wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 09:20 PM EDT

PDB ID	:	5I4L
Title	:	Crystal structure of Amicoumacin A bound to the yeast 80S ribosome
Authors	:	Prokhorova, I.V.; Yusupova, G.; Yusupov, M.
Deposited on	:	2016-02-12
Resolution	:	3.10 Å(reported)

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

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

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

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

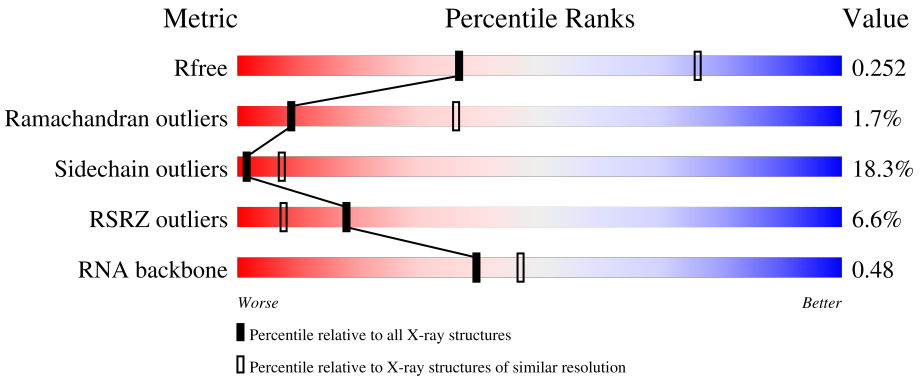
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	4% 70% 27%
1	6	1800	4% 72% 26%
2	S0	206	13% 83% 16%
2	s0	206	5% 80% 18%
3	S1	216	25% 79% 19%

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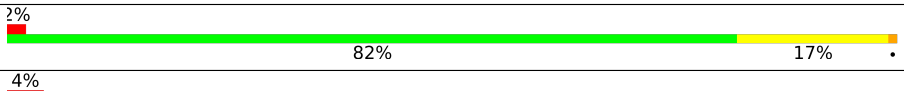
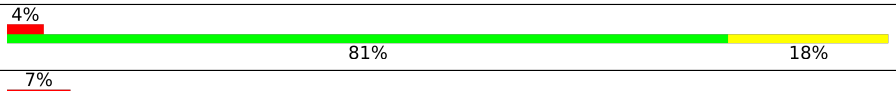
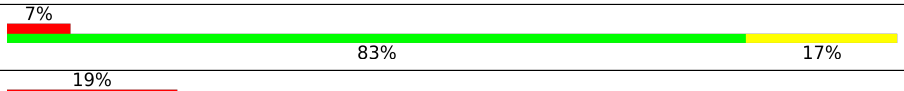
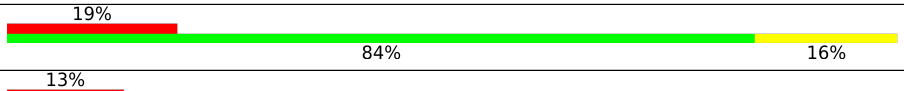
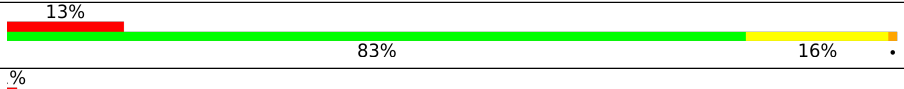
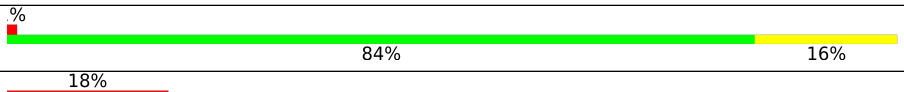
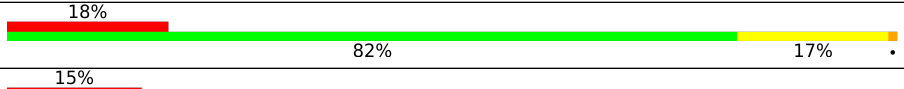
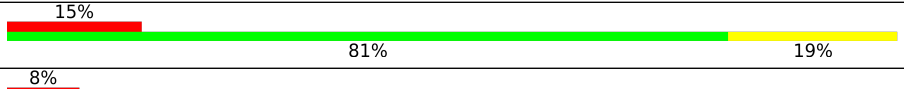
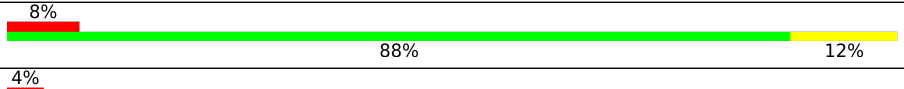
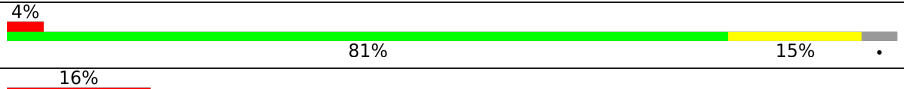
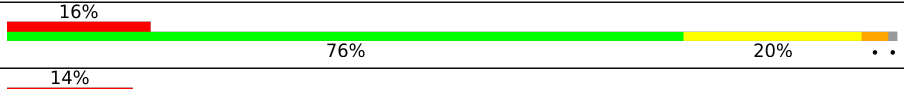
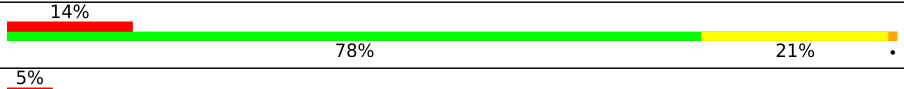
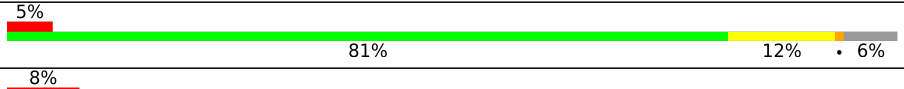
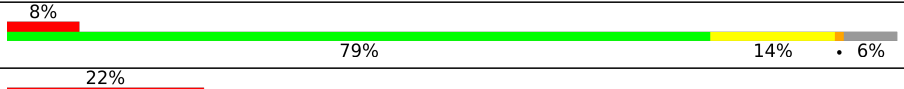
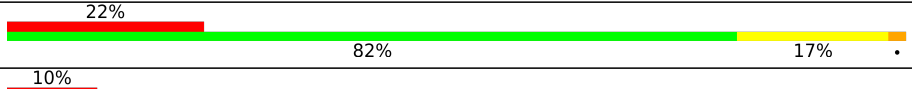
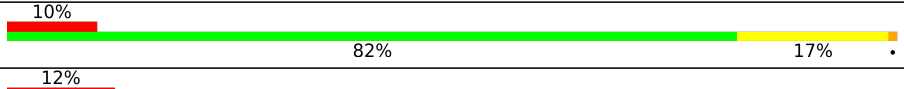
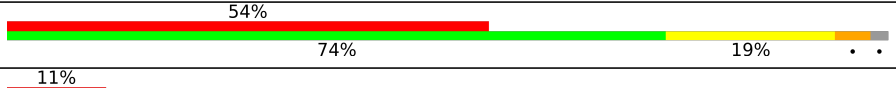
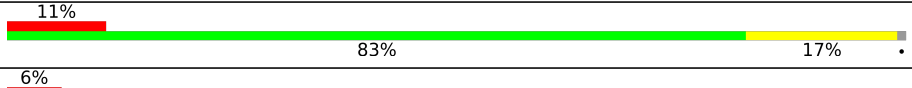
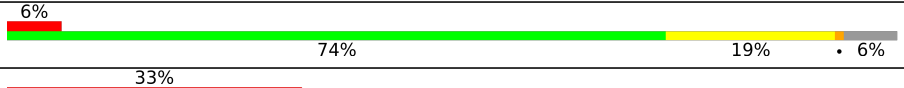
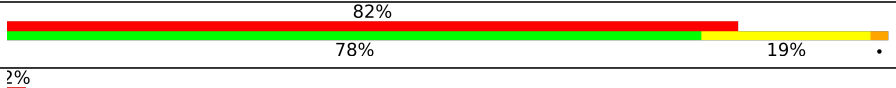
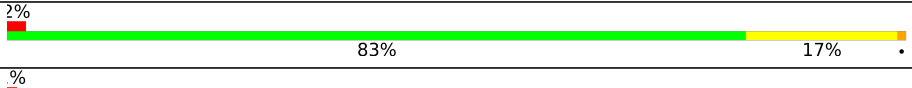
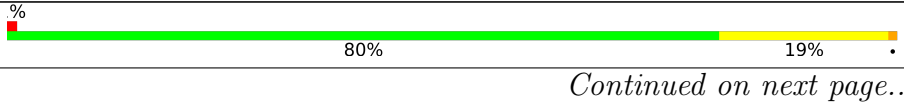
Mol	Chain	Length	Quality of chain
3	s1	216	
4	S2	217	
4	s2	217	
5	S3	223	
5	s3	223	
6	S4	260	
6	s4	260	
7	S5	206	
7	s5	206	
8	S6	226	
8	s6	226	
9	S7	186	
9	s7	186	
10	S8	200	
10	s8	200	
11	S9	185	
11	s9	185	
12	C0	98	
12	c0	98	
13	C1	156	
13	c1	156	
14	C2	124	
14	c2	124	
15	C3	150	
15	c3	150	

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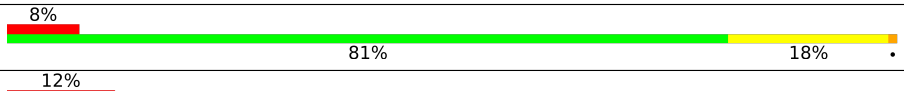
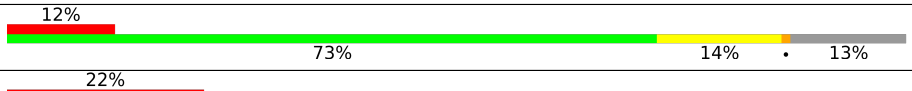
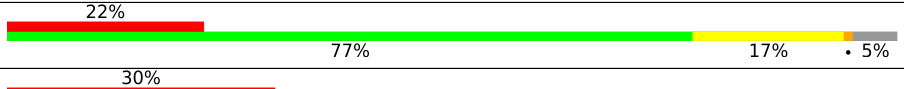
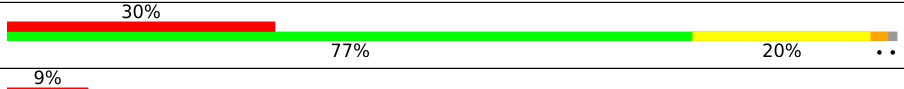
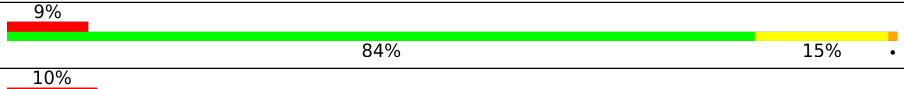
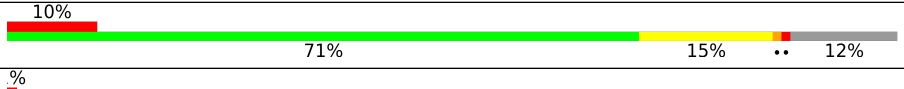
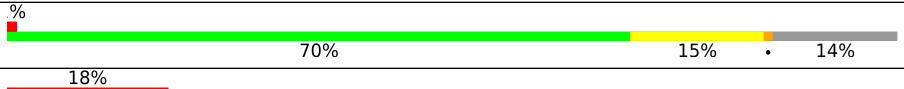
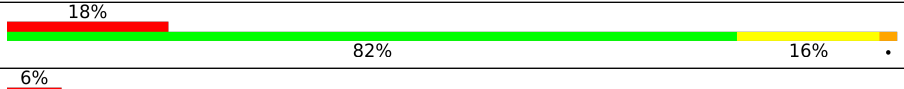
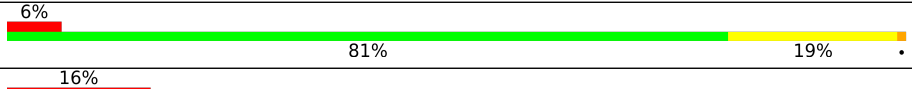
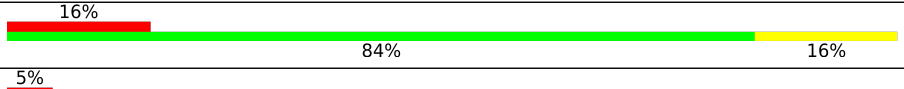
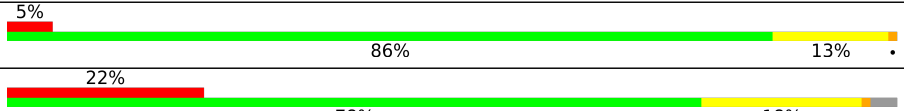
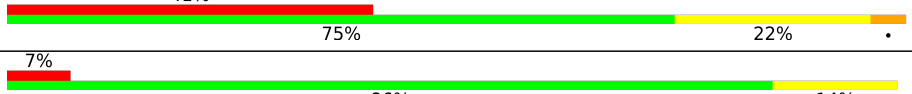
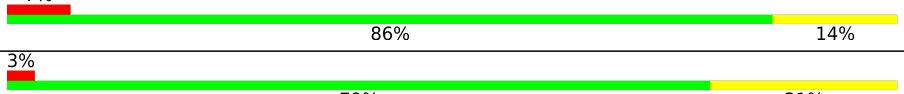
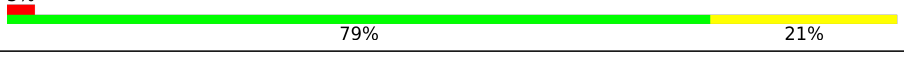
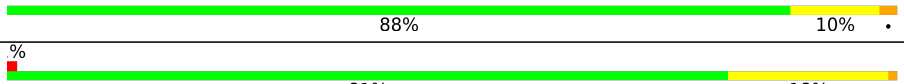
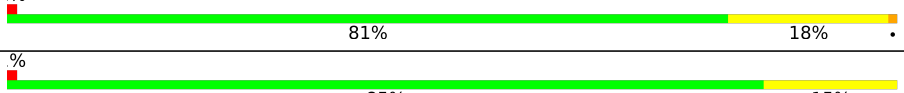
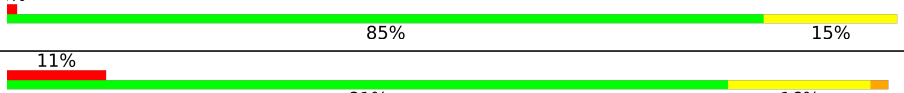
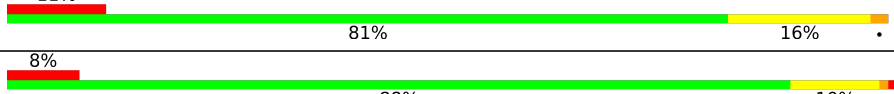
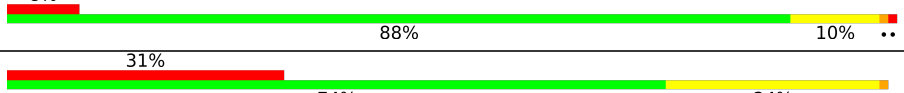
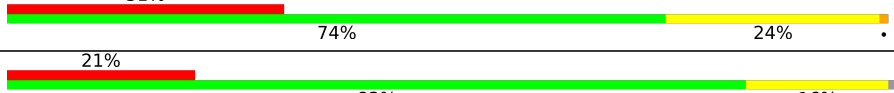
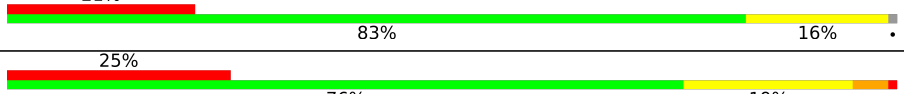
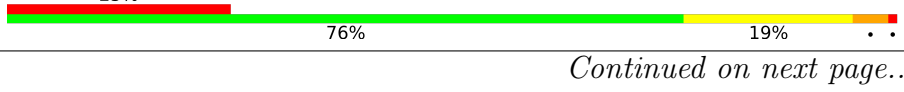
Mol	Chain	Length	Quality of chain
16	C4	128	
16	c4	128	
17	C5	142	
17	c5	142	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	110	
22	d0	110	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	70	
27	d5	70	
28	D6	97	

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Mol	Chain	Length	Quality of chain
28	d6	97	4% 80% 16%
29	D7	81	12% 85% 15%
29	d7	81	10% 84% 16%
30	D8	63	27% 78% 22%
30	d8	63	33% 81% 19%
31	D9	53	8% 74% 25%
31	d9	53	26% 75% 25%
32	E0	62	23% 81% 16%
32	e0	62	13% 79% 21%
33	E1	76	25% 68% 17% 8% 7%
33	e1	76	63% 68% 22% 8%
34	SR	318	21% 90% 10%
34	sR	318	25% 90% 10%
35	SM	176	12% 75% 15% 10%
36	1	3396	2% 71% 20% 7%
36	5	3396	% 71% 20% 7%
37	3	121	87% 13%
37	7	121	84% 15%
38	4	158	% 77% 22%
38	8	158	% 78% 20%
39	L2	252	% 88% 12%
39	l2	252	2% 83% 17%
40	L3	386	% 82% 18%
40	l3	386	% 85% 15%
41	L4	361	85% 14%

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Mol	Chain	Length	Quality of chain
41	l4	361	86% 13%
42	L5	296	11% 81% 18%
42	l5	296	2% 85% 13%
43	L6	176	% 79% 9% 11%
43	l6	176	% 76% 13% 11%
44	L7	223	87% 12%
44	l7	223	87% 13%
45	L8	233	4% 85% 14%
46	L9	191	3% 81% 19%
46	l9	191	% 82% 18%
47	M0	221	3% 83% 12% 5%
47	m0	221	2% 77% 19%
48	M1	169	7% 79% 20%
48	m1	169	% 81% 17%
49	M3	194	2% 81% 18%
49	m3	194	7% 83% 16%
50	M4	137	% 86% 12%
50	m4	137	% 88% 12%
51	M5	203	84% 16%
51	m5	203	84% 15%
52	M6	197	85% 15%
52	m6	197	% 85% 15%
53	M7	183	8% 86% 14%
53	m7	183	70% 14% 15%
54	M8	185	86% 12%

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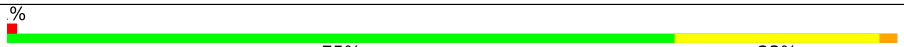
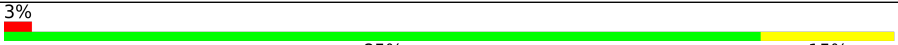
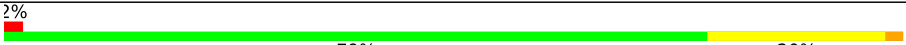
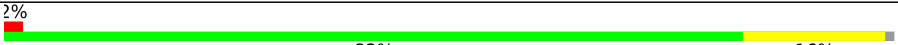
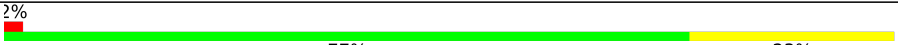
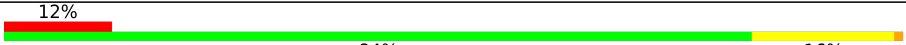
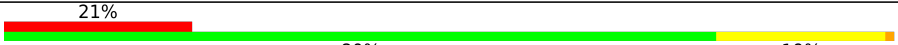
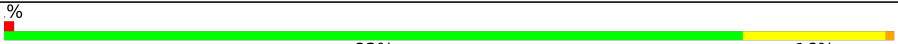
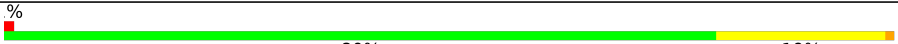
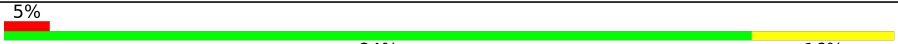
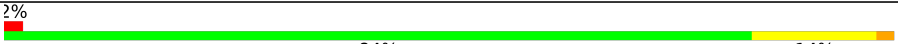
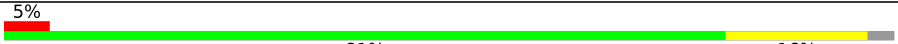
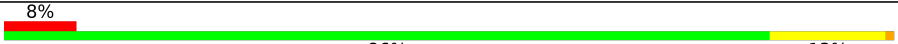
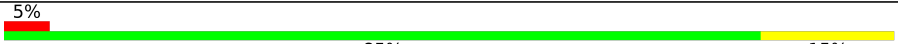
Mol	Chain	Length	Quality of chain
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	100	
58	n2	100	
59	N3	136	
59	n3	136	
60	N4	98	
61	N5	121	
61	n5	121	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	100	
66	o0	100	
67	O1	109	

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Mol	Chain	Length	Quality of chain
67	o1	109	3% 81% 19%
68	O2	127	2% 89% 11%
68	o2	127	2% 82% 18%
69	O3	106	89% 11%
69	o3	106	% 91% 9%
70	O4	112	4% 88% 12%
70	o4	112	3% 89% 11%
71	O5	119	3% 82% 18%
71	o5	119	3% 85% 15%
72	O6	99	6% 76% 24%
72	o6	99	12% 74% 25%
73	O7	87	3% 90% 10%
73	o7	87	2% 84% 16%
74	O8	77	9% 73% 27%
74	o8	77	18% 82% 18%
75	O9	50	90% 10%
75	o9	50	2% 86% 14%
76	Q0	52	10% 87% 13%
76	q0	52	81% 19%
77	Q1	25	80% 20%
77	q1	25	72% 28%
78	Q2	105	10% 83% 16%
78	q2	105	5% 81% 19%
79	Q3	91	85% 15%
79	q3	91	% 81% 18%

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Mol	Chain	Length	Quality of chain
80	sM	159	6% 56% 8% 35%
81	l8	231	9% 84% 16%
82	m2	155	94%
83	n4	135	15% 86% 13%
84	p0	312	13% 38% 8% 54%
85	p1	47	100%
85	p2	47	98%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	2	2027	-	-	-	X
86	OHX	6	2034	-	-	-	X
87	MG	1	3716	-	-	-	X
87	MG	1	3718	-	-	-	X
87	MG	1	3750	-	-	-	X
87	MG	1	3759	-	-	-	X
87	MG	1	3767	-	-	-	X
87	MG	1	3784	-	-	-	X
87	MG	1	3853	-	-	-	X
87	MG	1	3912	-	-	-	X
87	MG	1	3918	-	-	-	X
87	MG	1	3922	-	-	-	X
87	MG	1	3944	-	-	-	X
87	MG	1	3962	-	-	-	X
87	MG	1	3986	-	-	-	X
87	MG	1	4000	-	-	-	X
87	MG	1	4035	-	-	-	X
87	MG	1	4037	-	-	-	X
87	MG	1	4043	-	-	-	X
87	MG	1	4050	-	-	-	X
87	MG	2	2047	-	-	-	X
87	MG	2	2050	-	-	-	X
87	MG	2	2060	-	-	-	X
87	MG	2	2068	-	-	-	X
87	MG	2	2072	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	2	2083	-	-	-	X
87	MG	2	2089	-	-	-	X
87	MG	2	2095	-	-	-	X
87	MG	2	2097	-	-	-	X
87	MG	2	2108	-	-	-	X
87	MG	2	2112	-	-	-	X
87	MG	3	215	-	-	-	X
87	MG	4	227	-	-	-	X
87	MG	5	3805	-	-	-	X
87	MG	5	3864	-	-	-	X
87	MG	5	3869	-	-	-	X
87	MG	5	3875	-	-	-	X
87	MG	5	3919	-	-	-	X
87	MG	5	3935	-	-	-	X
87	MG	5	3946	-	-	-	X
87	MG	5	3950	-	-	-	X
87	MG	5	3954	-	-	-	X
87	MG	5	3985	-	-	-	X
87	MG	5	4074	-	-	-	X
87	MG	5	4093	-	-	-	X
87	MG	5	4104	-	-	-	X
87	MG	6	2040	-	-	-	X
87	MG	6	2054	-	-	-	X
87	MG	6	2056	-	-	-	X
87	MG	6	2067	-	-	-	X
87	MG	6	2091	-	-	-	X
87	MG	6	2092	-	-	-	X
87	MG	6	2124	-	-	-	X
87	MG	6	2130	-	-	-	X
87	MG	6	2132	-	-	-	X
87	MG	8	224	-	-	-	X
87	MG	M3	201	-	-	-	X
87	MG	N8	202	-	-	-	X
87	MG	d6	102	-	-	-	X
88	ZN	D7	101	-	-	-	X

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 410475 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	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			
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
			772	499	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- 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
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	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
			2437	1541	418	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2438	1541	417	472	8			

- Molecule 35 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
80	sM	104	Total	C	N	O	0	0	0
			680	403	140	137			

- Molecule 81 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 82 is a protein called 60S ribosomal protein L12.

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

- Molecule 83 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

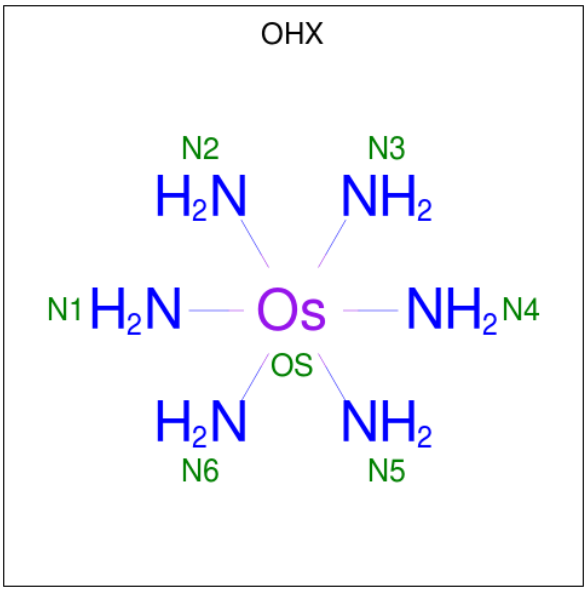
- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 85 is a protein called Ribosomal protein P1 alpha, P2 beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
85	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			
85	p2	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



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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	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	S9	1	Total N Os 7 6 1	0	0
86	C1	1	Total N Os 7 6 1	0	0
86	C3	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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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	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	M0	1	Total N Os 7 6 1	0	0
86	M5	1	Total N Os 7 6 1	0	0
86	M7	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	N9	1	Total N Os 7 6 1	0	0
86	O1	1	Total N Os 7 6 1	0	0
86	O3	1	Total N Os 7 6 1	0	0
86	Q2	1	Total N Os 7 6 1	0	0
86	6	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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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	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	l5	1	Total N Os 7 6 1	0	0
86	l5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	l9	1	Total N Os 7 6 1	0	0
86	m0	1	Total N Os 7 6 1	0	0
86	m0	1	Total N Os 7 6 1	0	0
86	m4	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	n1	1	Total N Os 7 6 1	0	0
86	n3	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	o3	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	2	91	Total Mg 91 91	0	0
87	S2	1	Total Mg 1 1	0	0
87	D3	1	Total Mg 1 1	0	0
87	1	353	Total Mg 353 353	0	0
87	3	8	Total Mg 8 8	0	0
87	4	17	Total Mg 17 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	L2	2	Total Mg 2 2	0	0
87	L3	1	Total Mg 1 1	0	0
87	L4	1	Total Mg 1 1	0	0
87	L7	3	Total Mg 3 3	0	0
87	M0	1	Total Mg 1 1	0	0
87	M3	2	Total Mg 2 2	0	0
87	M5	2	Total Mg 2 2	0	0
87	M7	3	Total Mg 3 3	0	0
87	M9	1	Total Mg 1 1	0	0
87	N3	1	Total Mg 1 1	0	0
87	N8	2	Total Mg 2 2	0	0
87	O2	1	Total Mg 1 1	0	0
87	O7	1	Total Mg 1 1	0	0
87	Q2	1	Total Mg 1 1	0	0
87	6	98	Total Mg 98 98	0	0
87	c1	1	Total Mg 1 1	0	0
87	c6	1	Total Mg 1 1	0	0
87	d3	1	Total Mg 1 1	0	0
87	d6	1	Total Mg 1 1	0	0
87	sM	1	Total Mg 1 1	0	0
87	5	383	Total Mg 383 383	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	7	11	Total Mg 11 11	0	0
87	8	9	Total Mg 9 9	0	0
87	l2	3	Total Mg 3 3	0	0
87	l3	1	Total Mg 1 1	0	0
87	m5	3	Total Mg 3 3	0	0
87	m7	2	Total Mg 2 2	0	0
87	n3	1	Total Mg 1 1	0	0
87	n6	2	Total Mg 2 2	0	0
87	n8	2	Total Mg 2 2	0	0
87	n9	1	Total Mg 1 1	0	0
87	o7	2	Total Mg 2 2	0	0
87	q0	1	Total Mg 1 1	0	0
87	q1	1	Total Mg 1 1	0	0
87	q2	1	Total Mg 1 1	0	0

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	D6	1	Total Zn 1 1	0	0
88	D7	1	Total Zn 1 1	0	0
88	D9	1	Total Zn 1 1	0	0
88	E1	1	Total Zn 1 1	0	0
88	O7	1	Total Zn 1 1	0	0

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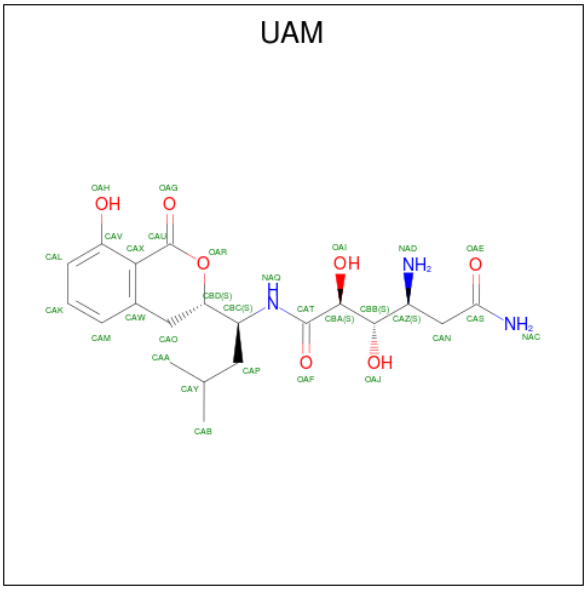
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	Q0	1	Total Zn 1 1	0	0
88	Q2	1	Total Zn 1 1	0	0
88	Q3	1	Total Zn 1 1	0	0
88	d6	1	Total Zn 1 1	0	0
88	d7	1	Total Zn 1 1	0	0
88	d9	1	Total Zn 1 1	0	0
88	e1	1	Total Zn 1 1	0	0
88	o7	1	Total Zn 1 1	0	0
88	q0	1	Total Zn 1 1	0	0
88	q2	1	Total Zn 1 1	0	0
88	q3	1	Total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

- Molecule 89 is Amicoumacin A (three-letter code: UAM) (formula: $C_{20}H_{29}N_3O_7$).



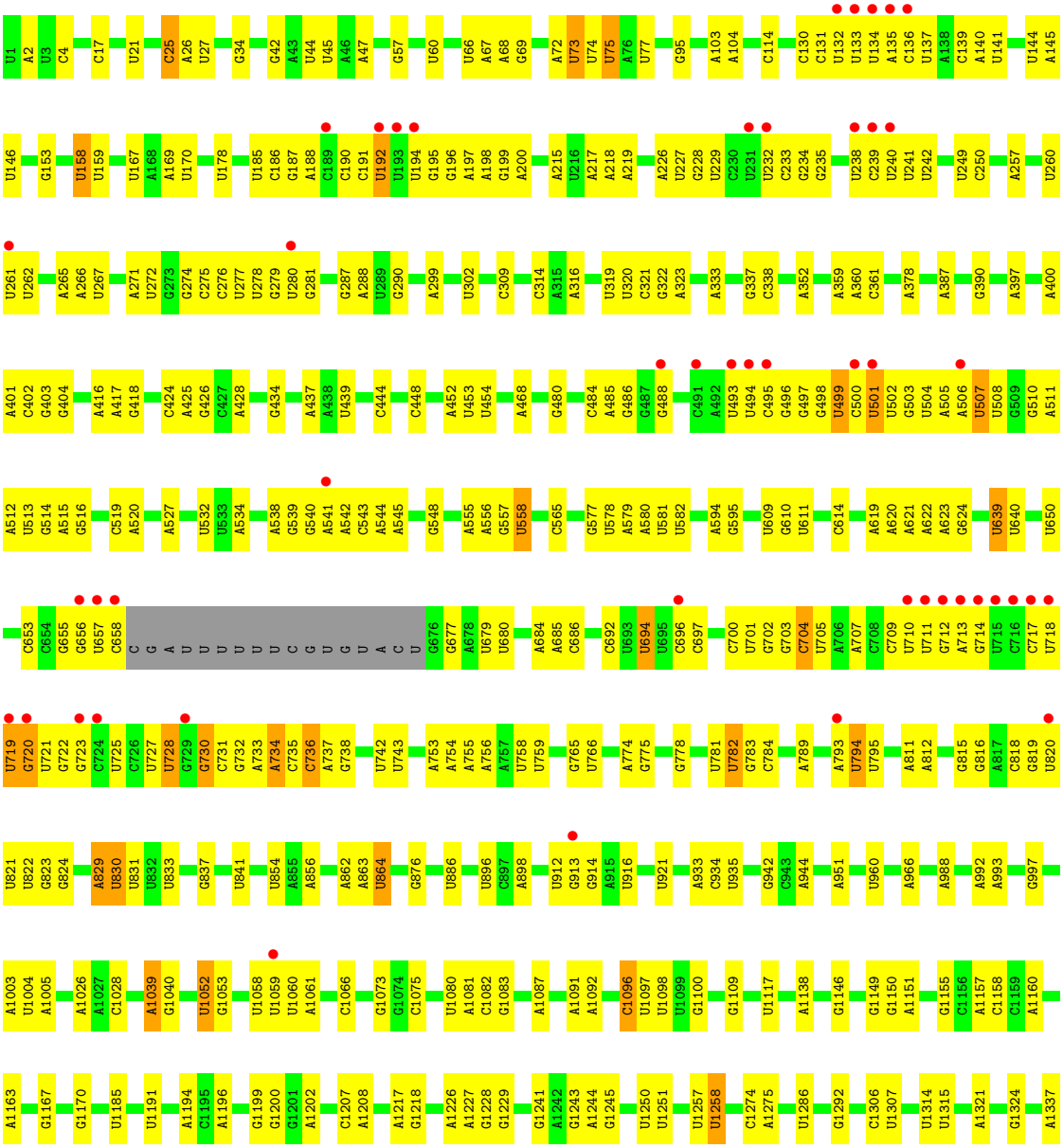
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	6	1	Total	C	N	O	0	0
			30	20	3	7		

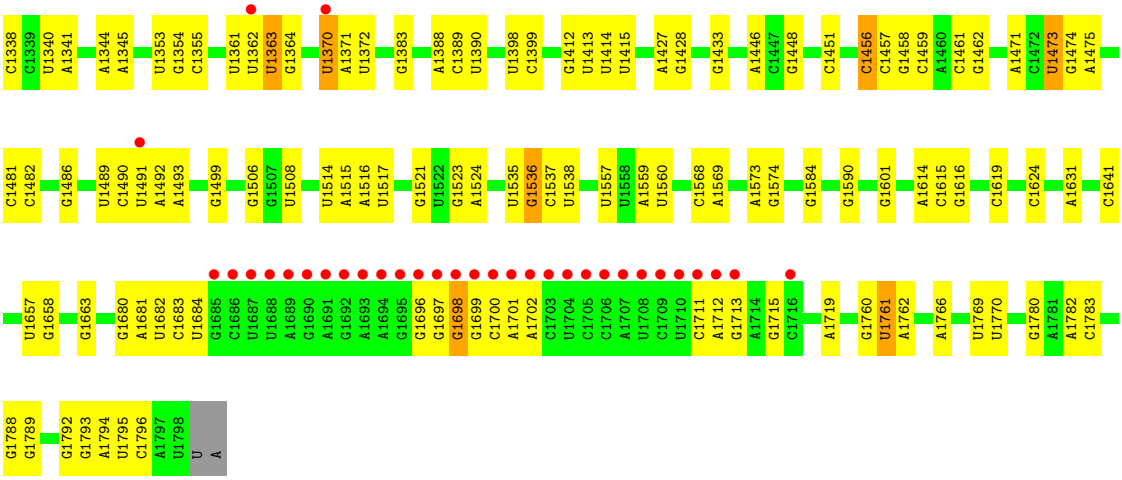
3 Residue-property plots (i)

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

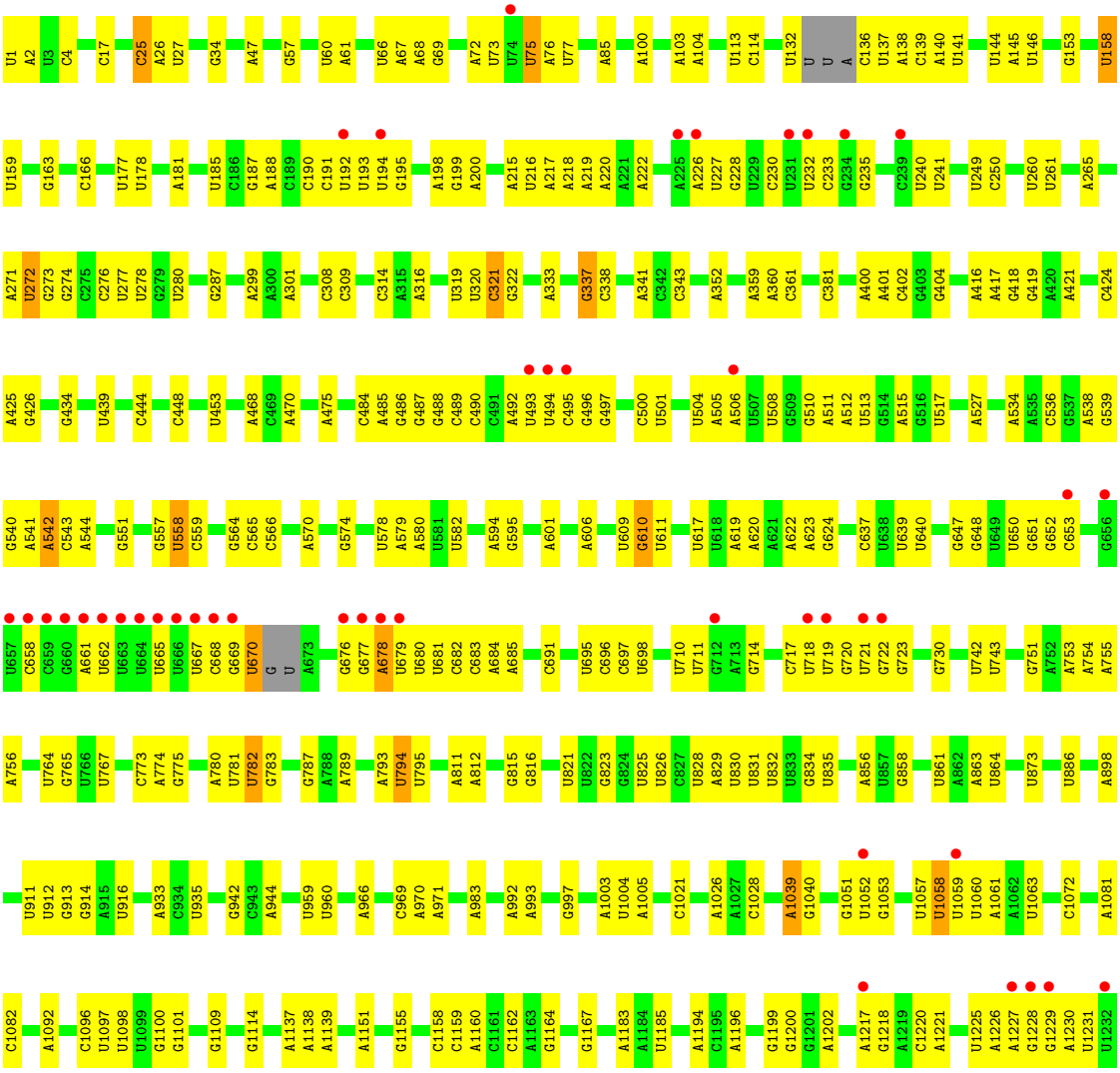
Chain 2:

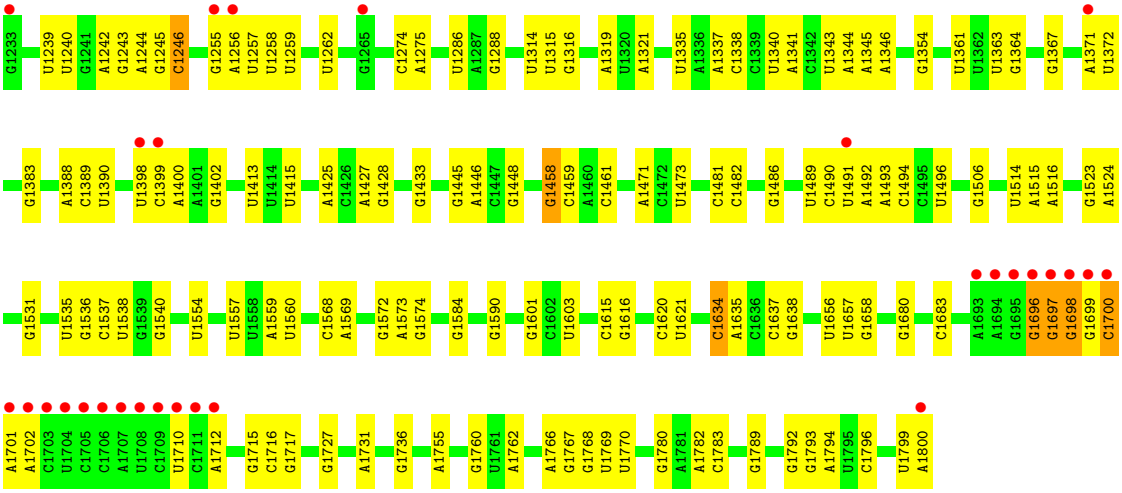




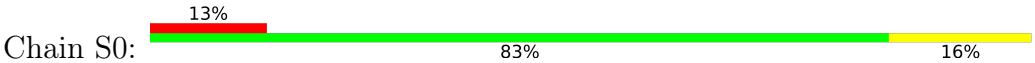
• Molecule 1: 18S ribosomal RNA

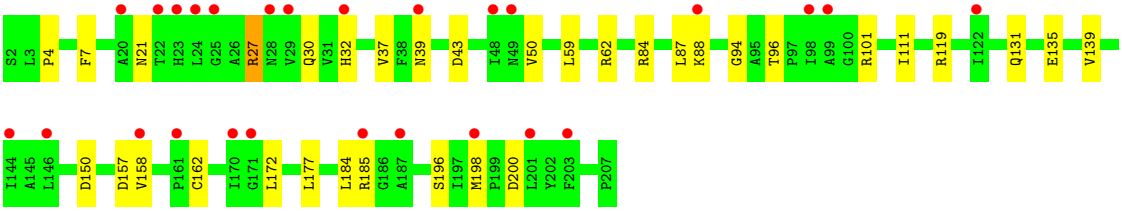
Chain 6:



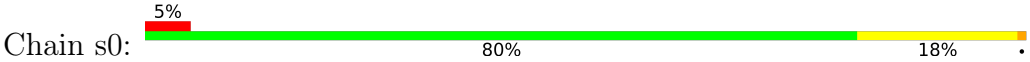


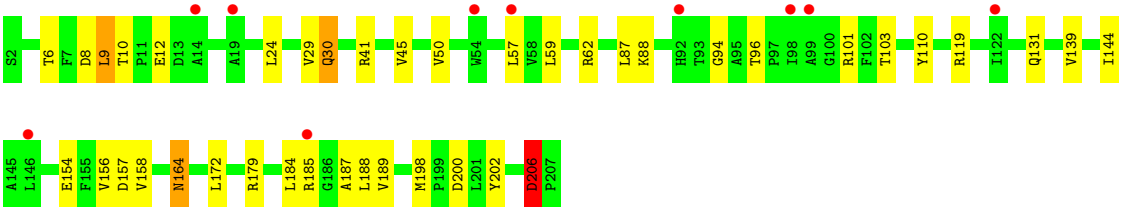
• Molecule 2: 40S ribosomal protein S0-A



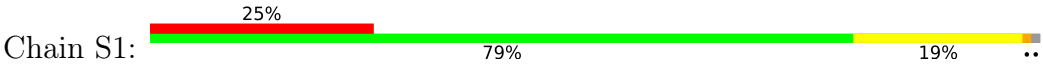


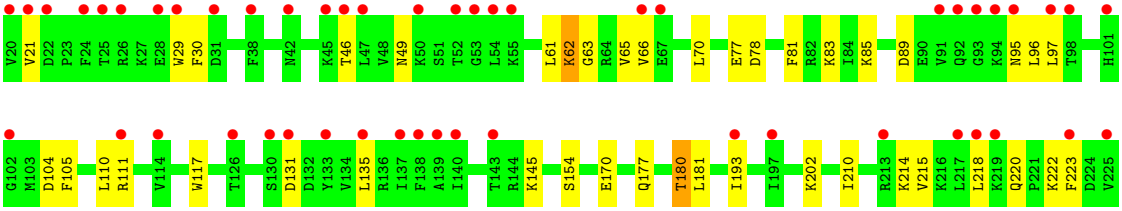
• Molecule 2: 40S ribosomal protein S0-A

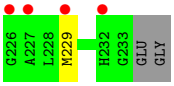




• Molecule 3: 40S ribosomal protein S1-A

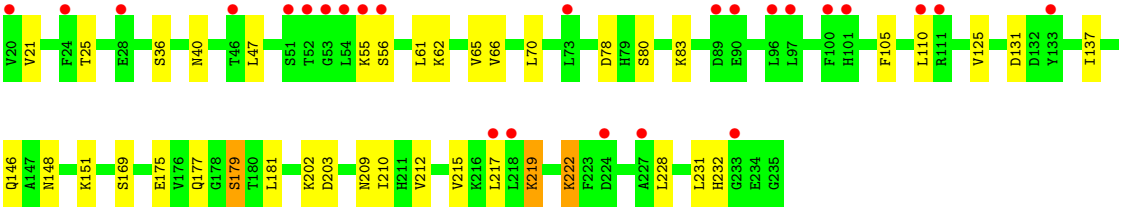






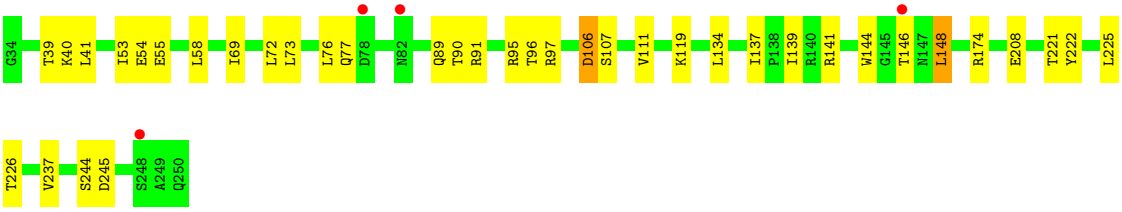
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



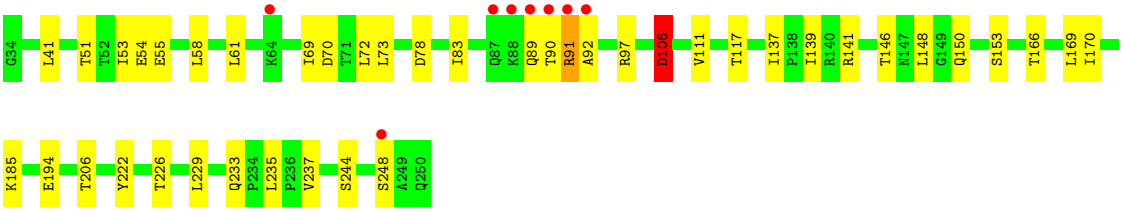
• Molecule 4: 40S ribosomal protein S2

Chain S2:



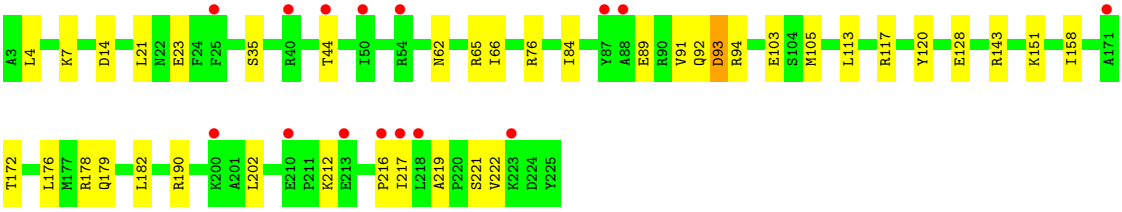
• Molecule 4: 40S ribosomal protein S2

Chain s2:



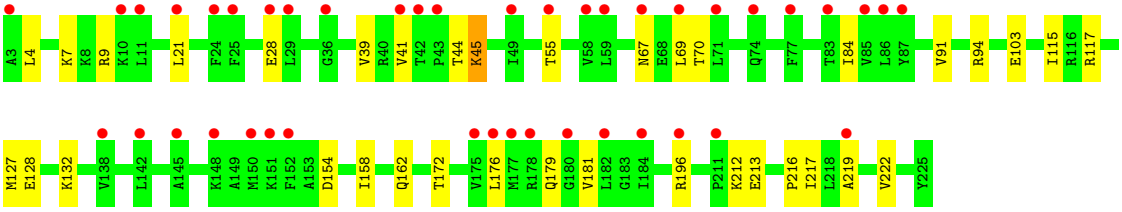
• Molecule 5: 40S ribosomal protein S3

Chain S3:

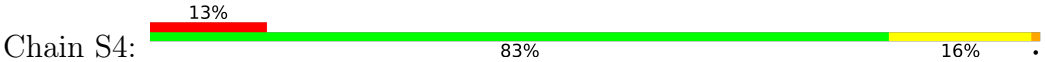


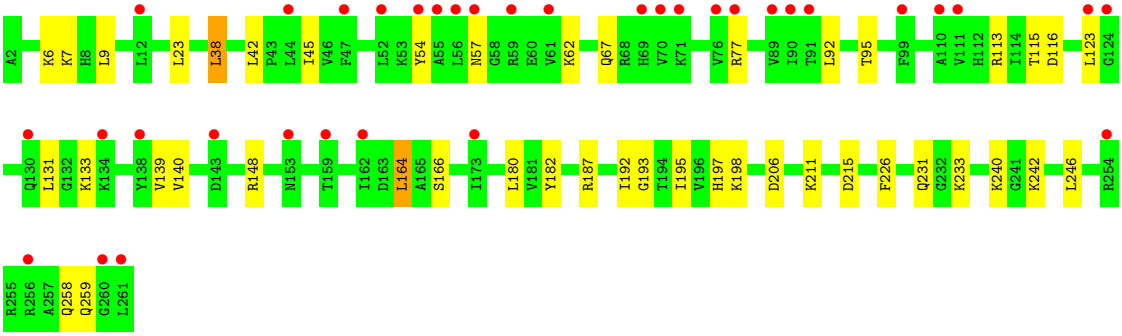
• Molecule 5: 40S ribosomal protein S3

Chain s3:

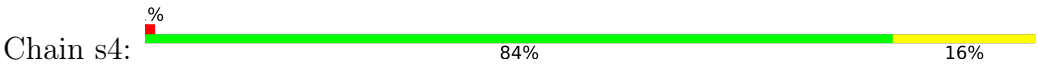


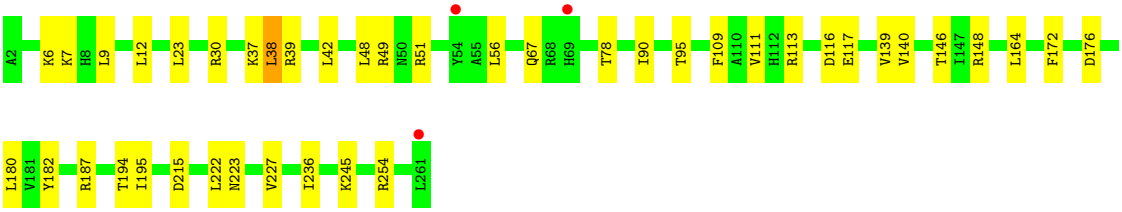
• Molecule 6: 40S ribosomal protein S4-A



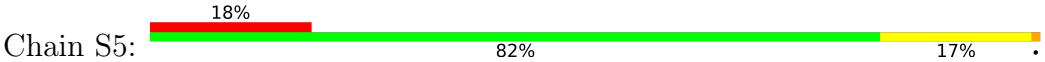


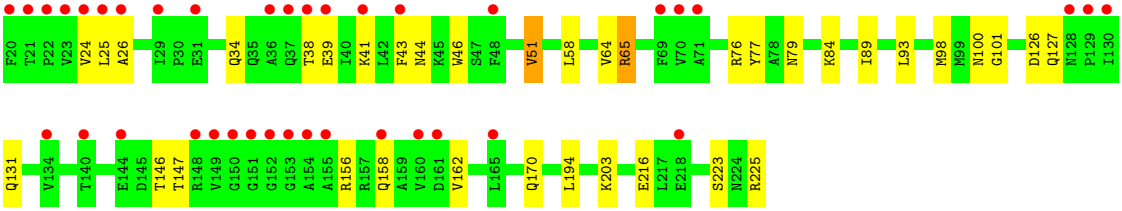
• Molecule 6: 40S ribosomal protein S4-A



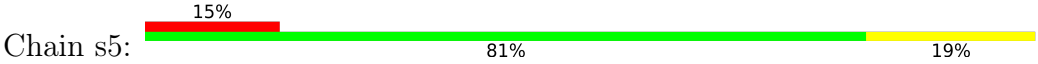


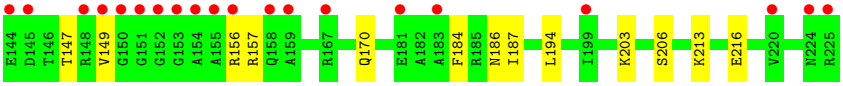
• Molecule 7: 40S ribosomal protein S5



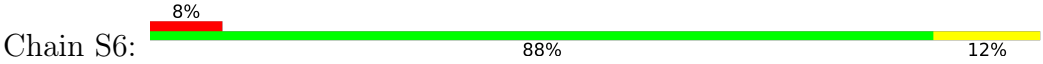


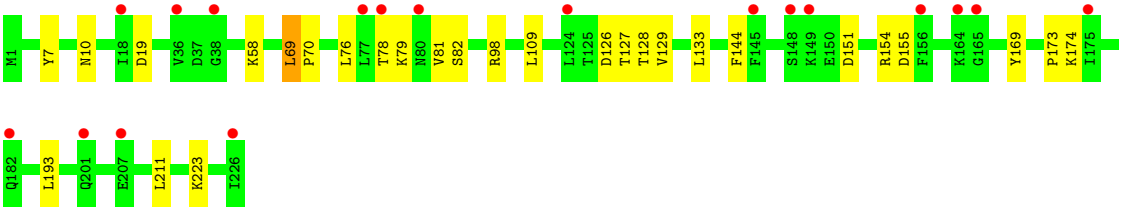
• Molecule 7: 40S ribosomal protein S5



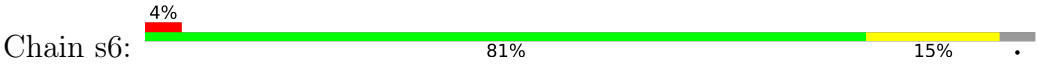


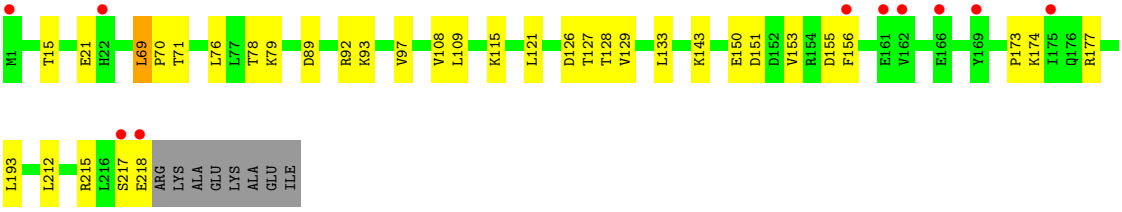
• Molecule 8: 40S ribosomal protein S6-A



