wwPDB EM Validation Summary Report

Mar 3, 2024 – 11:28 AM EST

PDB ID	:	6BY7
EMDB ID	:	EMD-7304
Title	:	Folding DNA into a lipid-conjugated nano-barrel for controlled reconstitution of membrane proteins
Authors	:	Dong, Y.; Chen, S.; Zhang, S.; Sodroski, J.; Yang, Z.; Liu, D.; Mao, Y.
Deposited on	:	2017-12-20
Resolution	:	7.50 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

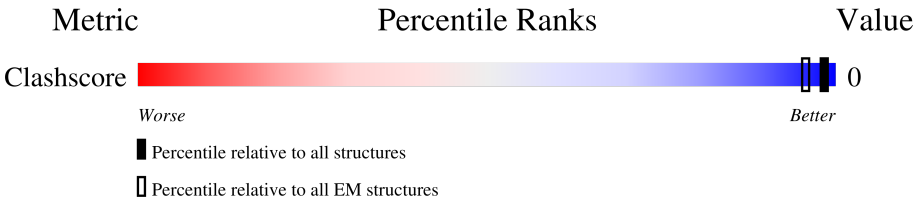
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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)	EM structures (#Entries)
Clashscore	158937	4297

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	52	48% 83% 17%
2	1B	55	60% 69% 27% .
3	1C	16	100% 88% 12%
4	1D	59	71% 80% 20%
5	1E	51	73% 84% 14% .
6	1F	46	100% 67% 28% .
7	1G	16	88% 81% 12% 6%
8	1H	48	56% 79% 19% .
9	1I	47	83% 79% 19% .
10	1J	24	58% 83% 17%

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Mol	Chain	Length	Quality of chain
11	1K	46	100% 67% 28%
12	1L	16	100% 81% 19%
13	1M	32	50% 88% 9%
14	1O	40	58% 75% 25%
15	1P	46	100% 72% 24%
16	1Q	37	78% 84% 16%
17	1R	48	58% 73% 25%
18	1S	37	65% 76% 22%
19	1T	16	100% 94% 6%
20	1U	40	38% 90% 8%
21	1V	26	100% 85% 15%
22	1W	40	80% 85% 15%
23	1X	48	56% 85% 12%
24	1Y	27	85% 89% 11%
25	1Z	26	100% 88% 8%
26	1a	47	85% 85% 15%
27	1b	32	41% 75% 25%
28	1c	40	32% 92% 8%
29	1d	40	75% 92% 8%
30	1e	26	100% 92% 8%
31	1f	40	38% 85% 15%
32	1g	48	44% 92% 6%
33	1h	48	31% 83% 17%
34	1i	48	98% 90% 10%
35	1j	32	53% 91% 9%

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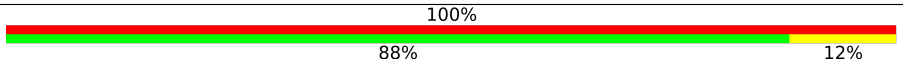
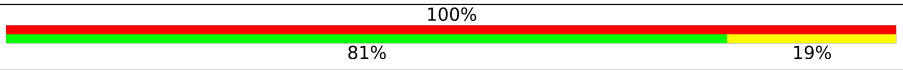
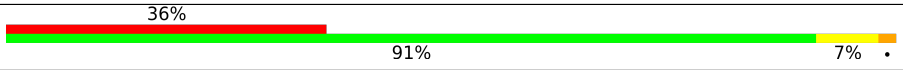
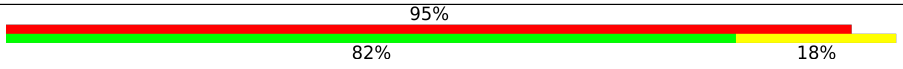
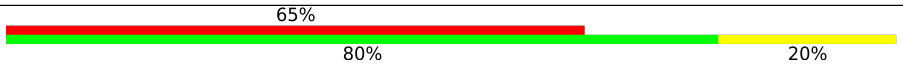
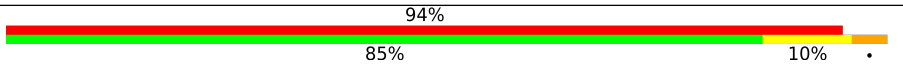
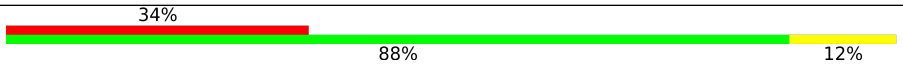
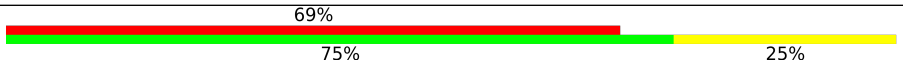
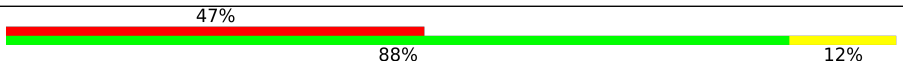
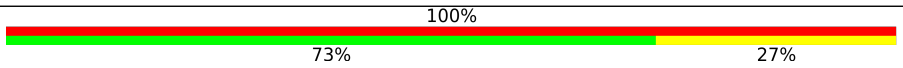
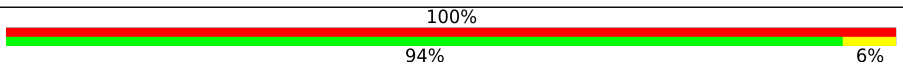
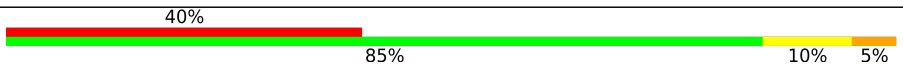
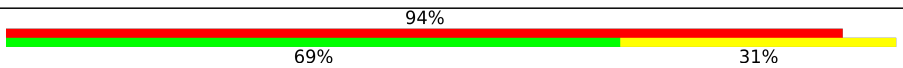
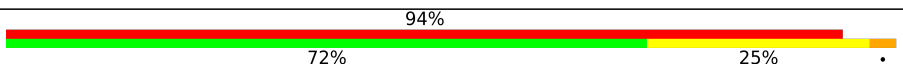
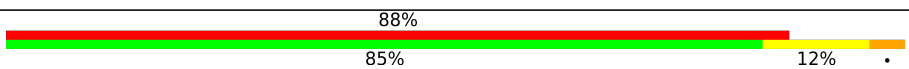
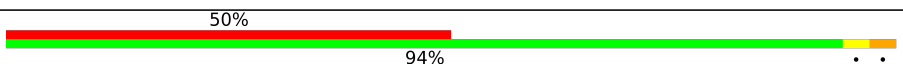
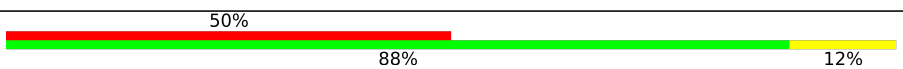
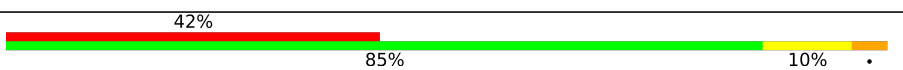
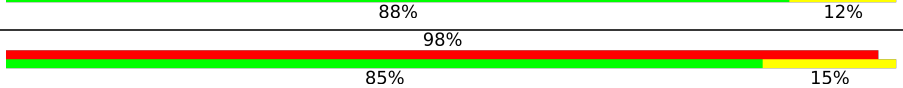
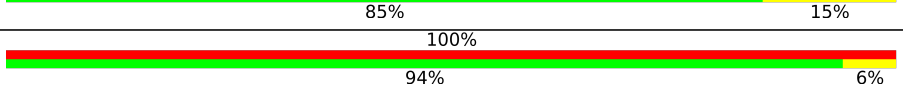
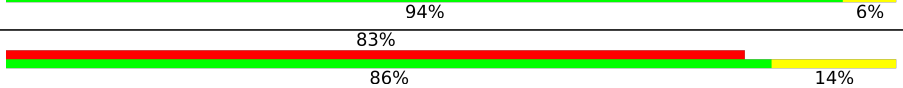
Mol	Chain	Length	Quality of chain
36	1k	40	
37	1l	48	
38	1m	16	
39	1n	56	
40	1o	40	
41	1p	40	
42	1q	48	
43	1r	32	
44	1s	32	
45	1t	32	
46	1u	48	
47	1v	16	
48	1w	40	
49	1x	16	
50	2N	36	
51	2A	32	
52	2B	48	
53	2C	26	
54	2D	32	
55	2E	40	
56	2F	48	
57	2G	40	
58	2H	40	
59	2I	16	
60	2J	29	

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Mol	Chain	Length	Quality of chain
61	2K	24	38% 83% 17%
62	2L	32	69% 91% 9%
63	2M	24	92% 96%
64	2O	26	88% 77% 12% 8%
65	2P	40	35% 75% 25%
66	2Q	40	58% 92% 5%
67	2R	40	42% 82% 18%
68	2S	58	86% 81% 19%
69	2T	24	96% 96%
70	2U	52	48% 88% 12%
71	2V	40	40% 88% 12%
72	2W	48	46% 88% 12%
73	2X	48	40% 85% 15%
74	2Y	32	16% 91% 6%
75	2Z	40	58% 82% 18%
76	2a	58	83% 88% 12%
77	2b	56	32% 84% 14%
78	2c	45	84% 93%
79	2d	52	35% 88% 10%
80	2e	37	97% 84% 14%
81	2f	48	48% 90% 10%
82	2g	48	60% 90% 10%
83	2h	56	34% 91% 5%
84	2i	32	47% 78% 22%
85	2j	16	100% 81% 19%

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Mol	Chain	Length	Quality of chain
86	2k	32	44% 91% 9%
87	2l	48	40% 88% 10%
88	2m	48	81% 94% 6%
89	2n	16	100% 81% 19%
90	2o	32	88% 91% 9%
91	2p	32	44% 88% 12%
92	2q	40	55% 80% 20%
93	2r	24	71% 79% 12% 8%
94	2s	32	56% 91% 9%
95	2t	40	100% 78% 22%
96	2u	32	72% 88% 12%
97	2v	32	50% 81% 19%
98	2w	47	74% 77% 23%
99	2x	16	100% 94% 6%
100	3N	4346	66% 83% 16%
101	3A	40	82% 88% 12%
102	3B	40	42% 80% 15% 5%
103	3C	48	46% 83% 17%
104	3D	48	46% 81% 15%
105	3E	48	54% 85% 15%
106	3F	56	32% 88% 9%
107	3G	16	100% 88% 12%
108	3H	56	71% 79% 20%
109	3I	36	42% 78% 19%
110	3J	35	100% 83% 14%

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Mol	Chain	Length	Quality of chain
111	3S	32	78% 88% 12%
112	3K	48	63% 90% 8%
113	3L	37	65% 95% 5%
114	3M	55	65% 80% 20%
115	3O	48	75% 83% 15%
116	3P	38	100% 97%
117	3Q	26	88% 81% 15%
118	3R	32	22% 84% 16%

2 Entry composition (i)

There are 118 unique types of molecules in this entry. The entry contains 180167 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA chain called DNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1A	52	1082	516	213	302	51	0	0

- Molecule 2 is a DNA chain called DNA (55-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1B	55	1137	540	219	324	54	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*AP*TP*AP*AP*CP*GP*GP*CP*TP*CP*AP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	1C	16	327	156	66	90	15	0	0

- Molecule 4 is a DNA chain called DNA (59-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	1D	59	1220	584	229	349	58	0	0

- Molecule 5 is a DNA chain called DNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	1E	51	1052	502	206	294	50	0	0

- Molecule 6 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	46	Total	C	N	O	P	0	0
			950	455	181	269	45		

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*CP*AP*AP*CP*CP*GP*AP*GP*CP*TP*TP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	16	Total	C	N	O	P	0	0
			321	155	55	96	15		

- Molecule 8 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	48	Total	C	N	O	P	0	0
			970	465	177	281	47		

- Molecule 9 is a DNA chain called DNA (47-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	47	Total	C	N	O	P	0	0
			971	462	183	280	46		

- Molecule 10 is a DNA chain called DNA (5'-D(*TP*AP*TP*TP*AP*GP*CP*GP*AP*GP*AP*TP*GP*GP*TP*TP*TP*TP*AP*TP*TP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	24	Total	C	N	O	P	0	0
			492	238	86	145	23		

- Molecule 11 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	46	Total	C	N	O	P	0	0
			945	450	177	273	45		

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*GP*AP*CP*AP*GP*AP*AP*TP*GP*AP*AP*AP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	16	Total	C	N	O	P	0	0
			333	158	73	87	15		

- Molecule 13 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	32	Total	C	N	O	P	0	0
			645	306	120	188	31		

- Molecule 14 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1O	40	Total	C	N	O	P	0	0
			808	386	154	229	39		

- Molecule 15 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1P	46	Total	C	N	O	P	0	0
			948	451	182	270	45		

- Molecule 16 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1Q	37	Total	C	N	O	P	0	0
			752	358	149	209	36		

- Molecule 17 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1R	48	Total	C	N	O	P	0	0
			976	464	181	284	47		

- Molecule 18 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1S	37	Total	C	N	O	P	0	0
			763	365	145	217	36		

- Molecule 19 is a DNA chain called DNA (5'-D(*CP*GP*CP*CP*AP*CP*CP*AP*GP*AP *TP*TP*CP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1T	16	Total	C	N	O	P	0	0
			318	153	57	93	15		

- Molecule 20 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1U	40	Total	C	N	O	P	0	0
			826	393	168	226	39		

- Molecule 21 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	26	Total	C	N	O	P	0	0
			521	252	84	160	25		

- Molecule 22 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	40	Total	C	N	O	P	0	0
			830	397	158	236	39		

- Molecule 23 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	48	Total	C	N	O	P	0	0
			983	468	192	276	47		

- Molecule 24 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Y	27	Total	C	N	O	P	0	0
			544	262	92	164	26		

- Molecule 25 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Z	26	Total	C	N	O	P	0	0
			531	254	100	152	25		

- Molecule 26 is a DNA chain called DNA (47-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1a	47	Total	C	N	O	P	0	0
			965	465	183	271	46		

- Molecule 27 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1b	32	Total	C	N	O	P	0	0
			665	317	133	184	31		

- Molecule 28 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1c	40	Total	C	N	O	P	0	0
			820	395	151	235	39		

- Molecule 29 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1d	40	Total	C	N	O	P	0	0
			826	396	162	229	39		

- Molecule 30 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1e	26	Total	C	N	O	P	0	0
			524	252	96	151	25		

- Molecule 31 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1f	40	Total	C	N	O	P	0	0
			804	387	141	237	39		

- Molecule 32 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1g	48	Total	C	N	O	P	0	0
			982	469	191	275	47		

- Molecule 33 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1h	48	Total	C	N	O	P	0	0
			993	474	192	280	47		

- Molecule 34 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	48	Total	C	N	O	P	0	0
			986	473	184	282	47		

- Molecule 35 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1j	32	Total	C	N	O	P	0	0
			659	314	130	184	31		

- Molecule 36 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1k	40	Total	C	N	O	P	0	0
			827	397	152	239	39		

- Molecule 37 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1l	48	Total	C	N	O	P	0	0
			980	470	175	288	47		

- Molecule 38 is a DNA chain called DNA (5'-D(P*TP*CP*GP*AP*GP*GP*TP*GP*AP*TP*TP*CP*GP*CP*GP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1m	16	Total	C	N	O	P	0	0
			328	157	59	97	15		

- Molecule 39 is a DNA chain called DNA (56-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1n	56	Total	C	N	O	P	0	0
			1148	548	217	328	55		

- Molecule 40 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1o	40	Total	C	N	O	P	0	0
			821	390	156	236	39		

- Molecule 41 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	40	Total	C	N	O	P	0	0
			816	389	157	231	39		

- Molecule 42 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1q	48	Total	C	N	O	P	0	0
			981	468	183	283	47		

- Molecule 43 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	32	Total	C	N	O	P	0	0
			654	310	125	188	31		

- Molecule 44 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	32	Total	C	N	O	P	0	0
			649	312	117	189	31		

- Molecule 45 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1t	32	Total	C	N	O	P	0	0
			651	310	119	191	31		

- Molecule 46 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1u	48	Total	C	N	O	P	0	0
			982	469	176	290	47		

- Molecule 47 is a DNA chain called DNA (5'-D(P*CP*CP*CP*CP*CP*AP*GP*CP*TP*GP*GP*TP*CP*AP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1v	16	Total	C	N	O	P	0	0
			319	153	57	94	15		

- Molecule 48 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1w	40	Total	C	N	O	P	0	0
			808	387	144	238	39		

- Molecule 49 is a DNA chain called DNA (5'-D(P*GP*AP*CP*AP*GP*AP*TP*GP*CP*GP*TP*GP*CP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1x	16	Total	C	N	O	P	0	0
			329	156	66	92	15		

- Molecule 50 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2N	36	Total	C	N	O	P	0	0
			736	353	133	215	35		

- Molecule 51 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
51	2A	32	Total	C	N	O	P	0	0
			665	315	135	184	31		

- Molecule 52 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2B	48	Total	C	N	O	P	0	0
			975	465	186	277	47		

- Molecule 53 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2C	26	Total	C	N	O	P	0	0
			527	256	83	163	25		

- Molecule 54 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2D	32	Total	C	N	O	P	0	0
			652	314	124	183	31		

- Molecule 55 is a DNA chain called DNA (5'-D(P*CP*AP*TP*AP*AP*CP*GP*CP*AP*TP*AP*AP*AP*AP*CP*GP*AP*GP*GP*AP*GP*GP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2E	40	Total 816	C 393	N 147	O 237	P 39	0	0

- Molecule 56 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	2F	48	Total 988	C 473	N 181	O 287	P 47	0	0

- Molecule 57 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	2G	40	Total 820	C 393	N 147	O 241	P 39	0	0

- Molecule 58 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
58	2H	40	Total 807	C 389	N 148	O 231	P 39	0	0

- Molecule 59 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
59	2I	16	Total 328	C 158	N 61	O 94	P 15	0	0

- Molecule 60 is a DNA chain called DNA (58-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
60	2J	29	Total 599	C 285	N 117	O 169	P 28	0	0

- Molecule 61 is a DNA chain called DNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
61	2K	24	Total 495	C 236	N 100	O 136	P 23	0	0

- Molecule 62 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
62	2L	32	Total	C	N	O	P	0	0
			653	314	121	187	31		

- Molecule 63 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
63	2M	24	Total	C	N	O	P	0	0
			488	233	94	138	23		

- Molecule 64 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
64	2O	26	Total	C	N	O	P	0	0
			532	257	97	153	25		

- Molecule 65 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
65	2P	40	Total	C	N	O	P	0	0
			822	390	162	231	39		

- Molecule 66 is a DNA chain called DNA (58-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
66	2Q	40	Total	C	N	O	P	0	0
			818	392	151	236	39		

- Molecule 67 is a DNA chain called DNA (56-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
67	2R	40	Total	C	N	O	P	0	0
			822	394	155	234	39		

- Molecule 68 is a DNA chain called DNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
68	2S	58	Total	C	N	O	P	0	0
			1192	566	232	337	57		

