2146	7/7	0.83	0.20	115,115,115,115	0
86	OHX	1	4204	7/7	0.83	0.24	109,109,109,109	0
85	MG	1	3666	1/1	0.83	0.10	30,30,30,30	0
86	OHX	1	4211	7/7	0.83	0.26	106,106,106,106	0
86	OHX	4	234	7/7	0.83	0.21	116,116,116,116	0
85	MG	5	3630	1/1	0.83	0.46	75,75,75,75	0
85	MG	1	3672	1/1	0.83	0.16	36,36,36,36	0
85	MG	3	203	1/1	0.83	0.25	75,75,75,75	0
85	MG	2	1948	1/1	0.83	0.43	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	2	1987	1/1	0.83	0.27	91,91,91,91	0
86	OHX	6	2148	7/7	0.83	0.19	108,108,108,108	0
86	OHX	1	4203	7/7	0.84	0.23	108,108,108,108	0
85	MG	5	3672	1/1	0.84	0.16	57,57,57,57	0
85	MG	2	1965	1/1	0.84	0.30	74,74,74,74	0
85	MG	7	214	1/1	0.84	0.25	54,54,54,54	0
86	OHX	1	4214	7/7	0.84	0.24	103,103,103,103	0
86	OHX	1	4215	7/7	0.84	0.22	118,118,118,118	0
85	MG	6	1910	1/1	0.84	0.24	54,54,54,54	0
86	OHX	4	235	7/7	0.84	0.21	108,108,108,108	0
85	MG	5	3696	1/1	0.84	0.18	36,36,36,36	0
86	OHX	L3	404	7/7	0.84	0.19	128,128,128,128	0
85	MG	1	3852	1/1	0.84	0.17	43,43,43,43	0
86	OHX	M7	207	7/7	0.84	0.30	83,83,83,83	0
85	MG	l5	303	1/1	0.84	0.19	51,51,51,51	0
85	MG	6	1915	1/1	0.84	0.23	57,57,57,57	0
85	MG	1	3417	1/1	0.84	0.27	34,34,34,34	0
85	MG	5	3731	1/1	0.84	0.10	37,37,37,37	0
86	OHX	2	2116	7/7	0.84	0.20	111,111,111,111	0
85	MG	1	3732	1/1	0.84	0.13	37,37,37,37	0
86	OHX	2	2138	7/7	0.84	0.17	132,132,132,132	0
86	OHX	2	2144	7/7	0.84	0.23	105,105,105,105	0
85	MG	5	3737	1/1	0.84	0.14	36,36,36,36	0
86	OHX	2	2157	7/7	0.84	0.14	195,195,195,195	0
85	MG	5	3738	1/1	0.84	0.35	61,61,61,61	0
86	OHX	6	2187	7/7	0.84	0.16	136,136,136,136	0
85	MG	6	2041	1/1	0.84	0.47	65,65,65,65	0
85	MG	6	1933	1/1	0.84	0.37	53,53,53,53	0
85	MG	5	3761	1/1	0.84	0.22	64,64,64,64	0
86	OHX	6	2191	7/7	0.84	0.19	131,131,131,131	0
86	OHX	6	2192	7/7	0.84	0.18	130,130,130,130	0
85	MG	2	1910	1/1	0.84	0.30	48,48,48,48	0
85	MG	2	1999	1/1	0.84	0.10	83,83,83,83	0
85	MG	2	1929	1/1	0.84	0.34	51,51,51,51	0
85	MG	5	3769	1/1	0.84	0.14	86,86,86,86	0
86	OHX	2	2176	7/7	0.84	0.20	125,125,125,125	0
85	MG	5	3412	1/1	0.84	0.12	26,26,26,26	0
86	OHX	5	4145	7/7	0.84	0.24	93,93,93,93	0
86	OHX	5	4159	7/7	0.84	0.22	101,101,101,101	0
85	MG	6	1941	1/1	0.84	0.20	41,41,41,41	0
86	OHX	5	4181	7/7	0.84	0.20	107,107,107,107	0
86	OHX	2	2180	7/7	0.84	0.21	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3447	1/1	0.84	0.27	44,44,44,44	0
86	OHX	1	4066	7/7	0.84	0.23	106,106,106,106	0
86	OHX	5	4194	7/7	0.84	0.19	116,116,116,116	0
86	OHX	5	4200	7/7	0.84	0.19	114,114,114,114	0
86	OHX	5	4202	7/7	0.84	0.22	112,112,112,112	0
85	MG	1	3547	1/1	0.84	0.11	32,32,32,32	0
86	OHX	1	4135	7/7	0.84	0.24	95,95,95,95	0
86	OHX	1	4141	7/7	0.84	0.21	113,113,113,113	0
85	MG	1	3548	1/1	0.84	0.33	42,42,42,42	0
85	MG	2	1952	1/1	0.84	0.38	75,75,75,75	0
86	OHX	1	4148	7/7	0.84	0.20	118,118,118,118	0
86	OHX	1	4152	7/7	0.84	0.18	124,124,124,124	0
85	MG	1	3566	1/1	0.84	0.33	33,33,33,33	0
85	MG	1	3801	1/1	0.84	0.11	41,41,41,41	0
85	MG	1	3462	1/1	0.84	0.17	23,23,23,23	0
85	MG	1	3464	1/1	0.84	0.10	31,31,31,31	0
85	MG	5	3805	1/1	0.84	0.19	87,87,87,87	0
85	MG	5	3489	1/1	0.84	0.13	42,42,42,42	0
85	MG	5	3814	1/1	0.84	0.22	53,53,53,53	0
85	MG	6	1981	1/1	0.84	0.21	47,47,47,47	0
85	MG	5	3837	1/1	0.84	0.16	40,40,40,40	0
85	MG	2	2005	1/1	0.84	0.17	59,59,59,59	0
85	MG	4	216	1/1	0.84	0.13	55,55,55,55	0
85	MG	5	3578	1/1	0.84	0.21	28,28,28,28	0
85	MG	6	1992	1/1	0.84	0.12	40,40,40,40	0
85	MG	2	1963	1/1	0.84	0.29	65,65,65,65	0
86	OHX	5	4245	7/7	0.84	0.22	119,119,119,119	0
85	MG	1	3696	1/1	0.84	0.12	35,35,35,35	0
86	OHX	5	4247	7/7	0.84	0.22	102,102,102,102	0
85	MG	5	3627	1/1	0.84	0.24	52,52,52,52	0
85	MG	1	3700	1/1	0.84	0.11	31,31,31,31	0
86	OHX	1	4193	7/7	0.84	0.22	110,110,110,110	0
85	MG	1	3471	1/1	0.84	0.12	35,35,35,35	0
85	MG	2	1941	1/1	0.84	0.21	50,50,50,50	0
85	MG	N8	201	1/1	0.84	0.10	26,26,26,26	0
85	MG	1	3622	1/1	0.84	0.21	42,42,42,42	0
85	MG	6	2027	1/1	0.84	0.26	61,61,61,61	0
85	MG	1	3478	1/1	0.84	0.17	36,36,36,36	0
87	ZN	d7	101	1/1	0.84	0.21	119,119,119,119	0
86	OHX	1	4182	7/7	0.85	0.22	106,106,106,106	0
85	MG	4	219	1/1	0.85	0.18	45,45,45,45	0
86	OHX	6	2194	7/7	0.85	0.16	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4184	7/7	0.85	0.25	86,86,86,86	0
86	OHX	2	2141	7/7	0.85	0.18	133,133,133,133	0
85	MG	5	3855	1/1	0.85	0.19	42,42,42,42	0
85	MG	6	1975	1/1	0.85	0.27	53,53,53,53	0
86	OHX	s9	201	7/7	0.85	0.22	102,102,102,102	0
86	OHX	2	2150	7/7	0.85	0.16	134,134,134,134	0
86	OHX	5	4139	7/7	0.85	0.23	105,105,105,105	0
85	MG	5	3422	1/1	0.85	0.24	47,47,47,47	0
86	OHX	5	4146	7/7	0.85	0.23	100,100,100,100	0
85	MG	5	3424	1/1	0.85	0.17	34,34,34,34	0
85	MG	5	3872	1/1	0.85	0.27	34,34,34,34	0
85	MG	5	3873	1/1	0.85	0.40	47,47,47,47	0
86	OHX	2	2162	7/7	0.85	0.19	126,126,126,126	0
85	MG	5	3640	1/1	0.85	0.11	32,32,32,32	0
85	MG	1	3751	1/1	0.85	0.12	34,34,34,34	0
85	MG	1	3708	1/1	0.85	0.15	34,34,34,34	0
85	MG	1	3480	1/1	0.85	0.27	57,57,57,57	0
86	OHX	2	2170	7/7	0.85	0.20	126,126,126,126	0
85	MG	1	3488	1/1	0.85	0.13	42,42,42,42	0
85	MG	5	3888	1/1	0.85	0.14	32,32,32,32	0
85	MG	1	3769	1/1	0.85	0.24	53,53,53,53	0
86	OHX	5	4209	7/7	0.85	0.24	91,91,91,91	0
86	OHX	1	4206	7/7	0.85	0.22	106,106,106,106	0
86	OHX	5	4214	7/7	0.85	0.22	110,110,110,110	0
85	MG	5	3478	1/1	0.85	0.28	50,50,50,50	0
85	MG	2	1996	1/1	0.85	0.41	48,48,48,48	0
85	MG	2	1959	1/1	0.85	0.46	66,66,66,66	0
86	OHX	3	224	7/7	0.85	0.17	132,132,132,132	0
86	OHX	5	4222	7/7	0.85	0.25	101,101,101,101	0
85	MG	5	3897	1/1	0.85	0.18	44,44,44,44	0
85	MG	5	3689	1/1	0.85	0.13	45,45,45,45	0
86	OHX	1	4134	7/7	0.85	0.19	127,127,127,127	0
85	MG	6	2042	1/1	0.85	0.39	65,65,65,65	0
85	MG	5	3701	1/1	0.85	0.20	56,56,56,56	0
85	MG	1	3790	1/1	0.85	0.10	33,33,33,33	0
85	MG	8	202	1/1	0.85	0.12	47,47,47,47	0
86	OHX	1	4147	7/7	0.85	0.20	120,120,120,120	0
86	OHX	5	4235	7/7	0.85	0.25	106,106,106,106	0
85	MG	8	205	1/1	0.85	0.13	59,59,59,59	0
86	OHX	6	2136	7/7	0.85	0.22	105,105,105,105	0
85	MG	5	3527	1/1	0.85	0.11	26,26,26,26	0
86	OHX	6	2165	7/7	0.85	0.19	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	2	1909	1/1	0.85	0.35	59,59,59,59	0
86	OHX	6	2174	7/7	0.85	0.24	101,101,101,101	0
86	OHX	1	4166	7/7	0.85	0.18	130,130,130,130	0
86	OHX	6	2179	7/7	0.85	0.17	123,123,123,123	0
86	OHX	5	4248	7/7	0.85	0.19	126,126,126,126	0
85	MG	1	3406	1/1	0.85	0.10	26,26,26,26	0
85	MG	n6	201	1/1	0.85	0.16	52,52,52,52	0
86	OHX	1	4171	7/7	0.85	0.25	91,91,91,91	0
85	MG	5	3816	1/1	0.85	0.13	37,37,37,37	0
85	MG	c7	201	1/1	0.85	0.37	63,63,63,63	0
85	MG	5	3822	1/1	0.85	0.26	78,78,78,78	0
86	OHX	1	4177	7/7	0.85	0.19	114,114,114,114	0
85	MG	1	3592	1/1	0.85	0.33	43,43,43,43	0
86	OHX	2	2120	7/7	0.85	0.19	111,111,111,111	0
85	MG	1	3528	1/1	0.85	0.25	37,37,37,37	0
86	OHX	1	4116	7/7	0.86	0.27	91,91,91,91	0
85	MG	4	202	1/1	0.86	0.26	48,48,48,48	0
86	OHX	6	2175	7/7	0.86	0.19	122,122,122,122	0
86	OHX	1	4132	7/7	0.86	0.16	129,129,129,129	0
86	OHX	1	4133	7/7	0.86	0.19	121,121,121,121	0
85	MG	1	3421	1/1	0.86	0.24	37,37,37,37	0
85	MG	2	2008	1/1	0.86	0.36	40,40,40,40	0
86	OHX	1	4136	7/7	0.86	0.21	106,106,106,106	0
86	OHX	1	4138	7/7	0.86	0.23	91,91,91,91	0
85	MG	5	3880	1/1	0.86	0.25	45,45,45,45	0
85	MG	5	3691	1/1	0.86	0.14	38,38,38,38	0
85	MG	1	3542	1/1	0.86	0.28	27,27,27,27	0
86	OHX	1	4145	7/7	0.86	0.18	110,110,110,110	0
86	OHX	1	4146	7/7	0.86	0.24	94,94,94,94	0
85	MG	1	3634	1/1	0.86	0.33	60,60,60,60	0
85	MG	5	3702	1/1	0.86	0.11	44,44,44,44	0
85	MG	1	3546	1/1	0.86	0.28	52,52,52,52	0
85	MG	6	1972	1/1	0.86	0.11	46,46,46,46	0
85	MG	1	3427	1/1	0.86	0.17	27,27,27,27	0
85	MG	L3	402	1/1	0.86	0.15	43,43,43,43	0
86	OHX	6	2199	7/7	0.86	0.21	110,110,110,110	0
86	OHX	6	2200	7/7	0.86	0.21	115,115,115,115	0
86	OHX	1	4168	7/7	0.86	0.13	161,161,161,161	0
85	MG	L5	301	1/1	0.86	0.35	50,50,50,50	0
86	OHX	s1	303	7/7	0.86	0.18	128,128,128,128	0
86	OHX	1	4170	7/7	0.86	0.23	95,95,95,95	0
85	MG	5	3455	1/1	0.86	0.21	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4109	7/7	0.86	0.29	93,93,93,93	0
85	MG	2	1980	1/1	0.86	0.19	55,55,55,55	0
85	MG	6	1986	1/1	0.86	0.08	39,39,39,39	0
85	MG	5	3742	1/1	0.86	0.14	32,32,32,32	0
86	OHX	5	4151	7/7	0.86	0.25	92,92,92,92	0
86	OHX	5	4152	7/7	0.86	0.25	95,95,95,95	0
85	MG	5	3746	1/1	0.86	0.28	51,51,51,51	0
86	OHX	5	4162	7/7	0.86	0.20	115,115,115,115	0
85	MG	5	3474	1/1	0.86	0.29	64,64,64,64	0
86	OHX	5	4164	7/7	0.86	0.20	111,111,111,111	0
86	OHX	5	4174	7/7	0.86	0.22	109,109,109,109	0
85	MG	M3	204	1/1	0.86	0.09	24,24,24,24	0
85	MG	1	3553	1/1	0.86	0.17	46,46,46,46	0
85	MG	8	208	1/1	0.86	0.12	34,34,34,34	0
85	MG	5	3764	1/1	0.86	0.16	30,30,30,30	0
85	MG	1	3554	1/1	0.86	0.19	21,21,21,21	0
86	OHX	5	4195	7/7	0.86	0.24	95,95,95,95	0
85	MG	6	2000	1/1	0.86	0.15	42,42,42,42	0
86	OHX	5	4201	7/7	0.86	0.24	104,104,104,104	0
85	MG	5	3485	1/1	0.86	0.12	41,41,41,41	0
85	MG	1	3560	1/1	0.86	0.28	28,28,28,28	0
85	MG	5	3494	1/1	0.86	0.11	23,23,23,23	0
85	MG	q1	101	1/1	0.86	0.20	39,39,39,39	0
85	MG	5	3776	1/1	0.86	0.23	56,56,56,56	0
86	OHX	5	4210	7/7	0.86	0.21	109,109,109,109	0
86	OHX	5	4211	7/7	0.86	0.19	118,118,118,118	0
85	MG	5	3496	1/1	0.86	0.17	39,39,39,39	0
85	MG	2	2012	1/1	0.86	0.35	57,57,57,57	0
85	MG	5	3782	1/1	0.86	0.13	64,64,64,64	0
86	OHX	2	2140	7/7	0.86	0.19	125,125,125,125	0
85	MG	5	3503	1/1	0.86	0.27	45,45,45,45	0
85	MG	1	3858	1/1	0.86	0.23	36,36,36,36	0
85	MG	1	3484	1/1	0.86	0.32	38,38,38,38	0
85	MG	5	3566	1/1	0.86	0.28	24,24,24,24	0
85	MG	2	1944	1/1	0.86	0.14	53,53,53,53	0
86	OHX	5	4225	7/7	0.86	0.22	105,105,105,105	0
85	MG	2	1945	1/1	0.86	0.20	51,51,51,51	0
85	MG	2	1919	1/1	0.86	0.37	62,62,62,62	0
85	MG	6	1920	1/1	0.86	0.38	58,58,58,58	0
86	OHX	1	4207	7/7	0.86	0.23	111,111,111,111	0
86	OHX	1	4210	7/7	0.86	0.25	100,100,100,100	0
85	MG	1	3686	1/1	0.86	0.20	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	2	1977	1/1	0.86	0.27	73,73,73,73	0
85	MG	6	1930	1/1	0.86	0.17	46,46,46,46	0
86	OHX	5	4237	7/7	0.86	0.17	116,116,116,116	0
85	MG	2	1947	1/1	0.86	0.21	50,50,50,50	0
86	OHX	4	232	7/7	0.86	0.21	93,93,93,93	0
86	OHX	4	233	7/7	0.86	0.17	121,121,121,121	0
86	OHX	5	4241	7/7	0.86	0.28	81,81,81,81	0
85	MG	6	2038	1/1	0.86	0.37	48,48,48,48	0
85	MG	5	3839	1/1	0.86	0.09	30,30,30,30	0
85	MG	3	208	1/1	0.86	0.24	66,66,66,66	0
85	MG	1	3507	1/1	0.86	0.24	22,22,22,22	0
85	MG	6	1937	1/1	0.86	0.26	36,36,36,36	0
85	MG	1	3508	1/1	0.86	0.25	19,19,19,19	0
85	MG	5	3858	1/1	0.86	0.26	70,70,70,70	0
86	OHX	8	224	7/7	0.86	0.21	108,108,108,108	0
85	MG	1	3515	1/1	0.86	0.34	29,29,29,29	0
85	MG	4	201	1/1	0.86	0.32	50,50,50,50	0
86	OHX	1	4073	7/7	0.86	0.23	94,94,94,94	0
86	OHX	m0	302	7/7	0.86	0.24	96,96,96,96	0
86	OHX	1	4092	7/7	0.86	0.27	88,88,88,88	0
86	OHX	6	2152	7/7	0.86	0.19	126,126,126,126	0
86	OHX	6	2159	7/7	0.86	0.20	96,96,96,96	0
86	OHX	1	4096	7/7	0.86	0.16	123,123,123,123	0
86	OHX	6	2169	7/7	0.86	0.18	124,124,124,124	0
86	OHX	2	2137	7/7	0.87	0.21	104,104,104,104	0
86	OHX	6	2198	7/7	0.87	0.20	117,117,117,117	0
85	MG	5	3808	1/1	0.87	0.12	59,59,59,59	0
85	MG	1	3635	1/1	0.87	0.33	55,55,55,55	0
85	MG	5	3436	1/1	0.87	0.20	36,36,36,36	0
85	MG	5	3663	1/1	0.87	0.10	35,35,35,35	0
85	MG	1	3685	1/1	0.87	0.15	45,45,45,45	0
86	OHX	s8	303	7/7	0.87	0.18	129,129,129,129	0
85	MG	1	3502	1/1	0.87	0.28	35,35,35,35	0
86	OHX	2	2152	7/7	0.87	0.15	145,145,145,145	0
86	OHX	d4	201	7/7	0.87	0.17	120,120,120,120	0
86	OHX	2	2156	7/7	0.87	0.19	114,114,114,114	0
86	OHX	5	4137	7/7	0.87	0.24	101,101,101,101	0
86	OHX	5	4138	7/7	0.87	0.18	111,111,111,111	0
85	MG	5	3834	1/1	0.87	0.09	31,31,31,31	0
85	MG	5	3465	1/1	0.87	0.21	48,48,48,48	0
85	MG	1	3428	1/1	0.87	0.19	41,41,41,41	0
86	OHX	5	4147	7/7	0.87	0.21	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3467	1/1	0.87	0.20	31,31,31,31	0
85	MG	4	214	1/1	0.87	0.12	43,43,43,43	0
86	OHX	5	4155	7/7	0.87	0.18	111,111,111,111	0
86	OHX	5	4157	7/7	0.87	0.24	87,87,87,87	0
85	MG	5	3854	1/1	0.87	0.10	54,54,54,54	0
85	MG	1	3746	1/1	0.87	0.16	50,50,50,50	0
85	MG	1	3689	1/1	0.87	0.07	25,25,25,25	0
85	MG	1	3841	1/1	0.87	0.28	37,37,37,37	0
86	OHX	5	4167	7/7	0.87	0.21	108,108,108,108	0
85	MG	5	3705	1/1	0.87	0.14	41,41,41,41	0
86	OHX	5	4179	7/7	0.87	0.20	113,113,113,113	0
86	OHX	5	4180	7/7	0.87	0.18	120,120,120,120	0
86	OHX	2	2172	7/7	0.87	0.19	119,119,119,119	0
86	OHX	5	4182	7/7	0.87	0.22	98,98,98,98	0
86	OHX	5	4185	7/7	0.87	0.24	94,94,94,94	0