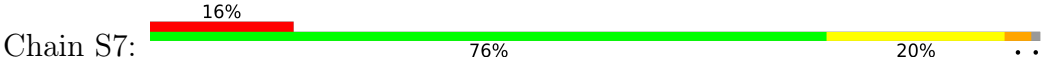


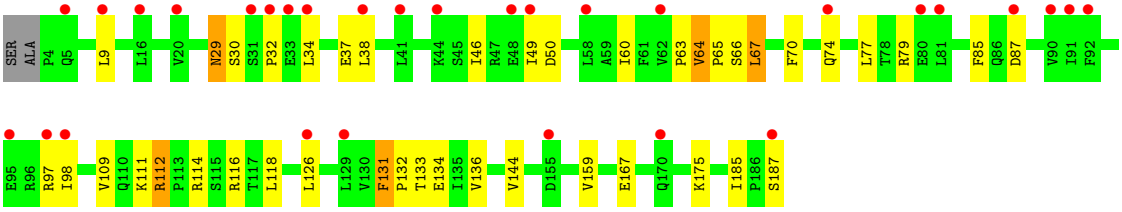
• Molecule 8: 40S ribosomal protein S6-A



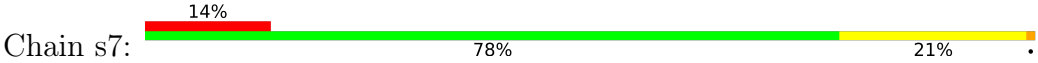


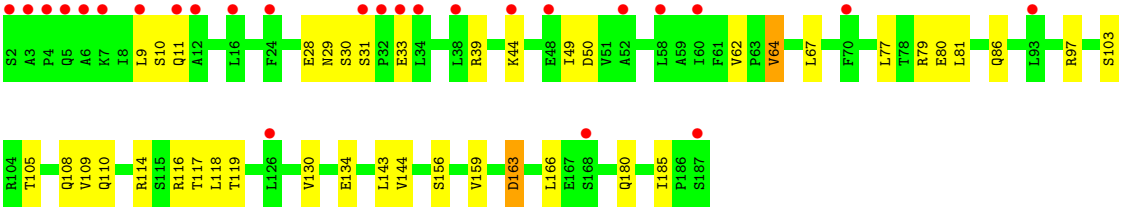
• Molecule 9: 40S ribosomal protein S7-A



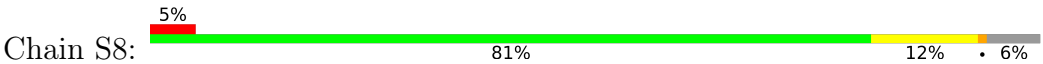


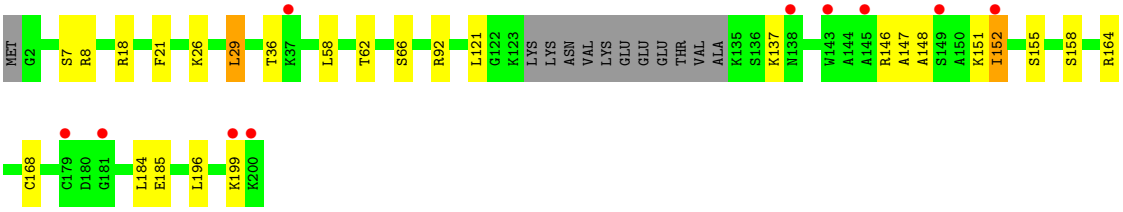
• Molecule 9: 40S ribosomal protein S7-A



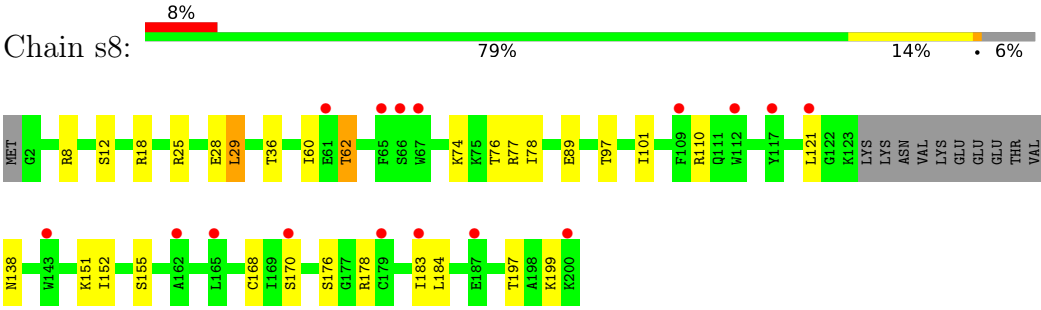


• Molecule 10: 40S ribosomal protein S8-A

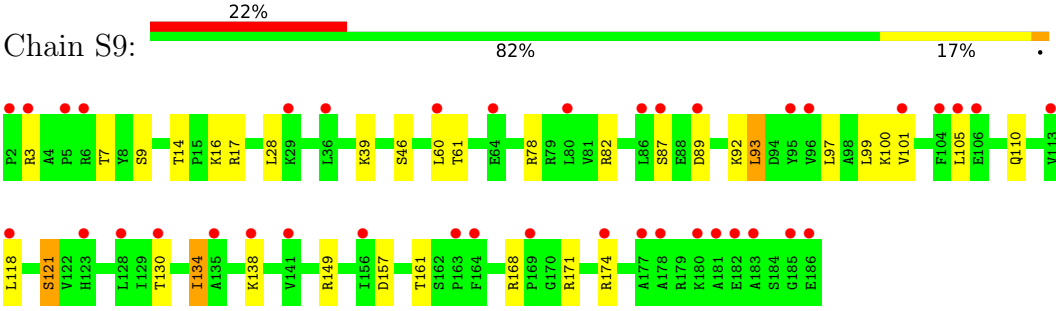




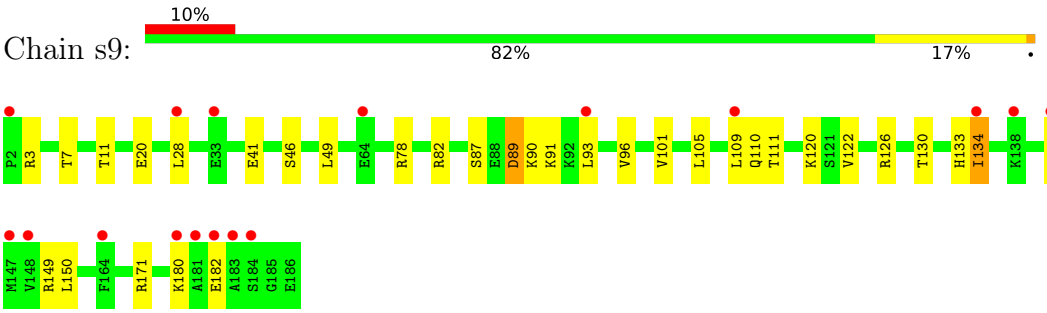
• Molecule 10: 40S ribosomal protein S8-A



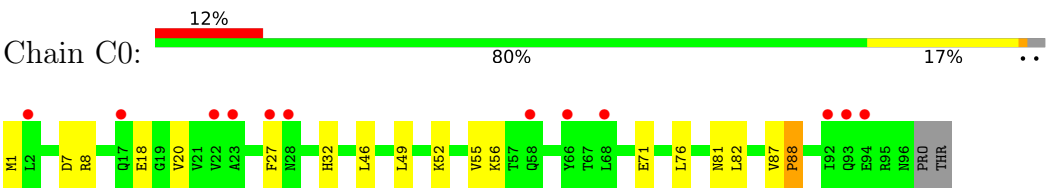
• Molecule 11: 40S ribosomal protein S9-A



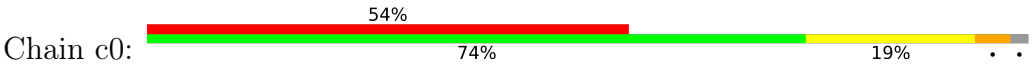
• Molecule 11: 40S ribosomal protein S9-A

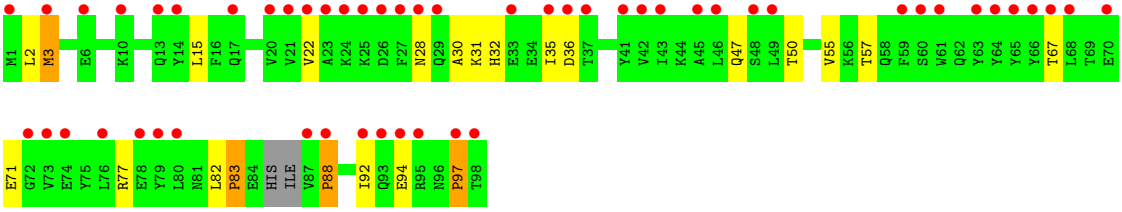


• Molecule 12: 40S ribosomal protein S10-A



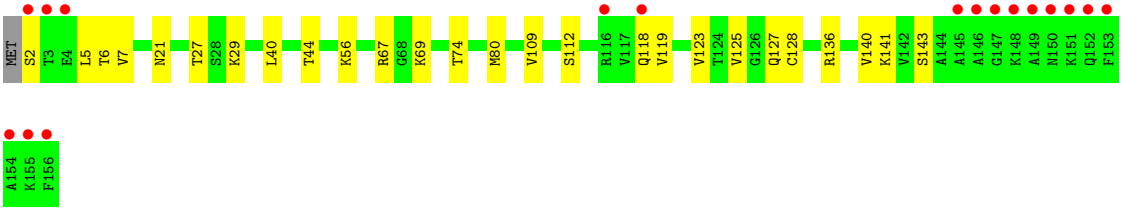
• Molecule 12: 40S ribosomal protein S10-A





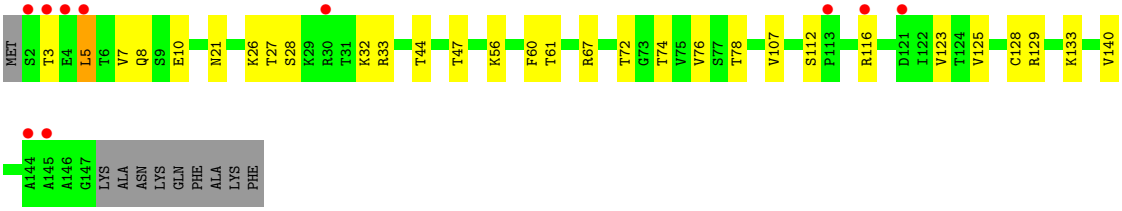
• Molecule 13: 40S ribosomal protein S11-A

Chain C1:



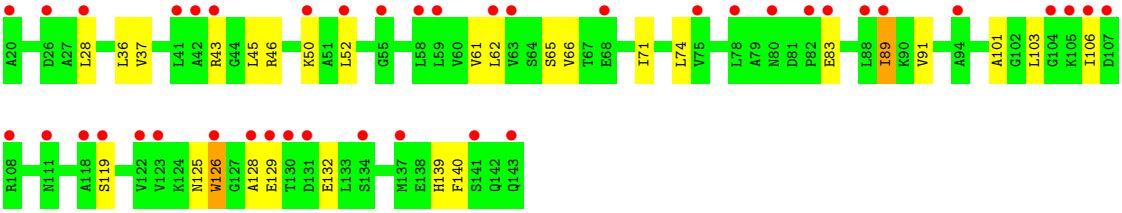
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



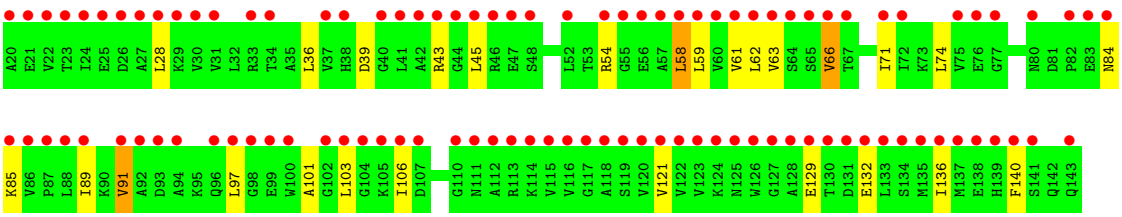
• Molecule 14: 40S ribosomal protein S12

Chain C2:



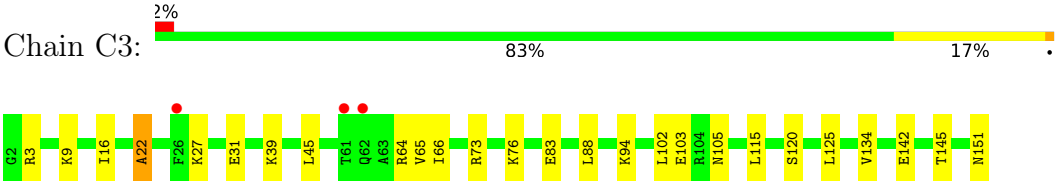
• Molecule 14: 40S ribosomal protein S12

Chain c2:



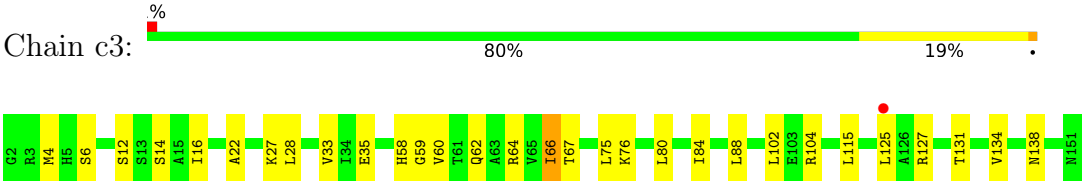
• Molecule 15: 40S ribosomal protein S13

Chain C3:



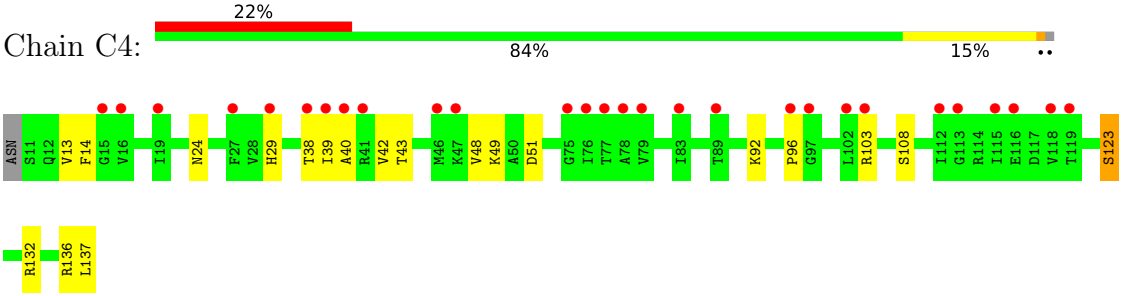
• Molecule 15: 40S ribosomal protein S13

Chain c3:



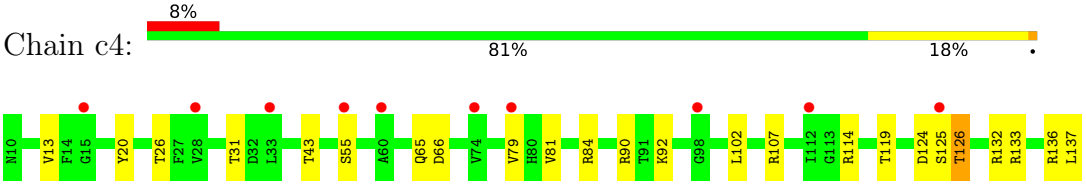
• Molecule 16: 40S ribosomal protein S14-B

Chain C4:



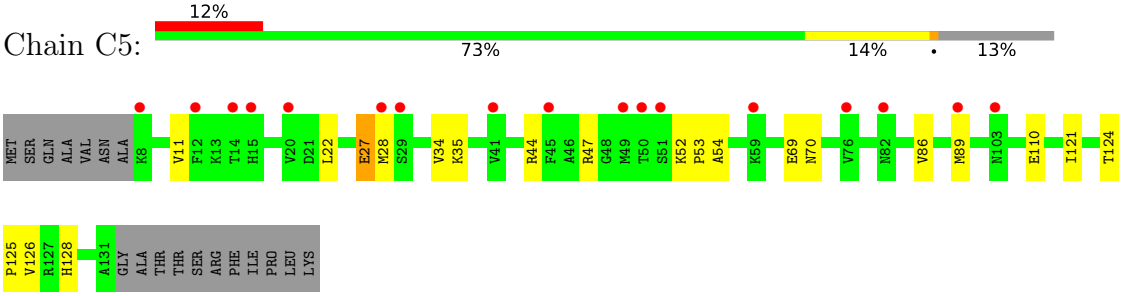
• Molecule 16: 40S ribosomal protein S14-B

Chain c4:



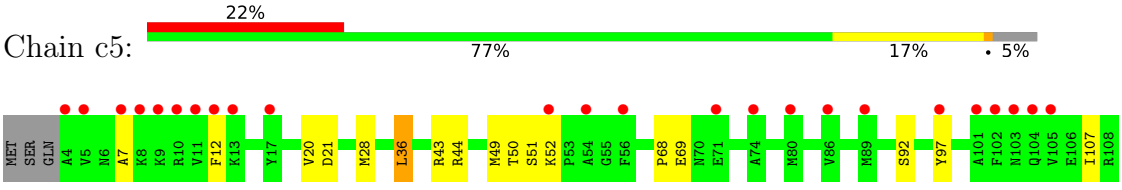
• Molecule 17: 40S ribosomal protein S15

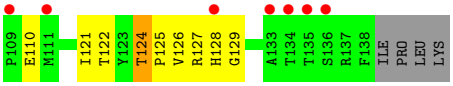
Chain C5:



• Molecule 17: 40S ribosomal protein S15

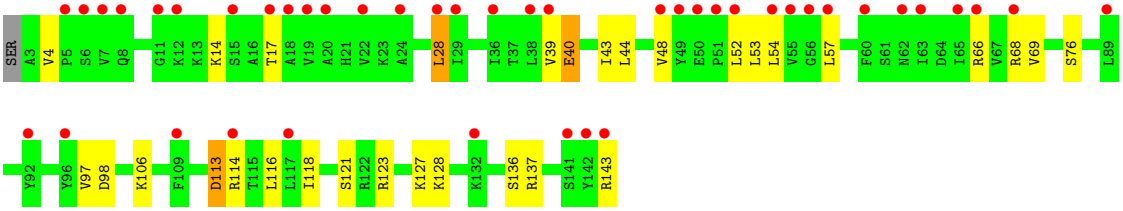
Chain c5:





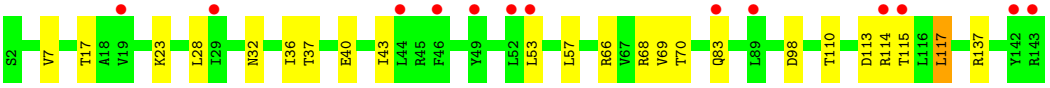
• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



• Molecule 18: 40S ribosomal protein S16-A

Chain c6:

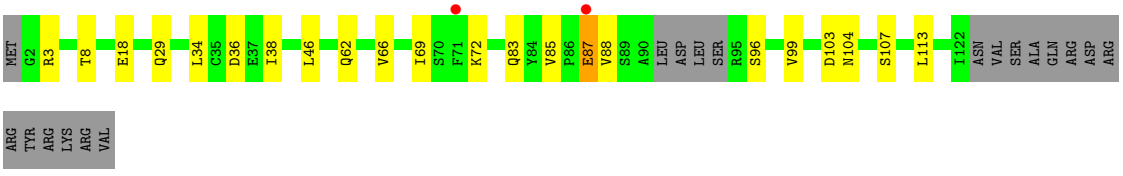


• Molecule 19: 40S ribosomal protein S17-A

Chain C7:

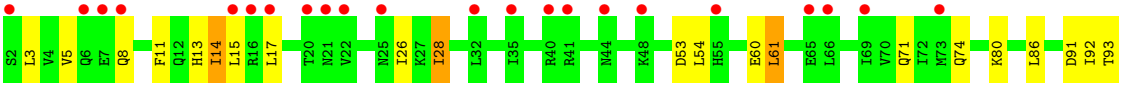
• Molecule 19: 40S ribosomal protein S17-A

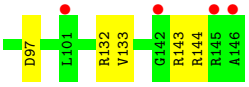
Chain c7:



• Molecule 20: 40S ribosomal protein S18-A

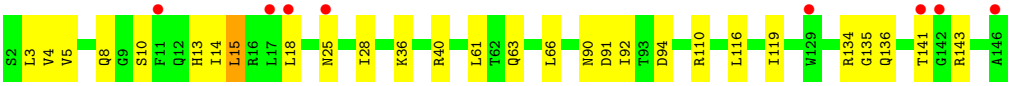
Chain C8:





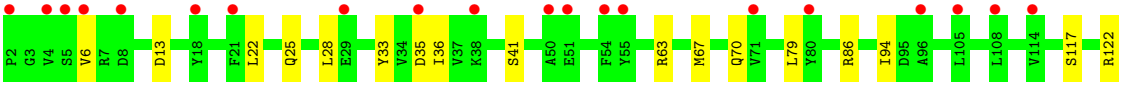
• Molecule 20: 40S ribosomal protein S18-A

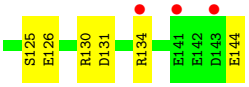
Chain c8:



• Molecule 21: 40S ribosomal protein S19-A

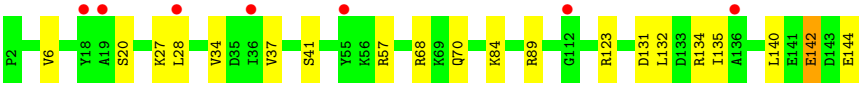
Chain C9:





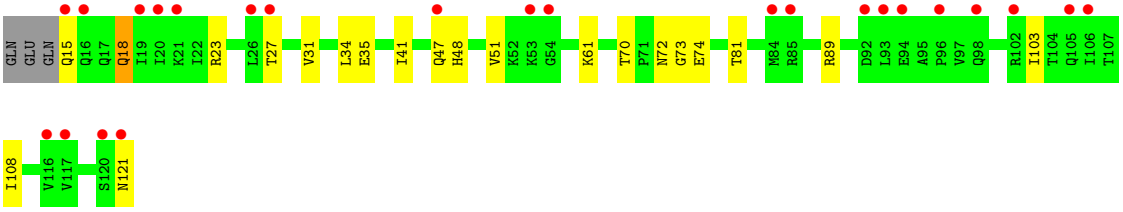
• Molecule 21: 40S ribosomal protein S19-A

Chain c9:



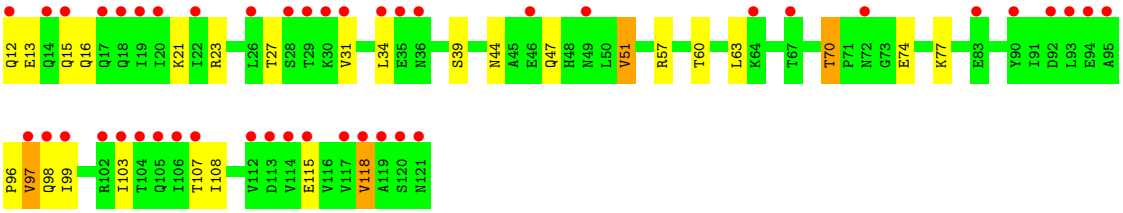
• Molecule 22: 40S ribosomal protein S20

Chain D0:



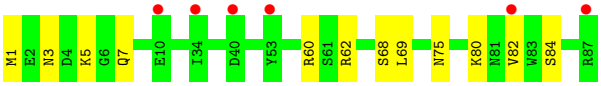
• Molecule 22: 40S ribosomal protein S20

Chain d0:



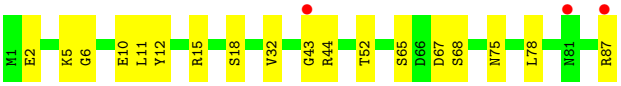
• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



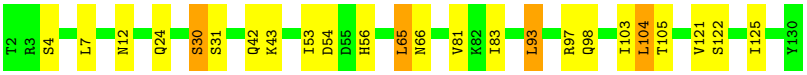
• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



• Molecule 24: 40S ribosomal protein S22-A

Chain D2:

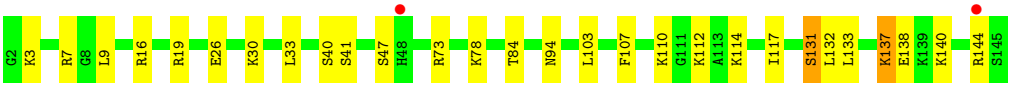


• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

• Molecule 25: 40S ribosomal protein S23-A

Chain D3:

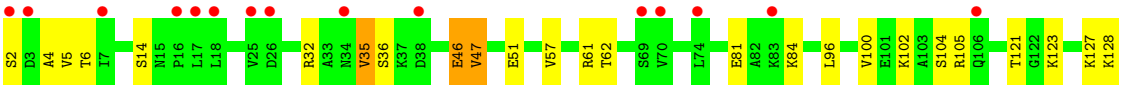


• Molecule 25: 40S ribosomal protein S23-A

Chain d3:

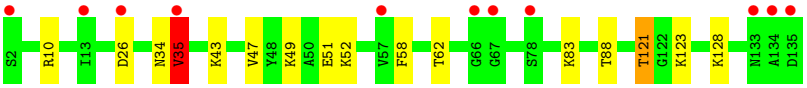
• Molecule 26: 40S ribosomal protein S24-A

Chain D4:



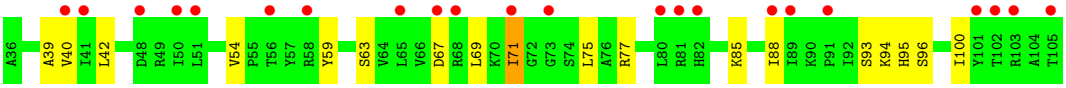
• Molecule 26: 40S ribosomal protein S24-A

Chain d4:



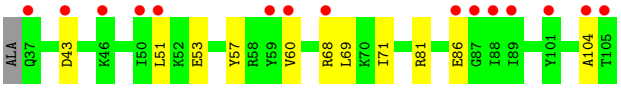
• Molecule 27: 40S ribosomal protein S25-A

Chain D5:



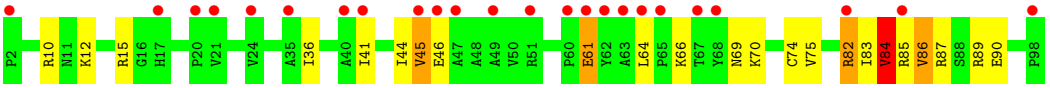
• Molecule 27: 40S ribosomal protein S25-A

Chain d5:



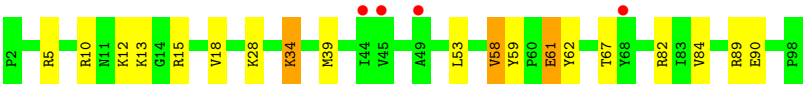
• Molecule 28: 40S ribosomal protein S26-B

Chain D6:



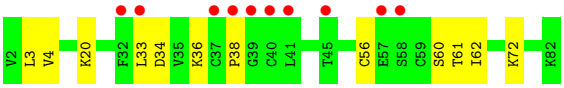
• Molecule 28: 40S ribosomal protein S26-B

Chain d6:



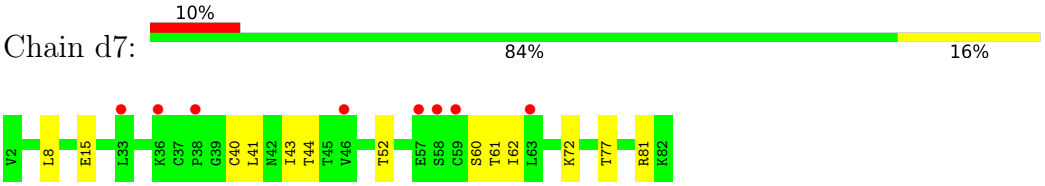
• Molecule 29: 40S ribosomal protein S27-A

Chain D7:



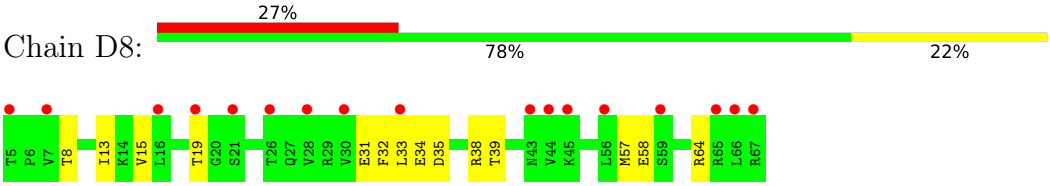
• Molecule 29: 40S ribosomal protein S27-A

Chain d7:



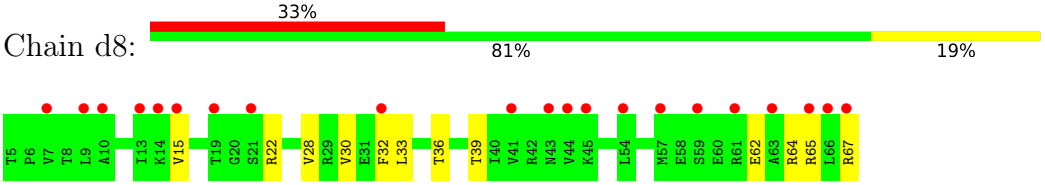
• Molecule 30: 40S ribosomal protein S28-A

Chain D8:



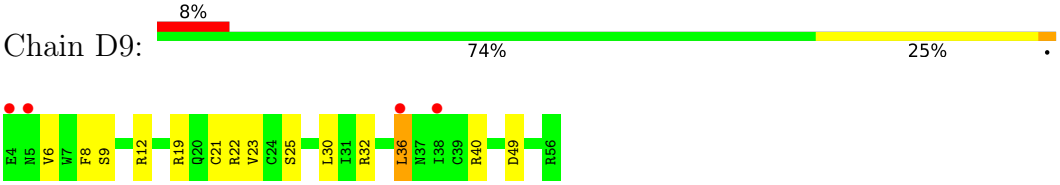
• Molecule 30: 40S ribosomal protein S28-A

Chain d8:



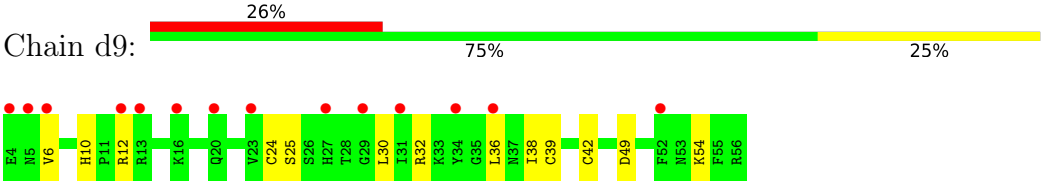
• Molecule 31: 40S ribosomal protein S29-A

Chain D9:



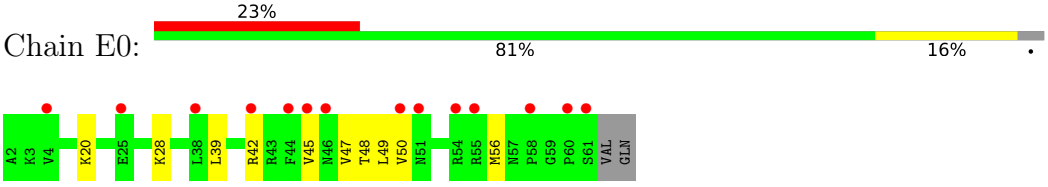
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



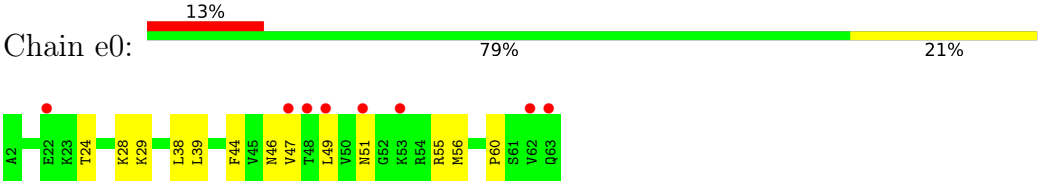
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



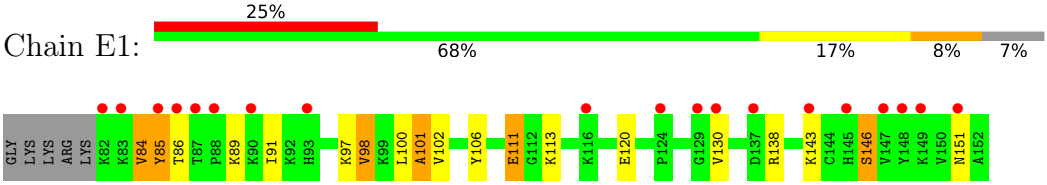
• Molecule 32: 40S ribosomal protein S30-A

Chain e0:



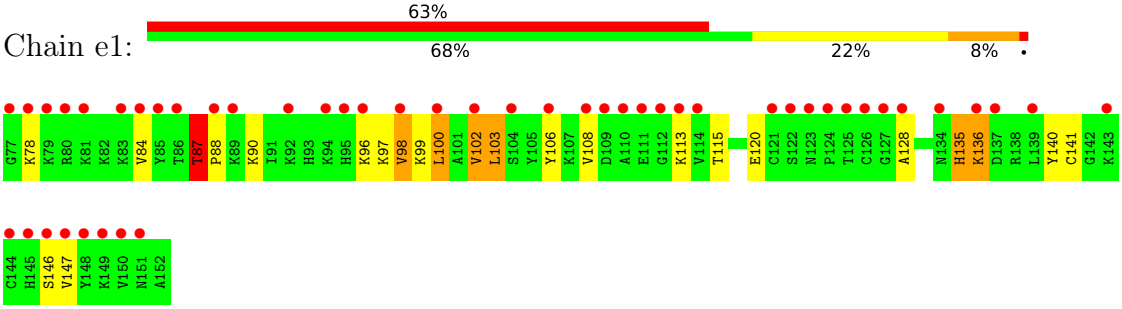
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



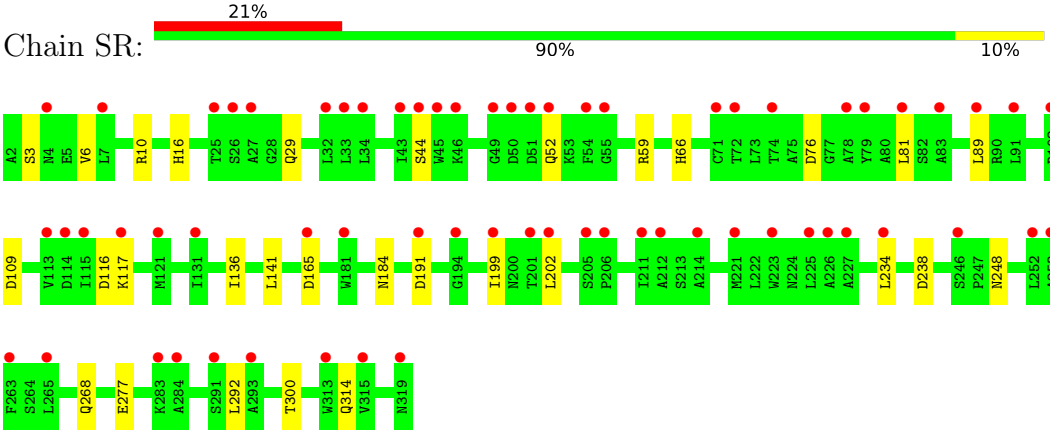
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:



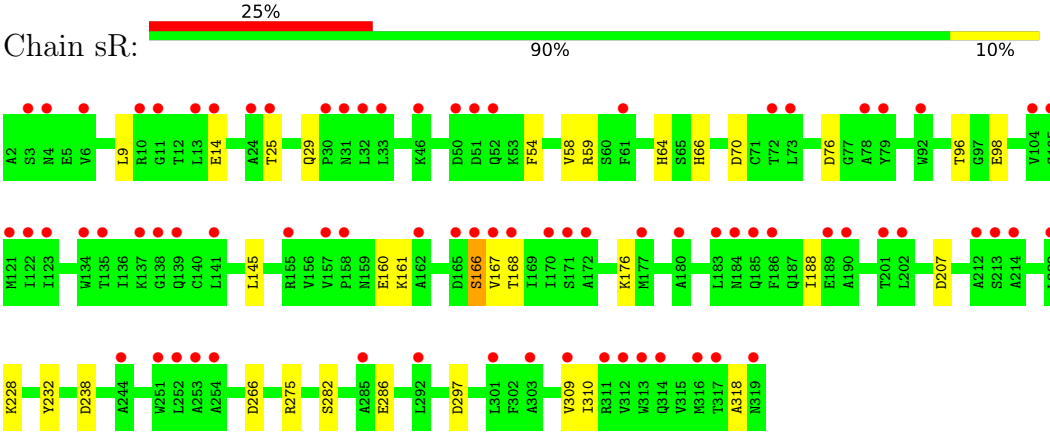
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



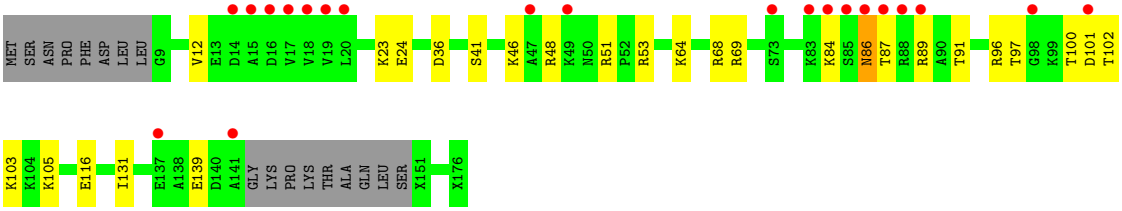
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



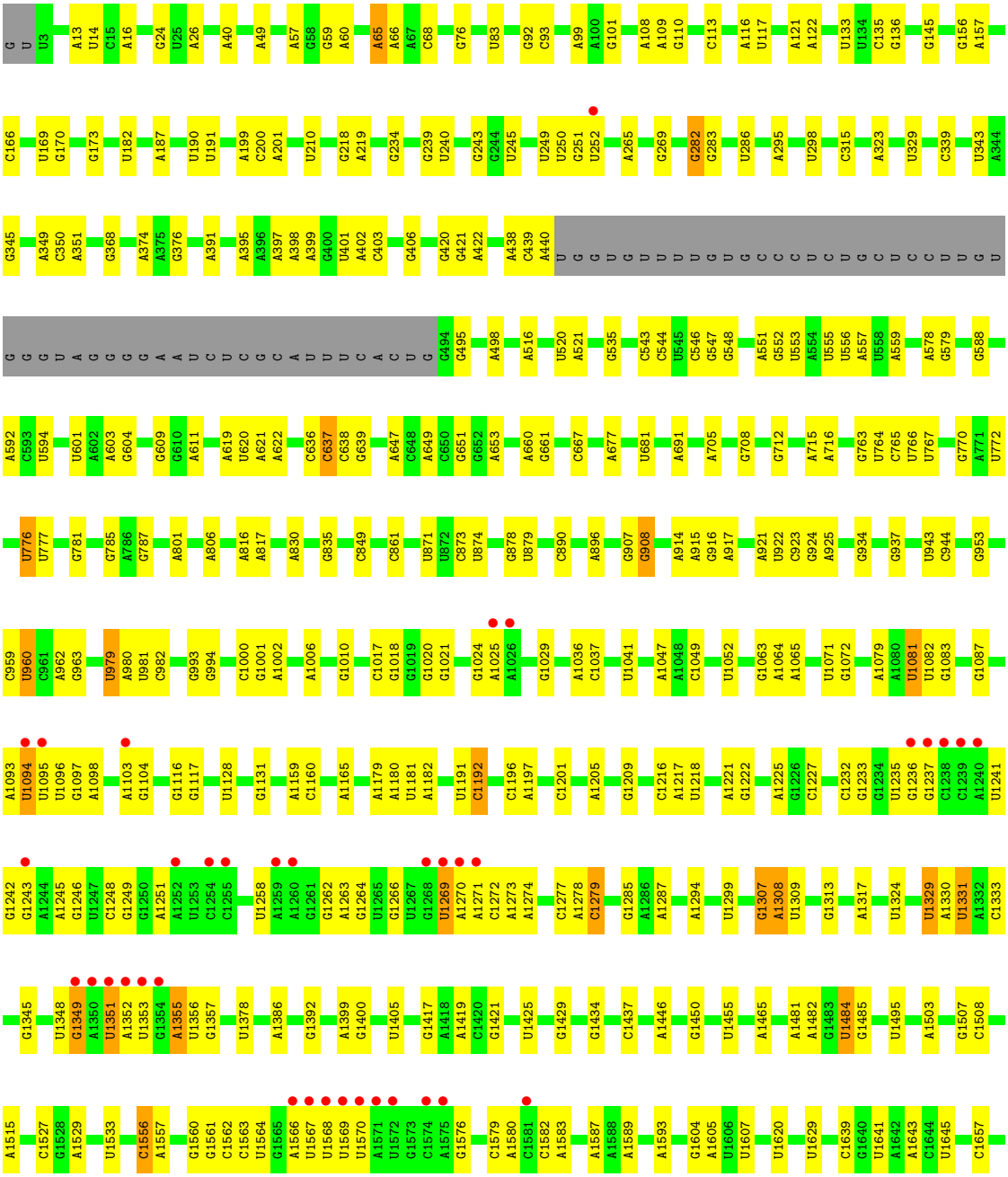
• Molecule 35: Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1

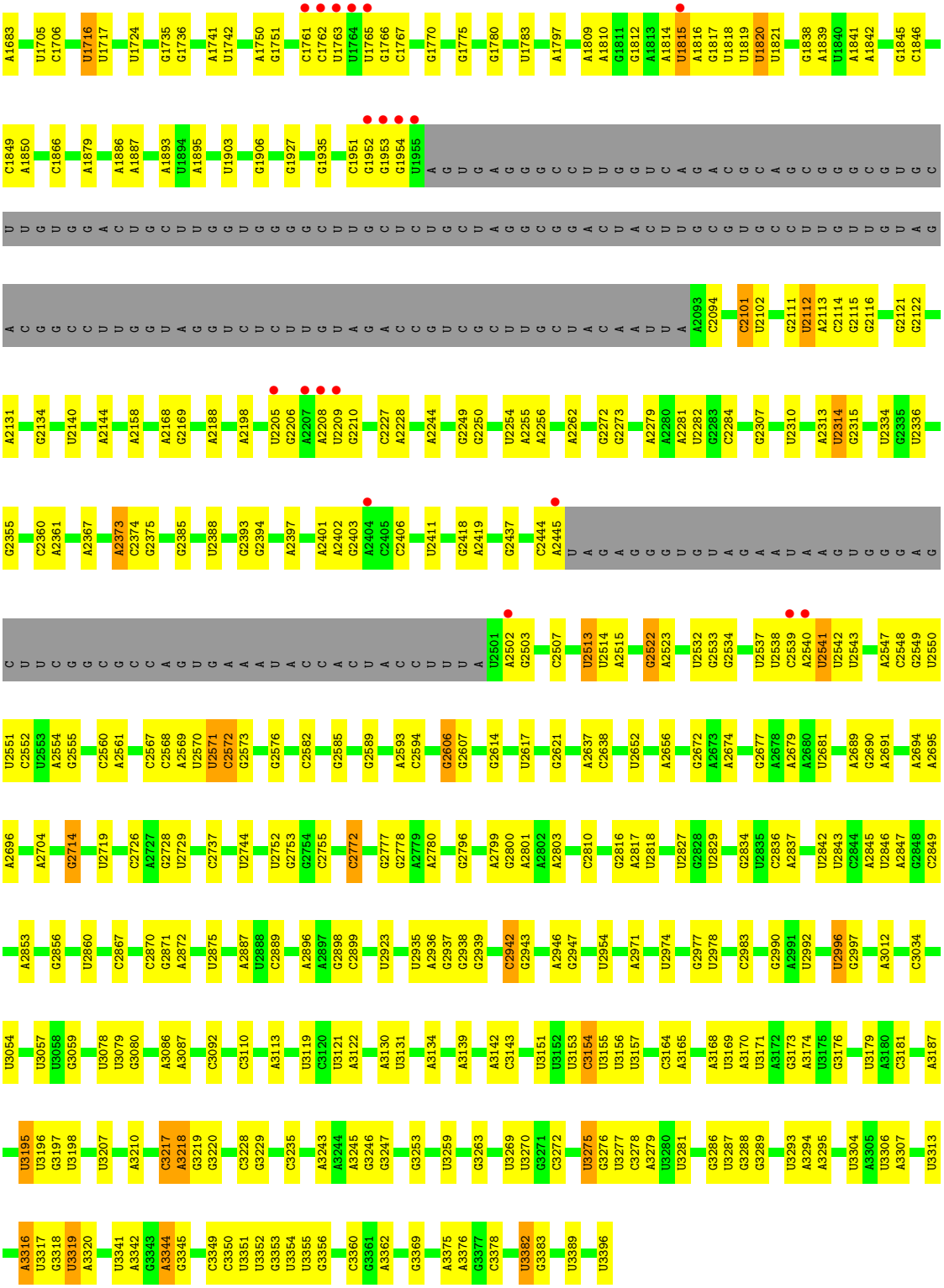
Chain SM:



• Molecule 36: 25S ribosomal RNA

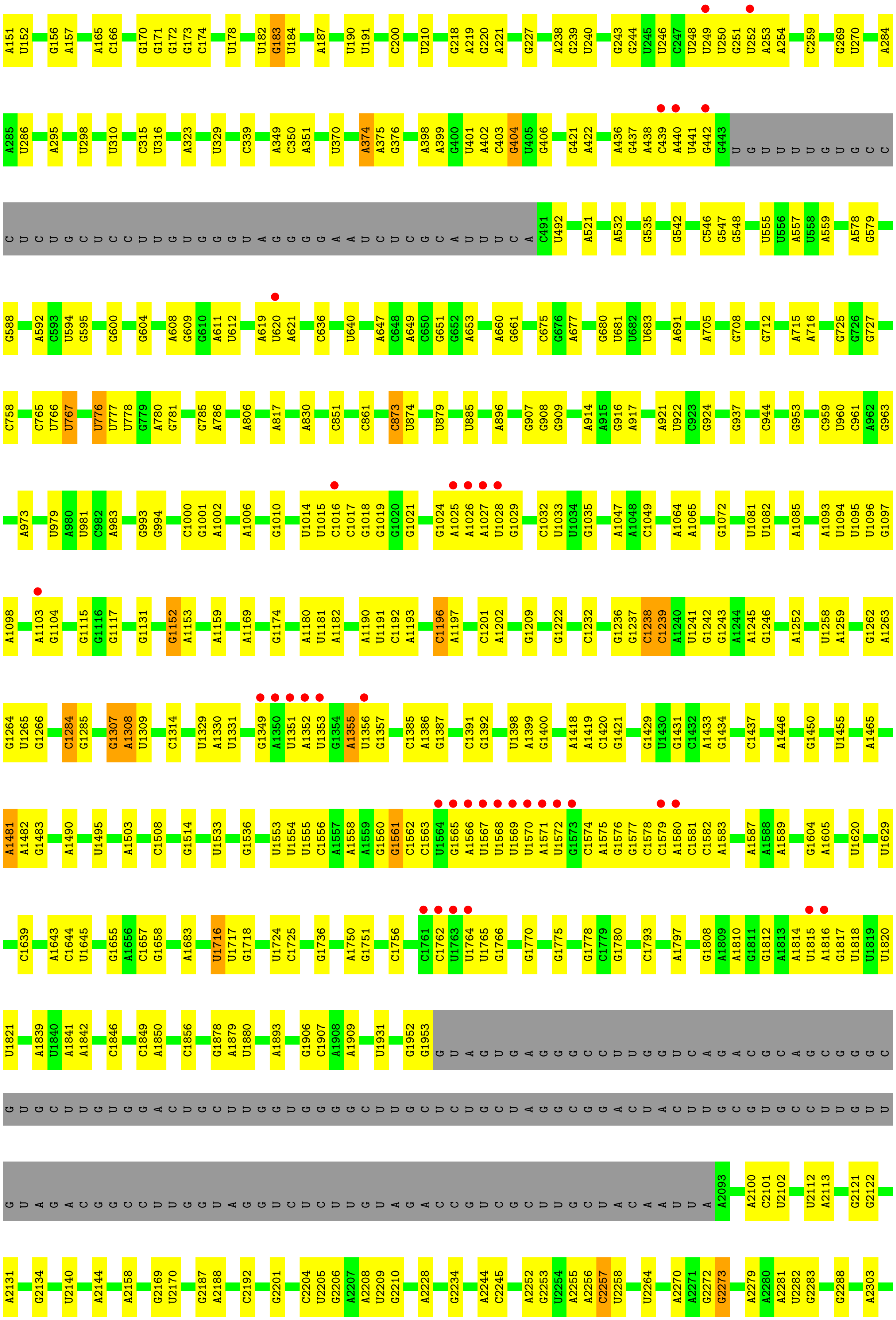
Chain 1:





• Molecule 36: 25S ribosomal RNA

Chain 5: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A285 U286 A295 U298 U310 C315 U316 A323 U329 C339 A349 C350 A351 U370 A374 A375 G376 A398 A399 G400 U401 A402 C403 G404 U405 G406 G421 A422 A436 G437 A438 C439 A440 U441 G442 G443 U G U U U U G U G C C
C U C U G C U C C U U G U G G G U A G G G G A A U C U C G C A U U U C A C491 U492 A521 A532 G535 G542 C546 G547 G548 U555 U556 A557 U558 A559 A578 G579
G588 A592 C593 U594 G595 G600 G604 A608 G609 G610 A611 U612 A619 U620 A621 C636 U640 A647 C648 A649 C650 G651 G652 A653 A660 G661 C675 G676 A677 G680 U681 U682 U683 A691 A705 G708 G712 A715 A716 G725 G726 G727
C758 C765 U766 U767 U776 U777 U778 G779 A780 G781 G785 A786 A806 A817 A830 C851 C861 C873 U874 U879 U885 A896 G907 G908 G909 A914 A915 G916 A917 A921 U922 C923 G924 G937 C944 G953 C959 U960 C961 A962 G963
A973 U979 A980 U981 C982 A983 G993 G994 C1000 G1001 A1002 A1006 G1010 U1014 U1015 C1016 C1017 G1018 G1019 G1020 G1021 G1024 A1025 A1026 A1027 U1028 G1029 C1032 U1033 U1034 G1035 A1047 A1048 C1049 A1064 A1065 G1072 U1081 U1082 A1085 A1093 U1094 U1095 U1096 G1097
A1098 A1103 G1104 G1115 G1116 G1117 G1131 G1152 A1153 A1159 A1169 G1174 A1180 U1181 A1182 A1190 U1191 C1192 A1193 C1196 A1197 C1201 A1202 G1209 G1222 C1232 G1236 G1237 C1238 C1239 A1240 U1241 G1242 G1243 A1244 A1245 G1246 A1252 U1258 A1259 G1262 A1263
G1264 U1265 G1266 C1284 G1285 G1307 A1308 U1309 C1314 U1329 A1330 U1331 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 C1385 A1386 G1387 C1391 G1392 U1398 A1399 G1400 A1418 A1419 C1420 G1421 G1429 U1430 G1431 C1432 A1433 G1434 C1437 A1446 G1450 U1455 A1465
A1481 A1482 G1483 A1490 U1495 A1503 C1508 G1514 U1533 G1536 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 G1604 A1605 U1620 U1629
C1639 A1643 C1644 U1645 G1655 A1656 C1657 G1658 A1683 U1716 U1717 G1718 U1724 C1725 G1736 A1750 G1751 C1756 C1761 C1762 U1763 U1764 U1765 G1766 G1770 G1775 G1778 C1779 G1780 C1793 A1797 G1808 A1809 A1810 G1811 G1812 A1813 A1814 U1815 A1816 G1817 U1818 U1819 U1820
U1821 A1839 U1840 A1841 A1842 C1846 C1849 A1850 C1856 G1878 A1879 U1880 A1893 G1906 C1907 A1908 A1909 U1931 G1952 G1953 G U A G U G A G G G C C U U G G G U C A G A C C G U G C A G C C G G G C
G U G C U U G U G G A C U G C U U G G U G G G G C U U G C U C U G G C U A G G C G G A C U A C U U G G C G U G C C U U G U U
G U A G A C G G C C U U G G U A G G U C U C U U G U A G A C C G U C G C U U G C U A C A A U U A A2093 A2100 C2101 U2102 U2112 A2113 G2121 G2122
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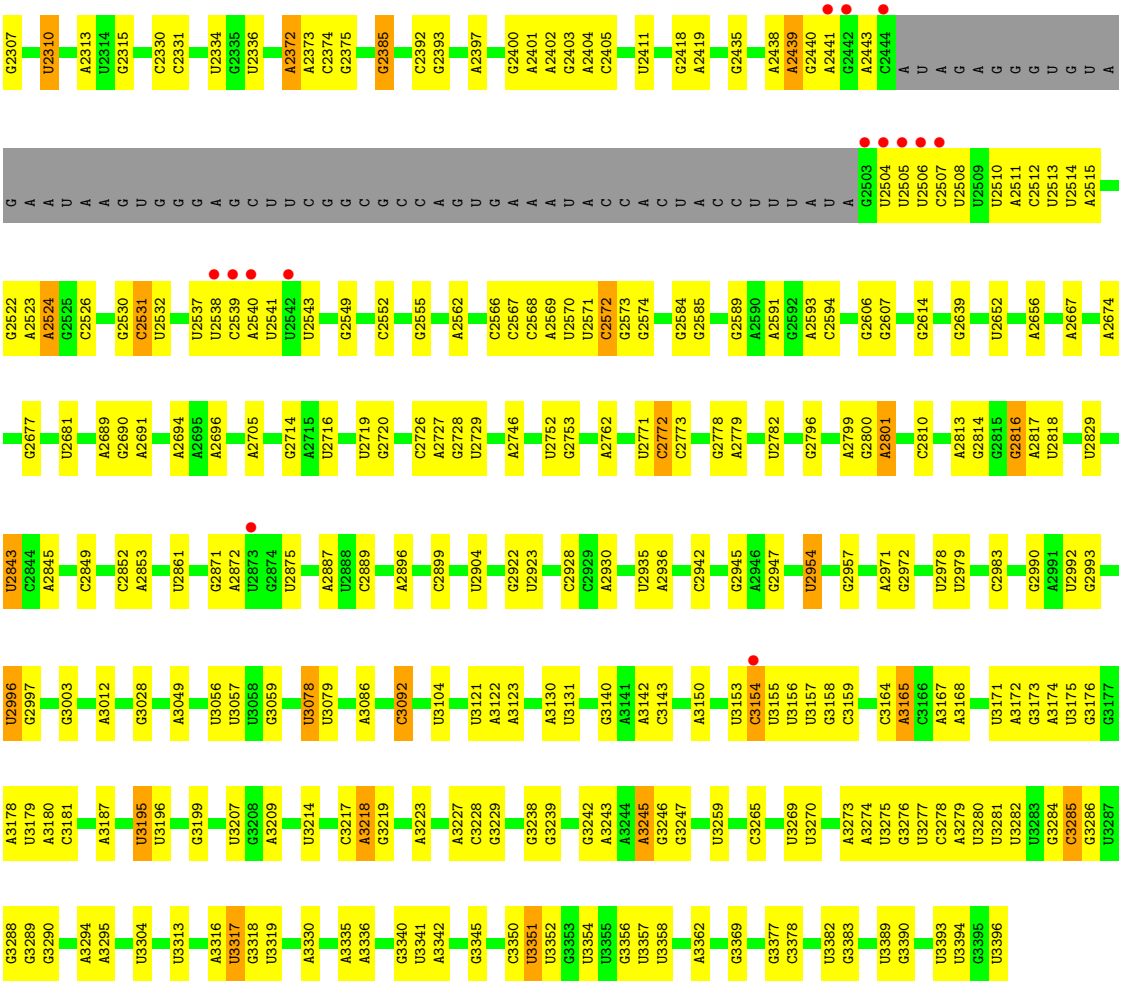
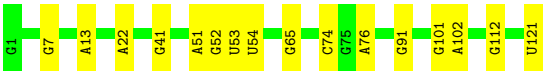