- Molecule 69 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
69	2T	24	Total	C	N	O	P	0	0
			494	236	94	141	23		

- Molecule 70 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
70	2U	52	Total	C	N	O	P	0	0
			1059	508	191	309	51		

- Molecule 71 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
71	2V	40	Total	C	N	O	P	0	0
			815	393	141	242	39		

- Molecule 72 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
72	2W	48	Total	C	N	O	P	0	0
			987	472	185	283	47		

- Molecule 73 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
73	2X	48	Total	C	N	O	P	0	0
			974	463	179	285	47		

- Molecule 74 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
74	2Y	32	Total	C	N	O	P	0	0
			656	312	126	187	31		

- Molecule 75 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
75	2Z	40	Total	C	N	O	P	0	0
			818	394	146	239	39		

- Molecule 76 is a DNA chain called DNA (5'-D(P*TP*TP*TP*GP*TP*TP*AP*AP*AP*AP*CP*CP*GP*AP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
76	2a	58	Total	C	N	O	P	0	0
			1179	566	214	342	57		

- Molecule 77 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
77	2b	56	Total	C	N	O	P	0	0
			1149	549	213	332	55		

- Molecule 78 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
78	2c	45	Total	C	N	O	P	0	0
			914	441	165	264	44		

- Molecule 79 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
79	2d	52	Total	C	N	O	P	0	0
			1075	508	218	298	51		

- Molecule 80 is a DNA chain called DNA (5'-D(P*CP*TP*GP*GP*CP*CP*TP*TP*CP*C P*TP*GP*TP*AP*GP*CP*CP*AP*AP*AP*AP*AP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
80	2e	37	Total	C	N	O	P	0	0
			766	367	143	220	36		

- Molecule 81 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
81	2f	48	Total	C	N	O	P	0	0
			976	467	184	278	47		

- Molecule 82 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
82	2g	48	Total	C	N	O	P	0	0
			972	464	184	277	47		

- Molecule 83 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
83	2h	56	Total	C	N	O	P	0	0
			1156	551	223	327	55		

- Molecule 84 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
84	2i	32	Total	C	N	O	P	0	0
			661	315	135	180	31		

- Molecule 85 is a DNA chain called DNA (47-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
85	2j	16	Total	C	N	O	P	0	0
			326	157	59	95	15		

- Molecule 86 is a DNA chain called DNA (5'-D(P*CP*CP*AP*GP*TP*GP*CP*CP*AP*AP*AP*TP*CP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
86	2k	32	Total	C	N	O	P	0	0
			652	312	123	186	31		

- Molecule 87 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
87	2l	48	Total	C	N	O	P	0	0
			980	466	191	276	47		

- Molecule 88 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
88	2m	48	Total	C	N	O	P	0	0
			984	472	185	280	47		

- Molecule 89 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
89	2n	16	Total	C	N	O	P	0	0
			325	158	58	94	15		

- Molecule 90 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
90	2o	32	Total	C	N	O	P	0	0
			653	314	112	196	31		

- Molecule 91 is a DNA chain called DNA (56-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
91	2p	32	Total	C	N	O	P	0	0
			656	312	120	193	31		

- Molecule 92 is a DNA chain called DNA (56-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
92	2q	40	Total	C	N	O	P	0	0
			805	386	136	244	39		

- Molecule 93 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
93	2r	24	Total	C	N	O	P	0	0
			485	233	88	141	23		

- Molecule 94 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
94	2s	32	Total	C	N	O	P	0	0
			655	311	130	183	31		

- Molecule 95 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
95	2t	40	Total	C	N	O	P	0	0
			824	391	164	230	39		

- Molecule 96 is a DNA chain called DNA (55-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
96	2u	32	Total	C	N	O	P	0	0
			652	311	121	189	31		

- Molecule 97 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
97	2v	32	Total	C	N	O	P	0	0
			651	313	107	200	31		

- Molecule 98 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
98	2w	47	Total	C	N	O	P	0	0
			974	464	202	262	46		

- Molecule 99 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
99	2x	16	Total	C	N	O	P	0	0
			320	153	60	92	15		

- Molecule 100 is a DNA chain called DNA (4346-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
100	3N	4346	Total	C	N	O	P	0	0
			88890	42499	15686	26368	4337		

- Molecule 101 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
101	3A	40	Total	C	N	O	P	0	0
			841	395	175	232	39		

- Molecule 102 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
102	3B	40	Total	C	N	O	P	0	0
			818	389	157	233	39		

- Molecule 103 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
103	3C	48	Total	C	N	O	P	0	0
			982	469	185	281	47		

- Molecule 104 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
104	3D	48	Total	C	N	O	P	0	0
			999	473	193	286	47		

- Molecule 105 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
105	3E	48	Total	C	N	O	P	0	0
			991	468	198	278	47		

- Molecule 106 is a DNA chain called DNA (56-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
106	3F	56	Total	C	N	O	P	0	0
			1131	544	197	335	55		

- Molecule 107 is a DNA chain called DNA (5'-D(*GP*TP*GP*CP*CP*TP*AP*AP*GP*GP*AP*TP*AP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
107	3G	16	Total	C	N	O	P	0	0
			326	157	59	95	15		

- Molecule 108 is a DNA chain called DNA (56-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
108	3H	56	Total	C	N	O	P	0	0
			1142	546	210	331	55		

- Molecule 109 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
109	3I	36	Total	C	N	O	P	0	0
			736	350	139	212	35		

- Molecule 110 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
110	3J	35	Total	C	N	O	P	0	0
			714	341	133	206	34		

- Molecule 111 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
111	3S	32	Total	C	N	O	P	0	0
			655	314	121	189	31		

- Molecule 112 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
112	3K	48	Total	C	N	O	P	0	0
			988	469	197	275	47		

- Molecule 113 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
113	3L	37	Total	C	N	O	P	0	0
			760	358	146	220	36		

- Molecule 114 is a DNA chain called DNA (55-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
114	3M	55	Total	C	N	O	P	0	0
			1129	539	214	322	54		

- Molecule 115 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
115	3O	48	Total	C	N	O	P	0	0
			985	471	189	278	47		

- Molecule 116 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
116	3P	38	Total	C	N	O	P	0	0
			785	375	150	223	37		

- Molecule 117 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
117	3Q	26	Total	C	N	O	P	0	0
			539	255	114	145	25		

- Molecule 118 is a DNA chain called DNA (32-MER).

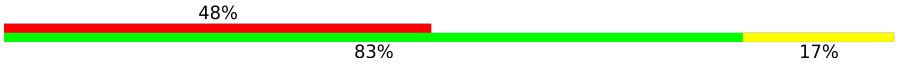
Mol	Chain	Residues	Atoms					AltConf	Trace
118	3R	32	Total	C	N	O	P	0	0
			666	317	127	191	31		

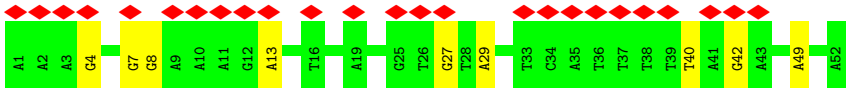
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: DNA (52-MER)

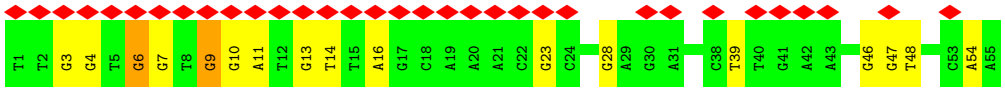
Chain 1A:





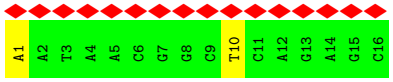
• Molecule 2: DNA (55-MER)

Chain 1B:



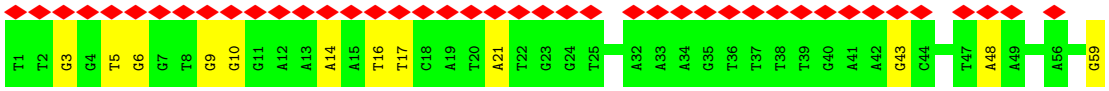
• Molecule 3: DNA (5'-D(*AP*AP*TP*AP*AP*CP*GP*GP*CP*TP*CP*AP*GP*AP*GP*C)-3')

Chain 1C:



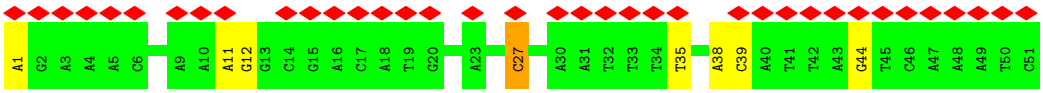
• Molecule 4: DNA (59-MER)

Chain 1D:



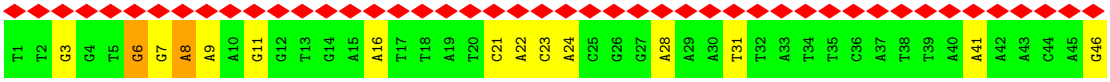
• Molecule 5: DNA (51-MER)

Chain 1E:



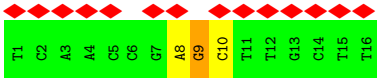
• Molecule 6: DNA (46-MER)

Chain 1F:



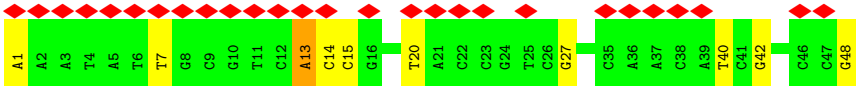
• Molecule 7: DNA (5'-D(*TP*CP*AP*AP*CP*CP*GP*AP*GP*CP*TP*TP*GP*CP*TP*T)-3')

Chain 1G:



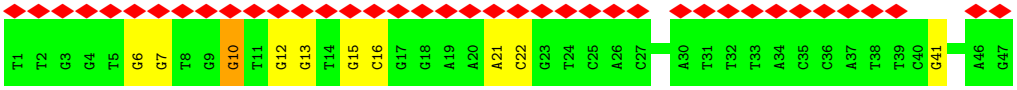
• Molecule 8: DNA (48-MER)

Chain 1H:



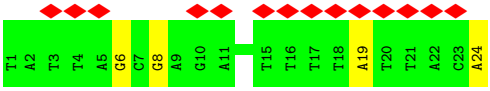
• Molecule 9: DNA (47-MER)

Chain 1I:



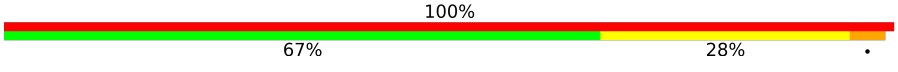
• Molecule 10: DNA (5'-D(*TP*AP*TP*TP*AP*GP*CP*GP*AP*GP*AP*TP*GP*GP*TP*TP*TP*TP*AP*TP*TP*AP*CP*A)-3')

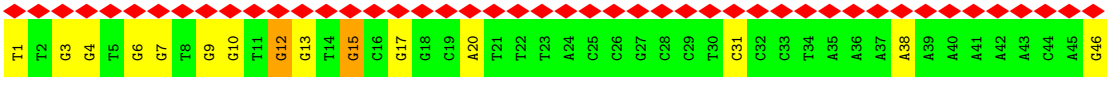
Chain 1J:



• Molecule 11: DNA (46-MER)

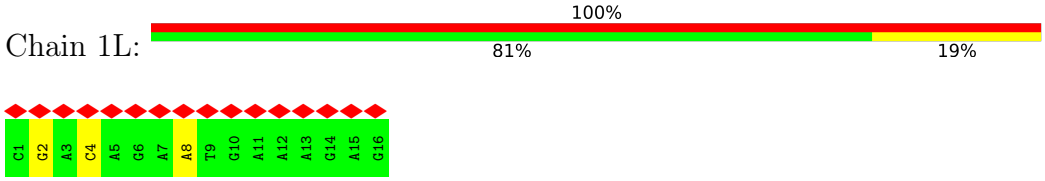
Chain 1K:





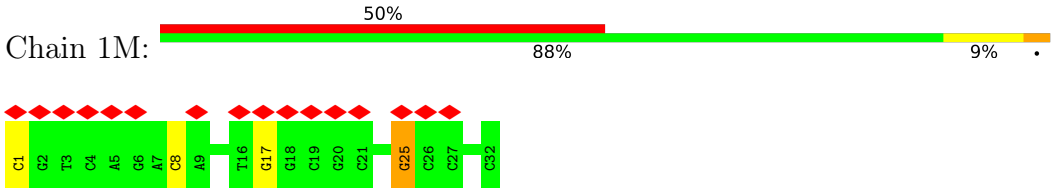
• Molecule 12: DNA (5'-D(*CP*GP*AP*CP*AP*GP*AP*AP*TP*GP*AP*AP*AP*GP*AP*G)-3')

Chain 1L:



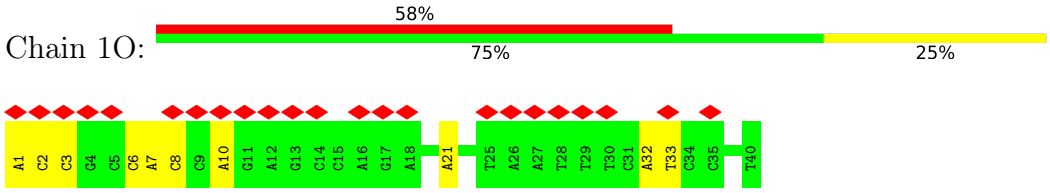
• Molecule 13: DNA (32-MER)

Chain 1M:



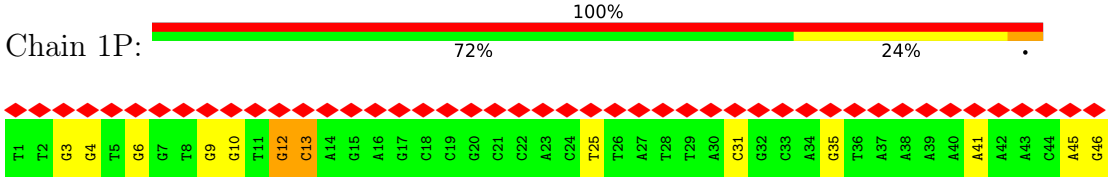
• Molecule 14: DNA (40-MER)

Chain 1O:



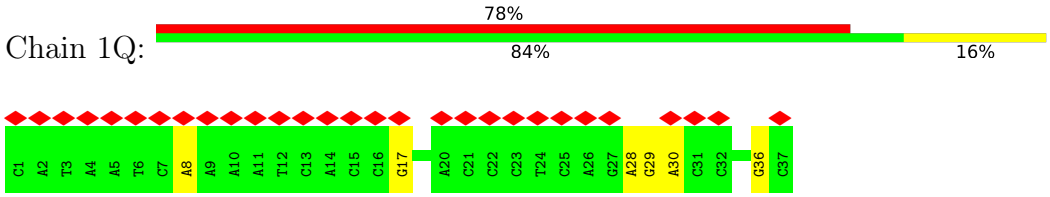
• Molecule 15: DNA (46-MER)

Chain 1P:



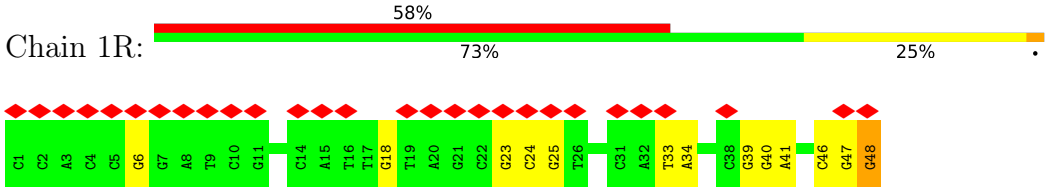
• Molecule 16: DNA (37-MER)

Chain 1Q:



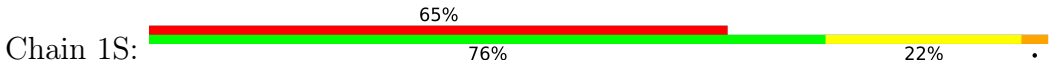
• Molecule 17: DNA (48-MER)

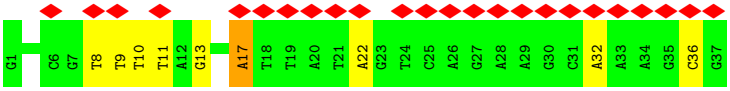
Chain 1R:



• Molecule 18: DNA (37-MER)

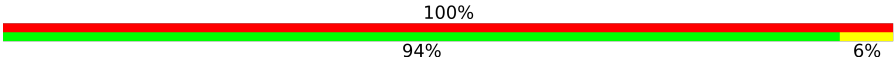
Chain 1S:

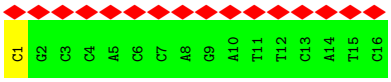




• Molecule 19: DNA (5'-D(*CP*GP*CP*CP*AP*CP*CP*AP*GP*AP*TP*TP*CP*AP*TP*C)-3')

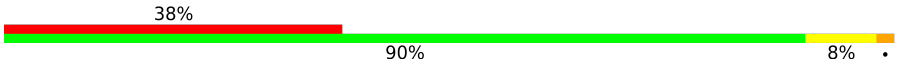
Chain 1T:

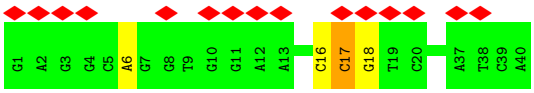




• Molecule 20: DNA (40-MER)

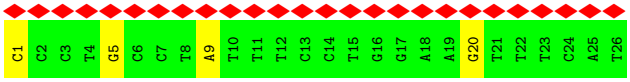
Chain 1U:





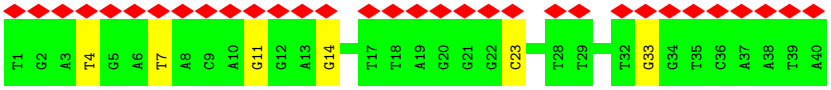
• Molecule 21: DNA (26-MER)

Chain 1V:



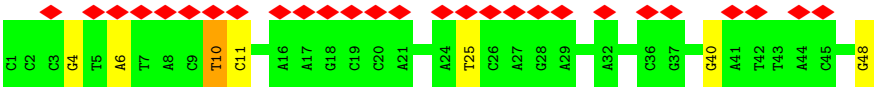
• Molecule 22: DNA (40-MER)

Chain 1W:



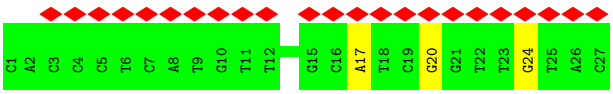
• Molecule 23: DNA (48-MER)

Chain 1X:



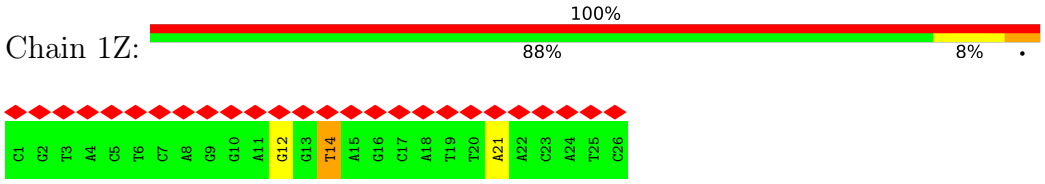
• Molecule 24: DNA (27-MER)