86	OHX	1	4201	7/7	0.87	0.21	100,100,100,100	0
86	OHX	5	4188	7/7	0.87	0.18	111,111,111,111	0
85	MG	1	3690	1/1	0.87	0.29	49,49,49,49	0
85	MG	5	3712	1/1	0.87	0.11	38,38,38,38	0
85	MG	1	3481	1/1	0.87	0.25	31,31,31,31	0
85	MG	5	3718	1/1	0.87	0.10	49,49,49,49	0
85	MG	1	3758	1/1	0.87	0.09	23,23,23,23	0
85	MG	5	3488	1/1	0.87	0.18	41,41,41,41	0
86	OHX	S8	302	7/7	0.87	0.17	126,126,126,126	0
85	MG	6	1964	1/1	0.87	0.25	44,44,44,44	0
86	OHX	1	4213	7/7	0.87	0.16	128,128,128,128	0
85	MG	6	2036	1/1	0.87	0.32	62,62,62,62	0
86	OHX	5	4208	7/7	0.87	0.20	110,110,110,110	0
86	OHX	1	4085	7/7	0.87	0.17	114,114,114,114	0
85	MG	1	3649	1/1	0.87	0.11	19,19,19,19	0
86	OHX	1	4093	7/7	0.87	0.19	109,109,109,109	0
85	MG	1	3703	1/1	0.87	0.25	49,49,49,49	0
86	OHX	1	4099	7/7	0.87	0.17	115,115,115,115	0
86	OHX	5	4216	7/7	0.87	0.20	113,113,113,113	0
86	OHX	1	4111	7/7	0.87	0.21	110,110,110,110	0
85	MG	1	3773	1/1	0.87	0.12	37,37,37,37	0
86	OHX	1	4119	7/7	0.87	0.21	103,103,103,103	0
86	OHX	1	4128	7/7	0.87	0.25	96,96,96,96	0
86	OHX	5	4221	7/7	0.87	0.19	113,113,113,113	0
85	MG	1	3429	1/1	0.87	0.20	36,36,36,36	0
85	MG	5	3748	1/1	0.87	0.24	29,29,29,29	0
85	MG	5	3542	1/1	0.87	0.28	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3785	1/1	0.87	0.28	55,55,55,55	0
85	MG	5	3564	1/1	0.87	0.31	38,38,38,38	0
85	MG	1	3617	1/1	0.87	0.22	48,48,48,48	0
85	MG	1	3420	1/1	0.87	0.44	57,57,57,57	0
85	MG	1	3795	1/1	0.87	0.19	51,51,51,51	0
86	OHX	6	2160	7/7	0.87	0.24	103,103,103,103	0
86	OHX	6	2164	7/7	0.87	0.13	153,153,153,153	0
85	MG	5	3580	1/1	0.87	0.31	36,36,36,36	0
85	MG	5	3588	1/1	0.87	0.29	30,30,30,30	0
85	MG	1	3414	1/1	0.87	0.18	28,28,28,28	0
86	OHX	6	2173	7/7	0.87	0.20	116,116,116,116	0
85	MG	1	3448	1/1	0.87	0.12	32,32,32,32	0
85	MG	5	3403	1/1	0.87	0.37	53,53,53,53	0
86	OHX	6	2177	7/7	0.87	0.24	97,97,97,97	0
86	OHX	5	4242	7/7	0.87	0.17	124,124,124,124	0
85	MG	5	3409	1/1	0.87	0.23	39,39,39,39	0
86	OHX	1	4150	7/7	0.87	0.19	111,111,111,111	0
86	OHX	6	2180	7/7	0.87	0.22	106,106,106,106	0
85	MG	1	3718	1/1	0.87	0.18	33,33,33,33	0
85	MG	5	3635	1/1	0.87	0.23	39,39,39,39	0
86	OHX	5	4250	7/7	0.87	0.17	128,128,128,128	0
86	OHX	1	4163	7/7	0.87	0.18	118,118,118,118	0
86	OHX	1	4165	7/7	0.87	0.17	123,123,123,123	0
85	MG	n8	202	1/1	0.87	0.11	19,19,19,19	0
85	MG	6	1918	1/1	0.87	0.43	57,57,57,57	0
86	OHX	l4	402	7/7	0.87	0.19	103,103,103,103	0
85	MG	6	1996	1/1	0.87	0.27	62,62,62,62	0
85	MG	5	3643	1/1	0.87	0.13	37,37,37,37	0
86	OHX	2	2094	7/7	0.87	0.16	119,119,119,119	0
85	MG	2	1992	1/1	0.87	0.10	50,50,50,50	0
85	MG	2	1970	1/1	0.87	0.25	60,60,60,60	0
86	OHX	m7	206	7/7	0.87	0.23	99,99,99,99	0
85	MG	5	3653	1/1	0.87	0.15	46,46,46,46	0
86	OHX	2	2136	7/7	0.87	0.19	107,107,107,107	0
86	OHX	1	4176	7/7	0.87	0.15	133,133,133,133	0
85	MG	1	3582	1/1	0.88	0.25	30,30,30,30	0
85	MG	6	2028	1/1	0.88	0.38	56,56,56,56	0
86	OHX	1	4155	7/7	0.88	0.18	115,115,115,115	0
85	MG	5	3526	1/1	0.88	0.31	42,42,42,42	0
85	MG	1	3521	1/1	0.88	0.32	60,60,60,60	0
85	MG	5	3536	1/1	0.88	0.19	27,27,27,27	0
85	MG	1	3781	1/1	0.88	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3547	1/1	0.88	0.30	32,32,32,32	0
85	MG	6	1925	1/1	0.88	0.33	34,34,34,34	0
85	MG	6	1928	1/1	0.88	0.34	54,54,54,54	0
85	MG	1	3591	1/1	0.88	0.28	34,34,34,34	0
85	MG	5	3567	1/1	0.88	0.20	26,26,26,26	0
86	OHX	5	4108	7/7	0.88	0.23	95,95,95,95	0
85	MG	1	3641	1/1	0.88	0.11	32,32,32,32	0
86	OHX	5	4131	7/7	0.88	0.13	147,147,147,147	0
86	OHX	5	4136	7/7	0.88	0.19	103,103,103,103	0
86	OHX	2	2108	7/7	0.88	0.18	110,110,110,110	0
85	MG	1	3457	1/1	0.88	0.19	21,21,21,21	0
85	MG	1	3459	1/1	0.88	0.29	55,55,55,55	0
86	OHX	5	4140	7/7	0.88	0.19	101,101,101,101	0
85	MG	3	213	1/1	0.88	0.38	49,49,49,49	0
86	OHX	2	2134	7/7	0.88	0.14	127,127,127,127	0
86	OHX	2	2135	7/7	0.88	0.19	108,108,108,108	0
86	OHX	5	4148	7/7	0.88	0.17	119,119,119,119	0
85	MG	5	3590	1/1	0.88	0.24	21,21,21,21	0
85	MG	1	3538	1/1	0.88	0.15	31,31,31,31	0
85	MG	1	3608	1/1	0.88	0.19	50,50,50,50	0
85	MG	6	1951	1/1	0.88	0.36	55,55,55,55	0
86	OHX	5	4158	7/7	0.88	0.22	110,110,110,110	0
85	MG	1	3805	1/1	0.88	0.18	49,49,49,49	0
85	MG	1	3806	1/1	0.88	0.17	48,48,48,48	0
85	MG	c1	201	1/1	0.88	0.14	41,41,41,41	0
86	OHX	2	2148	7/7	0.88	0.14	142,142,142,142	0
86	OHX	2	2149	7/7	0.88	0.22	96,96,96,96	0
86	OHX	5	4169	7/7	0.88	0.16	130,130,130,130	0
85	MG	2	1966	1/1	0.88	0.24	49,49,49,49	0
86	OHX	5	4176	7/7	0.88	0.26	86,86,86,86	0
86	OHX	2	2151	7/7	0.88	0.17	134,134,134,134	0
85	MG	4	212	1/1	0.88	0.09	29,29,29,29	0
86	OHX	1	4194	7/7	0.88	0.18	114,114,114,114	0
86	OHX	2	2153	7/7	0.88	0.17	118,118,118,118	0
86	OHX	2	2154	7/7	0.88	0.17	131,131,131,131	0
86	OHX	2	2155	7/7	0.88	0.17	114,114,114,114	0
85	MG	5	3641	1/1	0.88	0.25	47,47,47,47	0
85	MG	2	2021	1/1	0.88	0.45	61,61,61,61	0
86	OHX	5	4191	7/7	0.88	0.21	97,97,97,97	0
85	MG	4	215	1/1	0.88	0.16	60,60,60,60	0
85	MG	1	3410	1/1	0.88	0.24	36,36,36,36	0
85	MG	5	3828	1/1	0.88	0.24	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3832	1/1	0.88	0.08	37,37,37,37	0
85	MG	6	1969	1/1	0.88	0.14	49,49,49,49	0
85	MG	1	3724	1/1	0.88	0.10	43,43,43,43	0
85	MG	2	1912	1/1	0.88	0.23	53,53,53,53	0
85	MG	1	3670	1/1	0.88	0.26	65,65,65,65	0
86	OHX	2	2167	7/7	0.88	0.15	132,132,132,132	0
86	OHX	5	4207	7/7	0.88	0.25	89,89,89,89	0
85	MG	5	3851	1/1	0.88	0.23	46,46,46,46	0
85	MG	1	3412	1/1	0.88	0.33	37,37,37,37	0
85	MG	5	3431	1/1	0.88	0.25	37,37,37,37	0
86	OHX	2	2175	7/7	0.88	0.15	128,128,128,128	0
86	OHX	4	231	7/7	0.88	0.18	115,115,115,115	0
85	MG	5	3676	1/1	0.88	0.22	81,81,81,81	0
86	OHX	2	2177	7/7	0.88	0.21	113,113,113,113	0
85	MG	5	3432	1/1	0.88	0.28	49,49,49,49	0
85	MG	1	3674	1/1	0.88	0.36	50,50,50,50	0
85	MG	5	3861	1/1	0.88	0.09	30,30,30,30	0
85	MG	5	3863	1/1	0.88	0.25	44,44,44,44	0
85	MG	5	3437	1/1	0.88	0.20	45,45,45,45	0
85	MG	L8	301	1/1	0.88	0.33	54,54,54,54	0
85	MG	5	3693	1/1	0.88	0.22	59,59,59,59	0
85	MG	1	3737	1/1	0.88	0.26	54,54,54,54	0
85	MG	2	2011	1/1	0.88	0.38	59,59,59,59	0
86	OHX	6	2135	7/7	0.88	0.16	116,116,116,116	0
85	MG	6	1991	1/1	0.88	0.26	56,56,56,56	0
86	OHX	5	4228	7/7	0.88	0.15	141,141,141,141	0
85	MG	1	3683	1/1	0.88	0.12	32,32,32,32	0
85	MG	1	3625	1/1	0.88	0.17	27,27,27,27	0
86	OHX	5	4231	7/7	0.88	0.14	137,137,137,137	0
86	OHX	6	2156	7/7	0.88	0.16	119,119,119,119	0
85	MG	5	3885	1/1	0.88	0.30	59,59,59,59	0
86	OHX	1	4115	7/7	0.88	0.20	106,106,106,106	0
85	MG	2	1993	1/1	0.88	0.12	46,46,46,46	0
86	OHX	1	4117	7/7	0.88	0.15	136,136,136,136	0
86	OHX	6	2167	7/7	0.88	0.15	140,140,140,140	0
86	OHX	6	2168	7/7	0.88	0.24	97,97,97,97	0
85	MG	2	1917	1/1	0.88	0.32	46,46,46,46	0
86	OHX	1	4122	7/7	0.88	0.20	103,103,103,103	0
86	OHX	1	4123	7/7	0.88	0.22	94,94,94,94	0
86	OHX	1	4124	7/7	0.88	0.21	104,104,104,104	0
86	OHX	1	4126	7/7	0.88	0.20	110,110,110,110	0
85	MG	6	2001	1/1	0.88	0.15	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4129	7/7	0.88	0.17	118,118,118,118	0
85	MG	5	3889	1/1	0.88	0.10	31,31,31,31	0
85	MG	5	3721	1/1	0.88	0.28	46,46,46,46	0
85	MG	5	3722	1/1	0.88	0.10	39,39,39,39	0
86	OHX	6	2182	7/7	0.88	0.19	109,109,109,109	0
85	MG	1	3688	1/1	0.88	0.13	39,39,39,39	0
85	MG	1	3761	1/1	0.88	0.11	42,42,42,42	0
86	OHX	8	228	7/7	0.88	0.20	101,101,101,101	0
86	OHX	8	229	7/7	0.88	0.20	108,108,108,108	0
86	OHX	l3	404	7/7	0.88	0.19	112,112,112,112	0
85	MG	1	3762	1/1	0.88	0.09	24,24,24,24	0
86	OHX	1	4137	7/7	0.88	0.20	89,89,89,89	0
85	MG	1	3862	1/1	0.88	0.11	41,41,41,41	0
85	MG	7	209	1/1	0.88	0.32	35,35,35,35	0
85	MG	7	211	1/1	0.88	0.17	46,46,46,46	0
85	MG	7	212	1/1	0.88	0.16	64,64,64,64	0
85	MG	1	3763	1/1	0.88	0.11	38,38,38,38	0
85	MG	6	2018	1/1	0.88	0.09	44,44,44,44	0
85	MG	2	1974	1/1	0.88	0.25	59,59,59,59	0
85	MG	5	3745	1/1	0.88	0.22	33,33,33,33	0
88	3H3	1	4216	33/33	0.88	0.14	26,26,26,26	0
86	OHX	1	4149	7/7	0.89	0.18	105,105,105,105	0
85	MG	2	1995	1/1	0.89	0.45	75,75,75,75	0
85	MG	m1	201	1/1	0.89	0.25	51,51,51,51	0
85	MG	1	3585	1/1	0.89	0.35	40,40,40,40	0
86	OHX	1	4160	7/7	0.89	0.18	114,114,114,114	0
85	MG	n6	202	1/1	0.89	0.13	34,34,34,34	0
85	MG	2	1920	1/1	0.89	0.14	48,48,48,48	0
85	MG	6	2022	1/1	0.89	0.14	71,71,71,71	0
85	MG	5	3491	1/1	0.89	0.11	34,34,34,34	0
86	OHX	5	4096	7/7	0.89	0.17	115,115,115,115	0
86	OHX	5	4098	7/7	0.89	0.17	114,114,114,114	0
86	OHX	5	4101	7/7	0.89	0.16	121,121,121,121	0
85	MG	6	2025	1/1	0.89	0.17	52,52,52,52	0
85	MG	1	3784	1/1	0.89	0.12	29,29,29,29	0
86	OHX	5	4123	7/7	0.89	0.15	116,116,116,116	0
85	MG	5	3498	1/1	0.89	0.25	27,27,27,27	0
85	MG	1	3516	1/1	0.89	0.26	28,28,28,28	0
85	MG	2	2014	1/1	0.89	0.40	61,61,61,61	0
85	MG	5	3516	1/1	0.89	0.29	20,20,20,20	0
85	MG	5	3517	1/1	0.89	0.22	18,18,18,18	0
86	OHX	2	2128	7/7	0.89	0.19	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4142	7/7	0.89	0.21	96,96,96,96	0
85	MG	1	3788	1/1	0.89	0.23	48,48,48,48	0
85	MG	2	2015	1/1	0.89	0.35	59,59,59,59	0
85	MG	6	2032	1/1	0.89	0.22	56,56,56,56	0
85	MG	1	3719	1/1	0.89	0.07	30,30,30,30	0
85	MG	2	1985	1/1	0.89	0.09	45,45,45,45	0
85	MG	5	3548	1/1	0.89	0.32	44,44,44,44	0
86	OHX	5	4154	7/7	0.89	0.19	106,106,106,106	0
85	MG	2	1998	1/1	0.89	0.21	60,60,60,60	0
85	MG	5	3552	1/1	0.89	0.24	23,23,23,23	0
85	MG	5	3554	1/1	0.89	0.20	31,31,31,31	0
86	OHX	1	4186	7/7	0.89	0.17	120,120,120,120	0
85	MG	5	3556	1/1	0.89	0.19	36,36,36,36	0
85	MG	1	3727	1/1	0.89	0.15	51,51,51,51	0
85	MG	1	3609	1/1	0.89	0.32	54,54,54,54	0
86	OHX	5	4166	7/7	0.89	0.16	120,120,120,120	0
85	MG	1	3455	1/1	0.89	0.24	45,45,45,45	0
85	MG	5	3802	1/1	0.89	0.11	40,40,40,40	0
86	OHX	5	4173	7/7	0.89	0.20	110,110,110,110	0
85	MG	1	3671	1/1	0.89	0.18	40,40,40,40	0
85	MG	5	3570	1/1	0.89	0.28	30,30,30,30	0
86	OHX	5	4177	7/7	0.89	0.19	110,110,110,110	0
85	MG	5	3575	1/1	0.89	0.30	33,33,33,33	0
85	MG	6	1957	1/1	0.89	0.44	48,48,48,48	0
85	MG	6	2044	1/1	0.89	0.36	44,44,44,44	0
86	OHX	2	2158	7/7	0.89	0.21	93,93,93,93	0
85	MG	5	3586	1/1	0.89	0.27	52,52,52,52	0
85	MG	5	3587	1/1	0.89	0.27	21,21,21,21	0
85	MG	1	3544	1/1	0.89	0.21	32,32,32,32	0
86	OHX	5	4189	7/7	0.89	0.19	100,100,100,100	0
85	MG	5	3825	1/1	0.89	0.12	31,31,31,31	0
85	MG	6	1959	1/1	0.89	0.40	52,52,52,52	0
85	MG	s6	301	1/1	0.89	0.39	59,59,59,59	0
85	MG	1	3545	1/1	0.89	0.24	37,37,37,37	0
85	MG	2	1927	1/1	0.89	0.35	46,46,46,46	0
85	MG	5	3617	1/1	0.89	0.09	32,32,32,32	0
86	OHX	1	4208	7/7	0.89	0.22	100,100,100,100	0
86	OHX	1	4209	7/7	0.89	0.20	104,104,104,104	0
86	OHX	2	2168	7/7	0.89	0.14	135,135,135,135	0
85	MG	5	3844	1/1	0.89	0.12	22,22,22,22	0
85	MG	5	3620	1/1	0.89	0.07	25,25,25,25	0
85	MG	5	3847	1/1	0.89	0.24	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3739	1/1	0.89	0.25	53,53,53,53	0
85	MG	d6	102	1/1	0.89	0.16	47,47,47,47	0
86	OHX	3	225	7/7	0.89	0.22	103,103,103,103	0
86	OHX	3	226	7/7	0.89	0.19	113,113,113,113	0
85	MG	1	3740	1/1	0.89	0.14	49,49,49,49	0
86	OHX	5	4213	7/7	0.89	0.11	166,166,166,166	0
85	MG	2	1940	1/1	0.89	0.26	53,53,53,53	0
85	MG	5	3407	1/1	0.89	0.15	32,32,32,32	0
85	MG	2	1932	1/1	0.89	0.38	48,48,48,48	0
85	MG	2	1942	1/1	0.89	0.25	63,63,63,63	0
85	MG	5	3413	1/1	0.89	0.20	25,25,25,25	0
86	OHX	1	4020	7/7	0.89	0.12	127,127,127,127	0
86	OHX	L4	404	7/7	0.89	0.19	103,103,103,103	0
86	OHX	1	4024	7/7	0.89	0.20	94,94,94,94	0
86	OHX	1	4031	7/7	0.89	0.22	88,88,88,88	0
85	MG	M1	201	1/1	0.89	0.22	61,61,61,61	0
85	MG	2	1943	1/1	0.89	0.26	55,55,55,55	0
86	OHX	1	4084	7/7	0.89	0.22	89,89,89,89	0
86	OHX	6	2105	7/7	0.89	0.19	97,97,97,97	0
85	MG	5	3868	1/1	0.89	0.43	32,32,32,32	0
85	MG	5	3871	1/1	0.89	0.44	47,47,47,47	0
85	MG	1	3629	1/1	0.89	0.12	30,30,30,30	0
85	MG	5	3656	1/1	0.89	0.08	35,35,35,35	0
86	OHX	1	4098	7/7	0.89	0.19	103,103,103,103	0
85	MG	6	1979	1/1	0.89	0.31	51,51,51,51	0
86	OHX	1	4103	7/7	0.89	0.20	98,98,98,98	0
86	OHX	1	4104	7/7	0.89	0.16	119,119,119,119	0
85	MG	M5	301	1/1	0.89	0.11	43,43,43,43	0
86	OHX	1	4113	7/7	0.89	0.19	106,106,106,106	0
85	MG	5	3666	1/1	0.89	0.09	21,21,21,21	0
85	MG	5	3430	1/1	0.89	0.15	27,27,27,27	0
85	MG	M5	302	1/1	0.89	0.11	46,46,46,46	0
85	MG	M7	202	1/1	0.89	0.21	26,26,26,26	0
86	OHX	5	4243	7/7	0.89	0.19	109,109,109,109	0
85	MG	5	3678	1/1	0.89	0.12	37,37,37,37	0
85	MG	5	3433	1/1	0.89	0.28	64,64,64,64	0
86	OHX	6	2176	7/7	0.89	0.23	87,87,87,87	0
85	MG	2	1933	1/1	0.89	0.32	57,57,57,57	0
85	MG	6	1990	1/1	0.89	0.29	58,58,58,58	0
86	OHX	5	4249	7/7	0.89	0.18	109,109,109,109	0
85	MG	5	3441	1/1	0.89	0.28	26,26,26,26	0