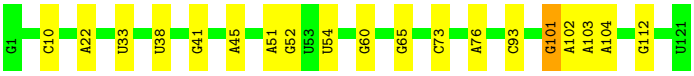
• Molecule 37: 5S ribosomal RNA

Chain 3:



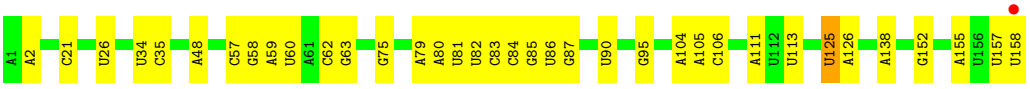
• Molecule 37: 5S ribosomal RNA

Chain 7:



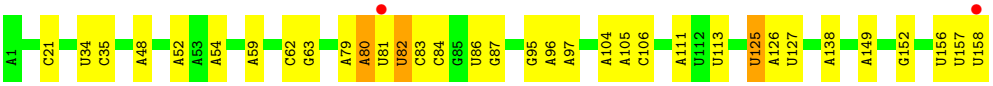
• Molecule 38: 5.8S ribosomal RNA

Chain 4:



• Molecule 38: 5.8S ribosomal RNA

Chain 8:

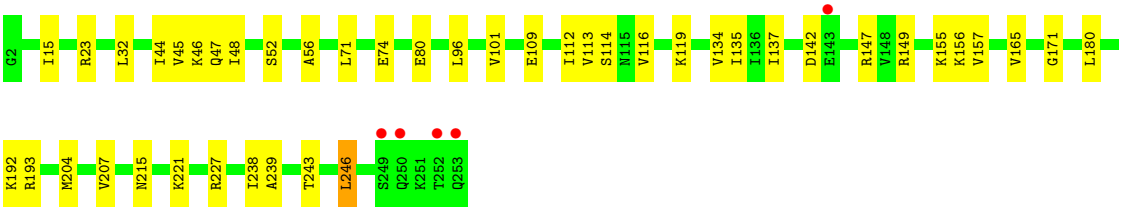


• Molecule 39: 60S ribosomal protein L2-A

Chain L2:

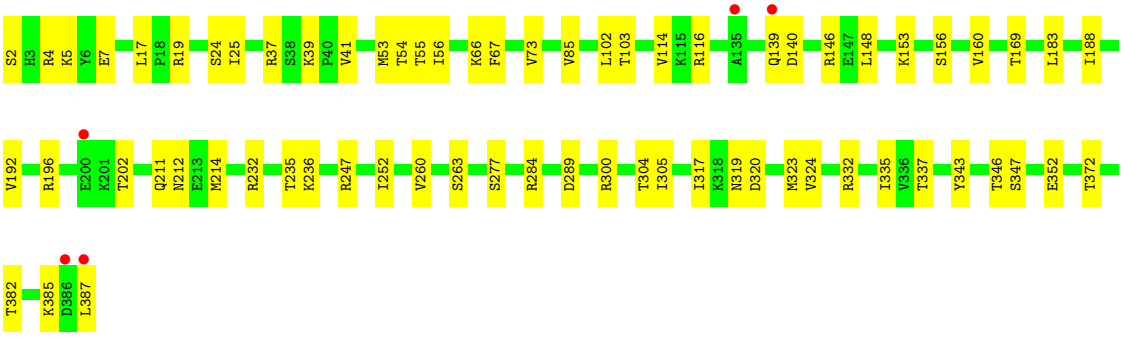
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:



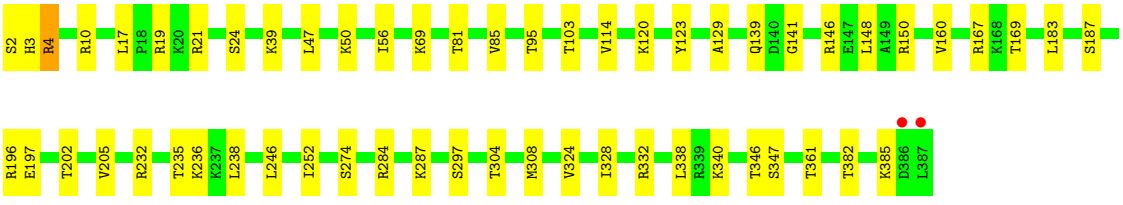
• Molecule 40: 60S ribosomal protein L3

Chain L3:



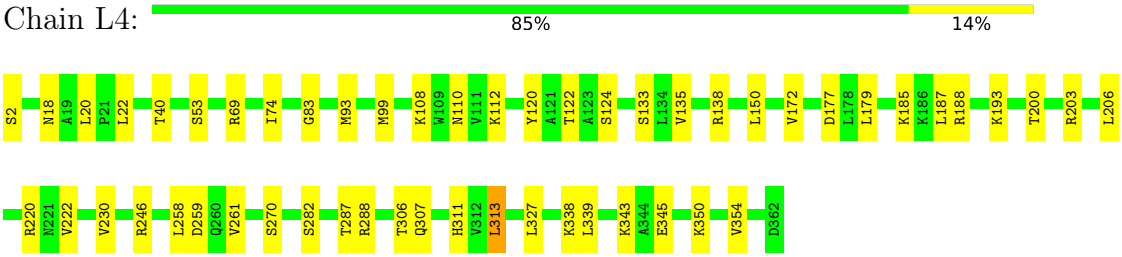
• Molecule 40: 60S ribosomal protein L3

Chain l3:



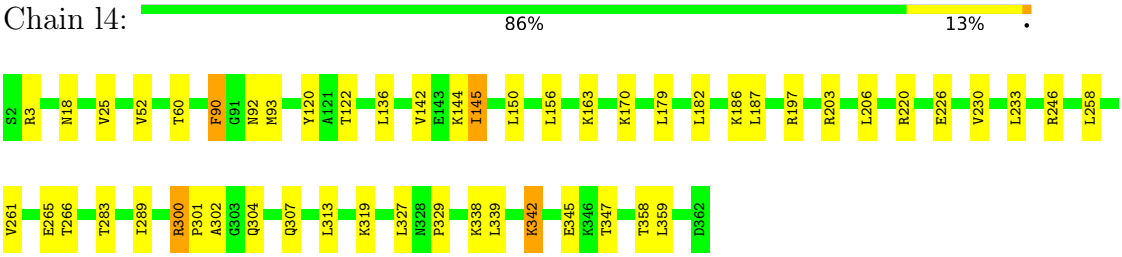
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



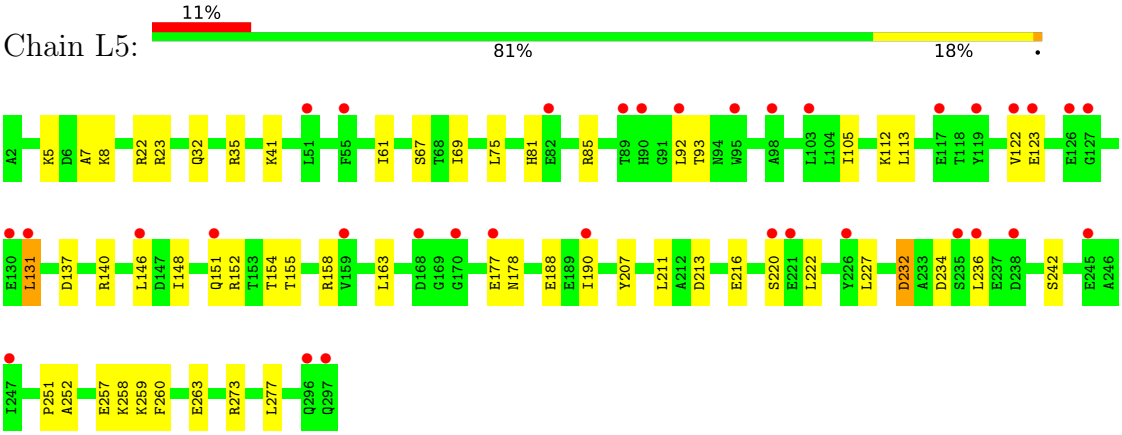
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:



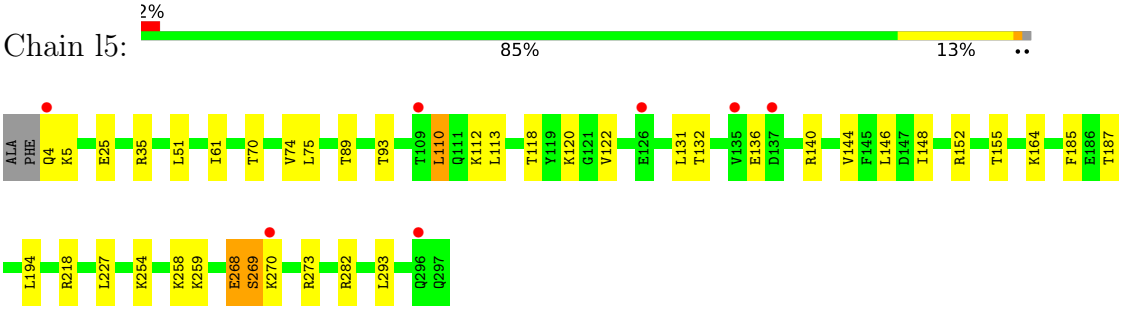
• Molecule 42: 60S ribosomal protein L5

Chain L5:



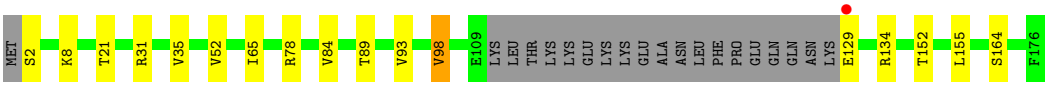
• Molecule 42: 60S ribosomal protein L5

Chain l5:



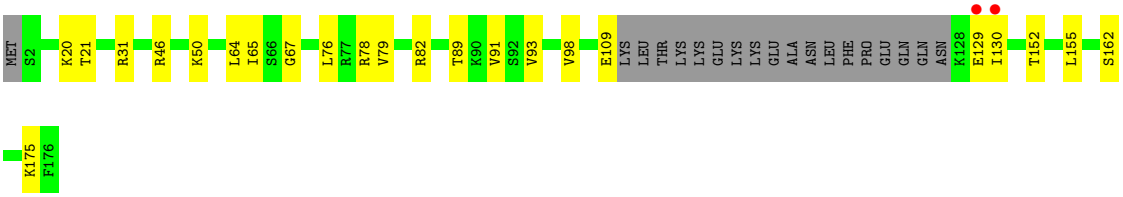
• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



• Molecule 43: 60S ribosomal protein L6-A

Chain l6:



• Molecule 44: 60S ribosomal protein L7-A

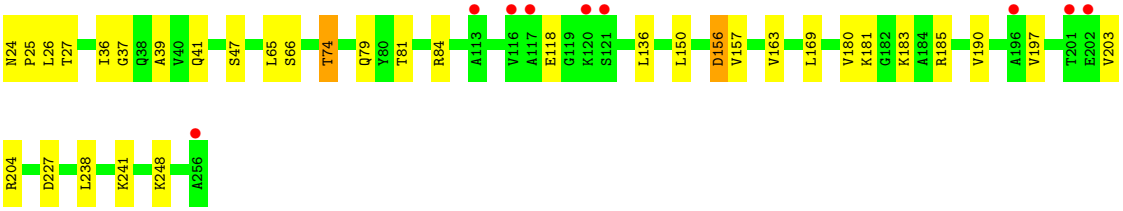
Chain L7:

• Molecule 44: 60S ribosomal protein L7-A

Chain l7:

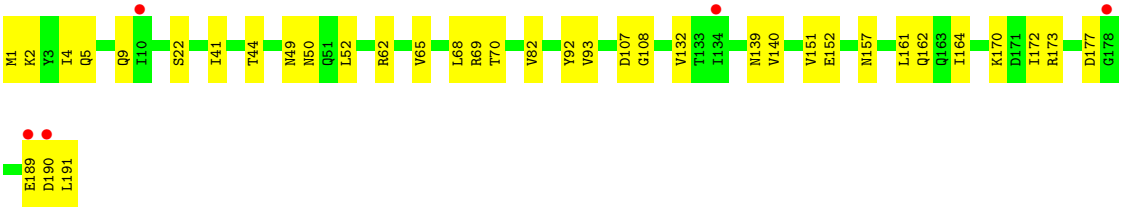
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



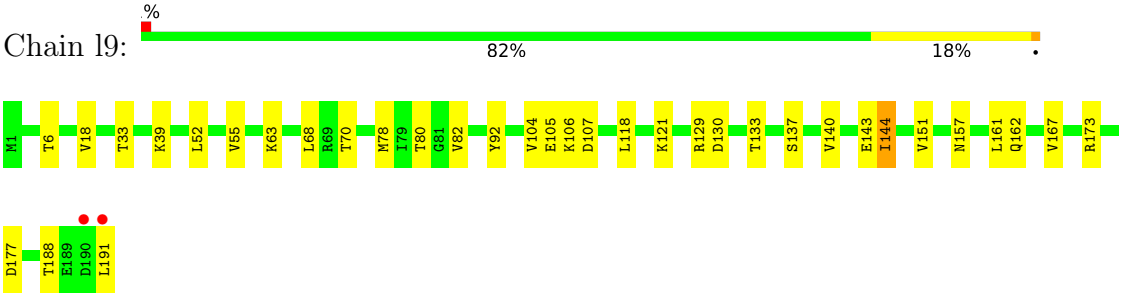
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



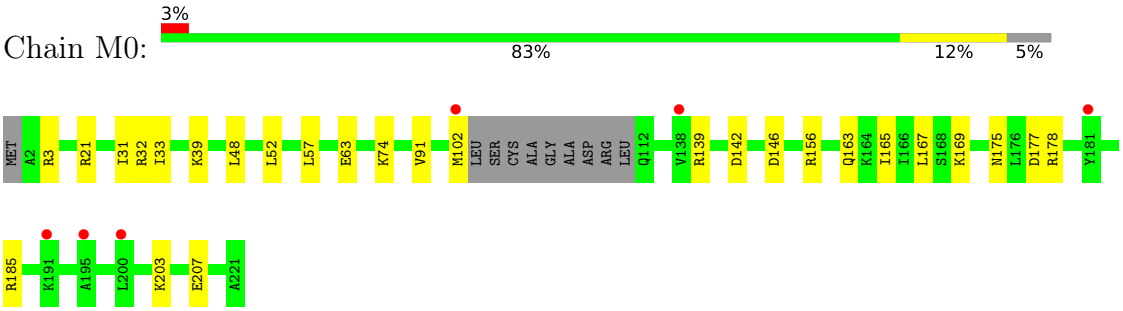
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



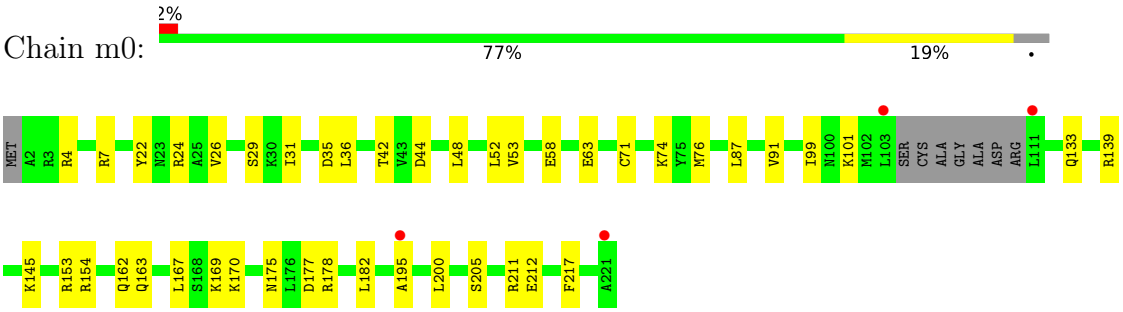
• Molecule 47: 60S ribosomal protein L10

Chain M0:



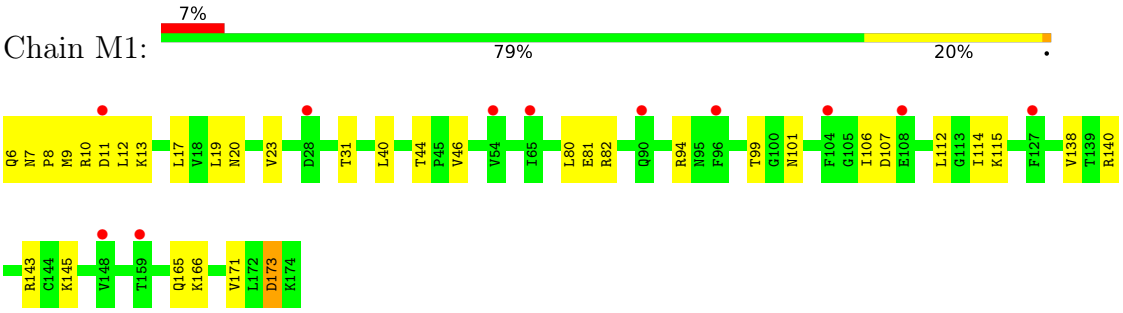
• Molecule 47: 60S ribosomal protein L10

Chain m0:



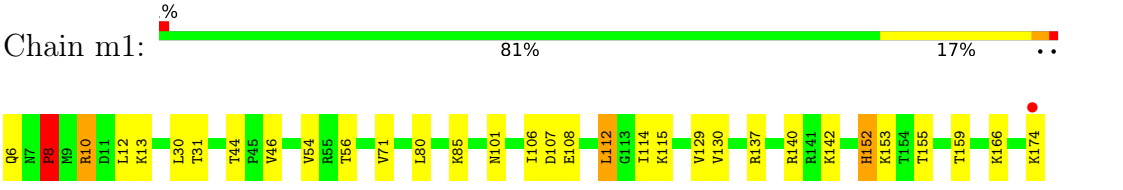
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



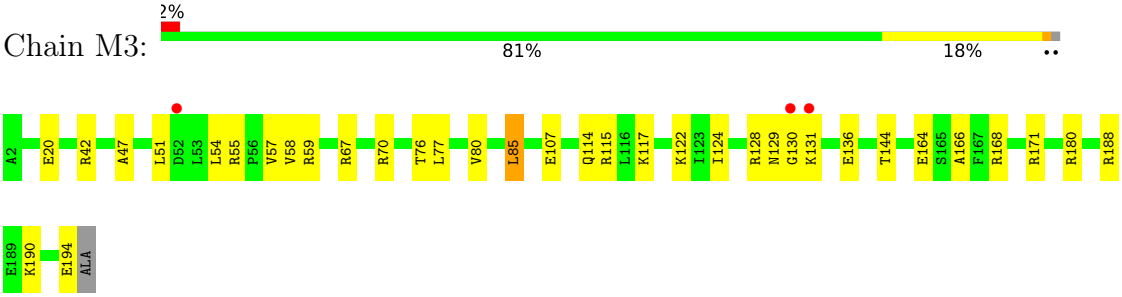
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



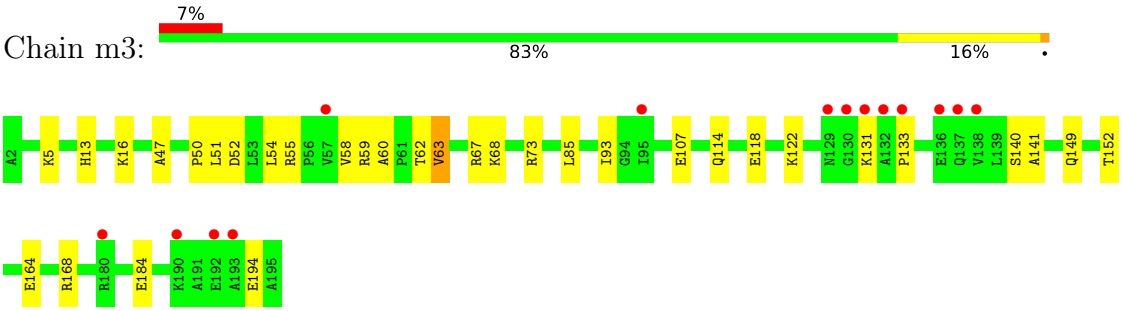
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



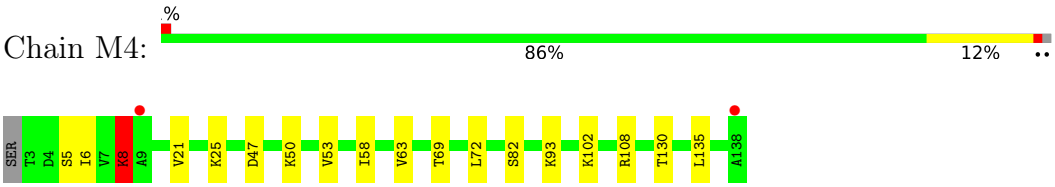
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



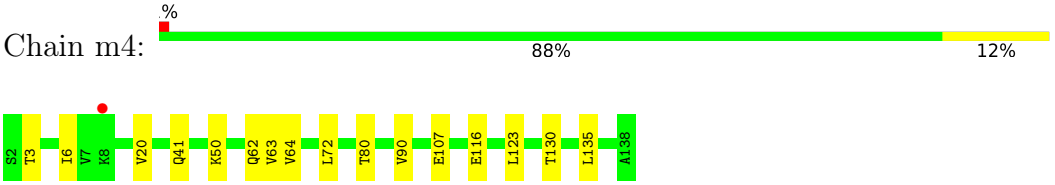
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



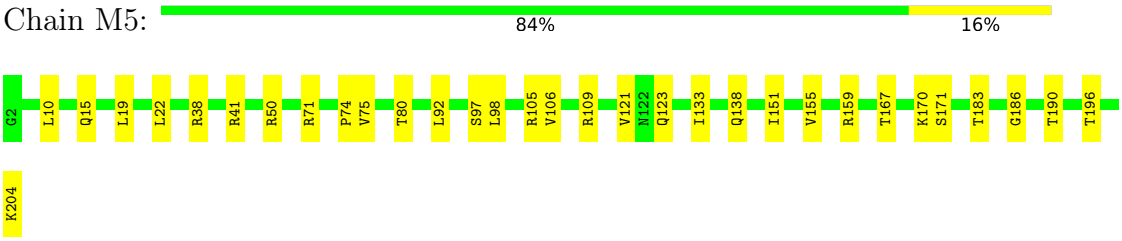
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



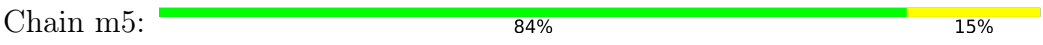
• Molecule 51: 60S ribosomal protein L15-A

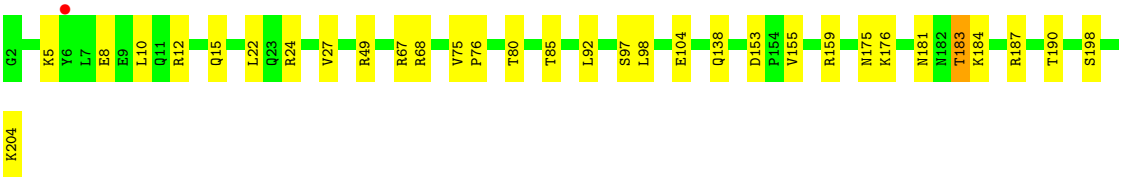
Chain M5:



• Molecule 51: 60S ribosomal protein L15-A

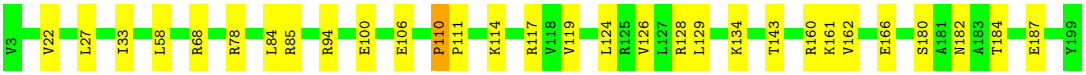
Chain m5:





• 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

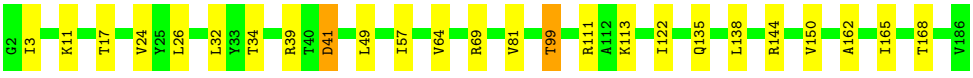
Chain M7:

• 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

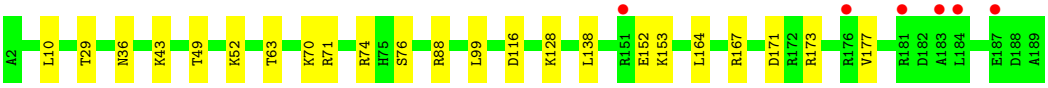
Chain m8:

• Molecule 55: 60S ribosomal protein L19-A

Chain M9:

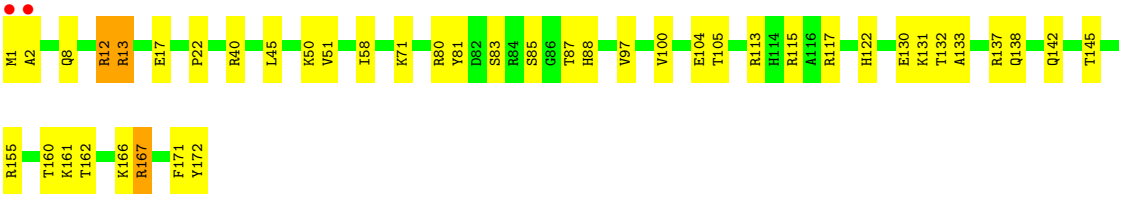
• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



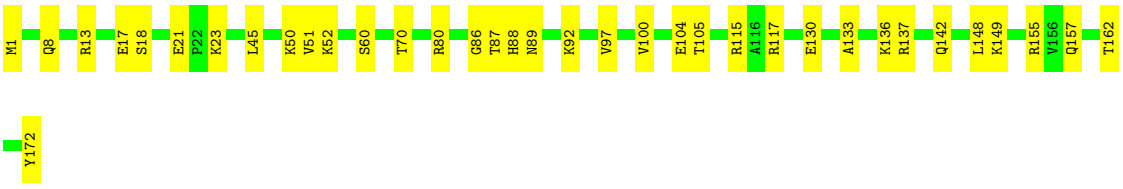
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



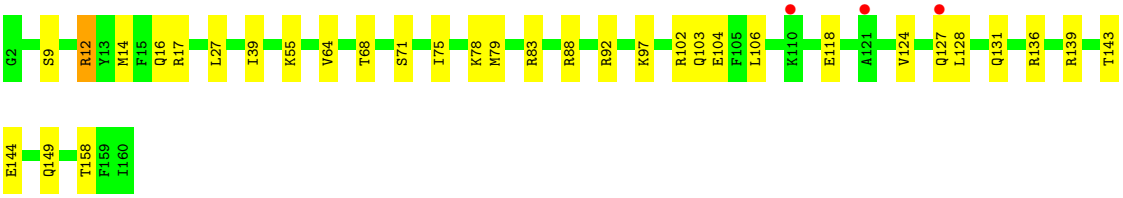
• Molecule 56: 60S ribosomal protein L20-A

Chain n0:



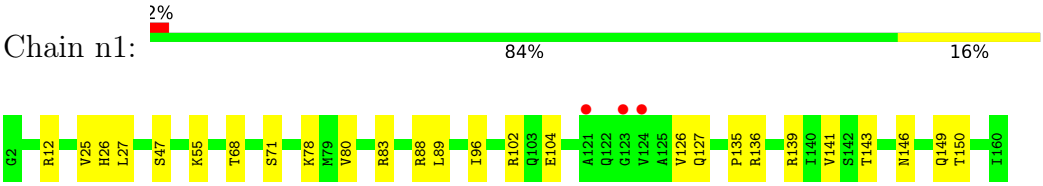
• Molecule 57: 60S ribosomal protein L21-A

Chain N1:



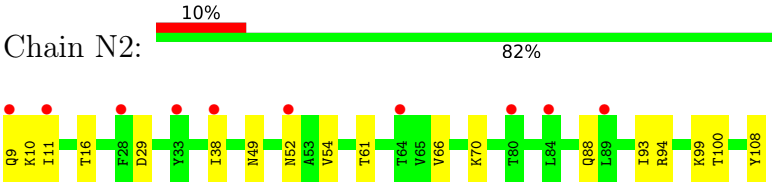
• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



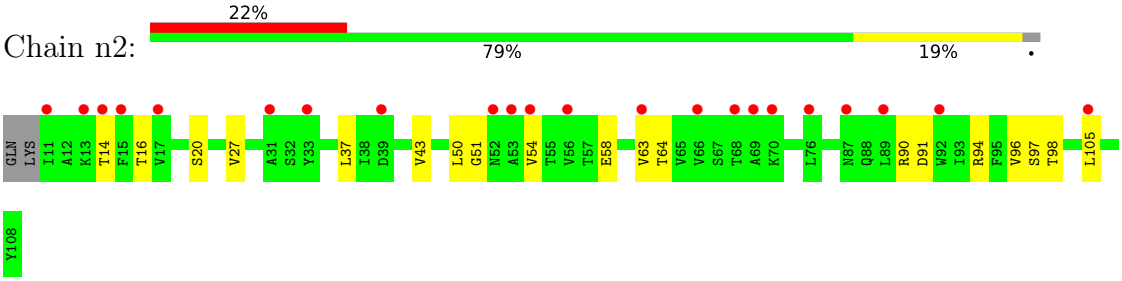
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



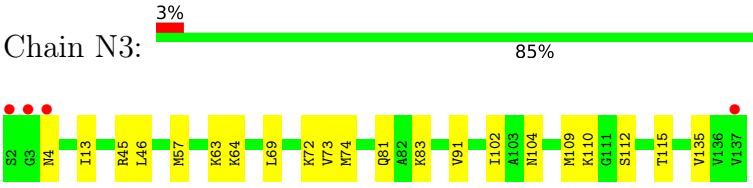
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



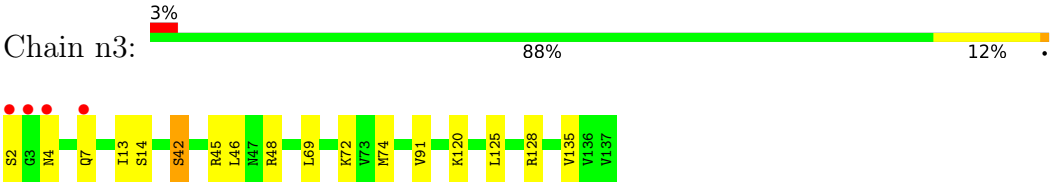
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



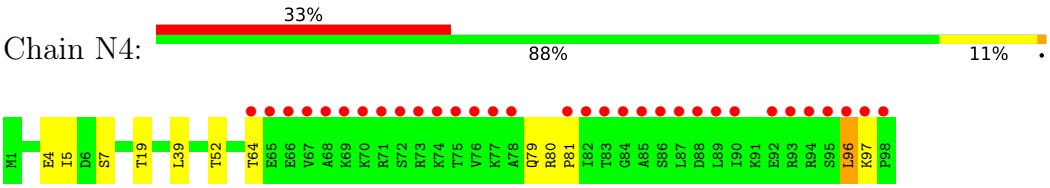
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



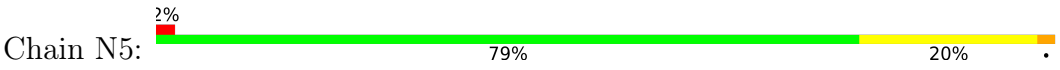
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



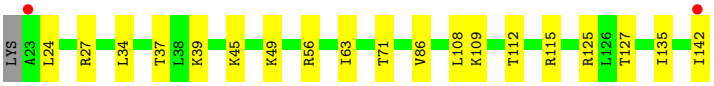
• Molecule 61: 60S ribosomal protein L25

Chain N5:



• Molecule 61: 60S ribosomal protein L25

Chain n5:

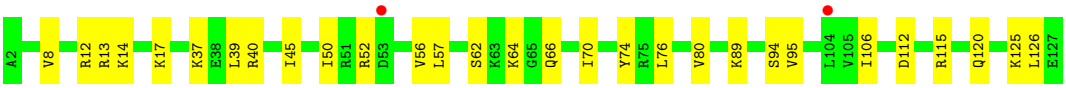


• Molecule 62: 60S ribosomal protein L26-A

Chain N6:

• Molecule 62: 60S ribosomal protein L26-A

Chain n6:

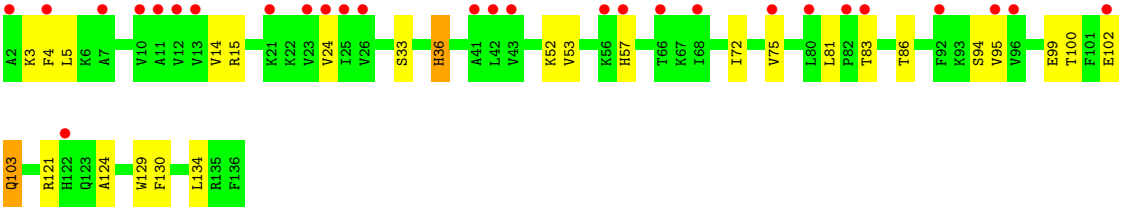


• Molecule 63: 60S ribosomal protein L27-A

Chain N7:

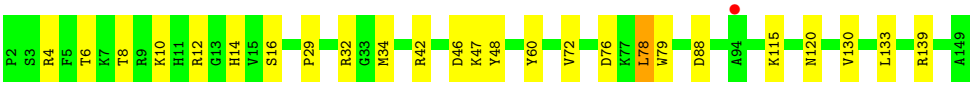
• Molecule 63: 60S ribosomal protein L27-A

Chain n7:

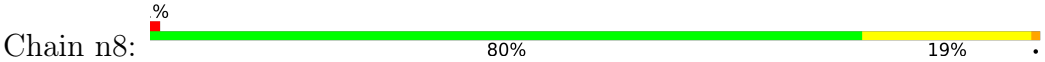


• Molecule 64: 60S ribosomal protein L28

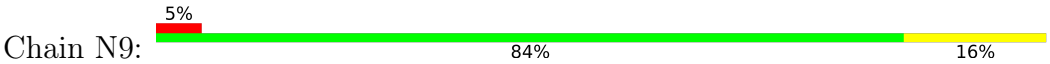
Chain N8:

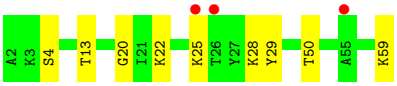


• Molecule 64: 60S ribosomal protein L28

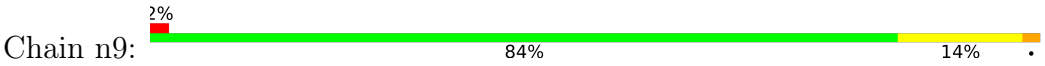


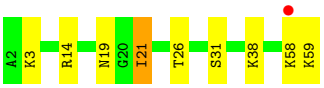
• Molecule 65: 60S ribosomal protein L29



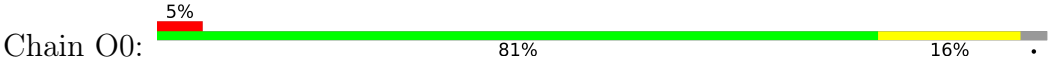


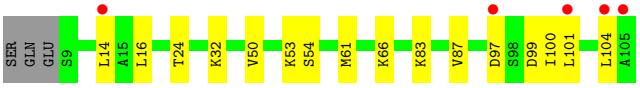
• Molecule 65: 60S ribosomal protein L29



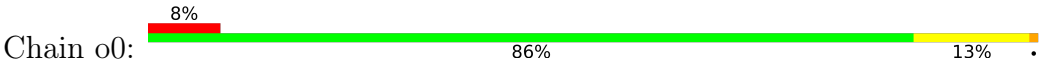


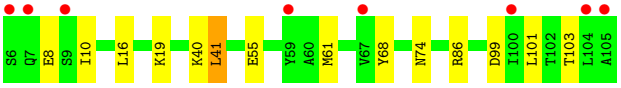
• Molecule 66: 60S ribosomal protein L30



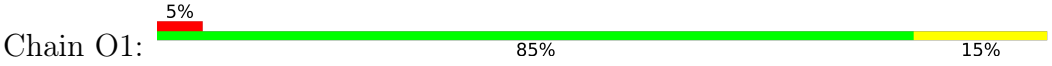


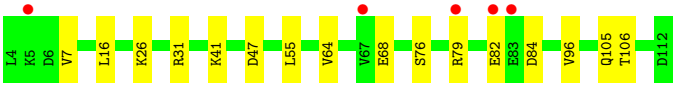
• Molecule 66: 60S ribosomal protein L30





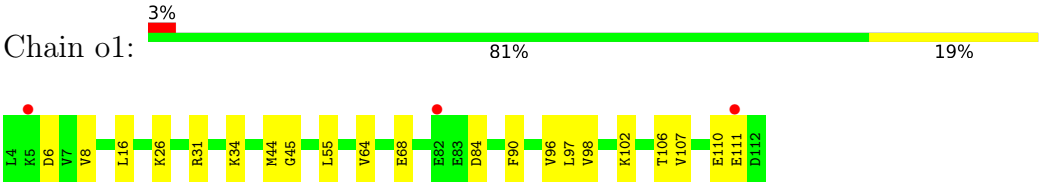
• Molecule 67: 60S ribosomal protein L31-A





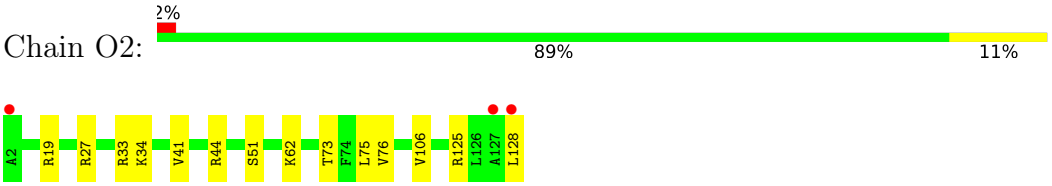
• Molecule 67: 60S ribosomal protein L31-A

Chain o1:



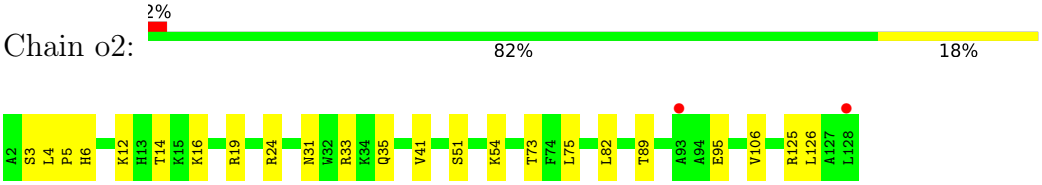
• Molecule 68: 60S ribosomal protein L32

Chain O2:



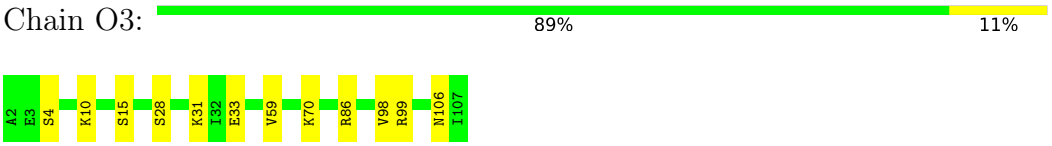
• Molecule 68: 60S ribosomal protein L32

Chain o2:



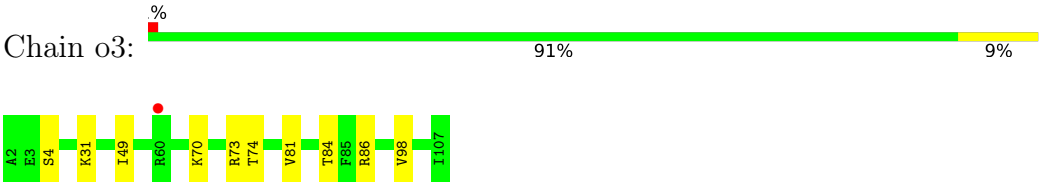
• Molecule 69: 60S ribosomal protein L33-A

Chain O3:



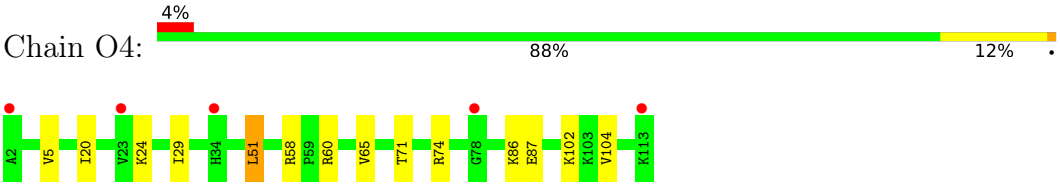
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



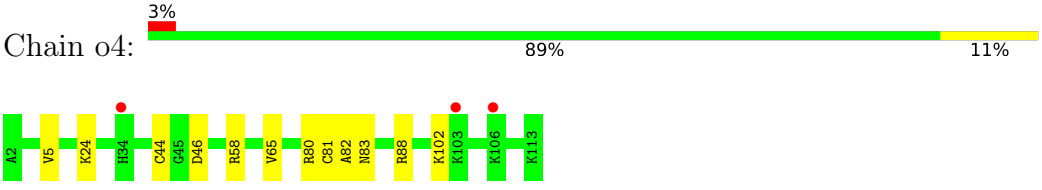
• Molecule 70: 60S ribosomal protein L34-A

Chain O4:



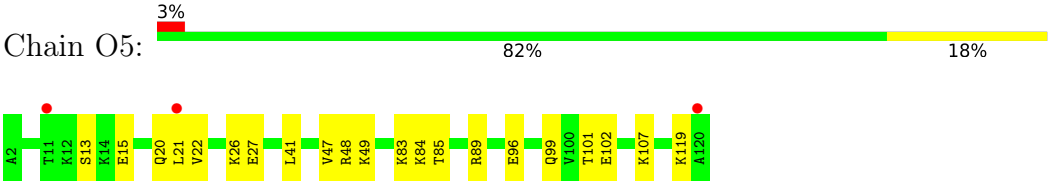
• Molecule 70: 60S ribosomal protein L34-A

Chain o4:



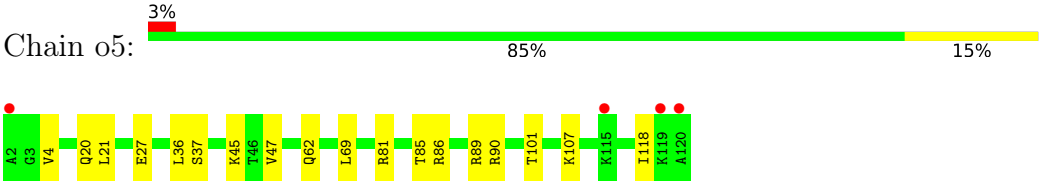
• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



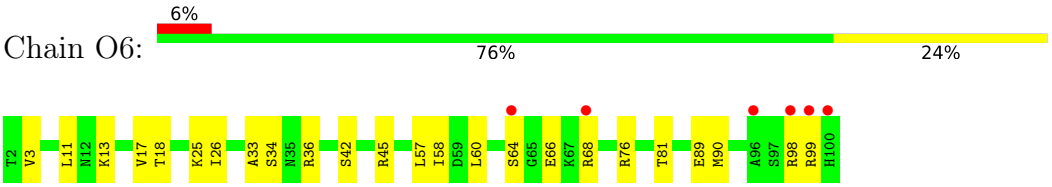
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



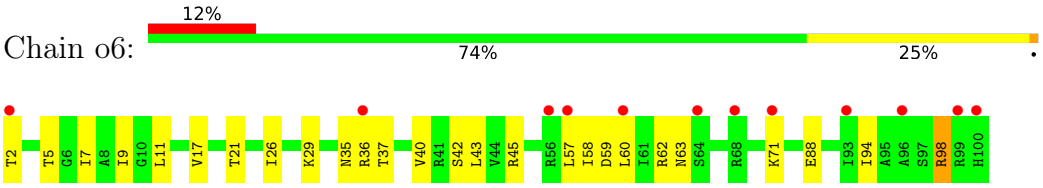
• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



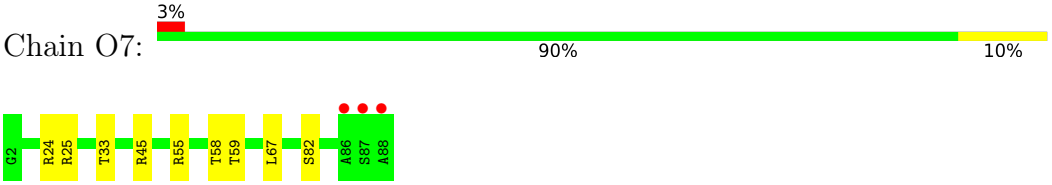
• Molecule 72: 60S ribosomal protein L36-A

Chain o6:



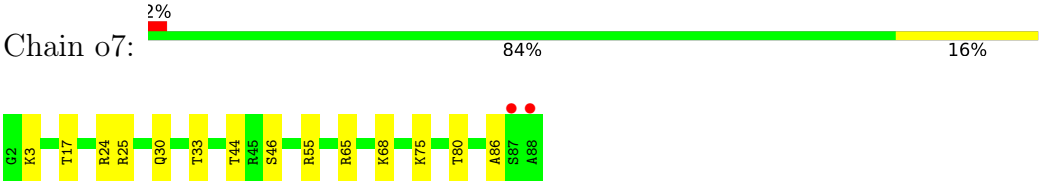
• Molecule 73: 60S ribosomal protein L37-A

Chain O7:



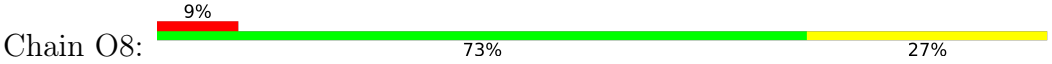
• Molecule 73: 60S ribosomal protein L37-A

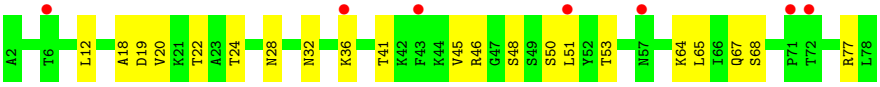
Chain o7:



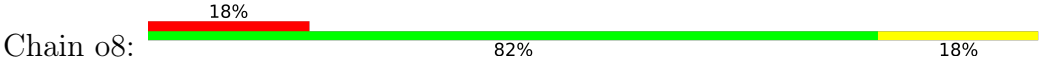
• Molecule 74: 60S ribosomal protein L38

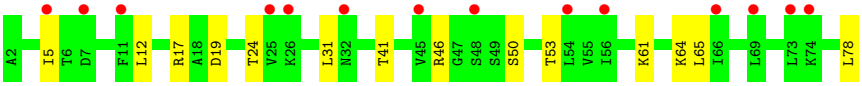
Chain O8:



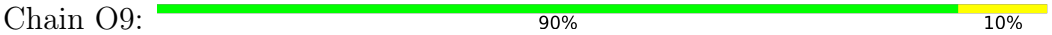


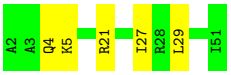
• Molecule 74: 60S ribosomal protein L38



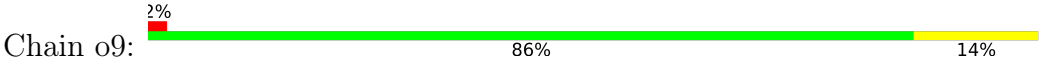


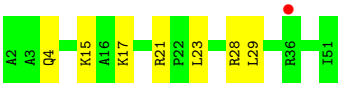
• Molecule 75: 60S ribosomal protein L39



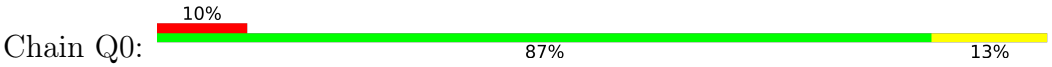


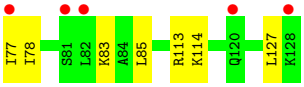
• Molecule 75: 60S ribosomal protein L39



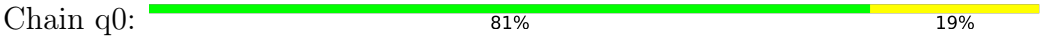


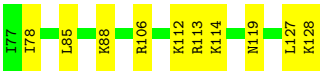
• Molecule 76: Ubiquitin-60S ribosomal protein L40



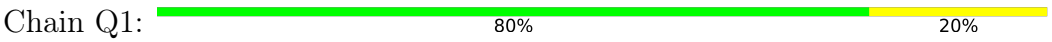


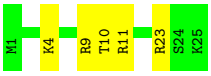
• Molecule 76: Ubiquitin-60S ribosomal protein L40





• Molecule 77: 60S ribosomal protein L41-A



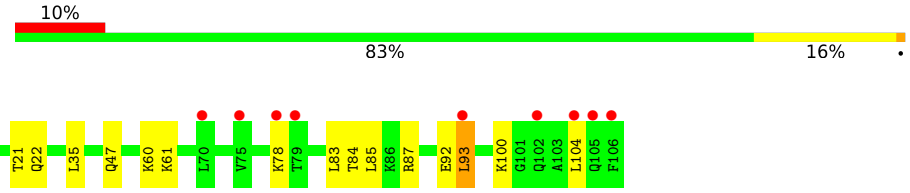


• Molecule 77: 60S ribosomal protein L41-A

Chain q1:

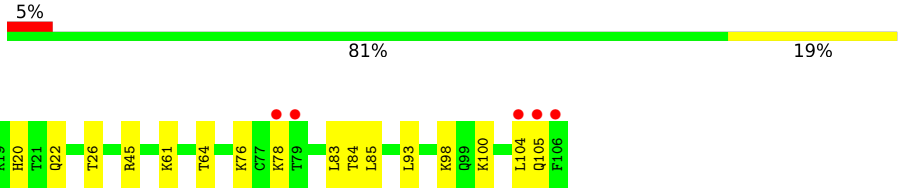
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



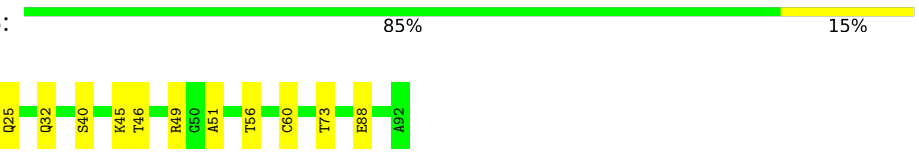
• Molecule 78: 60S ribosomal protein L42-A

Chain q2:



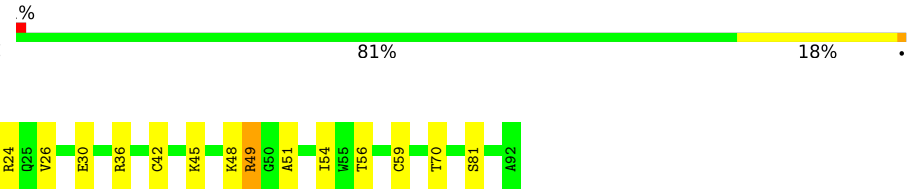
• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



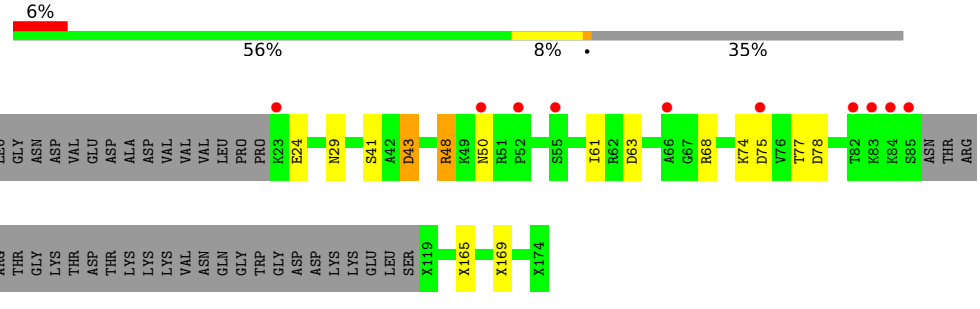
• Molecule 79: 60S ribosomal protein L43-A

Chain q3:



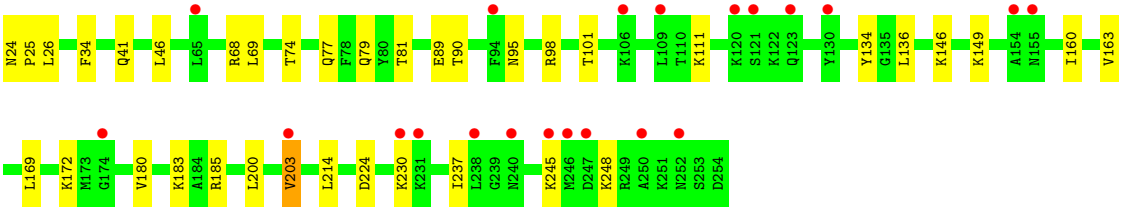
• Molecule 80: Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1

Chain sM:



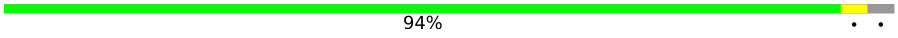
• Molecule 81: 60S ribosomal protein L8-A

Chain l8:



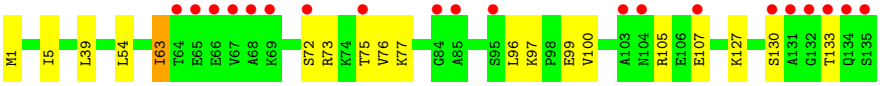
• Molecule 82: 60S ribosomal protein L12

Chain m2:



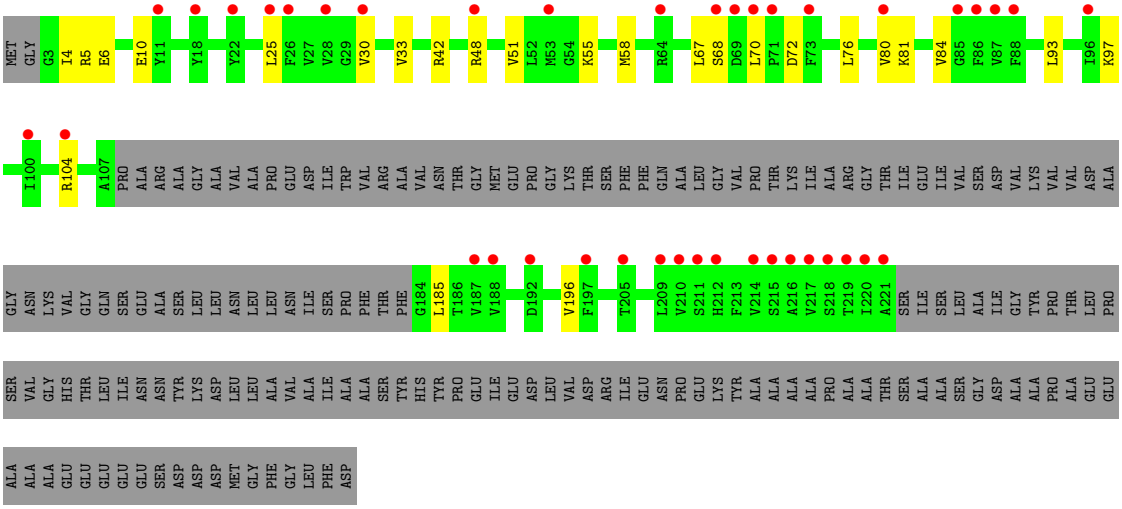
• Molecule 83: 60S ribosomal protein L24-A

Chain n4:



• Molecule 84: 60S acidic ribosomal protein P0

Chain p0:



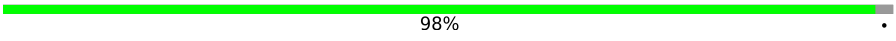
• Molecule 85: Ribosomal protein P1 alpha, P2 beta

Chain p1:

There are no outlier residues recorded for this chain.