Chain 1Y:



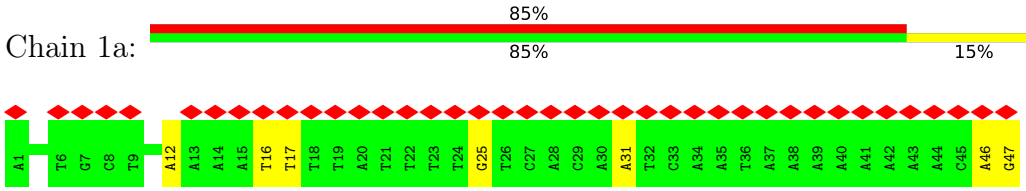
• Molecule 25: DNA (26-MER)

Chain 1Z:



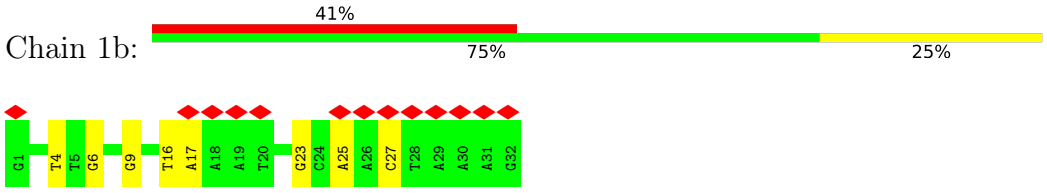
• Molecule 26: DNA (47-MER)

Chain 1a:



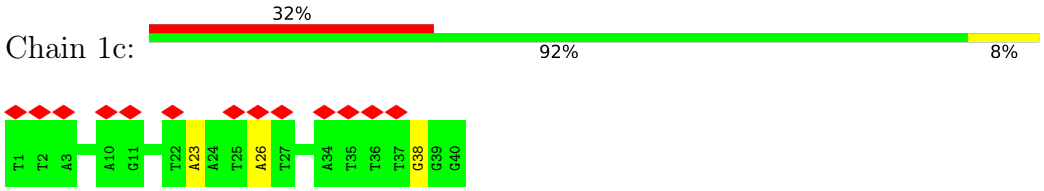
• Molecule 27: DNA (32-MER)

Chain 1b:



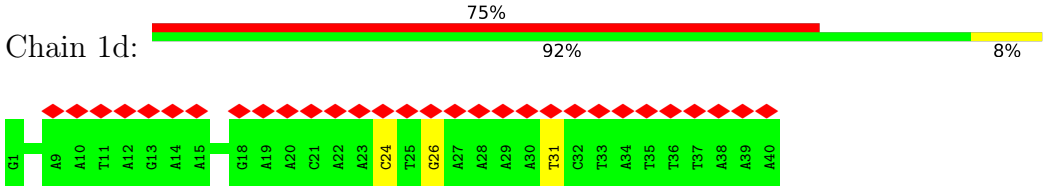
• Molecule 28: DNA (40-MER)

Chain 1c:



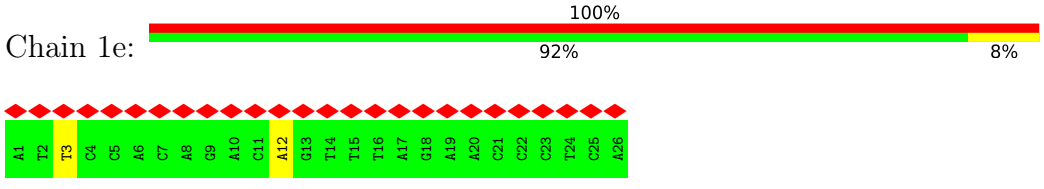
• Molecule 29: DNA (40-MER)

Chain 1d:



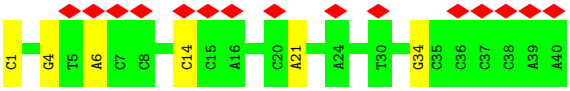
• Molecule 30: DNA (26-MER)

Chain 1e:



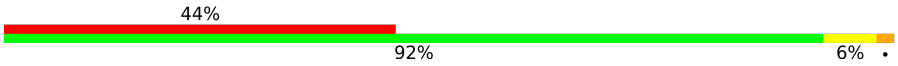
• Molecule 31: DNA (40-MER)

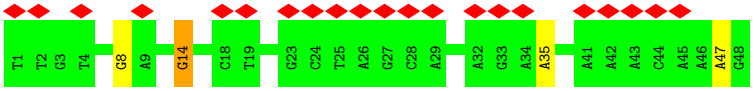
Chain 1f:



• Molecule 32: DNA (48-MER)

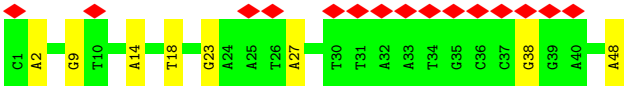
Chain 1g:





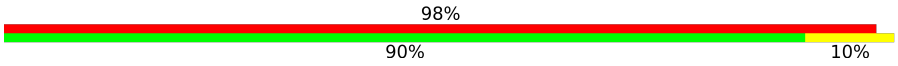
• Molecule 33: DNA (48-MER)

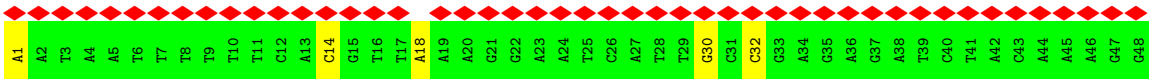
Chain 1h:



• Molecule 34: DNA (48-MER)

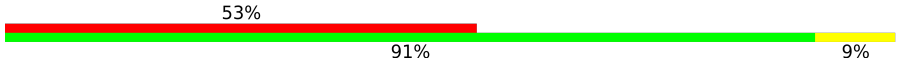
Chain 1i:

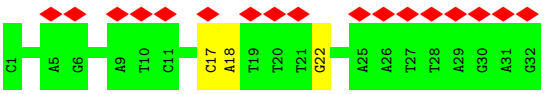




• Molecule 35: DNA (32-MER)

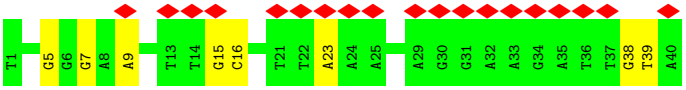
Chain 1j:





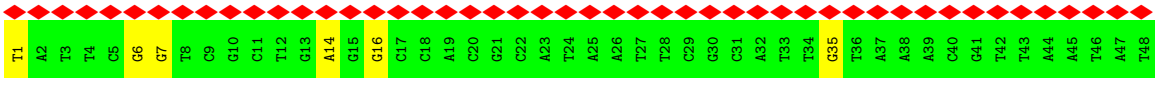
• Molecule 36: DNA (40-MER)

Chain 1k:



• Molecule 37: DNA (48-MER)

Chain 1l:

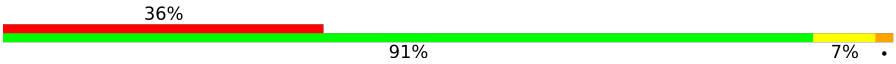


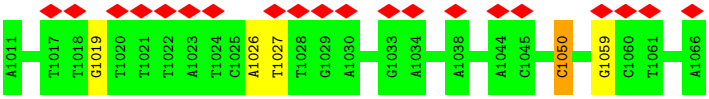
• Molecule 38: DNA (5'-D(P*TP*CP*GP*AP*GP*GP*TP*GP*AP*TP*TP*CP*GP*CP*GP*T)-3')

Chain 1m:

• Molecule 39: DNA (56-MER)

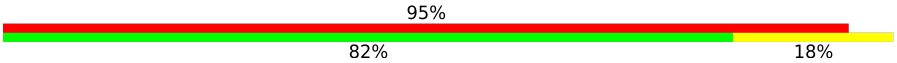
Chain 1n:

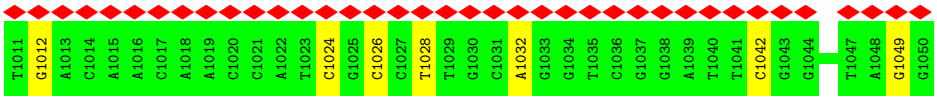




• Molecule 40: DNA (40-MER)

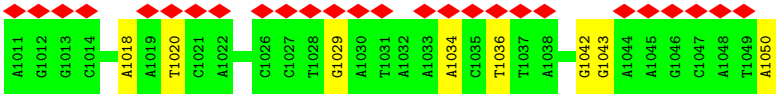
Chain 1o:





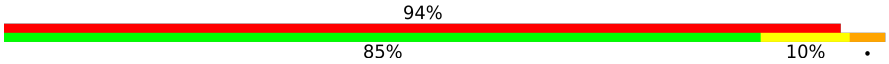
• Molecule 41: DNA (40-MER)

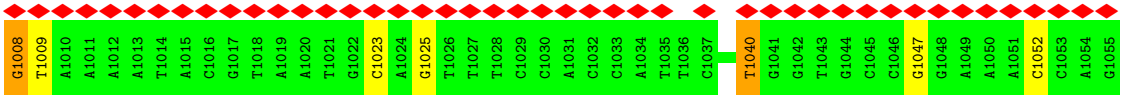
Chain 1p:



• Molecule 42: DNA (48-MER)

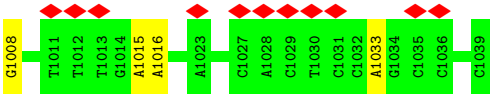
Chain 1q:





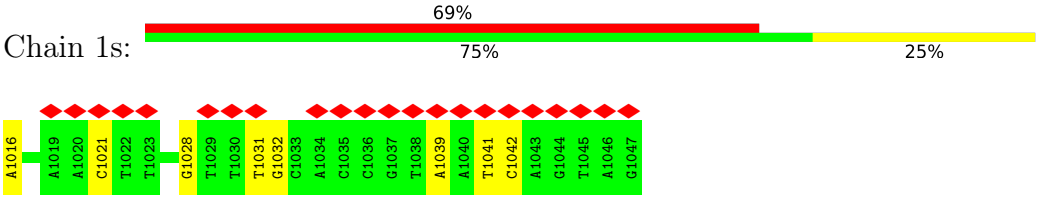
• Molecule 43: DNA (32-MER)

Chain 1r:



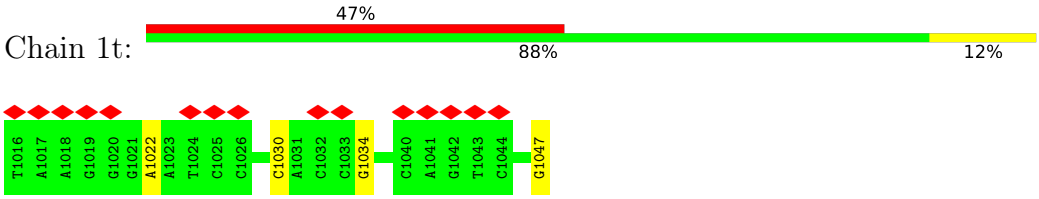
• Molecule 44: DNA (32-MER)

Chain 1s:



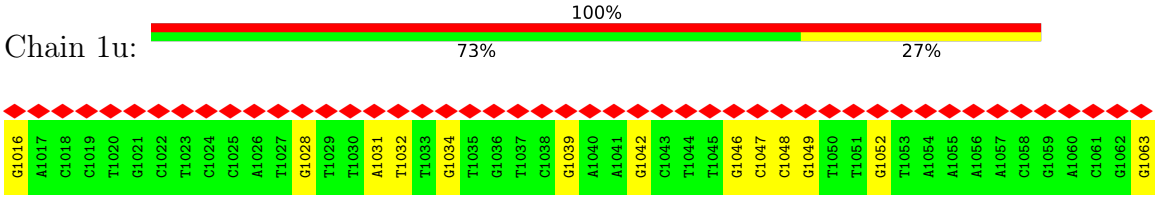
• Molecule 45: DNA (32-MER)

Chain 1t:



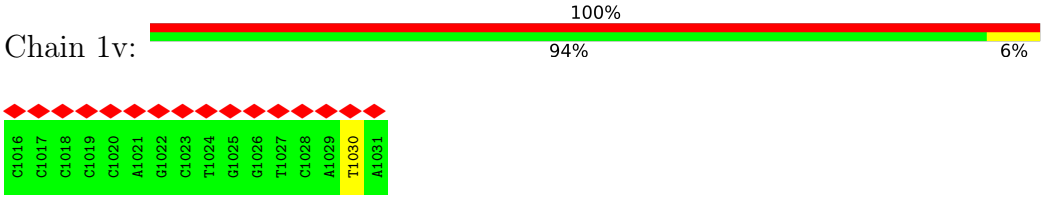
• Molecule 46: DNA (48-MER)

Chain 1u:



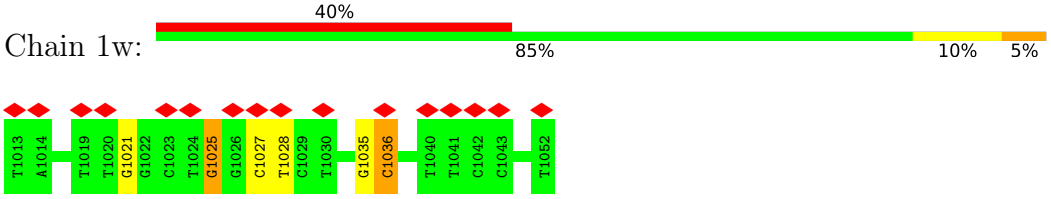
• Molecule 47: DNA (5'-D(P*CP*CP*CP*CP*CP*AP*GP*CP*TP*GP*GP*TP*CP*AP*TP*A)-3')

Chain 1v:



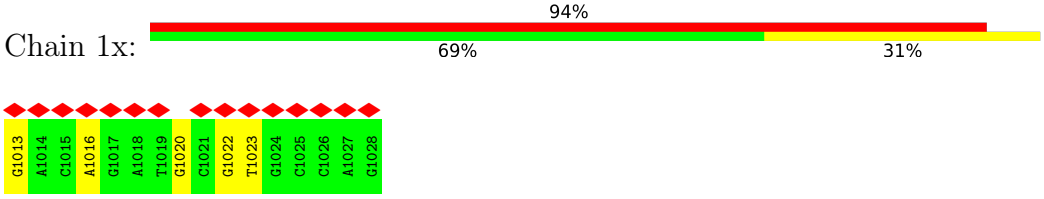
• Molecule 48: DNA (40-MER)

Chain 1w:



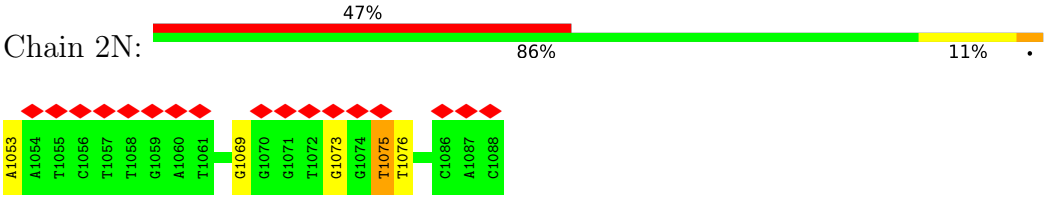
• Molecule 49: DNA (5'-D(P*GP*AP*CP*AP*GP*AP*TP*GP*CP*GP*TP*GP*CP*CP*AP*G)-3')

Chain 1x:



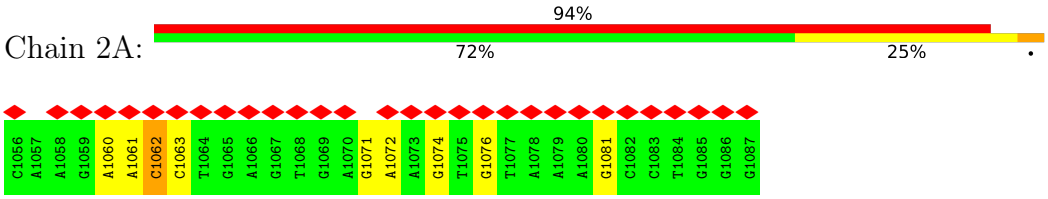
• Molecule 50: DNA (48-MER)

Chain 2N:



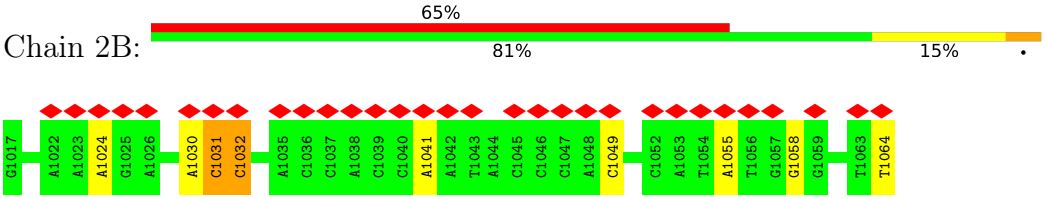
• Molecule 51: DNA (40-MER)

Chain 2A:



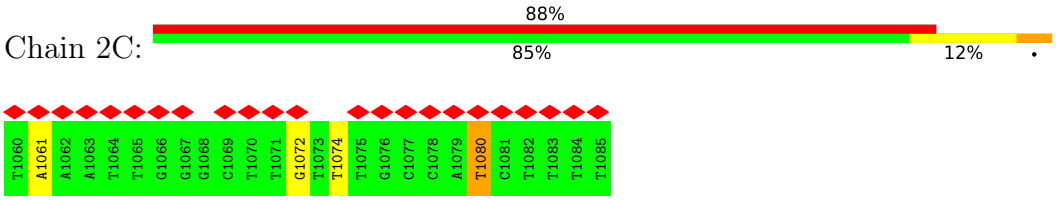
• Molecule 52: DNA (48-MER)

Chain 2B:



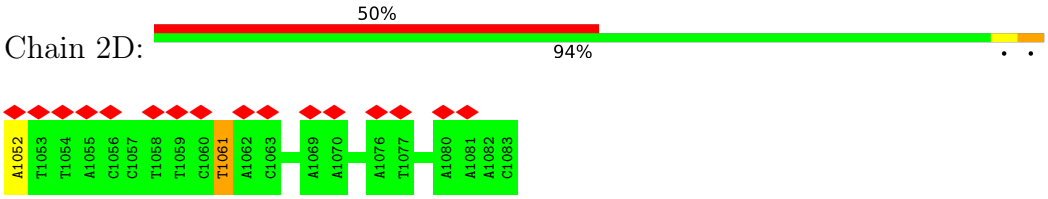
• Molecule 53: DNA (40-MER)

Chain 2C:



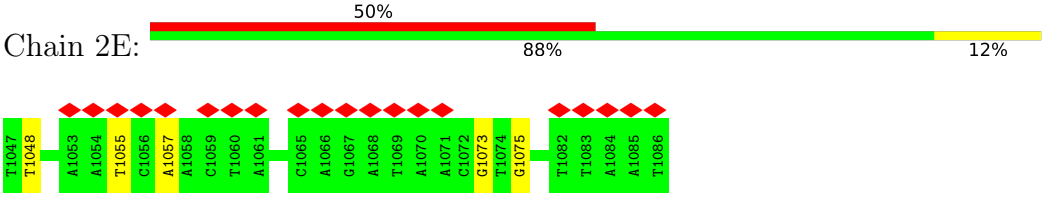
• Molecule 54: DNA (29-MER)