85	MG	1	3563	1/1	0.89	0.22	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3451	1/1	0.89	0.10	25,25,25,25	0
86	OHX	1	4131	7/7	0.89	0.22	102,102,102,102	0
85	MG	1	3856	1/1	0.89	0.10	22,22,22,22	0
85	MG	5	3460	1/1	0.89	0.08	24,24,24,24	0
85	MG	5	3464	1/1	0.89	0.08	30,30,30,30	0
85	MG	Q2	502	1/1	0.89	0.25	50,50,50,50	0
85	MG	1	3857	1/1	0.89	0.12	59,59,59,59	0
85	MG	1	3468	1/1	0.89	0.21	37,37,37,37	0
86	OHX	l5	304	7/7	0.89	0.15	116,116,116,116	0
85	MG	1	3766	1/1	0.89	0.20	32,32,32,32	0
85	MG	5	3473	1/1	0.89	0.23	44,44,44,44	0
85	MG	1	3565	1/1	0.89	0.12	27,27,27,27	0
86	OHX	1	4143	7/7	0.89	0.19	107,107,107,107	0
85	MG	1	3469	1/1	0.89	0.31	56,56,56,56	0
85	MG	1	3770	1/1	0.89	0.19	75,75,75,75	0
85	MG	6	1916	1/1	0.89	0.39	54,54,54,54	0
85	MG	5	3734	1/1	0.89	0.32	58,58,58,58	0
85	MG	l2	301	1/1	0.89	0.24	43,43,43,43	0
86	OHX	1	4140	7/7	0.90	0.21	100,100,100,100	0
85	MG	1	3698	1/1	0.90	0.33	62,62,62,62	0
86	OHX	6	2197	7/7	0.90	0.18	113,113,113,113	0
85	MG	O3	201	1/1	0.90	0.07	28,28,28,28	0
85	MG	6	2008	1/1	0.90	0.12	41,41,41,41	0
85	MG	5	3720	1/1	0.90	0.09	31,31,31,31	0
85	MG	1	3587	1/1	0.90	0.30	26,26,26,26	0
85	MG	6	1902	1/1	0.90	0.20	47,47,47,47	0
85	MG	l5	302	1/1	0.90	0.28	54,54,54,54	0
85	MG	6	2017	1/1	0.90	0.17	58,58,58,58	0
85	MG	l7	301	1/1	0.90	0.22	32,32,32,32	0
85	MG	1	3526	1/1	0.90	0.24	21,21,21,21	0
86	OHX	c5	201	7/7	0.90	0.14	127,127,127,127	0
86	OHX	1	4151	7/7	0.90	0.16	113,113,113,113	0
86	OHX	5	4017	7/7	0.90	0.15	128,128,128,128	0
86	OHX	5	4027	7/7	0.90	0.17	83,83,83,83	0
86	OHX	5	4062	7/7	0.90	0.18	99,99,99,99	0
86	OHX	5	4063	7/7	0.90	0.17	106,106,106,106	0
85	MG	m1	202	1/1	0.90	0.16	49,49,49,49	0
86	OHX	1	4154	7/7	0.90	0.19	109,109,109,109	0
85	MG	5	3495	1/1	0.90	0.17	26,26,26,26	0
86	OHX	5	4105	7/7	0.90	0.23	87,87,87,87	0
85	MG	6	2020	1/1	0.90	0.12	40,40,40,40	0
86	OHX	1	4161	7/7	0.90	0.18	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4122	7/7	0.90	0.17	114,114,114,114	0
85	MG	2	1989	1/1	0.90	0.29	65,65,65,65	0
85	MG	1	3483	1/1	0.90	0.22	39,39,39,39	0
86	OHX	1	4164	7/7	0.90	0.19	108,108,108,108	0
85	MG	n8	203	1/1	0.90	0.24	38,38,38,38	0
85	MG	5	3739	1/1	0.90	0.16	31,31,31,31	0
85	MG	2	1901	1/1	0.90	0.45	57,57,57,57	0
85	MG	5	3514	1/1	0.90	0.19	22,22,22,22	0
85	MG	1	3650	1/1	0.90	0.10	35,35,35,35	0
85	MG	6	1914	1/1	0.90	0.25	29,29,29,29	0
86	OHX	2	2112	7/7	0.90	0.16	130,130,130,130	0
85	MG	1	3774	1/1	0.90	0.23	45,45,45,45	0
85	MG	1	3780	1/1	0.90	0.20	53,53,53,53	0
86	OHX	5	4149	7/7	0.90	0.23	96,96,96,96	0
86	OHX	5	4150	7/7	0.90	0.17	113,113,113,113	0
85	MG	5	3531	1/1	0.90	0.24	31,31,31,31	0
85	MG	6	1917	1/1	0.90	0.29	44,44,44,44	0
85	MG	5	3763	1/1	0.90	0.15	26,26,26,26	0
85	MG	5	3540	1/1	0.90	0.29	28,28,28,28	0
86	OHX	5	4156	7/7	0.90	0.18	107,107,107,107	0
85	MG	1	3598	1/1	0.90	0.29	33,33,33,33	0
85	MG	5	3544	1/1	0.90	0.32	41,41,41,41	0
86	OHX	1	4181	7/7	0.90	0.08	192,192,192,192	0
85	MG	5	3545	1/1	0.90	0.24	42,42,42,42	0
86	OHX	2	2139	7/7	0.90	0.16	112,112,112,112	0
85	MG	5	3546	1/1	0.90	0.22	39,39,39,39	0
85	MG	5	3771	1/1	0.90	0.15	55,55,55,55	0
86	OHX	2	2143	7/7	0.90	0.17	113,113,113,113	0
85	MG	1	3486	1/1	0.90	0.09	39,39,39,39	0
86	OHX	5	4172	7/7	0.90	0.21	102,102,102,102	0
85	MG	1	4219	1/1	0.90	0.19	24,24,24,24	0
85	MG	5	3778	1/1	0.90	0.10	52,52,52,52	0
86	OHX	5	4175	7/7	0.90	0.19	105,105,105,105	0
85	MG	1	4221	1/1	0.90	0.10	36,36,36,36	0
85	MG	6	2037	1/1	0.90	0.29	52,52,52,52	0
85	MG	2	1911	1/1	0.90	0.34	50,50,50,50	0
85	MG	5	3783	1/1	0.90	0.11	50,50,50,50	0
85	MG	6	1926	1/1	0.90	0.23	40,40,40,40	0
85	MG	1	3436	1/1	0.90	0.16	35,35,35,35	0
86	OHX	5	4183	7/7	0.90	0.20	100,100,100,100	0
86	OHX	5	4184	7/7	0.90	0.21	98,98,98,98	0
85	MG	1	3722	1/1	0.90	0.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3492	1/1	0.90	0.15	42,42,42,42	0
85	MG	1	3613	1/1	0.90	0.27	36,36,36,36	0
85	MG	6	1935	1/1	0.90	0.29	46,46,46,46	0
85	MG	6	2046	1/1	0.90	0.47	66,66,66,66	0
85	MG	5	3576	1/1	0.90	0.35	36,36,36,36	0
85	MG	3	211	1/1	0.90	0.14	62,62,62,62	0
85	MG	1	3668	1/1	0.90	0.09	43,43,43,43	0
85	MG	1	3799	1/1	0.90	0.28	21,21,21,21	0
85	MG	2	2182	1/1	0.90	0.18	54,54,54,54	0
85	MG	1	3444	1/1	0.90	0.29	49,49,49,49	0
85	MG	c8	202	1/1	0.90	0.31	54,54,54,54	0
85	MG	5	3593	1/1	0.90	0.36	34,34,34,34	0
85	MG	5	3596	1/1	0.90	0.27	25,25,25,25	0
85	MG	1	3445	1/1	0.90	0.20	39,39,39,39	0
85	MG	6	1955	1/1	0.90	0.32	32,32,32,32	0
85	MG	5	3604	1/1	0.90	0.18	33,33,33,33	0
86	OHX	2	2174	7/7	0.90	0.17	115,115,115,115	0
85	MG	1	3619	1/1	0.90	0.27	53,53,53,53	0
85	MG	5	3616	1/1	0.90	0.14	36,36,36,36	0
85	MG	5	3845	1/1	0.90	0.10	44,44,44,44	0
85	MG	4	210	1/1	0.90	0.12	43,43,43,43	0
85	MG	5	3618	1/1	0.90	0.18	37,37,37,37	0
85	MG	1	3408	1/1	0.90	0.27	27,27,27,27	0
85	MG	6	1960	1/1	0.90	0.31	38,38,38,38	0
85	MG	2	2000	1/1	0.90	0.25	53,53,53,53	0
86	OHX	C3	202	7/7	0.90	0.15	131,131,131,131	0
85	MG	5	3631	1/1	0.90	0.07	33,33,33,33	0
85	MG	1	3450	1/1	0.90	0.27	35,35,35,35	0
85	MG	5	3857	1/1	0.90	0.07	37,37,37,37	0
86	OHX	1	4065	7/7	0.90	0.16	113,113,113,113	0
85	MG	1	3514	1/1	0.90	0.21	29,29,29,29	0
86	OHX	1	4067	7/7	0.90	0.21	100,100,100,100	0
86	OHX	1	4071	7/7	0.90	0.20	99,99,99,99	0
85	MG	1	3750	1/1	0.90	0.09	38,38,38,38	0
85	MG	5	3862	1/1	0.90	0.09	33,33,33,33	0
85	MG	1	3825	1/1	0.90	0.15	31,31,31,31	0
86	OHX	6	2144	7/7	0.90	0.17	105,105,105,105	0
86	OHX	1	4086	7/7	0.90	0.19	101,101,101,101	0
86	OHX	1	4091	7/7	0.90	0.20	98,98,98,98	0
86	OHX	6	2153	7/7	0.90	0.16	118,118,118,118	0
86	OHX	6	2154	7/7	0.90	0.13	117,117,117,117	0
85	MG	5	3642	1/1	0.90	0.08	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2158	7/7	0.90	0.16	112,112,112,112	0
85	MG	1	3826	1/1	0.90	0.25	59,59,59,59	0
85	MG	1	3627	1/1	0.90	0.14	58,58,58,58	0
86	OHX	6	2163	7/7	0.90	0.19	106,106,106,106	0
85	MG	6	1971	1/1	0.90	0.28	54,54,54,54	0
85	MG	1	3831	1/1	0.90	0.08	39,39,39,39	0
86	OHX	1	4101	7/7	0.90	0.16	122,122,122,122	0
85	MG	6	1973	1/1	0.90	0.14	43,43,43,43	0
85	MG	5	3435	1/1	0.90	0.07	28,28,28,28	0
86	OHX	1	4106	7/7	0.90	0.17	113,113,113,113	0
86	OHX	6	2172	7/7	0.90	0.17	114,114,114,114	0
85	MG	5	3658	1/1	0.90	0.08	38,38,38,38	0
85	MG	1	3453	1/1	0.90	0.21	37,37,37,37	0
85	MG	L6	201	1/1	0.90	0.13	35,35,35,35	0
85	MG	L7	301	1/1	0.90	0.16	29,29,29,29	0
85	MG	1	3425	1/1	0.90	0.13	21,21,21,21	0
85	MG	1	3837	1/1	0.90	0.10	30,30,30,30	0
85	MG	M3	201	1/1	0.90	0.14	37,37,37,37	0
86	OHX	8	227	7/7	0.90	0.20	108,108,108,108	0
85	MG	1	3757	1/1	0.90	0.17	35,35,35,35	0
85	MG	6	1988	1/1	0.90	0.05	36,36,36,36	0
86	OHX	1	4125	7/7	0.90	0.24	85,85,85,85	0
85	MG	5	3681	1/1	0.90	0.08	29,29,29,29	0
85	MG	1	3519	1/1	0.90	0.28	31,31,31,31	0
85	MG	1	3843	1/1	0.90	0.28	46,46,46,46	0
85	MG	2	1988	1/1	0.90	0.30	62,62,62,62	0
86	OHX	l9	600	7/7	0.90	0.19	105,105,105,105	0
85	MG	7	202	1/1	0.90	0.20	27,27,27,27	0
85	MG	M7	201	1/1	0.90	0.43	52,52,52,52	0
85	MG	5	3471	1/1	0.90	0.08	40,40,40,40	0
85	MG	5	3698	1/1	0.90	0.16	44,44,44,44	0
85	MG	1	3847	1/1	0.90	0.29	49,49,49,49	0
86	OHX	o4	203	7/7	0.90	0.20	104,104,104,104	0
85	MG	1	3849	1/1	0.90	0.19	33,33,33,33	0
85	MG	N3	203	1/1	0.90	0.22	40,40,40,40	0
85	MG	1	3851	1/1	0.90	0.28	50,50,50,50	0
85	MG	2	1938	1/1	0.91	0.33	48,48,48,48	0
85	MG	5	3729	1/1	0.91	0.33	61,61,61,61	0
85	MG	2	2009	1/1	0.91	0.32	46,46,46,46	0
85	MG	M6	201	1/1	0.91	0.08	39,39,39,39	0
85	MG	5	3733	1/1	0.91	0.15	32,32,32,32	0
85	MG	d2	201	1/1	0.91	0.26	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3735	1/1	0.91	0.08	31,31,31,31	0
85	MG	1	3638	1/1	0.91	0.20	49,49,49,49	0
85	MG	1	3522	1/1	0.91	0.31	27,27,27,27	0
85	MG	M9	201	1/1	0.91	0.25	52,52,52,52	0
85	MG	6	1974	1/1	0.91	0.17	45,45,45,45	0
85	MG	m7	203	1/1	0.91	0.17	26,26,26,26	0
85	MG	m7	205	1/1	0.91	0.07	26,26,26,26	0
85	MG	2	1956	1/1	0.91	0.20	53,53,53,53	0
85	MG	1	3860	1/1	0.91	0.28	43,43,43,43	0
85	MG	1	3527	1/1	0.91	0.31	27,27,27,27	0
85	MG	5	3416	1/1	0.91	0.21	21,21,21,21	0
86	OHX	5	3995	7/7	0.91	0.15	86,86,86,86	0
85	MG	5	3753	1/1	0.91	0.10	42,42,42,42	0
85	MG	5	3417	1/1	0.91	0.10	21,21,21,21	0
86	OHX	5	4037	7/7	0.91	0.18	94,94,94,94	0
85	MG	o4	201	1/1	0.91	0.18	41,41,41,41	0
85	MG	5	3569	1/1	0.91	0.25	20,20,20,20	0
86	OHX	5	4089	7/7	0.91	0.25	84,84,84,84	0
86	OHX	1	4153	7/7	0.91	0.18	92,92,92,92	0
85	MG	1	3646	1/1	0.91	0.18	30,30,30,30	0
86	OHX	5	4099	7/7	0.91	0.19	94,94,94,94	0
86	OHX	2	2082	7/7	0.91	0.17	110,110,110,110	0
86	OHX	5	4103	7/7	0.91	0.13	123,123,123,123	0
86	OHX	1	4157	7/7	0.91	0.20	105,105,105,105	0
86	OHX	5	4107	7/7	0.91	0.19	103,103,103,103	0
86	OHX	2	2087	7/7	0.91	0.20	93,93,93,93	0
85	MG	2	1981	1/1	0.91	0.31	52,52,52,52	0
86	OHX	5	4118	7/7	0.91	0.19	94,94,94,94	0
86	OHX	2	2100	7/7	0.91	0.17	115,115,115,115	0
85	MG	1	3716	1/1	0.91	0.08	39,39,39,39	0
86	OHX	5	4124	7/7	0.91	0.15	119,119,119,119	0
86	OHX	5	4126	7/7	0.91	0.18	103,103,103,103	0
86	OHX	5	4127	7/7	0.91	0.18	100,100,100,100	0
85	MG	2	1982	1/1	0.91	0.24	59,59,59,59	0
86	OHX	5	4132	7/7	0.91	0.19	96,96,96,96	0
86	OHX	5	4135	7/7	0.91	0.17	109,109,109,109	0
85	MG	5	3579	1/1	0.91	0.27	28,28,28,28	0
85	MG	5	3428	1/1	0.91	0.11	21,21,21,21	0
86	OHX	2	2122	7/7	0.91	0.16	116,116,116,116	0
86	OHX	2	2123	7/7	0.91	0.17	114,114,114,114	0
85	MG	5	3581	1/1	0.91	0.26	36,36,36,36	0
86	OHX	2	2127	7/7	0.91	0.15	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4143	7/7	0.91	0.20	106,106,106,106	0
85	MG	5	3583	1/1	0.91	0.30	27,27,27,27	0
85	MG	5	3585	1/1	0.91	0.21	20,20,20,20	0
85	MG	6	1903	1/1	0.91	0.28	36,36,36,36	0
85	MG	1	3531	1/1	0.91	0.18	19,19,19,19	0
85	MG	1	3536	1/1	0.91	0.35	42,42,42,42	0
85	MG	2	1922	1/1	0.91	0.31	55,55,55,55	0
85	MG	1	3656	1/1	0.91	0.19	39,39,39,39	0
85	MG	1	3802	1/1	0.91	0.16	74,74,74,74	0
85	MG	5	3785	1/1	0.91	0.07	31,31,31,31	0
85	MG	3	204	1/1	0.91	0.43	51,51,51,51	0
85	MG	2	1984	1/1	0.91	0.13	60,60,60,60	0
85	MG	5	3790	1/1	0.91	0.09	41,41,41,41	0
86	OHX	2	2147	7/7	0.91	0.16	105,105,105,105	0
85	MG	5	3603	1/1	0.91	0.07	19,19,19,19	0
86	OHX	5	4161	7/7	0.91	0.22	94,94,94,94	0
85	MG	2	1908	1/1	0.91	0.26	60,60,60,60	0
85	MG	5	3795	1/1	0.91	0.14	42,42,42,42	0
85	MG	6	2004	1/1	0.91	0.14	62,62,62,62	0
86	OHX	5	4165	7/7	0.91	0.18	102,102,102,102	0
85	MG	5	3609	1/1	0.91	0.11	24,24,24,24	0
85	MG	5	3610	1/1	0.91	0.20	40,40,40,40	0
86	OHX	5	4168	7/7	0.91	0.11	154,154,154,154	0
85	MG	5	3613	1/1	0.91	0.25	36,36,36,36	0
85	MG	1	3439	1/1	0.91	0.23	34,34,34,34	0
85	MG	5	3454	1/1	0.91	0.16	37,37,37,37	0
85	MG	5	3813	1/1	0.91	0.10	47,47,47,47	0
85	MG	1	3667	1/1	0.91	0.38	62,62,62,62	0
85	MG	5	3619	1/1	0.91	0.26	34,34,34,34	0
85	MG	5	3457	1/1	0.91	0.21	35,35,35,35	0
85	MG	1	3818	1/1	0.91	0.20	48,48,48,48	0
85	MG	6	2009	1/1	0.91	0.07	40,40,40,40	0
85	MG	6	2011	1/1	0.91	0.37	54,54,54,54	0
85	MG	5	3831	1/1	0.91	0.15	59,59,59,59	0
85	MG	6	1921	1/1	0.91	0.29	36,36,36,36	0
85	MG	6	1922	1/1	0.91	0.35	42,42,42,42	0
85	MG	5	3468	1/1	0.91	0.14	29,29,29,29	0
85	MG	2	1918	1/1	0.91	0.33	46,46,46,46	0
86	OHX	5	4187	7/7	0.91	0.19	97,97,97,97	0
85	MG	5	3470	1/1	0.91	0.23	25,25,25,25	0
85	MG	1	3501	1/1	0.91	0.26	22,22,22,22	0
85	MG	5	3645	1/1	0.91	0.29	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	2	1913	1/1	0.91	0.43	64,64,64,64	0
85	MG	1	3505	1/1	0.91	0.19	25,25,25,25	0
86	OHX	1	4212	7/7	0.91	0.22	98,98,98,98	0
85	MG	5	3476	1/1	0.91	0.16	19,19,19,19	0
85	MG	4	208	1/1	0.91	0.21	42,42,42,42	0
85	MG	6	1929	1/1	0.91	0.25	49,49,49,49	0
86	OHX	3	222	7/7	0.91	0.14	119,119,119,119	0
85	MG	1	3673	1/1	0.91	0.41	56,56,56,56	0
85	MG	5	3480	1/1	0.91	0.17	29,29,29,29	0
85	MG	5	3481	1/1	0.91	0.40	57,57,57,57	0
86	OHX	5	4206	7/7	0.91	0.15	121,121,121,121	0
85	MG	5	3483	1/1	0.91	0.10	34,34,34,34	0
85	MG	1	3742	1/1	0.91	0.29	53,53,53,53	0
86	OHX	1	4003	7/7	0.91	0.20	90,90,90,90	0
85	MG	1	3827	1/1	0.91	0.15	33,33,33,33	0
86	OHX	1	4022	7/7	0.91	0.16	105,105,105,105	0
85	MG	5	3674	1/1	0.91	0.16	33,33,33,33	0
85	MG	2	1916	1/1	0.91	0.30	44,44,44,44	0
86	OHX	1	4039	7/7	0.91	0.18	98,98,98,98	0
85	MG	1	3623	1/1	0.91	0.18	42,42,42,42	0
85	MG	5	3869	1/1	0.91	0.21	28,28,28,28	0
85	MG	5	3490	1/1	0.91	0.33	53,53,53,53	0
85	MG	5	3680	1/1	0.91	0.41	68,68,68,68	0
85	MG	1	3678	1/1	0.91	0.13	36,36,36,36	0
86	OHX	1	4074	7/7	0.91	0.15	105,105,105,105	0
86	OHX	6	2117	7/7	0.91	0.17	108,108,108,108	0
86	OHX	6	2127	7/7	0.91	0.18	98,98,98,98	0
86	OHX	1	4079	7/7	0.91	0.18	99,99,99,99	0