• Molecule 85: Ribosomal protein P1 alpha, P2 beta

Chain p2:




X1
X46
UNK

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	434.23Å 287.91Å 304.12Å 90.00° 99.11° 90.00°	Depositor
Resolution (Å)	103.62 – 3.10 103.62 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (103.62-3.10) 91.8 (103.62-3.10)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.94 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.251 0.213 , 0.252	Depositor DCC
R_{free} test set	26600 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	410475	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: ZN, MG, UAM, OHX

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	0.37	0/42442	0.93	91/66130 (0.1%)
1	6	0.42	1/42765 (0.0%)	0.93	69/66634 (0.1%)
2	S0	0.33	0/1617	0.59	0/2215
2	s0	0.33	0/1623	0.60	1/2222 (0.0%)
3	S1	0.30	0/1735	0.61	0/2335
3	s1	0.32	1/1748 (0.1%)	0.61	0/2352
4	S2	0.32	0/1665	0.59	0/2263
4	s2	0.33	0/1665	0.62	0/2263
5	S3	0.31	0/1759	0.56	0/2368
5	s3	0.31	0/1759	0.57	0/2368
6	S4	0.32	0/2109	0.63	2/2839 (0.1%)
6	s4	0.34	0/2109	0.66	3/2839 (0.1%)
7	S5	0.28	0/1629	0.56	0/2202
7	s5	0.30	0/1629	0.57	0/2202
8	S6	0.31	0/1823	0.53	0/2439
8	s6	0.34	0/1779	0.58	0/2379
9	S7	0.32	0/1506	0.66	1/2028 (0.0%)
9	s7	0.31	0/1516	0.63	1/2043 (0.0%)
10	S8	0.33	0/1514	0.60	1/2021 (0.0%)
10	s8	0.35	0/1514	0.59	1/2021 (0.0%)
11	S9	0.31	0/1519	0.57	1/2035 (0.0%)
11	s9	0.33	0/1519	0.60	0/2035
12	C0	0.30	0/789	0.67	1/1067 (0.1%)
12	c0	0.30	0/776	0.70	3/1047 (0.3%)
13	C1	0.35	0/1239	0.60	0/1673
13	c1	0.39	1/1194 (0.1%)	0.61	1/1610 (0.1%)
14	C2	0.31	0/898	0.69	1/1220 (0.1%)
14	c2	0.28	0/898	0.67	1/1220 (0.1%)
15	C3	0.33	0/1215	0.55	1/1638 (0.1%)
15	c3	0.31	0/1215	0.60	1/1638 (0.1%)
16	C4	0.30	0/901	0.62	0/1217
16	c4	0.32	0/960	0.57	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.33	0/998	0.60	0/1341
17	c5	0.31	0/1060	0.65	1/1426 (0.1%)
18	C6	0.30	0/1125	0.66	2/1510 (0.1%)
18	c6	0.31	0/1131	0.57	1/1518 (0.1%)
19	C7	0.36	0/935	0.72	2/1254 (0.2%)
19	c7	0.31	0/914	0.60	0/1224
20	C8	0.30	0/1211	0.58	0/1628
20	c8	0.31	0/1211	0.59	1/1628 (0.1%)
21	C9	0.30	0/1130	0.52	0/1517
21	c9	0.35	0/1130	0.55	0/1517
22	D0	0.32	0/865	0.60	0/1169
22	d0	0.32	0/892	0.60	0/1205
23	D1	0.31	0/693	0.58	0/935
23	d1	0.31	0/693	0.58	0/935
24	D2	0.32	0/1038	0.62	3/1395 (0.2%)
24	d2	0.35	0/1038	0.61	1/1395 (0.1%)
25	D3	0.37	0/1139	0.61	0/1518
25	d3	0.38	0/1139	0.60	0/1518
26	D4	0.32	0/1087	0.57	0/1449
26	d4	0.34	0/1087	0.64	1/1449 (0.1%)
27	D5	0.31	0/571	0.62	0/768
27	d5	0.31	0/566	0.51	0/761
28	D6	0.32	0/782	0.67	1/1047 (0.1%)
28	d6	0.34	0/782	0.58	0/1047
29	D7	0.28	0/620	0.61	0/838
29	d7	0.30	0/620	0.63	0/838
30	D8	0.27	0/499	0.54	0/670
30	d8	0.31	0/499	0.59	0/670
31	D9	0.40	0/452	0.68	1/600 (0.2%)
31	d9	0.32	0/452	0.57	0/600
32	E0	0.30	0/483	0.55	0/643
32	e0	0.35	0/499	0.66	0/665
33	E1	0.33	0/577	0.87	1/770 (0.1%)
33	e1	0.35	0/619	0.91	3/822 (0.4%)
34	SR	0.29	0/2490	0.55	0/3389
34	sR	0.28	0/2491	0.56	0/3391
35	SM	0.32	0/984	0.60	0/1323
36	1	0.53	0/75394	0.99	140/117545 (0.1%)
36	5	0.54	1/75414 (0.0%)	0.99	107/117575 (0.1%)
37	3	0.41	0/2883	0.86	1/4491 (0.0%)
37	7	0.52	0/2883	0.96	2/4491 (0.0%)
38	4	0.52	0/3746	0.97	3/5832 (0.1%)
38	8	0.44	0/3746	0.90	5/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	L2	0.38	0/1948	0.63	0/2617
39	l2	0.37	0/1946	0.65	1/2614 (0.0%)
40	L3	0.38	0/3146	0.63	0/4228
40	l3	0.43	0/3146	0.65	1/4228 (0.0%)
41	L4	0.41	0/2800	0.66	3/3790 (0.1%)
41	l4	0.38	0/2800	0.65	1/3790 (0.0%)
42	L5	0.34	0/2425	0.60	1/3271 (0.0%)
42	l5	0.39	0/2408	0.59	1/3248 (0.0%)
43	L6	0.37	0/1260	0.58	0/1694
43	l6	0.40	0/1269	0.62	1/1705 (0.1%)
44	L7	0.38	0/1821	0.58	0/2451
44	l7	0.41	0/1828	0.62	2/2461 (0.1%)
45	L8	0.33	0/1836	0.54	0/2481
46	L9	0.33	0/1539	0.56	0/2073
46	l9	0.39	0/1539	0.58	0/2073
47	M0	0.38	0/1741	0.60	1/2335 (0.0%)
47	m0	0.42	0/1758	0.65	0/2358
48	M1	0.32	0/1374	0.56	0/1842
48	m1	0.36	0/1374	0.67	3/1842 (0.2%)
49	M3	0.39	0/1568	0.65	1/2106 (0.0%)
49	m3	0.36	0/1573	0.62	0/2113
50	M4	0.36	0/1068	0.55	0/1438
50	m4	0.40	0/1074	0.56	0/1446
51	M5	0.38	0/1757	0.60	0/2354
51	m5	0.35	0/1757	0.59	0/2354
52	M6	0.42	0/1585	0.57	0/2128
52	m6	0.52	0/1585	0.61	0/2128
53	M7	0.39	0/1443	0.63	0/1944
53	m7	0.43	0/1250	0.61	0/1683
54	M8	0.39	0/1465	0.63	1/1965 (0.1%)
54	m8	0.38	0/1465	0.61	0/1965
55	M9	0.31	0/1538	0.51	1/2050 (0.0%)
55	m9	0.34	0/1538	0.47	0/2050
56	N0	0.37	0/1481	0.62	0/1990
56	n0	0.42	0/1481	0.58	0/1990
57	N1	0.39	0/1300	0.60	0/1743
57	n1	0.43	0/1300	0.59	0/1743
58	N2	0.33	0/812	0.59	0/1099
58	n2	0.32	0/794	0.56	0/1076
59	N3	0.38	0/1018	0.60	0/1369
59	n3	0.43	0/1018	0.65	0/1369
60	N4	0.34	0/712	0.62	2/958 (0.2%)
61	N5	0.35	0/979	0.62	2/1321 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
61	n5	0.34	0/974	0.58	0/1314
62	N6	0.38	0/1004	0.65	1/1341 (0.1%)
62	n6	0.36	0/1004	0.63	0/1341
63	N7	0.33	0/1118	0.54	0/1497
63	n7	0.40	1/1118 (0.1%)	0.53	0/1497
64	N8	0.41	0/1204	0.67	1/1612 (0.1%)
64	n8	0.40	0/1204	0.71	1/1612 (0.1%)
65	N9	0.38	0/473	0.57	0/629
65	n9	0.39	0/473	0.64	0/629
66	O0	0.31	0/751	0.52	0/1008
66	o0	0.30	0/775	0.54	1/1040 (0.1%)
67	O1	0.36	0/890	0.55	0/1196
67	o1	0.40	0/897	0.63	0/1205
68	O2	0.46	1/1041 (0.1%)	0.60	0/1394
68	o2	0.42	0/1041	0.65	0/1394
69	O3	0.43	0/868	0.60	0/1168
69	o3	0.46	0/868	0.67	0/1168
70	O4	0.33	0/890	0.59	1/1189 (0.1%)
70	o4	0.33	0/890	0.58	0/1189
71	O5	0.37	0/978	0.60	1/1301 (0.1%)
71	o5	0.33	0/974	0.51	0/1297
72	O6	0.34	0/778	0.57	0/1034
72	o6	0.34	0/777	0.58	0/1033
73	O7	0.41	0/696	0.70	0/923
73	o7	0.38	0/696	0.67	0/923
74	O8	0.33	0/618	0.55	0/826
74	o8	0.31	0/614	0.56	0/822
75	O9	0.41	0/443	0.65	0/588
75	o9	0.38	0/443	0.57	0/588
76	Q0	0.38	0/423	0.62	0/562
76	q0	0.47	0/423	0.66	0/562
77	Q1	0.33	0/234	0.54	0/300
77	q1	0.39	0/234	0.58	0/300
78	Q2	0.39	0/860	0.64	1/1136 (0.1%)
78	q2	0.38	0/860	0.58	0/1136
79	Q3	0.39	0/701	0.62	0/934
79	q3	0.40	0/701	0.63	0/934
80	sM	0.34	0/480	0.64	0/642
81	l8	0.33	0/1795	0.55	0/2429
83	n4	0.37	0/1052	0.63	1/1398 (0.1%)
84	p0	0.33	0/1092	0.55	0/1474
All	All	0.44	6/430471 (0.0%)	0.84	486/632040 (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
2	s0	0	3
3	S1	0	1
3	s1	0	1
4	S2	0	1
4	s2	0	2
5	S3	0	1
5	s3	0	1
6	S4	0	1
7	S5	0	3
7	s5	0	4
9	S7	0	2
9	s7	0	3
10	S8	0	2
10	s8	0	1
11	s9	0	1
14	c2	0	1
15	c3	0	1
16	C4	0	3
16	c4	0	2
17	C5	0	2
17	c5	0	3
18	C6	0	2
18	c6	0	2
19	C7	0	1
19	c7	0	3
20	c8	0	1
22	D0	0	1
22	d0	0	1
23	d1	0	1
24	D2	0	1
24	d2	0	1
25	D3	0	1
25	d3	0	1
26	D4	0	1
26	d4	0	1
27	D5	0	2
27	d5	0	2
28	D6	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	e0	0	1
33	E1	0	3
33	e1	0	3
34	sR	0	1
39	l2	0	1
40	l3	0	2
41	L4	0	1
41	l4	0	1
42	L5	0	3
42	l5	0	3
43	l6	0	1
44	l7	0	1
45	L8	0	2
46	L9	0	1
48	m1	0	1
49	M3	0	1
49	m3	0	1
50	M4	0	1
50	m4	0	1
51	M5	0	1
51	m5	0	1
52	M6	0	1
52	m6	0	1
53	m7	0	1
56	N0	0	3
56	n0	0	2
57	N1	0	1
58	n2	0	1
60	N4	0	2
63	n7	0	2
64	n8	0	1
65	N9	0	1
65	n9	0	1
66	o0	0	1
67	o1	0	1
70	o4	0	1
71	o5	0	1
79	Q3	0	1
79	q3	0	1
80	sM	0	2
81	l8	0	1
82	m2	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	126

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-8.63	1.31	1.38
63	n7	36	HIS	C-N	7.01	1.47	1.34
68	O2	51	SER	C-N	-6.35	1.19	1.34
1	6	163	G	N9-C4	-5.93	1.33	1.38
13	c1	128	CYS	CB-SG	-5.29	1.73	1.81

The worst 5 of 486 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	N3-C4-N9	-16.34	116.20	126.00
36	5	1152	G	N3-C4-C5	15.93	136.56	128.60
1	6	163	G	N3-C4-N9	-11.53	119.08	126.00
36	1	1308	A	C8-N9-C4	-11.40	101.24	105.80
36	5	2726	C	C6-N1-C2	-10.77	115.99	120.30

There are no chirality outliers.

5 of 126 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S0	94	GLY	Peptide
3	S1	131	ASP	Peptide
4	S2	106	ASP	Peptide
5	S3	219	ALA	Peptide
6	S4	57	ASN	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	S0	204/206 (99%)	173 (85%)	27 (13%)	4 (2%)	7 31
2	s0	204/206 (99%)	175 (86%)	21 (10%)	8 (4%)	3 18
3	S1	212/216 (98%)	167 (79%)	40 (19%)	5 (2%)	6 27
3	s1	214/216 (99%)	182 (85%)	29 (14%)	3 (1%)	11 40
4	S2	215/217 (99%)	200 (93%)	11 (5%)	4 (2%)	8 33
4	s2	215/217 (99%)	195 (91%)	17 (8%)	3 (1%)	11 40
5	S3	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	8 34
5	s3	221/223 (99%)	185 (84%)	31 (14%)	5 (2%)	6 28
6	S4	258/260 (99%)	232 (90%)	24 (9%)	2 (1%)	19 54
6	s4	258/260 (99%)	230 (89%)	25 (10%)	3 (1%)	13 44
7	S5	204/206 (99%)	181 (89%)	15 (7%)	8 (4%)	3 18
7	s5	204/206 (99%)	182 (89%)	19 (9%)	3 (2%)	10 39
8	S6	224/226 (99%)	207 (92%)	14 (6%)	3 (1%)	12 42
8	s6	216/226 (96%)	198 (92%)	14 (6%)	4 (2%)	8 33
9	S7	182/186 (98%)	148 (81%)	20 (11%)	14 (8%)	1 5
9	s7	184/186 (99%)	154 (84%)	27 (15%)	3 (2%)	9 37
10	S8	184/200 (92%)	161 (88%)	21 (11%)	2 (1%)	14 46
10	s8	184/200 (92%)	170 (92%)	11 (6%)	3 (2%)	9 37
11	S9	183/185 (99%)	163 (89%)	16 (9%)	4 (2%)	6 29
11	s9	183/185 (99%)	164 (90%)	18 (10%)	1 (0%)	29 64
12	C0	94/98 (96%)	75 (80%)	17 (18%)	2 (2%)	7 30
12	c0	92/98 (94%)	67 (73%)	14 (15%)	11 (12%)	0 1
13	C1	153/156 (98%)	131 (86%)	20 (13%)	2 (1%)	12 42
13	c1	144/156 (92%)	124 (86%)	15 (10%)	5 (4%)	3 20
14	C2	122/124 (98%)	89 (73%)	27 (22%)	6 (5%)	2 14
14	c2	122/124 (98%)	85 (70%)	33 (27%)	4 (3%)	4 21
15	C3	148/150 (99%)	138 (93%)	9 (6%)	1 (1%)	22 57
15	c3	148/150 (99%)	130 (88%)	15 (10%)	3 (2%)	7 31
16	C4	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	9 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	c4	126/128 (98%)	111 (88%)	14 (11%)	1 (1%)	19 54
17	C5	122/142 (86%)	102 (84%)	14 (12%)	6 (5%)	2 14
17	c5	133/142 (94%)	109 (82%)	17 (13%)	7 (5%)	2 12
18	C6	139/142 (98%)	124 (89%)	13 (9%)	2 (1%)	11 40
18	c6	140/142 (99%)	131 (94%)	9 (6%)	0	100 100
19	C7	116/136 (85%)	100 (86%)	11 (10%)	5 (4%)	2 16
19	c7	113/136 (83%)	99 (88%)	11 (10%)	3 (3%)	5 25
20	C8	143/145 (99%)	120 (84%)	18 (13%)	5 (4%)	3 20
20	c8	143/145 (99%)	121 (85%)	17 (12%)	5 (4%)	3 20
21	C9	141/143 (99%)	127 (90%)	14 (10%)	0	100 100
21	c9	141/143 (99%)	125 (89%)	14 (10%)	2 (1%)	11 40
22	D0	105/110 (96%)	91 (87%)	13 (12%)	1 (1%)	15 49
22	d0	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	2 15
23	D1	85/87 (98%)	71 (84%)	13 (15%)	1 (1%)	13 44
23	d1	85/87 (98%)	75 (88%)	9 (11%)	1 (1%)	13 44
24	D2	127/129 (98%)	118 (93%)	6 (5%)	3 (2%)	6 27
24	d2	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19 54
25	D3	142/144 (99%)	118 (83%)	19 (13%)	5 (4%)	3 20
25	d3	142/144 (99%)	131 (92%)	11 (8%)	0	100 100
26	D4	132/134 (98%)	117 (89%)	9 (7%)	6 (4%)	2 15
26	d4	132/134 (98%)	111 (84%)	18 (14%)	3 (2%)	6 28
27	D5	68/70 (97%)	51 (75%)	14 (21%)	3 (4%)	2 15
27	d5	67/70 (96%)	58 (87%)	8 (12%)	1 (2%)	10 39
28	D6	95/97 (98%)	70 (74%)	19 (20%)	6 (6%)	1 8
28	d6	95/97 (98%)	76 (80%)	12 (13%)	7 (7%)	1 6
29	D7	79/81 (98%)	69 (87%)	8 (10%)	2 (2%)	5 27
29	d7	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	12 42
30	D8	61/63 (97%)	54 (88%)	7 (12%)	0	100 100
30	d8	61/63 (97%)	49 (80%)	12 (20%)	0	100 100
31	D9	51/53 (96%)	47 (92%)	4 (8%)	0	100 100
31	d9	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	7 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	E0	58/62 (94%)	49 (84%)	7 (12%)	2 (3%)	3 21
32	e0	60/62 (97%)	51 (85%)	7 (12%)	2 (3%)	4 21
33	E1	69/76 (91%)	45 (65%)	18 (26%)	6 (9%)	1 4
33	e1	74/76 (97%)	49 (66%)	18 (24%)	7 (10%)	0 3
34	SR	316/318 (99%)	288 (91%)	28 (9%)	0	100 100
34	sR	316/318 (99%)	286 (90%)	26 (8%)	4 (1%)	12 42
35	SM	131/176 (74%)	108 (82%)	17 (13%)	6 (5%)	2 15
39	L2	250/252 (99%)	234 (94%)	15 (6%)	1 (0%)	34 69
39	l2	250/252 (99%)	225 (90%)	22 (9%)	3 (1%)	13 44
40	L3	384/386 (100%)	356 (93%)	24 (6%)	4 (1%)	15 49
40	l3	384/386 (100%)	362 (94%)	20 (5%)	2 (0%)	29 64
41	L4	359/361 (99%)	327 (91%)	32 (9%)	0	100 100
41	l4	359/361 (99%)	327 (91%)	25 (7%)	7 (2%)	8 33
42	L5	294/296 (99%)	257 (87%)	33 (11%)	4 (1%)	11 40
42	l5	292/296 (99%)	275 (94%)	17 (6%)	0	100 100
43	L6	152/176 (86%)	145 (95%)	6 (4%)	1 (1%)	22 57
43	l6	153/176 (87%)	139 (91%)	12 (8%)	2 (1%)	12 42
44	L7	220/223 (99%)	208 (94%)	11 (5%)	1 (0%)	29 64
44	l7	221/223 (99%)	208 (94%)	11 (5%)	2 (1%)	17 52
45	L8	231/233 (99%)	203 (88%)	22 (10%)	6 (3%)	5 26
46	L9	189/191 (99%)	171 (90%)	17 (9%)	1 (0%)	29 64
46	l9	189/191 (99%)	175 (93%)	12 (6%)	2 (1%)	14 46
47	M0	207/221 (94%)	188 (91%)	19 (9%)	0	100 100
47	m0	209/221 (95%)	188 (90%)	18 (9%)	3 (1%)	11 40
48	M1	167/169 (99%)	141 (84%)	20 (12%)	6 (4%)	3 20
48	m1	167/169 (99%)	143 (86%)	18 (11%)	6 (4%)	3 20
49	M3	191/194 (98%)	171 (90%)	14 (7%)	6 (3%)	4 23
49	m3	192/194 (99%)	166 (86%)	17 (9%)	9 (5%)	2 14
50	M4	134/137 (98%)	125 (93%)	7 (5%)	2 (2%)	10 39
50	m4	135/137 (98%)	132 (98%)	3 (2%)	0	100 100
51	M5	201/203 (99%)	191 (95%)	8 (4%)	2 (1%)	15 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	m5	201/203 (99%)	186 (92%)	12 (6%)	3 (2%)	10 39
52	M6	195/197 (99%)	189 (97%)	4 (2%)	2 (1%)	15 49
52	m6	195/197 (99%)	184 (94%)	11 (6%)	0	100 100
53	M7	181/183 (99%)	169 (93%)	12 (7%)	0	100 100
53	m7	153/183 (84%)	146 (95%)	7 (5%)	0	100 100
54	M8	183/185 (99%)	169 (92%)	12 (7%)	2 (1%)	14 46
54	m8	183/185 (99%)	169 (92%)	13 (7%)	1 (0%)	29 64
55	M9	186/188 (99%)	175 (94%)	9 (5%)	2 (1%)	14 46
55	m9	186/188 (99%)	173 (93%)	13 (7%)	0	100 100
56	N0	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	8 34
56	n0	170/172 (99%)	163 (96%)	7 (4%)	0	100 100
57	N1	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	12 42
57	n1	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12 42
58	N2	98/100 (98%)	85 (87%)	12 (12%)	1 (1%)	15 49
58	n2	96/100 (96%)	91 (95%)	4 (4%)	1 (1%)	15 49
59	N3	134/136 (98%)	128 (96%)	6 (4%)	0	100 100
59	n3	134/136 (98%)	130 (97%)	3 (2%)	1 (1%)	22 57
60	N4	96/98 (98%)	84 (88%)	10 (10%)	2 (2%)	7 30
61	N5	119/121 (98%)	113 (95%)	6 (5%)	0	100 100
61	n5	118/121 (98%)	104 (88%)	14 (12%)	0	100 100
62	N6	124/126 (98%)	115 (93%)	9 (7%)	0	100 100
62	n6	124/126 (98%)	119 (96%)	3 (2%)	2 (2%)	9 37
63	N7	133/135 (98%)	124 (93%)	6 (4%)	3 (2%)	6 28
63	n7	133/135 (98%)	115 (86%)	15 (11%)	3 (2%)	6 28
64	N8	146/148 (99%)	131 (90%)	12 (8%)	3 (2%)	7 30
64	n8	146/148 (99%)	131 (90%)	13 (9%)	2 (1%)	11 40
65	N9	56/58 (97%)	49 (88%)	7 (12%)	0	100 100
65	n9	56/58 (97%)	46 (82%)	9 (16%)	1 (2%)	8 34
66	O0	95/100 (95%)	93 (98%)	2 (2%)	0	100 100
66	o0	98/100 (98%)	89 (91%)	9 (9%)	0	100 100
67	O1	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	17 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
67	o1	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	17 52
68	O2	125/127 (98%)	121 (97%)	4 (3%)	0	100 100
68	o2	125/127 (98%)	116 (93%)	6 (5%)	3 (2%)	6 27
69	O3	104/106 (98%)	99 (95%)	5 (5%)	0	100 100
69	o3	104/106 (98%)	97 (93%)	7 (7%)	0	100 100
70	O4	110/112 (98%)	104 (94%)	6 (6%)	0	100 100
70	o4	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	17 52
71	O5	117/119 (98%)	108 (92%)	9 (8%)	0	100 100
71	o5	117/119 (98%)	106 (91%)	11 (9%)	0	100 100
72	O6	97/99 (98%)	79 (81%)	15 (16%)	3 (3%)	4 23
72	o6	97/99 (98%)	87 (90%)	8 (8%)	2 (2%)	7 30
73	O7	85/87 (98%)	78 (92%)	7 (8%)	0	100 100
73	o7	85/87 (98%)	78 (92%)	6 (7%)	1 (1%)	13 44
74	O8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	3 17
74	o8	75/77 (97%)	67 (89%)	7 (9%)	1 (1%)	12 42
75	O9	48/50 (96%)	46 (96%)	2 (4%)	0	100 100
75	o9	48/50 (96%)	44 (92%)	4 (8%)	0	100 100
76	Q0	50/52 (96%)	47 (94%)	3 (6%)	0	100 100
76	q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	7 31
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%)	89 (86%)	14 (14%)	0	100 100
78	q2	103/105 (98%)	96 (93%)	6 (6%)	1 (1%)	15 49
79	Q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	14 46
79	q3	89/91 (98%)	85 (96%)	3 (3%)	1 (1%)	14 46
80	sM	61/159 (38%)	50 (82%)	8 (13%)	3 (5%)	2 14
81	l8	229/231 (99%)	197 (86%)	28 (12%)	4 (2%)	9 36
83	n4	133/135 (98%)	111 (84%)	16 (12%)	6 (4%)	2 15
84	p0	139/312 (45%)	126 (91%)	12 (9%)	1 (1%)	22 57
All	All	22272/23122 (96%)	19937 (90%)	1963 (9%)	372 (2%)	9 36

5 of 372 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	S7	64	VAL
9	S7	111	LYS
9	S7	131	PHE
9	S7	133	THR
12	C0	87	VAL

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	164/173 (95%)	134 (82%)	30 (18%)	1 7
2	s0	165/173 (95%)	131 (79%)	34 (21%)	1 5
3	S1	191/192 (100%)	152 (80%)	39 (20%)	1 5
3	s1	192/192 (100%)	154 (80%)	38 (20%)	1 5
4	S2	176/176 (100%)	141 (80%)	35 (20%)	1 5
4	s2	176/176 (100%)	136 (77%)	40 (23%)	1 3
5	S3	182/182 (100%)	147 (81%)	35 (19%)	1 6
5	s3	182/182 (100%)	151 (83%)	31 (17%)	2 9
6	S4	221/221 (100%)	180 (81%)	41 (19%)	1 7
6	s4	221/221 (100%)	184 (83%)	37 (17%)	2 9
7	S5	173/173 (100%)	145 (84%)	28 (16%)	2 10
7	s5	173/173 (100%)	141 (82%)	32 (18%)	1 7
8	S6	188/193 (97%)	162 (86%)	26 (14%)	3 16
8	s6	187/193 (97%)	155 (83%)	32 (17%)	2 9
9	S7	165/166 (99%)	135 (82%)	30 (18%)	1 7
9	s7	165/166 (99%)	129 (78%)	36 (22%)	1 4
10	S8	150/161 (93%)	127 (85%)	23 (15%)	2 12
10	s8	150/161 (93%)	123 (82%)	27 (18%)	1 7
11	S9	158/158 (100%)	126 (80%)	32 (20%)	1 5
11	s9	158/158 (100%)	124 (78%)	34 (22%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	C0	77/91 (85%)	61 (79%)	16 (21%)	1 5
12	c0	73/91 (80%)	60 (82%)	13 (18%)	2 8
13	C1	129/137 (94%)	105 (81%)	24 (19%)	1 7
13	c1	129/137 (94%)	105 (81%)	24 (19%)	1 7
14	C2	88/100 (88%)	65 (74%)	23 (26%)	0 1
14	c2	88/100 (88%)	64 (73%)	24 (27%)	0 1
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1 6
15	c3	127/127 (100%)	101 (80%)	26 (20%)	1 5
16	C4	81/97 (84%)	65 (80%)	16 (20%)	1 5
16	c4	97/97 (100%)	75 (77%)	22 (23%)	1 3
17	C5	101/118 (86%)	87 (86%)	14 (14%)	3 15
17	c5	103/118 (87%)	86 (84%)	17 (16%)	2 10
18	C6	117/118 (99%)	89 (76%)	28 (24%)	0 2
18	c6	118/118 (100%)	97 (82%)	21 (18%)	2 8
19	C7	94/124 (76%)	72 (77%)	22 (23%)	1 3
19	c7	92/124 (74%)	75 (82%)	17 (18%)	1 7
20	C8	128/128 (100%)	104 (81%)	24 (19%)	1 6
20	c8	128/128 (100%)	106 (83%)	22 (17%)	2 9
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1 5
21	c9	115/115 (100%)	96 (84%)	19 (16%)	2 10
22	D0	100/103 (97%)	80 (80%)	20 (20%)	1 5
22	d0	103/103 (100%)	77 (75%)	26 (25%)	0 1
23	D1	74/74 (100%)	63 (85%)	11 (15%)	3 13
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1 4
24	D2	110/110 (100%)	89 (81%)	21 (19%)	1 6
24	d2	110/110 (100%)	96 (87%)	14 (13%)	4 18
25	D3	119/119 (100%)	95 (80%)	24 (20%)	1 5
25	d3	119/119 (100%)	99 (83%)	20 (17%)	2 9
26	D4	112/112 (100%)	91 (81%)	21 (19%)	1 6
26	d4	112/112 (100%)	98 (88%)	14 (12%)	4 18
27	D5	61/61 (100%)	47 (77%)	14 (23%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	d5	61/61 (100%)	53 (87%)	8 (13%)	4 17
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0 2
28	d6	83/83 (100%)	68 (82%)	15 (18%)	1 7
29	D7	70/70 (100%)	60 (86%)	10 (14%)	3 14
29	d7	70/70 (100%)	58 (83%)	12 (17%)	2 9
30	D8	56/56 (100%)	42 (75%)	14 (25%)	0 2
30	d8	56/56 (100%)	44 (79%)	12 (21%)	1 4
31	D9	47/47 (100%)	33 (70%)	14 (30%)	0 1
31	d9	47/47 (100%)	35 (74%)	12 (26%)	0 1
32	E0	51/53 (96%)	43 (84%)	8 (16%)	2 11
32	e0	53/53 (100%)	43 (81%)	10 (19%)	1 6
33	E1	62/66 (94%)	47 (76%)	15 (24%)	0 2
33	e1	66/66 (100%)	47 (71%)	19 (29%)	0 1
34	SR	259/261 (99%)	228 (88%)	31 (12%)	5 20
34	sR	259/261 (99%)	230 (89%)	29 (11%)	6 24
35	SM	97/122 (80%)	75 (77%)	22 (23%)	1 3
39	L2	193/194 (100%)	163 (84%)	30 (16%)	2 11
39	l2	192/194 (99%)	152 (79%)	40 (21%)	1 5
40	L3	320/322 (99%)	256 (80%)	64 (20%)	1 5
40	l3	319/322 (99%)	266 (83%)	53 (17%)	2 9
41	L4	288/288 (100%)	238 (83%)	50 (17%)	2 9
41	l4	288/288 (100%)	241 (84%)	47 (16%)	2 10
42	L5	244/244 (100%)	194 (80%)	50 (20%)	1 5
42	l5	243/244 (100%)	203 (84%)	40 (16%)	2 10
43	L6	134/153 (88%)	117 (87%)	17 (13%)	4 18
43	l6	135/153 (88%)	116 (86%)	19 (14%)	3 15
44	L7	186/187 (100%)	160 (86%)	26 (14%)	3 15
44	l7	187/187 (100%)	159 (85%)	28 (15%)	3 12
45	L8	187/191 (98%)	159 (85%)	28 (15%)	3 12
46	L9	171/171 (100%)	136 (80%)	35 (20%)	1 5
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	M0	177/187 (95%)	151 (85%)	26 (15%)	3 13
47	m0	179/187 (96%)	139 (78%)	40 (22%)	1 3
48	M1	147/147 (100%)	117 (80%)	30 (20%)	1 5
48	m1	147/147 (100%)	120 (82%)	27 (18%)	1 7
49	M3	154/154 (100%)	126 (82%)	28 (18%)	1 7
49	m3	154/154 (100%)	130 (84%)	24 (16%)	2 11
50	M4	107/108 (99%)	90 (84%)	17 (16%)	2 11
50	m4	108/108 (100%)	93 (86%)	15 (14%)	3 15
51	M5	175/175 (100%)	146 (83%)	29 (17%)	2 9
51	m5	175/175 (100%)	146 (83%)	29 (17%)	2 9
52	M6	160/160 (100%)	132 (82%)	28 (18%)	2 8
52	m6	160/160 (100%)	132 (82%)	28 (18%)	2 8
53	M7	140/145 (97%)	115 (82%)	25 (18%)	2 8
53	m7	125/145 (86%)	100 (80%)	25 (20%)	1 5
54	M8	150/150 (100%)	126 (84%)	24 (16%)	2 11
54	m8	150/150 (100%)	124 (83%)	26 (17%)	2 9
55	M9	153/153 (100%)	134 (88%)	19 (12%)	4 19
55	m9	153/153 (100%)	130 (85%)	23 (15%)	3 12
56	N0	156/156 (100%)	116 (74%)	40 (26%)	0 1
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1 4
57	N1	136/136 (100%)	105 (77%)	31 (23%)	1 3
57	n1	136/136 (100%)	112 (82%)	24 (18%)	2 8
58	N2	87/87 (100%)	70 (80%)	17 (20%)	1 6
58	n2	85/87 (98%)	68 (80%)	17 (20%)	1 5
59	N3	104/104 (100%)	83 (80%)	21 (20%)	1 5
59	n3	104/104 (100%)	87 (84%)	17 (16%)	2 10
60	N4	57/86 (66%)	50 (88%)	7 (12%)	4 19
61	N5	104/105 (99%)	78 (75%)	26 (25%)	0 2
61	n5	104/105 (99%)	85 (82%)	19 (18%)	1 7
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1 5
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
63	N7	115/115 (100%)	95 (83%)	20 (17%)	2 9
63	n7	115/115 (100%)	92 (80%)	23 (20%)	1 5
64	N8	118/118 (100%)	96 (81%)	22 (19%)	1 7
64	n8	118/118 (100%)	90 (76%)	28 (24%)	1 2
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2 9
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2 9
66	O0	81/84 (96%)	65 (80%)	16 (20%)	1 5
66	o0	84/84 (100%)	71 (84%)	13 (16%)	2 11
67	O1	92/96 (96%)	77 (84%)	15 (16%)	2 10
67	o1	94/96 (98%)	75 (80%)	19 (20%)	1 5
68	O2	109/109 (100%)	96 (88%)	13 (12%)	5 20
68	o2	109/109 (100%)	89 (82%)	20 (18%)	1 7
69	O3	90/90 (100%)	78 (87%)	12 (13%)	4 16
69	o3	90/90 (100%)	80 (89%)	10 (11%)	6 24
70	O4	95/95 (100%)	81 (85%)	14 (15%)	3 13
70	o4	95/95 (100%)	85 (90%)	10 (10%)	7 26
71	O5	104/104 (100%)	84 (81%)	20 (19%)	1 6
71	o5	103/104 (99%)	86 (84%)	17 (16%)	2 10
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0 1
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0 0
73	O7	70/70 (100%)	61 (87%)	9 (13%)	4 18
73	o7	70/70 (100%)	57 (81%)	13 (19%)	1 7
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0 1
74	o8	67/68 (98%)	54 (81%)	13 (19%)	1 6
75	O9	45/45 (100%)	40 (89%)	5 (11%)	6 24
75	o9	45/45 (100%)	38 (84%)	7 (16%)	2 11
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3 13
76	q0	47/47 (100%)	38 (81%)	9 (19%)	1 6
77	Q1	23/23 (100%)	18 (78%)	5 (22%)	1 4
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0 0
78	Q2	90/90 (100%)	72 (80%)	18 (20%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1 5
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2 9
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1 3
80	sM	54/103 (52%)	42 (78%)	12 (22%)	1 4
81	l8	177/190 (93%)	144 (81%)	33 (19%)	1 7
83	n4	100/114 (88%)	87 (87%)	13 (13%)	4 18
84	p0	105/254 (41%)	81 (77%)	24 (23%)	1 3
All	All	18725/19364 (97%)	15293 (82%)	3432 (18%)	1 7

5 of 3432 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	s4	38	LEU
24	d2	6	VAL
64	n8	124	ILE
7	s5	156	ARG
6	s4	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
33	e1	93	HIS
70	o4	3	GLN
34	sR	314	GLN
46	l9	8	GLN
76	q0	119	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	480 (27%)	60 (3%)
1	6	1793/1800 (99%)	466 (25%)	52 (2%)
36	1	3145/3396 (92%)	667 (21%)	76 (2%)
36	5	3145/3396 (92%)	677 (21%)	67 (2%)
37	3	120/121 (99%)	15 (12%)	0
37	7	120/121 (99%)	19 (15%)	0
38	4	157/158 (99%)	35 (22%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
38	8	157/158 (99%)	34 (21%)	3 (1%)
All	All	10414/10950 (95%)	2393 (22%)	260 (2%)