Chain 2D:



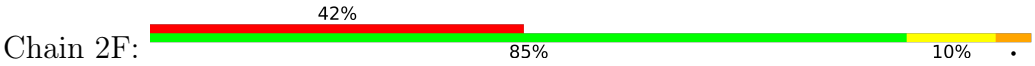
• Molecule 55: DNA (5'-D(P*CP*AP*TP*AP*AP*CP*GP*CP*AP*TP*AP*AP*AP*AP*CP*GP*AP*GP*GP*AP*GP*GP*TP*T)-3')

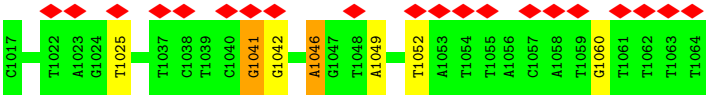
Chain 2E:



• Molecule 56: DNA (32-MER)

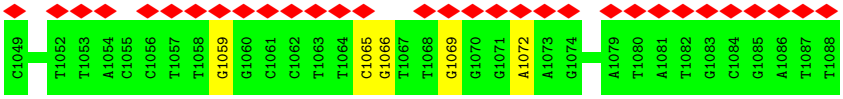
Chain 2F:





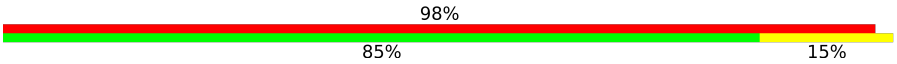
• Molecule 57: DNA (26-MER)

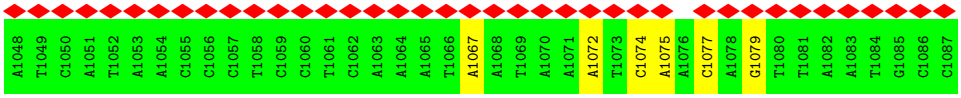
Chain 2G:



• Molecule 58: DNA (40-MER)

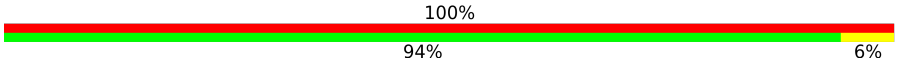
Chain 2H:

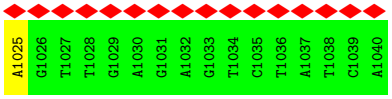




• Molecule 59: DNA (40-MER)

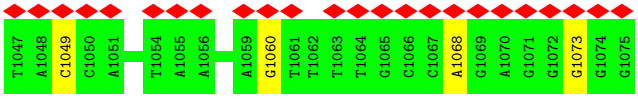
Chain 2I:





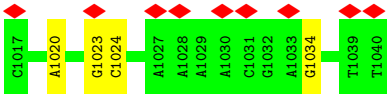
• Molecule 60: DNA (58-MER)

Chain 2J:



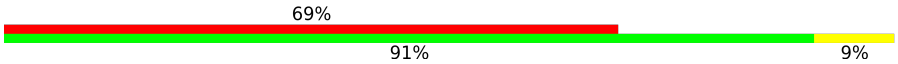
• Molecule 61: DNA (52-MER)

Chain 2K:



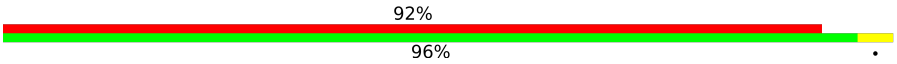
• Molecule 62: DNA (40-MER)

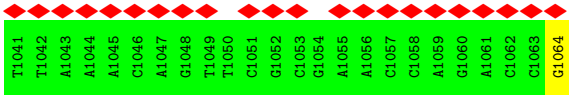
Chain 2L:



• Molecule 63: DNA (48-MER)

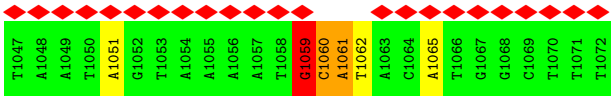
Chain 2M:





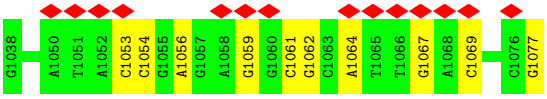
• Molecule 64: DNA (48-MER)

Chain 2O:



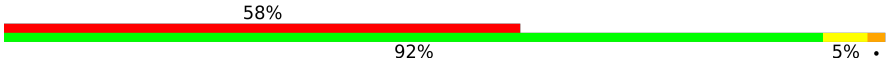
• Molecule 65: DNA (32-MER)

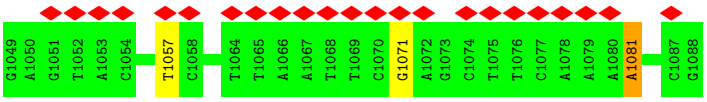
Chain 2P:



• Molecule 66: DNA (58-MER)

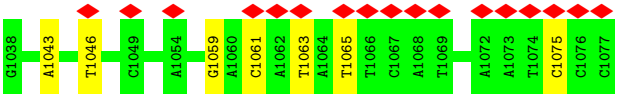
Chain 2Q:





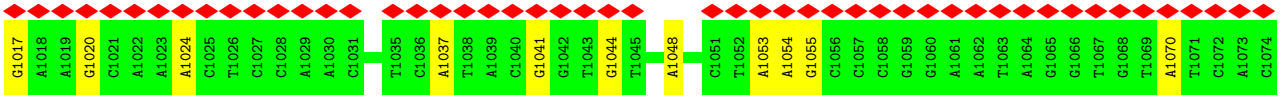
• Molecule 67: DNA (56-MER)

Chain 2R:



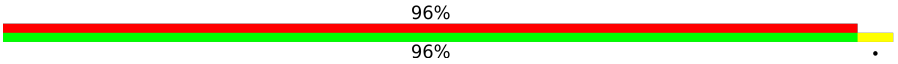
• Molecule 68: DNA (52-MER)

Chain 2S:



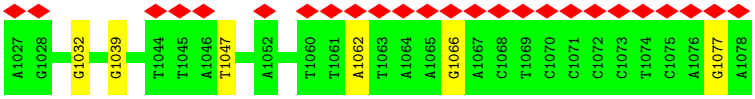
• Molecule 69: DNA (37-MER)

Chain 2T:



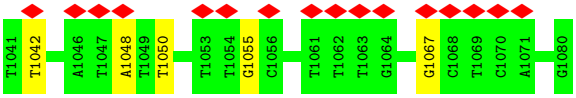
• Molecule 70: DNA (48-MER)

Chain 2U:



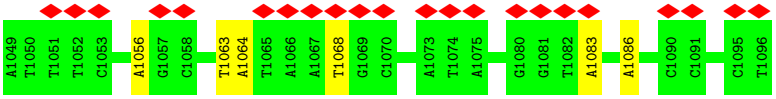
• Molecule 71: DNA (48-MER)

Chain 2V:



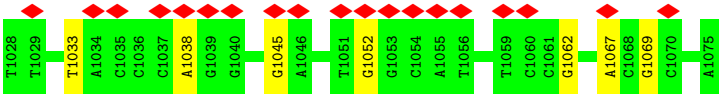
• Molecule 72: DNA (32-MER)

Chain 2W:



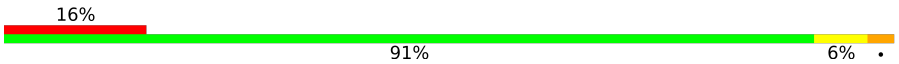
• Molecule 73: DNA (32-MER)

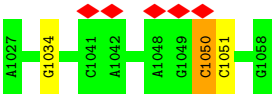
Chain 2X:



• Molecule 74: DNA (48-MER)

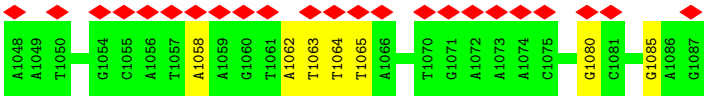
Chain 2Y:





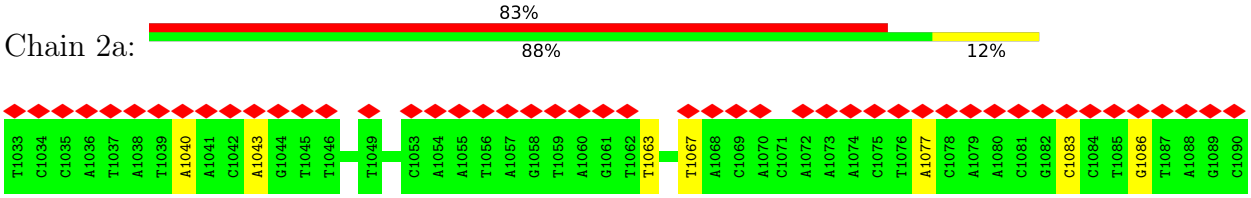
• Molecule 75: DNA (48-MER)

Chain 2Z:



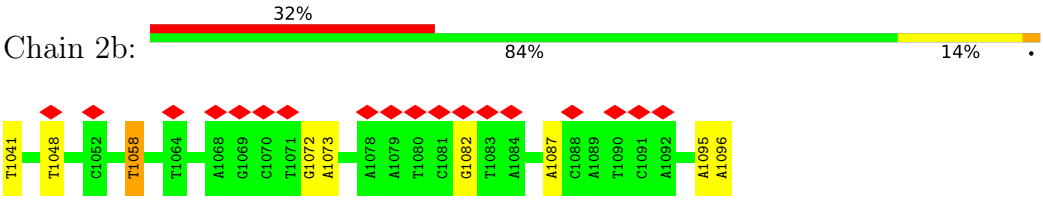
• Molecule 76: DNA (5'-D(P*TP*TP*TP*GP*TP*TP*AP*AP*AP*AP*CP*CP*GP*AP*TP*A)-3')

Chain 2a:



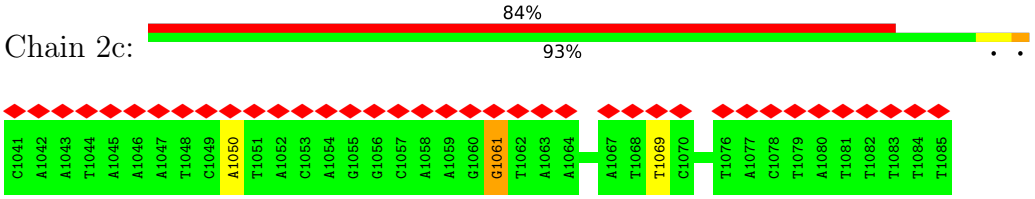
• Molecule 77: DNA (32-MER)

Chain 2b:



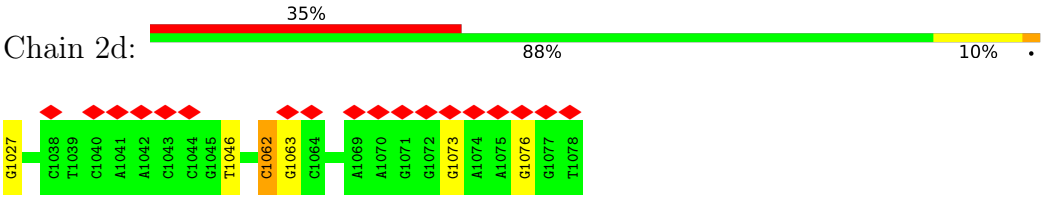
• Molecule 78: DNA (32-MER)

Chain 2c:



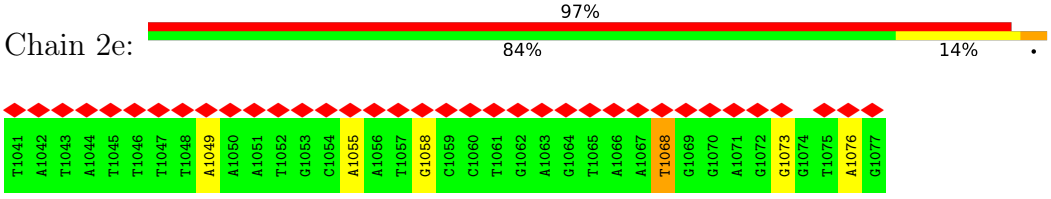
• Molecule 79: DNA (40-MER)

Chain 2d:



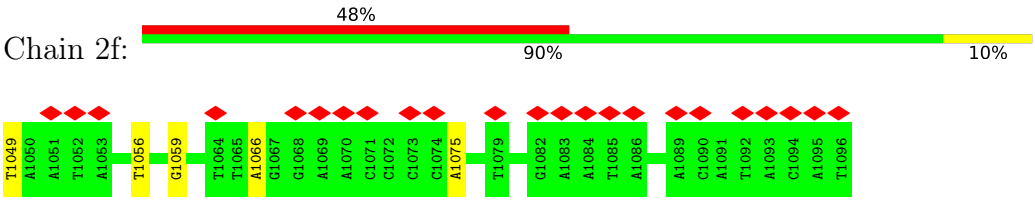
• Molecule 80: DNA (5'-D(P*CP*TP*GP*GP*CP*CP*TP*TP*CP*CP*TP*GP*TP*AP*GP*CP*CP*AP*AP*AP*AP*AP*TP*A)-3')

Chain 2e:



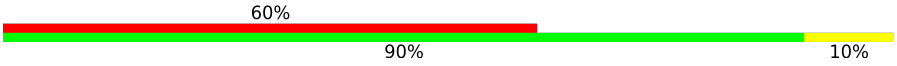
• Molecule 81: DNA (32-MER)

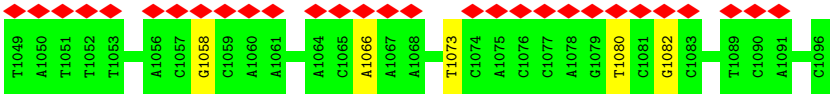
Chain 2f:



• Molecule 82: DNA (40-MER)

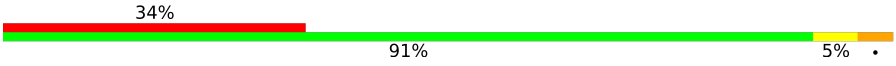
Chain 2g:

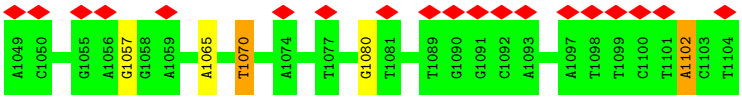




• Molecule 83: DNA (32-MER)

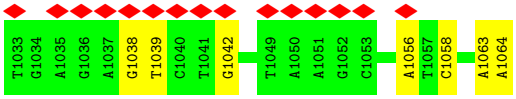
Chain 2h:





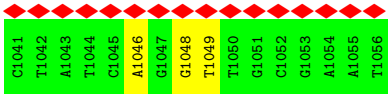
• Molecule 84: DNA (32-MER)

Chain 2i:



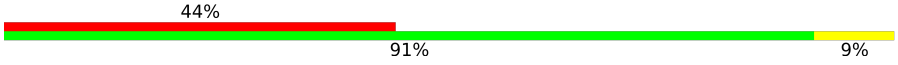
• Molecule 85: DNA (47-MER)

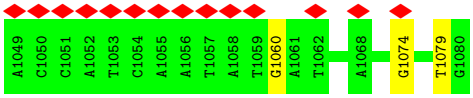
Chain 2j:



• Molecule 86: DNA (5'-D(P*CP*CP*AP*GP*TP*GP*CP*CP*AP*AP*AP*TP*CP*CP*GP*C)-3')

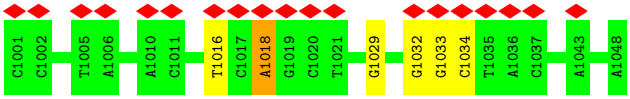
Chain 2k:





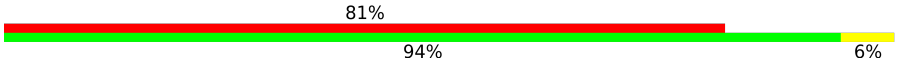
• Molecule 87: DNA (40-MER)

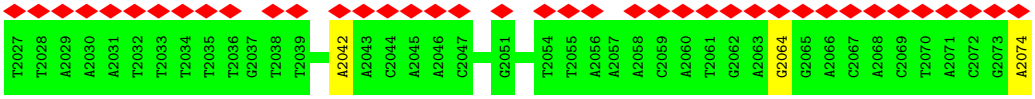
Chain 2l:



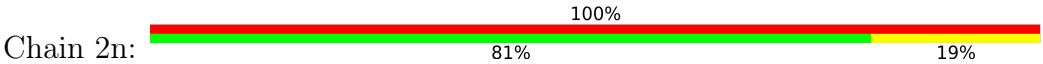
• Molecule 88: DNA (48-MER)

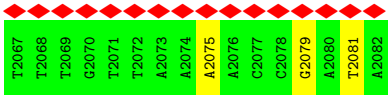
Chain 2m:



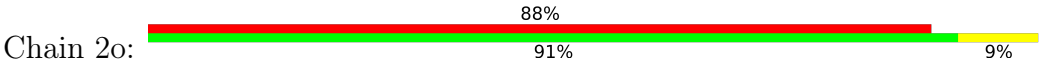


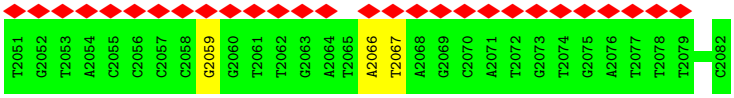
• Molecule 89: DNA (48-MER)



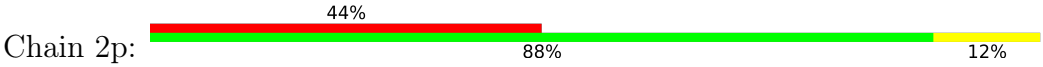


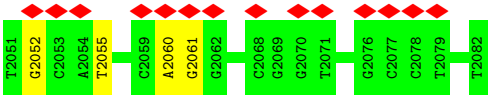
• Molecule 90: DNA (48-MER)



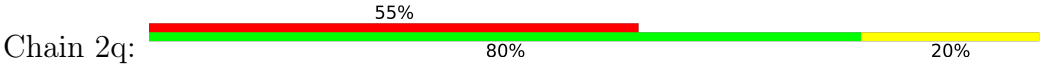


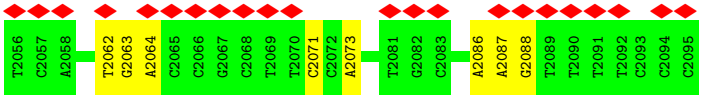
• Molecule 91: DNA (56-MER)