86	OHX	1	4081	7/7	0.91	0.21	96,96,96,96	0
86	OHX	6	2140	7/7	0.91	0.18	111,111,111,111	0
86	OHX	6	2143	7/7	0.91	0.15	117,117,117,117	0
85	MG	1	3680	1/1	0.91	0.07	30,30,30,30	0
86	OHX	6	2145	7/7	0.91	0.17	110,110,110,110	0
86	OHX	6	2146	7/7	0.91	0.16	109,109,109,109	0
86	OHX	6	2147	7/7	0.91	0.22	90,90,90,90	0
85	MG	5	3688	1/1	0.91	0.12	33,33,33,33	0
86	OHX	6	2151	7/7	0.91	0.20	92,92,92,92	0
85	MG	1	3681	1/1	0.91	0.15	56,56,56,56	0
86	OHX	1	4087	7/7	0.91	0.15	120,120,120,120	0
85	MG	5	3883	1/1	0.91	0.15	48,48,48,48	0
85	MG	6	1944	1/1	0.91	0.41	50,50,50,50	0
86	OHX	6	2157	7/7	0.91	0.19	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	1947	1/1	0.91	0.31	50,50,50,50	0
85	MG	1	3416	1/1	0.91	0.11	21,21,21,21	0
86	OHX	1	4097	7/7	0.91	0.15	115,115,115,115	0
86	OHX	6	2161	7/7	0.91	0.19	101,101,101,101	0
85	MG	2	1921	1/1	0.91	0.32	44,44,44,44	0
85	MG	5	3700	1/1	0.91	0.17	47,47,47,47	0
86	OHX	1	4100	7/7	0.91	0.16	116,116,116,116	0
86	OHX	6	2166	7/7	0.91	0.15	115,115,115,115	0
85	MG	L4	401	1/1	0.91	0.10	32,32,32,32	0
85	MG	5	3890	1/1	0.91	0.07	21,21,21,21	0
85	MG	1	3449	1/1	0.91	0.12	32,32,32,32	0
86	OHX	1	4105	7/7	0.91	0.18	101,101,101,101	0
86	OHX	6	2171	7/7	0.91	0.22	90,90,90,90	0
85	MG	5	3704	1/1	0.91	0.09	41,41,41,41	0
86	OHX	1	4107	7/7	0.91	0.20	98,98,98,98	0
86	OHX	8	226	7/7	0.91	0.16	115,115,115,115	0
86	OHX	1	4108	7/7	0.91	0.20	97,97,97,97	0
85	MG	2	1937	1/1	0.91	0.29	46,46,46,46	0
85	MG	5	3706	1/1	0.91	0.20	42,42,42,42	0
86	OHX	1	4114	7/7	0.91	0.25	87,87,87,87	0
85	MG	1	3845	1/1	0.91	0.12	43,43,43,43	0
85	MG	1	3517	1/1	0.91	0.22	22,22,22,22	0
85	MG	7	203	1/1	0.91	0.24	43,43,43,43	0
86	OHX	l5	305	7/7	0.91	0.17	112,112,112,112	0
85	MG	5	3716	1/1	0.91	0.20	44,44,44,44	0
86	OHX	1	4120	7/7	0.91	0.17	105,105,105,105	0
86	OHX	1	4121	7/7	0.91	0.18	102,102,102,102	0
85	MG	7	207	1/1	0.91	0.12	43,43,43,43	0
85	MG	7	208	1/1	0.91	0.22	42,42,42,42	0
85	MG	1	3848	1/1	0.91	0.26	45,45,45,45	0
85	MG	5	3532	1/1	0.91	0.17	39,39,39,39	0
85	MG	1	3578	1/1	0.91	0.25	20,20,20,20	0
85	MG	1	3632	1/1	0.91	0.21	50,50,50,50	0
85	MG	1	3581	1/1	0.91	0.11	29,29,29,29	0
85	MG	5	3725	1/1	0.91	0.10	41,41,41,41	0
86	OHX	s4	301	7/7	0.92	0.16	122,122,122,122	0
86	OHX	2	2117	7/7	0.92	0.15	110,110,110,110	0
86	OHX	2	2119	7/7	0.92	0.15	110,110,110,110	0
85	MG	5	3482	1/1	0.92	0.28	30,30,30,30	0
85	MG	5	3638	1/1	0.92	0.19	29,29,29,29	0
85	MG	6	1949	1/1	0.92	0.28	40,40,40,40	0
86	OHX	sR	401	7/7	0.92	0.13	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3555	1/1	0.92	0.31	25,25,25,25	0
86	OHX	5	3999	7/7	0.92	0.15	91,91,91,91	0
86	OHX	5	4006	7/7	0.92	0.16	87,87,87,87	0
86	OHX	2	2126	7/7	0.92	0.18	103,103,103,103	0
86	OHX	1	4156	7/7	0.92	0.19	105,105,105,105	0
85	MG	1	3699	1/1	0.92	0.22	31,31,31,31	0
86	OHX	5	4042	7/7	0.92	0.16	100,100,100,100	0
86	OHX	5	4043	7/7	0.92	0.18	96,96,96,96	0
85	MG	1	3768	1/1	0.92	0.20	45,45,45,45	0
86	OHX	2	2129	7/7	0.92	0.15	121,121,121,121	0
86	OHX	5	4071	7/7	0.92	0.19	106,106,106,106	0
86	OHX	5	4075	7/7	0.92	0.20	91,91,91,91	0
86	OHX	2	2133	7/7	0.92	0.15	119,119,119,119	0
86	OHX	5	4092	7/7	0.92	0.19	93,93,93,93	0
86	OHX	5	4095	7/7	0.92	0.15	104,104,104,104	0
85	MG	5	3804	1/1	0.92	0.09	27,27,27,27	0
85	MG	1	3497	1/1	0.92	0.17	33,33,33,33	0
85	MG	5	3807	1/1	0.92	0.15	29,29,29,29	0
85	MG	1	3850	1/1	0.92	0.26	41,41,41,41	0
86	OHX	5	4102	7/7	0.92	0.20	82,82,82,82	0
85	MG	5	3810	1/1	0.92	0.15	32,32,32,32	0
86	OHX	5	4104	7/7	0.92	0.17	107,107,107,107	0
85	MG	1	3415	1/1	0.92	0.07	36,36,36,36	0
86	OHX	5	4106	7/7	0.92	0.20	88,88,88,88	0
85	MG	5	3652	1/1	0.92	0.26	55,55,55,55	0
85	MG	5	3492	1/1	0.92	0.06	22,22,22,22	0
85	MG	2	1962	1/1	0.92	0.24	44,44,44,44	0
86	OHX	5	4115	7/7	0.92	0.14	118,118,118,118	0
86	OHX	5	4117	7/7	0.92	0.17	96,96,96,96	0
85	MG	6	1961	1/1	0.92	0.36	60,60,60,60	0
86	OHX	5	4119	7/7	0.92	0.18	99,99,99,99	0
86	OHX	5	4121	7/7	0.92	0.17	111,111,111,111	0
85	MG	5	3821	1/1	0.92	0.22	32,32,32,32	0
85	MG	5	3657	1/1	0.92	0.13	30,30,30,30	0
85	MG	5	3823	1/1	0.92	0.23	51,51,51,51	0
85	MG	2	1935	1/1	0.92	0.31	60,60,60,60	0
85	MG	1	3658	1/1	0.92	0.26	36,36,36,36	0
85	MG	5	3499	1/1	0.92	0.23	24,24,24,24	0
85	MG	1	3855	1/1	0.92	0.13	41,41,41,41	0
86	OHX	5	4133	7/7	0.92	0.18	102,102,102,102	0
85	MG	1	3418	1/1	0.92	0.26	41,41,41,41	0
85	MG	5	3668	1/1	0.92	0.08	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3670	1/1	0.92	0.30	44,44,44,44	0
85	MG	5	3504	1/1	0.92	0.20	26,26,26,26	0
85	MG	5	3673	1/1	0.92	0.29	37,37,37,37	0
85	MG	5	3507	1/1	0.92	0.24	33,33,33,33	0
86	OHX	5	4141	7/7	0.92	0.17	108,108,108,108	0
85	MG	5	3513	1/1	0.92	0.14	27,27,27,27	0
85	MG	5	3850	1/1	0.92	0.09	56,56,56,56	0
85	MG	1	3660	1/1	0.92	0.22	40,40,40,40	0
85	MG	5	3515	1/1	0.92	0.20	28,28,28,28	0
85	MG	1	3714	1/1	0.92	0.08	25,25,25,25	0
85	MG	1	3621	1/1	0.92	0.08	32,32,32,32	0
85	MG	5	3524	1/1	0.92	0.13	36,36,36,36	0
85	MG	5	3685	1/1	0.92	0.16	37,37,37,37	0
85	MG	1	3664	1/1	0.92	0.06	39,39,39,39	0
85	MG	1	3567	1/1	0.92	0.27	24,24,24,24	0
85	MG	1	3577	1/1	0.92	0.12	17,17,17,17	0
86	OHX	2	2171	7/7	0.92	0.16	110,110,110,110	0
85	MG	5	3692	1/1	0.92	0.11	39,39,39,39	0
85	MG	1	3793	1/1	0.92	0.15	73,73,73,73	0
85	MG	5	3695	1/1	0.92	0.20	46,46,46,46	0
85	MG	5	3867	1/1	0.92	0.31	31,31,31,31	0
86	OHX	5	4160	7/7	0.92	0.21	93,93,93,93	0
85	MG	N8	202	1/1	0.92	0.09	37,37,37,37	0
85	MG	1	3794	1/1	0.92	0.15	45,45,45,45	0
85	MG	1	3866	1/1	0.92	0.24	49,49,49,49	0
85	MG	5	3410	1/1	0.92	0.29	47,47,47,47	0
85	MG	1	3867	1/1	0.92	0.08	21,21,21,21	0
85	MG	1	3534	1/1	0.92	0.24	31,31,31,31	0
85	MG	1	3797	1/1	0.92	0.08	16,16,16,16	0
85	MG	1	3535	1/1	0.92	0.24	41,41,41,41	0
86	OHX	C5	201	7/7	0.92	0.13	136,136,136,136	0
86	OHX	1	3957	7/7	0.92	0.20	80,80,80,80	0
86	OHX	1	3967	7/7	0.92	0.18	82,82,82,82	0
86	OHX	1	3970	7/7	0.92	0.13	94,94,94,94	0
86	OHX	1	3981	7/7	0.92	0.23	79,79,79,79	0
86	OHX	3	223	7/7	0.92	0.20	96,96,96,96	0
85	MG	2	1979	1/1	0.92	0.28	45,45,45,45	0
86	OHX	1	4007	7/7	0.92	0.20	90,90,90,90	0
86	OHX	1	4012	7/7	0.92	0.17	101,101,101,101	0
86	OHX	4	226	7/7	0.92	0.18	91,91,91,91	0
86	OHX	4	229	7/7	0.92	0.13	121,121,121,121	0
86	OHX	1	4014	7/7	0.92	0.17	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4015	7/7	0.92	0.15	98,98,98,98	0
85	MG	5	3709	1/1	0.92	0.21	74,74,74,74	0
85	MG	5	3551	1/1	0.92	0.32	39,39,39,39	0
85	MG	5	3713	1/1	0.92	0.10	41,41,41,41	0
85	MG	1	3460	1/1	0.92	0.21	26,26,26,26	0
85	MG	2	2016	1/1	0.92	0.40	59,59,59,59	0
86	OHX	1	4045	7/7	0.92	0.18	94,94,94,94	0
86	OHX	1	4053	7/7	0.92	0.20	87,87,87,87	0
86	OHX	5	4192	7/7	0.92	0.13	135,135,135,135	0
85	MG	5	3423	1/1	0.92	0.13	36,36,36,36	0
85	MG	1	3630	1/1	0.92	0.07	21,21,21,21	0
85	MG	5	3425	1/1	0.92	0.15	30,30,30,30	0
86	OHX	O3	202	7/7	0.92	0.21	91,91,91,91	0
85	MG	1	3676	1/1	0.92	0.12	59,59,59,59	0
86	OHX	6	2095	7/7	0.92	0.16	100,100,100,100	0
85	MG	6	1998	1/1	0.92	0.21	49,49,49,49	0
86	OHX	6	2107	7/7	0.92	0.18	96,96,96,96	0
85	MG	1	3735	1/1	0.92	0.29	55,55,55,55	0
86	OHX	6	2125	7/7	0.92	0.17	106,106,106,106	0
86	OHX	1	4075	7/7	0.92	0.15	113,113,113,113	0
86	OHX	6	2133	7/7	0.92	0.13	126,126,126,126	0
85	MG	1	3588	1/1	0.92	0.21	21,21,21,21	0
86	OHX	1	4080	7/7	0.92	0.16	106,106,106,106	0
86	OHX	6	2138	7/7	0.92	0.16	100,100,100,100	0
85	MG	5	4252	1/1	0.92	0.18	25,25,25,25	0
85	MG	7	201	1/1	0.92	0.37	36,36,36,36	0
85	MG	2	2017	1/1	0.92	0.40	58,58,58,58	0
85	MG	1	3679	1/1	0.92	0.10	38,38,38,38	0
85	MG	1	3424	1/1	0.92	0.14	37,37,37,37	0
85	MG	7	206	1/1	0.92	0.11	36,36,36,36	0
85	MG	2	2184	1/1	0.92	0.14	78,78,78,78	0
86	OHX	6	2150	7/7	0.92	0.15	115,115,115,115	0
85	MG	2	1936	1/1	0.92	0.36	42,42,42,42	0
85	MG	5	3736	1/1	0.92	0.10	36,36,36,36	0
85	MG	7	210	1/1	0.92	0.13	28,28,28,28	0
85	MG	4	205	1/1	0.92	0.24	41,41,41,41	0
85	MG	5	3443	1/1	0.92	0.21	20,20,20,20	0
85	MG	1	3749	1/1	0.92	0.12	43,43,43,43	0
85	MG	6	2010	1/1	0.92	0.07	36,36,36,36	0
86	OHX	1	4102	7/7	0.92	0.21	90,90,90,90	0
85	MG	4	209	1/1	0.92	0.11	37,37,37,37	0
85	MG	5	3744	1/1	0.92	0.06	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2162	7/7	0.92	0.20	96,96,96,96	0
85	MG	2	1971	1/1	0.92	0.33	56,56,56,56	0
85	MG	1	3606	1/1	0.92	0.09	42,42,42,42	0
85	MG	8	207	1/1	0.92	0.09	53,53,53,53	0
85	MG	5	3458	1/1	0.92	0.20	54,54,54,54	0
85	MG	5	3595	1/1	0.92	0.28	27,27,27,27	0
86	OHX	1	4112	7/7	0.92	0.17	102,102,102,102	0
85	MG	6	2016	1/1	0.92	0.12	38,38,38,38	0
85	MG	5	3757	1/1	0.92	0.25	49,49,49,49	0
85	MG	5	3462	1/1	0.92	0.23	27,27,27,27	0
85	MG	1	3549	1/1	0.92	0.22	27,27,27,27	0
85	MG	6	1931	1/1	0.92	0.40	54,54,54,54	0
86	OHX	1	4118	7/7	0.92	0.20	95,95,95,95	0
85	MG	6	2019	1/1	0.92	0.32	48,48,48,48	0
85	MG	m4	201	1/1	0.92	0.23	46,46,46,46	0
85	MG	4	213	1/1	0.92	0.09	50,50,50,50	0
85	MG	5	3608	1/1	0.92	0.17	29,29,29,29	0
85	MG	n0	202	1/1	0.92	0.11	32,32,32,32	0
85	MG	1	3451	1/1	0.92	0.26	34,34,34,34	0
85	MG	1	3834	1/1	0.92	0.25	16,16,16,16	0
86	OHX	7	226	7/7	0.92	0.21	92,92,92,92	0
85	MG	6	2023	1/1	0.92	0.13	41,41,41,41	0
86	OHX	1	4127	7/7	0.92	0.14	120,120,120,120	0
85	MG	1	3525	1/1	0.92	0.20	20,20,20,20	0
85	MG	6	2026	1/1	0.92	0.11	69,69,69,69	0
85	MG	n9	3801	1/1	0.92	0.07	24,24,24,24	0
85	MG	5	3777	1/1	0.92	0.18	45,45,45,45	0
85	MG	o3	201	1/1	0.92	0.18	40,40,40,40	0
85	MG	1	3648	1/1	0.92	0.09	35,35,35,35	0
85	MG	1	3760	1/1	0.92	0.07	30,30,30,30	0
85	MG	6	1940	1/1	0.92	0.48	70,70,70,70	0
85	MG	5	3625	1/1	0.92	0.16	53,53,53,53	0
85	MG	1	3691	1/1	0.92	0.12	28,28,28,28	0
86	OHX	2	2089	7/7	0.92	0.17	100,100,100,100	0
86	OHX	2	2093	7/7	0.92	0.23	94,94,94,94	0
85	MG	5	3784	1/1	0.92	0.21	22,22,22,22	0
85	MG	5	3629	1/1	0.92	0.15	37,37,37,37	0
86	OHX	2	2103	7/7	0.92	0.16	112,112,112,112	0
86	OHX	2	2104	7/7	0.92	0.11	169,169,169,169	0
86	OHX	2	2105	7/7	0.92	0.17	97,97,97,97	0
86	OHX	6	2201	7/7	0.92	0.17	116,116,116,116	0
85	MG	6	1942	1/1	0.92	0.20	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3610	1/1	0.92	0.18	34,34,34,34	0
85	MG	1	3697	1/1	0.92	0.11	45,45,45,45	0
86	OHX	2	2145	7/7	0.93	0.11	133,133,133,133	0
85	MG	5	3518	1/1	0.93	0.32	32,32,32,32	0
85	MG	1	3701	1/1	0.93	0.07	34,34,34,34	0
85	MG	M3	202	1/1	0.93	0.10	34,34,34,34	0
85	MG	5	3848	1/1	0.93	0.17	34,34,34,34	0
85	MG	1	3702	1/1	0.93	0.19	39,39,39,39	0
86	OHX	5	4079	7/7	0.93	0.17	99,99,99,99	0
86	OHX	5	4084	7/7	0.93	0.13	112,112,112,112	0
86	OHX	5	4087	7/7	0.93	0.15	105,105,105,105	0
85	MG	5	3530	1/1	0.93	0.30	40,40,40,40	0
85	MG	5	3684	1/1	0.93	0.25	61,61,61,61	0
85	MG	1	3523	1/1	0.93	0.21	22,22,22,22	0
85	MG	5	3687	1/1	0.93	0.18	45,45,45,45	0
86	OHX	5	4097	7/7	0.93	0.19	93,93,93,93	0
85	MG	1	3494	1/1	0.93	0.18	30,30,30,30	0
85	MG	5	3535	1/1	0.93	0.24	32,32,32,32	0
86	OHX	5	4100	7/7	0.93	0.16	100,100,100,100	0
85	MG	1	3776	1/1	0.93	0.26	53,53,53,53	0
85	MG	1	3706	1/1	0.93	0.07	30,30,30,30	0
85	MG	1	3653	1/1	0.93	0.19	49,49,49,49	0
85	MG	1	3556	1/1	0.93	0.26	30,30,30,30	0
85	MG	5	3864	1/1	0.93	0.29	52,52,52,52	0
85	MG	M7	204	1/1	0.93	0.07	27,27,27,27	0
85	MG	M7	205	1/1	0.93	0.07	34,34,34,34	0
85	MG	1	3783	1/1	0.93	0.17	36,36,36,36	0
85	MG	5	3414	1/1	0.93	0.20	39,39,39,39	0
86	OHX	5	4110	7/7	0.93	0.16	103,103,103,103	0
86	OHX	5	4111	7/7	0.93	0.17	104,104,104,104	0
86	OHX	5	4113	7/7	0.93	0.19	92,92,92,92	0
86	OHX	5	4114	7/7	0.93	0.18	95,95,95,95	0
85	MG	1	3859	1/1	0.93	0.18	54,54,54,54	0
85	MG	5	3870	1/1	0.93	0.09	39,39,39,39	0
85	MG	N3	202	1/1	0.93	0.21	51,51,51,51	0
85	MG	6	1977	1/1	0.93	0.20	40,40,40,40	0
85	MG	1	3558	1/1	0.93	0.23	40,40,40,40	0
85	MG	5	3421	1/1	0.93	0.16	33,33,33,33	0
85	MG	5	3878	1/1	0.93	0.16	27,27,27,27	0
85	MG	1	3612	1/1	0.93	0.11	37,37,37,37	0
85	MG	5	3711	1/1	0.93	0.11	51,51,51,51	0
86	OHX	1	4196	7/7	0.93	0.13	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4128	7/7	0.93	0.15	112,112,112,112	0
85	MG	1	3438	1/1	0.93	0.14	36,36,36,36	0
85	MG	1	3562	1/1	0.93	0.27	22,22,22,22	0
85	MG	5	3715	1/1	0.93	0.13	58,58,58,58	0
86	OHX	5	4134	7/7	0.93	0.19	99,99,99,99	0
85	MG	6	1985	1/1	0.93	0.24	59,59,59,59	0
85	MG	1	3423	1/1	0.93	0.13	28,28,28,28	0
85	MG	O4	201	1/1	0.93	0.21	45,45,45,45	0
85	MG	5	3572	1/1	0.93	0.36	34,34,34,34	0
85	MG	5	3574	1/1	0.93	0.31	40,40,40,40	0
85	MG	1	3792	1/1	0.93	0.11	58,58,58,58	0
86	OHX	D9	102	7/7	0.93	0.15	109,109,109,109	0
86	OHX	1	3915	7/7	0.93	0.19	73,73,73,73	0
86	OHX	1	3956	7/7	0.93	0.14	86,86,86,86	0