5 of 2393 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	21	U
1	2	25	C

5 of 260 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	2373	A
36	5	2772	C
36	1	1716	U
36	1	1562	C
36	5	3078	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2029 ligands modelled in this entry, 1035 are monoatomic - leaving 994 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	6	1993	-	0,6,6	-	-	-		
86	OHX	1	3466	-	0,6,6	-	-	-		
86	OHX	5	3435	-	0,6,6	-	-	-		
86	OHX	1	3462	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	1	3614	-	0,6,6	-	-	-		
86	OHX	1	3653	-	0,6,6	-	-	-		
86	OHX	5	3440	-	0,6,6	-	-	-		
86	OHX	2	2013	-	0,6,6	-	-	-		
86	OHX	5	3553	-	0,6,6	-	-	-		
86	OHX	1	3472	-	0,6,6	-	-	-		
86	OHX	5	3425	-	0,6,6	-	-	-		
86	OHX	5	3705	-	0,6,6	-	-	-		
86	OHX	5	3544	-	0,6,6	-	-	-		
86	OHX	1	3565	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	5	3489	-	0,6,6	-	-	-		
86	OHX	1	3533	-	0,6,6	-	-	-		
86	OHX	1	3588	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	6	2033	-	0,6,6	-	-	-		
86	OHX	6	1946	-	0,6,6	-	-	-		
86	OHX	1	3464	-	0,6,6	-	-	-		
86	OHX	2	1913	-	0,6,6	-	-	-		
86	OHX	5	3500	-	0,6,6	-	-	-		
86	OHX	6	1981	-	0,6,6	-	-	-		
86	OHX	1	3432	-	0,6,6	-	-	-		
86	OHX	5	3412	-	0,6,6	-	-	-		
86	OHX	5	3638	-	0,6,6	-	-	-		
86	OHX	5	3711	-	0,6,6	-	-	-		
86	OHX	8	204	-	0,6,6	-	-	-		
86	OHX	5	3530	-	0,6,6	-	-	-		
86	OHX	2	1981	-	0,6,6	-	-	-		
86	OHX	2	1964	-	0,6,6	-	-	-		
86	OHX	1	3642	-	0,6,6	-	-	-		
86	OHX	6	1921	-	0,6,6	-	-	-		
86	OHX	5	3713	-	0,6,6	-	-	-		
86	OHX	2	1905	-	0,6,6	-	-	-		
86	OHX	4	207	-	0,6,6	-	-	-		
86	OHX	5	3471	-	0,6,6	-	-	-		
86	OHX	2	1936	-	0,6,6	-	-	-		
86	OHX	5	3542	-	0,6,6	-	-	-		
86	OHX	2	1901	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3709	-	0,6,6	-	-	-		
86	OHX	5	3589	-	0,6,6	-	-	-		
86	OHX	5	3506	-	0,6,6	-	-	-		
86	OHX	5	3693	-	0,6,6	-	-	-		
86	OHX	6	2001	-	0,6,6	-	-	-		
86	OHX	5	3503	-	0,6,6	-	-	-		
86	OHX	5	3543	-	0,6,6	-	-	-		
86	OHX	5	3581	-	0,6,6	-	-	-		
86	OHX	6	2007	-	0,6,6	-	-	-		
86	OHX	l9	201	-	0,6,6	-	-	-		
86	OHX	5	3618	-	0,6,6	-	-	-		
86	OHX	4	214	-	0,6,6	-	-	-		
86	OHX	5	3654	-	0,6,6	-	-	-		
86	OHX	1	3540	-	0,6,6	-	-	-		
86	OHX	5	3653	-	0,6,6	-	-	-		
86	OHX	m6	201	-	0,6,6	-	-	-		
86	OHX	5	3629	-	0,6,6	-	-	-		
86	OHX	2	1929	-	0,6,6	-	-	-		
86	OHX	2	1966	-	0,6,6	-	-	-		
86	OHX	5	3547	-	0,6,6	-	-	-		
86	OHX	5	3584	-	0,6,6	-	-	-		
86	OHX	1	3523	-	0,6,6	-	-	-		
86	OHX	2	1991	-	0,6,6	-	-	-		
86	OHX	6	1911	-	0,6,6	-	-	-		
86	OHX	5	3665	-	0,6,6	-	-	-		
86	OHX	5	3703	-	0,6,6	-	-	-		
86	OHX	6	2002	-	0,6,6	-	-	-		
86	OHX	1	3438	-	0,6,6	-	-	-		
86	OHX	5	3421	-	0,6,6	-	-	-		
86	OHX	5	3602	-	0,6,6	-	-	-		
86	OHX	M5	301	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	5	3566	-	0,6,6	-	-	-		
86	OHX	1	3442	-	0,6,6	-	-	-		
86	OHX	1	3587	-	0,6,6	-	-	-		
86	OHX	1	3536	-	0,6,6	-	-	-		
86	OHX	1	3634	-	0,6,6	-	-	-		
86	OHX	1	3613	-	0,6,6	-	-	-		
86	OHX	5	3473	-	0,6,6	-	-	-		
86	OHX	5	3409	-	0,6,6	-	-	-		
86	OHX	1	3546	-	0,6,6	-	-	-		
86	OHX	5	3507	-	0,6,6	-	-	-		
86	OHX	5	3538	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3453	-	0,6,6	-	-	-		
86	OHX	1	3627	-	0,6,6	-	-	-		
86	OHX	1	3494	-	0,6,6	-	-	-		
86	OHX	6	1971	-	0,6,6	-	-	-		
86	OHX	5	3458	-	0,6,6	-	-	-		
86	OHX	6	1922	-	0,6,6	-	-	-		
86	OHX	5	3712	-	0,6,6	-	-	-		
86	OHX	5	3656	-	0,6,6	-	-	-		
86	OHX	5	3449	-	0,6,6	-	-	-		
86	OHX	1	3605	-	0,6,6	-	-	-		
86	OHX	1	3643	-	0,6,6	-	-	-		
86	OHX	5	3512	-	0,6,6	-	-	-		
86	OHX	o3	201	-	0,6,6	-	-	-		
86	OHX	5	3698	-	0,6,6	-	-	-		
86	OHX	5	3586	-	0,6,6	-	-	-		
86	OHX	2	2001	-	0,6,6	-	-	-		
86	OHX	6	1927	1	0,6,6	-	-	-		
86	OHX	5	3683	-	0,6,6	-	-	-		
86	OHX	1	3434	-	0,6,6	-	-	-		
86	OHX	5	3488	-	0,6,6	-	-	-		
86	OHX	5	3695	-	0,6,6	-	-	-		
86	OHX	1	3498	-	0,6,6	-	-	-		
86	OHX	s8	301	-	0,6,6	-	-	-		
86	OHX	5	3674	-	0,6,6	-	-	-		
86	OHX	4	208	-	0,6,6	-	-	-		
86	OHX	1	3622	-	0,6,6	-	-	-		
86	OHX	2	1909	1	0,6,6	-	-	-		
86	OHX	1	3620	-	0,6,6	-	-	-		
86	OHX	5	3525	-	0,6,6	-	-	-		
86	OHX	8	211	-	0,6,6	-	-	-		
86	OHX	1	3493	-	0,6,6	-	-	-		
86	OHX	1	3638	-	0,6,6	-	-	-		
86	OHX	2	2002	-	0,6,6	-	-	-		
86	OHX	4	213	-	0,6,6	-	-	-		
86	OHX	5	3590	-	0,6,6	-	-	-		
86	OHX	6	2010	-	0,6,6	-	-	-		
86	OHX	5	3461	-	0,6,6	-	-	-		
86	OHX	7	208	-	0,6,6	-	-	-		
86	OHX	5	3645	-	0,6,6	-	-	-		
86	OHX	6	2025	-	0,6,6	-	-	-		
86	OHX	1	3569	-	0,6,6	-	-	-		
86	OHX	2	1918	-	0,6,6	-	-	-		
86	OHX	6	1905	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3550	-	0,6,6	-	-	-		
86	OHX	2	1935	-	0,6,6	-	-	-		
86	OHX	1	3676	-	0,6,6	-	-	-		
86	OHX	2	1977	-	0,6,6	-	-	-		
86	OHX	6	1973	-	0,6,6	-	-	-		
86	OHX	5	3594	-	0,6,6	-	-	-		
86	OHX	7	202	-	0,6,6	-	-	-		
86	OHX	5	3575	-	0,6,6	-	-	-		
86	OHX	1	3692	-	0,6,6	-	-	-		
86	OHX	L3	402	-	0,6,6	-	-	-		
86	OHX	2	1956	-	0,6,6	-	-	-		
86	OHX	6	1933	-	0,6,6	-	-	-		
86	OHX	8	209	-	0,6,6	-	-	-		
86	OHX	1	3673	-	0,6,6	-	-	-		
86	OHX	2	1959	-	0,6,6	-	-	-		
86	OHX	5	3448	-	0,6,6	-	-	-		
86	OHX	2	1984	-	0,6,6	-	-	-		
86	OHX	5	3450	-	0,6,6	-	-	-		
86	OHX	2	1924	-	0,6,6	-	-	-		
86	OHX	2	1922	-	0,6,6	-	-	-		
86	OHX	1	3444	-	0,6,6	-	-	-		
86	OHX	5	3492	-	0,6,6	-	-	-		
86	OHX	1	3668	-	0,6,6	-	-	-		
86	OHX	5	3611	-	0,6,6	-	-	-		
86	OHX	6	1931	-	0,6,6	-	-	-		
86	OHX	1	3629	-	0,6,6	-	-	-		
86	OHX	6	1919	-	0,6,6	-	-	-		
86	OHX	1	3457	-	0,6,6	-	-	-		
86	OHX	6	1968	-	0,6,6	-	-	-		
86	OHX	l5	302	-	0,6,6	-	-	-		
86	OHX	5	3608	-	0,6,6	-	-	-		
86	OHX	2	1910	-	0,6,6	-	-	-		
86	OHX	5	3514	-	0,6,6	-	-	-		
86	OHX	1	3644	-	0,6,6	-	-	-		
86	OHX	n3	201	-	0,6,6	-	-	-		
86	OHX	5	3493	-	0,6,6	-	-	-		
86	OHX	1	3497	-	0,6,6	-	-	-		
86	OHX	1	3534	-	0,6,6	-	-	-		
86	OHX	1	3706	-	0,6,6	-	-	-		
86	OHX	5	3443	-	0,6,6	-	-	-		
86	OHX	5	3652	-	0,6,6	-	-	-		
86	OHX	5	3650	-	0,6,6	-	-	-		
86	OHX	6	1955	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3598	-	0,6,6	-	-	-		
86	OHX	6	1983	-	0,6,6	-	-	-		
86	OHX	2	1921	-	0,6,6	-	-	-		
86	OHX	2	2004	-	0,6,6	-	-	-		
86	OHX	2	2010	-	0,6,6	-	-	-		
86	OHX	1	3602	-	0,6,6	-	-	-		
86	OHX	6	2016	-	0,6,6	-	-	-		
86	OHX	5	3460	-	0,6,6	-	-	-		
86	OHX	1	3471	-	0,6,6	-	-	-		
86	OHX	7	209	-	0,6,6	-	-	-		
86	OHX	1	3712	-	0,6,6	-	-	-		
86	OHX	2	1954	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	2	1974	-	0,6,6	-	-	-		
86	OHX	6	2019	-	0,6,6	-	-	-		
86	OHX	5	3655	-	0,6,6	-	-	-		
86	OHX	2	1973	-	0,6,6	-	-	-		
86	OHX	1	3437	-	0,6,6	-	-	-		
86	OHX	1	3698	-	0,6,6	-	-	-		
86	OHX	1	3691	-	0,6,6	-	-	-		
86	OHX	1	3618	-	0,6,6	-	-	-		
86	OHX	1	3412	-	0,6,6	-	-	-		
86	OHX	5	3636	-	0,6,6	-	-	-		
86	OHX	5	3431	-	0,6,6	-	-	-		
86	OHX	5	3540	-	0,6,6	-	-	-		
86	OHX	6	1961	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	5	3579	-	0,6,6	-	-	-		
86	OHX	2	1992	-	0,6,6	-	-	-		
86	OHX	1	3701	-	0,6,6	-	-	-		
86	OHX	C1	201	-	0,6,6	-	-	-		
86	OHX	6	1926	-	0,6,6	-	-	-		
86	OHX	7	203	-	0,6,6	-	-	-		
86	OHX	8	205	-	0,6,6	-	-	-		
86	OHX	2	1931	-	0,6,6	-	-	-		
86	OHX	1	3688	-	0,6,6	-	-	-		
86	OHX	1	3515	-	0,6,6	-	-	-		
86	OHX	2	1998	-	0,6,6	-	-	-		
86	OHX	1	3633	-	0,6,6	-	-	-		
86	OHX	1	3631	-	0,6,6	-	-	-		
86	OHX	5	3568	-	0,6,6	-	-	-		
86	OHX	5	3646	-	0,6,6	-	-	-		
86	OHX	5	3640	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	5	3582	-	0,6,6	-	-	-		
86	OHX	L4	401	-	0,6,6	-	-	-		
86	OHX	1	3461	-	0,6,6	-	-	-		
86	OHX	5	3691	-	0,6,6	-	-	-		
86	OHX	2	1995	-	0,6,6	-	-	-		
86	OHX	1	3560	-	0,6,6	-	-	-		
86	OHX	1	3473	-	0,6,6	-	-	-		
86	OHX	5	3508	-	0,6,6	-	-	-		
86	OHX	2	1945	-	0,6,6	-	-	-		
86	OHX	5	3459	-	0,6,6	-	-	-		
86	OHX	1	3609	-	0,6,6	-	-	-		
86	OHX	1	3508	-	0,6,6	-	-	-		
86	OHX	5	3494	-	0,6,6	-	-	-		
86	OHX	5	3559	-	0,6,6	-	-	-		
86	OHX	1	3454	-	0,6,6	-	-	-		
86	OHX	6	2035	-	0,6,6	-	-	-		
86	OHX	5	3404	-	0,6,6	-	-	-		
86	OHX	1	3580	-	0,6,6	-	-	-		
86	OHX	5	3499	-	0,6,6	-	-	-		
86	OHX	5	3511	-	0,6,6	-	-	-		
86	OHX	c8	201	-	0,6,6	-	-	-		
86	OHX	6	1956	-	0,6,6	-	-	-		
86	OHX	1	3458	-	0,6,6	-	-	-		
86	OHX	1	3532	-	0,6,6	-	-	-		
86	OHX	6	1932	-	0,6,6	-	-	-		
86	OHX	5	3554	-	0,6,6	-	-	-		
86	OHX	5	3510	-	0,6,6	-	-	-		
86	OHX	5	3587	-	0,6,6	-	-	-		
86	OHX	l4	401	-	0,6,6	-	-	-		
86	OHX	6	1924	-	0,6,6	-	-	-		
86	OHX	5	3617	-	0,6,6	-	-	-		
86	OHX	1	3492	-	0,6,6	-	-	-		
86	OHX	1	3645	-	0,6,6	-	-	-		
86	OHX	5	3411	-	0,6,6	-	-	-		
86	OHX	1	3416	-	0,6,6	-	-	-		
86	OHX	1	3679	-	0,6,6	-	-	-		
86	OHX	1	3522	-	0,6,6	-	-	-		
86	OHX	5	3642	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	6	1910	-	0,6,6	-	-	-		
86	OHX	2	2017	-	0,6,6	-	-	-		
86	OHX	1	3490	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3514	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	3	206	-	0,6,6	-	-	-		
86	OHX	5	3552	-	0,6,6	-	-	-		
86	OHX	5	3724	-	0,6,6	-	-	-		
86	OHX	5	3558	-	0,6,6	-	-	-		
86	OHX	1	3591	-	0,6,6	-	-	-		
86	OHX	4	217	-	0,6,6	-	-	-		
86	OHX	6	1957	-	0,6,6	-	-	-		
86	OHX	5	3630	-	0,6,6	-	-	-		
86	OHX	1	3443	-	0,6,6	-	-	-		
86	OHX	5	3632	-	0,6,6	-	-	-		
86	OHX	5	3475	-	0,6,6	-	-	-		
86	OHX	1	3652	-	0,6,6	-	-	-		
86	OHX	1	3407	-	0,6,6	-	-	-		
86	OHX	1	3463	-	0,6,6	-	-	-		
86	OHX	1	3598	-	0,6,6	-	-	-		
86	OHX	5	3528	-	0,6,6	-	-	-		
86	OHX	5	3592	-	0,6,6	-	-	-		
86	OHX	6	1918	-	0,6,6	-	-	-		
86	OHX	6	1951	-	0,6,6	-	-	-		
86	OHX	5	3502	-	0,6,6	-	-	-		
86	OHX	1	3516	-	0,6,6	-	-	-		
86	OHX	1	3660	-	0,6,6	-	-	-		
86	OHX	1	3550	-	0,6,6	-	-	-		
86	OHX	5	3452	-	0,6,6	-	-	-		
86	OHX	1	3419	-	0,6,6	-	-	-		
86	OHX	6	1965	-	0,6,6	-	-	-		
86	OHX	2	1988	-	0,6,6	-	-	-		
86	OHX	1	3671	-	0,6,6	-	-	-		
86	OHX	1	3578	-	0,6,6	-	-	-		
86	OHX	1	3632	-	0,6,6	-	-	-		
86	OHX	5	3482	-	0,6,6	-	-	-		
86	OHX	5	3635	-	0,6,6	-	-	-		
86	OHX	5	3673	-	0,6,6	-	-	-		
86	OHX	5	3445	-	0,6,6	-	-	-		
86	OHX	1	3402	-	0,6,6	-	-	-		
86	OHX	2	1947	-	0,6,6	-	-	-		
86	OHX	8	208	-	0,6,6	-	-	-		
86	OHX	1	3583	36	0,6,6	-	-	-		
86	OHX	2	1904	-	0,6,6	-	-	-		
86	OHX	l3	402	-	0,6,6	-	-	-		
86	OHX	5	3441	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	1970	-	0,6,6	-	-	-		
86	OHX	5	3657	-	0,6,6	-	-	-		
86	OHX	3	201	-	0,6,6	-	-	-		
86	OHX	6	1979	-	0,6,6	-	-	-		
86	OHX	1	3568	-	0,6,6	-	-	-		
86	OHX	2	1912	-	0,6,6	-	-	-		
86	OHX	1	3646	-	0,6,6	-	-	-		
86	OHX	2	1932	-	0,6,6	-	-	-		
86	OHX	5	3681	-	0,6,6	-	-	-		
86	OHX	1	3422	-	0,6,6	-	-	-		
86	OHX	5	3680	-	0,6,6	-	-	-		
86	OHX	6	1964	-	0,6,6	-	-	-		
86	OHX	2	1972	-	0,6,6	-	-	-		
86	OHX	5	3722	-	0,6,6	-	-	-		
86	OHX	1	3535	-	0,6,6	-	-	-		
86	OHX	5	3659	-	0,6,6	-	-	-		
86	OHX	3	207	-	0,6,6	-	-	-		
86	OHX	1	3604	-	0,6,6	-	-	-		
86	OHX	5	3497	-	0,6,6	-	-	-		
86	OHX	5	3694	-	0,6,6	-	-	-		
86	OHX	6	1985	-	0,6,6	-	-	-		
86	OHX	1	3693	-	0,6,6	-	-	-		
86	OHX	6	2008	-	0,6,6	-	-	-		
86	OHX	1	3521	-	0,6,6	-	-	-		
86	OHX	5	3585	-	0,6,6	-	-	-		
86	OHX	5	3424	-	0,6,6	-	-	-		
86	OHX	5	3607	-	0,6,6	-	-	-		
86	OHX	5	3688	-	0,6,6	-	-	-		
86	OHX	2	1955	-	0,6,6	-	-	-		
86	OHX	5	3572	-	0,6,6	-	-	-		
86	OHX	1	3511	-	0,6,6	-	-	-		
86	OHX	2	2018	-	0,6,6	-	-	-		
86	OHX	1	3554	-	0,6,6	-	-	-		
86	OHX	6	2029	-	0,6,6	-	-	-		
86	OHX	5	3648	-	0,6,6	-	-	-		
86	OHX	1	3617	-	0,6,6	-	-	-		
86	OHX	6	1943	-	0,6,6	-	-	-		
86	OHX	2	1987	-	0,6,6	-	-	-		
86	OHX	6	2023	-	0,6,6	-	-	-		
86	OHX	1	3548	-	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	1	3455	-	0,6,6	-	-	-		
86	OHX	5	3593	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	1990	-	0,6,6	-	-	-		
86	OHX	5	3522	-	0,6,6	-	-	-		
86	OHX	3	202	-	0,6,6	-	-	-		
86	OHX	1	3556	-	0,6,6	-	-	-		
86	OHX	5	3718	-	0,6,6	-	-	-		
86	OHX	6	1963	-	0,6,6	-	-	-		
86	OHX	5	3513	-	0,6,6	-	-	-		
86	OHX	2	1990	-	0,6,6	-	-	-		
86	OHX	1	3625	-	0,6,6	-	-	-		
86	OHX	1	3524	-	0,6,6	-	-	-		
86	OHX	1	3592	-	0,6,6	-	-	-		
86	OHX	5	3649	-	0,6,6	-	-	-		
86	OHX	6	1998	-	0,6,6	-	-	-		
86	OHX	1	3418	-	0,6,6	-	-	-		
86	OHX	5	3601	-	0,6,6	-	-	-		
86	OHX	5	3633	-	0,6,6	-	-	-		
86	OHX	5	3631	-	0,6,6	-	-	-		
86	OHX	5	3416	-	0,6,6	-	-	-		
86	OHX	2	1958	-	0,6,6	-	-	-		
86	OHX	1	3696	-	0,6,6	-	-	-		
86	OHX	1	3619	-	0,6,6	-	-	-		
86	OHX	1	3557	-	0,6,6	-	-	-		
86	OHX	M0	301	-	0,6,6	-	-	-		
86	OHX	1	3711	-	0,6,6	-	-	-		
86	OHX	6	1939	-	0,6,6	-	-	-		
86	OHX	5	3676	-	0,6,6	-	-	-		
86	OHX	2	1920	-	0,6,6	-	-	-		
86	OHX	Q2	502	-	0,6,6	-	-	-		
86	OHX	2	1985	-	0,6,6	-	-	-		
86	OHX	5	3708	-	0,6,6	-	-	-		
86	OHX	2	1978	-	0,6,6	-	-	-		
86	OHX	1	3526	-	0,6,6	-	-	-		
86	OHX	1	3678	-	0,6,6	-	-	-		
86	OHX	1	3501	-	0,6,6	-	-	-		
86	OHX	1	3656	-	0,6,6	-	-	-		
86	OHX	1	3635	-	0,6,6	-	-	-		
86	OHX	1	3488	-	0,6,6	-	-	-		
86	OHX	5	3560	-	0,6,6	-	-	-		
86	OHX	1	3695	-	0,6,6	-	-	-		
86	OHX	5	3430	-	0,6,6	-	-	-		
86	OHX	5	3716	-	0,6,6	-	-	-		
86	OHX	1	3528	-	0,6,6	-	-	-		
86	OHX	6	1929	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	7	211	-	0,6,6	-	-	-		
86	OHX	1	3639	-	0,6,6	-	-	-		
86	OHX	1	3477	-	0,6,6	-	-	-		
86	OHX	1	3662	36	0,6,6	-	-	-		
86	OHX	1	3623	-	0,6,6	-	-	-		
86	OHX	5	3580	-	0,6,6	-	-	-		
86	OHX	1	3597	-	0,6,6	-	-	-		
86	OHX	1	3527	-	0,6,6	-	-	-		
86	OHX	5	3670	-	0,6,6	-	-	-		
86	OHX	5	3446	-	0,6,6	-	-	-		
86	OHX	3	204	-	0,6,6	-	-	-		
86	OHX	L3	401	-	0,6,6	-	-	-		
86	OHX	6	2000	-	0,6,6	-	-	-		
86	OHX	5	3574	-	0,6,6	-	-	-		
86	OHX	2	1963	-	0,6,6	-	-	-		
86	OHX	5	3467	-	0,6,6	-	-	-		
86	OHX	6	2022	-	0,6,6	-	-	-		
86	OHX	5	3429	-	0,6,6	-	-	-		
86	OHX	5	3612	-	0,6,6	-	-	-		
86	OHX	5	3483	-	0,6,6	-	-	-		
86	OHX	1	3439	-	0,6,6	-	-	-		
86	OHX	M7	202	-	0,6,6	-	-	-		
86	OHX	6	1972	-	0,6,6	-	-	-		
86	OHX	7	204	-	0,6,6	-	-	-		
86	OHX	6	1959	-	0,6,6	-	-	-		
86	OHX	2	1916	-	0,6,6	-	-	-		
86	OHX	6	2009	-	0,6,6	-	-	-		
86	OHX	1	3624	-	0,6,6	-	-	-		
86	OHX	1	3607	-	0,6,6	-	-	-		
86	OHX	2	2009	-	0,6,6	-	-	-		
86	OHX	1	3674	-	0,6,6	-	-	-		
86	OHX	5	3490	-	0,6,6	-	-	-		
86	OHX	5	3715	-	0,6,6	-	-	-		
86	OHX	1	3431	-	0,6,6	-	-	-		
86	OHX	1	3677	-	0,6,6	-	-	-		
86	OHX	8	210	-	0,6,6	-	-	-		
86	OHX	1	3448	-	0,6,6	-	-	-		
86	OHX	5	3591	-	0,6,6	-	-	-		
86	OHX	6	2018	-	0,6,6	-	-	-		
86	OHX	2	1961	-	0,6,6	-	-	-		
86	OHX	5	3531	-	0,6,6	-	-	-		
86	OHX	5	3527	-	0,6,6	-	-	-		
86	OHX	1	3576	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3414	-	0,6,6	-	-	-		
86	OHX	1	3517	-	0,6,6	-	-	-		
86	OHX	5	3720	-	0,6,6	-	-	-		
86	OHX	l5	301	-	0,6,6	-	-	-		
86	OHX	6	1987	-	0,6,6	-	-	-		
86	OHX	5	3699	-	0,6,6	-	-	-		
86	OHX	5	3520	-	0,6,6	-	-	-		
86	OHX	6	1930	-	0,6,6	-	-	-		
86	OHX	2	2012	-	0,6,6	-	-	-		
86	OHX	1	3555	-	0,6,6	-	-	-		
86	OHX	5	3684	-	0,6,6	-	-	-		
86	OHX	1	3476	-	0,6,6	-	-	-		
86	OHX	1	3478	-	0,6,6	-	-	-		
86	OHX	1	3482	-	0,6,6	-	-	-		
86	OHX	5	3451	-	0,6,6	-	-	-		
86	OHX	5	3562	-	0,6,6	-	-	-		
86	OHX	1	3606	-	0,6,6	-	-	-		
86	OHX	5	3634	-	0,6,6	-	-	-		
86	OHX	6	1967	-	0,6,6	-	-	-		
86	OHX	6	1901	-	0,6,6	-	-	-		
86	OHX	5	3408	-	0,6,6	-	-	-		
86	OHX	7	205	-	0,6,6	-	-	-		
86	OHX	2	2008	-	0,6,6	-	-	-		
86	OHX	5	3563	-	0,6,6	-	-	-		
86	OHX	6	2034	-	0,6,6	-	-	-		
86	OHX	6	1958	-	0,6,6	-	-	-		
86	OHX	8	202	-	0,6,6	-	-	-		
86	OHX	1	3542	-	0,6,6	-	-	-		
86	OHX	2	2000	-	0,6,6	-	-	-		
86	OHX	1	3460	-	0,6,6	-	-	-		
86	OHX	4	212	-	0,6,6	-	-	-		
86	OHX	1	3480	-	0,6,6	-	-	-		
86	OHX	5	3535	-	0,6,6	-	-	-		
86	OHX	5	3434	-	0,6,6	-	-	-		
86	OHX	5	3573	-	0,6,6	-	-	-		
86	OHX	5	3595	-	0,6,6	-	-	-		
86	OHX	5	3604	-	0,6,6	-	-	-		
86	OHX	6	1991	-	0,6,6	-	-	-		
86	OHX	2	1968	-	0,6,6	-	-	-		
86	OHX	1	3537	-	0,6,6	-	-	-		
86	OHX	1	3539	-	0,6,6	-	-	-		
86	OHX	1	3573	-	0,6,6	-	-	-		
86	OHX	6	1974	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3672	-	0,6,6	-	-	-		
86	OHX	1	3585	-	0,6,6	-	-	-		
86	OHX	1	3651	-	0,6,6	-	-	-		
86	OHX	1	3675	-	0,6,6	-	-	-		
86	OHX	6	1906	-	0,6,6	-	-	-		
86	OHX	5	3622	-	0,6,6	-	-	-		
86	OHX	6	1978	-	0,6,6	-	-	-		
86	OHX	6	2032	-	0,6,6	-	-	-		
86	OHX	2	1994	-	0,6,6	-	-	-		
86	OHX	1	3564	-	0,6,6	-	-	-		
86	OHX	5	3536	-	0,6,6	-	-	-		
86	OHX	6	2013	-	0,6,6	-	-	-		
86	OHX	1	3415	-	0,6,6	-	-	-		
86	OHX	1	3648	-	0,6,6	-	-	-		
86	OHX	4	205	-	0,6,6	-	-	-		
86	OHX	1	3420	-	0,6,6	-	-	-		
86	OHX	6	1928	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	2	1930	-	0,6,6	-	-	-		
86	OHX	5	3426	-	0,6,6	-	-	-		
86	OHX	5	3504	36	0,6,6	-	-	-		
86	OHX	5	3462	-	0,6,6	-	-	-		
86	OHX	1	3513	-	0,6,6	-	-	-		
86	OHX	2	1967	-	0,6,6	-	-	-		
86	OHX	5	3548	-	0,6,6	-	-	-		
86	OHX	5	3625	-	0,6,6	-	-	-		
86	OHX	1	3467	-	0,6,6	-	-	-		
86	OHX	5	3571	-	0,6,6	-	-	-		
86	OHX	4	210	-	0,6,6	-	-	-		
86	OHX	5	3541	-	0,6,6	-	-	-		
86	OHX	5	3672	-	0,6,6	-	-	-		
86	OHX	1	3636	-	0,6,6	-	-	-		
86	OHX	5	3578	-	0,6,6	-	-	-		
86	OHX	1	3601	-	0,6,6	-	-	-		
86	OHX	2	1923	-	0,6,6	-	-	-		
86	OHX	6	1992	-	0,6,6	-	-	-		
86	OHX	2	1993	-	0,6,6	-	-	-		
86	OHX	5	3710	-	0,6,6	-	-	-		
86	OHX	1	3626	-	0,6,6	-	-	-		
86	OHX	5	3565	-	0,6,6	-	-	-		
86	OHX	6	1916	-	0,6,6	-	-	-		
86	OHX	1	3417	-	0,6,6	-	-	-		
86	OHX	5	3588	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	2	1976	-	0,6,6	-	-	-		
86	OHX	1	3479	-	0,6,6	-	-	-		
86	OHX	5	3457	-	0,6,6	-	-	-		
86	OHX	1	3641	-	0,6,6	-	-	-		
86	OHX	1	3403	-	0,6,6	-	-	-		
86	OHX	5	3667	-	0,6,6	-	-	-		
86	OHX	1	3665	-	0,6,6	-	-	-		
86	OHX	5	3432	-	0,6,6	-	-	-		
86	OHX	2	1941	-	0,6,6	-	-	-		
86	OHX	6	1954	-	0,6,6	-	-	-		
86	OHX	1	3485	-	0,6,6	-	-	-		
86	OHX	1	3499	-	0,6,6	-	-	-		
86	OHX	2	1944	-	0,6,6	-	-	-		
86	OHX	1	3552	-	0,6,6	-	-	-		
86	OHX	1	3603	-	0,6,6	-	-	-		
86	OHX	6	1995	-	0,6,6	-	-	-		
86	OHX	1	3683	-	0,6,6	-	-	-		
86	OHX	2	1960	-	0,6,6	-	-	-		
86	OHX	5	3696	-	0,6,6	-	-	-		
86	OHX	6	1940	-	0,6,6	-	-	-		
86	OHX	5	3534	-	0,6,6	-	-	-		
86	OHX	1	3451	-	0,6,6	-	-	-		
86	OHX	1	3562	-	0,6,6	-	-	-		
86	OHX	6	1909	-	0,6,6	-	-	-		
86	OHX	1	3558	-	0,6,6	-	-	-		
86	OHX	6	1935	-	0,6,6	-	-	-		
86	OHX	6	1977	-	0,6,6	-	-	-		
86	OHX	5	3637	-	0,6,6	-	-	-		
86	OHX	5	3447	-	0,6,6	-	-	-		
86	OHX	1	3456	-	0,6,6	-	-	-		
86	OHX	1	3489	-	0,6,6	-	-	-		
86	OHX	6	2036	-	0,6,6	-	-	-		
86	OHX	5	3495	-	0,6,6	-	-	-		
86	OHX	5	3532	-	0,6,6	-	-	-		
86	OHX	5	3623	-	0,6,6	-	-	-		
86	OHX	5	3403	-	0,6,6	-	-	-		
86	OHX	1	3654	-	0,6,6	-	-	-		
86	OHX	1	3584	-	0,6,6	-	-	-		
86	OHX	1	3468	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	3438	-	0,6,6	-	-	-		
86	OHX	5	3610	-	0,6,6	-	-	-		
86	OHX	5	3496	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3429	36	0,6,6	-	-	-		
86	OHX	1	3612	-	0,6,6	-	-	-		
86	OHX	1	3615	-	0,6,6	-	-	-		
86	OHX	7	201	-	0,6,6	-	-	-		
86	OHX	1	3566	-	0,6,6	-	-	-		
86	OHX	1	3616	-	0,6,6	-	-	-		
86	OHX	1	3440	-	0,6,6	-	-	-		
86	OHX	6	1936	-	0,6,6	-	-	-		
86	OHX	1	3481	-	0,6,6	-	-	-		
86	OHX	6	2014	-	0,6,6	-	-	-		
86	OHX	2	1943	-	0,6,6	-	-	-		
86	OHX	6	1953	-	0,6,6	-	-	-		
86	OHX	2	1902	-	0,6,6	-	-	-		
86	OHX	1	3445	-	0,6,6	-	-	-		
86	OHX	5	3600	-	0,6,6	-	-	-		
86	OHX	2	1962	-	0,6,6	-	-	-		
86	OHX	1	3405	-	0,6,6	-	-	-		
86	OHX	1	3621	-	0,6,6	-	-	-		
86	OHX	3	205	-	0,6,6	-	-	-		
86	OHX	1	3507	-	0,6,6	-	-	-		
86	OHX	5	3433	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	5	3682	-	0,6,6	-	-	-		
86	OHX	5	3401	-	0,6,6	-	-	-		
86	OHX	5	3555	-	0,6,6	-	-	-		
86	OHX	7	206	-	0,6,6	-	-	-		
86	OHX	1	3670	-	0,6,6	-	-	-		
86	OHX	5	3436	-	0,6,6	-	-	-		
86	OHX	6	2030	-	0,6,6	-	-	-		
86	OHX	1	3483	-	0,6,6	-	-	-		
86	OHX	1	3509	-	0,6,6	-	-	-		
86	OHX	6	2004	-	0,6,6	-	-	-		
86	OHX	5	3487	-	0,6,6	-	-	-		
86	OHX	5	3557	-	0,6,6	-	-	-		
86	OHX	5	3583	-	0,6,6	-	-	-		
86	OHX	5	3605	-	0,6,6	-	-	-		
86	OHX	6	1912	-	0,6,6	-	-	-		
86	OHX	2	1997	-	0,6,6	-	-	-		
86	OHX	5	3677	-	0,6,6	-	-	-		
86	OHX	5	3454	-	0,6,6	-	-	-		
86	OHX	6	1975	-	0,6,6	-	-	-		
86	OHX	6	2011	-	0,6,6	-	-	-		
86	OHX	1	3571	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3506	-	0,6,6	-	-	-		
86	OHX	6	1945	-	0,6,6	-	-	-		
86	OHX	6	2003	-	0,6,6	-	-	-		
86	OHX	2	1975	-	0,6,6	-	-	-		
86	OHX	1	3581	-	0,6,6	-	-	-		
86	OHX	5	3714	-	0,6,6	-	-	-		
86	OHX	5	3702	-	0,6,6	-	-	-		
86	OHX	6	2015	-	0,6,6	-	-	-		
86	OHX	1	3570	-	0,6,6	-	-	-		
86	OHX	1	3704	-	0,6,6	-	-	-		
86	OHX	5	3679	-	0,6,6	-	-	-		
86	OHX	2	1937	-	0,6,6	-	-	-		
86	OHX	4	211	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	5	3491	-	0,6,6	-	-	-		
86	OHX	1	3567	-	0,6,6	-	-	-		
86	OHX	1	3595	-	0,6,6	-	-	-		
86	OHX	6	1941	-	0,6,6	-	-	-		
86	OHX	5	3466	-	0,6,6	-	-	-		
86	OHX	2	1979	-	0,6,6	-	-	-		
86	OHX	2	2007	-	0,6,6	-	-	-		
86	OHX	1	3486	-	0,6,6	-	-	-		
86	OHX	1	3435	-	0,6,6	-	-	-		
86	OHX	2	2014	-	0,6,6	-	-	-		
86	OHX	1	3594	-	0,6,6	-	-	-		
86	OHX	5	3546	-	0,6,6	-	-	-		
86	OHX	5	3658	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	2	1953	-	0,6,6	-	-	-		
86	OHX	1	3669	-	0,6,6	-	-	-		
86	OHX	S8	301	-	0,6,6	-	-	-		
86	OHX	2	1957	-	0,6,6	-	-	-		
86	OHX	4	209	-	0,6,6	-	-	-		
86	OHX	5	3692	-	0,6,6	-	-	-		
86	OHX	1	3544	-	0,6,6	-	-	-		
86	OHX	6	1948	-	0,6,6	-	-	-		
86	OHX	2	1938	-	0,6,6	-	-	-		
86	OHX	6	1913	-	0,6,6	-	-	-		
86	OHX	5	3516	-	0,6,6	-	-	-		
86	OHX	5	3643	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	5	3668	-	0,6,6	-	-	-		
86	OHX	1	3426	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3419	-	0,6,6	-	-	-		
86	OHX	1	3504	-	0,6,6	-	-	-		
86	OHX	1	3608	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	1	3496	-	0,6,6	-	-	-		
86	OHX	1	3484	-	0,6,6	-	-	-		
86	OHX	2	2003	-	0,6,6	-	-	-		
86	OHX	6	2027	1	0,6,6	-	-	-		
86	OHX	5	3663	-	0,6,6	-	-	-		
86	OHX	3	203	-	0,6,6	-	-	-		
86	OHX	5	3551	-	0,6,6	-	-	-		
86	OHX	5	3644	-	0,6,6	-	-	-		
89	UAM	6	2134	-	31,31,31	0.18	0	38,44,44	0.55	1 (2%)
86	OHX	1	3700	-	0,6,6	-	-	-		
86	OHX	5	3519	-	0,6,6	-	-	-		
86	OHX	2	1915	-	0,6,6	-	-	-		
86	OHX	5	3481	-	0,6,6	-	-	-		
86	OHX	1	3543	-	0,6,6	-	-	-		
86	OHX	5	3479	-	0,6,6	-	-	-		
86	OHX	1	3650	-	0,6,6	-	-	-		
86	OHX	6	2024	-	0,6,6	-	-	-		
86	OHX	6	1902	-	0,6,6	-	-	-		
86	OHX	1	3667	-	0,6,6	-	-	-		
86	OHX	5	3671	-	0,6,6	-	-	-		
86	OHX	6	1980	-	0,6,6	-	-	-		
86	OHX	O1	201	-	0,6,6	-	-	-		
86	OHX	1	3610	-	0,6,6	-	-	-		
86	OHX	5	3596	-	0,6,6	-	-	-		
86	OHX	2	1999	-	0,6,6	-	-	-		
86	OHX	1	3611	-	0,6,6	-	-	-		
86	OHX	5	3647	-	0,6,6	-	-	-		
86	OHX	6	1960	-	0,6,6	-	-	-		
86	OHX	5	3469	-	0,6,6	-	-	-		
86	OHX	1	3411	-	0,6,6	-	-	-		
86	OHX	5	3616	-	0,6,6	-	-	-		
86	OHX	2	2005	-	0,6,6	-	-	-		
86	OHX	8	206	-	0,6,6	-	-	-		
86	OHX	5	3509	-	0,6,6	-	-	-		
86	OHX	1	3574	-	0,6,6	-	-	-		
86	OHX	6	1997	-	0,6,6	-	-	-		
86	OHX	5	3413	-	0,6,6	-	-	-		
86	OHX	1	3637	-	0,6,6	-	-	-		
86	OHX	1	3541	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	1	3628	-	0,6,6	-	-	-		
86	OHX	6	1988	-	0,6,6	-	-	-		
86	OHX	1	3531	-	0,6,6	-	-	-		
86	OHX	5	3485	-	0,6,6	-	-	-		
86	OHX	8	212	-	0,6,6	-	-	-		
86	OHX	5	3701	-	0,6,6	-	-	-		
86	OHX	1	3682	-	0,6,6	-	-	-		
86	OHX	5	3407	-	0,6,6	-	-	-		
86	OHX	1	3538	-	0,6,6	-	-	-		
86	OHX	5	3484	-	0,6,6	-	-	-		
86	OHX	5	3468	-	0,6,6	-	-	-		
86	OHX	5	3515	-	0,6,6	-	-	-		
86	OHX	5	3444	-	0,6,6	-	-	-		
86	OHX	5	3545	-	0,6,6	-	-	-		
86	OHX	5	3474	-	0,6,6	-	-	-		
86	OHX	5	3556	-	0,6,6	-	-	-		
86	OHX	2	1926	-	0,6,6	-	-	-		
86	OHX	5	3442	-	0,6,6	-	-	-		
86	OHX	5	3624	-	0,6,6	-	-	-		
86	OHX	1	3512	-	0,6,6	-	-	-		
86	OHX	5	3706	-	0,6,6	-	-	-		
86	OHX	5	3418	-	0,6,6	-	-	-		
86	OHX	2	1969	-	0,6,6	-	-	-		
86	OHX	2	2022	-	0,6,6	-	-	-		
86	OHX	1	3630	-	0,6,6	-	-	-		
86	OHX	2	1980	-	0,6,6	-	-	-		
86	OHX	5	3464	-	0,6,6	-	-	-		
86	OHX	1	3408	-	0,6,6	-	-	-		
86	OHX	5	3626	-	0,6,6	-	-	-		
86	OHX	1	3709	-	0,6,6	-	-	-		
86	OHX	1	3495	-	0,6,6	-	-	-		
86	OHX	1	3433	-	0,6,6	-	-	-		
86	OHX	1	3661	-	0,6,6	-	-	-		
86	OHX	2	1971	-	0,6,6	-	-	-		
86	OHX	1	3687	-	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	S9	201	-	0,6,6	-	-	-		
86	OHX	5	3619	-	0,6,6	-	-	-		
86	OHX	1	3430	-	0,6,6	-	-	-		
86	OHX	1	3710	-	0,6,6	-	-	-		
86	OHX	1	3518	-	0,6,6	-	-	-		
86	OHX	1	3590	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3452	-	0,6,6	-	-	-		
86	OHX	6	1938	-	0,6,6	-	-	-		
86	OHX	M9	201	-	0,6,6	-	-	-		
86	OHX	1	3505	-	0,6,6	-	-	-		
86	OHX	5	3437	-	0,6,6	-	-	-		
86	OHX	6	1920	-	0,6,6	-	-	-		
86	OHX	5	3690	-	0,6,6	-	-	-		
86	OHX	5	3621	-	0,6,6	-	-	-		
86	OHX	2	1996	-	0,6,6	-	-	-		
86	OHX	5	3463	36	0,6,6	-	-	-		
86	OHX	6	1969	-	0,6,6	-	-	-		
86	OHX	5	3570	-	0,6,6	-	-	-		
86	OHX	1	3425	-	0,6,6	-	-	-		
86	OHX	5	3627	-	0,6,6	-	-	-		
86	OHX	1	3519	-	0,6,6	-	-	-		
86	OHX	6	1915	-	0,6,6	-	-	-		
86	OHX	5	3477	-	0,6,6	-	-	-		
86	OHX	5	3577	-	0,6,6	-	-	-		
86	OHX	5	3639	-	0,6,6	-	-	-		
86	OHX	6	1982	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	5	3717	-	0,6,6	-	-	-		
86	OHX	1	3549	-	0,6,6	-	-	-		
86	OHX	5	3410	-	0,6,6	-	-	-		
86	OHX	2	1933	-	0,6,6	-	-	-		
86	OHX	6	1994	-	0,6,6	-	-	-		
86	OHX	5	3537	-	0,6,6	-	-	-		
86	OHX	1	3491	-	0,6,6	-	-	-		
86	OHX	1	3572	-	0,6,6	-	-	-		
86	OHX	5	3518	-	0,6,6	-	-	-		
86	OHX	1	3596	-	0,6,6	-	-	-		
86	OHX	1	3436	-	0,6,6	-	-	-		
86	OHX	6	2021	-	0,6,6	-	-	-		
86	OHX	5	3439	-	0,6,6	-	-	-		
86	OHX	n1	201	-	0,6,6	-	-	-		
86	OHX	1	3686	-	0,6,6	-	-	-		
86	OHX	5	3599	-	0,6,6	-	-	-		
86	OHX	5	3402	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	2	2016	-	0,6,6	-	-	-		
86	OHX	1	3529	-	0,6,6	-	-	-		
86	OHX	1	3428	-	0,6,6	-	-	-		
86	OHX	6	1934	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3526	-	0,6,6	-	-	-		
86	OHX	2	1927	-	0,6,6	-	-	-		
86	OHX	2	1934	-	0,6,6	-	-	-		
86	OHX	2	1949	-	0,6,6	-	-	-		
86	OHX	6	2026	-	0,6,6	-	-	-		
86	OHX	1	3657	-	0,6,6	-	-	-		
86	OHX	7	210	-	0,6,6	-	-	-		
86	OHX	2	1986	-	0,6,6	-	-	-		
86	OHX	6	2020	-	0,6,6	-	-	-		
86	OHX	5	3476	-	0,6,6	-	-	-		
86	OHX	2	2006	-	0,6,6	-	-	-		
86	OHX	5	3422	-	0,6,6	-	-	-		
86	OHX	1	3413	-	0,6,6	-	-	-		
86	OHX	5	3478	-	0,6,6	-	-	-		
86	OHX	1	3427	-	0,6,6	-	-	-		
86	OHX	6	2017	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	5	3666	-	0,6,6	-	-	-		
86	OHX	1	3659	-	0,6,6	-	-	-		
86	OHX	1	3663	-	0,6,6	-	-	-		
86	OHX	6	2037	-	0,6,6	-	-	-		
86	OHX	6	2028	-	0,6,6	-	-	-		
86	OHX	5	3501	36	0,6,6	-	-	-		
86	OHX	5	3498	-	0,6,6	-	-	-		
86	OHX	1	3655	-	0,6,6	-	-	-		
86	OHX	2	2019	-	0,6,6	-	-	-		
86	OHX	1	3423	-	0,6,6	-	-	-		
86	OHX	5	3697	-	0,6,6	-	-	-		
86	OHX	6	1984	-	0,6,6	-	-	-		
86	OHX	1	3424	-	0,6,6	-	-	-		
86	OHX	2	1982	-	0,6,6	-	-	-		
86	OHX	1	3681	-	0,6,6	-	-	-		
86	OHX	5	3561	-	0,6,6	-	-	-		
86	OHX	5	3521	-	0,6,6	-	-	-		
86	OHX	2	1914	-	0,6,6	-	-	-		
86	OHX	2	1951	-	0,6,6	-	-	-		
86	OHX	1	3465	-	0,6,6	-	-	-		
86	OHX	1	3647	-	0,6,6	-	-	-		
86	OHX	5	3661	-	0,6,6	-	-	-		
86	OHX	5	3689	-	0,6,6	-	-	-		
86	OHX	4	203	-	0,6,6	-	-	-		
86	OHX	O3	201	-	0,6,6	-	-	-		
86	OHX	5	3480	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2021	-	0,6,6	-	-	-		
86	OHX	5	3687	-	0,6,6	-	-	-		
86	OHX	5	3707	-	0,6,6	-	-	-		
86	OHX	1	3689	-	0,6,6	-	-	-		
86	OHX	2	1907	-	0,6,6	-	-	-		
86	OHX	5	3524	-	0,6,6	-	-	-		
86	OHX	1	3708	-	0,6,6	-	-	-		
86	OHX	5	3567	-	0,6,6	-	-	-		
86	OHX	1	3450	-	0,6,6	-	-	-		
86	OHX	1	3640	-	0,6,6	-	-	-		
86	OHX	1	3690	-	0,6,6	-	-	-		
86	OHX	5	3529	-	0,6,6	-	-	-		
86	OHX	5	3651	-	0,6,6	-	-	-		
86	OHX	1	3449	-	0,6,6	-	-	-		
86	OHX	5	3675	-	0,6,6	-	-	-		
86	OHX	6	1903	-	0,6,6	-	-	-		
86	OHX	5	3455	-	0,6,6	-	-	-		
86	OHX	1	3582	-	0,6,6	-	-	-		
86	OHX	1	3553	-	0,6,6	-	-	-		
86	OHX	6	1996	-	0,6,6	-	-	-		
86	OHX	1	3649	-	0,6,6	-	-	-		
86	OHX	5	3415	-	0,6,6	-	-	-		
86	OHX	5	3472	-	0,6,6	-	-	-		
86	OHX	6	2005	-	0,6,6	-	-	-		
86	OHX	6	1908	-	0,6,6	-	-	-		
86	OHX	n3	202	-	0,6,6	-	-	-		
86	OHX	2	1908	-	0,6,6	-	-	-		
86	OHX	2	1928	-	0,6,6	-	-	-		
86	OHX	2	1919	-	0,6,6	-	-	-		
86	OHX	1	3559	-	0,6,6	-	-	-		
86	OHX	5	3628	-	0,6,6	-	-	-		
86	OHX	2	2020	-	0,6,6	-	-	-		
86	OHX	5	3685	-	0,6,6	-	-	-		
86	OHX	5	3505	-	0,6,6	-	-	-		
86	OHX	1	3474	-	0,6,6	-	-	-		
86	OHX	1	3589	-	0,6,6	-	-	-		
86	OHX	3	208	-	0,6,6	-	-	-		
86	OHX	5	3664	-	0,6,6	-	-	-		
86	OHX	1	3510	-	0,6,6	-	-	-		
86	OHX	2	1906	-	0,6,6	-	-	-		
86	OHX	1	3500	-	0,6,6	-	-	-		
86	OHX	1	3530	-	0,6,6	-	-	-		
86	OHX	8	203	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3401	-	0,6,6	-	-	-		
86	OHX	5	3723	-	0,6,6	-	-	-		
86	OHX	1	3487	-	0,6,6	-	-	-		
86	OHX	5	3719	-	0,6,6	-	-	-		
86	OHX	5	3721	-	0,6,6	-	-	-		
86	OHX	6	1917	-	0,6,6	-	-	-		
86	OHX	6	1966	-	0,6,6	-	-	-		
86	OHX	1	3406	-	0,6,6	-	-	-		
86	OHX	5	3417	-	0,6,6	-	-	-		
86	OHX	5	3686	-	0,6,6	-	-	-		
86	OHX	6	1976	-	0,6,6	-	-	-		
86	OHX	5	3597	-	0,6,6	-	-	-		
86	OHX	2	1925	-	0,6,6	-	-	-		
86	OHX	5	3700	-	0,6,6	-	-	-		
86	OHX	5	3641	-	0,6,6	-	-	-		
86	OHX	2	1939	-	0,6,6	-	-	-		
86	OHX	1	3545	-	0,6,6	-	-	-		
86	OHX	2	1942	-	0,6,6	-	-	-		
86	OHX	4	215	-	0,6,6	-	-	-		
86	OHX	1	3702	-	0,6,6	-	-	-		
86	OHX	5	3428	-	0,6,6	-	-	-		
86	OHX	2	1948	-	0,6,6	-	-	-		
86	OHX	5	3564	-	0,6,6	-	-	-		
86	OHX	6	1949	-	0,6,6	-	-	-		
86	OHX	5	3603	-	0,6,6	-	-	-		
86	OHX	1	3520	-	0,6,6	-	-	-		
86	OHX	5	3614	-	0,6,6	-	-	-		
86	OHX	1	3446	-	0,6,6	-	-	-		
86	OHX	6	1986	-	0,6,6	-	-	-		
86	OHX	1	3475	-	0,6,6	-	-	-		
86	OHX	1	3600	-	0,6,6	-	-	-		
86	OHX	6	1989	-	0,6,6	-	-	-		
86	OHX	1	3547	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	2	1940	-	0,6,6	-	-	-		
86	OHX	2	1989	-	0,6,6	-	-	-		
86	OHX	1	3470	-	0,6,6	-	-	-		
86	OHX	6	1952	-	0,6,6	-	-	-		
86	OHX	5	3606	-	0,6,6	-	-	-		
86	OHX	1	3502	-	0,6,6	-	-	-		
86	OHX	5	3660	-	0,6,6	-	-	-		
86	OHX	1	3453	-	0,6,6	-	-	-		
86	OHX	5	3609	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3456	-	0,6,6	-	-	-		
86	OHX	m5	302	-	0,6,6	-	-	-		
86	OHX	1	3447	-	0,6,6	-	-	-		
86	OHX	1	3577	-	0,6,6	-	-	-		
86	OHX	5	3406	-	0,6,6	-	-	-		
86	OHX	5	3533	-	0,6,6	-	-	-		
86	OHX	5	3423	-	0,6,6	-	-	-		
86	OHX	5	3576	-	0,6,6	-	-	-		
86	OHX	1	3404	-	0,6,6	-	-	-		
86	OHX	1	3503	-	0,6,6	-	-	-		
86	OHX	1	3697	-	0,6,6	-	-	-		
86	OHX	4	206	-	0,6,6	-	-	-		
86	OHX	1	3410	-	0,6,6	-	-	-		
86	OHX	l3	401	-	0,6,6	-	-	-		
86	OHX	2	2011	-	0,6,6	-	-	-		
86	OHX	6	2012	-	0,6,6	-	-	-		
86	OHX	2	1946	-	0,6,6	-	-	-		
86	OHX	4	216	-	0,6,6	-	-	-		
86	OHX	1	3409	-	0,6,6	-	-	-		
86	OHX	6	1923	-	0,6,6	-	-	-		
86	OHX	5	3613	-	0,6,6	-	-	-		
86	OHX	6	1914	-	0,6,6	-	-	-		
86	OHX	2	2015	-	0,6,6	-	-	-		
86	OHX	1	3459	-	0,6,6	-	-	-		
86	OHX	1	3586	-	0,6,6	-	-	-		
86	OHX	1	3707	-	0,6,6	-	-	-		
86	OHX	6	1950	-	0,6,6	-	-	-		
86	OHX	5	3615	-	0,6,6	-	-	-		
86	OHX	1	3699	-	0,6,6	-	-	-		
86	OHX	6	1907	-	0,6,6	-	-	-		
86	OHX	1	3441	-	0,6,6	-	-	-		
86	OHX	5	3517	-	0,6,6	-	-	-		
86	OHX	2	1983	-	0,6,6	-	-	-		
86	OHX	2	1917	-	0,6,6	-	-	-		
86	OHX	1	3599	-	0,6,6	-	-	-		
86	OHX	5	3569	-	0,6,6	-	-	-		
86	OHX	1	3421	-	0,6,6	-	-	-		
86	OHX	1	3561	-	0,6,6	-	-	-		
86	OHX	1	3680	-	0,6,6	-	-	-		
86	OHX	8	207	-	0,6,6	-	-	-		
86	OHX	6	1962	-	0,6,6	-	-	-		
86	OHX	1	3414	-	0,6,6	-	-	-		
86	OHX	1	3694	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3669	-	0,6,6	-	-	-		
86	OHX	1	3684	-	0,6,6	-	-	-		
86	OHX	5	3678	-	0,6,6	-	-	-		
86	OHX	5	3405	-	0,6,6	-	-	-		
86	OHX	5	3662	-	0,6,6	-	-	-		
86	OHX	1	3563	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	5	3470	-	0,6,6	-	-	-		
86	OHX	6	2006	-	0,6,6	-	-	-		
86	OHX	5	3620	-	0,6,6	-	-	-		
86	OHX	6	1944	-	0,6,6	-	-	-		
86	OHX	5	3486	-	0,6,6	-	-	-		
86	OHX	1	3685	-	0,6,6	-	-	-		
86	OHX	5	3523	-	0,6,6	-	-	-		
86	OHX	5	3427	-	0,6,6	-	-	-		
86	OHX	1	3525	-	0,6,6	-	-	-		
86	OHX	2	1911	-	0,6,6	-	-	-		
86	OHX	1	3664	-	0,6,6	-	-	-		
86	OHX	1	3703	-	0,6,6	-	-	-		
86	OHX	8	213	-	0,6,6	-	-	-		
86	OHX	2	1952	-	0,6,6	-	-	-		
86	OHX	6	1999	-	0,6,6	-	-	-		
86	OHX	1	3469	-	0,6,6	-	-	-		
86	OHX	2	1965	-	0,6,6	-	-	-		
86	OHX	1	3579	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	6	1947	-	0,6,6	-	-	-		
86	OHX	5	3420	-	0,6,6	-	-	-		
86	OHX	2	1903	-	0,6,6	-	-	-		
86	OHX	1	3593	-	0,6,6	-	-	-		
86	OHX	5	3539	-	0,6,6	-	-	-		
86	OHX	1	3705	-	0,6,6	-	-	-		
86	OHX	1	3551	-	0,6,6	-	-	-		
86	OHX	6	1904	-	0,6,6	-	-	-		
86	OHX	5	3704	-	0,6,6	-	-	-		
86	OHX	5	3465	-	0,6,6	-	-	-		
86	OHX	6	1925	-	0,6,6	-	-	-		
86	OHX	1	3658	-	0,6,6	-	-	-		
86	OHX	4	204	-	0,6,6	-	-	-		
86	OHX	6	1937	-	0,6,6	-	-	-		
86	OHX	1	3575	-	0,6,6	-	-	-		
86	OHX	6	2031	-	0,6,6	-	-	-		
86	OHX	6	1942	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	2	1950	-	0,6,6	-	-	-		
86	OHX	5	3549	-	0,6,6	-	-	-		
86	OHX	2	1970	-	0,6,6	-	-	-		
86	OHX	7	207	-	0,6,6	-	-	-		
86	OHX	1	3666	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	UAM	6	2134	-	-	14/28/40/40	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
89	6	2134	UAM	CAZ-CAN-CAS	2.30	115.82	112.65

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	6	2134	UAM	NAQ-CAT-CBA-OAI
89	6	2134	UAM	NAQ-CAT-CBA-CBB
89	6	2134	UAM	OAF-CAT-CBA-OAI
89	6	2134	UAM	OAF-CAT-CBA-CBB
89	6	2134	UAM	CAT-CBA-CBB-OAJ

There are no ring outliers.

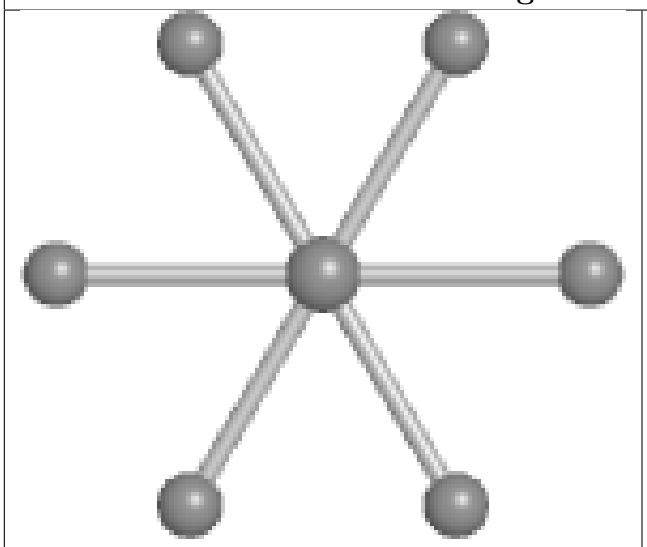
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	C8	201	OHX	0	1

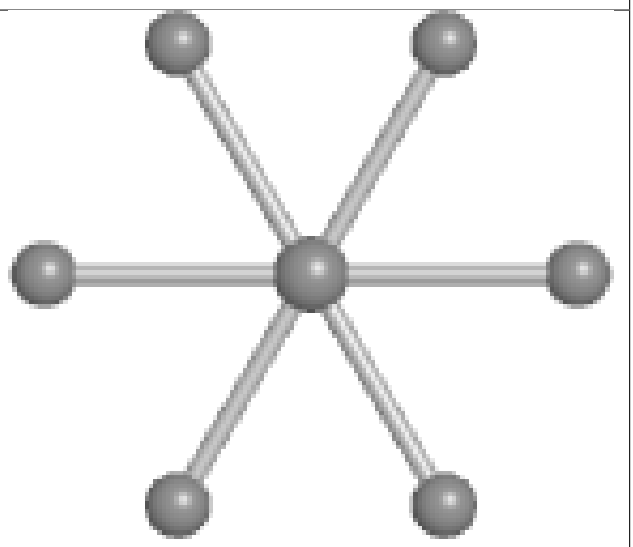
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

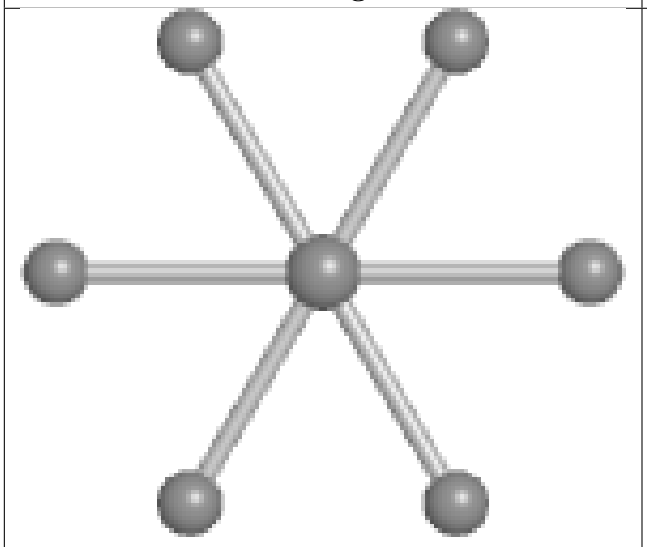
Ligand OHX 2 2027



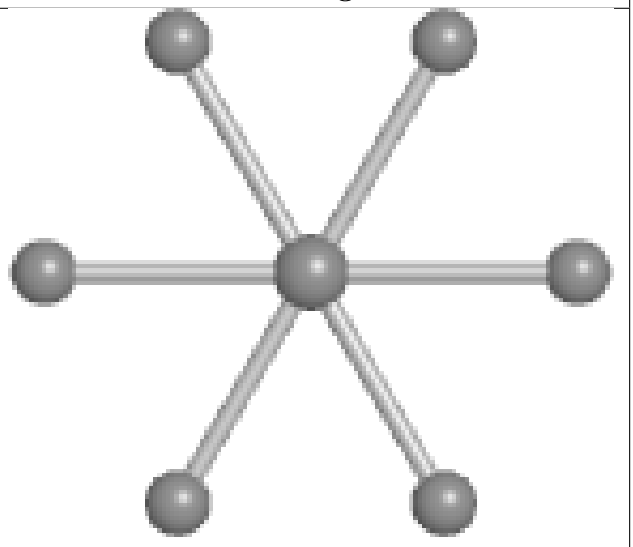
Bond lengths



Bond angles

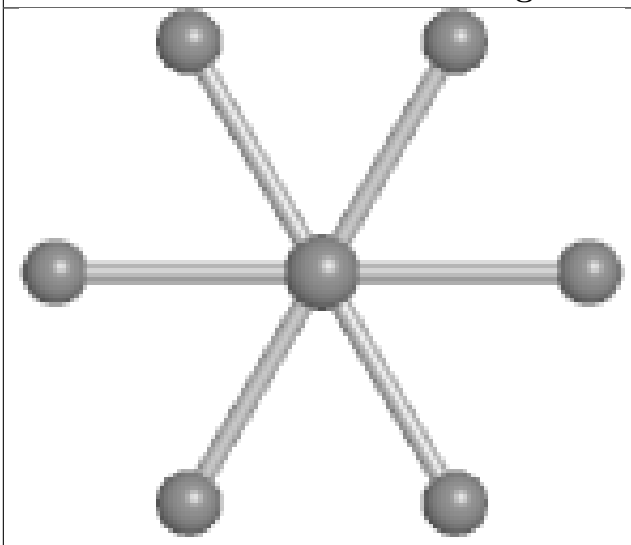


Torsions

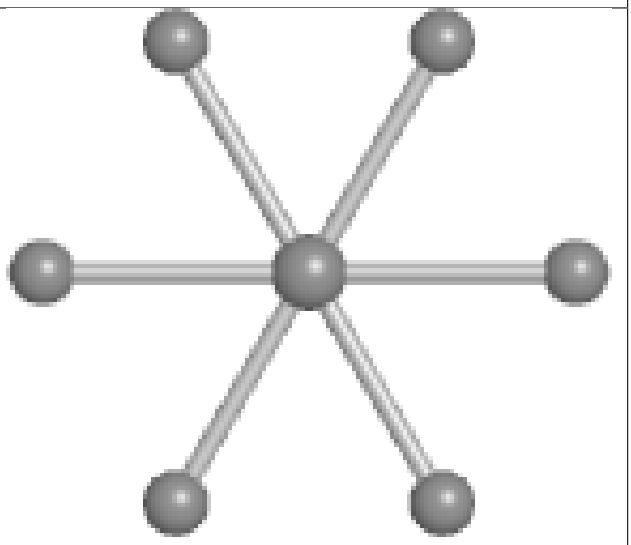


Rings

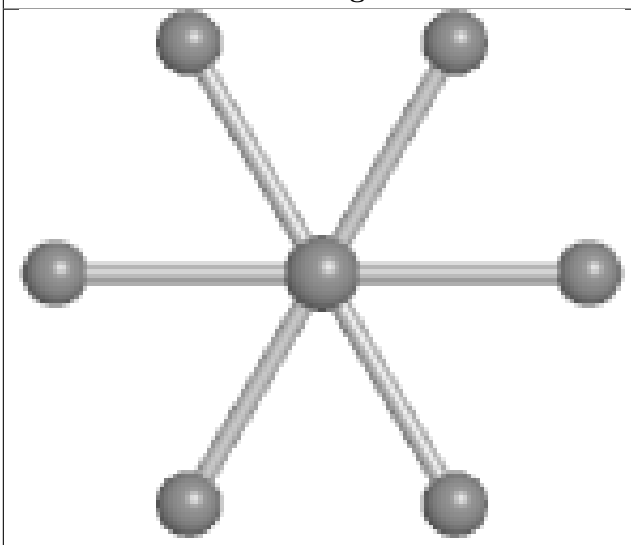
Ligand OHX 6 2034



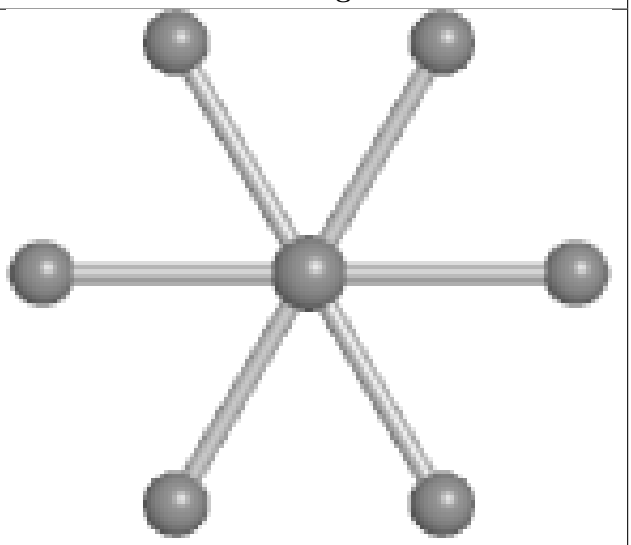
Bond lengths



Bond angles

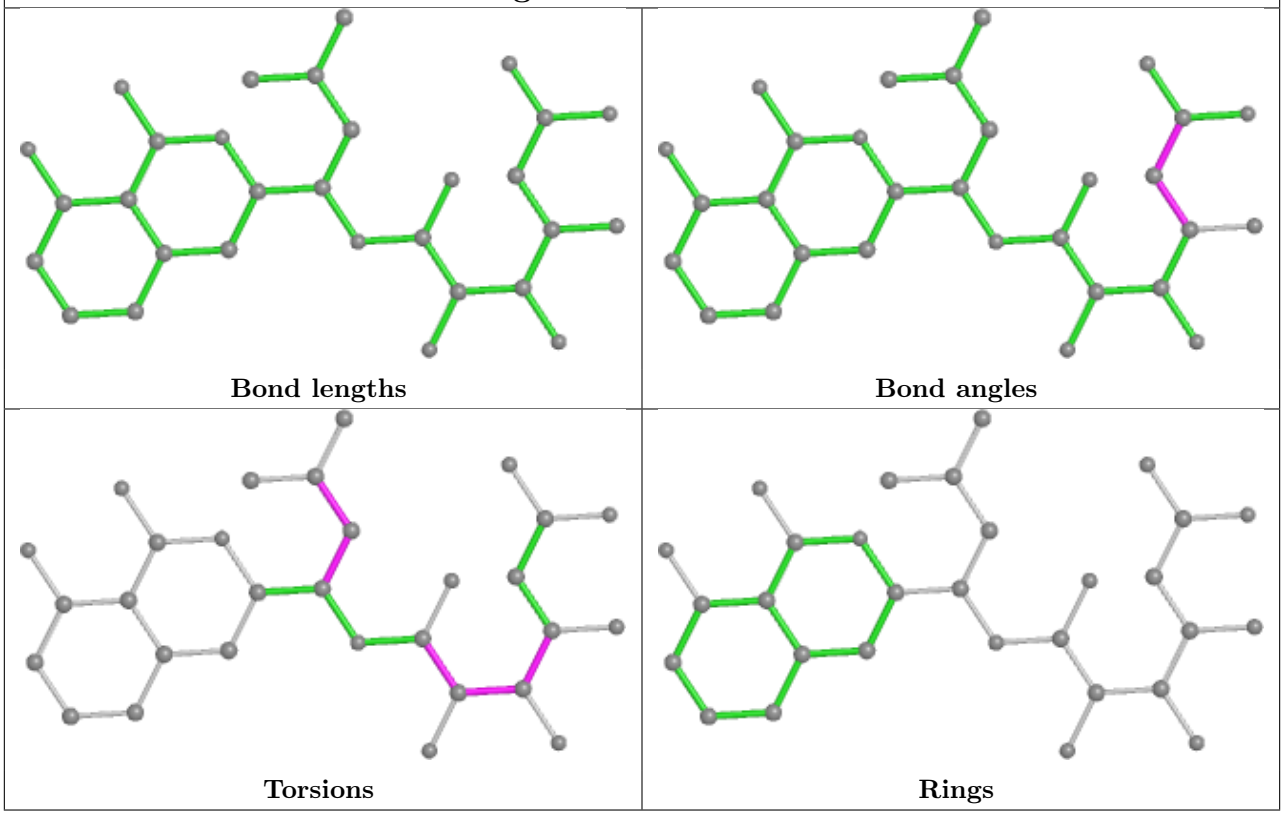


Torsions



Rings

Ligand UAM 6 2134



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2
82	m2	2
80	sM	1
68	O2	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	139:UNK	C	155:UNK	N	37.77
1	2	1716:C	O3'	1717:G	P	4.09
1	m2	23:UNK	C	28:UNK	N	3.84
1	m2	52:UNK	C	54:UNK	N	3.47