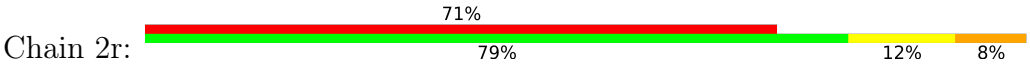


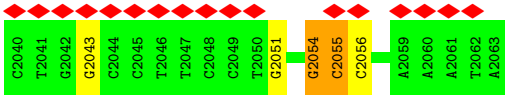
• Molecule 92: DNA (56-MER)



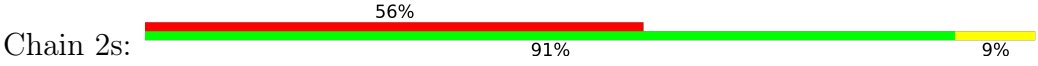


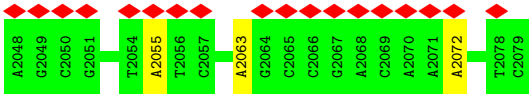
• Molecule 93: DNA (32-MER)





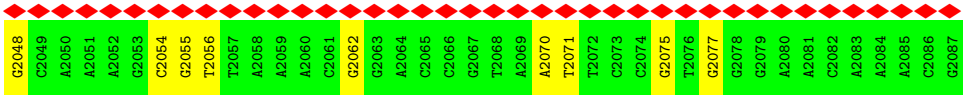
• Molecule 94: DNA (48-MER)





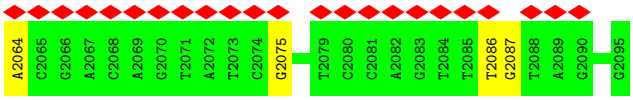
• Molecule 95: DNA (37-MER)

Chain 2t:



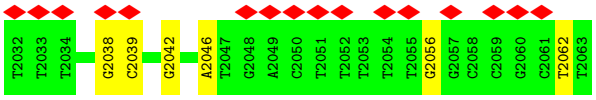
• Molecule 96: DNA (55-MER)

Chain 2u:



• Molecule 97: DNA (48-MER)

Chain 2v:



• Molecule 98: DNA (38-MER)

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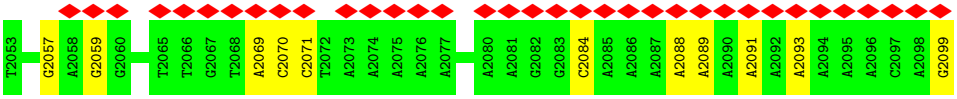
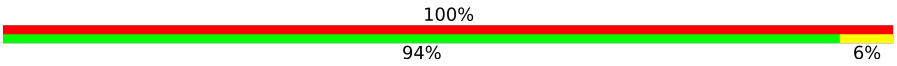
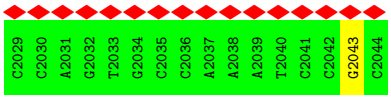


• Molecule 99: DNA (32-MER)

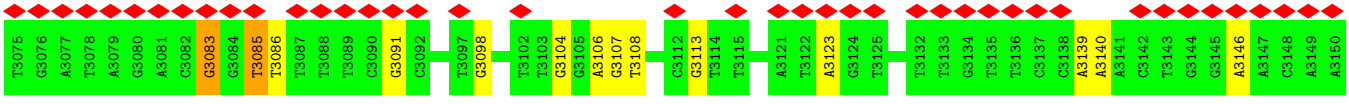
Chain 2x:

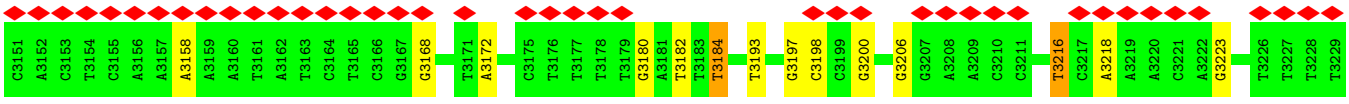


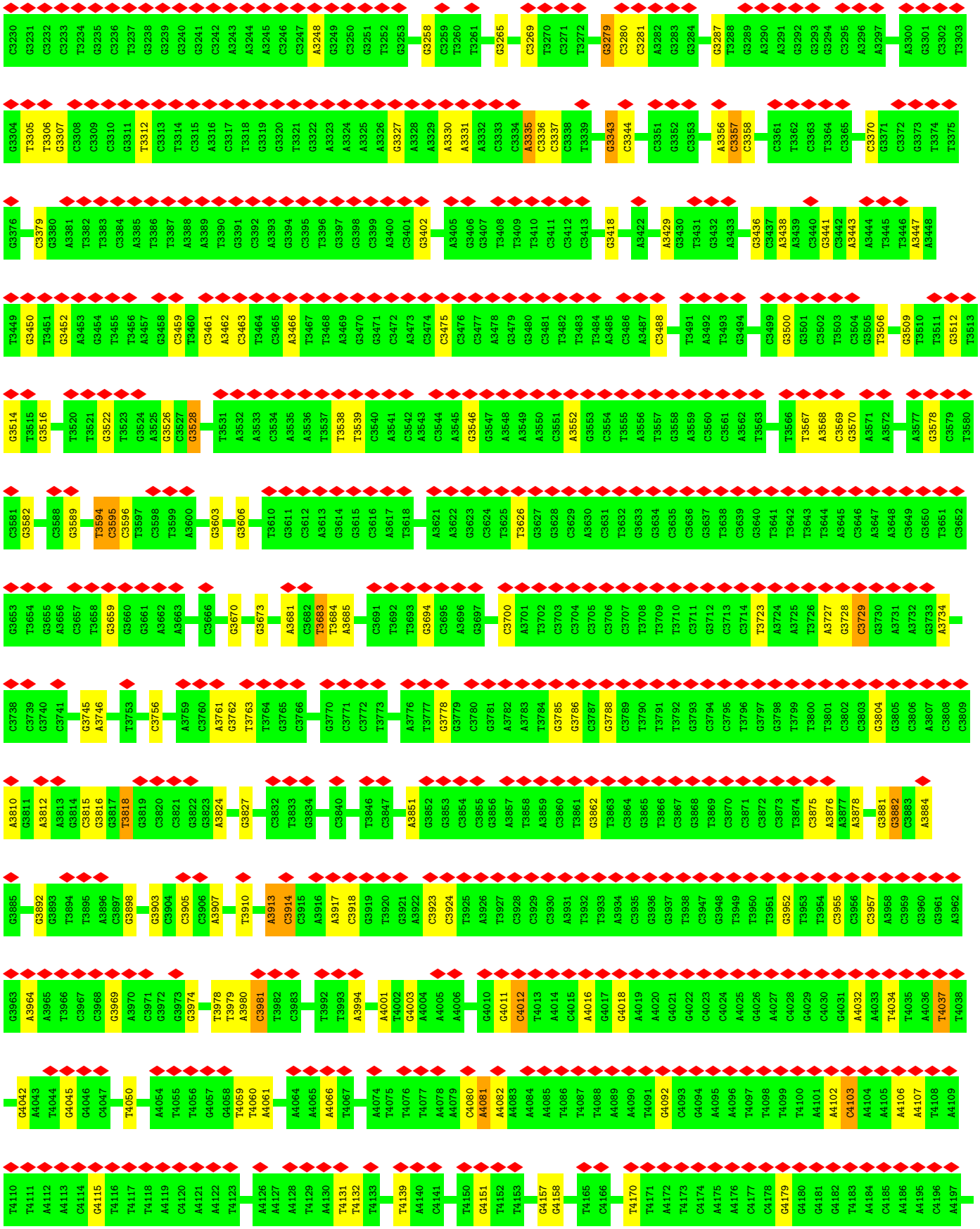


• Molecule 100: DNA (4346-MER)

Chain 3N:



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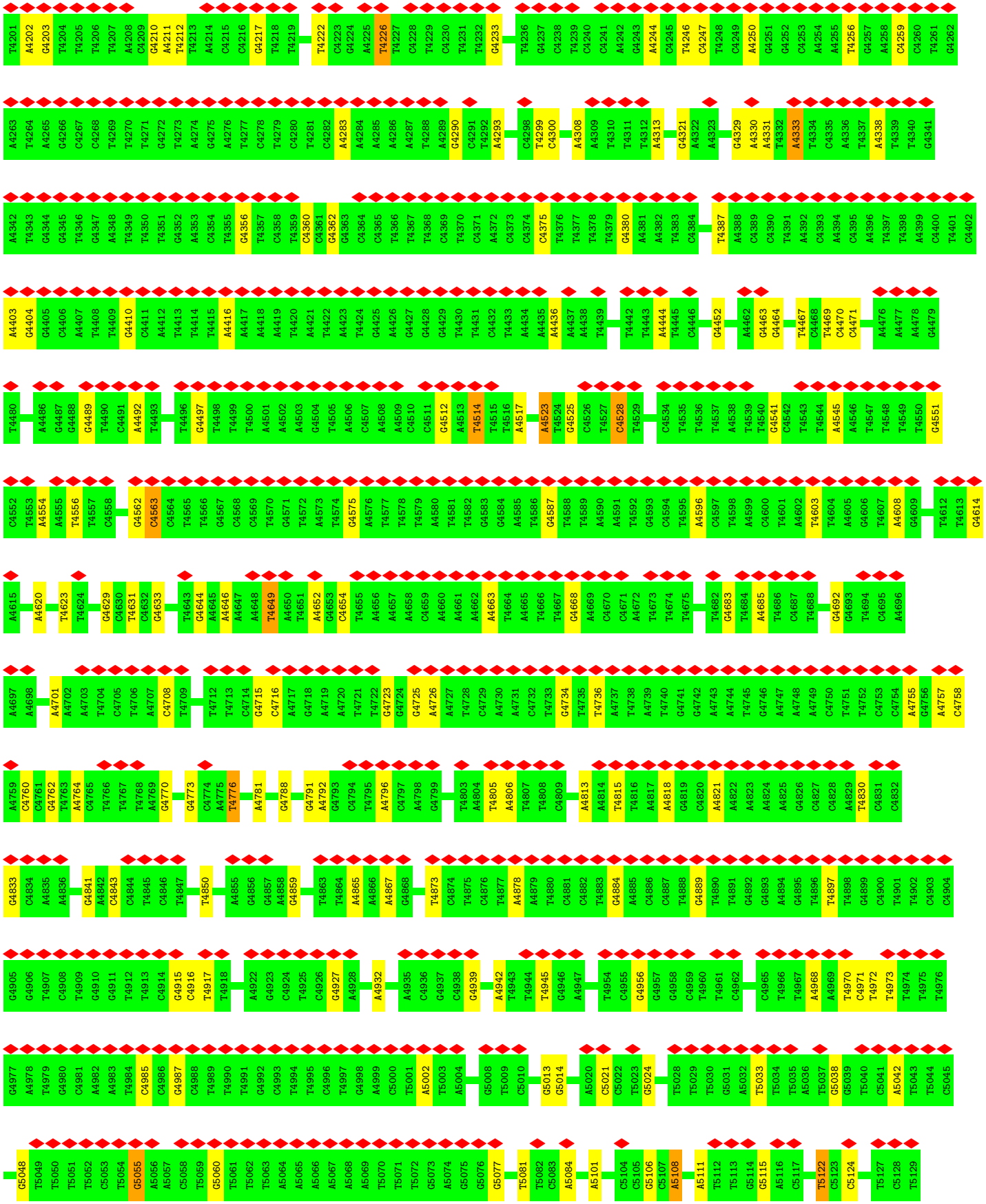
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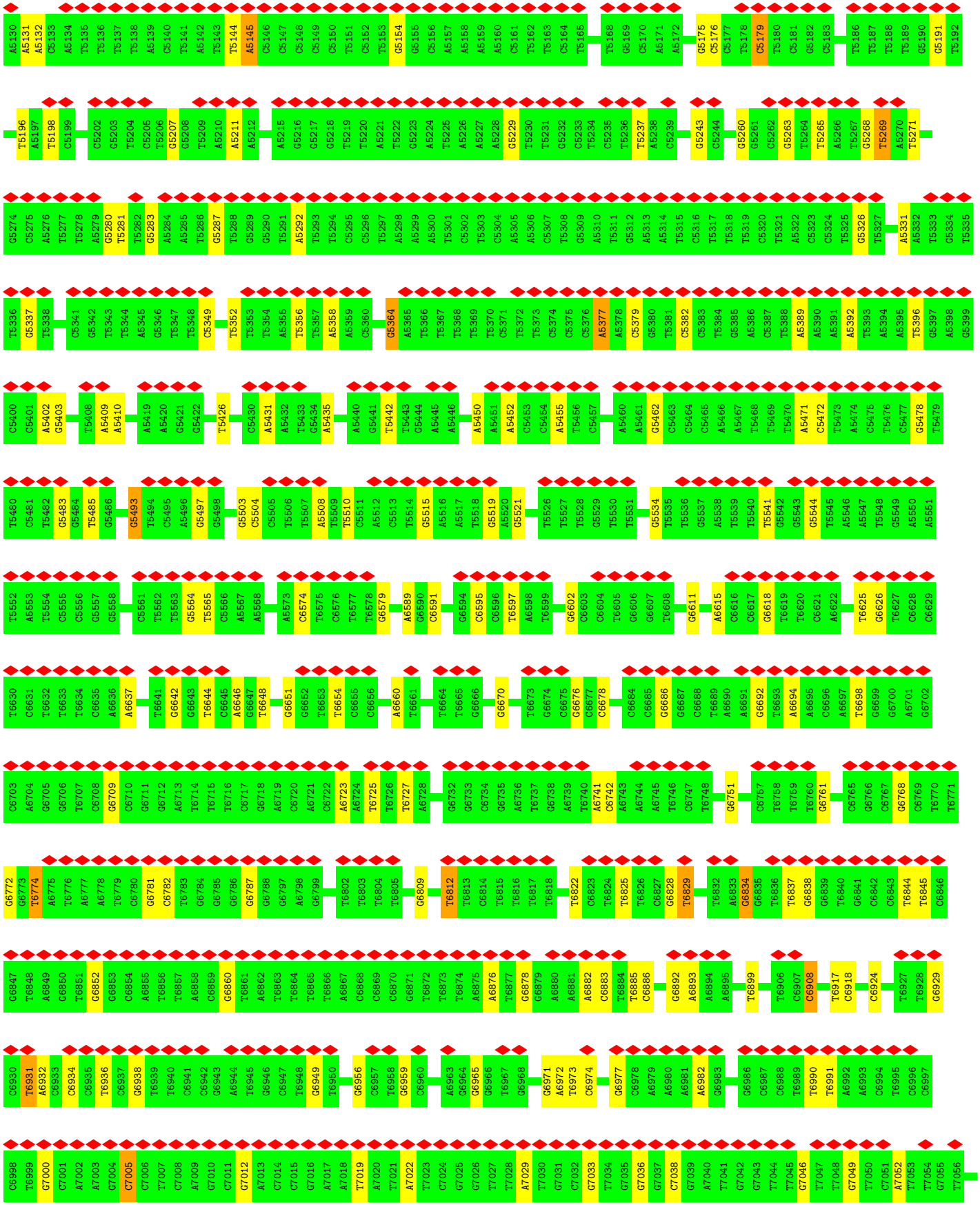
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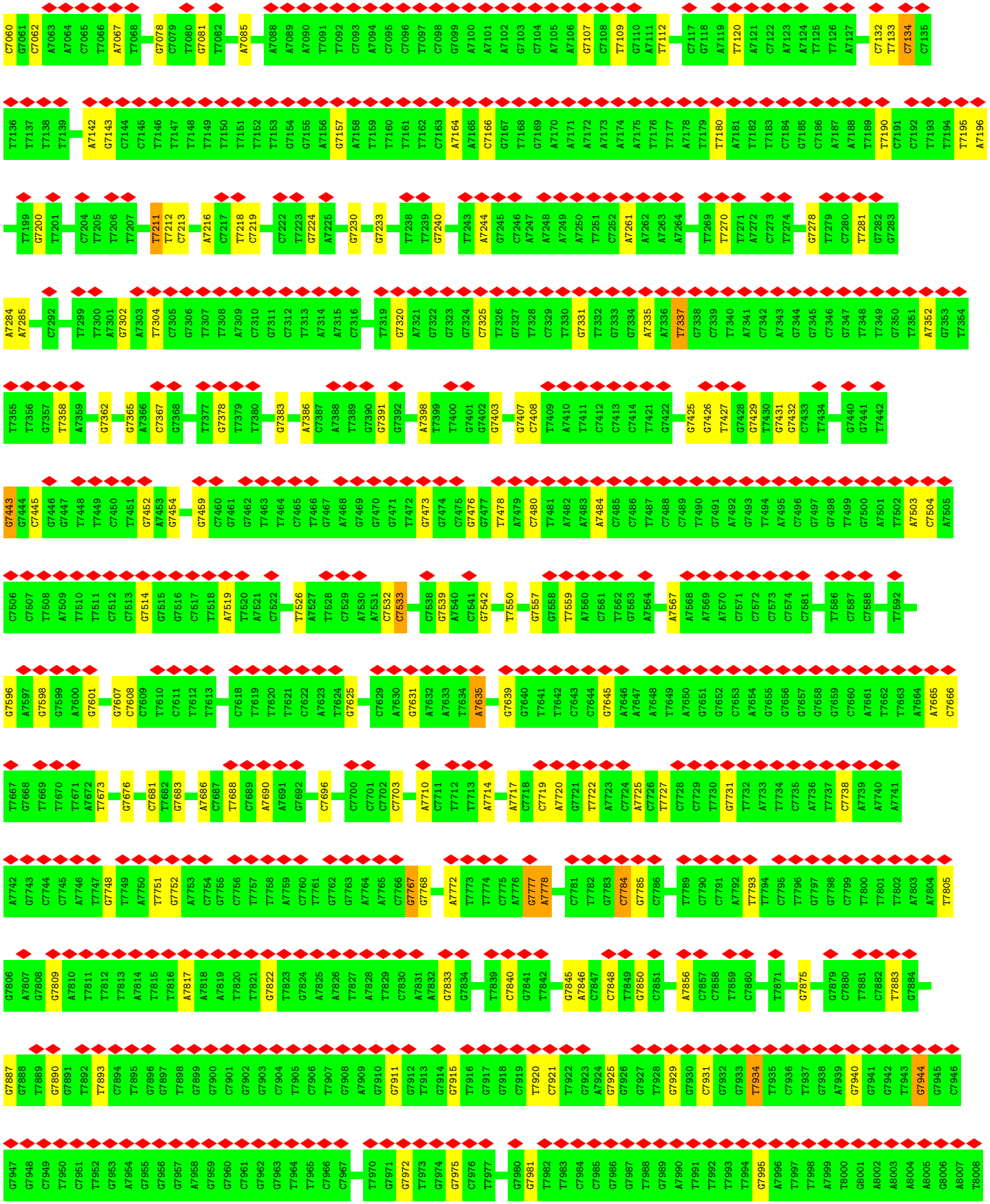
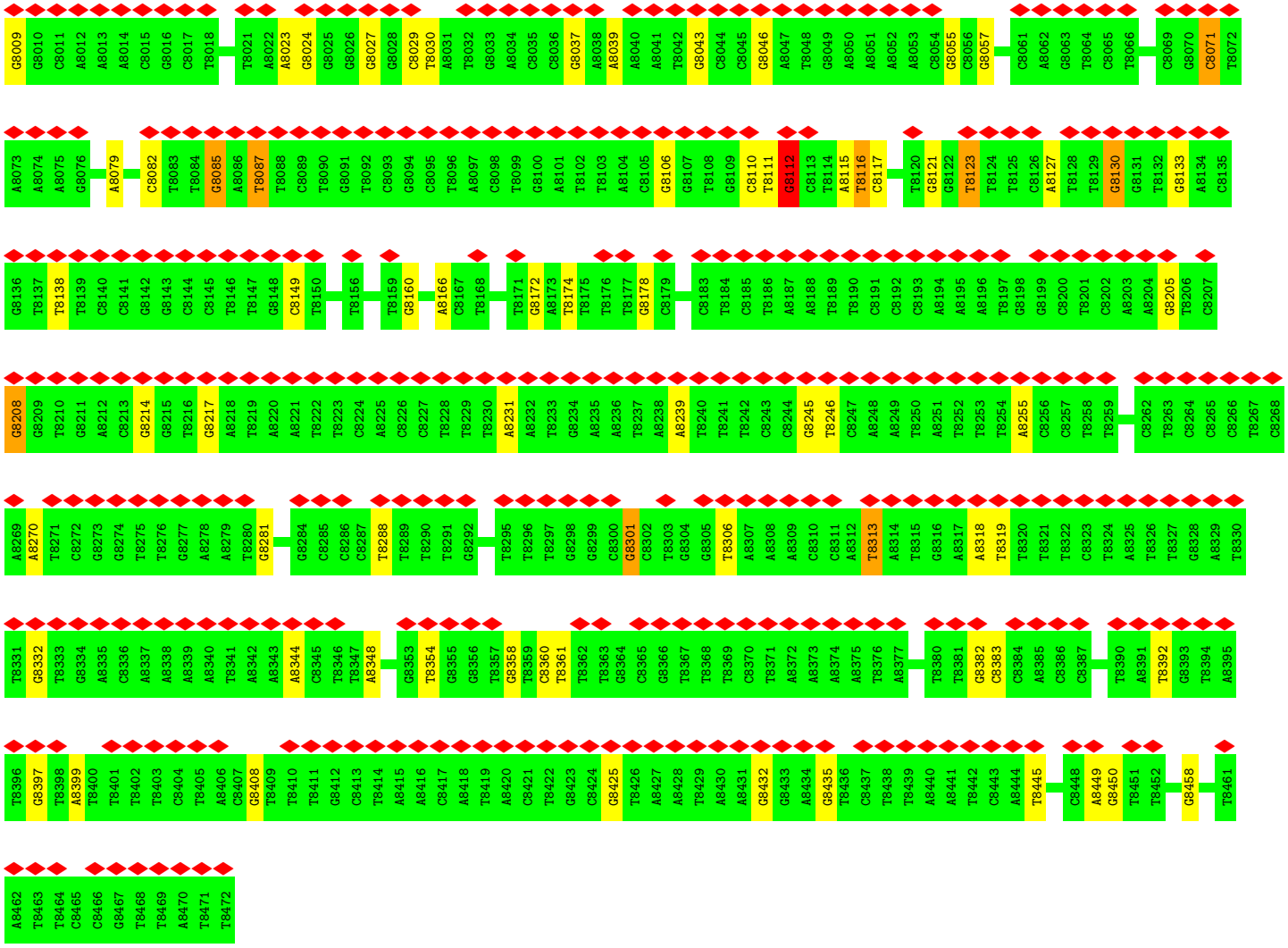
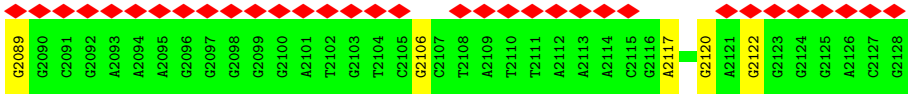