85	MG	1	3463	1/1	0.93	0.29	19,19,19,19	0
85	MG	1	3440	1/1	0.93	0.08	31,31,31,31	0
85	MG	5	3728	1/1	0.93	0.15	20,20,20,20	0
85	MG	1	3620	1/1	0.93	0.19	55,55,55,55	0
86	OHX	1	4001	7/7	0.93	0.15	133,133,133,133	0
85	MG	6	1993	1/1	0.93	0.19	42,42,42,42	0
85	MG	5	4256	1/1	0.93	0.10	23,23,23,23	0
85	MG	5	4257	1/1	0.93	0.30	22,22,22,22	0
85	MG	6	1994	1/1	0.93	0.19	51,51,51,51	0
85	MG	6	1905	1/1	0.93	0.27	49,49,49,49	0
85	MG	5	3438	1/1	0.93	0.34	58,58,58,58	0
85	MG	1	4220	1/1	0.93	0.10	23,23,23,23	0
85	MG	1	3482	1/1	0.93	0.27	22,22,22,22	0
85	MG	5	3446	1/1	0.93	0.11	30,30,30,30	0
86	OHX	1	4032	7/7	0.93	0.15	108,108,108,108	0
85	MG	5	3589	1/1	0.93	0.19	33,33,33,33	0
86	OHX	1	4040	7/7	0.93	0.13	114,114,114,114	0
86	OHX	1	4042	7/7	0.93	0.17	97,97,97,97	0
85	MG	1	3726	1/1	0.93	0.14	33,33,33,33	0
85	MG	5	3592	1/1	0.93	0.25	29,29,29,29	0
86	OHX	1	4063	7/7	0.93	0.15	102,102,102,102	0
86	OHX	1	4064	7/7	0.93	0.12	123,123,123,123	0
85	MG	1	3669	1/1	0.93	0.11	37,37,37,37	0
85	MG	6	1913	1/1	0.93	0.28	46,46,46,46	0
85	MG	1	3729	1/1	0.93	0.12	61,61,61,61	0
86	OHX	1	4070	7/7	0.93	0.20	88,88,88,88	0
85	MG	1	3533	1/1	0.93	0.09	24,24,24,24	0
85	MG	3	206	1/1	0.93	0.32	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2077	7/7	0.93	0.17	92,92,92,92	0
86	OHX	6	2085	7/7	0.93	0.13	109,109,109,109	0
86	OHX	5	4178	7/7	0.93	0.13	126,126,126,126	0
86	OHX	6	2091	7/7	0.93	0.18	94,94,94,94	0
85	MG	5	3750	1/1	0.93	0.09	34,34,34,34	0
85	MG	8	204	1/1	0.93	0.17	42,42,42,42	0
86	OHX	1	4076	7/7	0.93	0.34	81,81,81,81	0
85	MG	3	207	1/1	0.93	0.34	55,55,55,55	0
85	MG	5	3754	1/1	0.93	0.19	38,38,38,38	0
85	MG	1	3569	1/1	0.93	0.25	21,21,21,21	0
86	OHX	1	4083	7/7	0.93	0.18	100,100,100,100	0
86	OHX	6	2134	7/7	0.93	0.15	101,101,101,101	0
85	MG	6	1919	1/1	0.93	0.27	34,34,34,34	0
85	MG	1	3807	1/1	0.93	0.12	26,26,26,26	0
85	MG	8	210	1/1	0.93	0.15	50,50,50,50	0
86	OHX	6	2139	7/7	0.93	0.17	106,106,106,106	0
85	MG	8	211	1/1	0.93	0.11	79,79,79,79	0
86	OHX	1	4088	7/7	0.93	0.16	104,104,104,104	0
86	OHX	1	4090	7/7	0.93	0.15	102,102,102,102	0
85	MG	1	3571	1/1	0.93	0.29	35,35,35,35	0
85	MG	l3	401	1/1	0.93	0.29	22,22,22,22	0
85	MG	l5	301	1/1	0.93	0.23	36,36,36,36	0
86	OHX	1	4095	7/7	0.93	0.20	95,95,95,95	0
86	OHX	6	2149	7/7	0.93	0.19	87,87,87,87	0
85	MG	1	3504	1/1	0.93	0.34	39,39,39,39	0
85	MG	5	3612	1/1	0.93	0.10	26,26,26,26	0
85	MG	1	3810	1/1	0.93	0.23	26,26,26,26	0
85	MG	1	3413	1/1	0.93	0.30	52,52,52,52	0
85	MG	1	3467	1/1	0.93	0.14	38,38,38,38	0
86	OHX	6	2155	7/7	0.93	0.18	93,93,93,93	0
85	MG	1	3485	1/1	0.93	0.23	35,35,35,35	0
85	MG	6	1927	1/1	0.93	0.28	39,39,39,39	0
85	MG	1	3584	1/1	0.93	0.17	31,31,31,31	0
85	MG	5	3621	1/1	0.93	0.09	46,46,46,46	0
85	MG	n3	201	1/1	0.93	0.24	21,21,21,21	0
85	MG	5	3623	1/1	0.93	0.21	33,33,33,33	0
85	MG	1	3511	1/1	0.93	0.14	21,21,21,21	0
85	MG	1	3543	1/1	0.93	0.28	29,29,29,29	0
86	OHX	1	4109	7/7	0.93	0.11	120,120,120,120	0
86	OHX	1	4110	7/7	0.93	0.18	92,92,92,92	0
85	MG	6	2024	1/1	0.93	0.17	40,40,40,40	0
85	MG	1	3745	1/1	0.93	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3633	1/1	0.93	0.14	35,35,35,35	0
85	MG	n9	3802	1/1	0.93	0.18	31,31,31,31	0
85	MG	5	3632	1/1	0.93	0.07	30,30,30,30	0
85	MG	1	3454	1/1	0.93	0.22	30,30,30,30	0
85	MG	o3	202	1/1	0.93	0.11	24,24,24,24	0
85	MG	1	3589	1/1	0.93	0.28	25,25,25,25	0
85	MG	1	3832	1/1	0.93	0.17	31,31,31,31	0
85	MG	q0	202	1/1	0.93	0.08	34,34,34,34	0
85	MG	1	3487	1/1	0.93	0.16	27,27,27,27	0
86	OHX	2	2041	7/7	0.93	0.17	85,85,85,85	0
86	OHX	2	2069	7/7	0.93	0.12	125,125,125,125	0
86	OHX	2	2076	7/7	0.93	0.14	115,115,115,115	0
85	MG	6	1938	1/1	0.93	0.24	35,35,35,35	0
85	MG	5	3487	1/1	0.93	0.09	23,23,23,23	0
85	MG	2	1958	1/1	0.93	0.30	62,62,62,62	0
85	MG	5	3644	1/1	0.93	0.26	29,29,29,29	0
85	MG	6	2033	1/1	0.93	0.08	45,45,45,45	0
85	MG	1	3489	1/1	0.93	0.17	22,22,22,22	0
85	MG	1	3836	1/1	0.93	0.18	23,23,23,23	0
85	MG	1	3432	1/1	0.93	0.28	36,36,36,36	0
85	MG	2	1953	1/1	0.93	0.21	76,76,76,76	0
85	MG	1	3645	1/1	0.93	0.08	54,54,54,54	0
85	MG	5	3809	1/1	0.93	0.09	62,62,62,62	0
86	OHX	2	2114	7/7	0.93	0.15	124,124,124,124	0
85	MG	6	1948	1/1	0.93	0.25	37,37,37,37	0
85	MG	5	3811	1/1	0.93	0.08	29,29,29,29	0
86	OHX	1	4139	7/7	0.93	0.17	87,87,87,87	0
86	OHX	7	223	7/7	0.93	0.14	106,106,106,106	0
86	OHX	2	2118	7/7	0.93	0.13	129,129,129,129	0
85	MG	1	3694	1/1	0.93	0.12	27,27,27,27	0
85	MG	6	1950	1/1	0.93	0.21	35,35,35,35	0
86	OHX	8	221	7/7	0.93	0.17	95,95,95,95	0
85	MG	5	3659	1/1	0.93	0.24	22,22,22,22	0
85	MG	5	3660	1/1	0.93	0.16	39,39,39,39	0
85	MG	L4	402	1/1	0.93	0.15	51,51,51,51	0
85	MG	5	3819	1/1	0.93	0.11	47,47,47,47	0
85	MG	5	3662	1/1	0.93	0.12	54,54,54,54	0
85	MG	6	2043	1/1	0.93	0.19	39,39,39,39	0
85	MG	1	3604	1/1	0.93	0.21	27,27,27,27	0
86	OHX	2	2130	7/7	0.93	0.12	150,150,150,150	0
86	OHX	2	2132	7/7	0.93	0.17	103,103,103,103	0
85	MG	1	3647	1/1	0.93	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3826	1/1	0.93	0.06	29,29,29,29	0
85	MG	5	3827	1/1	0.93	0.17	20,20,20,20	0
85	MG	5	3509	1/1	0.93	0.22	22,22,22,22	0
86	OHX	d9	102	7/7	0.93	0.14	117,117,117,117	0
85	MG	5	3669	1/1	0.93	0.09	26,26,26,26	0
85	MG	6	1956	1/1	0.93	0.31	38,38,38,38	0
85	MG	6	2205	1/1	0.93	0.23	42,42,42,42	0
85	MG	1	3605	1/1	0.93	0.12	29,29,29,29	0
85	MG	1	3552	1/1	0.93	0.37	32,32,32,32	0
85	MG	5	3840	1/1	0.93	0.10	43,43,43,43	0
86	OHX	5	4035	7/7	0.93	0.15	102,102,102,102	0
87	ZN	q2	501	1/1	0.93	0.14	59,59,59,59	0
85	MG	1	3437	1/1	0.93	0.19	22,22,22,22	0
88	3H3	5	4251	33/33	0.93	0.10	29,29,29,29	0
86	OHX	5	4116	7/7	0.94	0.19	82,82,82,82	0
86	OHX	6	2064	7/7	0.94	0.15	80,80,80,80	0
85	MG	1	3442	1/1	0.94	0.16	19,19,19,19	0
85	MG	1	3503	1/1	0.94	0.16	17,17,17,17	0
86	OHX	5	4120	7/7	0.94	0.12	118,118,118,118	0
85	MG	5	3599	1/1	0.94	0.10	31,31,31,31	0
85	MG	5	3800	1/1	0.94	0.11	35,35,35,35	0
86	OHX	6	2100	7/7	0.94	0.14	127,127,127,127	0
85	MG	1	3614	1/1	0.94	0.23	29,29,29,29	0
85	MG	5	3694	1/1	0.94	0.06	35,35,35,35	0
86	OHX	6	2112	7/7	0.94	0.14	99,99,99,99	0
86	OHX	6	2114	7/7	0.94	0.16	102,102,102,102	0
86	OHX	5	4130	7/7	0.94	0.16	95,95,95,95	0
86	OHX	6	2116	7/7	0.94	0.13	100,100,100,100	0
85	MG	6	1976	1/1	0.94	0.14	33,33,33,33	0
86	OHX	6	2122	7/7	0.94	0.13	115,115,115,115	0
86	OHX	6	2123	7/7	0.94	0.14	114,114,114,114	0
85	MG	1	3551	1/1	0.94	0.26	25,25,25,25	0
86	OHX	6	2126	7/7	0.94	0.34	81,81,81,81	0
85	MG	1	3430	1/1	0.94	0.27	41,41,41,41	0
86	OHX	6	2131	7/7	0.94	0.13	119,119,119,119	0
86	OHX	6	2132	7/7	0.94	0.15	100,100,100,100	0
85	MG	5	3699	1/1	0.94	0.07	30,30,30,30	0
85	MG	8	201	1/1	0.94	0.28	31,31,31,31	0
85	MG	1	3431	1/1	0.94	0.26	41,41,41,41	0
85	MG	6	1980	1/1	0.94	0.32	60,60,60,60	0
86	OHX	5	4144	7/7	0.94	0.19	97,97,97,97	0
86	OHX	6	2137	7/7	0.94	0.17	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3618	1/1	0.94	0.27	48,48,48,48	0
85	MG	6	1932	1/1	0.94	0.20	37,37,37,37	0
85	MG	2	2013	1/1	0.94	0.23	44,44,44,44	0
85	MG	5	3520	1/1	0.94	0.18	24,24,24,24	0
85	MG	5	3614	1/1	0.94	0.08	32,32,32,32	0
85	MG	5	3708	1/1	0.94	0.11	36,36,36,36	0
85	MG	5	3523	1/1	0.94	0.26	23,23,23,23	0
85	MG	8	212	1/1	0.94	0.22	47,47,47,47	0
85	MG	1	3458	1/1	0.94	0.16	30,30,30,30	0
86	OHX	2	2169	7/7	0.94	0.19	96,96,96,96	0
85	MG	5	3445	1/1	0.94	0.24	33,33,33,33	0
85	MG	1	3510	1/1	0.94	0.26	25,25,25,25	0
85	MG	5	3528	1/1	0.94	0.25	22,22,22,22	0
85	MG	5	3529	1/1	0.94	0.26	25,25,25,25	0
85	MG	1	3472	1/1	0.94	0.06	29,29,29,29	0
85	MG	1	3474	1/1	0.94	0.20	20,20,20,20	0
85	MG	5	3719	1/1	0.94	0.12	31,31,31,31	0
85	MG	4	206	1/1	0.94	0.26	28,28,28,28	0
85	MG	m7	202	1/1	0.94	0.20	25,25,25,25	0
85	MG	4	207	1/1	0.94	0.12	32,32,32,32	0
85	MG	1	3435	1/1	0.94	0.09	32,32,32,32	0
85	MG	1	3765	1/1	0.94	0.19	40,40,40,40	0
85	MG	2	2004	1/1	0.94	0.12	67,67,67,67	0
85	MG	n3	202	1/1	0.94	0.10	35,35,35,35	0
85	MG	5	3634	1/1	0.94	0.26	33,33,33,33	0
85	MG	5	3841	1/1	0.94	0.27	37,37,37,37	0
85	MG	5	3843	1/1	0.94	0.09	25,25,25,25	0
86	OHX	1	3924	7/7	0.94	0.16	94,94,94,94	0
86	OHX	1	3932	7/7	0.94	0.17	82,82,82,82	0
85	MG	5	3543	1/1	0.94	0.13	23,23,23,23	0
85	MG	O7	102	1/1	0.94	0.11	32,32,32,32	0
85	MG	5	3463	1/1	0.94	0.26	44,44,44,44	0
85	MG	6	1946	1/1	0.94	0.30	52,52,52,52	0
85	MG	1	3595	1/1	0.94	0.24	22,22,22,22	0
86	OHX	1	3984	7/7	0.94	0.16	94,94,94,94	0
86	OHX	1	4000	7/7	0.94	0.19	82,82,82,82	0
85	MG	1	3815	1/1	0.94	0.07	26,26,26,26	0
85	MG	6	2002	1/1	0.94	0.09	43,43,43,43	0
85	MG	s8	302	1/1	0.94	0.11	40,40,40,40	0
86	OHX	1	4008	7/7	0.94	0.15	99,99,99,99	0
86	OHX	1	4010	7/7	0.94	0.20	82,82,82,82	0
85	MG	5	3853	1/1	0.94	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3817	1/1	0.94	0.26	40,40,40,40	0
85	MG	5	3647	1/1	0.94	0.16	41,41,41,41	0
85	MG	q3	502	1/1	0.94	0.25	45,45,45,45	0
86	OHX	1	4021	7/7	0.94	0.14	99,99,99,99	0
85	MG	5	3553	1/1	0.94	0.28	37,37,37,37	0
85	MG	5	3741	1/1	0.94	0.08	46,46,46,46	0
85	MG	1	3541	1/1	0.94	0.19	19,19,19,19	0
86	OHX	2	2080	7/7	0.94	0.19	98,98,98,98	0
85	MG	5	3859	1/1	0.94	0.09	44,44,44,44	0
85	MG	5	3555	1/1	0.94	0.23	20,20,20,20	0
85	MG	1	3601	1/1	0.94	0.15	18,18,18,18	0
86	OHX	2	2090	7/7	0.94	0.17	89,89,89,89	0
86	OHX	2	2092	7/7	0.94	0.15	103,103,103,103	0
86	OHX	1	4054	7/7	0.94	0.17	94,94,94,94	0
86	OHX	1	4057	7/7	0.94	0.14	114,114,114,114	0
86	OHX	1	4058	7/7	0.94	0.22	80,80,80,80	0
86	OHX	1	4061	7/7	0.94	0.17	97,97,97,97	0
85	MG	1	3693	1/1	0.94	0.27	36,36,36,36	0
85	MG	5	3747	1/1	0.94	0.15	47,47,47,47	0
85	MG	5	3655	1/1	0.94	0.29	45,45,45,45	0
86	OHX	2	2101	7/7	0.94	0.14	116,116,116,116	0
85	MG	5	3565	1/1	0.94	0.26	22,22,22,22	0
85	MG	d3	201	1/1	0.94	0.16	39,39,39,39	0
85	MG	6	1908	1/1	0.94	0.23	41,41,41,41	0
86	OHX	1	4072	7/7	0.94	0.18	103,103,103,103	0
86	OHX	2	2106	7/7	0.94	0.15	111,111,111,111	0
86	OHX	2	2107	7/7	0.94	0.15	96,96,96,96	0
85	MG	sM	301	1/1	0.94	0.06	33,33,33,33	0
86	OHX	2	2109	7/7	0.94	0.12	123,123,123,123	0
86	OHX	1	4077	7/7	0.94	0.14	97,97,97,97	0
86	OHX	1	4078	7/7	0.94	0.16	101,101,101,101	0
86	OHX	5	3955	7/7	0.94	0.12	79,79,79,79	0
86	OHX	2	2110	7/7	0.94	0.14	113,113,113,113	0
85	MG	1	3461	1/1	0.94	0.20	20,20,20,20	0
85	MG	5	3758	1/1	0.94	0.24	46,46,46,46	0
86	OHX	1	4082	7/7	0.94	0.16	93,93,93,93	0
86	OHX	5	4026	7/7	0.94	0.17	83,83,83,83	0
85	MG	5	3760	1/1	0.94	0.06	35,35,35,35	0
86	OHX	5	4030	7/7	0.94	0.16	94,94,94,94	0
86	OHX	5	4032	7/7	0.94	0.18	88,88,88,88	0
85	MG	1	3822	1/1	0.94	0.18	48,48,48,48	0
85	MG	1	3695	1/1	0.94	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4041	7/7	0.94	0.13	126,126,126,126	0
85	MG	5	3573	1/1	0.94	0.28	26,26,26,26	0
85	MG	6	2012	1/1	0.94	0.21	41,41,41,41	0
86	OHX	5	4051	7/7	0.94	0.16	88,88,88,88	0
86	OHX	2	2121	7/7	0.94	0.14	116,116,116,116	0
85	MG	2	1957	1/1	0.94	0.30	47,47,47,47	0
86	OHX	5	4069	7/7	0.94	0.13	108,108,108,108	0
85	MG	5	3766	1/1	0.94	0.12	35,35,35,35	0
86	OHX	5	4072	7/7	0.94	0.17	96,96,96,96	0
86	OHX	5	4073	7/7	0.94	0.16	93,93,93,93	0
86	OHX	2	2124	7/7	0.94	0.14	116,116,116,116	0
86	OHX	5	4076	7/7	0.94	0.16	99,99,99,99	0
86	OHX	3	221	7/7	0.94	0.14	102,102,102,102	0
86	OHX	7	224	7/7	0.94	0.18	92,92,92,92	0
86	OHX	5	4083	7/7	0.94	0.16	94,94,94,94	0
85	MG	6	2014	1/1	0.94	0.12	53,53,53,53	0
86	OHX	1	4094	7/7	0.94	0.11	129,129,129,129	0
86	OHX	8	219	7/7	0.94	0.19	91,91,91,91	0
86	OHX	5	4088	7/7	0.94	0.18	91,91,91,91	0
85	MG	1	3778	1/1	0.94	0.09	41,41,41,41	0
86	OHX	5	4091	7/7	0.94	0.19	92,92,92,92	0
85	MG	1	3779	1/1	0.94	0.14	24,24,24,24	0
86	OHX	5	4094	7/7	0.94	0.15	101,101,101,101	0
85	MG	2	2007	1/1	0.94	0.42	52,52,52,52	0
85	MG	5	3772	1/1	0.94	0.12	23,23,23,23	0
86	OHX	4	227	7/7	0.94	0.18	86,86,86,86	0
85	MG	1	3568	1/1	0.94	0.20	19,19,19,19	0
85	MG	5	3582	1/1	0.94	0.31	27,27,27,27	0
85	MG	1	3409	1/1	0.94	0.27	30,30,30,30	0
85	MG	2	1906	1/1	0.94	0.23	39,39,39,39	0
85	MG	5	3420	1/1	0.94	0.24	29,29,29,29	0
85	MG	M0	302	1/1	0.94	0.08	37,37,37,37	0
86	OHX	m0	301	7/7	0.94	0.14	105,105,105,105	0
85	MG	1	3574	1/1	0.94	0.29	30,30,30,30	0
86	OHX	L3	403	7/7	0.94	0.17	90,90,90,90	0
85	MG	1	3741	1/1	0.94	0.17	43,43,43,43	0
85	MG	5	4253	1/1	0.94	0.19	28,28,28,28	0
85	MG	1	3524	1/1	0.94	0.06	20,20,20,20	0
86	OHX	M0	303	7/7	0.94	0.15	86,86,86,86	0
85	MG	3	205	1/1	0.94	0.23	28,28,28,28	0
85	MG	5	3686	1/1	0.94	0.15	32,32,32,32	0
85	MG	5	3787	1/1	0.94	0.14	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3427	1/1	0.94	0.17	23,23,23,23	0