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1685:G	O3'	1686:C	P	3.06

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	1781/1800 (98%)	0.24	80 (4%) 33 16	54, 93, 190, 248	0
1	6	1795/1800 (99%)	0.13	73 (4%) 37 18	41, 80, 181, 246	0
2	S0	206/206 (100%)	0.69	26 (12%) 3 1	92, 107, 120, 134	0
2	s0	206/206 (100%)	0.60	10 (4%) 29 14	77, 95, 110, 124	0
3	S1	214/216 (99%)	1.28	54 (25%) 0 0	101, 136, 157, 161	0
3	s1	216/216 (100%)	0.89	25 (11%) 4 2	79, 98, 118, 131	0
4	S2	217/217 (100%)	0.30	4 (1%) 68 47	75, 88, 102, 114	0
4	s2	217/217 (100%)	0.30	8 (3%) 41 21	62, 78, 91, 106	0
5	S3	223/223 (100%)	0.67	15 (6%) 17 7	82, 97, 126, 136	0
5	s3	223/223 (100%)	1.08	42 (18%) 1 0	82, 119, 148, 156	0
6	S4	260/260 (100%)	0.92	35 (13%) 3 1	65, 93, 104, 136	0
6	s4	260/260 (100%)	0.46	3 (1%) 79 61	52, 76, 92, 126	0
7	S5	206/206 (100%)	1.07	38 (18%) 1 0	102, 125, 135, 149	0
7	s5	206/206 (100%)	0.92	30 (14%) 2 1	76, 104, 123, 130	0
8	S6	226/226 (100%)	0.72	18 (7%) 12 5	68, 109, 126, 143	0
8	s6	218/226 (96%)	0.36	10 (4%) 32 16	52, 86, 103, 121	0
9	S7	184/186 (98%)	0.94	30 (16%) 1 1	84, 117, 140, 147	0
9	s7	186/186 (100%)	0.79	26 (13%) 2 1	71, 111, 139, 148	0
10	S8	188/200 (94%)	0.48	10 (5%) 26 12	59, 77, 113, 129	0
10	s8	188/200 (94%)	0.63	17 (9%) 9 3	49, 71, 110, 133	0
11	S9	185/185 (100%)	1.30	41 (22%) 0 0	84, 101, 137, 158	0
11	s9	185/185 (100%)	0.81	18 (9%) 7 2	65, 82, 117, 141	0
12	C0	96/98 (97%)	1.00	12 (12%) 3 1	89, 114, 145, 157	0
12	c0	96/98 (97%)	2.72	53 (55%) 0 0	116, 151, 162, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	C1	155/156 (99%)	0.73	17 (10%) 5 2	61, 76, 122, 126	0
13	c1	146/156 (93%)	0.56	10 (6%) 17 7	50, 68, 96, 120	0
14	C2	124/124 (100%)	1.62	41 (33%) 0 0	147, 156, 166, 169	0
14	c2	124/124 (100%)	3.32	102 (82%) 0 0	196, 205, 216, 219	0
15	C3	150/150 (100%)	0.29	3 (2%) 65 44	70, 89, 102, 109	0
15	c3	150/150 (100%)	0.13	1 (0%) 87 75	63, 80, 98, 102	0
16	C4	127/128 (99%)	1.06	28 (22%) 0 0	71, 126, 142, 143	0
16	c4	128/128 (100%)	0.82	10 (7%) 13 5	57, 95, 104, 113	0
17	C5	124/142 (87%)	0.98	17 (13%) 3 1	88, 106, 128, 144	0
17	c5	135/142 (95%)	1.30	31 (22%) 0 0	77, 113, 129, 134	0
18	C6	141/142 (99%)	1.44	43 (30%) 0 0	84, 113, 119, 123	0
18	c6	142/142 (100%)	0.69	13 (9%) 9 3	72, 96, 114, 138	0
19	C7	120/136 (88%)	0.73	13 (10%) 5 2	93, 109, 132, 135	0
19	c7	117/136 (86%)	0.39	2 (1%) 70 49	83, 101, 117, 122	0
20	C8	145/145 (100%)	0.99	26 (17%) 1 0	84, 114, 141, 149	0
20	c8	145/145 (100%)	0.44	8 (5%) 25 11	78, 97, 115, 124	0
21	C9	143/143 (100%)	1.07	23 (16%) 1 1	96, 110, 124, 132	0
21	c9	143/143 (100%)	0.38	7 (4%) 29 14	70, 86, 106, 118	0
22	D0	107/110 (97%)	1.19	24 (22%) 0 0	78, 112, 139, 142	0
22	d0	110/110 (100%)	1.92	45 (40%) 0 0	78, 118, 151, 154	0
23	D1	87/87 (100%)	0.62	6 (6%) 16 7	88, 96, 111, 119	0
23	d1	87/87 (100%)	0.37	3 (3%) 45 24	71, 83, 106, 117	0
24	D2	129/129 (100%)	0.36	0 100 100	69, 83, 90, 99	0
24	d2	129/129 (100%)	0.15	0 100 100	56, 68, 78, 85	0
25	D3	144/144 (100%)	0.37	2 (1%) 75 56	61, 69, 83, 101	0
25	d3	144/144 (100%)	0.19	2 (1%) 75 56	51, 56, 70, 87	0
26	D4	134/134 (100%)	0.90	15 (11%) 5 2	83, 104, 120, 126	0
26	d4	134/134 (100%)	0.59	11 (8%) 11 4	61, 87, 101, 110	0
27	D5	70/70 (100%)	1.55	22 (31%) 0 0	123, 140, 145, 146	0
27	d5	69/70 (98%)	1.39	15 (21%) 0 0	92, 113, 123, 126	0
28	D6	97/97 (100%)	1.27	24 (24%) 0 0	78, 96, 144, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	d6	97/97 (100%)	0.48	4 (4%) 37 18	62, 78, 106, 112	0
29	D7	81/81 (100%)	0.83	10 (12%) 4 1	86, 104, 137, 138	0
29	d7	81/81 (100%)	0.66	8 (9%) 7 2	74, 92, 133, 136	0
30	D8	63/63 (100%)	1.42	17 (26%) 0 0	111, 131, 140, 142	0
30	d8	63/63 (100%)	1.66	21 (33%) 0 0	96, 115, 125, 132	0
31	D9	53/53 (100%)	0.64	4 (7%) 14 5	81, 86, 112, 118	0
31	d9	53/53 (100%)	1.37	14 (26%) 0 0	77, 94, 143, 158	0
32	E0	60/62 (96%)	1.43	14 (23%) 0 0	70, 103, 131, 136	0
32	e0	62/62 (100%)	0.82	8 (12%) 3 1	56, 84, 115, 127	0
33	E1	71/76 (93%)	1.53	19 (26%) 0 0	110, 142, 152, 154	0
33	e1	76/76 (100%)	3.08	48 (63%) 0 0	120, 187, 198, 200	0
34	SR	318/318 (100%)	1.12	67 (21%) 1 0	107, 124, 138, 158	0
34	sR	318/318 (100%)	1.32	79 (24%) 0 0	108, 128, 144, 156	0
35	SM	133/176 (75%)	0.99	21 (15%) 2 1	62, 94, 148, 159	0
36	1	3149/3396 (92%)	0.01	56 (1%) 68 47	31, 56, 138, 237	0
36	5	3150/3396 (92%)	-0.02	50 (1%) 72 51	29, 54, 127, 213	0
37	3	121/121 (100%)	-0.17	0 100 100	45, 83, 107, 113	0
37	7	121/121 (100%)	-0.26	0 100 100	36, 59, 72, 85	0
38	4	158/158 (100%)	-0.10	1 (0%) 89 78	36, 56, 97, 138	0
38	8	158/158 (100%)	-0.02	2 (1%) 77 59	42, 65, 107, 142	0
39	L2	252/252 (100%)	0.08	3 (1%) 79 61	37, 54, 70, 85	0
39	l2	252/252 (100%)	0.16	5 (1%) 65 44	40, 61, 80, 87	0
40	L3	386/386 (100%)	0.05	5 (1%) 77 59	39, 64, 80, 97	0
40	l3	386/386 (100%)	-0.16	2 (0%) 91 81	30, 46, 64, 92	0
41	L4	361/361 (100%)	-0.18	0 100 100	33, 49, 70, 78	0
41	l4	361/361 (100%)	-0.04	0 100 100	38, 57, 76, 87	0
42	L5	296/296 (100%)	0.73	34 (11%) 4 2	58, 91, 113, 136	0
42	l5	294/296 (99%)	0.16	7 (2%) 59 37	42, 64, 88, 109	0
43	L6	156/176 (88%)	0.02	1 (0%) 89 78	44, 55, 73, 84	0
43	l6	157/176 (89%)	0.05	2 (1%) 77 59	48, 56, 79, 92	0
44	L7	222/223 (99%)	-0.07	1 (0%) 91 81	39, 49, 80, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	l7	223/223 (100%)	-0.14	0 100 100	35, 45, 86, 119	0
45	L8	233/233 (100%)	0.53	9 (3%) 39 20	62, 79, 117, 130	0
46	L9	191/191 (100%)	0.19	5 (2%) 56 33	64, 76, 90, 106	0
46	l9	191/191 (100%)	-0.10	2 (1%) 82 67	43, 52, 72, 86	0
47	M0	211/221 (95%)	0.49	6 (2%) 53 30	44, 67, 103, 110	0
47	m0	213/221 (96%)	0.24	4 (1%) 66 46	37, 55, 83, 102	0
48	M1	169/169 (100%)	0.53	11 (6%) 18 8	75, 94, 108, 118	0
48	m1	169/169 (100%)	0.08	1 (0%) 89 78	47, 69, 81, 85	0
49	M3	193/194 (99%)	0.11	3 (1%) 72 51	36, 60, 100, 131	0
49	m3	194/194 (100%)	0.62	14 (7%) 15 6	42, 72, 112, 125	0
50	M4	136/137 (99%)	-0.08	2 (1%) 73 54	51, 61, 78, 91	0
50	m4	137/137 (100%)	-0.25	1 (0%) 87 75	44, 51, 68, 84	0
51	M5	203/203 (100%)	-0.02	0 100 100	36, 50, 61, 64	0
51	m5	203/203 (100%)	0.21	1 (0%) 91 81	45, 63, 76, 80	0
52	M6	197/197 (100%)	-0.06	0 100 100	39, 50, 72, 78	0
52	m6	197/197 (100%)	-0.14	1 (0%) 91 81	31, 37, 68, 76	0
53	M7	183/183 (100%)	0.54	14 (7%) 13 5	40, 49, 107, 132	0
53	m7	155/183 (84%)	-0.01	0 100 100	36, 45, 61, 89	0
54	M8	185/185 (100%)	-0.10	0 100 100	39, 49, 65, 85	0
54	m8	185/185 (100%)	-0.01	0 100 100	38, 56, 68, 74	0
55	M9	188/188 (100%)	0.41	10 (5%) 26 12	57, 72, 146, 153	0
55	m9	188/188 (100%)	0.21	6 (3%) 47 25	52, 66, 133, 143	0
56	N0	172/172 (100%)	0.14	2 (1%) 79 61	50, 60, 75, 81	0
56	n0	172/172 (100%)	-0.10	0 100 100	37, 45, 59, 73	0
57	N1	159/159 (100%)	0.20	3 (1%) 66 46	43, 57, 103, 110	0
57	n1	159/159 (100%)	0.04	3 (1%) 66 46	40, 47, 91, 97	0
58	N2	100/100 (100%)	0.65	10 (10%) 7 2	90, 104, 113, 114	0
58	n2	98/100 (98%)	1.22	22 (22%) 0 0	80, 92, 102, 105	0
59	N3	136/136 (100%)	0.36	4 (2%) 51 28	46, 60, 74, 83	0
59	n3	136/136 (100%)	0.23	4 (2%) 51 28	32, 43, 59, 67	0
60	N4	98/98 (100%)	2.05	32 (32%) 0 0	59, 72, 144, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
61	N5	121/121 (100%)	0.29	3 (2%) 57 34	50, 66, 79, 104	0
61	n5	120/121 (99%)	0.37	2 (1%) 70 49	56, 72, 90, 106	0
62	N6	126/126 (100%)	0.29	5 (3%) 38 19	42, 58, 72, 85	0
62	n6	126/126 (100%)	0.43	2 (1%) 72 51	50, 67, 84, 91	0
63	N7	135/135 (100%)	0.98	16 (11%) 4 2	75, 91, 103, 109	0
63	n7	135/135 (100%)	1.15	28 (20%) 1 0	87, 102, 115, 123	0
64	N8	148/148 (100%)	0.01	1 (0%) 87 75	30, 52, 77, 86	0
64	n8	148/148 (100%)	0.15	1 (0%) 87 75	34, 58, 80, 84	0
65	N9	58/58 (100%)	0.33	3 (5%) 27 12	37, 60, 105, 119	0
65	n9	58/58 (100%)	0.11	1 (1%) 70 49	37, 58, 83, 93	0
66	O0	97/100 (97%)	0.45	5 (5%) 27 12	75, 85, 106, 114	0
66	o0	100/100 (100%)	0.68	8 (8%) 12 5	79, 90, 114, 122	0
67	O1	109/109 (100%)	0.56	5 (4%) 32 16	55, 68, 96, 104	0
67	o1	109/109 (100%)	0.35	3 (2%) 53 30	44, 58, 91, 114	0
68	O2	127/127 (100%)	0.11	3 (2%) 59 37	34, 45, 59, 78	0
68	o2	127/127 (100%)	0.21	2 (1%) 72 51	33, 52, 68, 89	0
69	O3	106/106 (100%)	-0.10	0 100 100	40, 46, 68, 83	0
69	o3	106/106 (100%)	-0.00	1 (0%) 84 69	35, 43, 68, 84	0
70	O4	112/112 (100%)	0.49	5 (4%) 33 16	49, 70, 107, 115	0
70	o4	112/112 (100%)	0.34	3 (2%) 54 31	53, 74, 114, 119	0
71	O5	119/119 (100%)	0.25	3 (2%) 57 34	47, 68, 77, 80	0
71	o5	119/119 (100%)	0.36	4 (3%) 45 24	60, 78, 88, 98	0
72	O6	99/99 (100%)	0.54	6 (6%) 21 9	57, 68, 99, 114	0
72	o6	99/99 (100%)	0.77	12 (12%) 4 1	66, 79, 100, 115	0
73	O7	87/87 (100%)	0.00	3 (3%) 45 24	39, 44, 65, 77	0
73	o7	87/87 (100%)	0.20	2 (2%) 60 39	40, 51, 81, 100	0
74	O8	77/77 (100%)	0.84	7 (9%) 9 3	80, 92, 104, 107	0
74	o8	77/77 (100%)	1.29	14 (18%) 1 0	85, 96, 106, 108	0
75	O9	50/50 (100%)	0.07	0 100 100	46, 52, 58, 59	0
75	o9	50/50 (100%)	0.15	1 (2%) 65 44	48, 56, 67, 70	0
76	Q0	52/52 (100%)	0.48	5 (9%) 8 2	55, 65, 84, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
76	q0	52/52 (100%)	-0.11	0 100 100	38, 43, 58, 62	0
77	Q1	25/25 (100%)	0.49	0 100 100	57, 59, 62, 62	0
77	q1	25/25 (100%)	0.29	0 100 100	46, 52, 57, 60	0
78	Q2	105/105 (100%)	0.85	10 (9%) 8 2	42, 63, 90, 117	0
78	q2	105/105 (100%)	0.33	5 (4%) 30 14	46, 61, 83, 105	0
79	Q3	91/91 (100%)	0.03	0 100 100	45, 58, 76, 83	0
79	q3	91/91 (100%)	0.14	1 (1%) 80 64	43, 62, 77, 89	0
80	sM	63/159 (39%)	1.31	10 (15%) 1 1	53, 109, 119, 121	0
81	l8	231/231 (100%)	0.80	21 (9%) 9 3	77, 92, 121, 130	0
82	m2	0/155	-	-	-	-
83	n4	135/135 (100%)	0.86	20 (14%) 2 1	43, 90, 125, 142	0
84	p0	143/312 (45%)	1.46	40 (27%) 0 0	91, 112, 173, 175	0
85	p1	0/47	-	-	-	-
85	p2	0/47	-	-	-	-
All	All	33027/34321 (96%)	0.38	2176 (6%) 18 7	29, 74, 138, 248	0

The worst 5 of 2176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	c0	98	THR	15.8
60	N4	86	SER	15.2
60	N4	85	ALA	13.6
1	2	1702	A	13.5
1	2	1693	A	12.9