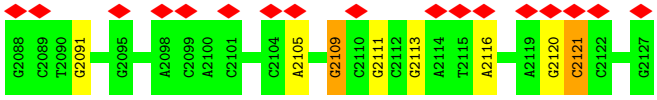
• Molecule 101: DNA (40-MER)

Chain 3A:



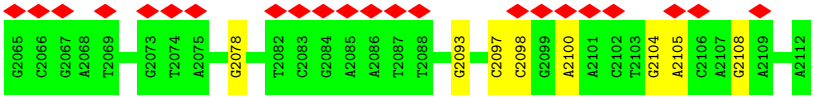
• Molecule 102: DNA (40-MER)

Chain 3B:



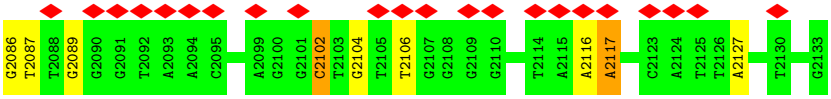
• Molecule 103: DNA (48-MER)

Chain 3C:



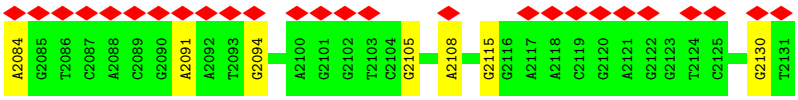
• Molecule 104: DNA (48-MER)

Chain 3D:



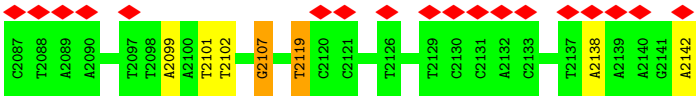
• Molecule 105: DNA (48-MER)

Chain 3E:



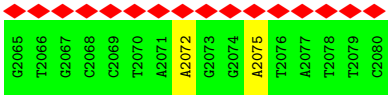
• Molecule 106: DNA (56-MER)

Chain 3F:



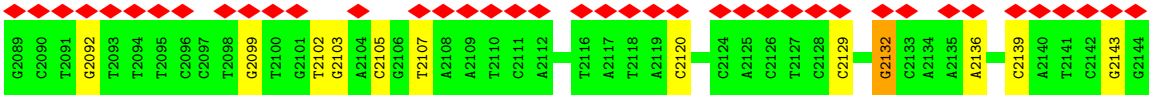
• Molecule 107: DNA (5'-D(*GP*TP*GP*CP*CP*TP*AP*AP*GP*GP*AP*TP*AP*TP*TP*C)-3')

Chain 3G:



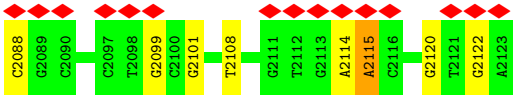
• Molecule 108: DNA (56-MER)

Chain 3H:

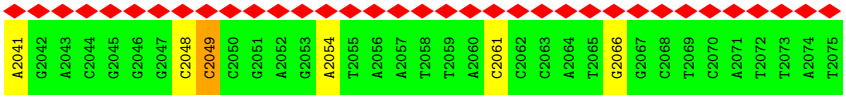


• Molecule 109: DNA (36-MER)

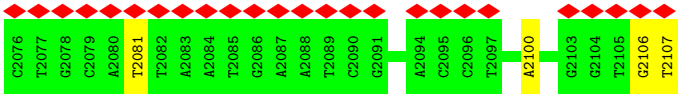
Chain 3I:



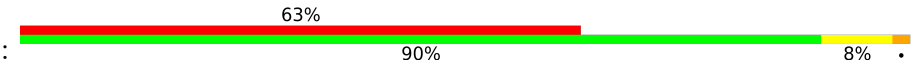
• Molecule 110: DNA (35-MER)

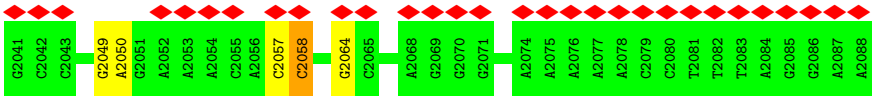


• Molecule 111: DNA (32-MER)

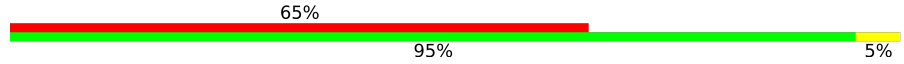


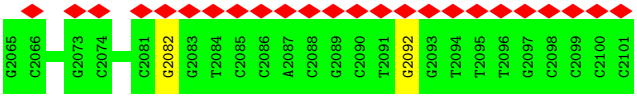
• Molecule 112: DNA (48-MER)



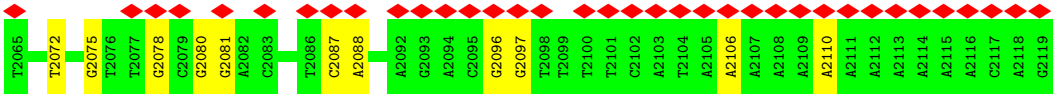


• Molecule 113: DNA (37-MER)

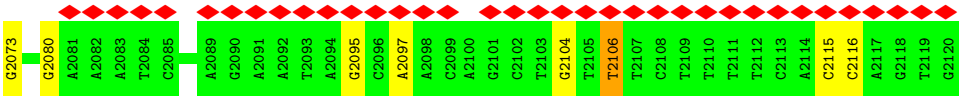




• Molecule 114: DNA (55-MER)

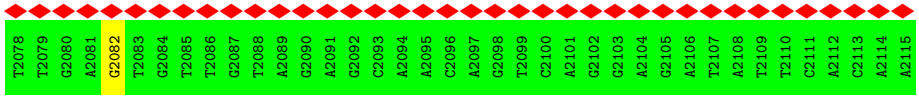


• Molecule 115: DNA (48-MER)



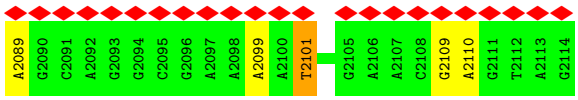
• Molecule 116: DNA (38-MER)

Chain 3P:



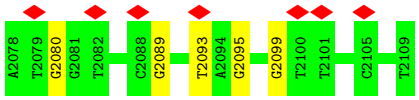
• Molecule 117: DNA (26-MER)

Chain 3Q:



• Molecule 118: DNA (32-MER)

Chain 3R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	108931	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	23500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.005	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	456.0, 456.0, 456.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.76, 0.76, 0.76	Depositor

5 Model quality

5.1 Standard geometry

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	1A	1.12	0/1220	1.18	9/1885 (0.5%)
2	1B	1.16	0/1279	1.27	12/1975 (0.6%)
3	1C	1.13	0/368	1.28	5/566 (0.9%)
4	1D	1.12	0/1372	1.16	9/2119 (0.4%)
5	1E	1.12	0/1185	1.14	5/1828 (0.3%)
6	1F	1.15	0/1069	1.43	15/1650 (0.9%)
7	1G	1.10	0/358	1.30	4/550 (0.7%)
8	1H	1.11	0/1087	1.29	10/1671 (0.6%)
9	1I	1.19	0/1091	1.27	6/1685 (0.4%)
10	1J	1.10	0/551	1.13	3/850 (0.4%)
11	1K	1.18	0/1061	1.39	12/1637 (0.7%)
12	1L	1.11	0/377	1.18	2/581 (0.3%)
13	1M	1.15	0/722	1.31	7/1110 (0.6%)
14	1O	1.13	0/907	1.20	3/1394 (0.2%)
15	1P	1.15	0/1066	1.36	13/1645 (0.8%)
16	1Q	1.09	0/846	1.23	5/1301 (0.4%)
17	1R	1.17	0/1094	1.35	13/1685 (0.8%)
18	1S	1.16	0/858	1.27	9/1324 (0.7%)
19	1T	1.08	0/355	1.28	2/544 (0.4%)
20	1U	1.14	1/932 (0.1%)	1.73	9/1437 (0.6%)
21	1V	1.11	0/580	1.19	6/892 (0.7%)
22	1W	1.12	0/934	1.18	7/1443 (0.5%)
23	1X	1.13	0/1106	1.18	2/1704 (0.1%)
24	1Y	1.11	0/607	1.15	3/934 (0.3%)
25	1Z	1.10	0/596	1.23	5/918 (0.5%)
26	1a	1.08	0/1086	1.19	4/1674 (0.2%)
27	1b	1.12	0/750	1.27	9/1158 (0.8%)
28	1c	1.10	0/921	1.14	5/1420 (0.4%)
29	1d	1.10	0/931	1.15	2/1436 (0.1%)
30	1e	1.09	0/587	1.13	2/902 (0.2%)
31	1f	1.14	0/899	1.27	9/1382 (0.7%)
32	1g	1.11	0/1105	1.19	6/1702 (0.4%)
33	1h	1.11	0/1118	1.16	6/1726 (0.3%)
34	1i	1.10	0/1108	1.18	6/1709 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	1j	1.13	0/742	1.15	4/1144 (0.3%)
36	1k	1.10	0/929	1.15	7/1435 (0.5%)
37	1l	1.12	0/1098	1.16	7/1693 (0.4%)
38	1m	1.15	0/367	1.35	4/566 (0.7%)
39	1n	1.12	0/1290	1.23	6/1989 (0.3%)
40	1o	1.16	0/922	1.25	5/1422 (0.4%)
41	1p	1.14	0/917	1.34	10/1412 (0.7%)
42	1q	1.12	0/1101	1.18	10/1697 (0.6%)
43	1r	1.12	0/734	1.26	5/1131 (0.4%)
44	1s	1.11	0/727	1.34	8/1119 (0.7%)
45	1t	1.15	0/729	1.28	7/1123 (0.6%)
46	1u	1.15	0/1100	1.35	17/1697 (1.0%)
47	1v	1.12	0/356	1.10	0/546
48	1w	1.12	0/904	1.32	7/1391 (0.5%)
49	1x	1.17	0/370	1.29	5/570 (0.9%)
50	2N	1.11	0/825	1.20	7/1272 (0.6%)
51	2A	1.16	0/750	1.32	10/1158 (0.9%)
52	2B	1.14	0/1095	1.28	5/1685 (0.3%)
53	2C	1.11	0/587	1.20	5/905 (0.6%)
54	2D	1.09	0/733	1.19	5/1128 (0.4%)
55	2E	1.10	0/915	1.22	9/1410 (0.6%)
56	2F	1.12	0/1109	1.11	4/1712 (0.2%)
57	2G	1.10	0/919	1.16	5/1418 (0.4%)
58	2H	1.09	0/905	1.27	8/1391 (0.6%)
59	2I	1.07	0/368	1.16	3/567 (0.5%)
60	2J	1.13	0/674	1.22	5/1040 (0.5%)
61	2K	1.12	0/558	1.15	3/860 (0.3%)
62	2L	1.10	0/733	1.18	5/1129 (0.4%)
63	2M	1.10	0/548	1.14	1/843 (0.1%)
64	2O	1.18	2/597 (0.3%)	1.48	10/920 (1.1%)
65	2P	1.12	0/925	1.64	12/1426 (0.8%)
66	2Q	1.10	0/918	1.21	5/1415 (0.4%)
67	2R	1.11	0/924	1.23	8/1425 (0.6%)
68	2S	1.12	0/1341	1.51	18/2068 (0.9%)
69	2T	1.10	0/555	1.16	4/856 (0.5%)
70	2U	1.10	1/1187 (0.1%)	1.15	4/1829 (0.2%)
71	2V	1.11	0/912	1.15	5/1406 (0.4%)
72	2W	1.11	0/1109	1.10	4/1711 (0.2%)
73	2X	1.13	0/1091	1.23	6/1680 (0.4%)
74	2Y	1.13	0/737	1.19	4/1136 (0.4%)
75	2Z	1.11	0/917	1.24	7/1414 (0.5%)
76	2a	1.09	0/1322	1.23	11/2036 (0.5%)
77	2b	1.12	0/1290	1.55	15/1990 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
78	2c	1.07	0/1025	1.08	3/1578 (0.2%)
79	2d	1.13	0/1212	1.24	9/1870 (0.5%)
80	2e	1.08	0/861	1.11	6/1330 (0.5%)
81	2f	1.11	0/1096	1.24	7/1687 (0.4%)
82	2g	1.12	0/1091	1.27	7/1678 (0.4%)
83	2h	1.12	0/1301	1.18	6/2008 (0.3%)
84	2i	1.12	0/746	1.21	4/1150 (0.3%)
85	2j	1.14	0/365	1.11	1/562 (0.2%)
86	2k	1.11	0/732	1.15	3/1127 (0.3%)
87	2l	1.11	0/1102	1.18	6/1697 (0.4%)
88	2m	1.10	0/1106	1.10	2/1705 (0.1%)
89	2n	1.11	0/364	1.23	2/560 (0.4%)
90	2o	1.10	0/730	1.10	2/1126 (0.2%)
91	2p	1.13	0/735	1.25	4/1134 (0.4%)
92	2q	1.12	0/898	1.24	8/1382 (0.6%)
93	2r	1.15	0/543	1.48	10/835 (1.2%)
94	2s	1.14	0/737	1.24	3/1135 (0.3%)
95	2t	1.14	0/928	1.44	14/1431 (1.0%)
96	2u	1.13	0/731	1.27	6/1126 (0.5%)
97	2v	1.14	0/726	1.31	5/1120 (0.4%)
98	2w	1.14	0/1101	1.33	14/1698 (0.8%)
99	2x	1.10	0/358	1.17	1/549 (0.2%)
100	3N	1.12	0/99584	1.25	838/153695 (0.5%)
101	3A	1.14	0/950	1.14	4/1470 (0.3%)
102	3B	1.13	0/919	1.22	8/1416 (0.6%)
103	3C	1.12	0/1103	1.22	7/1700 (0.4%)
104	3D	1.15	0/1124	1.28	12/1738 (0.7%)
105	3E	1.14	0/1116	1.34	15/1722 (0.9%)
106	3F	1.09	0/1265	1.21	7/1947 (0.4%)
107	3G	1.12	0/365	1.15	1/562 (0.2%)
108	3H	1.14	0/1281	1.30	12/1974 (0.6%)
109	3I	1.15	0/826	1.30	9/1273 (0.7%)
110	3J	1.14	0/801	1.26	7/1234 (0.6%)
111	3S	1.11	0/735	1.25	4/1133 (0.4%)
112	3K	1.12	0/1113	1.14	1/1716 (0.1%)
113	3L	1.13	0/853	1.21	3/1316 (0.2%)
114	3M	1.13	0/1269	1.29	11/1957 (0.6%)
115	3O	1.09	0/1108	1.19	11/1708 (0.6%)
116	3P	1.10	0/883	1.10	2/1363 (0.1%)
117	3Q	1.12	0/609	1.25	3/939 (0.3%)
118	3R	1.13	0/749	1.29	8/1158 (0.7%)
All	All	1.12	4/202097 (0.0%)	1.25	1601/311711 (0.5%)

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
1	1A	0	2
2	1B	0	9
4	1D	0	5
5	1E	0	3
6	1F	0	5
7	1G	0	1
8	1H	0	4
9	1I	0	6
10	1J	0	1
11	1K	0	8
12	1L	0	1
13	1M	0	1
14	1O	0	5
15	1P	0	9
16	1Q	0	1
17	1R	0	3
18	1S	0	2
20	1U	0	1
22	1W	0	1
23	1X	0	4
25	1Z	0	1
26	1a	0	4
27	1b	0	2
29	1d	0	1
31	1f	0	1
32	1g	0	1
33	1h	0	3
34	1i	0	1
35	1j	0	1
36	1k	0	3
37	1l	0	2
39	1n	0	1
40	1o	0	2
41	1p	0	2
42	1q	0	3
44	1s	0	3
46	1u	0	1
47	1v	0	1
48	1w	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
50	2N	0	2
52	2B	0	4
53	2C	0	1
54	2D	0	1
56	2F	0	5
57	2G	0	2
58	2H	0	1
60	2J	0	1
64	2O	0	3
65	2P	0	3
66	2Q	0	2
67	2R	0	2
68	2S	0	2
70	2U	0	1
71	2V	0	1
72	2W	0	2
73	2X	0	1
74	2Y	0	1
75	2Z	0	1
77	2b	0	3
78	2c	0	2
79	2d	0	1
80	2e	0	1
82	2g	0	1
83	2h	0	4
84	2i	0	3
85	2j	0	2
87	2l	0	2
88	2m	0	1
89	2n	0	1
90	2o	0	1
91	2p	0	1
92	2q	0	4
93	2r	0	2
95	2t	0	1
96	2u	0	1
97	2v	0	2
98	2w	0	3
100	3N	0	176
101	3A	0	2
102	3B	0	1
103	3C	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
104	3D	0	3
106	3F	0	4
107	3G	0	1
108	3H	0	5
109	3I	0	2
110	3J	0	2
111	3S	0	1
112	3K	0	3
114	3M	0	2
115	3O	0	1
117	3Q	0	4
All	All	0	390

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	2O	1059	DG	C5'-C4'	5.71	1.57	1.51
20	1U	17	DC	N1-C6	5.49	1.40	1.37
64	2O	1060	DC	C5'-C4'	5.38	1.57	1.51
70	2U	1047	DT	C5'-C4'	5.03	1.56	1.51

The worst 5 of 1601 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1U	17	DC	C6-N1-C2	-42.12	103.45	120.30
77	2b	1073	DA	O5'-P-OP1	-26.14	79.33	110.70
65	2P	1062	DG	O5'-P-OP1	-24.68	81.09	110.70
68	2S	1054	DA	O5'-P-OP1	-24.15	81.72	110.70
77	2b	1073	DA	O5'-P-OP2	-23.92	81.99	110.70

There are no chirality outliers.