85	MG	5	3594	1/1	0.94	0.36	26,26,26,26	0
85	MG	1	3771	1/1	0.95	0.12	36,36,36,36	0
85	MG	1	3575	1/1	0.95	0.23	22,22,22,22	0
85	MG	1	3491	1/1	0.95	0.16	23,23,23,23	0
86	OHX	6	2098	7/7	0.95	0.12	103,103,103,103	0
85	MG	1	3520	1/1	0.95	0.14	23,23,23,23	0
85	MG	5	3703	1/1	0.95	0.06	32,32,32,32	0
85	MG	1	3777	1/1	0.95	0.16	55,55,55,55	0
86	OHX	6	2111	7/7	0.95	0.13	104,104,104,104	0
85	MG	5	3806	1/1	0.95	0.06	30,30,30,30	0
85	MG	1	3665	1/1	0.95	0.17	37,37,37,37	0
85	MG	5	3444	1/1	0.95	0.10	21,21,21,21	0
85	MG	8	203	1/1	0.95	0.26	37,37,37,37	0
85	MG	2	1903	1/1	0.95	0.30	40,40,40,40	0
85	MG	1	3557	1/1	0.95	0.17	38,38,38,38	0
86	OHX	6	2124	7/7	0.95	0.15	87,87,87,87	0
85	MG	1	3736	1/1	0.95	0.20	32,32,32,32	0
85	MG	5	3710	1/1	0.95	0.05	28,28,28,28	0
85	MG	5	3449	1/1	0.95	0.37	53,53,53,53	0
86	OHX	5	4125	7/7	0.95	0.12	113,113,113,113	0
86	OHX	6	2128	7/7	0.95	0.12	109,109,109,109	0
86	OHX	6	2129	7/7	0.95	0.13	113,113,113,113	0
85	MG	5	3450	1/1	0.95	0.11	20,20,20,20	0
86	OHX	5	4129	7/7	0.95	0.12	114,114,114,114	0
85	MG	5	3622	1/1	0.95	0.26	29,29,29,29	0
85	MG	5	3817	1/1	0.95	0.06	33,33,33,33	0
85	MG	5	3714	1/1	0.95	0.16	42,42,42,42	0
85	MG	6	1989	1/1	0.95	0.12	60,60,60,60	0
85	MG	1	3506	1/1	0.95	0.29	37,37,37,37	0
85	MG	5	3533	1/1	0.95	0.22	29,29,29,29	0
85	MG	1	3559	1/1	0.95	0.20	18,18,18,18	0
85	MG	5	3456	1/1	0.95	0.18	21,21,21,21	0
85	MG	1	3637	1/1	0.95	0.25	41,41,41,41	0
86	OHX	6	2141	7/7	0.95	0.11	127,127,127,127	0
85	MG	2	2001	1/1	0.95	0.18	63,63,63,63	0
85	MG	5	3633	1/1	0.95	0.46	71,71,71,71	0
85	MG	5	3723	1/1	0.95	0.10	32,32,32,32	0
85	MG	m7	201	1/1	0.95	0.16	24,24,24,24	0
85	MG	5	3724	1/1	0.95	0.15	28,28,28,28	0
85	MG	5	3833	1/1	0.95	0.12	26,26,26,26	0
85	MG	m7	204	1/1	0.95	0.05	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3459	1/1	0.95	0.11	23,23,23,23	0
85	MG	n0	201	1/1	0.95	0.07	33,33,33,33	0
85	MG	2	2006	1/1	0.95	0.19	45,45,45,45	0
85	MG	N3	201	1/1	0.95	0.25	25,25,25,25	0
85	MG	1	3509	1/1	0.95	0.20	34,34,34,34	0
85	MG	5	3730	1/1	0.95	0.15	41,41,41,41	0
85	MG	C3	201	1/1	0.95	0.39	56,56,56,56	0
85	MG	4	203	1/1	0.95	0.32	44,44,44,44	0
85	MG	5	3549	1/1	0.95	0.23	24,24,24,24	0
85	MG	1	3791	1/1	0.95	0.15	19,19,19,19	0
85	MG	6	1945	1/1	0.95	0.33	43,43,43,43	0
85	MG	c8	201	1/1	0.95	0.31	57,57,57,57	0
86	OHX	1	3939	7/7	0.95	0.14	84,84,84,84	0
86	OHX	1	3951	7/7	0.95	0.14	72,72,72,72	0
85	MG	5	3849	1/1	0.95	0.16	40,40,40,40	0
85	MG	1	3477	1/1	0.95	0.10	30,30,30,30	0
85	MG	1	3513	1/1	0.95	0.23	18,18,18,18	0
85	MG	1	3401	1/1	0.95	0.29	33,33,33,33	0
86	OHX	1	3972	7/7	0.95	0.12	107,107,107,107	0
85	MG	5	3472	1/1	0.95	0.10	23,23,23,23	0
85	MG	5	3563	1/1	0.95	0.19	17,17,17,17	0
86	OHX	1	4159	7/7	0.95	0.13	92,92,92,92	0
86	OHX	5	4170	7/7	0.95	0.31	81,81,81,81	0
86	OHX	1	3992	7/7	0.95	0.15	94,94,94,94	0
86	OHX	1	3995	7/7	0.95	0.14	81,81,81,81	0
85	MG	6	2006	1/1	0.95	0.16	46,46,46,46	0
85	MG	1	3709	1/1	0.95	0.14	28,28,28,28	0
85	MG	5	3475	1/1	0.95	0.27	25,25,25,25	0
86	OHX	1	4005	7/7	0.95	0.23	79,79,79,79	0
86	OHX	1	4006	7/7	0.95	0.13	102,102,102,102	0
86	OHX	2	2044	7/7	0.95	0.14	96,96,96,96	0
86	OHX	2	2068	7/7	0.95	0.11	113,113,113,113	0
86	OHX	1	4009	7/7	0.95	0.14	93,93,93,93	0
85	MG	sM	302	1/1	0.95	0.13	31,31,31,31	0
85	MG	1	3594	1/1	0.95	0.23	22,22,22,22	0
86	OHX	1	4013	7/7	0.95	0.14	105,105,105,105	0
86	OHX	2	2078	7/7	0.95	0.13	100,100,100,100	0
86	OHX	2	2079	7/7	0.95	0.12	107,107,107,107	0
86	OHX	1	4016	7/7	0.95	0.12	105,105,105,105	0
86	OHX	1	4017	7/7	0.95	0.16	97,97,97,97	0
86	OHX	1	4019	7/7	0.95	0.14	89,89,89,89	0
85	MG	1	3798	1/1	0.95	0.17	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	2081	7/7	0.95	0.10	127,127,127,127	0
85	MG	5	3404	1/1	0.95	0.11	32,32,32,32	0
86	OHX	2	2086	7/7	0.95	0.12	112,112,112,112	0
86	OHX	1	4025	7/7	0.95	0.15	91,91,91,91	0
86	OHX	1	4026	7/7	0.95	0.12	116,116,116,116	0
86	OHX	5	4197	7/7	0.95	0.15	92,92,92,92	0
86	OHX	5	4198	7/7	0.95	0.14	98,98,98,98	0
86	OHX	5	4199	7/7	0.95	0.16	98,98,98,98	0
86	OHX	1	4027	7/7	0.95	0.12	112,112,112,112	0
86	OHX	1	4029	7/7	0.95	0.13	102,102,102,102	0
85	MG	5	3751	1/1	0.95	0.25	49,49,49,49	0
85	MG	5	3752	1/1	0.95	0.20	36,36,36,36	0
86	OHX	1	4033	7/7	0.95	0.11	103,103,103,103	0
86	OHX	1	4035	7/7	0.95	0.15	99,99,99,99	0
86	OHX	1	4037	7/7	0.95	0.16	86,86,86,86	0
85	MG	5	3571	1/1	0.95	0.26	27,27,27,27	0
85	MG	5	3406	1/1	0.95	0.12	26,26,26,26	0
85	MG	5	3755	1/1	0.95	0.27	47,47,47,47	0
85	MG	1	3754	1/1	0.95	0.06	29,29,29,29	0
86	OHX	1	4049	7/7	0.95	0.17	87,87,87,87	0
86	OHX	c1	202	7/7	0.95	0.14	108,108,108,108	0
86	OHX	1	4050	7/7	0.95	0.17	92,92,92,92	0
86	OHX	2	2097	7/7	0.95	0.10	131,131,131,131	0
86	OHX	5	4215	7/7	0.95	0.16	85,85,85,85	0
86	OHX	2	2098	7/7	0.95	0.11	126,126,126,126	0
86	OHX	2	2099	7/7	0.95	0.17	94,94,94,94	0
85	MG	5	3664	1/1	0.95	0.12	37,37,37,37	0
85	MG	6	1953	1/1	0.95	0.33	55,55,55,55	0
86	OHX	5	3974	7/7	0.95	0.12	89,89,89,89	0
86	OHX	5	3977	7/7	0.95	0.13	81,81,81,81	0
85	MG	1	3800	1/1	0.95	0.18	42,42,42,42	0
85	MG	2	1973	1/1	0.95	0.19	57,57,57,57	0
85	MG	6	1906	1/1	0.95	0.28	43,43,43,43	0
85	MG	5	3874	1/1	0.95	0.40	41,41,41,41	0
86	OHX	5	4020	7/7	0.95	0.17	85,85,85,85	0
86	OHX	5	4023	7/7	0.95	0.16	89,89,89,89	0
85	MG	5	3486	1/1	0.95	0.22	28,28,28,28	0
86	OHX	1	4069	7/7	0.95	0.10	119,119,119,119	0
86	OHX	5	4029	7/7	0.95	0.22	76,76,76,76	0
85	MG	1	3596	1/1	0.95	0.27	20,20,20,20	0
86	OHX	5	4232	7/7	0.95	0.24	82,82,82,82	0
85	MG	5	3879	1/1	0.95	0.13	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4033	7/7	0.95	0.18	85,85,85,85	0
85	MG	1	3715	1/1	0.95	0.05	31,31,31,31	0
86	OHX	5	4036	7/7	0.95	0.12	105,105,105,105	0
86	OHX	2	2111	7/7	0.95	0.15	93,93,93,93	0
85	MG	1	3759	1/1	0.95	0.11	35,35,35,35	0
85	MG	5	3675	1/1	0.95	0.07	28,28,28,28	0
85	MG	4	217	1/1	0.95	0.24	48,48,48,48	0
86	OHX	5	4048	7/7	0.95	0.14	94,94,94,94	0
86	OHX	5	4050	7/7	0.95	0.11	111,111,111,111	0
86	OHX	3	216	7/7	0.95	0.16	87,87,87,87	0
86	OHX	5	4052	7/7	0.95	0.17	83,83,83,83	0
86	OHX	5	4053	7/7	0.95	0.25	80,80,80,80	0
86	OHX	5	4056	7/7	0.95	0.16	87,87,87,87	0
86	OHX	5	4057	7/7	0.95	0.13	105,105,105,105	0
86	OHX	5	4058	7/7	0.95	0.12	109,109,109,109	0
86	OHX	5	4061	7/7	0.95	0.23	80,80,80,80	0
85	MG	6	1911	1/1	0.95	0.21	38,38,38,38	0
85	MG	4	218	1/1	0.95	0.07	34,34,34,34	0
86	OHX	5	4064	7/7	0.95	0.10	125,125,125,125	0
86	OHX	5	4067	7/7	0.95	0.12	105,105,105,105	0
85	MG	5	3493	1/1	0.95	0.17	21,21,21,21	0
85	MG	1	3597	1/1	0.95	0.23	22,22,22,22	0
86	OHX	8	218	7/7	0.95	0.12	97,97,97,97	0
85	MG	5	3775	1/1	0.95	0.11	21,21,21,21	0
85	MG	1	3717	1/1	0.95	0.18	56,56,56,56	0
86	OHX	8	223	7/7	0.95	0.14	99,99,99,99	0
85	MG	5	3892	1/1	0.95	0.24	38,38,38,38	0
85	MG	1	3684	1/1	0.95	0.25	41,41,41,41	0
85	MG	5	3591	1/1	0.95	0.20	26,26,26,26	0
86	OHX	5	4082	7/7	0.95	0.18	85,85,85,85	0
86	OHX	4	230	7/7	0.95	0.12	113,113,113,113	0
85	MG	5	3779	1/1	0.95	0.07	38,38,38,38	0
86	OHX	5	4085	7/7	0.95	0.15	95,95,95,95	0
86	OHX	5	4086	7/7	0.95	0.16	98,98,98,98	0
85	MG	1	3532	1/1	0.95	0.25	34,34,34,34	0
85	MG	1	3764	1/1	0.95	0.15	42,42,42,42	0
85	MG	1	3452	1/1	0.95	0.13	23,23,23,23	0
85	MG	L4	403	1/1	0.95	0.07	25,25,25,25	0
85	MG	5	4255	1/1	0.95	0.23	23,23,23,23	0
85	MG	5	3690	1/1	0.95	0.07	36,36,36,36	0
85	MG	1	3603	1/1	0.95	0.07	24,24,24,24	0
85	MG	5	4258	1/1	0.95	0.09	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3505	1/1	0.95	0.32	30,30,30,30	0
85	MG	1	3723	1/1	0.95	0.09	43,43,43,43	0
85	MG	1	3572	1/1	0.95	0.22	24,24,24,24	0
85	MG	5	3512	1/1	0.95	0.24	20,20,20,20	0
85	MG	7	205	1/1	0.95	0.30	23,23,23,23	0
87	ZN	Q2	501	1/1	0.95	0.14	63,63,63,63	0
85	MG	1	3628	1/1	0.95	0.09	52,52,52,52	0
86	OHX	2	2142	7/7	0.95	0.12	127,127,127,127	0
85	MG	5	3697	1/1	0.95	0.13	26,26,26,26	0
85	MG	2	1925	1/1	0.95	0.34	60,60,60,60	0
86	OHX	1	3987	7/7	0.96	0.13	80,80,80,80	0
86	OHX	5	4112	7/7	0.96	0.29	79,79,79,79	0
86	OHX	1	3990	7/7	0.96	0.11	97,97,97,97	0
86	OHX	1	3991	7/7	0.96	0.13	92,92,92,92	0
85	MG	5	3559	1/1	0.96	0.22	21,21,21,21	0
86	OHX	1	3993	7/7	0.96	0.15	84,84,84,84	0
86	OHX	1	3994	7/7	0.96	0.14	92,92,92,92	0
85	MG	5	3796	1/1	0.96	0.19	27,27,27,27	0
86	OHX	6	2142	7/7	0.96	0.13	108,108,108,108	0
86	OHX	1	3996	7/7	0.96	0.14	93,93,93,93	0
86	OHX	1	3997	7/7	0.96	0.11	111,111,111,111	0
85	MG	5	3891	1/1	0.96	0.07	64,64,64,64	0
85	MG	5	3798	1/1	0.96	0.26	62,62,62,62	0
85	MG	5	3799	1/1	0.96	0.10	39,39,39,39	0
86	OHX	2	2096	7/7	0.96	0.11	121,121,121,121	0
85	MG	1	3775	1/1	0.96	0.08	29,29,29,29	0
85	MG	1	3657	1/1	0.96	0.11	23,23,23,23	0
85	MG	1	3710	1/1	0.96	0.06	25,25,25,25	0
85	MG	1	3403	1/1	0.96	0.19	27,27,27,27	0
85	MG	5	3439	1/1	0.96	0.14	24,24,24,24	0
86	OHX	1	4011	7/7	0.96	0.14	89,89,89,89	0
85	MG	5	3440	1/1	0.96	0.16	31,31,31,31	0
85	MG	5	4254	1/1	0.96	0.25	19,19,19,19	0
85	MG	1	3743	1/1	0.96	0.20	36,36,36,36	0
85	MG	1	3823	1/1	0.96	0.12	30,30,30,30	0
86	OHX	1	4158	7/7	0.96	0.16	84,84,84,84	0
85	MG	L2	301	1/1	0.96	0.05	26,26,26,26	0
85	MG	5	3651	1/1	0.96	0.06	31,31,31,31	0
85	MG	5	3726	1/1	0.96	0.12	31,31,31,31	0
85	MG	L3	401	1/1	0.96	0.16	28,28,28,28	0
85	MG	5	3501	1/1	0.96	0.19	30,30,30,30	0
85	MG	6	1954	1/1	0.96	0.29	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4023	7/7	0.96	0.14	93,93,93,93	0
86	OHX	2	2113	7/7	0.96	0.12	108,108,108,108	0
85	MG	1	3600	1/1	0.96	0.21	25,25,25,25	0
85	MG	5	3815	1/1	0.96	0.18	36,36,36,36	0
85	MG	1	3539	1/1	0.96	0.21	17,17,17,17	0
85	MG	1	3747	1/1	0.96	0.13	22,22,22,22	0
86	OHX	1	4030	7/7	0.96	0.11	103,103,103,103	0
85	MG	5	3508	1/1	0.96	0.28	24,24,24,24	0
85	MG	1	3748	1/1	0.96	0.16	28,28,28,28	0
85	MG	5	3510	1/1	0.96	0.06	20,20,20,20	0
86	OHX	5	4153	7/7	0.96	0.15	95,95,95,95	0
86	OHX	1	4034	7/7	0.96	0.14	86,86,86,86	0
85	MG	5	3511	1/1	0.96	0.30	45,45,45,45	0
85	MG	1	3602	1/1	0.96	0.14	21,21,21,21	0
86	OHX	1	4038	7/7	0.96	0.10	119,119,119,119	0
85	MG	1	4222	1/1	0.96	0.07	45,45,45,45	0
85	MG	1	3830	1/1	0.96	0.07	16,16,16,16	0
86	OHX	1	4041	7/7	0.96	0.15	85,85,85,85	0
85	MG	6	1962	1/1	0.96	0.16	37,37,37,37	0
85	MG	1	3540	1/1	0.96	0.35	48,48,48,48	0
86	OHX	1	4047	7/7	0.96	0.14	85,85,85,85	0
85	MG	5	3830	1/1	0.96	0.13	46,46,46,46	0
85	MG	1	3640	1/1	0.96	0.06	28,28,28,28	0
86	OHX	1	4051	7/7	0.96	0.13	99,99,99,99	0
85	MG	6	1965	1/1	0.96	0.07	52,52,52,52	0
86	OHX	2	2131	7/7	0.96	0.15	93,93,93,93	0
86	OHX	1	4055	7/7	0.96	0.13	104,104,104,104	0
86	OHX	1	4056	7/7	0.96	0.11	112,112,112,112	0
86	OHX	5	4171	7/7	0.96	0.33	73,73,73,73	0
85	MG	5	3461	1/1	0.96	0.05	29,29,29,29	0
85	MG	5	3522	1/1	0.96	0.25	31,31,31,31	0
86	OHX	1	4059	7/7	0.96	0.12	117,117,117,117	0
85	MG	1	3466	1/1	0.96	0.28	49,49,49,49	0
86	OHX	1	4062	7/7	0.96	0.09	133,133,133,133	0
85	MG	5	3838	1/1	0.96	0.08	53,53,53,53	0
85	MG	1	3642	1/1	0.96	0.07	36,36,36,36	0
85	MG	5	3525	1/1	0.96	0.21	30,30,30,30	0
85	MG	1	3755	1/1	0.96	0.14	18,18,18,18	0
86	OHX	6	2202	7/7	0.96	0.08	159,159,159,159	0
85	MG	8	213	1/1	0.96	0.31	31,31,31,31	0
85	MG	5	3842	1/1	0.96	0.20	42,42,42,42	0
85	MG	l2	302	1/1	0.96	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3677	1/1	0.96	0.17	34,34,34,34	0
85	MG	1	3586	1/1	0.96	0.32	38,38,38,38	0
85	MG	1	3441	1/1	0.96	0.10	30,30,30,30	0
85	MG	5	3601	1/1	0.96	0.10	35,35,35,35	0
85	MG	1	3839	1/1	0.96	0.25	28,28,28,28	0
85	MG	1	3476	1/1	0.96	0.11	21,21,21,21	0
86	OHX	c8	203	7/7	0.96	0.11	113,113,113,113	0
85	MG	1	3570	1/1	0.96	0.19	13,13,13,13	0
85	MG	5	3759	1/1	0.96	0.13	32,32,32,32	0
85	MG	1	3842	1/1	0.96	0.20	22,22,22,22	0
86	OHX	5	3949	7/7	0.96	0.14	84,84,84,84	0
85	MG	5	3415	1/1	0.96	0.20	19,19,19,19	0
86	OHX	5	3960	7/7	0.96	0.13	61,61,61,61	0
86	OHX	5	3963	7/7	0.96	0.13	77,77,77,77	0
85	MG	1	3725	1/1	0.96	0.05	35,35,35,35	0
85	MG	1	3512	1/1	0.96	0.29	22,22,22,22	0
86	OHX	5	3994	7/7	0.96	0.12	102,102,102,102	0
86	OHX	3	219	7/7	0.96	0.11	96,96,96,96	0
86	OHX	3	220	7/7	0.96	0.11	101,101,101,101	0
85	MG	5	3611	1/1	0.96	0.04	22,22,22,22	0
86	OHX	5	4013	7/7	0.96	0.10	129,129,129,129	0
85	MG	5	3537	1/1	0.96	0.21	33,33,33,33	0
85	MG	5	3538	1/1	0.96	0.23	19,19,19,19	0
86	OHX	5	4022	7/7	0.96	0.14	87,87,87,87	0
85	MG	SM	301	1/1	0.96	0.19	38,38,38,38	0
86	OHX	5	4025	7/7	0.96	0.14	88,88,88,88	0
85	MG	5	3768	1/1	0.96	0.14	36,36,36,36	0
85	MG	5	3615	1/1	0.96	0.23	30,30,30,30	0
86	OHX	1	4089	7/7	0.96	0.09	159,159,159,159	0
85	MG	5	3541	1/1	0.96	0.20	22,22,22,22	0
86	OHX	5	4031	7/7	0.96	0.12	110,110,110,110	0