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	3963	1/1	0.28	0.33	74,74,74,74	0
87	MG	2	2032	1/1	0.38	0.34	77,77,77,77	0
88	ZN	D7	101	1/1	0.44	0.55	159,159,159,159	0
87	MG	6	2130	1/1	0.45	0.77	95,95,95,95	0
87	MG	1	3986	1/1	0.48	0.52	93,93,93,93	0
87	MG	1	4035	1/1	0.48	0.49	111,111,111,111	0
87	MG	1	3989	1/1	0.49	0.31	82,82,82,82	0
87	MG	6	2118	1/1	0.53	0.31	109,109,109,109	0
87	MG	6	2040	1/1	0.55	0.52	54,54,54,54	0
87	MG	2	2060	1/1	0.55	0.51	76,76,76,76	0
87	MG	5	3942	1/1	0.56	0.37	94,94,94,94	0
87	MG	1	4023	1/1	0.56	0.18	59,59,59,59	0
87	MG	2	2088	1/1	0.58	0.36	83,83,83,83	0
87	MG	5	3805	1/1	0.58	0.57	63,63,63,63	0
87	MG	c6	201	1/1	0.60	0.40	91,91,91,91	0
87	MG	7	218	1/1	0.61	0.32	67,67,67,67	0
87	MG	5	4096	1/1	0.61	0.21	73,73,73,73	0
87	MG	M3	201	1/1	0.62	0.43	98,98,98,98	0
87	MG	1	4000	1/1	0.62	0.47	39,39,39,39	0
87	MG	1	4021	1/1	0.64	0.37	43,43,43,43	1
87	MG	1	4062	1/1	0.64	0.23	56,56,56,56	0
87	MG	1	3962	1/1	0.64	0.59	59,59,59,59	0
87	MG	n9	101	1/1	0.65	0.35	46,46,46,46	0
87	MG	2	2108	1/1	0.65	0.88	131,131,131,131	0
87	MG	1	3795	1/1	0.66	0.38	77,77,77,77	0
87	MG	1	3951	1/1	0.66	0.33	51,51,51,51	0
87	MG	1	4050	1/1	0.66	0.63	55,55,55,55	0
87	MG	7	221	1/1	0.66	0.33	63,63,63,63	0
87	MG	2	2041	1/1	0.66	0.32	74,74,74,74	0
86	OHX	2	2022	7/7	0.66	0.16	250,250,250,254	7
87	MG	1	3944	1/1	0.67	1.26	59,59,59,59	0
87	MG	1	3750	1/1	0.67	0.43	46,46,46,46	0
87	MG	d6	102	1/1	0.68	0.44	66,66,66,66	0
87	MG	2	2114	1/1	0.68	0.23	105,105,105,105	0
87	MG	5	3985	1/1	0.69	0.58	50,50,50,50	0
87	MG	1	3853	1/1	0.69	0.52	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	3977	1/1	0.69	0.39	79,79,79,79	0
86	OHX	2	2027	7/7	0.70	0.49	72,73,74,103	7
87	MG	2	2072	1/1	0.70	0.50	99,99,99,99	0
87	MG	5	3954	1/1	0.70	0.60	65,65,65,65	0
87	MG	2	2047	1/1	0.70	0.51	61,61,61,61	0
87	MG	5	4093	1/1	0.70	0.45	78,78,78,78	0
87	MG	l2	303	1/1	0.71	0.38	44,44,44,44	0
87	MG	2	2078	1/1	0.71	0.38	68,68,68,68	0
87	MG	6	2132	1/1	0.71	0.45	85,85,85,85	0
87	MG	5	4104	1/1	0.72	0.44	52,52,52,52	0
87	MG	1	3981	1/1	0.72	0.18	66,66,66,66	0
87	MG	1	3922	1/1	0.72	0.66	63,63,63,63	0
87	MG	8	224	1/1	0.72	0.85	59,59,59,59	0
87	MG	1	3716	1/1	0.72	0.43	123,123,123,123	0
87	MG	6	2045	1/1	0.72	0.36	52,52,52,52	0
86	OHX	5	3681	7/7	0.72	0.33	96,97,98,130	7
87	MG	5	3731	1/1	0.73	0.34	49,49,49,49	0
87	MG	3	215	1/1	0.73	0.56	62,62,62,62	0
86	OHX	6	2034	7/7	0.74	0.48	84,85,86,112	7
87	MG	1	3923	1/1	0.74	0.13	69,69,69,69	0
87	MG	2	2050	1/1	0.74	0.67	67,67,67,67	0
87	MG	5	4099	1/1	0.75	0.34	41,41,41,41	0
87	MG	6	2121	1/1	0.75	0.30	49,49,49,49	0
87	MG	6	2124	1/1	0.75	0.57	84,84,84,84	0
87	MG	5	3729	1/1	0.75	0.40	41,41,41,41	0
87	MG	5	4059	1/1	0.75	0.34	47,47,47,47	1
87	MG	5	4074	1/1	0.75	0.81	55,55,55,55	0
87	MG	1	3918	1/1	0.75	0.58	58,58,58,58	0
86	OHX	5	3724	7/7	0.75	0.20	181,181,182,194	7
87	MG	5	4060	1/1	0.76	0.27	54,54,54,54	0
87	MG	6	2135	1/1	0.76	0.18	61,61,61,61	0
87	MG	1	3784	1/1	0.76	0.73	54,54,54,54	0
86	OHX	1	3688	7/7	0.76	0.24	158,158,159,172	7
87	MG	2	2068	1/1	0.76	0.57	86,86,86,86	0
87	MG	6	2056	1/1	0.76	0.92	64,64,64,64	0
87	MG	2	2055	1/1	0.76	0.38	86,86,86,86	0
87	MG	1	3752	1/1	0.76	0.26	68,68,68,68	0
87	MG	5	3943	1/1	0.76	0.40	84,84,84,84	0
87	MG	1	3759	1/1	0.76	0.48	48,48,48,48	0
87	MG	1	3767	1/1	0.76	0.73	59,59,59,59	0
87	MG	4	231	1/1	0.76	0.32	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	3982	1/1	0.77	0.25	52,52,52,52	0
87	MG	1	3915	1/1	0.77	0.36	63,63,63,63	0
86	OHX	6	2029	7/7	0.77	0.29	125,126,128,147	7
87	MG	6	2054	1/1	0.77	0.47	69,69,69,69	0
87	MG	5	4067	1/1	0.77	0.17	68,68,68,68	0
87	MG	1	4043	1/1	0.77	0.40	54,54,54,54	0
87	MG	1	3726	1/1	0.77	0.34	52,52,52,52	0
87	MG	1	3727	1/1	0.77	0.26	50,50,50,50	0
87	MG	5	3864	1/1	0.77	0.51	60,60,60,60	0
87	MG	5	3875	1/1	0.77	0.47	48,48,48,48	0
87	MG	5	3919	1/1	0.77	0.55	46,46,46,46	0
87	MG	2	2095	1/1	0.77	0.40	69,69,69,69	0
87	MG	1	3845	1/1	0.77	0.23	73,73,73,73	0
87	MG	5	3950	1/1	0.77	0.69	61,61,61,61	0
87	MG	5	3951	1/1	0.77	0.37	57,57,57,57	0
87	MG	2	2118	1/1	0.77	0.16	75,75,75,75	0
87	MG	5	3946	1/1	0.78	0.61	50,50,50,50	0
87	MG	2	2089	1/1	0.78	0.90	84,84,84,84	0
87	MG	1	4064	1/1	0.78	0.13	66,66,66,66	0
87	MG	1	3909	1/1	0.78	0.15	71,71,71,71	0
87	MG	5	3958	1/1	0.78	0.19	48,48,48,48	0
87	MG	4	227	1/1	0.78	0.49	56,56,56,56	0
87	MG	1	3994	1/1	0.78	0.38	58,58,58,58	0
87	MG	5	3986	1/1	0.78	0.17	49,49,49,49	0
87	MG	2	2092	1/1	0.78	0.25	61,61,61,61	0
87	MG	1	4019	1/1	0.78	0.36	40,40,40,40	0
87	MG	2	2083	1/1	0.78	0.57	98,98,98,98	0
87	MG	5	3737	1/1	0.78	0.29	49,49,49,49	0
87	MG	5	3774	1/1	0.78	0.35	46,46,46,46	0
87	MG	5	3793	1/1	0.78	0.38	43,43,43,43	0
87	MG	1	3973	1/1	0.78	0.14	57,57,57,57	0
87	MG	2	2098	1/1	0.78	0.19	107,107,107,107	0
87	MG	5	3869	1/1	0.78	0.45	47,47,47,47	0
87	MG	6	2110	1/1	0.78	0.16	49,49,49,49	0
87	MG	6	2115	1/1	0.78	0.17	56,56,56,56	0
87	MG	5	3935	1/1	0.78	0.42	43,43,43,43	0
87	MG	1	3757	1/1	0.78	0.23	50,50,50,50	0
87	MG	1	3982	1/1	0.78	0.40	56,56,56,56	0
87	MG	1	3946	1/1	0.79	0.29	32,32,32,32	0
87	MG	1	3718	1/1	0.79	0.67	46,46,46,46	0
87	MG	5	3760	1/1	0.79	0.29	42,42,42,42	0
87	MG	2	2112	1/1	0.79	0.50	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	N8	202	1/1	0.79	0.50	41,41,41,41	0
86	OHX	6	2037	7/7	0.79	0.23	115,116,117,137	7
87	MG	1	4059	1/1	0.79	0.39	69,69,69,69	0
87	MG	2	2103	1/1	0.79	0.28	93,93,93,93	0
87	MG	2	2074	1/1	0.79	0.34	107,107,107,107	0
87	MG	6	2092	1/1	0.79	0.48	61,61,61,61	0
87	MG	5	4000	1/1	0.79	0.15	61,61,61,61	0
87	MG	5	4024	1/1	0.79	0.19	55,55,55,55	0
87	MG	1	3717	1/1	0.79	0.24	45,45,45,45	0
88	ZN	q2	501	1/1	0.79	0.38	107,107,107,107	0
87	MG	5	3780	1/1	0.80	0.12	47,47,47,47	0
87	MG	1	3912	1/1	0.80	0.54	63,63,63,63	0
87	MG	5	3803	1/1	0.80	0.22	53,53,53,53	0
87	MG	1	3764	1/1	0.80	0.47	60,60,60,60	0
87	MG	5	3860	1/1	0.80	0.43	40,40,40,40	0
87	MG	2	2097	1/1	0.80	0.50	65,65,65,65	0
87	MG	2	2115	1/1	0.80	0.66	66,66,66,66	0
86	OHX	5	3710	7/7	0.80	0.24	106,106,107,137	7
87	MG	M7	203	1/1	0.80	0.45	69,69,69,69	0
87	MG	1	4036	1/1	0.80	0.55	54,54,54,54	0
87	MG	1	4037	1/1	0.80	0.49	62,62,62,62	0
87	MG	2	2040	1/1	0.80	0.50	80,80,80,80	0
86	OHX	5	3715	7/7	0.80	0.43	62,64,66,97	7
86	OHX	1	3685	7/7	0.80	0.26	106,107,109,129	7
87	MG	6	2067	1/1	0.80	0.72	65,65,65,65	0
87	MG	6	2077	1/1	0.80	0.65	75,75,75,75	0
87	MG	n6	201	1/1	0.80	0.28	69,69,69,69	0
87	MG	n8	202	1/1	0.80	0.29	51,51,51,51	0
87	MG	6	2091	1/1	0.80	0.49	60,60,60,60	0
87	MG	5	3981	1/1	0.80	0.26	84,84,84,84	0
87	MG	1	3958	1/1	0.80	0.36	45,45,45,45	0
87	MG	5	4039	1/1	0.81	0.44	45,45,45,45	0
87	MG	5	3887	1/1	0.81	0.55	37,37,37,37	0
87	MG	2	2037	1/1	0.81	0.38	77,77,77,77	0
87	MG	6	2063	1/1	0.81	0.40	52,52,52,52	0
86	OHX	1	3644	7/7	0.81	0.20	140,141,142,164	7
87	MG	6	2071	1/1	0.81	0.58	52,52,52,52	0
87	MG	1	3972	1/1	0.81	0.27	46,46,46,46	0
87	MG	4	220	1/1	0.81	0.58	53,53,53,53	0
87	MG	D3	201	1/1	0.81	0.18	64,64,64,64	0
87	MG	7	217	1/1	0.81	0.43	44,44,44,44	0
87	MG	1	4026	1/1	0.81	0.31	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	3930	1/1	0.81	0.29	50,50,50,50	0
87	MG	1	3943	1/1	0.81	0.37	78,78,78,78	0
87	MG	l2	302	1/1	0.81	0.38	51,51,51,51	0
87	MG	M9	202	1/1	0.81	0.21	79,79,79,79	0
86	OHX	6	2020	7/7	0.81	0.37	58,58,60,94	7
87	MG	2	2100	1/1	0.81	0.56	68,68,68,68	0
87	MG	1	3913	1/1	0.81	0.34	54,54,54,54	0
87	MG	5	4008	1/1	0.81	0.29	52,52,52,52	0
87	MG	1	3792	1/1	0.81	0.24	53,53,53,53	0
87	MG	5	3838	1/1	0.82	0.38	42,42,42,42	0
87	MG	5	4001	1/1	0.82	0.21	49,49,49,49	0
87	MG	5	4005	1/1	0.82	0.40	43,43,43,43	0
86	OHX	1	3667	7/7	0.82	0.41	57,58,60,89	7
87	MG	2	2116	1/1	0.82	0.30	64,64,64,64	0
86	OHX	5	3708	7/7	0.82	0.20	86,87,88,116	7
87	MG	1	4044	1/1	0.82	0.65	57,57,57,57	0
86	OHX	1	3596	7/7	0.82	0.21	84,84,87,118	7
86	OHX	2	1970	7/7	0.82	0.17	132,137,138,157	7
87	MG	5	3754	1/1	0.82	0.35	39,39,39,39	0
87	MG	5	3938	1/1	0.82	0.31	37,37,37,37	0
87	MG	1	3964	1/1	0.82	0.28	44,44,44,44	0
86	OHX	5	3716	7/7	0.82	0.33	61,64,65,102	7
87	MG	5	3777	1/1	0.82	0.34	32,32,32,32	0
87	MG	7	213	1/1	0.82	0.44	27,27,27,27	0
87	MG	1	3901	1/1	0.82	0.17	46,46,46,46	0
87	MG	5	3786	1/1	0.82	0.58	34,34,34,34	0
87	MG	5	3787	1/1	0.82	0.36	59,59,59,59	0
87	MG	5	3788	1/1	0.82	0.38	86,86,86,86	0
87	MG	5	3974	1/1	0.82	0.13	84,84,84,84	0
87	MG	5	3980	1/1	0.82	0.43	77,77,77,77	0
87	MG	5	3790	1/1	0.82	0.17	110,110,110,110	0
87	MG	1	3907	1/1	0.82	0.41	42,42,42,42	0
87	MG	6	2131	1/1	0.82	0.69	60,60,60,60	0
86	OHX	1	3693	7/7	0.82	0.38	55,57,58,91	7
87	MG	5	3998	1/1	0.82	0.85	71,71,71,71	0
86	OHX	5	3709	7/7	0.83	0.43	45,45,47,82	7
87	MG	1	3979	1/1	0.83	0.23	54,54,54,54	0
86	OHX	6	1989	7/7	0.83	0.30	72,73,75,105	7
87	MG	6	2123	1/1	0.83	0.16	62,62,62,62	0
87	MG	5	4071	1/1	0.83	0.37	55,55,55,55	0
87	MG	1	3945	1/1	0.83	0.53	57,57,57,57	0
86	OHX	6	2006	7/7	0.83	0.34	87,87,88,112	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	4047	1/1	0.83	0.46	59,59,59,59	0
86	OHX	5	3519	7/7	0.83	0.23	133,136,138,156	7
87	MG	1	4052	1/1	0.83	0.21	75,75,75,75	0
87	MG	1	3991	1/1	0.83	0.40	61,61,61,61	0
87	MG	1	3732	1/1	0.83	0.41	50,50,50,50	0
87	MG	1	3794	1/1	0.83	0.43	61,61,61,61	0
86	OHX	5	3722	7/7	0.83	0.33	69,69,70,99	7
87	MG	5	3995	1/1	0.83	0.39	53,53,53,53	0
86	OHX	2	2003	7/7	0.83	0.25	81,83,83,114	7
87	MG	5	3748	1/1	0.83	0.22	47,47,47,47	0
86	OHX	1	3703	7/7	0.83	0.34	55,57,58,89	7
87	MG	6	2102	1/1	0.83	0.36	61,61,61,61	0
87	MG	5	4007	1/1	0.83	0.20	56,56,56,56	0
87	MG	1	3879	1/1	0.83	0.43	39,39,39,39	0
87	MG	5	3941	1/1	0.83	0.21	53,53,53,53	0
87	MG	1	3733	1/1	0.84	0.27	51,51,51,51	0
86	OHX	2	2024	7/7	0.84	0.21	116,116,118,142	7
87	MG	5	3808	1/1	0.84	0.30	41,41,41,41	0
87	MG	2	2080	1/1	0.84	0.54	88,88,88,88	0
87	MG	5	4083	1/1	0.84	0.24	53,53,53,53	0
87	MG	5	3739	1/1	0.84	0.24	71,71,71,71	0
87	MG	5	3740	1/1	0.84	0.35	40,40,40,40	0
87	MG	1	3961	1/1	0.84	0.25	63,63,63,63	0
87	MG	1	3797	1/1	0.84	0.43	52,52,52,52	0
87	MG	2	2096	1/1	0.84	0.12	107,107,107,107	0
87	MG	5	3761	1/1	0.84	0.56	48,48,48,48	0
87	MG	6	2049	1/1	0.84	0.53	50,50,50,50	0
87	MG	1	4009	1/1	0.84	0.59	65,65,65,65	0
86	OHX	6	2030	7/7	0.84	0.38	68,69,70,102	7
87	MG	1	3927	1/1	0.84	0.24	50,50,50,50	0
86	OHX	1	3674	7/7	0.84	0.18	114,116,116,146	7
87	MG	2	2099	1/1	0.84	0.58	74,74,74,74	0
87	MG	5	4028	1/1	0.84	0.38	80,80,80,80	0
87	MG	1	3772	1/1	0.84	0.29	44,44,44,44	0
87	MG	5	4047	1/1	0.84	0.28	44,44,44,44	0
86	OHX	1	3659	7/7	0.84	0.16	131,131,133,156	7
89	UAM	6	2134	30/30	0.84	0.43	75,75,75,75	0
87	MG	6	2060	1/1	0.85	0.41	86,86,86,86	0
86	OHX	5	3644	7/7	0.85	0.24	53,57,59,103	7
86	OHX	5	3646	7/7	0.85	0.25	77,78,79,104	7
86	OHX	2	2026	7/7	0.85	0.27	104,105,106,127	7
87	MG	5	3921	1/1	0.85	0.48	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	4010	1/1	0.85	0.28	68,68,68,68	0
87	MG	6	2080	1/1	0.85	0.46	51,51,51,51	0
86	OHX	6	1958	7/7	0.85	0.25	67,68,70,109	7
86	OHX	6	2013	7/7	0.85	0.15	163,163,164,174	7
87	MG	5	4068	1/1	0.85	0.63	61,61,61,61	0
87	MG	1	3966	1/1	0.85	0.52	50,50,50,50	0
87	MG	5	4073	1/1	0.85	0.31	40,40,40,40	0
87	MG	L7	303	1/1	0.85	0.19	48,48,48,48	0
87	MG	5	4082	1/1	0.85	0.28	48,48,48,48	0
87	MG	1	3938	1/1	0.85	0.56	48,48,48,48	0
87	MG	1	3731	1/1	0.85	0.24	39,39,39,39	0
86	OHX	7	211	7/7	0.85	0.21	79,80,80,112	7
87	MG	2	2054	1/1	0.85	0.42	53,53,53,53	0
87	MG	6	2038	1/1	0.85	0.52	51,51,51,51	0
87	MG	5	3979	1/1	0.85	0.21	53,53,53,53	0
87	MG	1	3736	1/1	0.85	0.45	44,44,44,44	0
87	MG	1	3949	1/1	0.85	0.34	47,47,47,47	0
87	MG	6	2047	1/1	0.85	0.41	53,53,53,53	0
87	MG	1	3950	1/1	0.85	0.14	61,61,61,61	0
87	MG	c1	201	1/1	0.85	0.48	52,52,52,52	0
87	MG	5	3811	1/1	0.85	0.34	50,50,50,50	0
87	MG	5	3996	1/1	0.85	0.28	50,50,50,50	0
87	MG	5	3816	1/1	0.85	0.52	51,51,51,51	0
87	MG	5	3999	1/1	0.85	0.52	67,67,67,67	0
86	OHX	l4	401	7/7	0.85	0.28	62,62,63,86	7
87	MG	1	3954	1/1	0.85	0.36	54,54,54,54	0
87	MG	5	3728	1/1	0.85	0.15	46,46,46,46	0
86	OHX	m4	201	7/7	0.86	0.24	124,124,124,140	7
87	MG	1	3956	1/1	0.86	0.90	69,69,69,69	0
87	MG	5	3791	1/1	0.86	0.33	39,39,39,39	0
87	MG	2	2081	1/1	0.86	0.78	60,60,60,60	0
87	MG	5	3802	1/1	0.86	0.13	74,74,74,74	0
87	MG	6	2106	1/1	0.86	0.32	48,48,48,48	0
87	MG	1	3960	1/1	0.86	0.40	53,53,53,53	0
87	MG	1	3799	1/1	0.86	0.44	48,48,48,48	0
87	MG	1	3822	1/1	0.86	0.39	50,50,50,50	0
87	MG	5	3812	1/1	0.86	0.15	51,51,51,51	0
87	MG	5	4030	1/1	0.86	0.46	81,81,81,81	0
87	MG	2	2031	1/1	0.86	0.65	50,50,50,50	0
87	MG	2	2085	1/1	0.86	0.49	74,74,74,74	0
87	MG	5	4050	1/1	0.86	0.26	48,48,48,48	0
87	MG	5	4058	1/1	0.86	0.17	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	M9	201	7/7	0.86	0.16	98,98,99,123	7
86	OHX	5	3682	7/7	0.86	0.19	77,78,79,115	7
87	MG	5	4062	1/1	0.86	0.39	36,36,36,36	1
86	OHX	5	3689	7/7	0.86	0.28	80,80,81,104	7
86	OHX	2	1973	7/7	0.86	0.28	102,102,104,125	7
87	MG	L7	301	1/1	0.86	0.18	47,47,47,47	0
86	OHX	1	3555	7/7	0.86	0.23	90,92,93,115	7
86	OHX	6	2035	7/7	0.86	0.43	113,114,115,138	7
86	OHX	2	1989	7/7	0.86	0.26	94,95,97,121	7
87	MG	1	3985	1/1	0.86	0.56	44,44,44,44	0
86	OHX	1	3605	7/7	0.86	0.24	72,74,76,101	7
86	OHX	5	3720	7/7	0.86	0.42	75,76,77,111	7
86	OHX	5	3632	7/7	0.86	0.19	146,147,148,168	7
87	MG	1	3924	1/1	0.86	0.19	61,61,61,61	0
87	MG	1	3758	1/1	0.86	0.27	47,47,47,47	0
87	MG	5	3747	1/1	0.86	0.30	40,40,40,40	0
86	OHX	1	3705	7/7	0.86	0.23	61,62,64,96	7
87	MG	2	2111	1/1	0.86	0.42	91,91,91,91	0
87	MG	5	3756	1/1	0.86	0.33	61,61,61,61	0
87	MG	2	2073	1/1	0.86	0.35	101,101,101,101	0
87	MG	2	2113	1/1	0.86	0.53	61,61,61,61	0
87	MG	1	3781	1/1	0.86	0.37	42,42,42,42	0
86	OHX	6	2024	7/7	0.86	0.28	90,90,92,119	7
87	MG	1	3789	1/1	0.86	0.24	43,43,43,43	0
86	OHX	5	3651	7/7	0.86	0.29	47,47,49,84	7
88	ZN	d7	101	1/1	0.86	0.23	142,142,142,142	0
87	MG	5	3989	1/1	0.86	0.37	40,40,40,40	0
87	MG	2	2079	1/1	0.86	0.47	58,58,58,58	0
86	OHX	6	2004	7/7	0.87	0.17	96,97,99,128	7
87	MG	6	2101	1/1	0.87	0.30	72,72,72,72	0
86	OHX	1	3673	7/7	0.87	0.22	97,98,101,124	7
87	MG	2	2091	1/1	0.87	0.58	64,64,64,64	0
87	MG	6	2107	1/1	0.87	0.62	61,61,61,61	0
87	MG	2	2117	1/1	0.87	0.37	95,95,95,95	0
87	MG	6	2111	1/1	0.87	0.28	54,54,54,54	0
87	MG	5	4012	1/1	0.87	0.32	40,40,40,40	0
87	MG	1	3969	1/1	0.87	0.43	57,57,57,57	0
86	OHX	5	3684	7/7	0.87	0.16	73,74,76,109	7
87	MG	S2	301	1/1	0.87	0.81	68,68,68,68	0
87	MG	2	2093	1/1	0.87	0.72	61,61,61,61	0
87	MG	5	3844	1/1	0.87	0.26	48,48,48,48	0
87	MG	5	3847	1/1	0.87	0.40	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	4052	1/1	0.87	0.21	34,34,34,34	0
87	MG	5	4055	1/1	0.87	0.63	47,47,47,47	1
86	OHX	8	213	7/7	0.87	0.21	80,82,83,117	7
86	OHX	5	3687	7/7	0.87	0.14	143,144,145,163	7
86	OHX	1	3712	7/7	0.87	0.21	84,88,89,117	7
86	OHX	2	2012	7/7	0.87	0.19	128,128,129,143	7
86	OHX	1	3698	7/7	0.87	0.12	168,168,168,180	7
87	MG	M5	303	1/1	0.87	0.25	49,49,49,49	0
87	MG	5	4069	1/1	0.87	0.42	70,70,70,70	0
86	OHX	5	3639	7/7	0.87	0.17	84,84,85,116	7
87	MG	M7	204	1/1	0.87	0.41	42,42,42,42	0
87	MG	1	3942	1/1	0.87	0.45	47,47,47,47	0
86	OHX	6	1974	7/7	0.87	0.26	67,70,73,106	7
87	MG	1	3996	1/1	0.87	0.28	47,47,47,47	0
86	OHX	2	2019	7/7	0.87	0.18	112,113,113,139	7
87	MG	1	3825	1/1	0.87	0.43	38,38,38,38	0
87	MG	1	3835	1/1	0.87	0.47	58,58,58,58	0
87	MG	5	3741	1/1	0.87	0.14	29,29,29,29	0
87	MG	2	2082	1/1	0.87	0.57	60,60,60,60	0
87	MG	6	2051	1/1	0.87	0.43	75,75,75,75	0
87	MG	1	3852	1/1	0.87	0.51	38,38,38,38	0
87	MG	5	3978	1/1	0.87	0.22	39,39,39,39	0
86	OHX	5	3718	7/7	0.87	0.26	76,78,79,104	7
87	MG	l2	301	1/1	0.87	0.91	53,53,53,53	0
87	MG	1	3855	1/1	0.87	0.51	47,47,47,47	0
86	OHX	6	2032	7/7	0.87	0.28	76,77,78,101	7
87	MG	1	3957	1/1	0.87	0.34	50,50,50,50	0
87	MG	n8	201	1/1	0.87	0.36	53,53,53,53	0
87	MG	1	3880	1/1	0.87	0.10	51,51,51,51	0
87	MG	6	2073	1/1	0.87	0.53	94,94,94,94	0
87	MG	5	3988	1/1	0.87	0.12	64,64,64,64	0
87	MG	1	4039	1/1	0.87	0.22	55,55,55,55	0
87	MG	1	3887	1/1	0.87	0.46	39,39,39,39	0
87	MG	1	3889	1/1	0.87	0.75	45,45,45,45	0
87	MG	5	4044	1/1	0.88	0.35	42,42,42,42	0
87	MG	2	2090	1/1	0.88	0.36	60,60,60,60	0
87	MG	1	3998	1/1	0.88	0.26	44,44,44,44	0
86	OHX	1	3702	7/7	0.88	0.21	94,95,96,121	7
86	OHX	5	3677	7/7	0.88	0.20	99,100,102,127	7
87	MG	1	3810	1/1	0.88	0.42	48,48,48,48	0
87	MG	M3	202	1/1	0.88	0.40	38,38,38,38	0
87	MG	2	2076	1/1	0.88	0.51	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	2	2077	1/1	0.88	0.53	95,95,95,95	0
87	MG	5	3960	1/1	0.88	0.52	54,54,54,54	0
87	MG	1	4022	1/1	0.88	0.19	53,53,53,53	0
87	MG	5	3977	1/1	0.88	0.42	79,79,79,79	0
86	OHX	1	3627	7/7	0.88	0.20	94,94,96,126	7
87	MG	5	4072	1/1	0.88	0.36	67,67,67,67	0
87	MG	N8	201	1/1	0.88	0.31	33,33,33,33	0
87	MG	5	3796	1/1	0.88	0.23	36,36,36,36	0
87	MG	5	3801	1/1	0.88	0.59	37,37,37,37	0
87	MG	6	2128	1/1	0.88	0.55	54,54,54,54	0
86	OHX	1	3641	7/7	0.88	0.26	77,77,78,103	7
86	OHX	2	1968	7/7	0.88	0.26	113,114,115,142	7
86	OHX	5	3685	7/7	0.88	0.17	66,67,68,108	7
87	MG	1	3936	1/1	0.88	0.71	56,56,56,56	0
86	OHX	6	2017	7/7	0.88	0.21	96,96,98,122	7
87	MG	1	4042	1/1	0.88	0.32	55,55,55,55	0
87	MG	1	3862	1/1	0.88	0.38	38,38,38,38	0
87	MG	7	220	1/1	0.88	0.27	56,56,56,56	0
87	MG	1	3778	1/1	0.88	0.34	34,34,34,34	0
87	MG	8	219	1/1	0.88	0.68	62,62,62,62	0
87	MG	1	3980	1/1	0.88	0.35	53,53,53,53	0
86	OHX	4	217	7/7	0.88	0.40	61,63,64,98	7
87	MG	2	2104	1/1	0.88	0.31	65,65,65,65	0
87	MG	1	4058	1/1	0.88	0.24	38,38,38,38	0
86	OHX	1	3651	7/7	0.88	0.38	62,63,67,100	7
87	MG	n6	202	1/1	0.88	0.24	51,51,51,51	0
86	OHX	1	3604	7/7	0.88	0.29	54,56,56,93	7
87	MG	5	4021	1/1	0.88	0.28	44,44,44,44	0
87	MG	1	3903	1/1	0.88	0.31	68,68,68,68	0
87	MG	q0	202	1/1	0.88	0.20	53,53,53,53	0
87	MG	1	3905	1/1	0.88	0.35	51,51,51,51	0
87	MG	4	201	1/1	0.88	0.22	56,56,56,56	0
87	MG	5	4037	1/1	0.88	0.39	52,52,52,52	0
86	OHX	2	2023	7/7	0.88	0.31	76,77,79,101	7
87	MG	4	232	1/1	0.89	0.67	59,59,59,59	0
87	MG	1	3968	1/1	0.89	0.57	49,49,49,49	0
87	MG	1	3868	1/1	0.89	0.71	52,52,52,52	0
87	MG	5	3734	1/1	0.89	0.29	53,53,53,53	0
86	OHX	5	3706	7/7	0.89	0.30	57,58,59,88	7
86	OHX	2	2018	7/7	0.89	0.18	116,117,118,136	7
86	OHX	2	1953	7/7	0.89	0.20	85,86,88,118	7
86	OHX	2	2021	7/7	0.89	0.26	64,65,66,101	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	3743	1/1	0.89	0.52	74,74,74,74	0
86	OHX	O1	201	7/7	0.89	0.18	89,91,92,109	7
86	OHX	6	1928	7/7	0.89	0.15	138,141,142,159	7
87	MG	5	3753	1/1	0.89	0.17	65,65,65,65	0
87	MG	N3	201	1/1	0.89	0.28	43,43,43,43	0
86	OHX	s4	301	7/7	0.89	0.27	85,86,87,117	7
86	OHX	c3	201	7/7	0.89	0.19	102,103,104,130	7
87	MG	1	3908	1/1	0.89	0.38	42,42,42,42	0
87	MG	5	3772	1/1	0.89	0.39	41,41,41,41	1
87	MG	2	2087	1/1	0.89	0.45	84,84,84,84	0
87	MG	1	3743	1/1	0.89	0.17	53,53,53,53	0
87	MG	5	4017	1/1	0.89	0.10	68,68,68,68	0
87	MG	1	3745	1/1	0.89	0.26	44,44,44,44	0
86	OHX	2	1998	7/7	0.89	0.23	97,97,100,119	7
87	MG	5	4027	1/1	0.89	0.22	56,56,56,56	0
86	OHX	5	3572	7/7	0.89	0.32	61,63,65,101	7
87	MG	1	3920	1/1	0.89	0.28	44,44,44,44	0
86	OHX	5	3601	7/7	0.89	0.26	83,85,88,109	7
86	OHX	8	212	7/7	0.89	0.43	72,73,74,109	7
87	MG	5	4040	1/1	0.89	0.22	40,40,40,40	0
86	OHX	5	3604	7/7	0.89	0.12	110,112,113,139	7
87	MG	1	3925	1/1	0.89	0.37	44,44,44,44	0
87	MG	6	2069	1/1	0.89	0.66	72,72,72,72	0
86	OHX	8	216	7/7	0.89	0.24	84,85,86,112	7
86	OHX	5	3629	7/7	0.89	0.20	99,99,101,126	7
86	OHX	2	1974	7/7	0.89	0.25	101,101,104,126	7
86	OHX	1	3634	7/7	0.89	0.43	72,73,74,107	7
86	OHX	5	3640	7/7	0.89	0.35	63,63,66,91	7
86	OHX	6	1994	7/7	0.89	0.17	127,128,128,142	7
87	MG	5	4066	1/1	0.89	0.69	60,60,60,60	0
87	MG	6	2095	1/1	0.89	0.52	52,52,52,52	0
87	MG	5	3836	1/1	0.89	0.60	27,27,27,27	0
87	MG	6	2100	1/1	0.89	0.37	73,73,73,73	0
87	MG	2	2039	1/1	0.89	0.48	64,64,64,64	0
86	OHX	2	2006	7/7	0.89	0.16	114,116,116,135	7
86	OHX	1	3700	7/7	0.89	0.23	67,68,69,95	7
87	MG	2	2105	1/1	0.89	0.79	57,57,57,57	0
87	MG	5	4078	1/1	0.89	0.38	37,37,37,37	0
87	MG	2	2045	1/1	0.89	0.57	50,50,50,50	0
86	OHX	5	3658	7/7	0.89	0.25	56,57,60,98	7
87	MG	5	4091	1/1	0.89	0.42	52,52,52,52	0
87	MG	6	2113	1/1	0.89	0.31	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	4094	1/1	0.89	0.24	70,70,70,70	0
87	MG	5	3916	1/1	0.89	0.12	46,46,46,46	0
86	OHX	5	3668	7/7	0.89	0.39	101,102,103,131	7
86	OHX	6	2007	7/7	0.89	0.24	85,86,87,119	7
87	MG	5	3933	1/1	0.89	0.92	60,60,60,60	0
87	MG	7	215	1/1	0.89	0.53	30,30,30,30	0
87	MG	5	3934	1/1	0.89	0.52	52,52,52,52	0
87	MG	6	2120	1/1	0.89	0.81	58,58,58,58	0
86	OHX	2	1984	7/7	0.89	0.20	85,85,89,120	7
87	MG	1	3827	1/1	0.89	0.42	30,30,30,30	0
86	OHX	2	2013	7/7	0.89	0.14	120,120,121,141	7
87	MG	6	2126	1/1	0.89	0.51	63,63,63,63	0
87	MG	3	209	1/1	0.89	0.18	89,89,89,89	0
87	MG	5	3948	1/1	0.89	0.19	40,40,40,40	0
86	OHX	1	3704	7/7	0.89	0.26	68,69,70,101	7
86	OHX	S9	201	7/7	0.89	0.25	85,86,87,114	7
86	OHX	6	2027	7/7	0.89	0.21	82,82,85,113	7
87	MG	5	3957	1/1	0.89	0.35	65,65,65,65	0
87	MG	4	221	1/1	0.89	0.53	48,48,48,48	0
87	MG	4	223	1/1	0.89	0.77	31,31,31,31	0
87	MG	5	3963	1/1	0.89	0.40	55,55,55,55	0
87	MG	5	3964	1/1	0.89	0.68	49,49,49,49	0
88	ZN	Q2	501	1/1	0.89	0.27	107,107,107,107	0
86	OHX	1	3709	7/7	0.89	0.19	79,80,81,112	7
87	MG	5	3975	1/1	0.89	0.24	42,42,42,42	0
86	OHX	5	3702	7/7	0.89	0.21	79,80,80,110	7
87	MG	1	3965	1/1	0.90	0.34	46,46,46,46	0
86	OHX	1	3642	7/7	0.90	0.26	50,50,53,86	7
87	MG	1	3871	1/1	0.90	0.45	45,45,45,45	0
87	MG	5	3733	1/1	0.90	0.25	46,46,46,46	0
87	MG	L7	302	1/1	0.90	0.56	49,49,49,49	0
87	MG	5	3736	1/1	0.90	0.34	39,39,39,39	0
86	OHX	3	205	7/7	0.90	0.18	88,89,90,118	7
86	OHX	6	2014	7/7	0.90	0.27	94,95,97,120	7
87	MG	5	3987	1/1	0.90	0.36	43,43,43,43	0
86	OHX	5	3721	7/7	0.90	0.20	111,113,114,141	7
87	MG	1	3976	1/1	0.90	0.18	51,51,51,51	0
87	MG	5	3994	1/1	0.90	0.35	49,49,49,49	0
86	OHX	3	207	7/7	0.90	0.17	108,108,110,132	7
87	MG	5	3745	1/1	0.90	0.11	40,40,40,40	0
86	OHX	3	208	7/7	0.90	0.26	96,97,97,118	7
86	OHX	7	209	7/7	0.90	0.30	77,78,81,100	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	3742	1/1	0.90	0.36	44,44,44,44	0
86	OHX	2	2017	7/7	0.90	0.13	145,145,146,164	7
86	OHX	6	2026	7/7	0.90	0.32	64,64,66,98	7
86	OHX	S8	301	7/7	0.90	0.15	113,114,115,138	7
86	OHX	8	215	7/7	0.90	0.28	70,71,75,101	7
87	MG	6	2044	1/1	0.90	0.46	75,75,75,75	0
86	OHX	1	3696	7/7	0.90	0.28	45,47,49,83	7
87	MG	5	4020	1/1	0.90	0.18	47,47,47,47	0
86	OHX	5	3661	7/7	0.90	0.23	92,93,94,128	7
87	MG	5	4022	1/1	0.90	0.36	59,59,59,59	0
87	MG	5	3778	1/1	0.90	0.35	34,34,34,34	0
86	OHX	1	3653	7/7	0.90	0.23	48,50,53,92	7
86	OHX	6	1954	7/7	0.90	0.14	152,153,154,166	7
86	OHX	1	3606	7/7	0.90	0.32	39,40,42,80	7
87	MG	1	4007	1/1	0.90	0.38	52,52,52,52	0
87	MG	6	2057	1/1	0.90	0.47	48,48,48,48	0
87	MG	1	3771	1/1	0.90	0.38	33,33,33,33	0
87	MG	5	4042	1/1	0.90	0.12	39,39,39,39	0
87	MG	2	2036	1/1	0.90	0.32	82,82,82,82	0
87	MG	6	2065	1/1	0.90	0.69	61,61,61,61	0
87	MG	5	3798	1/1	0.90	0.45	71,71,71,71	0
86	OHX	6	1960	7/7	0.90	0.28	66,68,71,107	7
86	OHX	2	1945	7/7	0.90	0.13	110,111,113,137	7
86	OHX	6	1979	7/7	0.90	0.20	87,88,90,120	7
87	MG	1	3933	1/1	0.90	0.22	49,49,49,49	0
87	MG	6	2075	1/1	0.90	0.20	34,34,34,34	0
87	MG	1	4024	1/1	0.90	0.46	63,63,63,63	0
87	MG	5	4063	1/1	0.90	0.44	48,48,48,48	0
87	MG	1	3935	1/1	0.90	0.53	40,40,40,40	0
87	MG	6	2088	1/1	0.90	0.45	45,45,45,45	0
86	OHX	s8	301	7/7	0.90	0.14	105,105,106,130	7
86	OHX	2	2002	7/7	0.90	0.26	111,111,114,134	7
87	MG	6	2094	1/1	0.90	0.25	98,98,98,98	0
87	MG	2	2046	1/1	0.90	0.45	71,71,71,71	0
86	OHX	5	3692	7/7	0.90	0.26	55,57,59,90	7
86	OHX	5	3694	7/7	0.90	0.28	59,60,60,88	7
87	MG	2	2052	1/1	0.90	0.70	66,66,66,66	0
87	MG	5	4080	1/1	0.90	0.36	52,52,52,52	0
87	MG	5	3870	1/1	0.90	0.81	50,50,50,50	0
87	MG	5	3872	1/1	0.90	0.64	49,49,49,49	0
87	MG	1	3801	1/1	0.90	0.56	74,74,74,74	0
87	MG	1	3948	1/1	0.90	0.32	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	3889	1/1	0.90	0.47	45,45,45,45	0
86	OHX	5	3695	7/7	0.90	0.21	73,74,75,102	7
87	MG	1	4051	1/1	0.90	0.22	76,76,76,76	0
87	MG	5	4103	1/1	0.90	0.31	49,49,49,49	0
87	MG	5	3920	1/1	0.90	0.37	39,39,39,39	0
87	MG	5	4107	1/1	0.90	0.34	46,46,46,46	0
87	MG	6	2112	1/1	0.90	0.36	59,59,59,59	0
87	MG	1	3812	1/1	0.90	0.64	34,34,34,34	0
86	OHX	5	3696	7/7	0.90	0.24	68,69,69,96	7
87	MG	6	2117	1/1	0.90	0.57	69,69,69,69	0
86	OHX	c5	201	7/7	0.90	0.12	134,134,135,148	7
87	MG	2	2067	1/1	0.90	0.20	71,71,71,71	0
87	MG	7	222	1/1	0.90	0.17	59,59,59,59	0
86	OHX	sR	401	7/7	0.90	0.14	136,137,137,158	7
87	MG	8	223	1/1	0.90	0.57	55,55,55,55	0
86	OHX	2	1958	7/7	0.90	0.22	97,98,99,129	7
87	MG	3	210	1/1	0.90	0.59	47,47,47,47	0
87	MG	5	3947	1/1	0.90	0.90	52,52,52,52	0
87	MG	1	3959	1/1	0.90	0.49	45,45,45,45	0
87	MG	6	2127	1/1	0.90	0.45	49,49,49,49	0
86	OHX	5	3536	7/7	0.90	0.23	73,74,75,104	7
87	MG	4	202	1/1	0.90	0.24	53,53,53,53	0
87	MG	5	3955	1/1	0.90	0.26	36,36,36,36	0
86	OHX	1	3679	7/7	0.90	0.25	74,75,76,101	7
86	OHX	5	3712	7/7	0.90	0.25	94,95,95,113	7
86	OHX	1	3682	7/7	0.90	0.24	86,87,88,115	7
87	MG	4	225	1/1	0.90	0.64	50,50,50,50	0
87	MG	1	3867	1/1	0.90	0.48	25,25,25,25	0
87	MG	4	230	1/1	0.90	0.72	72,72,72,72	0
87	MG	sM	301	1/1	0.90	0.09	52,52,52,52	0
87	MG	5	3755	1/1	0.91	0.24	44,44,44,44	0
86	OHX	1	3665	7/7	0.91	0.16	59,60,61,105	7
87	MG	1	3941	1/1	0.91	0.27	44,44,44,44	0
86	OHX	6	1976	7/7	0.91	0.23	104,106,108,131	7
86	OHX	5	3697	7/7	0.91	0.18	111,111,112,137	7
87	MG	5	3773	1/1	0.91	0.37	35,35,35,35	0
86	OHX	5	3698	7/7	0.91	0.40	66,66,68,99	7
87	MG	5	3775	1/1	0.91	0.58	36,36,36,36	0
87	MG	2	2110	1/1	0.91	0.57	59,59,59,59	0
86	OHX	5	3508	7/7	0.91	0.34	79,80,82,117	7
87	MG	1	3947	1/1	0.91	0.69	51,51,51,51	0
87	MG	1	3807	1/1	0.91	0.74	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3703	7/7	0.91	0.42	50,52,53,85	7
86	OHX	5	3705	7/7	0.91	0.30	62,62,63,90	7
86	OHX	1	3625	7/7	0.91	0.15	102,103,105,121	7
87	MG	2	2057	1/1	0.91	0.25	66,66,66,66	0
87	MG	6	2082	1/1	0.91	0.57	58,58,58,58	0
87	MG	5	4013	1/1	0.91	0.28	49,49,49,49	0
87	MG	5	4014	1/1	0.91	0.40	47,47,47,47	0
87	MG	5	3794	1/1	0.91	0.33	56,56,56,56	0
87	MG	6	2086	1/1	0.91	0.54	67,67,67,67	0
87	MG	2	2059	1/1	0.91	0.51	63,63,63,63	0
87	MG	1	4053	1/1	0.91	0.20	64,64,64,64	0
86	OHX	6	1986	7/7	0.91	0.27	88,89,91,108	7
87	MG	6	2093	1/1	0.91	0.46	46,46,46,46	0
86	OHX	5	3564	7/7	0.91	0.22	88,89,91,122	7
87	MG	5	3807	1/1	0.91	0.63	39,39,39,39	0
86	OHX	1	3668	7/7	0.91	0.13	84,84,85,110	7
87	MG	5	3809	1/1	0.91	0.43	48,48,48,48	0
86	OHX	1	3707	7/7	0.91	0.16	84,84,85,114	7
87	MG	5	4041	1/1	0.91	0.38	66,66,66,66	0
86	OHX	1	3708	7/7	0.91	0.11	170,171,172,180	7
86	OHX	5	3620	7/7	0.91	0.20	76,77,78,110	7
87	MG	5	3833	1/1	0.91	0.29	38,38,38,38	0
87	MG	3	211	1/1	0.91	0.35	78,78,78,78	0
87	MG	3	212	1/1	0.91	0.52	40,40,40,40	0
87	MG	5	3840	1/1	0.91	0.44	34,34,34,34	0
87	MG	3	214	1/1	0.91	0.44	75,75,75,75	0
86	OHX	2	1995	7/7	0.91	0.28	75,76,78,101	7
87	MG	3	216	1/1	0.91	0.27	75,75,75,75	0
86	OHX	1	3710	7/7	0.91	0.16	93,94,94,124	7
87	MG	6	2114	1/1	0.91	0.15	76,76,76,76	0
86	OHX	1	3574	7/7	0.91	0.17	101,103,104,129	7
86	OHX	1	3677	7/7	0.91	0.30	68,69,69,96	7
86	OHX	6	2015	7/7	0.91	0.20	126,127,128,140	7
86	OHX	2	2008	7/7	0.91	0.23	111,113,114,139	7
87	MG	5	4070	1/1	0.91	0.15	45,45,45,45	0
87	MG	1	3971	1/1	0.91	0.29	39,39,39,39	0
87	MG	5	3898	1/1	0.91	0.41	39,39,39,39	0
87	MG	5	3907	1/1	0.91	0.53	39,39,39,39	0
87	MG	5	3915	1/1	0.91	0.08	47,47,47,47	0
87	MG	1	3734	1/1	0.91	0.22	42,42,42,42	0
87	MG	5	3918	1/1	0.91	0.40	45,45,45,45	0
87	MG	4	229	1/1	0.91	0.23	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	6	2125	1/1	0.91	0.25	69,69,69,69	0
87	MG	5	4090	1/1	0.91	0.68	41,41,41,41	0
86	OHX	2	2011	7/7	0.91	0.20	82,84,85,120	7
87	MG	1	3740	1/1	0.91	0.57	48,48,48,48	0
86	OHX	4	214	7/7	0.91	0.26	58,59,63,92	7
87	MG	5	4095	1/1	0.91	0.21	77,77,77,77	0
87	MG	L2	301	1/1	0.91	0.42	37,37,37,37	0
87	MG	5	3937	1/1	0.91	0.33	49,49,49,49	0
87	MG	5	4100	1/1	0.91	0.30	41,41,41,41	0
87	MG	L4	402	1/1	0.91	0.29	50,50,50,50	0
86	OHX	2	1990	7/7	0.91	0.19	101,102,106,126	7
86	OHX	8	214	7/7	0.91	0.19	104,105,107,129	7
86	OHX	1	3646	7/7	0.91	0.20	69,71,71,109	7
87	MG	M0	302	1/1	0.91	0.23	51,51,51,51	0
86	OHX	1	3545	7/7	0.91	0.25	68,69,71,105	7
86	OHX	1	3614	7/7	0.91	0.20	66,66,69,99	7
86	OHX	l5	301	7/7	0.91	0.11	104,105,106,134	7
86	OHX	m0	302	7/7	0.91	0.22	58,59,60,95	7
87	MG	1	3763	1/1	0.91	0.34	60,60,60,60	0
86	OHX	6	1932	7/7	0.91	0.26	75,82,85,110	7
87	MG	8	222	1/1	0.91	0.46	61,61,61,61	0
87	MG	2	2094	1/1	0.91	0.38	74,74,74,74	0
86	OHX	6	1950	7/7	0.91	0.27	92,93,95,123	7
86	OHX	6	1952	7/7	0.91	0.12	159,160,161,172	7
87	MG	5	3961	1/1	0.91	0.57	40,40,40,40	0
87	MG	1	3926	1/1	0.91	0.40	45,45,45,45	0
87	MG	1	3776	1/1	0.91	0.57	54,54,54,54	0
87	MG	5	3968	1/1	0.91	0.29	34,34,34,34	0
87	MG	5	3971	1/1	0.91	0.39	65,65,65,65	0
87	MG	5	3972	1/1	0.91	0.54	45,45,45,45	0
87	MG	6	2041	1/1	0.91	0.34	76,76,76,76	0
87	MG	6	2042	1/1	0.91	0.54	67,67,67,67	0
87	MG	q1	101	1/1	0.91	0.20	47,47,47,47	0
87	MG	q2	503	1/1	0.91	0.40	51,51,51,51	0
86	OHX	1	3658	7/7	0.91	0.32	93,93,94,127	7
87	MG	1	4014	1/1	0.91	0.19	55,55,55,55	0
86	OHX	1	3620	7/7	0.91	0.30	60,62,63,97	7
86	OHX	1	3663	7/7	0.91	0.30	73,74,75,117	7
86	OHX	6	1968	7/7	0.91	0.23	89,91,94,128	7
86	OHX	1	3706	7/7	0.92	0.25	51,52,54,82	7
87	MG	5	3965	1/1	0.92	0.28	48,48,48,48	0
87	MG	5	3966	1/1	0.92	0.25	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	2010	7/7	0.92	0.30	104,107,108,129	7
86	OHX	5	3707	7/7	0.92	0.36	63,64,66,96	7
87	MG	4	228	1/1	0.92	0.24	41,41,41,41	0
87	MG	5	3973	1/1	0.92	0.33	48,48,48,48	0
86	OHX	1	3666	7/7	0.92	0.25	67,69,72,97	7
87	MG	1	3955	1/1	0.92	0.34	38,38,38,38	0
87	MG	5	3976	1/1	0.92	0.15	57,57,57,57	0
87	MG	5	3738	1/1	0.92	0.58	34,34,34,34	0
86	OHX	5	3571	7/7	0.92	0.16	71,73,75,105	7
87	MG	2	2086	1/1	0.92	0.45	70,70,70,70	0
87	MG	1	3791	1/1	0.92	0.20	46,46,46,46	0
86	OHX	6	1991	7/7	0.92	0.15	79,80,81,108	7
86	OHX	5	3585	7/7	0.92	0.16	94,96,99,127	7
87	MG	5	3983	1/1	0.92	0.56	52,52,52,52	0
86	OHX	5	3595	7/7	0.92	0.17	69,70,73,104	7
86	OHX	5	3597	7/7	0.92	0.23	97,97,99,124	7
87	MG	5	3752	1/1	0.92	0.21	39,39,39,39	0
86	OHX	2	1911	7/7	0.92	0.19	109,111,116,131	7
86	OHX	5	3602	7/7	0.92	0.17	119,121,122,143	7
87	MG	5	3991	1/1	0.92	0.28	41,41,41,41	0
86	OHX	5	3603	7/7	0.92	0.33	49,50,53,92	7
87	MG	1	3808	1/1	0.92	0.55	35,35,35,35	0
87	MG	5	3758	1/1	0.92	0.24	77,77,77,77	0
86	OHX	1	3628	7/7	0.92	0.14	93,95,97,122	7
86	OHX	5	3609	7/7	0.92	0.18	66,67,70,97	7
87	MG	5	3771	1/1	0.92	0.16	46,46,46,46	0
87	MG	1	3820	1/1	0.92	0.64	41,41,41,41	0
87	MG	5	4004	1/1	0.92	0.13	65,65,65,65	0
86	OHX	5	3616	7/7	0.92	0.17	77,79,80,101	7
86	OHX	1	3632	7/7	0.92	0.18	105,105,106,124	7
86	OHX	5	3625	7/7	0.92	0.12	102,102,104,128	7
87	MG	O7	102	1/1	0.92	0.41	61,61,61,61	0
86	OHX	1	3568	7/7	0.92	0.29	71,72,73,98	7
87	MG	6	2039	1/1	0.92	0.31	60,60,60,60	0
87	MG	5	3783	1/1	0.92	0.65	45,45,45,45	0
87	MG	1	3843	1/1	0.92	0.25	34,34,34,34	0
86	OHX	6	2008	7/7	0.92	0.19	87,88,89,118	7
87	MG	1	3846	1/1	0.92	0.32	53,53,53,53	0
87	MG	5	4023	1/1	0.92	0.49	44,44,44,44	0
86	OHX	2	1977	7/7	0.92	0.25	85,88,88,112	7
86	OHX	2	1978	7/7	0.92	0.10	179,179,180,188	7
86	OHX	l3	402	7/7	0.92	0.17	86,87,88,111	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	3987	1/1	0.92	0.23	49,49,49,49	0
87	MG	5	4032	1/1	0.92	0.39	40,40,40,40	0
87	MG	5	4034	1/1	0.92	0.19	38,38,38,38	0
87	MG	5	4036	1/1	0.92	0.33	39,39,39,39	0
86	OHX	5	3642	7/7	0.92	0.22	65,67,68,98	7
87	MG	5	3797	1/1	0.92	0.36	37,37,37,37	0
87	MG	1	3990	1/1	0.92	0.25	58,58,58,58	0
87	MG	1	3864	1/1	0.92	0.37	49,49,49,49	0
86	OHX	5	3643	7/7	0.92	0.25	50,52,54,79	7
87	MG	5	4043	1/1	0.92	0.24	77,77,77,77	0
86	OHX	l5	302	7/7	0.92	0.15	101,102,102,130	7
87	MG	5	4045	1/1	0.92	0.61	29,29,29,29	0
86	OHX	l9	201	7/7	0.92	0.19	70,70,71,107	7
87	MG	1	3875	1/1	0.92	0.46	31,31,31,31	0
87	MG	1	4001	1/1	0.92	0.24	54,54,54,54	0
86	OHX	2	2014	7/7	0.92	0.21	62,65,67,103	7
87	MG	5	4056	1/1	0.92	0.38	48,48,48,48	0
86	OHX	4	215	7/7	0.92	0.20	87,88,89,114	7
86	OHX	5	3648	7/7	0.92	0.37	84,85,87,110	7
86	OHX	5	3650	7/7	0.92	0.26	44,46,47,79	7
87	MG	5	4061	1/1	0.92	0.23	55,55,55,55	0
87	MG	5	3825	1/1	0.92	0.73	39,39,39,39	0
86	OHX	2	1992	7/7	0.92	0.18	88,90,90,111	7
86	OHX	5	3654	7/7	0.92	0.18	83,84,84,117	7
86	OHX	L4	401	7/7	0.92	0.17	74,74,76,102	7
87	MG	1	3906	1/1	0.92	0.41	46,46,46,46	0
87	MG	5	3841	1/1	0.92	0.40	46,46,46,46	0
86	OHX	6	2025	7/7	0.92	0.20	94,94,95,122	7
86	OHX	5	3666	7/7	0.92	0.35	54,55,56,85	7
87	MG	5	3854	1/1	0.92	0.35	41,41,41,41	0
87	MG	2	2042	1/1	0.92	0.41	71,71,71,71	0
86	OHX	M7	202	7/7	0.92	0.25	69,69,70,100	7
87	MG	5	3865	1/1	0.92	0.29	58,58,58,58	0
87	MG	1	3723	1/1	0.92	0.47	51,51,51,51	0
87	MG	1	3914	1/1	0.92	0.30	47,47,47,47	0
87	MG	6	2099	1/1	0.92	0.40	91,91,91,91	0
87	MG	5	3873	1/1	0.92	0.73	46,46,46,46	0
87	MG	1	4040	1/1	0.92	0.19	62,62,62,62	0
87	MG	5	3882	1/1	0.92	0.32	30,30,30,30	0
86	OHX	5	3672	7/7	0.92	0.18	66,66,67,96	7
87	MG	1	3916	1/1	0.92	0.31	42,42,42,42	0
86	OHX	1	3686	7/7	0.92	0.27	74,75,76,104	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	3903	1/1	0.92	0.34	30,30,30,30	0
87	MG	1	3728	1/1	0.92	0.53	56,56,56,56	0
87	MG	1	4048	1/1	0.92	0.56	59,59,59,59	0
86	OHX	5	3678	7/7	0.92	0.23	71,71,74,106	7
87	MG	2	2051	1/1	0.92	0.62	80,80,80,80	0
86	OHX	1	3649	7/7	0.92	0.18	68,68,70,99	7
86	OHX	2	2007	7/7	0.92	0.17	101,101,104,120	7
87	MG	1	4055	1/1	0.92	0.62	51,51,51,51	0
87	MG	5	3929	1/1	0.92	0.18	52,52,52,52	0
86	OHX	1	3695	7/7	0.92	0.13	118,118,118,140	7
87	MG	1	3737	1/1	0.92	0.28	60,60,60,60	0
87	MG	1	4060	1/1	0.92	0.40	28,28,28,28	0
86	OHX	1	3613	7/7	0.92	0.21	62,65,66,97	7
87	MG	6	2122	1/1	0.92	0.40	70,70,70,70	0
87	MG	1	4063	1/1	0.92	0.38	34,34,34,34	0
86	OHX	1	3654	7/7	0.92	0.29	75,75,77,106	7
86	OHX	6	2036	7/7	0.92	0.13	101,103,104,124	7
86	OHX	1	3699	7/7	0.92	0.22	75,76,77,106	7
86	OHX	5	3693	7/7	0.92	0.19	64,66,67,88	7
87	MG	m5	304	1/1	0.92	0.23	50,50,50,50	0
87	MG	2	2071	1/1	0.92	0.23	60,60,60,60	0
87	MG	5	3949	1/1	0.92	0.19	57,57,57,57	0
86	OHX	2	1982	7/7	0.92	0.19	85,85,87,112	7
86	OHX	1	3616	7/7	0.92	0.34	58,58,61,88	7
86	OHX	s9	201	7/7	0.92	0.21	68,68,71,98	7
86	OHX	1	3660	7/7	0.92	0.23	61,62,63,93	7
87	MG	5	3956	1/1	0.92	0.31	61,61,61,61	0
86	OHX	6	1971	7/7	0.92	0.23	91,92,93,114	7
87	MG	4	218	1/1	0.92	0.63	53,53,53,53	0
87	MG	5	3959	1/1	0.92	0.32	56,56,56,56	0
87	MG	4	219	1/1	0.92	0.66	59,59,59,59	0
86	OHX	1	3661	7/7	0.92	0.21	55,58,60,89	7
86	OHX	C3	201	7/7	0.92	0.18	105,107,107,135	7
87	MG	1	4012	1/1	0.93	0.43	48,48,48,48	0
86	OHX	5	3559	7/7	0.93	0.19	105,106,107,129	7
87	MG	1	4018	1/1	0.93	0.29	54,54,54,54	0
86	OHX	1	3491	7/7	0.93	0.23	48,53,56,87	7
87	MG	1	3861	1/1	0.93	0.56	47,47,47,47	0
86	OHX	5	3569	7/7	0.93	0.26	58,61,64,89	7
86	OHX	1	3687	7/7	0.93	0.17	72,72,74,100	7
86	OHX	1	3509	7/7	0.93	0.23	51,52,55,75	7
87	MG	1	4025	1/1	0.93	0.24	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3713	7/7	0.93	0.27	44,44,45,87	7
87	MG	1	4028	1/1	0.93	0.24	39,39,39,39	0
86	OHX	5	3714	7/7	0.93	0.12	127,127,127,145	7
87	MG	1	3874	1/1	0.93	0.53	36,36,36,36	0
86	OHX	5	3577	7/7	0.93	0.18	67,68,71,100	7
87	MG	1	4038	1/1	0.93	0.45	41,41,41,41	0
87	MG	1	3876	1/1	0.93	0.45	36,36,36,36	0
86	OHX	6	1965	7/7	0.93	0.22	96,97,98,122	7
86	OHX	5	3717	7/7	0.93	0.15	121,122,123,139	7
86	OHX	1	3689	7/7	0.93	0.26	43,45,46,85	7
87	MG	1	3888	1/1	0.93	0.40	61,61,61,61	0
86	OHX	1	3691	7/7	0.93	0.32	60,61,62,98	7
87	MG	1	3896	1/1	0.93	0.18	47,47,47,47	0
87	MG	1	4049	1/1	0.93	0.08	79,79,79,79	0
86	OHX	6	1972	7/7	0.93	0.27	103,104,106,123	7
87	MG	d3	201	1/1	0.93	0.17	51,51,51,51	0
86	OHX	1	3692	7/7	0.93	0.20	70,71,71,92	7
86	OHX	5	3723	7/7	0.93	0.30	95,95,95,117	7
86	OHX	1	3512	7/7	0.93	0.19	69,72,76,102	7
87	MG	1	4054	1/1	0.93	0.59	48,48,48,48	0
87	MG	5	3730	1/1	0.93	0.33	42,42,42,42	0
86	OHX	7	208	7/7	0.93	0.30	51,53,55,82	7
86	OHX	2	1975	7/7	0.93	0.15	110,111,112,131	7
86	OHX	6	1984	7/7	0.93	0.16	100,102,102,129	7
86	OHX	2	1991	7/7	0.93	0.17	111,112,112,136	7
87	MG	1	4061	1/1	0.93	0.19	33,33,33,33	0
86	OHX	5	3618	7/7	0.93	0.26	68,68,71,92	7
86	OHX	5	3619	7/7	0.93	0.23	53,54,56,87	7
86	OHX	6	1988	7/7	0.93	0.30	96,97,97,128	7
86	OHX	5	3622	7/7	0.93	0.22	73,73,74,97	7
86	OHX	1	3643	7/7	0.93	0.22	51,52,53,83	7
86	OHX	1	3557	7/7	0.93	0.24	62,64,65,97	7
87	MG	5	3997	1/1	0.93	0.53	51,51,51,51	0
87	MG	1	3713	1/1	0.93	0.43	49,49,49,49	0
86	OHX	2	1909	7/7	0.93	0.19	99,102,106,112	0
86	OHX	5	3636	7/7	0.93	0.30	70,71,72,104	7
86	OHX	6	2002	7/7	0.93	0.28	90,90,91,117	7
87	MG	1	3722	1/1	0.93	0.50	42,42,42,42	0
86	OHX	m0	301	7/7	0.93	0.18	97,98,101,130	7
87	MG	1	3928	1/1	0.93	0.20	46,46,46,46	0
87	MG	1	3724	1/1	0.93	0.93	62,62,62,62	0
87	MG	5	4010	1/1	0.93	0.44	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3648	7/7	0.93	0.25	63,65,66,99	7
86	OHX	2	1940	7/7	0.93	0.17	94,96,98,118	7
86	OHX	1	3593	7/7	0.93	0.26	59,60,62,89	7
87	MG	5	4015	1/1	0.93	0.20	60,60,60,60	0
86	OHX	2	1971	7/7	0.93	0.19	153,154,154,170	7
87	MG	5	4018	1/1	0.93	0.27	38,38,38,38	0
87	MG	5	4019	1/1	0.93	0.21	53,53,53,53	0
87	MG	1	3940	1/1	0.93	0.24	55,55,55,55	0
87	MG	2	2033	1/1	0.93	0.55	63,63,63,63	0
87	MG	2	2034	1/1	0.93	0.44	63,63,63,63	0
86	OHX	1	3597	7/7	0.93	0.24	59,60,63,92	7
86	OHX	1	3657	7/7	0.93	0.21	85,85,86,119	7
86	OHX	2	1999	7/7	0.93	0.33	75,75,76,103	7
86	OHX	6	2016	7/7	0.93	0.30	64,65,67,102	7
87	MG	5	3785	1/1	0.93	0.41	53,53,53,53	0
87	MG	1	3741	1/1	0.93	0.44	49,49,49,49	0
86	OHX	5	3653	7/7	0.93	0.26	70,72,73,97	7
86	OHX	2	1944	7/7	0.93	0.17	104,104,108,128	7
86	OHX	2	1965	7/7	0.93	0.17	92,93,94,124	7
86	OHX	5	3659	7/7	0.93	0.21	48,50,52,90	7
87	MG	5	3792	1/1	0.93	0.35	53,53,53,53	0
87	MG	1	3952	1/1	0.93	0.45	52,52,52,52	0
86	OHX	6	2022	7/7	0.93	0.22	54,55,58,96	7
87	MG	5	3795	1/1	0.93	0.45	57,57,57,57	0
87	MG	2	2048	1/1	0.93	0.53	57,57,57,57	0
87	MG	2	2049	1/1	0.93	0.38	66,66,66,66	0
86	OHX	5	3665	7/7	0.93	0.29	69,69,71,102	7
87	MG	1	3760	1/1	0.93	0.31	39,39,39,39	0
86	OHX	1	3711	7/7	0.93	0.21	80,80,82,109	7
86	OHX	5	3667	7/7	0.93	0.12	134,134,135,149	7
86	OHX	1	3607	7/7	0.93	0.13	97,97,100,127	7
87	MG	O2	201	1/1	0.93	0.35	33,33,33,33	0
86	OHX	1	3610	7/7	0.93	0.16	84,85,86,112	7
87	MG	2	2056	1/1	0.93	0.34	68,68,68,68	0
87	MG	5	3810	1/1	0.93	0.23	51,51,51,51	0
86	OHX	5	3676	7/7	0.93	0.20	83,84,85,114	7
86	OHX	2	2028	7/7	0.93	0.14	130,130,131,153	7
87	MG	5	3814	1/1	0.93	0.33	42,42,42,42	0
86	OHX	2	2015	7/7	0.93	0.16	118,119,119,136	7
87	MG	5	3823	1/1	0.93	0.34	54,54,54,54	0
87	MG	1	3967	1/1	0.93	0.24	50,50,50,50	0
87	MG	2	2062	1/1	0.93	0.49	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	3788	1/1	0.93	0.37	54,54,54,54	0
87	MG	2	2064	1/1	0.93	0.55	61,61,61,61	0
87	MG	6	2048	1/1	0.93	0.35	91,91,91,91	0
87	MG	2	2065	1/1	0.93	0.40	77,77,77,77	0
87	MG	5	3842	1/1	0.93	0.45	40,40,40,40	0
86	OHX	2	2016	7/7	0.93	0.10	126,126,127,150	7
87	MG	5	3846	1/1	0.93	0.53	59,59,59,59	0
87	MG	1	3974	1/1	0.93	0.46	58,58,58,58	0
87	MG	1	3975	1/1	0.93	0.38	43,43,43,43	0
86	OHX	6	2031	7/7	0.93	0.18	81,82,83,108	7
86	OHX	1	3617	7/7	0.93	0.19	83,83,84,103	7
87	MG	6	2062	1/1	0.93	0.48	51,51,51,51	0
87	MG	5	3866	1/1	0.93	0.66	48,48,48,48	0
87	MG	1	3978	1/1	0.93	0.41	41,41,41,41	0
87	MG	6	2064	1/1	0.93	0.34	68,68,68,68	0
87	MG	5	3871	1/1	0.93	0.56	40,40,40,40	0
86	OHX	4	216	7/7	0.93	0.25	69,70,70,98	7
86	OHX	1	3671	7/7	0.93	0.21	69,69,70,100	7
87	MG	5	4106	1/1	0.93	0.62	50,50,50,50	0
87	MG	6	2068	1/1	0.93	0.21	83,83,83,83	0
87	MG	1	3800	1/1	0.93	0.38	35,35,35,35	0
87	MG	5	3883	1/1	0.93	0.44	44,44,44,44	0
87	MG	5	3885	1/1	0.93	0.36	29,29,29,29	0
86	OHX	5	3688	7/7	0.93	0.19	62,63,64,97	7
87	MG	1	3984	1/1	0.93	0.28	43,43,43,43	0
86	OHX	1	3618	7/7	0.93	0.19	74,76,78,102	7
86	OHX	M0	301	7/7	0.93	0.19	68,70,73,97	7
87	MG	8	217	1/1	0.93	0.47	60,60,60,60	0
87	MG	5	3904	1/1	0.93	0.54	40,40,40,40	0
86	OHX	1	3619	7/7	0.93	0.24	70,70,72,99	7
87	MG	5	3914	1/1	0.93	0.48	33,33,33,33	0
86	OHX	2	2005	7/7	0.93	0.21	81,81,81,110	7
86	OHX	1	3622	7/7	0.93	0.14	90,91,92,125	7
86	OHX	1	3681	7/7	0.93	0.19	56,60,61,86	7
87	MG	6	2089	1/1	0.93	0.57	48,48,48,48	0
86	OHX	C5	201	7/7	0.93	0.10	129,129,130,150	7
87	MG	m7	202	1/1	0.93	0.24	45,45,45,45	0
86	OHX	6	1940	7/7	0.93	0.15	118,121,123,134	7
87	MG	5	3927	1/1	0.93	0.11	40,40,40,40	0
87	MG	1	3834	1/1	0.93	0.65	38,38,38,38	0
87	MG	5	3931	1/1	0.93	0.45	44,44,44,44	0
86	OHX	5	3701	7/7	0.93	0.18	83,83,84,113	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	1949	7/7	0.93	0.17	99,100,102,117	7
87	MG	6	2098	1/1	0.93	0.21	87,87,87,87	0
87	MG	1	4004	1/1	0.93	0.26	52,52,52,52	0
86	OHX	1	3684	7/7	0.93	0.21	107,107,108,130	7
87	MG	5	3939	1/1	0.93	0.23	52,52,52,52	0
87	MG	1	4008	1/1	0.93	0.54	50,50,50,50	0
86	OHX	5	3528	7/7	0.93	0.21	52,54,57,86	7
86	OHX	1	3490	7/7	0.93	0.24	72,74,78,102	7
87	MG	5	3924	1/1	0.94	0.23	35,35,35,35	0
86	OHX	5	3544	7/7	0.94	0.29	58,60,63,99	7
87	MG	6	2097	1/1	0.94	0.71	59,59,59,59	0
87	MG	5	3930	1/1	0.94	0.33	49,49,49,49	0
86	OHX	5	3550	7/7	0.94	0.24	67,70,71,107	7
87	MG	5	3932	1/1	0.94	0.20	52,52,52,52	0
86	OHX	1	3655	7/7	0.94	0.29	87,87,87,115	7
87	MG	1	3832	1/1	0.94	0.47	35,35,35,35	0
86	OHX	5	3700	7/7	0.94	0.29	42,43,45,80	7
87	MG	1	4005	1/1	0.94	0.71	54,54,54,54	0
86	OHX	5	3561	7/7	0.94	0.15	112,112,114,136	7
87	MG	1	3841	1/1	0.94	0.50	40,40,40,40	0
87	MG	6	2108	1/1	0.94	0.24	51,51,51,51	0
86	OHX	1	3701	7/7	0.94	0.17	63,64,66,101	7
86	OHX	5	3566	7/7	0.94	0.27	66,67,67,94	7
86	OHX	5	3704	7/7	0.94	0.09	151,151,151,167	7
87	MG	1	3847	1/1	0.94	0.48	38,38,38,38	0
87	MG	1	4016	1/1	0.94	0.44	32,32,32,32	0
86	OHX	5	3568	7/7	0.94	0.14	78,79,80,116	7
86	OHX	6	1978	7/7	0.94	0.18	79,80,83,103	7
86	OHX	1	3656	7/7	0.94	0.16	83,84,85,110	7
87	MG	5	3953	1/1	0.94	0.26	57,57,57,57	0
86	OHX	6	1981	7/7	0.94	0.19	52,53,57,89	7
86	OHX	5	3575	7/7	0.94	0.27	65,68,69,94	7
86	OHX	6	1982	7/7	0.94	0.13	105,106,108,132	7
87	MG	1	3865	1/1	0.94	0.34	39,39,39,39	0
86	OHX	5	3711	7/7	0.94	0.27	67,70,71,97	7
87	MG	1	4027	1/1	0.94	0.16	53,53,53,53	0
86	OHX	6	1983	7/7	0.94	0.16	89,90,92,122	7
86	OHX	5	3586	7/7	0.94	0.20	62,63,64,98	7
87	MG	1	3873	1/1	0.94	0.52	29,29,29,29	0
87	MG	6	2129	1/1	0.94	0.44	77,77,77,77	0
86	OHX	1	3608	7/7	0.94	0.20	81,81,83,109	7
86	OHX	2	1921	7/7	0.94	0.25	93,94,101,115	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3599	7/7	0.94	0.18	83,84,87,112	7
87	MG	1	3878	1/1	0.94	0.30	39,39,39,39	0
87	MG	6	2136	1/1	0.94	0.12	76,76,76,76	0
87	MG	1	4041	1/1	0.94	0.35	58,58,58,58	0
86	OHX	6	1987	7/7	0.94	0.30	68,69,70,97	7
87	MG	2	2102	1/1	0.94	0.75	61,61,61,61	0
86	OHX	1	3611	7/7	0.94	0.19	59,60,62,92	7
87	MG	1	4045	1/1	0.94	0.57	42,42,42,42	0
86	OHX	1	3517	7/7	0.94	0.31	55,58,61,96	7
86	OHX	1	3520	7/7	0.94	0.22	60,60,63,89	7
87	MG	1	3894	1/1	0.94	0.68	41,41,41,41	0
86	OHX	5	3608	7/7	0.94	0.25	70,71,72,99	7
87	MG	5	3732	1/1	0.94	0.22	33,33,33,33	0
87	MG	1	3897	1/1	0.94	0.31	33,33,33,33	0
86	OHX	1	3662	7/7	0.94	0.19	63,64,66,94	7
87	MG	1	3902	1/1	0.94	0.08	58,58,58,58	0
86	OHX	5	3615	7/7	0.94	0.23	60,60,62,84	7
86	OHX	7	203	7/7	0.94	0.23	53,59,62,95	7
86	OHX	7	207	7/7	0.94	0.17	88,89,91,118	7
86	OHX	6	1997	7/7	0.94	0.18	103,104,105,124	7
87	MG	5	3993	1/1	0.94	0.20	88,88,88,88	0
86	OHX	1	3615	7/7	0.94	0.13	96,97,98,121	7
86	OHX	7	210	7/7	0.94	0.24	52,53,54,90	7
87	MG	1	3910	1/1	0.94	0.32	51,51,51,51	0
87	MG	5	3746	1/1	0.94	0.31	64,64,64,64	0
86	OHX	1	3535	7/7	0.94	0.12	125,125,126,142	7
86	OHX	8	207	7/7	0.94	0.20	96,97,99,122	7
86	OHX	1	3540	7/7	0.94	0.19	88,89,93,116	7
86	OHX	2	1959	7/7	0.94	0.24	96,99,100,120	7
86	OHX	5	3623	7/7	0.94	0.12	83,85,86,117	7
86	OHX	1	3549	7/7	0.94	0.18	88,88,90,108	7
86	OHX	5	3628	7/7	0.94	0.21	55,58,59,80	7
86	OHX	6	2009	7/7	0.94	0.17	66,67,70,99	7
87	MG	5	4009	1/1	0.94	0.48	72,72,72,72	0
87	MG	5	3759	1/1	0.94	0.24	31,31,31,31	0
87	MG	1	3721	1/1	0.94	0.42	49,49,49,49	0
86	OHX	5	3630	7/7	0.94	0.16	113,115,116,133	7
86	OHX	5	3631	7/7	0.94	0.20	74,76,78,110	7
86	OHX	1	3670	7/7	0.94	0.19	117,118,119,142	7
86	OHX	5	3634	7/7	0.94	0.28	62,63,64,90	7
86	OHX	2	2020	7/7	0.94	0.29	88,89,90,116	7
86	OHX	4	212	7/7	0.94	0.14	113,115,117,141	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	3931	1/1	0.94	0.52	51,51,51,51	0
87	MG	1	3932	1/1	0.94	0.65	110,110,110,110	0
87	MG	5	3779	1/1	0.94	0.60	52,52,52,52	0
87	MG	1	3730	1/1	0.94	0.70	42,42,42,42	0
86	OHX	1	3672	7/7	0.94	0.16	74,74,75,99	7
87	MG	2	2029	1/1	0.94	0.50	81,81,81,81	0
87	MG	1	3937	1/1	0.94	0.74	52,52,52,52	0
87	MG	2	2030	1/1	0.94	0.78	47,47,47,47	0
86	OHX	2	1951	7/7	0.94	0.13	134,135,136,149	7
87	MG	5	3789	1/1	0.94	0.25	33,33,33,33	0
86	OHX	6	2019	7/7	0.94	0.27	82,83,84,106	7
87	MG	L3	403	1/1	0.94	0.19	48,48,48,48	0
86	OHX	1	3562	7/7	0.94	0.15	96,98,99,118	7
86	OHX	6	2021	7/7	0.94	0.14	102,103,103,127	7
86	OHX	1	3626	7/7	0.94	0.17	89,91,92,118	7
86	OHX	6	2023	7/7	0.94	0.21	64,65,68,103	7