5 of 390 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	40	DT	Sidechain
1	1A	49	DA	Sidechain
2	1B	3	DG	Sidechain
2	1B	4	DG	Sidechain
2	1B	6	DG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	1082	0	587	0	0
2	1B	1137	0	619	0	0
3	1C	327	0	180	0	0
4	1D	1220	0	669	0	0
5	1E	1052	0	574	1	0
6	1F	950	0	521	1	0
7	1G	321	0	183	1	0
8	1H	970	0	541	0	0
9	1I	971	0	531	1	0
10	1J	492	0	276	0	0
11	1K	945	0	519	0	0
12	1L	333	0	179	0	0
13	1M	645	0	358	0	0
14	1O	808	0	448	1	0
15	1P	948	0	518	0	0
16	1Q	752	0	413	0	0
17	1R	976	0	539	0	0
18	1S	763	0	419	1	0
19	1T	318	0	181	0	0
20	1U	826	0	448	0	0
21	1V	521	0	298	0	0
22	1W	830	0	454	0	0
23	1X	983	0	538	1	0
24	1Y	544	0	308	0	0
25	1Z	531	0	294	0	0
26	1a	965	0	533	0	0
27	1b	665	0	361	0	0
28	1c	820	0	455	0	0
29	1d	826	0	452	0	0
30	1e	524	0	294	0	0
31	1f	804	0	453	0	0
32	1g	982	0	539	0	0
33	1h	993	0	542	0	0
34	1i	986	0	544	0	0
35	1j	659	0	360	0	0
36	1k	827	0	456	0	0
37	1l	980	0	545	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	1m	328	0	183	0	0
39	1n	1148	0	631	0	0
40	1o	821	0	450	0	0
41	1p	816	0	449	0	0
42	1q	981	0	541	0	0
43	1r	654	0	359	0	0
44	1s	649	0	363	0	0
45	1t	651	0	361	0	0
46	1u	982	0	544	0	0
47	1v	319	0	181	0	0
48	1w	808	0	452	0	0
49	1x	329	0	180	0	0
50	2N	736	0	409	0	0
51	2A	665	0	359	1	0
52	2B	975	0	538	1	0
53	2C	527	0	301	0	0
54	2D	652	0	362	0	0
55	2E	816	0	455	0	0
56	2F	988	0	545	0	0
57	2G	820	0	455	0	0
58	2H	807	0	452	0	0
59	2I	328	0	183	0	0
60	2J	599	0	327	0	0
61	2K	495	0	270	1	0
62	2L	653	0	363	0	0
63	2M	488	0	270	0	0
64	2O	532	0	297	2	0
65	2P	822	0	448	0	0
66	2Q	818	0	453	0	0
67	2R	822	0	453	0	0
68	2S	1192	0	650	0	0
69	2T	494	0	272	0	0
70	2U	1059	0	589	0	0
71	2V	815	0	457	0	0
72	2W	987	0	543	0	0
73	2X	974	0	539	0	0
74	2Y	656	0	360	0	0
75	2Z	818	0	456	0	0
76	2a	1179	0	656	0	0
77	2b	1149	0	633	0	0
78	2c	914	0	511	0	0
79	2d	1075	0	580	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	2e	766	0	421	0	0
81	2f	976	0	540	0	0
82	2g	972	0	538	0	0
83	2h	1156	0	631	0	0
84	2i	661	0	359	0	0
85	2j	326	0	183	0	0
86	2k	652	0	361	0	0
87	2l	980	0	537	0	0
88	2m	984	0	543	0	0
89	2n	325	0	184	0	0
90	2o	653	0	366	0	0
91	2p	656	0	362	0	0
92	2q	805	0	454	0	0
93	2r	485	0	272	0	0
94	2s	655	0	358	0	0
95	2t	824	0	448	0	0
96	2u	652	0	361	0	0
97	2v	651	0	367	0	0
98	2w	974	0	526	0	0
99	2x	320	0	180	0	0
100	3N	88890	0	49198	32	0
101	3A	841	0	447	0	0
102	3B	818	0	449	1	0
103	3C	982	0	541	0	0
104	3D	999	0	541	0	0
105	3E	991	0	536	0	0
106	3F	1131	0	635	0	0
107	3G	326	0	183	0	0
108	3H	1142	0	632	0	0
109	3I	736	0	405	0	0
110	3J	714	0	395	0	0
111	3S	655	0	363	0	0
112	3K	988	0	537	1	0
113	3L	760	0	414	0	0
114	3M	1129	0	620	0	0
115	3O	985	0	541	1	0
116	3P	785	0	430	0	0
117	3Q	539	0	290	0	0
118	3R	666	0	363	0	0
All	All	180167	0	99520	45	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 45 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
100:3N:3913:DA:H2"	100:3N:3914:DC:C6	2.46	0.50
18:1S:8:DT:H1'	64:2O:1060:DC:C5	2.48	0.49
61:2K:1023:DG:H2'	61:2K:1024:DC:C5	2.48	0.48
102:3B:2120:DG:H2'	102:3B:2121:DC:C6	2.49	0.47
100:3N:3568:DA:H2'	100:3N:3569:DC:C6	2.49	0.47

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

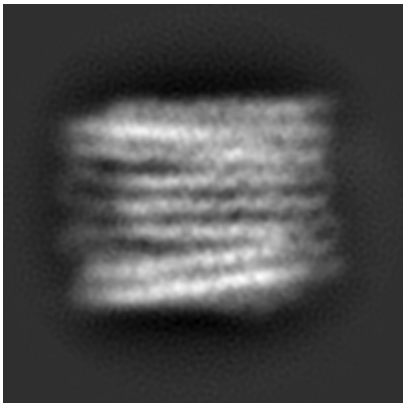
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7304. These allow visual inspection of the internal detail of the map and identification of artifacts.

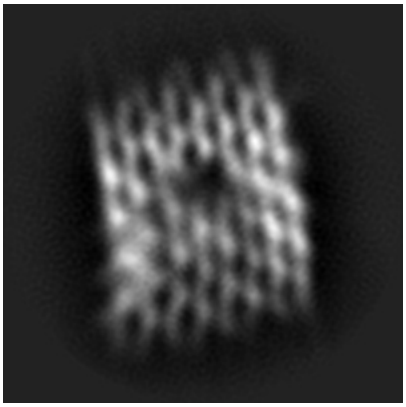
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

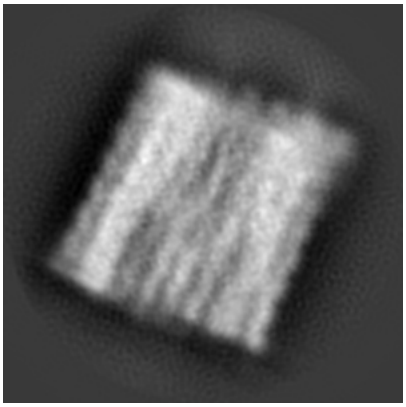
6.1.1 Primary map



X



Y

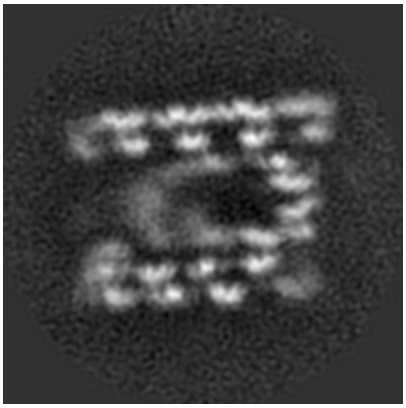


Z

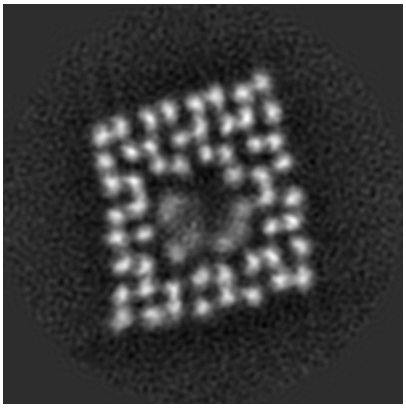
The images above show the map projected in three orthogonal directions.

6.2 Central slices

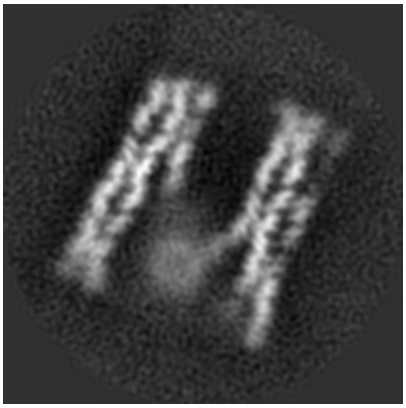
6.2.1 Primary map



X Index: 300



Y Index: 300

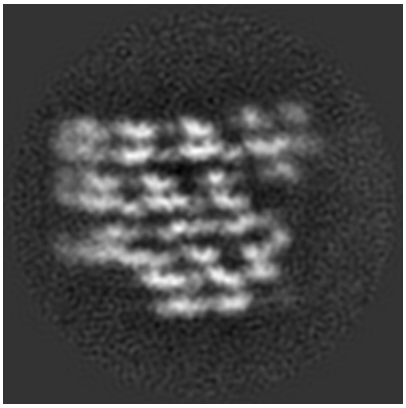


Z Index: 300

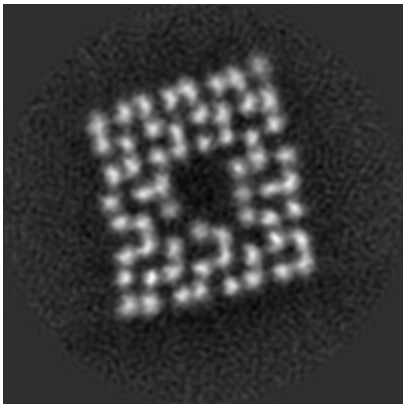
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

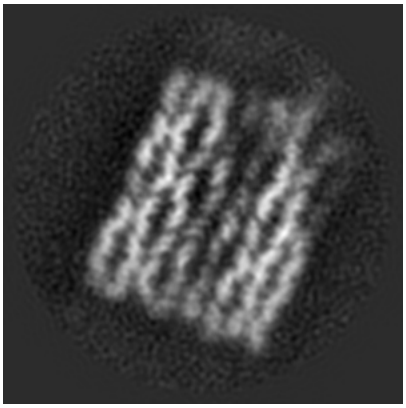
6.3.1 Primary map



X Index: 389



Y Index: 340

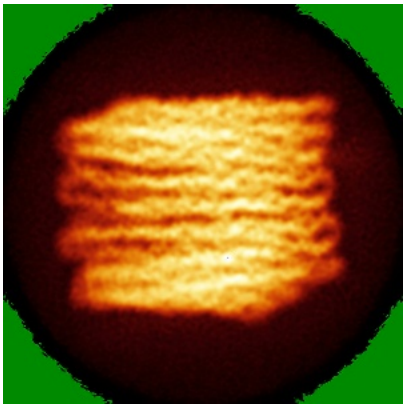


Z Index: 408

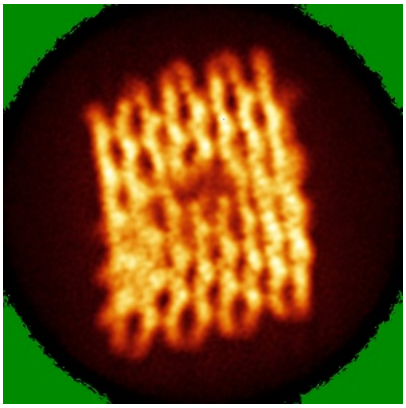
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

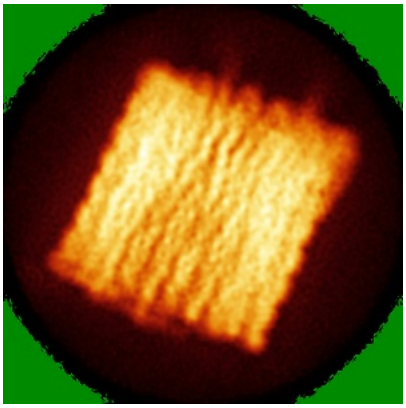
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

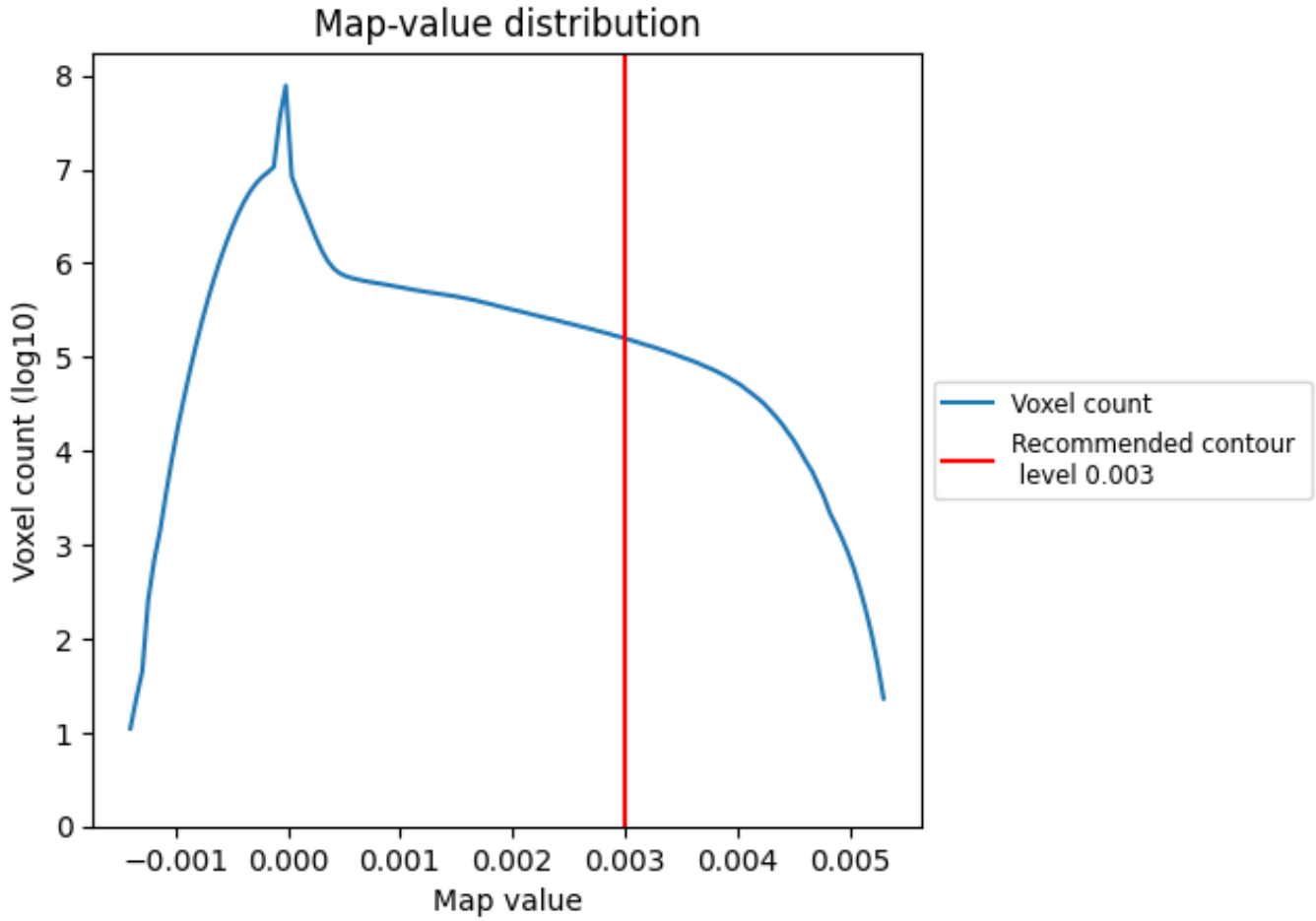
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