86	OHX	4	228	7/7	0.96	0.11	96,96,96,96	0
85	MG	2	1986	1/1	0.96	0.12	50,50,50,50	0
85	MG	1	3730	1/1	0.96	0.14	23,23,23,23	0
85	MG	1	3675	1/1	0.96	0.17	18,18,18,18	0
85	MG	2	1902	1/1	0.96	0.23	34,34,34,34	0
86	OHX	5	4040	7/7	0.96	0.13	103,103,103,103	0
85	MG	1	3433	1/1	0.96	0.13	29,29,29,29	0
85	MG	1	3537	1/1	0.96	0.34	25,25,25,25	0
85	MG	1	3654	1/1	0.96	0.15	33,33,33,33	0
86	OHX	5	4045	7/7	0.96	0.13	95,95,95,95	0
86	OHX	5	4046	7/7	0.96	0.21	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3624	1/1	0.96	0.14	18,18,18,18	0
85	MG	5	3426	1/1	0.96	0.25	37,37,37,37	0
85	MG	5	3626	1/1	0.96	0.17	42,42,42,42	0
85	MG	1	3705	1/1	0.96	0.15	47,47,47,47	0
85	MG	5	3628	1/1	0.96	0.15	32,32,32,32	0
86	OHX	5	4054	7/7	0.96	0.14	86,86,86,86	0
86	OHX	5	4055	7/7	0.96	0.15	86,86,86,86	0
85	MG	1	3579	1/1	0.96	0.35	33,33,33,33	0
86	OHX	M5	304	7/7	0.96	0.14	91,91,91,91	0
86	OHX	2	2038	7/7	0.96	0.14	97,97,97,97	0
86	OHX	5	4060	7/7	0.96	0.11	113,113,113,113	0
85	MG	5	3876	1/1	0.96	0.31	39,39,39,39	0
85	MG	1	3813	1/1	0.96	0.12	26,26,26,26	0
86	OHX	2	2054	7/7	0.96	0.10	107,107,107,107	0
86	OHX	2	2056	7/7	0.96	0.14	93,93,93,93	0
86	OHX	5	4065	7/7	0.96	0.12	91,91,91,91	0
86	OHX	2	2057	7/7	0.96	0.11	105,105,105,105	0
86	OHX	5	4068	7/7	0.96	0.14	81,81,81,81	0
86	OHX	2	2066	7/7	0.96	0.15	89,89,89,89	0
86	OHX	5	4070	7/7	0.96	0.14	98,98,98,98	0
86	OHX	2	2067	7/7	0.96	0.11	114,114,114,114	0
86	OHX	6	2086	7/7	0.96	0.12	88,88,88,88	0
85	MG	1	3580	1/1	0.96	0.24	34,34,34,34	0
86	OHX	5	4074	7/7	0.96	0.14	93,93,93,93	0
85	MG	6	1943	1/1	0.96	0.29	32,32,32,32	0
86	OHX	2	2070	7/7	0.96	0.14	89,89,89,89	0
86	OHX	5	4077	7/7	0.96	0.09	136,136,136,136	0
86	OHX	2	2074	7/7	0.96	0.10	111,111,111,111	0
86	OHX	8	216	7/7	0.96	0.13	86,86,86,86	0
86	OHX	5	4080	7/7	0.96	0.12	95,95,95,95	0
86	OHX	5	4081	7/7	0.96	0.14	87,87,87,87	0
86	OHX	8	220	7/7	0.96	0.12	101,101,101,101	0
86	OHX	6	2103	7/7	0.96	0.13	88,88,88,88	0
86	OHX	SR	401	7/7	0.96	0.10	136,136,136,136	0
86	OHX	6	2106	7/7	0.96	0.14	92,92,92,92	0
86	OHX	1	3900	7/7	0.96	0.14	65,65,65,65	0
86	OHX	6	2108	7/7	0.96	0.15	88,88,88,88	0
86	OHX	6	2109	7/7	0.96	0.12	98,98,98,98	0
86	OHX	2	2075	7/7	0.96	0.14	95,95,95,95	0
85	MG	5	3788	1/1	0.96	0.07	39,39,39,39	0
86	OHX	l3	403	7/7	0.96	0.14	87,87,87,87	0
86	OHX	6	2113	7/7	0.96	0.15	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	2077	7/7	0.96	0.13	98,98,98,98	0
86	OHX	5	4093	7/7	0.96	0.13	97,97,97,97	0
85	MG	5	3882	1/1	0.96	0.18	19,19,19,19	0
86	OHX	1	3944	7/7	0.96	0.12	87,87,87,87	0
86	OHX	6	2118	7/7	0.96	0.16	89,89,89,89	0
86	OHX	6	2119	7/7	0.96	0.12	107,107,107,107	0
86	OHX	6	2121	7/7	0.96	0.15	89,89,89,89	0
86	OHX	1	3950	7/7	0.96	0.13	89,89,89,89	0
85	MG	1	3816	1/1	0.96	0.14	38,38,38,38	0
86	OHX	1	3953	7/7	0.96	0.12	105,105,105,105	0
86	OHX	1	3954	7/7	0.96	0.13	98,98,98,98	0
85	MG	1	3682	1/1	0.96	0.23	50,50,50,50	0
86	OHX	o3	203	7/7	0.96	0.15	88,88,88,88	0
85	MG	5	3557	1/1	0.96	0.20	21,21,21,21	0
85	MG	5	3792	1/1	0.96	0.10	32,32,32,32	0
86	OHX	2	2085	7/7	0.96	0.14	95,95,95,95	0
85	MG	5	3793	1/1	0.96	0.05	36,36,36,36	0
87	ZN	e1	501	1/1	0.96	0.05	130,130,130,130	0
86	OHX	1	3977	7/7	0.96	0.14	85,85,85,85	0
85	MG	5	3558	1/1	0.96	0.23	24,24,24,24	0
86	OHX	2	2088	7/7	0.96	0.13	101,101,101,101	0
85	MG	1	3744	1/1	0.97	0.09	29,29,29,29	0
85	MG	1	3728	1/1	0.97	0.15	27,27,27,27	0
85	MG	1	3712	1/1	0.97	0.06	41,41,41,41	0
85	MG	1	3550	1/1	0.97	0.25	31,31,31,31	0
85	MG	1	3529	1/1	0.97	0.34	29,29,29,29	0
86	OHX	2	2115	7/7	0.97	0.14	100,100,100,100	0
86	OHX	1	3964	7/7	0.97	0.10	90,90,90,90	0
86	OHX	1	3965	7/7	0.97	0.11	85,85,85,85	0
86	OHX	1	3966	7/7	0.97	0.10	98,98,98,98	0
85	MG	5	3682	1/1	0.97	0.05	22,22,22,22	0
85	MG	n8	204	1/1	0.97	0.19	25,25,25,25	0
86	OHX	1	3971	7/7	0.97	0.16	75,75,75,75	0
86	OHX	3	217	7/7	0.97	0.13	86,86,86,86	0
86	OHX	3	218	7/7	0.97	0.15	81,81,81,81	0
85	MG	5	3584	1/1	0.97	0.30	19,19,19,19	0
86	OHX	1	3973	7/7	0.97	0.11	82,82,82,82	0
86	OHX	1	3974	7/7	0.97	0.10	86,86,86,86	0
86	OHX	1	3976	7/7	0.97	0.12	80,80,80,80	0
85	MG	5	3497	1/1	0.97	0.15	21,21,21,21	0
86	OHX	1	3978	7/7	0.97	0.10	101,101,101,101	0
86	OHX	1	3979	7/7	0.97	0.12	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3980	7/7	0.97	0.13	87,87,87,87	0
86	OHX	4	224	7/7	0.97	0.10	93,93,93,93	0
86	OHX	4	225	7/7	0.97	0.12	97,97,97,97	0
85	MG	1	3786	1/1	0.97	0.19	25,25,25,25	0
86	OHX	1	3983	7/7	0.97	0.12	89,89,89,89	0
85	MG	M7	206	1/1	0.97	0.10	42,42,42,42	0
85	MG	6	1995	1/1	0.97	0.06	32,32,32,32	0
85	MG	1	3496	1/1	0.97	0.19	26,26,26,26	0
85	MG	5	3637	1/1	0.97	0.12	35,35,35,35	0
85	MG	5	3502	1/1	0.97	0.26	28,28,28,28	0
85	MG	5	3639	1/1	0.97	0.17	40,40,40,40	0
85	MG	6	1997	1/1	0.97	0.07	43,43,43,43	0
86	OHX	2	2031	7/7	0.97	0.14	80,80,80,80	0
86	OHX	2	2034	7/7	0.97	0.15	88,88,88,88	0
86	OHX	2	2036	7/7	0.97	0.11	88,88,88,88	0
86	OHX	1	3998	7/7	0.97	0.11	96,96,96,96	0
86	OHX	1	3999	7/7	0.97	0.10	105,105,105,105	0
85	MG	5	3743	1/1	0.97	0.23	22,22,22,22	0
86	OHX	5	3926	7/7	0.97	0.14	59,59,59,59	0
86	OHX	5	3940	7/7	0.97	0.13	69,69,69,69	0
85	MG	5	3797	1/1	0.97	0.05	33,33,33,33	0
86	OHX	5	3950	7/7	0.97	0.11	67,67,67,67	0
86	OHX	5	3951	7/7	0.97	0.16	95,95,95,95	0
85	MG	1	3811	1/1	0.97	0.08	40,40,40,40	0
86	OHX	5	3956	7/7	0.97	0.12	76,76,76,76	0
86	OHX	5	3958	7/7	0.97	0.12	71,71,71,71	0
86	OHX	2	2049	7/7	0.97	0.10	94,94,94,94	0
86	OHX	2	2050	7/7	0.97	0.10	95,95,95,95	0
86	OHX	2	2051	7/7	0.97	0.12	91,91,91,91	0
86	OHX	5	3975	7/7	0.97	0.12	75,75,75,75	0
86	OHX	2	2053	7/7	0.97	0.11	94,94,94,94	0
86	OHX	5	3981	7/7	0.97	0.16	71,71,71,71	0
86	OHX	5	3986	7/7	0.97	0.16	72,72,72,72	0
86	OHX	5	3988	7/7	0.97	0.10	97,97,97,97	0
86	OHX	5	3990	7/7	0.97	0.12	84,84,84,84	0
86	OHX	5	3992	7/7	0.97	0.11	81,81,81,81	0
86	OHX	O7	103	7/7	0.97	0.13	77,77,77,77	0
85	MG	1	3812	1/1	0.97	0.10	27,27,27,27	0
86	OHX	5	3996	7/7	0.97	0.21	78,78,78,78	0
86	OHX	2	2055	7/7	0.97	0.10	100,100,100,100	0
86	OHX	5	4003	7/7	0.97	0.11	95,95,95,95	0
86	OHX	6	2066	7/7	0.97	0.15	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4007	7/7	0.97	0.09	101,101,101,101	0
86	OHX	5	4011	7/7	0.97	0.12	82,82,82,82	0
86	OHX	5	4012	7/7	0.97	0.13	82,82,82,82	0
86	OHX	6	2071	7/7	0.97	0.09	96,96,96,96	0
86	OHX	5	4015	7/7	0.97	0.12	83,83,83,83	0
86	OHX	5	4016	7/7	0.97	0.11	87,87,87,87	0
85	MG	5	3506	1/1	0.97	0.27	23,23,23,23	0
86	OHX	5	4018	7/7	0.97	0.11	101,101,101,101	0
86	OHX	5	4019	7/7	0.97	0.15	84,84,84,84	0
86	OHX	6	2078	7/7	0.97	0.16	76,76,76,76	0
86	OHX	5	4021	7/7	0.97	0.11	90,90,90,90	0
86	OHX	6	2084	7/7	0.97	0.11	96,96,96,96	0
85	MG	1	3518	1/1	0.97	0.27	19,19,19,19	0
86	OHX	2	2058	7/7	0.97	0.10	103,103,103,103	0
86	OHX	6	2089	7/7	0.97	0.10	108,108,108,108	0
86	OHX	2	2060	7/7	0.97	0.11	99,99,99,99	0
86	OHX	5	4028	7/7	0.97	0.21	73,73,73,73	0
86	OHX	2	2061	7/7	0.97	0.14	84,84,84,84	0
86	OHX	6	2096	7/7	0.97	0.10	105,105,105,105	0
86	OHX	6	2097	7/7	0.97	0.08	119,119,119,119	0
86	OHX	2	2062	7/7	0.97	0.10	105,105,105,105	0
86	OHX	6	2099	7/7	0.97	0.09	124,124,124,124	0
86	OHX	2	2063	7/7	0.97	0.10	95,95,95,95	0
86	OHX	6	2101	7/7	0.97	0.10	134,134,134,134	0
86	OHX	6	2102	7/7	0.97	0.09	96,96,96,96	0
86	OHX	5	4038	7/7	0.97	0.09	105,105,105,105	0
86	OHX	5	4039	7/7	0.97	0.28	67,67,67,67	0
86	OHX	1	4018	7/7	0.97	0.10	93,93,93,93	0
86	OHX	6	2104	7/7	0.97	0.10	100,100,100,100	0
86	OHX	2	2064	7/7	0.97	0.10	104,104,104,104	0
86	OHX	2	2065	7/7	0.97	0.12	87,87,87,87	0
86	OHX	5	4044	7/7	0.97	0.28	77,77,77,77	0
85	MG	1	3838	1/1	0.97	0.22	43,43,43,43	0
85	MG	5	3749	1/1	0.97	0.09	38,38,38,38	0
86	OHX	5	4047	7/7	0.97	0.11	97,97,97,97	0
85	MG	5	3646	1/1	0.97	0.19	35,35,35,35	0
86	OHX	5	4049	7/7	0.97	0.15	83,83,83,83	0
86	OHX	6	2110	7/7	0.97	0.13	93,93,93,93	0
85	MG	5	3598	1/1	0.97	0.17	30,30,30,30	0
85	MG	1	3789	1/1	0.97	0.17	26,26,26,26	0
86	OHX	2	2071	7/7	0.97	0.09	108,108,108,108	0
86	OHX	2	2072	7/7	0.97	0.12	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2115	7/7	0.97	0.11	95,95,95,95	0
86	OHX	1	4028	7/7	0.97	0.14	92,92,92,92	0
86	OHX	2	2073	7/7	0.97	0.11	95,95,95,95	0
85	MG	5	3434	1/1	0.97	0.18	24,24,24,24	0
86	OHX	5	4059	7/7	0.97	0.12	96,96,96,96	0
85	MG	5	3650	1/1	0.97	0.09	22,22,22,22	0
86	OHX	6	2120	7/7	0.97	0.11	93,93,93,93	0
85	MG	1	3661	1/1	0.97	0.07	30,30,30,30	0
85	MG	5	3402	1/1	0.97	0.13	16,16,16,16	0
85	MG	1	3404	1/1	0.97	0.33	46,46,46,46	0
85	MG	1	3753	1/1	0.97	0.13	44,44,44,44	0
86	OHX	1	4036	7/7	0.97	0.12	87,87,87,87	0
85	MG	5	3405	1/1	0.97	0.15	18,18,18,18	0
85	MG	5	3606	1/1	0.97	0.24	18,18,18,18	0
85	MG	1	3498	1/1	0.97	0.20	20,20,20,20	0
86	OHX	2	2083	7/7	0.97	0.09	114,114,114,114	0
86	OHX	6	2130	7/7	0.97	0.11	96,96,96,96	0
86	OHX	2	2084	7/7	0.97	0.11	111,111,111,111	0
85	MG	5	3561	1/1	0.97	0.38	31,31,31,31	0
86	OHX	1	4043	7/7	0.97	0.13	88,88,88,88	0
86	OHX	1	4044	7/7	0.97	0.10	109,109,109,109	0
85	MG	1	4217	1/1	0.97	0.19	19,19,19,19	0
86	OHX	1	4046	7/7	0.97	0.29	75,75,75,75	0
85	MG	5	3877	1/1	0.97	0.20	14,14,14,14	0
86	OHX	7	222	7/7	0.97	0.12	89,89,89,89	0
86	OHX	1	4048	7/7	0.97	0.12	86,86,86,86	0
85	MG	5	3442	1/1	0.97	0.16	27,27,27,27	0
85	MG	1	3583	1/1	0.97	0.26	31,31,31,31	0
85	MG	l4	401	1/1	0.97	0.10	28,28,28,28	0
86	OHX	1	4052	7/7	0.97	0.10	108,108,108,108	0
86	OHX	2	2091	7/7	0.97	0.12	100,100,100,100	0
86	OHX	8	217	7/7	0.97	0.10	102,102,102,102	0
85	MG	5	3521	1/1	0.97	0.30	34,34,34,34	0
85	MG	6	1901	1/1	0.97	0.23	37,37,37,37	0
85	MG	5	3411	1/1	0.97	0.18	30,30,30,30	0
86	OHX	5	4090	7/7	0.97	0.24	79,79,79,79	0
86	OHX	8	222	7/7	0.97	0.10	114,114,114,114	0
86	OHX	1	4175	7/7	0.97	0.14	86,86,86,86	0
86	OHX	2	2095	7/7	0.97	0.07	132,132,132,132	0
85	MG	5	3824	1/1	0.97	0.19	37,37,37,37	0
85	MG	1	3692	1/1	0.97	0.06	25,25,25,25	0
86	OHX	1	4060	7/7	0.97	0.24	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3447	1/1	0.97	0.10	29,29,29,29	0
85	MG	1	3573	1/1	0.97	0.37	32,32,32,32	0
86	OHX	C1	201	7/7	0.97	0.12	101,101,101,101	0
85	MG	m5	301	1/1	0.97	0.19	45,45,45,45	0
85	MG	6	1983	1/1	0.97	0.24	38,38,38,38	0
86	OHX	C8	201	7/7	0.97	0.12	91,91,91,91	0
86	OHX	2	2102	7/7	0.97	0.10	110,110,110,110	0
86	OHX	1	4068	7/7	0.97	0.26	78,78,78,78	0
85	MG	5	3829	1/1	0.97	0.14	59,59,59,59	0
85	MG	2	2022	1/1	0.97	0.07	66,66,66,66	0
86	OHX	1	3909	7/7	0.97	0.10	70,70,70,70	0
85	MG	1	3446	1/1	0.97	0.09	31,31,31,31	0
86	OHX	1	3916	7/7	0.97	0.10	71,71,71,71	0
86	OHX	1	3920	7/7	0.97	0.14	70,70,70,70	0
86	OHX	1	3921	7/7	0.97	0.11	79,79,79,79	0
85	MG	5	3453	1/1	0.97	0.30	34,34,34,34	0
86	OHX	1	3930	7/7	0.97	0.15	90,90,90,90	0
85	MG	1	3576	1/1	0.97	0.22	21,21,21,21	0
86	OHX	1	3937	7/7	0.97	0.10	88,88,88,88	0
85	MG	5	3577	1/1	0.97	0.24	23,23,23,23	0
86	OHX	1	3941	7/7	0.97	0.12	76,76,76,76	0
86	OHX	1	3942	7/7	0.97	0.15	78,78,78,78	0
86	OHX	1	3943	7/7	0.97	0.10	92,92,92,92	0
85	MG	1	3644	1/1	0.97	0.23	50,50,50,50	0
86	OHX	1	3948	7/7	0.97	0.10	90,90,90,90	0
86	OHX	O7	104	7/7	0.98	0.17	75,75,75,75	0
86	OHX	1	3952	7/7	0.98	0.09	90,90,90,90	0
86	OHX	Q2	503	7/7	0.98	0.18	64,64,64,64	0
86	OHX	6	2055	7/7	0.98	0.12	70,70,70,70	0
86	OHX	6	2059	7/7	0.98	0.13	81,81,81,81	0
86	OHX	5	4034	7/7	0.98	0.10	86,86,86,86	0
85	MG	5	3607	1/1	0.98	0.18	20,20,20,20	0
86	OHX	6	2065	7/7	0.98	0.09	78,78,78,78	0
86	OHX	2	2039	7/7	0.98	0.10	83,83,83,83	0
86	OHX	6	2069	7/7	0.98	0.10	79,79,79,79	0
86	OHX	2	2040	7/7	0.98	0.11	79,79,79,79	0
86	OHX	6	2072	7/7	0.98	0.15	67,67,67,67	0
86	OHX	6	2073	7/7	0.98	0.09	99,99,99,99	0
86	OHX	6	2074	7/7	0.98	0.10	103,103,103,103	0
85	MG	1	3814	1/1	0.98	0.05	38,38,38,38	0
86	OHX	1	3958	7/7	0.98	0.14	75,75,75,75	0
86	OHX	6	2079	7/7	0.98	0.09	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2083	7/7	0.98	0.09	98,98,98,98	0
86	OHX	1	3959	7/7	0.98	0.13	71,71,71,71	0
86	OHX	1	3960	7/7	0.98	0.10	78,78,78,78	0
86	OHX	1	3961	7/7	0.98	0.16	72,72,72,72	0
86	OHX	6	2087	7/7	0.98	0.10	91,91,91,91	0
86	OHX	6	2088	7/7	0.98	0.08	95,95,95,95	0
86	OHX	1	3963	7/7	0.98	0.10	88,88,88,88	0
86	OHX	6	2090	7/7	0.98	0.11	90,90,90,90	0
85	MG	m6	201	1/1	0.98	0.05	25,25,25,25	0
86	OHX	6	2092	7/7	0.98	0.10	94,94,94,94	0
86	OHX	6	2093	7/7	0.98	0.10	87,87,87,87	0
86	OHX	6	2094	7/7	0.98	0.08	105,105,105,105	0
86	OHX	2	2047	7/7	0.98	0.08	94,94,94,94	0
85	MG	5	3560	1/1	0.98	0.28	25,25,25,25	0
85	MG	1	3434	1/1	0.98	0.12	34,34,34,34	0
86	OHX	1	3968	7/7	0.98	0.18	65,65,65,65	0