86	OHX	2	1966	7/7	0.94	0.33	86,87,88,114	7
86	OHX	2	1997	7/7	0.94	0.29	69,70,72,98	7
86	OHX	1	3581	7/7	0.94	0.13	83,86,88,119	7
87	MG	5	3800	1/1	0.94	0.33	53,53,53,53	0
87	MG	5	4048	1/1	0.94	0.27	50,50,50,50	0
86	OHX	1	3588	7/7	0.94	0.16	104,104,106,123	7
87	MG	1	3754	1/1	0.94	0.22	51,51,51,51	0
87	MG	1	3755	1/1	0.94	0.18	53,53,53,53	0
86	OHX	1	3589	7/7	0.94	0.24	84,86,88,115	7
87	MG	5	4057	1/1	0.94	0.20	38,38,38,38	0
87	MG	1	3953	1/1	0.94	0.20	52,52,52,52	0
86	OHX	6	1919	7/7	0.94	0.19	62,64,67,98	7
86	OHX	5	3662	7/7	0.94	0.18	69,70,71,107	7
86	OHX	1	3466	7/7	0.94	0.20	81,83,86,117	7
87	MG	1	3762	1/1	0.94	0.45	43,43,43,43	0
87	MG	Q2	503	1/1	0.94	0.18	68,68,68,68	0
87	MG	5	4064	1/1	0.94	0.47	61,61,61,61	0
86	OHX	1	3473	7/7	0.94	0.20	77,80,82,116	7
86	OHX	2	1985	7/7	0.94	0.12	107,108,109,128	7
87	MG	5	3818	1/1	0.94	0.48	39,39,39,39	0
87	MG	5	3820	1/1	0.94	0.42	42,42,42,42	0
87	MG	5	3822	1/1	0.94	0.54	35,35,35,35	0
87	MG	1	3766	1/1	0.94	0.38	43,43,43,43	0
86	OHX	6	1946	7/7	0.94	0.24	62,64,66,99	7
86	OHX	5	3669	7/7	0.94	0.19	41,42,43,79	7
87	MG	5	3834	1/1	0.94	0.50	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	4076	1/1	0.94	0.42	43,43,43,43	0
87	MG	2	2053	1/1	0.94	0.57	84,84,84,84	0
87	MG	5	4079	1/1	0.94	0.38	45,45,45,45	0
87	MG	5	3837	1/1	0.94	0.45	28,28,28,28	0
87	MG	1	3775	1/1	0.94	0.22	44,44,44,44	0
86	OHX	1	3645	7/7	0.94	0.26	56,58,59,81	7
87	MG	5	4088	1/1	0.94	0.74	65,65,65,65	0
87	MG	5	4089	1/1	0.94	0.27	69,69,69,69	0
87	MG	1	3777	1/1	0.94	0.47	39,39,39,39	0
86	OHX	1	3690	7/7	0.94	0.23	72,73,73,110	7
87	MG	1	3779	1/1	0.94	0.52	26,26,26,26	0
87	MG	6	2052	1/1	0.94	0.40	61,61,61,61	0
86	OHX	1	3598	7/7	0.94	0.28	62,63,64,92	7
87	MG	1	3783	1/1	0.94	0.35	66,66,66,66	0
86	OHX	1	3647	7/7	0.94	0.17	73,75,76,102	7
87	MG	5	3861	1/1	0.94	0.43	40,40,40,40	0
87	MG	6	2058	1/1	0.94	0.38	61,61,61,61	0
86	OHX	5	3680	7/7	0.94	0.20	74,75,77,106	7
87	MG	5	4105	1/1	0.94	0.19	40,40,40,40	0
87	MG	6	2061	1/1	0.94	0.46	39,39,39,39	0
86	OHX	6	1955	7/7	0.94	0.12	169,169,170,177	7
87	MG	7	212	1/1	0.94	0.36	57,57,57,57	0
86	OHX	1	3601	7/7	0.94	0.19	45,45,49,77	7
87	MG	2	2063	1/1	0.94	0.73	57,57,57,57	0
86	OHX	5	3683	7/7	0.94	0.15	92,92,94,121	7
86	OHX	2	2025	7/7	0.94	0.22	98,98,100,121	7
87	MG	5	3874	1/1	0.94	0.50	34,34,34,34	0
86	OHX	6	1961	7/7	0.94	0.25	77,79,81,110	7
87	MG	5	3878	1/1	0.94	0.72	36,36,36,36	0
86	OHX	5	3500	7/7	0.94	0.17	74,78,81,100	7
86	OHX	1	3501	7/7	0.94	0.24	54,58,61,93	7
87	MG	6	2072	1/1	0.94	0.41	69,69,69,69	0
86	OHX	1	3697	7/7	0.94	0.20	75,76,77,104	7
87	MG	1	3983	1/1	0.94	0.23	41,41,41,41	0
87	MG	5	3893	1/1	0.94	0.38	38,38,38,38	0
87	MG	5	3896	1/1	0.94	0.39	38,38,38,38	0
87	MG	1	3803	1/1	0.94	0.63	47,47,47,47	0
87	MG	l3	403	1/1	0.94	0.43	28,28,28,28	0
87	MG	5	3899	1/1	0.94	0.59	43,43,43,43	0
86	OHX	5	3690	7/7	0.94	0.27	66,68,70,102	7
86	OHX	1	3504	7/7	0.94	0.15	85,86,89,113	7
87	MG	5	3906	1/1	0.94	0.36	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	6	2083	1/1	0.94	0.43	46,46,46,46	0
86	OHX	2	1931	7/7	0.94	0.12	112,112,116,133	7
86	OHX	5	3537	7/7	0.94	0.13	95,96,100,118	7
87	MG	o7	504	1/1	0.94	0.49	65,65,65,65	0
87	MG	1	3817	1/1	0.94	0.42	45,45,45,45	0
87	MG	5	3917	1/1	0.94	0.08	48,48,48,48	0
86	OHX	5	3543	7/7	0.94	0.16	62,62,64,85	7
87	MG	1	3992	1/1	0.94	0.17	56,56,56,56	0
87	MG	1	3993	1/1	0.94	0.23	40,40,40,40	0
87	MG	1	3821	1/1	0.94	0.40	38,38,38,38	0
87	MG	5	3922	1/1	0.94	0.40	32,32,32,32	0
87	MG	5	3923	1/1	0.94	0.40	36,36,36,36	0
86	OHX	2	1907	7/7	0.95	0.15	101,105,108,120	7
87	MG	5	3945	1/1	0.95	0.36	56,56,56,56	0
86	OHX	6	2028	7/7	0.95	0.16	74,76,76,101	7
87	MG	1	3899	1/1	0.95	0.13	41,41,41,41	0
86	OHX	1	3592	7/7	0.95	0.19	40,43,45,79	7
86	OHX	2	1918	7/7	0.95	0.19	82,83,87,106	7
87	MG	1	3719	1/1	0.95	0.61	40,40,40,40	0
87	MG	1	3720	1/1	0.95	0.45	42,42,42,42	0
86	OHX	5	3638	7/7	0.95	0.24	45,45,46,80	7
87	MG	5	3727	1/1	0.95	0.54	58,58,58,58	0
86	OHX	1	3594	7/7	0.95	0.36	70,70,72,100	7
86	OHX	2	1987	7/7	0.95	0.34	100,100,101,124	7
86	OHX	5	3641	7/7	0.95	0.23	68,69,70,102	7
86	OHX	1	3694	7/7	0.95	0.19	54,57,59,93	7
86	OHX	1	3523	7/7	0.95	0.15	83,84,87,111	7
86	OHX	6	1962	7/7	0.95	0.24	77,78,80,102	7
86	OHX	n3	202	7/7	0.95	0.18	60,62,65,94	7
86	OHX	5	3645	7/7	0.95	0.22	67,67,68,96	7
86	OHX	1	3533	7/7	0.95	0.24	59,60,62,92	7
87	MG	1	3917	1/1	0.95	0.55	43,43,43,43	0
86	OHX	6	1966	7/7	0.95	0.24	67,69,71,91	7
86	OHX	5	3649	7/7	0.95	0.22	63,64,66,91	7
87	MG	5	3969	1/1	0.95	0.29	39,39,39,39	0
87	MG	1	3921	1/1	0.95	0.44	69,69,69,69	0
86	OHX	1	3534	7/7	0.95	0.12	157,158,158,170	7
86	OHX	1	3652	7/7	0.95	0.36	80,81,82,112	7
87	MG	1	3738	1/1	0.95	0.57	51,51,51,51	0
86	OHX	1	3602	7/7	0.95	0.25	62,62,65,86	7
86	OHX	1	3603	7/7	0.95	0.23	69,69,70,99	7
87	MG	2	2038	1/1	0.95	0.55	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3656	7/7	0.95	0.26	46,48,50,85	7
86	OHX	5	3657	7/7	0.95	0.19	56,57,58,91	7
87	MG	1	3748	1/1	0.95	0.76	45,45,45,45	0
86	OHX	c8	201	7/7	0.95	0.18	107,107,108,127	7
87	MG	1	3751	1/1	0.95	0.46	31,31,31,31	0
87	MG	4	222	1/1	0.95	0.24	43,43,43,43	0
87	MG	5	3984	1/1	0.95	0.27	50,50,50,50	0
86	OHX	6	1975	7/7	0.95	0.22	105,106,106,128	7
87	MG	2	2043	1/1	0.95	0.57	57,57,57,57	0
87	MG	5	3764	1/1	0.95	0.70	44,44,44,44	0
87	MG	5	3769	1/1	0.95	0.38	49,49,49,49	0
87	MG	4	226	1/1	0.95	0.15	57,57,57,57	0
87	MG	2	2044	1/1	0.95	0.47	47,47,47,47	0
87	MG	5	3992	1/1	0.95	0.20	50,50,50,50	0
87	MG	1	3756	1/1	0.95	0.43	34,34,34,34	0
86	OHX	5	3481	7/7	0.95	0.23	74,75,78,94	7
86	OHX	2	1960	7/7	0.95	0.20	80,82,83,112	7
87	MG	5	3776	1/1	0.95	0.77	50,50,50,50	0
86	OHX	5	3501	7/7	0.95	0.23	48,49,52,80	7
86	OHX	5	3502	7/7	0.95	0.18	74,76,78,106	7
86	OHX	5	3505	7/7	0.95	0.21	78,79,83,110	7
86	OHX	1	3538	7/7	0.95	0.23	55,58,60,83	7
86	OHX	2	1961	7/7	0.95	0.20	65,66,71,98	7
87	MG	5	4003	1/1	0.95	0.57	43,43,43,43	0
87	MG	1	3765	1/1	0.95	0.38	35,35,35,35	0
86	OHX	5	3671	7/7	0.95	0.22	59,60,62,93	7
86	OHX	5	3523	7/7	0.95	0.20	47,49,55,86	7
86	OHX	5	3525	7/7	0.95	0.20	57,59,61,91	7
86	OHX	5	3527	7/7	0.95	0.16	69,74,75,104	7
87	MG	1	3774	1/1	0.95	0.51	53,53,53,53	0
86	OHX	1	3541	7/7	0.95	0.27	68,69,70,102	7
86	OHX	5	3534	7/7	0.95	0.23	56,58,61,96	7
86	OHX	2	1964	7/7	0.95	0.16	72,73,75,116	7
86	OHX	1	3609	7/7	0.95	0.18	72,74,75,102	7
87	MG	2	2061	1/1	0.95	0.57	59,59,59,59	0
86	OHX	5	3539	7/7	0.95	0.15	108,109,111,129	7
86	OHX	5	3541	7/7	0.95	0.21	65,68,69,97	7
86	OHX	2	1933	7/7	0.95	0.21	75,79,81,108	7
87	MG	5	3799	1/1	0.95	0.48	46,46,46,46	0
87	MG	1	3786	1/1	0.95	0.25	38,38,38,38	0
86	OHX	1	3477	7/7	0.95	0.13	96,98,104,122	7
87	MG	2	2066	1/1	0.95	0.43	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	4026	1/1	0.95	0.32	53,53,53,53	0
87	MG	1	3790	1/1	0.95	0.49	44,44,44,44	0
86	OHX	5	3547	7/7	0.95	0.20	48,52,54,83	7
87	MG	5	4029	1/1	0.95	0.21	43,43,43,43	0
86	OHX	1	3487	7/7	0.95	0.14	120,121,123,137	7
87	MG	2	2069	1/1	0.95	0.39	63,63,63,63	0
86	OHX	5	3553	7/7	0.95	0.18	54,55,56,87	7
86	OHX	5	3555	7/7	0.95	0.22	45,46,48,77	7
87	MG	1	3970	1/1	0.95	0.26	58,58,58,58	0
87	MG	1	3798	1/1	0.95	0.35	38,38,38,38	0
87	MG	5	3813	1/1	0.95	0.43	32,32,32,32	0
86	OHX	5	3558	7/7	0.95	0.18	97,97,98,125	7
86	OHX	1	3560	7/7	0.95	0.14	111,113,114,136	7
86	OHX	2	1934	7/7	0.95	0.16	97,98,99,115	7
86	OHX	5	3563	7/7	0.95	0.28	66,68,69,96	7
86	OHX	6	1990	7/7	0.95	0.16	89,91,93,122	7
87	MG	5	4046	1/1	0.95	0.17	49,49,49,49	0
86	OHX	1	3563	7/7	0.95	0.21	93,95,98,115	7
86	OHX	5	3699	7/7	0.95	0.17	68,69,70,100	7
87	MG	5	3826	1/1	0.95	0.58	27,27,27,27	0
87	MG	5	4051	1/1	0.95	0.52	40,40,40,40	0
87	MG	5	3827	1/1	0.95	0.34	44,44,44,44	0
86	OHX	6	1992	7/7	0.95	0.19	87,88,89,113	7
87	MG	1	3814	1/1	0.95	0.56	29,29,29,29	0
86	OHX	6	1993	7/7	0.95	0.17	85,86,89,116	7
86	OHX	5	3570	7/7	0.95	0.17	86,86,87,110	7
86	OHX	1	3564	7/7	0.95	0.29	49,51,52,90	7
87	MG	5	3839	1/1	0.95	0.70	42,42,42,42	0
86	OHX	3	206	7/7	0.95	0.18	96,97,98,122	7
86	OHX	6	1999	7/7	0.95	0.29	78,79,80,103	7
86	OHX	1	3565	7/7	0.95	0.14	75,76,77,108	7
87	MG	1	3828	1/1	0.95	0.66	40,40,40,40	0
87	MG	6	2070	1/1	0.95	0.44	44,44,44,44	0
87	MG	1	3988	1/1	0.95	0.23	39,39,39,39	0
87	MG	5	3851	1/1	0.95	0.41	34,34,34,34	0
87	MG	5	3852	1/1	0.95	0.26	56,56,56,56	0
87	MG	1	3829	1/1	0.95	0.21	50,50,50,50	0
87	MG	5	3856	1/1	0.95	0.25	50,50,50,50	0
87	MG	5	3857	1/1	0.95	0.44	31,31,31,31	0
87	MG	1	3830	1/1	0.95	0.52	40,40,40,40	0
87	MG	1	3831	1/1	0.95	0.30	51,51,51,51	0
87	MG	5	3863	1/1	0.95	0.32	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	4077	1/1	0.95	0.12	39,39,39,39	0
86	OHX	5	3581	7/7	0.95	0.14	84,84,86,111	7
86	OHX	6	2003	7/7	0.95	0.17	91,91,92,122	7
86	OHX	2	1979	7/7	0.95	0.18	63,64,65,94	7
87	MG	1	3840	1/1	0.95	0.41	30,30,30,30	0
87	MG	6	2084	1/1	0.95	0.39	79,79,79,79	0
87	MG	5	4084	1/1	0.95	0.48	33,33,33,33	0
87	MG	5	4087	1/1	0.95	0.29	42,42,42,42	0
87	MG	1	3997	1/1	0.95	0.70	58,58,58,58	0
87	MG	6	2087	1/1	0.95	0.42	55,55,55,55	0
86	OHX	1	3573	7/7	0.95	0.22	61,61,62,88	7
86	OHX	5	3596	7/7	0.95	0.18	68,70,72,98	7
87	MG	6	2090	1/1	0.95	0.49	61,61,61,61	0
87	MG	5	3876	1/1	0.95	0.35	37,37,37,37	0
86	OHX	2	1980	7/7	0.95	0.28	81,81,82,106	7
87	MG	1	4003	1/1	0.95	0.14	51,51,51,51	0
86	OHX	5	3598	7/7	0.95	0.26	52,52,54,77	7
86	OHX	1	3623	7/7	0.95	0.08	124,124,124,144	7
87	MG	5	4102	1/1	0.95	0.28	41,41,41,41	0
86	OHX	1	3675	7/7	0.95	0.16	63,64,65,94	7
86	OHX	6	2010	7/7	0.95	0.24	58,58,59,88	7
86	OHX	6	2011	7/7	0.95	0.21	64,65,66,95	7
87	MG	1	3858	1/1	0.95	0.69	34,34,34,34	0
87	MG	1	4011	1/1	0.95	0.41	41,41,41,41	0
87	MG	1	3860	1/1	0.95	0.30	51,51,51,51	0
86	OHX	1	3676	7/7	0.95	0.25	68,68,70,94	7
87	MG	6	2103	1/1	0.95	0.18	59,59,59,59	0
87	MG	6	2104	1/1	0.95	0.41	74,74,74,74	0
87	MG	1	4015	1/1	0.95	0.08	66,66,66,66	0
87	MG	5	3908	1/1	0.95	0.61	36,36,36,36	0
86	OHX	5	3719	7/7	0.95	0.32	57,57,58,94	7
87	MG	1	4017	1/1	0.95	0.32	37,37,37,37	0
87	MG	8	201	1/1	0.95	0.17	46,46,46,46	0
86	OHX	1	3575	7/7	0.95	0.19	63,64,65,85	7
87	MG	8	218	1/1	0.95	0.39	47,47,47,47	0
86	OHX	1	3678	7/7	0.95	0.38	57,57,58,89	7
87	MG	8	221	1/1	0.95	0.31	53,53,53,53	0
86	OHX	5	3611	7/7	0.95	0.14	83,84,86,106	7
87	MG	2	2106	1/1	0.95	0.32	87,87,87,87	0
87	MG	1	3870	1/1	0.95	0.49	29,29,29,29	0
86	OHX	1	3577	7/7	0.95	0.21	54,56,58,90	7
87	MG	6	2116	1/1	0.95	0.38	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3680	7/7	0.95	0.24	57,58,60,100	7
86	OHX	6	2018	7/7	0.95	0.16	75,75,76,108	7
87	MG	m5	303	1/1	0.95	0.61	45,45,45,45	0
87	MG	5	3925	1/1	0.95	0.32	44,44,44,44	0
87	MG	6	2119	1/1	0.95	0.66	49,49,49,49	0
87	MG	5	3928	1/1	0.95	0.24	37,37,37,37	0
86	OHX	1	3578	7/7	0.95	0.11	108,110,110,135	7
86	OHX	2	1935	7/7	0.95	0.24	98,100,101,122	7
87	MG	1	4030	1/1	0.95	0.34	45,45,45,45	0
87	MG	1	4031	1/1	0.95	0.27	96,96,96,96	0
87	MG	o7	503	1/1	0.95	0.39	78,78,78,78	0
86	OHX	1	3582	7/7	0.95	0.19	51,52,56,80	7
86	OHX	6	1929	7/7	0.95	0.18	137,138,140,147	7
86	OHX	1	3583	7/7	0.95	0.12	83,84,86,110	7
86	OHX	1	3636	7/7	0.95	0.27	58,58,61,85	7
86	OHX	8	210	7/7	0.95	0.25	86,87,88,113	7
88	ZN	E1	501	1/1	0.95	0.07	138,138,138,138	0
86	OHX	1	3586	7/7	0.95	0.21	69,71,72,101	7
87	MG	5	3940	1/1	0.95	0.45	42,42,42,42	0
87	MG	1	3890	1/1	0.95	0.61	30,30,30,30	0
86	OHX	2	2000	7/7	0.95	0.15	100,101,102,129	7
87	MG	1	3863	1/1	0.96	0.49	38,38,38,38	0
86	OHX	5	3587	7/7	0.96	0.24	59,60,61,91	7
86	OHX	5	3593	7/7	0.96	0.27	50,51,53,81	7
87	MG	1	3866	1/1	0.96	0.55	34,34,34,34	0
86	OHX	5	3594	7/7	0.96	0.25	79,79,81,107	7
86	OHX	2	1972	7/7	0.96	0.15	122,123,124,147	7
86	OHX	1	3483	7/7	0.96	0.15	79,81,83,107	7
87	MG	2	2109	1/1	0.96	0.58	57,57,57,57	0
87	MG	5	3952	1/1	0.96	0.33	38,38,38,38	0
86	OHX	2	1943	7/7	0.96	0.24	68,71,73,95	7
87	MG	5	3725	1/1	0.96	0.54	40,40,40,40	0
86	OHX	2	2004	7/7	0.96	0.21	70,71,71,94	7
86	OHX	6	1911	7/7	0.96	0.19	87,89,94,103	7
86	OHX	5	3600	7/7	0.96	0.24	51,53,54,89	7
87	MG	1	3877	1/1	0.96	0.36	43,43,43,43	0
86	OHX	2	1963	7/7	0.96	0.24	72,74,75,98	7
86	OHX	1	3566	7/7	0.96	0.09	104,105,105,128	7
86	OHX	1	3492	7/7	0.96	0.23	52,54,57,78	7
87	MG	5	3962	1/1	0.96	0.37	40,40,40,40	0
87	MG	1	3881	1/1	0.96	0.42	59,59,59,59	0
86	OHX	1	3500	7/7	0.96	0.16	101,104,108,126	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3605	7/7	0.96	0.20	73,75,77,112	7
86	OHX	5	3606	7/7	0.96	0.15	50,53,55,90	7
86	OHX	6	1933	7/7	0.96	0.18	51,53,58,84	7
87	MG	1	3891	1/1	0.96	0.66	33,33,33,33	0
86	OHX	2	1954	7/7	0.96	0.21	87,91,94,113	7
87	MG	1	3714	1/1	0.96	0.80	46,46,46,46	0
86	OHX	6	1941	7/7	0.96	0.19	72,72,76,96	7
87	MG	1	3898	1/1	0.96	0.36	35,35,35,35	0
86	OHX	5	3612	7/7	0.96	0.21	64,64,65,96	7
86	OHX	5	3613	7/7	0.96	0.23	41,43,45,72	7
87	MG	5	3751	1/1	0.96	0.27	32,32,32,32	0
86	OHX	5	3614	7/7	0.96	0.23	48,49,52,78	7
87	MG	1	4065	1/1	0.96	0.13	69,69,69,69	0
86	OHX	2	1956	7/7	0.96	0.20	76,76,78,103	7
87	MG	1	3904	1/1	0.96	0.40	67,67,67,67	0
86	OHX	1	3576	7/7	0.96	0.15	71,72,74,106	7
86	OHX	8	206	7/7	0.96	0.20	72,72,73,103	7
87	MG	3	213	1/1	0.96	0.58	38,38,38,38	0
86	OHX	1	3683	7/7	0.96	0.13	79,81,81,109	7
86	OHX	8	208	7/7	0.96	0.13	89,89,90,115	7
86	OHX	8	209	7/7	0.96	0.21	71,72,74,99	7
87	MG	5	3767	1/1	0.96	0.29	31,31,31,31	0
87	MG	5	3768	1/1	0.96	0.21	39,39,39,39	0
86	OHX	2	1957	7/7	0.96	0.12	136,137,137,147	7
87	MG	5	3770	1/1	0.96	0.21	43,43,43,43	0
87	MG	1	3911	1/1	0.96	0.22	41,41,41,41	1
86	OHX	8	211	7/7	0.96	0.10	114,114,115,137	7
87	MG	1	3729	1/1	0.96	0.34	78,78,78,78	0
86	OHX	1	3630	7/7	0.96	0.18	57,60,63,93	7
86	OHX	5	3621	7/7	0.96	0.13	92,93,95,111	7
86	OHX	6	2033	7/7	0.96	0.16	86,87,88,106	7
86	OHX	1	3631	7/7	0.96	0.18	61,64,65,94	7
86	OHX	5	3624	7/7	0.96	0.13	90,91,92,112	7
86	OHX	2	1993	7/7	0.96	0.12	114,114,115,138	7
87	MG	5	4002	1/1	0.96	0.19	42,42,42,42	0
86	OHX	5	3626	7/7	0.96	0.12	78,78,79,103	7
86	OHX	1	3579	7/7	0.96	0.18	60,61,63,89	7
87	MG	5	3784	1/1	0.96	0.60	39,39,39,39	0
86	OHX	1	3635	7/7	0.96	0.17	72,73,74,101	7
86	OHX	1	3513	7/7	0.96	0.27	56,59,62,84	7
86	OHX	1	3637	7/7	0.96	0.12	116,116,117,131	7
86	OHX	1	3638	7/7	0.96	0.12	67,69,70,105	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	3744	1/1	0.96	0.36	49,49,49,49	0
86	OHX	5	3633	7/7	0.96	0.17	75,76,79,99	7
87	MG	1	3747	1/1	0.96	0.35	50,50,50,50	0
86	OHX	m5	302	7/7	0.96	0.16	85,86,86,110	7
86	OHX	1	3639	7/7	0.96	0.19	79,80,81,109	7
86	OHX	5	3635	7/7	0.96	0.21	54,55,56,88	7
86	OHX	2	1994	7/7	0.96	0.14	89,90,91,113	7
87	MG	1	3753	1/1	0.96	0.51	45,45,45,45	0
86	OHX	2	1967	7/7	0.96	0.20	75,76,77,114	7
86	OHX	1	3584	7/7	0.96	0.09	106,106,108,131	7
87	MG	M7	201	1/1	0.96	0.59	33,33,33,33	0
86	OHX	5	3443	7/7	0.96	0.17	64,66,69,96	7
86	OHX	5	3459	7/7	0.96	0.19	57,59,65,93	7
86	OHX	5	3470	7/7	0.96	0.17	80,84,84,102	7
86	OHX	5	3475	7/7	0.96	0.17	81,83,88,104	7
87	MG	5	3804	1/1	0.96	0.75	46,46,46,46	0
86	OHX	1	3585	7/7	0.96	0.19	56,57,59,92	7
87	MG	5	3806	1/1	0.96	0.34	60,60,60,60	0
86	OHX	5	3489	7/7	0.96	0.18	95,96,99,122	7
86	OHX	5	3496	7/7	0.96	0.21	66,68,71,98	7
86	OHX	5	3647	7/7	0.96	0.18	50,52,54,92	7
87	MG	5	4038	1/1	0.96	0.28	54,54,54,54	0
86	OHX	1	3522	7/7	0.96	0.22	49,50,52,73	7
86	OHX	6	1977	7/7	0.96	0.19	61,62,64,90	7
86	OHX	2	1996	7/7	0.96	0.24	88,89,91,112	7
87	MG	1	3769	1/1	0.96	0.53	34,34,34,34	0
86	OHX	1	3528	7/7	0.96	0.22	53,54,57,85	7
86	OHX	5	3652	7/7	0.96	0.15	63,64,66,100	7
86	OHX	6	1980	7/7	0.96	0.20	61,62,63,100	7
86	OHX	5	3514	7/7	0.96	0.17	69,71,73,95	7
86	OHX	5	3655	7/7	0.96	0.20	61,64,64,89	7
86	OHX	1	3590	7/7	0.96	0.21	44,45,46,80	7
87	MG	5	4049	1/1	0.96	0.39	59,59,59,59	0
86	OHX	1	3531	7/7	0.96	0.24	56,59,60,98	7
86	OHX	1	3532	7/7	0.96	0.14	107,109,111,126	7
86	OHX	2	1927	7/7	0.96	0.19	98,99,102,123	7
87	MG	5	3829	1/1	0.96	0.58	32,32,32,32	0
87	MG	5	3830	1/1	0.96	0.23	39,39,39,39	0
87	MG	6	2053	1/1	0.96	0.50	61,61,61,61	0
87	MG	1	3782	1/1	0.96	0.61	47,47,47,47	0
86	OHX	6	1985	7/7	0.96	0.17	84,84,85,111	7
86	OHX	5	3529	7/7	0.96	0.27	48,51,53,92	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3663	7/7	0.96	0.23	51,52,54,83	7
87	MG	6	2059	1/1	0.96	0.27	67,67,67,67	0
86	OHX	5	3664	7/7	0.96	0.10	99,100,101,126	7
87	MG	2	2058	1/1	0.96	0.51	64,64,64,64	0
86	OHX	5	3530	7/7	0.96	0.22	41,43,48,79	7
86	OHX	5	3531	7/7	0.96	0.30	62,64,65,100	7
86	OHX	5	3532	7/7	0.96	0.15	113,114,116,129	7
87	MG	1	3793	1/1	0.96	0.48	38,38,38,38	0
87	MG	6	2066	1/1	0.96	0.36	51,51,51,51	0
86	OHX	1	3595	7/7	0.96	0.12	125,127,128,150	7
86	OHX	5	3535	7/7	0.96	0.21	65,68,72,92	7
87	MG	5	3855	1/1	0.96	0.84	41,41,41,41	0
86	OHX	C1	201	7/7	0.96	0.18	92,92,93,110	7
87	MG	5	4075	1/1	0.96	0.81	42,42,42,42	0
86	OHX	2	1981	7/7	0.96	0.17	74,75,77,106	7
87	MG	5	3859	1/1	0.96	0.42	35,35,35,35	0
86	OHX	5	3673	7/7	0.96	0.16	67,67,68,98	7
86	OHX	5	3675	7/7	0.96	0.09	132,133,134,150	7
87	MG	5	3862	1/1	0.96	0.93	59,59,59,59	0
87	MG	5	4081	1/1	0.96	0.53	44,44,44,44	0
86	OHX	5	3538	7/7	0.96	0.26	72,76,77,99	7
87	MG	6	2074	1/1	0.96	0.29	53,53,53,53	0
86	OHX	2	1915	7/7	0.96	0.15	118,121,121,123	7
87	MG	5	4085	1/1	0.96	0.55	51,51,51,51	0
87	MG	5	4086	1/1	0.96	0.69	45,45,45,45	0
87	MG	6	2076	1/1	0.96	0.44	42,42,42,42	0
87	MG	5	3867	1/1	0.96	0.51	55,55,55,55	0
86	OHX	SR	401	7/7	0.96	0.09	142,143,143,158	7
87	MG	6	2079	1/1	0.96	0.51	67,67,67,67	0
86	OHX	5	3679	7/7	0.96	0.23	55,56,59,90	7
87	MG	6	2081	1/1	0.96	0.52	44,44,44,44	0
87	MG	1	3809	1/1	0.96	0.64	29,29,29,29	0
86	OHX	1	3454	7/7	0.96	0.28	53,58,59,80	7
87	MG	1	3811	1/1	0.96	0.50	38,38,38,38	0
87	MG	5	4097	1/1	0.96	0.47	22,22,22,22	0
87	MG	5	4098	1/1	0.96	0.19	56,56,56,56	0
86	OHX	1	3543	7/7	0.96	0.19	59,62,64,100	7
87	MG	2	2075	1/1	0.96	0.31	63,63,63,63	0
87	MG	5	4101	1/1	0.96	0.45	34,34,34,34	0
87	MG	1	3815	1/1	0.96	0.54	36,36,36,36	0
86	OHX	1	3458	7/7	0.96	0.15	109,110,114,130	7
86	OHX	5	3548	7/7	0.96	0.17	83,84,86,107	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	3886	1/1	0.96	0.48	36,36,36,36	0
86	OHX	3	203	7/7	0.96	0.25	70,71,73,104	7
86	OHX	6	1995	7/7	0.96	0.14	91,93,94,119	7
87	MG	5	3892	1/1	0.96	0.59	40,40,40,40	0
87	MG	1	3823	1/1	0.96	0.55	40,40,40,40	0
87	MG	1	3824	1/1	0.96	0.62	34,34,34,34	0
86	OHX	5	3686	7/7	0.96	0.18	63,63,64,95	7
86	OHX	6	1996	7/7	0.96	0.14	102,103,104,128	7
87	MG	7	219	1/1	0.96	0.28	42,42,42,42	0
87	MG	5	3900	1/1	0.96	0.43	31,31,31,31	0
86	OHX	1	3547	7/7	0.96	0.25	72,73,74,106	7
86	OHX	1	3548	7/7	0.96	0.18	80,80,82,99	7
87	MG	2	2084	1/1	0.96	0.53	69,69,69,69	0
86	OHX	2	1922	7/7	0.96	0.21	72,74,76,104	7
86	OHX	1	3552	7/7	0.96	0.16	64,67,67,92	7
87	MG	5	3910	1/1	0.96	0.43	41,41,41,41	0
87	MG	1	4002	1/1	0.96	0.17	37,37,37,37	0
86	OHX	4	206	7/7	0.96	0.23	57,57,58,83	7
87	MG	6	2105	1/1	0.96	0.28	45,45,45,45	0
86	OHX	6	2005	7/7	0.96	0.18	67,68,71,103	7
87	MG	1	3836	1/1	0.96	0.50	48,48,48,48	0
87	MG	1	3837	1/1	0.96	0.71	35,35,35,35	0
87	MG	1	3838	1/1	0.96	0.37	42,42,42,42	0
86	OHX	4	207	7/7	0.96	0.13	77,78,81,100	7
86	OHX	4	209	7/7	0.96	0.16	59,62,64,92	7
87	MG	1	3842	1/1	0.96	0.55	43,43,43,43	0
86	OHX	1	3553	7/7	0.96	0.10	113,114,115,137	7
87	MG	1	3844	1/1	0.96	0.53	54,54,54,54	0
86	OHX	2	2001	7/7	0.96	0.17	74,75,77,107	7
86	OHX	1	3556	7/7	0.96	0.28	72,73,76,107	7
86	OHX	5	3574	7/7	0.96	0.15	62,63,64,95	7
87	MG	1	3850	1/1	0.96	0.59	40,40,40,40	0
87	MG	1	3851	1/1	0.96	0.28	57,57,57,57	0
87	MG	1	4020	1/1	0.96	0.24	43,43,43,43	0
86	OHX	1	3669	7/7	0.96	0.31	45,47,50,76	7
86	OHX	6	2012	7/7	0.96	0.22	66,66,67,88	7
86	OHX	5	3578	7/7	0.96	0.11	153,154,155,165	7
87	MG	1	3857	1/1	0.96	0.56	47,47,47,47	0
86	OHX	5	3580	7/7	0.96	0.30	60,61,61,91	7
86	OHX	1	3475	7/7	0.96	0.26	57,60,62,90	7
86	OHX	L3	402	7/7	0.96	0.17	74,75,79,102	7
88	ZN	e1	501	1/1	0.96	0.12	191,191,191,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3559	7/7	0.96	0.16	101,102,102,122	7
87	MG	1	4029	1/1	0.96	0.59	43,43,43,43	0
86	OHX	5	3495	7/7	0.97	0.14	86,87,88,111	7
86	OHX	1	3511	7/7	0.97	0.17	88,90,93,110	7
86	OHX	5	3499	7/7	0.97	0.18	77,79,80,102	7
86	OHX	2	1937	7/7	0.97	0.17	102,103,106,123	7
86	OHX	2	1983	7/7	0.97	0.15	100,102,103,115	7
86	OHX	1	3640	7/7	0.97	0.15	70,70,71,98	7
86	OHX	5	3503	7/7	0.97	0.17	49,53,55,75	7
87	MG	5	3967	1/1	0.97	0.33	37,37,37,37	0
87	MG	L2	302	1/1	0.97	0.42	39,39,39,39	0
86	OHX	5	3504	7/7	0.97	0.19	32,39,43,64	7
86	OHX	1	3514	7/7	0.97	0.24	41,46,51,81	7
86	OHX	1	3428	7/7	0.97	0.18	74,74,77,92	0
86	OHX	5	3509	7/7	0.97	0.13	103,104,106,124	7
86	OHX	5	3513	7/7	0.97	0.16	61,62,64,80	7
86	OHX	1	3519	7/7	0.97	0.16	85,85,87,108	7
86	OHX	5	3515	7/7	0.97	0.12	138,139,140,151	7
86	OHX	5	3516	7/7	0.97	0.23	42,45,50,70	7
86	OHX	1	3433	7/7	0.97	0.20	54,63,70,96	0
86	OHX	5	3520	7/7	0.97	0.14	103,104,106,122	7
86	OHX	1	3434	7/7	0.97	0.21	73,75,76,93	7
87	MG	5	3781	1/1	0.97	0.56	39,39,39,39	0
87	MG	5	3782	1/1	0.97	0.32	39,39,39,39	0
86	OHX	5	3524	7/7	0.97	0.21	68,71,73,95	7
86	OHX	1	3436	7/7	0.97	0.17	81,83,86,103	7
86	OHX	5	3660	7/7	0.97	0.28	42,46,48,80	7
86	OHX	1	3587	7/7	0.97	0.24	83,84,85,107	7
87	MG	1	3796	1/1	0.97	0.21	49,49,49,49	0
86	OHX	1	3525	7/7	0.97	0.16	80,81,84,112	7
86	OHX	1	3526	7/7	0.97	0.13	76,77,79,96	7
86	OHX	1	3650	7/7	0.97	0.16	53,53,55,79	7
86	OHX	1	3442	7/7	0.97	0.15	72,75,81,91	7
86	OHX	1	3591	7/7	0.97	0.12	106,107,108,136	7
86	OHX	5	3533	7/7	0.97	0.21	51,51,52,79	7
86	OHX	1	3447	7/7	0.97	0.22	54,55,59,84	7
87	MG	2	2070	1/1	0.97	0.30	94,94,94,94	0
87	MG	6	2043	1/1	0.97	0.41	47,47,47,47	0
86	OHX	3	201	7/7	0.97	0.20	82,89,90,102	7
86	OHX	1	3448	7/7	0.97	0.23	58,60,64,98	7
87	MG	6	2046	1/1	0.97	0.18	121,121,121,121	0
86	OHX	3	204	7/7	0.97	0.16	96,98,98,118	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3451	7/7	0.97	0.17	60,62,67,86	7
87	MG	1	3813	1/1	0.97	0.54	30,30,30,30	0
87	MG	6	2050	1/1	0.97	0.60	38,38,38,38	0
86	OHX	5	3674	7/7	0.97	0.31	70,71,72,102	7
87	MG	5	4006	1/1	0.97	0.23	34,34,34,34	0
86	OHX	2	1955	7/7	0.97	0.23	82,83,86,99	7
86	OHX	1	3455	7/7	0.97	0.14	76,78,82,100	7
86	OHX	5	3542	7/7	0.97	0.09	155,156,156,166	7
86	OHX	1	3536	7/7	0.97	0.17	50,55,57,76	7
87	MG	5	4011	1/1	0.97	0.36	43,43,43,43	0
86	OHX	4	204	7/7	0.97	0.22	59,60,63,80	7
86	OHX	5	3545	7/7	0.97	0.23	50,52,54,85	7
86	OHX	6	1998	7/7	0.97	0.28	76,77,78,103	7
86	OHX	1	3456	7/7	0.97	0.17	84,89,90,108	7
87	MG	5	4016	1/1	0.97	0.39	29,29,29,29	0
86	OHX	5	3549	7/7	0.97	0.22	59,60,60,86	7
86	OHX	6	2000	7/7	0.97	0.21	60,60,64,94	7
86	OHX	5	3551	7/7	0.97	0.08	113,114,115,135	7
86	OHX	6	2001	7/7	0.97	0.28	61,62,63,93	7
87	MG	5	3819	1/1	0.97	0.30	33,33,33,33	0
86	OHX	5	3554	7/7	0.97	0.21	54,57,58,90	7
86	OHX	1	3600	7/7	0.97	0.11	124,124,125,147	7
87	MG	1	3833	1/1	0.97	0.42	38,38,38,38	0
87	MG	5	4025	1/1	0.97	0.17	56,56,56,56	0
87	MG	5	3824	1/1	0.97	0.46	34,34,34,34	0
86	OHX	5	3556	7/7	0.97	0.18	58,59,60,83	7
86	OHX	1	3539	7/7	0.97	0.18	45,48,50,72	7
86	OHX	5	3691	7/7	0.97	0.17	51,53,55,88	7
87	MG	5	3828	1/1	0.97	0.49	31,31,31,31	0
86	OHX	4	210	7/7	0.97	0.15	82,83,85,107	7
87	MG	5	4033	1/1	0.97	0.22	45,45,45,45	0
86	OHX	4	211	7/7	0.97	0.22	45,47,49,83	7
87	MG	5	4035	1/1	0.97	0.35	42,42,42,42	0
87	MG	5	3831	1/1	0.97	0.25	47,47,47,47	0
87	MG	1	3839	1/1	0.97	0.66	29,29,29,29	0
86	OHX	1	3457	7/7	0.97	0.30	52,56,59,79	7
87	MG	5	3835	1/1	0.97	0.37	41,41,41,41	0
86	OHX	4	213	7/7	0.97	0.11	102,103,104,129	7
87	MG	1	3995	1/1	0.97	0.37	35,35,35,35	0
86	OHX	5	3565	7/7	0.97	0.09	124,125,127,141	7
87	MG	6	2078	1/1	0.97	0.50	42,42,42,42	0
86	OHX	2	1969	7/7	0.97	0.09	133,134,134,153	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3542	7/7	0.97	0.20	72,73,74,96	7
87	MG	1	3999	1/1	0.97	0.39	32,32,32,32	0
87	MG	5	3843	1/1	0.97	0.26	32,32,32,32	0
86	OHX	2	1986	7/7	0.97	0.14	90,91,92,113	7
87	MG	2	2101	1/1	0.97	0.33	78,78,78,78	0
86	OHX	1	3544	7/7	0.97	0.16	60,61,64,88	7
87	MG	5	3848	1/1	0.97	0.44	33,33,33,33	0
87	MG	6	2085	1/1	0.97	0.39	66,66,66,66	0
87	MG	5	4053	1/1	0.97	0.16	48,48,48,48	0
86	OHX	1	3467	7/7	0.97	0.12	91,92,95,114	7
86	OHX	1	3546	7/7	0.97	0.17	69,70,70,95	7
86	OHX	5	3573	7/7	0.97	0.17	64,65,68,85	7
86	OHX	2	1929	7/7	0.97	0.15	69,71,74,86	7
87	MG	1	3854	1/1	0.97	0.59	41,41,41,41	0
87	MG	5	3858	1/1	0.97	0.73	30,30,30,30	0
86	OHX	M5	301	7/7	0.97	0.18	70,70,72,103	7
86	OHX	2	1942	7/7	0.97	0.17	76,79,80,96	7
86	OHX	2	1910	7/7	0.97	0.18	88,89,92,110	7
86	OHX	1	3551	7/7	0.97	0.15	77,78,80,101	7
87	MG	1	4013	1/1	0.97	0.32	42,42,42,42	0
87	MG	6	2096	1/1	0.97	0.31	61,61,61,61	0
86	OHX	2	1932	7/7	0.97	0.18	92,93,94,116	7
86	OHX	5	3583	7/7	0.97	0.26	48,49,50,65	7
86	OHX	1	3485	7/7	0.97	0.15	88,89,90,107	7
86	OHX	6	1926	7/7	0.97	0.15	96,100,101,114	7
86	OHX	6	1927	7/7	0.97	0.20	55,58,62,72	7
86	OHX	5	3588	7/7	0.97	0.19	77,78,78,101	7
86	OHX	5	3589	7/7	0.97	0.18	48,50,52,84	7
86	OHX	5	3590	7/7	0.97	0.16	44,45,46,87	7
86	OHX	1	3554	7/7	0.97	0.13	69,69,70,97	7
86	OHX	2	1925	7/7	0.97	0.10	125,126,127,140	7
86	OHX	1	3488	7/7	0.97	0.16	110,110,114,130	7
86	OHX	2	2009	7/7	0.97	0.10	133,134,134,148	7
87	MG	5	3880	1/1	0.97	0.76	40,40,40,40	0
87	MG	6	2109	1/1	0.97	0.17	89,89,89,89	0
86	OHX	6	1938	7/7	0.97	0.12	89,90,93,109	7
86	OHX	6	1939	7/7	0.97	0.17	79,80,82,113	7
86	OHX	2	1946	7/7	0.97	0.14	125,126,127,136	7
86	OHX	2	1962	7/7	0.97	0.19	89,89,91,118	7
87	MG	5	3888	1/1	0.97	0.49	26,26,26,26	0
86	OHX	7	202	7/7	0.97	0.19	58,63,64,77	7
86	OHX	6	1943	7/7	0.97	0.13	87,88,89,109	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	1	4032	1/1	0.97	0.23	68,68,68,68	0
87	MG	1	4034	1/1	0.97	0.65	57,57,57,57	0
86	OHX	6	1945	7/7	0.97	0.17	71,72,74,100	7
87	MG	5	4092	1/1	0.97	0.34	42,42,42,42	0
87	MG	1	3882	1/1	0.97	0.47	51,51,51,51	0
87	MG	1	3883	1/1	0.97	0.58	48,48,48,48	0
87	MG	1	3886	1/1	0.97	0.35	43,43,43,43	0
86	OHX	1	3495	7/7	0.97	0.16	56,56,60,79	7
87	MG	5	3905	1/1	0.97	0.53	34,34,34,34	0
87	MG	1	3725	1/1	0.97	0.51	38,38,38,38	0
86	OHX	1	3624	7/7	0.97	0.23	54,54,55,85	7
86	OHX	1	3498	7/7	0.97	0.19	68,71,72,92	7
87	MG	5	3909	1/1	0.97	0.58	37,37,37,37	0
86	OHX	6	1951	7/7	0.97	0.10	115,116,117,131	7
87	MG	5	3913	1/1	0.97	0.53	41,41,41,41	0
86	OHX	8	205	7/7	0.97	0.24	71,71,74,91	7
86	OHX	5	3607	7/7	0.97	0.21	47,48,50,84	7
86	OHX	2	1947	7/7	0.97	0.20	68,69,70,98	7
86	OHX	2	1949	7/7	0.97	0.23	95,97,98,122	7
86	OHX	1	3503	7/7	0.97	0.17	65,66,70,87	7
86	OHX	6	1957	7/7	0.97	0.10	90,92,94,115	7
87	MG	6	2133	1/1	0.97	0.23	58,58,58,58	0
87	MG	7	216	1/1	0.97	0.37	37,37,37,37	0
86	OHX	1	3629	7/7	0.97	0.12	104,104,106,123	7
86	OHX	6	1959	7/7	0.97	0.19	84,86,87,109	7
86	OHX	1	3567	7/7	0.97	0.25	55,56,58,78	7
86	OHX	2	1917	7/7	0.97	0.16	81,82,84,103	7
86	OHX	5	3617	7/7	0.97	0.18	52,53,54,77	7
87	MG	5	3926	1/1	0.97	0.36	51,51,51,51	0
87	MG	1	4056	1/1	0.97	0.27	43,43,43,43	0
87	MG	1	4057	1/1	0.97	0.40	44,44,44,44	0
86	OHX	5	3434	7/7	0.97	0.18	102,104,108,113	0
87	MG	5	3726	1/1	0.97	0.24	34,34,34,34	0
86	OHX	1	3505	7/7	0.97	0.27	46,48,52,85	7
86	OHX	5	3447	7/7	0.97	0.18	44,46,52,76	7
86	OHX	5	3450	7/7	0.97	0.16	81,84,87,105	7
86	OHX	5	3451	7/7	0.97	0.21	57,59,60,78	7
86	OHX	5	3457	7/7	0.97	0.16	69,75,78,101	7
87	MG	5	3936	1/1	0.97	0.29	51,51,51,51	0
87	MG	1	3749	1/1	0.97	0.73	40,40,40,40	0
86	OHX	1	3633	7/7	0.97	0.18	69,70,72,98	7
87	MG	m5	301	1/1	0.97	0.40	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3463	7/7	0.97	0.15	73,74,77,102	7
87	MG	5	3735	1/1	0.97	0.46	37,37,37,37	0
87	MG	m7	201	1/1	0.97	0.65	35,35,35,35	0
86	OHX	5	3464	7/7	0.97	0.25	64,65,67,98	7
86	OHX	5	3627	7/7	0.97	0.25	57,58,59,90	7
86	OHX	5	3467	7/7	0.97	0.15	90,93,94,113	7
87	MG	1	3919	1/1	0.97	0.40	51,51,51,51	0
86	OHX	1	3506	7/7	0.97	0.17	103,104,108,129	7
86	OHX	5	3471	7/7	0.97	0.15	83,83,85,102	7
86	OHX	5	3474	7/7	0.97	0.22	46,48,51,76	7
86	OHX	1	3508	7/7	0.97	0.18	65,65,69,95	7
86	OHX	5	3476	7/7	0.97	0.22	76,79,82,100	7
86	OHX	5	3480	7/7	0.97	0.27	63,64,66,87	7
87	MG	2	2035	1/1	0.97	0.52	64,64,64,64	0
87	MG	5	3750	1/1	0.97	0.28	39,39,39,39	0
86	OHX	6	1970	7/7	0.97	0.17	90,91,92,111	7
86	OHX	5	3488	7/7	0.97	0.15	71,71,75,93	7
87	MG	1	3929	1/1	0.97	0.26	40,40,40,40	0
86	OHX	5	3637	7/7	0.97	0.10	59,61,61,95	7
86	OHX	2	1928	7/7	0.97	0.24	74,74,76,99	7
86	OHX	5	3494	7/7	0.97	0.23	46,47,50,70	7
86	OHX	5	3448	7/7	0.98	0.14	70,73,77,93	7
86	OHX	2	1912	7/7	0.98	0.13	105,106,108,115	7
86	OHX	2	1988	7/7	0.98	0.16	89,89,91,111	7
87	MG	5	3757	1/1	0.98	0.52	39,39,39,39	0
86	OHX	5	3452	7/7	0.98	0.13	109,110,112,119	0
86	OHX	5	3453	7/7	0.98	0.15	77,79,80,99	7
86	OHX	8	203	7/7	0.98	0.18	53,53,58,80	7
87	MG	1	3735	1/1	0.98	0.20	46,46,46,46	0
87	MG	5	3762	1/1	0.98	0.35	57,57,57,57	0
87	MG	5	3763	1/1	0.98	0.49	35,35,35,35	0
86	OHX	8	204	7/7	0.98	0.14	88,89,92,114	7
87	MG	5	3765	1/1	0.98	0.42	37,37,37,37	0
87	MG	5	3766	1/1	0.98	0.42	43,43,43,43	0
86	OHX	5	3455	7/7	0.98	0.19	81,84,85,99	7
86	OHX	5	3456	7/7	0.98	0.22	73,75,77,107	7
87	MG	1	3739	1/1	0.98	0.53	60,60,60,60	0
87	MG	4	224	1/1	0.98	0.39	37,37,37,37	0
86	OHX	6	1963	7/7	0.98	0.21	83,83,84,109	7
86	OHX	6	1964	7/7	0.98	0.12	57,60,61,83	7
86	OHX	5	3460	7/7	0.98	0.20	54,55,57,76	7
86	OHX	5	3462	7/7	0.98	0.16	65,67,69,94	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3486	7/7	0.98	0.22	63,65,68,95	7
86	OHX	2	1913	7/7	0.98	0.16	84,85,88,111	7
87	MG	1	3746	1/1	0.98	0.34	39,39,39,39	0
86	OHX	5	3466	7/7	0.98	0.16	95,96,98,108	0
86	OHX	5	3610	7/7	0.98	0.23	52,54,55,76	7
86	OHX	6	1967	7/7	0.98	0.19	56,57,59,80	7
86	OHX	5	3469	7/7	0.98	0.18	62,63,66,75	7
86	OHX	l3	401	7/7	0.98	0.18	54,57,59,83	7
86	OHX	2	1924	7/7	0.98	0.14	87,88,90,111	7
86	OHX	6	1969	7/7	0.98	0.13	79,80,80,104	7
86	OHX	5	3473	7/7	0.98	0.18	45,47,51,71	7
86	OHX	1	3599	7/7	0.98	0.15	49,50,51,76	7
86	OHX	1	3437	7/7	0.98	0.19	61,64,67,86	7
87	MG	5	3990	1/1	0.98	0.52	52,52,52,52	0
86	OHX	3	202	7/7	0.98	0.22	62,64,67,94	7
87	MG	M5	302	1/1	0.98	0.47	41,41,41,41	0
86	OHX	5	3477	7/7	0.98	0.18	68,69,71,94	7
86	OHX	5	3478	7/7	0.98	0.27	62,63,66,102	7
86	OHX	6	1973	7/7	0.98	0.15	76,78,80,103	7
87	MG	1	3761	1/1	0.98	0.47	52,52,52,52	0
87	MG	1	3934	1/1	0.98	0.42	39,39,39,39	0
86	OHX	m6	201	7/7	0.98	0.23	47,49,55,78	7
86	OHX	1	3440	7/7	0.98	0.16	77,79,81,87	7
86	OHX	o7	502	7/7	0.98	0.21	67,68,69,92	7
86	OHX	q2	502	7/7	0.98	0.20	53,55,61,84	7
86	OHX	5	3482	7/7	0.98	0.24	49,52,55,72	7
86	OHX	5	3487	7/7	0.98	0.19	45,47,49,69	7
86	OHX	2	1906	7/7	0.98	0.22	92,93,98,110	0
87	MG	1	3770	1/1	0.98	0.50	28,28,28,28	0
86	OHX	1	3445	7/7	0.98	0.17	59,62,63,91	7
86	OHX	5	3491	7/7	0.98	0.25	64,66,69,94	7
87	MG	1	3773	1/1	0.98	0.39	46,46,46,46	0
86	OHX	5	3492	7/7	0.98	0.25	61,64,66,88	7
86	OHX	5	3493	7/7	0.98	0.16	67,68,71,91	7
86	OHX	1	3496	7/7	0.98	0.19	43,45,49,65	7
86	OHX	1	3497	7/7	0.98	0.19	83,85,87,105	7
86	OHX	1	3550	7/7	0.98	0.22	73,74,75,100	7
86	OHX	5	3497	7/7	0.98	0.14	49,52,55,74	7
87	MG	1	3780	1/1	0.98	0.27	41,41,41,41	0
86	OHX	1	3446	7/7	0.98	0.16	78,81,85,98	0
86	OHX	4	205	7/7	0.98	0.23	61,63,64,91	7
87	MG	5	3815	1/1	0.98	0.49	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	3664	7/7	0.98	0.26	62,63,65,93	7
86	OHX	1	3499	7/7	0.98	0.17	58,59,63,83	7
87	MG	1	3785	1/1	0.98	0.54	45,45,45,45	0
87	MG	6	2055	1/1	0.98	0.48	44,44,44,44	0
87	MG	5	3821	1/1	0.98	0.23	48,48,48,48	0
86	OHX	4	208	7/7	0.98	0.18	82,83,85,104	7
87	MG	1	3787	1/1	0.98	0.53	54,54,54,54	0
86	OHX	2	1976	7/7	0.98	0.09	108,108,109,127	7
86	OHX	2	1916	7/7	0.98	0.15	82,86,87,105	7
86	OHX	5	3506	7/7	0.98	0.19	51,54,59,67	7
86	OHX	5	3507	7/7	0.98	0.18	62,64,65,95	7
86	OHX	1	3449	7/7	0.98	0.16	71,73,75,99	7
87	MG	5	4031	1/1	0.98	0.83	60,60,60,60	0
86	OHX	1	3612	7/7	0.98	0.15	62,63,64,83	7
86	OHX	5	3511	7/7	0.98	0.27	43,43,48,78	7
86	OHX	2	1948	7/7	0.98	0.09	107,108,109,129	7
86	OHX	1	3452	7/7	0.98	0.21	65,67,69,96	7
86	OHX	1	3558	7/7	0.98	0.21	59,60,62,84	7
86	OHX	1	3453	7/7	0.98	0.15	79,80,82,101	7
86	OHX	5	3517	7/7	0.98	0.17	65,67,68,97	7
86	OHX	5	3518	7/7	0.98	0.19	65,65,68,94	7
86	OHX	1	3507	7/7	0.98	0.15	79,79,82,95	7
87	MG	1	3802	1/1	0.98	0.46	28,28,28,28	0
86	OHX	L3	401	7/7	0.98	0.17	65,67,68,91	7
87	MG	1	3804	1/1	0.98	0.59	32,32,32,32	0
87	MG	1	3805	1/1	0.98	0.38	43,43,43,43	0
86	OHX	5	3521	7/7	0.98	0.19	45,45,47,69	7
86	OHX	5	3522	7/7	0.98	0.20	58,59,63,80	7
86	OHX	1	3561	7/7	0.98	0.22	54,54,56,73	7
86	OHX	2	1936	7/7	0.98	0.16	70,71,74,96	7
86	OHX	2	1903	7/7	0.98	0.20	83,89,95,96	0
87	MG	5	3849	1/1	0.98	0.84	36,36,36,36	0
86	OHX	1	3621	7/7	0.98	0.23	49,51,52,68	7
86	OHX	2	1952	7/7	0.98	0.17	68,69,71,98	7
87	MG	5	3853	1/1	0.98	0.61	40,40,40,40	0
87	MG	5	4054	1/1	0.98	0.29	30,30,30,30	0
86	OHX	2	1938	7/7	0.98	0.23	65,67,70,93	7
86	OHX	2	1939	7/7	0.98	0.15	98,99,100,120	7
87	MG	1	3816	1/1	0.98	0.48	39,39,39,39	0
86	OHX	O3	201	7/7	0.98	0.20	54,55,57,74	7
86	OHX	Q2	502	7/7	0.98	0.20	41,45,48,82	7
86	OHX	6	1905	7/7	0.98	0.19	74,77,79,87	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	1907	7/7	0.98	0.16	79,82,84,95	0
86	OHX	6	1909	7/7	0.98	0.18	86,86,90,100	7
86	OHX	1	3460	7/7	0.98	0.20	73,74,77,86	7
86	OHX	6	1913	7/7	0.98	0.19	76,77,80,94	7
87	MG	5	4065	1/1	0.98	0.53	59,59,59,59	0
87	MG	1	3826	1/1	0.98	0.39	36,36,36,36	0
86	OHX	5	3670	7/7	0.98	0.17	44,48,50,73	7
86	OHX	6	1914	7/7	0.98	0.13	94,95,96,108	7
86	OHX	1	3515	7/7	0.98	0.19	47,50,52,75	7
87	MG	5	3868	1/1	0.98	0.63	41,41,41,41	0
86	OHX	6	1920	7/7	0.98	0.16	79,80,82,104	7
86	OHX	6	1921	7/7	0.98	0.14	125,126,127,128	0
86	OHX	6	1922	7/7	0.98	0.25	56,58,60,81	7
86	OHX	6	1924	7/7	0.98	0.19	76,81,82,103	7
86	OHX	6	1925	7/7	0.98	0.19	59,59,62,76	7
86	OHX	5	3546	7/7	0.98	0.12	70,71,73,96	7
87	MG	1	4006	1/1	0.98	0.21	46,46,46,46	0
86	OHX	1	3569	7/7	0.98	0.17	49,53,56,82	7
87	MG	5	3877	1/1	0.98	0.50	37,37,37,37	0
86	OHX	1	3571	7/7	0.98	0.18	121,121,122,139	7
86	OHX	1	3572	7/7	0.98	0.16	45,46,49,72	7
87	MG	5	3881	1/1	0.98	0.57	34,34,34,34	0
86	OHX	1	3516	7/7	0.98	0.22	61,61,64,85	7
86	OHX	6	1931	7/7	0.98	0.17	70,72,75,96	7
86	OHX	5	3552	7/7	0.98	0.14	57,57,59,84	7
86	OHX	1	3461	7/7	0.98	0.23	50,52,60,78	7
86	OHX	1	3518	7/7	0.98	0.27	40,44,47,82	7
86	OHX	6	1934	7/7	0.98	0.17	86,87,89,102	7
86	OHX	6	1935	7/7	0.98	0.23	66,67,69,92	7
87	MG	5	3890	1/1	0.98	0.42	30,30,30,30	0
87	MG	5	3891	1/1	0.98	0.36	37,37,37,37	0
86	OHX	5	3557	7/7	0.98	0.19	58,58,60,83	7
86	OHX	6	1936	7/7	0.98	0.14	68,69,73,88	7
87	MG	5	3894	1/1	0.98	0.54	35,35,35,35	0
87	MG	5	3895	1/1	0.98	0.47	28,28,28,28	0
87	MG	1	3848	1/1	0.98	0.35	49,49,49,49	0
87	MG	1	3849	1/1	0.98	0.54	33,33,33,33	0
86	OHX	1	3462	7/7	0.98	0.22	67,68,71,90	7
86	OHX	5	3560	7/7	0.98	0.14	57,59,60,79	7
87	MG	5	3901	1/1	0.98	0.57	36,36,36,36	0
86	OHX	2	1908	7/7	0.98	0.19	96,98,99,106	0
86	OHX	5	3562	7/7	0.98	0.21	46,48,49,75	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	1941	7/7	0.98	0.14	98,98,100,115	7
86	OHX	1	3469	7/7	0.98	0.17	62,65,69,89	7
87	MG	1	3856	1/1	0.98	0.43	31,31,31,31	0
86	OHX	6	1942	7/7	0.98	0.18	84,84,85,102	7
86	OHX	1	3524	7/7	0.98	0.20	63,65,67,94	7
87	MG	1	3859	1/1	0.98	0.54	33,33,33,33	0
87	MG	5	3911	1/1	0.98	0.47	39,39,39,39	0
87	MG	7	214	1/1	0.98	0.40	59,59,59,59	0
86	OHX	5	3567	7/7	0.98	0.17	68,69,71,99	7
86	OHX	6	1944	7/7	0.98	0.15	111,111,113,127	7
87	MG	2	2107	1/1	0.98	0.68	71,71,71,71	0
86	OHX	1	3470	7/7	0.98	0.24	66,69,72,89	7
86	OHX	1	3472	7/7	0.98	0.18	52,55,56,86	7
86	OHX	6	1947	7/7	0.98	0.16	80,81,83,106	7
86	OHX	C8	201	7/7	0.98	0.14	114,115,117,130	7
86	OHX	1	3529	7/7	0.98	0.13	123,125,126,138	7
86	OHX	1	3530	7/7	0.98	0.18	76,76,78,96	7
87	MG	1	3869	1/1	0.98	0.50	36,36,36,36	0
86	OHX	1	3474	7/7	0.98	0.18	68,70,71,83	7
86	OHX	5	3576	7/7	0.98	0.14	51,52,53,76	7
87	MG	8	220	1/1	0.98	0.66	44,44,44,44	0
86	OHX	6	1953	7/7	0.98	0.16	88,89,91,115	7
86	OHX	2	1930	7/7	0.98	0.12	74,75,76,94	7
87	MG	1	4046	1/1	0.98	0.40	94,94,94,94	0
86	OHX	1	3476	7/7	0.98	0.28	55,57,59,91	7
87	MG	2	2119	1/1	0.98	0.15	93,93,93,93	0
86	OHX	6	1956	7/7	0.98	0.09	157,158,158,169	7
86	OHX	5	3582	7/7	0.98	0.20	58,60,63,83	7
86	OHX	1	3416	7/7	0.98	0.19	61,67,69,82	7
86	OHX	5	3584	7/7	0.98	0.17	53,53,56,68	7
87	MG	1	3715	1/1	0.98	0.35	45,45,45,45	0
86	OHX	5	3428	7/7	0.98	0.17	49,51,57,88	0
86	OHX	5	3433	7/7	0.98	0.17	48,50,55,73	7
87	MG	1	3884	1/1	0.98	0.85	36,36,36,36	0
87	MG	1	3885	1/1	0.98	0.49	35,35,35,35	0
86	OHX	1	3478	7/7	0.98	0.21	64,65,70,91	7
86	OHX	5	3440	7/7	0.98	0.19	75,76,77,89	7
86	OHX	5	3441	7/7	0.98	0.19	63,65,71,95	7
86	OHX	1	3481	7/7	0.98	0.16	85,88,90,104	7
87	MG	5	3742	1/1	0.98	0.58	26,26,26,26	0
87	MG	5	3944	1/1	0.98	0.25	43,43,43,43	0
86	OHX	5	3591	7/7	0.98	0.15	47,47,50,76	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	3744	1/1	0.98	0.61	43,43,43,43	0
86	OHX	5	3592	7/7	0.98	0.17	54,57,58,85	7
88	ZN	D6	500	1/1	0.98	0.08	85,85,85,85	0
87	MG	1	3893	1/1	0.98	0.61	31,31,31,31	0
88	ZN	D9	101	1/1	0.98	0.09	85,85,85,85	0
86	OHX	5	3444	7/7	0.98	0.16	48,54,57,83	7
88	ZN	Q0	500	1/1	0.98	0.14	56,56,56,56	0
86	OHX	5	3445	7/7	0.98	0.13	78,79,86,98	7
86	OHX	1	3482	7/7	0.98	0.12	61,66,70,88	7
86	OHX	7	204	7/7	0.98	0.20	49,50,53,71	7
86	OHX	7	206	7/7	0.98	0.15	69,69,72,96	7
87	MG	1	3900	1/1	0.98	0.30	39,39,39,39	0
86	OHX	6	1915	7/7	0.99	0.20	57,58,63,80	7
86	OHX	6	1916	7/7	0.99	0.17	62,62,65,81	7
86	OHX	6	1917	7/7	0.99	0.16	65,66,68,84	7
86	OHX	6	1918	7/7	0.99	0.15	61,62,65,83	7
86	OHX	1	3411	7/7	0.99	0.18	41,47,50,78	0
86	OHX	5	3479	7/7	0.99	0.15	49,53,56,81	7
87	MG	1	4033	1/1	0.99	0.39	40,40,40,40	0
86	OHX	1	3510	7/7	0.99	0.19	52,53,54,83	7
87	MG	5	3845	1/1	0.99	0.75	41,41,41,41	0
86	OHX	1	3570	7/7	0.99	0.16	52,55,56,78	7
86	OHX	1	3413	7/7	0.99	0.18	52,54,56,71	7
86	OHX	5	3483	7/7	0.99	0.14	48,49,51,67	7
86	OHX	5	3484	7/7	0.99	0.15	54,58,62,71	7
87	MG	5	3850	1/1	0.99	0.50	43,43,43,43	0
86	OHX	5	3485	7/7	0.99	0.12	54,55,58,74	7
86	OHX	5	3486	7/7	0.99	0.17	55,55,61,72	7
87	MG	1	3892	1/1	0.99	0.72	31,31,31,31	0
86	OHX	6	1923	7/7	0.99	0.15	65,67,69,79	7
86	OHX	1	3414	7/7	0.99	0.18	46,50,52,58	7
87	MG	1	3895	1/1	0.99	0.62	16,16,16,16	0
86	OHX	1	3415	7/7	0.99	0.17	64,64,69,79	0
86	OHX	5	3490	7/7	0.99	0.20	55,55,59,86	7
86	OHX	2	1919	7/7	0.99	0.16	77,80,82,97	7
86	OHX	1	3459	7/7	0.99	0.22	57,61,62,77	7
86	OHX	n1	201	7/7	0.99	0.17	39,45,52,70	7
86	OHX	n3	201	7/7	0.99	0.14	57,59,60,76	7
86	OHX	1	3417	7/7	0.99	0.18	41,42,48,68	7
86	OHX	n9	102	7/7	0.99	0.20	55,56,60,80	7
86	OHX	o3	201	7/7	0.99	0.16	56,56,59,85	7
86	OHX	1	3418	7/7	0.99	0.17	53,56,62,84	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	1930	7/7	0.99	0.23	56,57,60,77	7
86	OHX	1	3419	7/7	0.99	0.18	51,55,56,76	7
86	OHX	1	3463	7/7	0.99	0.22	49,53,53,61	7
86	OHX	5	3498	7/7	0.99	0.17	100,101,103,125	7
86	OHX	1	3580	7/7	0.99	0.20	51,52,55,82	7
86	OHX	1	3464	7/7	0.99	0.14	102,103,104,112	7
86	OHX	1	3521	7/7	0.99	0.24	45,46,47,84	7
86	OHX	1	3465	7/7	0.99	0.17	62,65,68,81	7
86	OHX	6	1937	7/7	0.99	0.15	72,72,75,85	7
87	MG	1	3768	1/1	0.99	0.58	40,40,40,40	0
86	OHX	1	3420	7/7	0.99	0.18	39,41,44,64	7
86	OHX	1	3421	7/7	0.99	0.18	63,65,66,82	7
87	MG	5	3879	1/1	0.99	0.52	32,32,32,32	0
86	OHX	1	3468	7/7	0.99	0.23	50,52,55,62	7
86	OHX	1	3422	7/7	0.99	0.17	64,65,67,75	7
86	OHX	1	3527	7/7	0.99	0.17	57,59,59,72	7
86	OHX	1	3423	7/7	0.99	0.20	63,65,70,86	7
87	MG	5	3884	1/1	0.99	0.60	33,33,33,33	0
86	OHX	5	3510	7/7	0.99	0.24	40,44,48,69	7
86	OHX	1	3471	7/7	0.99	0.14	89,90,92,113	7
86	OHX	5	3512	7/7	0.99	0.19	65,66,70,89	7
86	OHX	1	3424	7/7	0.99	0.15	78,79,81,89	0
86	OHX	1	3425	7/7	0.99	0.20	54,59,64,84	0
86	OHX	1	3426	7/7	0.99	0.17	53,55,62,79	7
86	OHX	6	1948	7/7	0.99	0.16	69,69,71,98	7
86	OHX	1	3427	7/7	0.99	0.15	85,86,90,94	0
86	OHX	2	1920	7/7	0.99	0.19	82,84,86,96	7
86	OHX	1	3429	7/7	0.99	0.18	54,57,59,73	7
86	OHX	1	3430	7/7	0.99	0.14	69,72,74,80	7
86	OHX	1	3537	7/7	0.99	0.23	48,50,52,69	7
87	MG	5	3897	1/1	0.99	0.46	35,35,35,35	0
86	OHX	4	203	7/7	0.99	0.18	40,44,48,69	7
86	OHX	1	3479	7/7	0.99	0.20	52,53,55,79	7
86	OHX	1	3480	7/7	0.99	0.18	53,54,59,81	7
86	OHX	1	3431	7/7	0.99	0.25	55,56,62,63	7
87	MG	5	3902	1/1	0.99	0.71	29,29,29,29	0
86	OHX	5	3526	7/7	0.99	0.16	93,95,96,119	7
87	MG	1	3939	1/1	0.99	0.08	38,38,38,38	0
86	OHX	1	3432	7/7	0.99	0.25	49,50,52,69	7
86	OHX	2	1914	7/7	0.99	0.23	65,66,66,82	7
87	MG	5	3749	1/1	0.99	0.52	44,44,44,44	0
86	OHX	1	3484	7/7	0.99	0.15	52,56,59,80	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	1902	7/7	0.99	0.16	77,77,81,93	0
86	OHX	1	3435	7/7	0.99	0.19	69,70,70,74	7
86	OHX	2	1950	7/7	0.99	0.15	83,84,86,106	7
87	MG	5	3912	1/1	0.99	0.49	27,27,27,27	0
86	OHX	2	1923	7/7	0.99	0.18	76,77,78,105	7
86	OHX	1	3489	7/7	0.99	0.18	64,66,67,88	7
86	OHX	5	3401	7/7	0.99	0.16	48,50,57,65	0
86	OHX	5	3402	7/7	0.99	0.16	34,39,46,63	0
86	OHX	5	3404	7/7	0.99	0.16	30,36,40,66	0
86	OHX	5	3405	7/7	0.99	0.16	57,58,60,69	0
86	OHX	5	3406	7/7	0.99	0.16	54,56,62,75	0
86	OHX	5	3540	7/7	0.99	0.17	49,50,52,75	7
87	MG	1	3806	1/1	0.99	0.30	39,39,39,39	0
86	OHX	5	3407	7/7	0.99	0.16	51,57,59,69	0
86	OHX	5	3408	7/7	0.99	0.18	43,49,52,69	7
86	OHX	5	3409	7/7	0.99	0.21	55,56,60,79	7
86	OHX	5	3410	7/7	0.99	0.16	54,56,59,70	7
86	OHX	5	3412	7/7	0.99	0.16	74,75,80,87	0
86	OHX	5	3413	7/7	0.99	0.17	43,45,51,64	7
86	OHX	5	3414	7/7	0.99	0.18	61,63,64,73	0
86	OHX	5	3415	7/7	0.99	0.19	52,52,55,73	7
86	OHX	5	3416	7/7	0.99	0.22	46,47,50,76	7
86	OHX	5	3417	7/7	0.99	0.16	55,58,60,79	7
86	OHX	5	3418	7/7	0.99	0.18	44,50,54,67	7
87	MG	1	3818	1/1	0.99	0.45	32,32,32,32	0
87	MG	1	3819	1/1	0.99	0.61	35,35,35,35	0
86	OHX	5	3419	7/7	0.99	0.16	40,45,51,71	7
86	OHX	5	3420	7/7	0.99	0.16	64,65,66,78	7
86	OHX	5	3421	7/7	0.99	0.17	67,68,73,82	0
86	OHX	5	3422	7/7	0.99	0.18	56,58,60,65	7
86	OHX	5	3423	7/7	0.99	0.17	59,62,62,79	7
86	OHX	5	3424	7/7	0.99	0.20	67,70,71,78	7
86	OHX	5	3425	7/7	0.99	0.20	57,61,62,83	0
86	OHX	5	3426	7/7	0.99	0.16	45,48,49,69	7
86	OHX	1	3438	7/7	0.99	0.16	51,54,60,75	7
86	OHX	5	3429	7/7	0.99	0.17	61,62,66,78	7
86	OHX	5	3430	7/7	0.99	0.15	54,55,59,67	7
86	OHX	5	3431	7/7	0.99	0.25	48,50,53,62	7
86	OHX	5	3432	7/7	0.99	0.18	48,48,52,66	7
86	OHX	1	3439	7/7	0.99	0.15	63,65,67,81	7
86	OHX	2	1901	7/7	0.99	0.16	71,74,79,94	0
86	OHX	5	3435	7/7	0.99	0.22	48,49,53,79	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3436	7/7	0.99	0.17	57,57,60,76	7
86	OHX	5	3437	7/7	0.99	0.26	60,62,65,79	7
86	OHX	5	3438	7/7	0.99	0.18	50,54,58,71	7
86	OHX	5	3439	7/7	0.99	0.16	82,83,86,93	0
86	OHX	1	3493	7/7	0.99	0.17	56,57,58,82	7
86	OHX	1	3494	7/7	0.99	0.13	71,71,74,88	7
86	OHX	5	3442	7/7	0.99	0.18	59,61,63,72	7
86	OHX	1	3441	7/7	0.99	0.18	49,52,56,62	7
86	OHX	2	1904	7/7	0.99	0.16	80,86,89,94	7
86	OHX	1	3443	7/7	0.99	0.16	57,58,59,81	7
86	OHX	5	3446	7/7	0.99	0.18	50,53,56,67	7
86	OHX	5	3579	7/7	0.99	0.20	56,58,59,80	7
86	OHX	1	3444	7/7	0.99	0.16	74,75,75,104	7
86	OHX	2	1926	7/7	0.99	0.12	85,87,88,100	7
86	OHX	5	3449	7/7	0.99	0.12	80,81,83,107	7
86	OHX	N9	101	7/7	0.99	0.23	50,50,57,72	7
86	OHX	2	1905	7/7	0.99	0.21	65,66,67,82	7
86	OHX	1	3404	7/7	0.99	0.14	56,60,63,69	0
86	OHX	1	3502	7/7	0.99	0.23	38,40,44,66	7
87	MG	5	3970	1/1	0.99	0.55	51,51,51,51	0
86	OHX	5	3454	7/7	0.99	0.16	44,46,48,64	7
86	OHX	6	1901	7/7	0.99	0.15	60,64,68,72	0
86	OHX	6	1902	7/7	0.99	0.20	76,79,84,89	0
86	OHX	6	1903	7/7	0.99	0.16	64,67,68,80	0
86	OHX	5	3458	7/7	0.99	0.17	59,60,62,82	7
86	OHX	7	201	7/7	0.99	0.19	64,69,70,92	7
87	MG	n3	203	1/1	0.99	0.47	31,31,31,31	0
87	MG	5	3817	1/1	0.99	0.26	40,40,40,40	0
86	OHX	6	1904	7/7	0.99	0.15	67,69,74,78	7
86	OHX	1	3405	7/7	0.99	0.17	62,63,71,80	0
86	OHX	5	3461	7/7	0.99	0.18	40,43,48,69	7
86	OHX	7	205	7/7	0.99	0.20	70,72,74,91	7
86	OHX	6	1906	7/7	0.99	0.21	57,58,60,80	7
86	OHX	1	3407	7/7	0.99	0.15	61,66,69,75	0
86	OHX	6	1908	7/7	0.99	0.16	66,67,72,92	0
86	OHX	5	3465	7/7	0.99	0.23	55,56,58,64	7
86	OHX	1	3450	7/7	0.99	0.19	69,69,69,89	7
86	OHX	6	1910	7/7	0.99	0.19	62,62,66,82	7
86	OHX	8	202	7/7	0.99	0.17	45,50,55,70	7
87	MG	1	3872	1/1	0.99	0.67	31,31,31,31	0
86	OHX	5	3468	7/7	0.99	0.20	61,61,66,78	7
86	OHX	1	3408	7/7	0.99	0.17	42,47,53,66	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	5	3832	1/1	0.99	0.56	33,33,33,33	0
88	ZN	Q3	501	1/1	0.99	0.10	71,71,71,71	0
88	ZN	d6	101	1/1	0.99	0.13	67,67,67,67	0
86	OHX	6	1912	7/7	0.99	0.16	62,63,66,82	7
88	ZN	d9	101	1/1	0.99	0.10	98,98,98,98	0
86	OHX	1	3409	7/7	0.99	0.18	57,59,61,75	7
86	OHX	5	3472	7/7	0.99	0.21	53,54,57,75	7
86	OHX	1	3410	7/7	0.99	0.17	56,58,60,73	7
86	OHX	1	3401	7/7	1.00	0.17	37,41,45,62	0
86	OHX	5	3411	7/7	1.00	0.17	40,41,45,59	7
86	OHX	1	3402	7/7	1.00	0.16	47,49,55,67	0
86	OHX	5	3427	7/7	1.00	0.18	41,42,45,56	7
86	OHX	1	3406	7/7	1.00	0.18	41,44,49,68	0
86	OHX	1	3403	7/7	1.00	0.15	44,45,48,62	0
86	OHX	1	3412	7/7	1.00	0.22	57,62,65,72	7
88	ZN	o7	501	1/1	1.00	0.18	57,57,57,57	0
88	ZN	q0	201	1/1	1.00	0.13	41,41,41,41	0
86	OHX	5	3403	7/7	1.00	0.16	32,33,41,65	0
88	ZN	q3	501	1/1	1.00	0.10	76,76,76,76	0
88	ZN	O7	101	1/1	1.00	0.17	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.