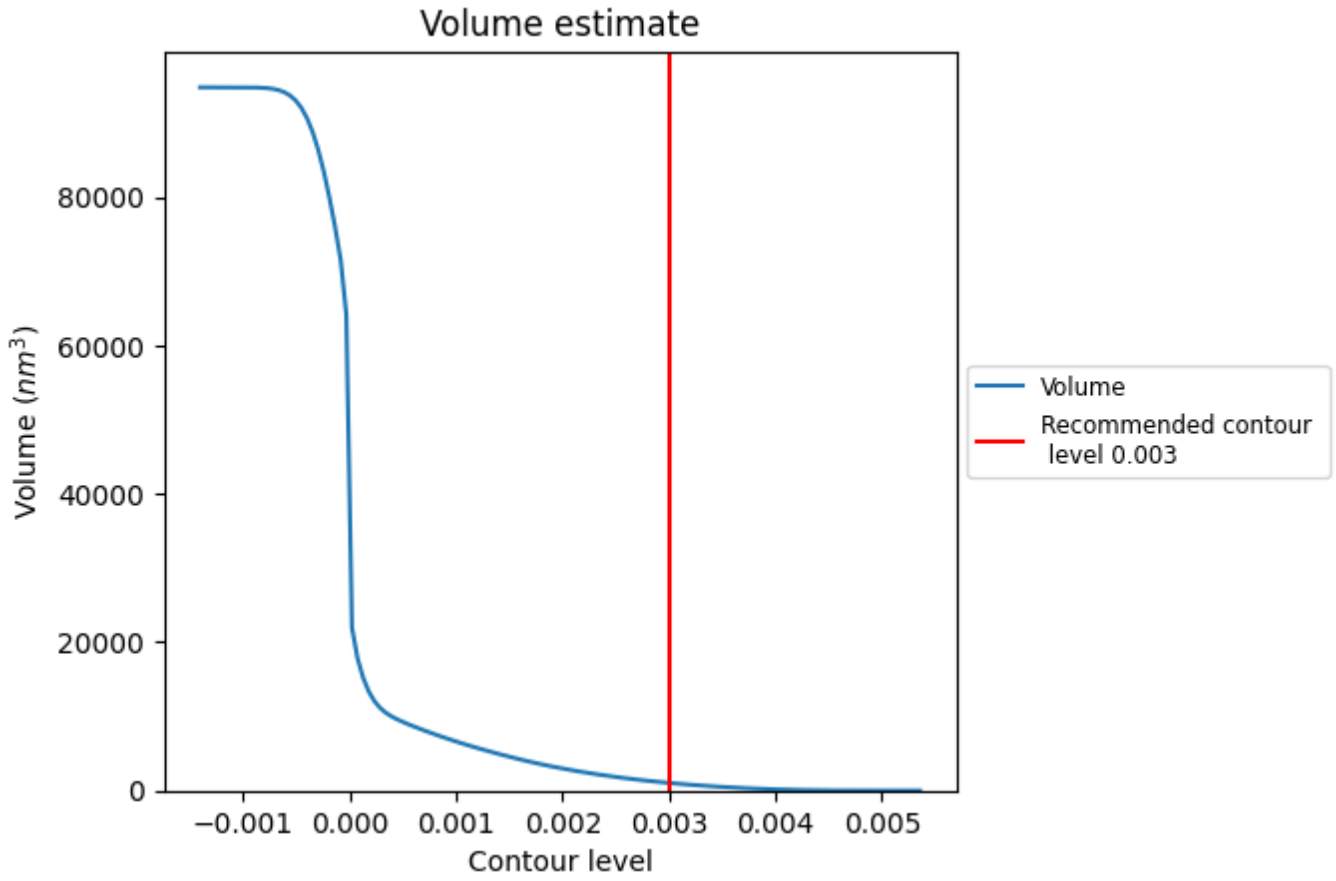
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

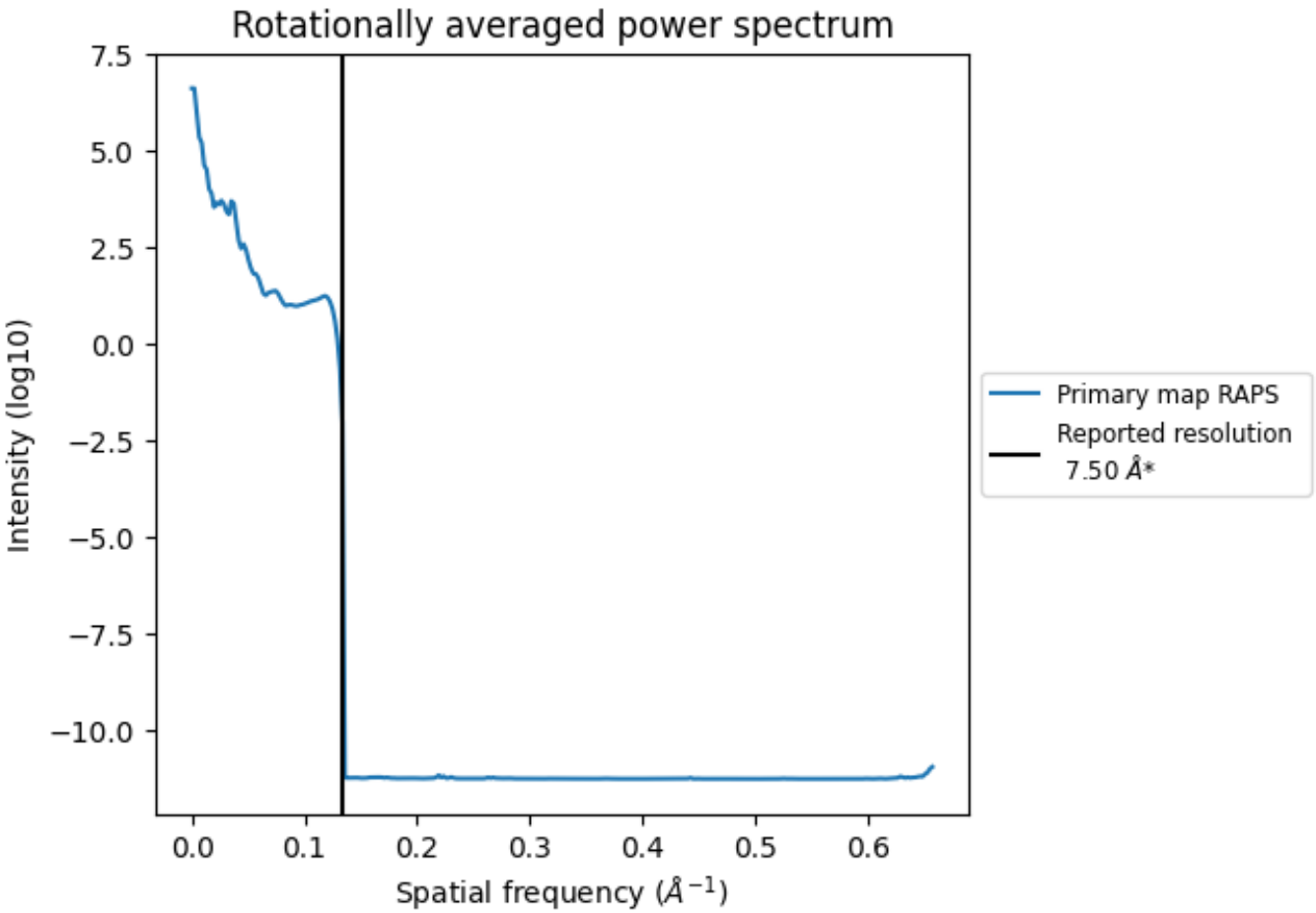
7.2 Volume estimate (i)



The volume at the recommended contour level is 1031 nm^3; this corresponds to an approximate mass of 931 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

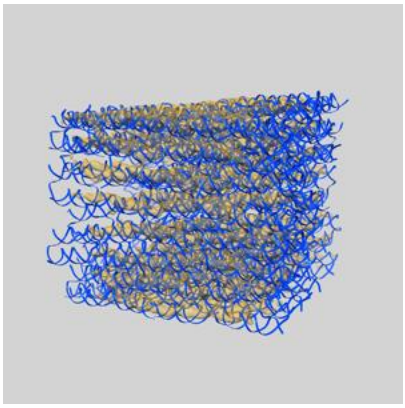
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

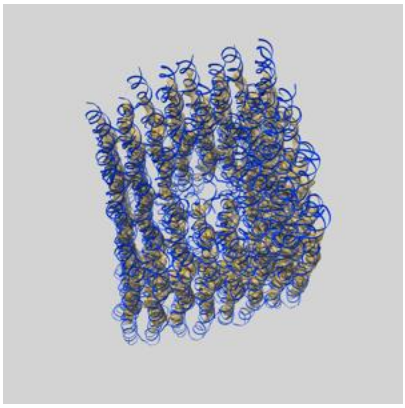
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7304 and PDB model 6BY7. Per-residue inclusion information can be found in section 3 on page 26.

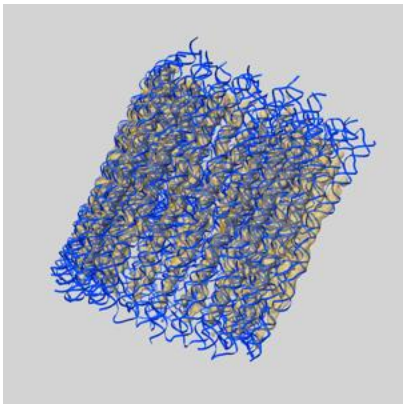
9.1 Map-model overlay



X



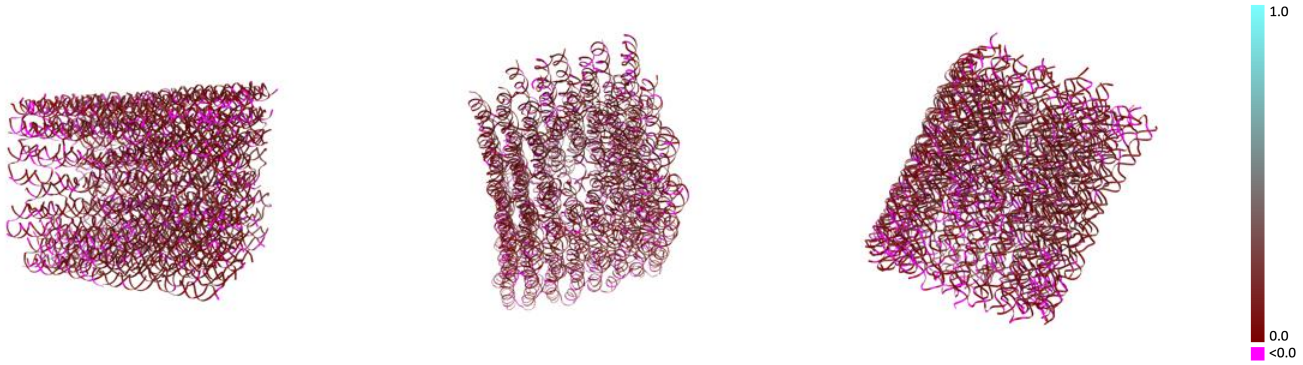
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

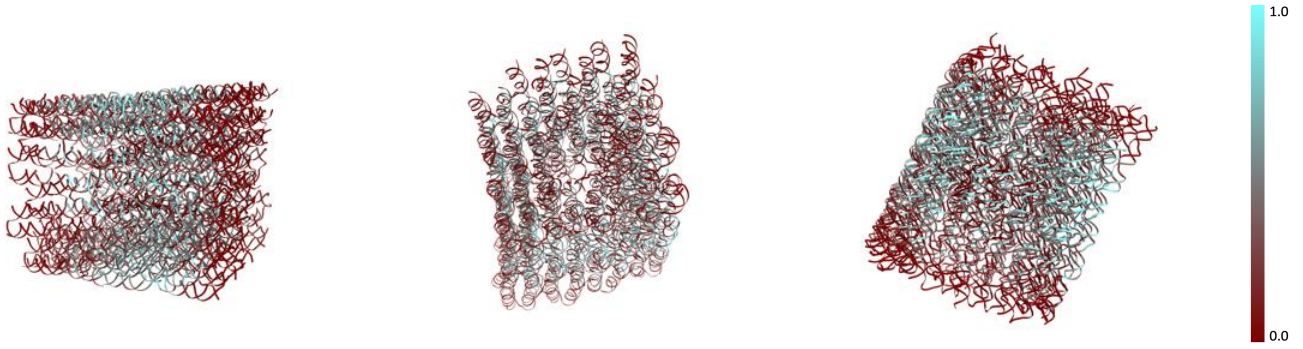
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

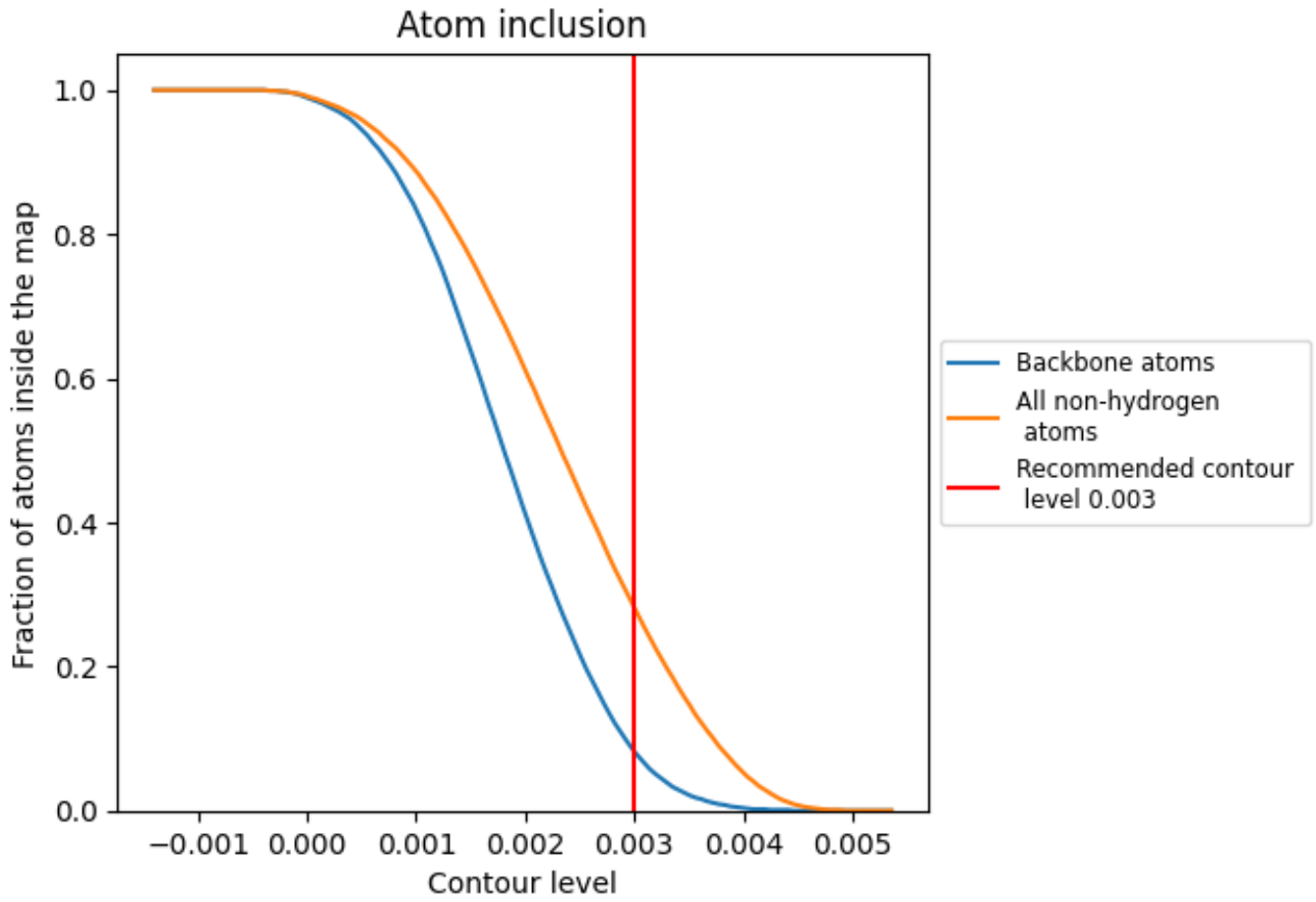
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.003).

9.4 Atom inclusion (i)



At the recommended contour level, 8% of all backbone atoms, 28% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2810	0.0890
1A	0.4310	0.1180
1B	0.2710	0.0740
1C	0.0090	0.0780
1D	0.2440	0.0490
1E	0.2150	0.1140
1F	0.0000	0.0400
1G	0.1310	0.1220
1H	0.3330	0.1020
1I	0.1670	0.0980
1J	0.4170	0.1090
1K	0.0060	0.0470
1L	0.0000	0.0590
1M	0.4420	0.0990
1O	0.3720	0.0990
1P	0.0000	-0.0000
1Q	0.1900	0.1280
1R	0.3400	0.0950
1S	0.2880	0.0950
1T	0.0000	0.0930
1U	0.4590	0.0920
1V	0.0190	0.0310
1W	0.2050	0.0910
1X	0.3410	0.1020
1Y	0.1410	0.0670
1Z	0.0000	0.0670
1a	0.1320	0.0190
1b	0.4160	0.0830
1c	0.4730	0.1360
1d	0.2360	0.0650
1e	0.0000	0.0700
1f	0.4650	0.1250
1g	0.4400	0.1200
1h	0.4660	0.1120
1i	0.0270	0.0570

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Chain	Atom inclusion	Q-score
1j	0.3660	0.1510
1k	0.4220	0.0920
1l	0.0000	0.0510
1m	0.0150	0.0160
1n	0.4120	0.1210
1o	0.1020	0.0550
1p	0.3240	0.1090
1q	0.0650	0.0510
1r	0.4910	0.1130
1s	0.2310	0.0940
1t	0.4460	0.0900
1u	0.0370	0.0790
1v	0.0060	0.0500
1w	0.4860	0.1150
1x	0.0270	0.0500
2A	0.1130	0.0550
2B	0.3330	0.1370
2C	0.1330	0.0840
2D	0.4220	0.0860
2E	0.4060	0.0880
2F	0.4860	0.0980
2G	0.2410	0.0520
2H	0.0320	0.0470
2I	0.0000	0.0590
2J	0.1800	0.1170
2K	0.5330	0.1140
2L	0.2740	0.0640
2M	0.1070	0.0640
2N	0.3650	0.0790
2O	0.1090	0.0950
2P	0.4960	0.1150
2Q	0.4020	0.1040
2R	0.3980	0.0720
2S	0.1370	0.0570
2T	0.0470	0.0780
2U	0.4040	0.1100
2V	0.5040	0.1000
2W	0.4220	0.1050
2X	0.4410	0.1060
2Y	0.5840	0.1150
2Z	0.4140	0.1130
2a	0.1150	0.0650

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Chain	Atom inclusion	Q-score
2b	0.5060	0.1260
2c	0.1120	0.0940
2d	0.4400	0.1170
2e	0.0870	0.0930
2f	0.4360	0.1190
2g	0.3300	0.0640
2h	0.4520	0.0990
2i	0.3190	0.1180
2j	0.0000	0.0590
2k	0.3600	0.1290
2l	0.4580	0.1040
2m	0.2300	0.0840
2n	0.0000	0.0420
2o	0.1590	0.1100
2p	0.4670	0.1170
2q	0.3700	0.0680
2r	0.2310	0.1120
2s	0.3540	0.0890
2t	0.0010	0.0280
2u	0.2620	0.1180
2v	0.4100	0.0770
2w	0.2390	0.0630
2x	0.0000	0.0770
3A	0.1330	0.1130
3B	0.4440	0.1230
3C	0.4110	0.0930
3D	0.4550	0.1100
3E	0.3490	0.0990
3F	0.5350	0.1310
3G	0.0030	0.0640
3H	0.2690	0.1010
3I	0.4480	0.1130
3J	0.0270	0.0240
3K	0.3320	0.0900
3L	0.2530	0.0910
3M	0.2930	0.0720
3N	0.2820	0.0900
3O	0.2050	0.0530
3P	0.0200	0.0660
3Q	0.0760	0.0580
3R	0.5480	0.1200
3S	0.2170	0.0700