86	OHX	1	3969	7/7	0.98	0.13	80,80,80,80	0
85	MG	5	3539	1/1	0.98	0.26	19,19,19,19	0
86	OHX	5	4196	7/7	0.98	0.20	65,65,65,65	0
86	OHX	2	2052	7/7	0.98	0.09	83,83,83,83	0
85	MG	M7	203	1/1	0.98	0.19	28,28,28,28	0
86	OHX	5	4066	7/7	0.98	0.10	97,97,97,97	0
85	MG	5	3519	1/1	0.98	0.22	35,35,35,35	0
85	MG	5	3860	1/1	0.98	0.08	51,51,51,51	0
86	OHX	1	3975	7/7	0.98	0.13	88,88,88,88	0
85	MG	6	1982	1/1	0.98	0.12	31,31,31,31	0
85	MG	5	3665	1/1	0.98	0.13	19,19,19,19	0
85	MG	5	3774	1/1	0.98	0.06	27,27,27,27	0
86	OHX	2	2059	7/7	0.98	0.09	91,91,91,91	0
85	MG	5	3408	1/1	0.98	0.13	17,17,17,17	0
85	MG	1	3561	1/1	0.98	0.24	30,30,30,30	0
86	OHX	1	3982	7/7	0.98	0.27	69,69,69,69	0
85	MG	L7	302	1/1	0.98	0.19	29,29,29,29	0
86	OHX	5	4078	7/7	0.98	0.20	78,78,78,78	0
85	MG	1	4218	1/1	0.98	0.13	17,17,17,17	0
86	OHX	1	3985	7/7	0.98	0.19	69,69,69,69	0
85	MG	M0	301	1/1	0.98	0.17	25,25,25,25	0
86	OHX	1	3988	7/7	0.98	0.19	73,73,73,73	0
86	OHX	1	3989	7/7	0.98	0.21	72,72,72,72	0
85	MG	5	3671	1/1	0.98	0.21	21,21,21,21	0
86	OHX	1	3894	7/7	0.98	0.13	64,64,64,64	0
85	MG	1	3422	1/1	0.98	0.13	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3929	7/7	0.98	0.09	50,50,50,50	0
86	OHX	5	3931	7/7	0.98	0.10	60,60,60,60	0
86	OHX	5	3932	7/7	0.98	0.15	77,77,77,77	0
86	OHX	5	3939	7/7	0.98	0.14	76,76,76,76	0
86	OHX	1	3901	7/7	0.98	0.12	65,65,65,65	0
86	OHX	5	3943	7/7	0.98	0.09	64,64,64,64	0
86	OHX	5	3944	7/7	0.98	0.11	71,71,71,71	0
86	OHX	5	3946	7/7	0.98	0.10	62,62,62,62	0
86	OHX	5	3947	7/7	0.98	0.09	72,72,72,72	0
86	OHX	3	215	7/7	0.98	0.10	79,79,79,79	0
86	OHX	1	3903	7/7	0.98	0.13	68,68,68,68	0
86	OHX	1	3904	7/7	0.98	0.11	70,70,70,70	0
86	OHX	5	3952	7/7	0.98	0.09	83,83,83,83	0
85	MG	1	3796	1/1	0.98	0.37	31,31,31,31	0
86	OHX	1	3912	7/7	0.98	0.10	66,66,66,66	0
86	OHX	1	3913	7/7	0.98	0.11	72,72,72,72	0
85	MG	5	3597	1/1	0.98	0.12	28,28,28,28	0
85	MG	1	3803	1/1	0.98	0.04	41,41,41,41	0
86	OHX	5	3964	7/7	0.98	0.20	66,66,66,66	0
86	OHX	5	3965	7/7	0.98	0.10	82,82,82,82	0
86	OHX	5	3966	7/7	0.98	0.10	83,83,83,83	0
86	OHX	5	3967	7/7	0.98	0.12	70,70,70,70	0
86	OHX	5	3968	7/7	0.98	0.09	74,74,74,74	0
86	OHX	5	3969	7/7	0.98	0.09	76,76,76,76	0
86	OHX	5	3972	7/7	0.98	0.14	66,66,66,66	0
86	OHX	1	3918	7/7	0.98	0.10	72,72,72,72	0
86	OHX	1	4002	7/7	0.98	0.08	115,115,115,115	0
86	OHX	1	3919	7/7	0.98	0.10	79,79,79,79	0
86	OHX	5	3978	7/7	0.98	0.19	65,65,65,65	0
86	OHX	5	3979	7/7	0.98	0.11	76,76,76,76	0
86	OHX	5	3980	7/7	0.98	0.10	81,81,81,81	0
86	OHX	7	216	7/7	0.98	0.12	73,73,73,73	0
86	OHX	7	217	7/7	0.98	0.10	68,68,68,68	0
86	OHX	7	218	7/7	0.98	0.12	84,84,84,84	0
86	OHX	7	220	7/7	0.98	0.18	76,76,76,76	0
86	OHX	7	221	7/7	0.98	0.09	82,82,82,82	0
86	OHX	1	4004	7/7	0.98	0.21	72,72,72,72	0
86	OHX	5	3983	7/7	0.98	0.18	77,77,77,77	0
86	OHX	5	3984	7/7	0.98	0.17	71,71,71,71	0
86	OHX	4	223	7/7	0.98	0.16	77,77,77,77	0
86	OHX	5	3987	7/7	0.98	0.10	80,80,80,80	0
85	MG	5	3452	1/1	0.98	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	8	215	7/7	0.98	0.09	90,90,90,90	0
85	MG	3	210	1/1	0.98	0.22	50,50,50,50	0
85	MG	1	3720	1/1	0.98	0.22	42,42,42,42	0
86	OHX	5	3993	7/7	0.98	0.19	66,66,66,66	0
86	OHX	1	3925	7/7	0.98	0.12	66,66,66,66	0
86	OHX	1	3926	7/7	0.98	0.10	72,72,72,72	0
86	OHX	1	3928	7/7	0.98	0.09	72,72,72,72	0
86	OHX	5	3997	7/7	0.98	0.08	98,98,98,98	0
86	OHX	5	3998	7/7	0.98	0.08	91,91,91,91	0
85	MG	1	4223	1/1	0.98	0.13	20,20,20,20	0
86	OHX	5	4000	7/7	0.98	0.09	94,94,94,94	0
86	OHX	5	4001	7/7	0.98	0.20	79,79,79,79	0
86	OHX	5	4002	7/7	0.98	0.19	58,58,58,58	0
85	MG	1	4224	1/1	0.98	0.18	19,19,19,19	0
86	OHX	5	4004	7/7	0.98	0.13	69,69,69,69	0
86	OHX	5	4005	7/7	0.98	0.14	80,80,80,80	0
86	OHX	1	3933	7/7	0.98	0.10	86,86,86,86	0
86	OHX	1	3934	7/7	0.98	0.12	68,68,68,68	0
86	OHX	5	4009	7/7	0.98	0.21	74,74,74,74	0
86	OHX	5	4010	7/7	0.98	0.10	88,88,88,88	0
86	OHX	1	3936	7/7	0.98	0.10	76,76,76,76	0
85	MG	5	3534	1/1	0.98	0.29	24,24,24,24	0
86	OHX	2	2026	7/7	0.98	0.15	69,69,69,69	0
86	OHX	5	4014	7/7	0.98	0.15	77,77,77,77	0
86	OHX	1	3940	7/7	0.98	0.09	80,80,80,80	0
86	OHX	2	2030	7/7	0.98	0.11	80,80,80,80	0
85	MG	1	3846	1/1	0.98	0.18	24,24,24,24	0
86	OHX	m5	302	7/7	0.98	0.10	98,98,98,98	0
86	OHX	m6	202	7/7	0.98	0.14	73,73,73,73	0
86	OHX	2	2032	7/7	0.98	0.09	89,89,89,89	0
86	OHX	2	2033	7/7	0.98	0.11	75,75,75,75	0
86	OHX	o2	201	7/7	0.98	0.16	78,78,78,78	0
86	OHX	1	3945	7/7	0.98	0.09	82,82,82,82	0
86	OHX	M6	202	7/7	0.98	0.12	80,80,80,80	0
86	OHX	o7	502	7/7	0.98	0.15	80,80,80,80	0
86	OHX	1	3946	7/7	0.98	0.16	71,71,71,71	0
87	ZN	E1	501	1/1	0.98	0.04	100,100,100,100	0
85	MG	5	3820	1/1	0.98	0.05	52,52,52,52	0
86	OHX	5	4024	7/7	0.98	0.09	95,95,95,95	0
86	OHX	1	3949	7/7	0.98	0.10	78,78,78,78	0
86	OHX	O2	201	7/7	0.98	0.18	74,74,74,74	0
86	OHX	2	2035	7/7	0.98	0.13	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3599	1/1	0.98	0.31	20,20,20,20	0
86	OHX	5	3935	7/7	0.99	0.06	56,56,56,56	0
86	OHX	5	3936	7/7	0.99	0.07	54,54,54,54	0
86	OHX	5	3937	7/7	0.99	0.09	62,62,62,62	0
86	OHX	5	3938	7/7	0.99	0.10	71,71,71,71	0
86	OHX	6	2062	7/7	0.99	0.08	71,71,71,71	0
86	OHX	6	2063	7/7	0.99	0.07	71,71,71,71	0
86	OHX	5	3941	7/7	0.99	0.08	67,67,67,67	0
86	OHX	5	3942	7/7	0.99	0.09	75,75,75,75	0
86	OHX	2	2027	7/7	0.99	0.09	69,69,69,69	0
86	OHX	2	2045	7/7	0.99	0.08	82,82,82,82	0
86	OHX	5	3945	7/7	0.99	0.08	61,61,61,61	0
86	OHX	1	3927	7/7	0.99	0.09	56,56,56,56	0
86	OHX	6	2067	7/7	0.99	0.15	70,70,70,70	0
86	OHX	5	3948	7/7	0.99	0.07	85,85,85,85	0
86	OHX	6	2068	7/7	0.99	0.13	71,71,71,71	0
86	OHX	2	2046	7/7	0.99	0.06	86,86,86,86	0
86	OHX	6	2070	7/7	0.99	0.12	67,67,67,67	0
86	OHX	1	3929	7/7	0.99	0.16	63,63,63,63	0
86	OHX	5	3954	7/7	0.99	0.08	74,74,74,74	0
86	OHX	2	2028	7/7	0.99	0.06	62,62,62,62	0
86	OHX	1	3986	7/7	0.99	0.08	93,93,93,93	0
86	OHX	5	3957	7/7	0.99	0.08	65,65,65,65	0
86	OHX	1	3931	7/7	0.99	0.09	68,68,68,68	0
86	OHX	5	3959	7/7	0.99	0.08	58,58,58,58	0
86	OHX	6	2075	7/7	0.99	0.12	69,69,69,69	0
86	OHX	5	3961	7/7	0.99	0.09	72,72,72,72	0
86	OHX	5	3962	7/7	0.99	0.06	73,73,73,73	0
86	OHX	6	2076	7/7	0.99	0.08	86,86,86,86	0
86	OHX	2	2048	7/7	0.99	0.05	104,104,104,104	0
86	OHX	1	3872	7/7	0.99	0.15	46,46,46,46	0
86	OHX	1	3874	7/7	0.99	0.12	48,48,48,48	0
86	OHX	6	2080	7/7	0.99	0.13	79,79,79,79	0
86	OHX	6	2081	7/7	0.99	0.11	78,78,78,78	0
86	OHX	6	2082	7/7	0.99	0.07	83,83,83,83	0
86	OHX	5	3970	7/7	0.99	0.06	77,77,77,77	0
86	OHX	5	3971	7/7	0.99	0.11	65,65,65,65	0
86	OHX	1	3935	7/7	0.99	0.08	68,68,68,68	0
86	OHX	5	3973	7/7	0.99	0.08	62,62,62,62	0
86	OHX	1	3877	7/7	0.99	0.10	46,46,46,46	0
86	OHX	1	3878	7/7	0.99	0.12	51,51,51,51	0
86	OHX	5	3976	7/7	0.99	0.08	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3938	7/7	0.99	0.09	58,58,58,58	0
86	OHX	1	3879	7/7	0.99	0.08	50,50,50,50	0
86	OHX	1	3880	7/7	0.99	0.08	44,44,44,44	0
86	OHX	1	3882	7/7	0.99	0.08	53,53,53,53	0
86	OHX	1	3883	7/7	0.99	0.12	52,52,52,52	0
86	OHX	5	3982	7/7	0.99	0.13	63,63,63,63	0
86	OHX	1	3885	7/7	0.99	0.09	55,55,55,55	0
86	OHX	1	3886	7/7	0.99	0.10	53,53,53,53	0
86	OHX	5	3985	7/7	0.99	0.13	71,71,71,71	0
86	OHX	1	3889	7/7	0.99	0.09	56,56,56,56	0
86	OHX	1	3891	7/7	0.99	0.12	65,65,65,65	0
86	OHX	1	3947	7/7	0.99	0.17	70,70,70,70	0
86	OHX	5	3989	7/7	0.99	0.09	62,62,62,62	0
86	OHX	1	3893	7/7	0.99	0.07	52,52,52,52	0
86	OHX	5	3991	7/7	0.99	0.13	69,69,69,69	0
86	OHX	2	2029	7/7	0.99	0.09	75,75,75,75	0
86	OHX	1	3895	7/7	0.99	0.07	54,54,54,54	0
86	OHX	1	3897	7/7	0.99	0.09	60,60,60,60	0
86	OHX	1	3898	7/7	0.99	0.09	55,55,55,55	0
85	MG	5	3562	1/1	0.99	0.30	24,24,24,24	0
85	MG	1	3662	1/1	0.99	0.04	22,22,22,22	0
86	OHX	1	3955	7/7	0.99	0.09	80,80,80,80	0
86	OHX	1	3902	7/7	0.99	0.08	59,59,59,59	0
85	MG	1	3500	1/1	0.99	0.34	51,51,51,51	0
85	MG	1	3829	1/1	0.99	0.07	47,47,47,47	0
86	OHX	1	3905	7/7	0.99	0.09	52,52,52,52	0
86	OHX	1	3906	7/7	0.99	0.06	57,57,57,57	0
86	OHX	1	3907	7/7	0.99	0.07	61,61,61,61	0
86	OHX	1	3962	7/7	0.99	0.16	59,59,59,59	0
86	OHX	1	3908	7/7	0.99	0.05	54,54,54,54	0
85	MG	1	3804	1/1	0.99	0.08	45,45,45,45	0
86	OHX	7	219	7/7	0.99	0.14	76,76,76,76	0
86	OHX	5	4008	7/7	0.99	0.14	64,64,64,64	0
86	OHX	1	3910	7/7	0.99	0.08	66,66,66,66	0
86	OHX	1	3911	7/7	0.99	0.08	70,70,70,70	0
86	OHX	M5	303	7/7	0.99	0.07	68,68,68,68	0
85	MG	1	3772	1/1	0.99	0.10	47,47,47,47	0
85	MG	1	3473	1/1	0.99	0.22	18,18,18,18	0
86	OHX	1	3914	7/7	0.99	0.06	58,58,58,58	0
86	OHX	2	2037	7/7	0.99	0.09	71,71,71,71	0
86	OHX	8	214	7/7	0.99	0.09	47,47,47,47	0
85	MG	5	3835	1/1	0.99	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	N9	101	7/7	0.99	0.11	48,48,48,48	0
86	OHX	1	3917	7/7	0.99	0.09	70,70,70,70	0
86	OHX	2	2024	7/7	0.99	0.11	62,62,62,62	0
86	OHX	2	2025	7/7	0.99	0.10	66,66,66,66	0
85	MG	5	3836	1/1	0.99	0.09	22,22,22,22	0
86	OHX	s1	302	7/7	0.99	0.14	67,67,67,67	0
86	OHX	2	2042	7/7	0.99	0.09	79,79,79,79	0
86	OHX	1	3922	7/7	0.99	0.08	77,77,77,77	0
86	OHX	6	2048	7/7	0.99	0.13	60,60,60,60	0
86	OHX	6	2049	7/7	0.99	0.09	51,51,51,51	0
86	OHX	6	2050	7/7	0.99	0.10	60,60,60,60	0
86	OHX	6	2051	7/7	0.99	0.11	60,60,60,60	0
86	OHX	6	2053	7/7	0.99	0.11	61,61,61,61	0
86	OHX	6	2054	7/7	0.99	0.10	69,69,69,69	0
86	OHX	l3	402	7/7	0.99	0.11	79,79,79,79	0
86	OHX	1	3923	7/7	0.99	0.07	69,69,69,69	0
86	OHX	6	2056	7/7	0.99	0.07	57,57,57,57	0
86	OHX	6	2057	7/7	0.99	0.07	63,63,63,63	0
86	OHX	5	3898	7/7	0.99	0.12	37,37,37,37	0
86	OHX	5	3902	7/7	0.99	0.14	43,43,43,43	0
86	OHX	5	3904	7/7	0.99	0.09	47,47,47,47	0
86	OHX	5	3905	7/7	0.99	0.09	45,45,45,45	0
86	OHX	5	3906	7/7	0.99	0.09	49,49,49,49	0
86	OHX	5	3907	7/7	0.99	0.11	44,44,44,44	0
86	OHX	5	3909	7/7	0.99	0.14	53,53,53,53	0
86	OHX	5	3910	7/7	0.99	0.08	48,48,48,48	0
86	OHX	5	3912	7/7	0.99	0.10	49,49,49,49	0
86	OHX	5	3913	7/7	0.99	0.10	54,54,54,54	0
86	OHX	5	3914	7/7	0.99	0.11	53,53,53,53	0
86	OHX	5	3916	7/7	0.99	0.07	51,51,51,51	0
86	OHX	5	3918	7/7	0.99	0.08	56,56,56,56	0
86	OHX	n3	203	7/7	0.99	0.09	69,69,69,69	0
86	OHX	n9	3803	7/7	0.99	0.10	52,52,52,52	0
86	OHX	5	3920	7/7	0.99	0.07	51,51,51,51	0
86	OHX	5	3921	7/7	0.99	0.09	49,49,49,49	0
86	OHX	5	3922	7/7	0.99	0.09	53,53,53,53	0
86	OHX	5	3923	7/7	0.99	0.10	57,57,57,57	0
86	OHX	q2	502	7/7	0.99	0.16	67,67,67,67	0
86	OHX	5	3924	7/7	0.99	0.07	52,52,52,52	0
86	OHX	6	2058	7/7	0.99	0.08	61,61,61,61	0
86	OHX	5	3927	7/7	0.99	0.06	59,59,59,59	0
87	ZN	Q3	501	1/1	0.99	0.02	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3928	7/7	0.99	0.06	55,55,55,55	0
86	OHX	2	2043	7/7	0.99	0.07	80,80,80,80	0
86	OHX	6	2060	7/7	0.99	0.06	69,69,69,69	0
86	OHX	6	2061	7/7	0.99	0.07	65,65,65,65	0
86	OHX	5	3933	7/7	0.99	0.07	60,60,60,60	0
86	OHX	1	3896	7/7	1.00	0.04	52,52,52,52	0
86	OHX	5	3911	7/7	1.00	0.06	44,44,44,44	0
86	OHX	1	3875	7/7	1.00	0.06	41,41,41,41	0
86	OHX	4	222	7/7	1.00	0.09	46,46,46,46	0
86	OHX	6	2047	7/7	1.00	0.10	47,47,47,47	0
86	OHX	5	3915	7/7	1.00	0.07	53,53,53,53	0
86	OHX	1	3884	7/7	1.00	0.05	50,50,50,50	0
86	OHX	5	3917	7/7	1.00	0.06	49,49,49,49	0
86	OHX	1	3899	7/7	1.00	0.06	48,48,48,48	0
86	OHX	5	3919	7/7	1.00	0.07	53,53,53,53	0
86	OHX	1	3876	7/7	1.00	0.10	50,50,50,50	0
86	OHX	1	3870	7/7	1.00	0.10	35,35,35,35	0
86	OHX	6	2052	7/7	1.00	0.07	56,56,56,56	0
86	OHX	5	3953	7/7	1.00	0.06	55,55,55,55	0
86	OHX	1	3887	7/7	1.00	0.05	49,49,49,49	0
86	OHX	1	3888	7/7	1.00	0.08	56,56,56,56	0
86	OHX	5	3925	7/7	1.00	0.04	46,46,46,46	0
86	OHX	1	3871	7/7	1.00	0.12	43,43,43,43	0
86	OHX	5	3899	7/7	1.00	0.11	34,34,34,34	0
86	OHX	5	3900	7/7	1.00	0.11	35,35,35,35	0
86	OHX	5	3901	7/7	1.00	0.10	37,37,37,37	0
86	OHX	5	3930	7/7	1.00	0.04	48,48,48,48	0
87	ZN	D6	500	1/1	1.00	0.01	67,67,67,67	0
86	OHX	1	3890	7/7	1.00	0.06	53,53,53,53	0
87	ZN	D9	101	1/1	1.00	0.02	60,60,60,60	0
86	OHX	5	3903	7/7	1.00	0.11	43,43,43,43	0
87	ZN	O7	101	1/1	1.00	0.01	25,25,25,25	0
87	ZN	Q0	500	1/1	1.00	0.02	35,35,35,35	0
86	OHX	1	3868	7/7	1.00	0.11	35,35,35,35	0
86	OHX	5	3934	7/7	1.00	0.06	62,62,62,62	0
87	ZN	d6	101	1/1	1.00	0.01	48,48,48,48	0
86	OHX	1	3892	7/7	1.00	0.05	56,56,56,56	0
87	ZN	d9	101	1/1	1.00	0.02	60,60,60,60	0
86	OHX	1	3873	7/7	1.00	0.08	42,42,42,42	0
87	ZN	o7	501	1/1	1.00	0.01	29,29,29,29	0
87	ZN	q0	201	1/1	1.00	0.02	23,23,23,23	0
86	OHX	1	3881	7/7	1.00	0.04	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	ZN	q3	501	1/1	1.00	0.02	50,50,50,50	0
86	OHX	5	3908	7/7	1.00	0.06	39,39,39,39	0
86	OHX	1	3869	7/7	1.00	0.09	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.