Computational Identification and Illustrative Standard for Representation of Unimolecular G-Quadruplex Secondary Structures (CIIS-GQ)

Modified Bases Included in pdb Structures

The structures with modified guanine bases were also used for the study. The algorithm was designed to regard a set of predefined modified bases as a guanine base during Hoogsteen base pair discovery. These modified bases are GFL[20-22], 8OG [23], 0G [24], GF2 [22,25,27], LCG [27-29], GF0 [25] and BGM. [30- 38]

Comparison with ONZ classification

We have compared CIIS-GQ results with the ONZ classification method. Among all DNA structures, we have 13 NNN, 29 OO, 79 OOO, 1 ZZ, 9 OOOO, 3 NNNN, 6 OOZ, 11 NN, 7 NNO, 1 NOO, 2 ONN, 1 ZZZ, 2 ZZO, 1 ZO classes were identified. Analysis of these structures also showed consistent patterns between the types of the loops and types of ONZ classifications. Firstly, it was observed that if a loop occurs after all tetrads are visited since the last loop or the sequence beginning, there is always a single ONZ class identified for all tetrads. This is actually an expected result. When all of the tetrads have the same ONZ class, the order of guanines in sequence goes from minimum to maximum sequentially from the bottom tetrad through the top one for each region between two consecutive loops. Therefore, loop occurs after each guanine from all tetrads is visited.

Among 13 NNN classes, all structures have 3 loops, where the first and the third are lateral or reversal, and the second one is diagonal. Among 3 NNNN and 11 NN classes, all contain lateral, diagonal and lateral loops in that order. It was apparent that for any G-quadruplex containing only N type tetrad, a diagonal loop is consistently present.

Among 29 OO classes, 27 structures have 3 loops and 2 of them which contain proteins have 4 loops. 22 of them have only lateral loops, while 5 of them have only reversal loops, and 2 contain both reversal and lateral ones. Among 79 OOO classes, 50 of them are structures which contain 3 reversal loops. 2 of them contain 3 lateral loops and the rest contain a mixture of lateral and reversal. Additionally, 78 of these structures contain 3 loops while only 1 of them contains 4 loops. Among 9 OOOO classes, 7 of them contain only reversal loops which have a number at least 6. And 2 of them contain 3 lateral loops. It was surprising to see that with the all-O type G-quadruplexes, we observed that the diagonal loop was absent and the reversal loop was dominant.

There were only 2 all-Z type G-quadruplexes. One being ZZZ and the other ZZ, both consist of diagonal, reversal and diagonal loops. For all-Z and all-N type structures, it is expected that two guanines that lay across to each other in a tetrad to be consecutive in the sequence order. For

Z-types this is possible if there are two diagonal loops, while in N-type, only one diagonal is adequate. This is in accordance with our observations where N-types have exactly one diagonal.

On the other hand, mixed type G-quadruplexes showed characteristics independent from their uniform type counterparts. 7 NNO G-quadruplexes, where all of them followed a lateral, lateral, reversal and reversal loop pattern. In the meanwhile, among 6 OOZ classes, all structures have 4 loops which are reversal, reversal, reversal and diagonal. Other classes which contain Z types also contain at least one diagonal loop. It is apparent that containing N or Z-type tetrad alone did not determine the existence of a diagonal loop. However, it can be said that when N and Z classes are in the structure, the probability of observing the diagonal loop is high.

Comparison with DSSR

DSSR is a stand alone tool which does not require any other software to find base pairs, tetrads and loops however, it utilises other tools for visualisation purposes, such as PyMol. In comparison CIIS-GQ is capable of generating a depiction using python's turtle library. DSSR has a detailed explanation of strands, tetrads and loops. However, the comprehensive output of DSSR is often hard to understand and grasp the details of the structure. The plain 2D illustration generated by CIIS-GQ presents an advantage, where tetrads can be identified horizontally, and stacking guanines can be distinguished vertically. Additionally, DSSR requires licensing to get annotation results for G-quadruplex structures. Fortunately, the annotation results for a number of G-quadruplexes were already published at DSSR-G4DB[1] (46) and we were able to compare. DSSR has three types of loops which are lateral, diagonal and propeller, which corresponds to lateral, diagonal and reversal in CIIS-GQ, respectively.

Another advantage of CIIS-GQ is that it requires only two thresholds, the thresholds of distance and angle parameters that can be modified to detect loosely connected tetrads. Due to this advantage, the identification of the tetrads were possible in at least two structures. In case of 1OZ8, DSSR found three tetrads (G1-G4-G7-G10, G13-G16-G19-G22 and G14-G17-G20-G23) as shown at the result page[2] (47) while CIIS-GQ has found one more tetrad which is G2-G5-G8-G11. In comparison DSSR highlighted G5-G8-G11 as a multiplet, omitting the G2. Based on this difference, loop classification differs with CIIS-GQ. DSSR has identified 3 stem reversal loops and 3 non-stem lateral loops while we have identified 7 reversal loops. Stem loop is defined as any loop that also forms a duplex within itself.

A similar difference exists in 6T2G. DSSR could find 2 tetrads in this structure (G2-G6-G11-G26 and G4-G9-G13-G28) as shown at the result page[3] (47) while CIIS-GQ found one more tetrad, G3-G7-G12-G27. DSSR is able to show these four guanines as a multiplet in the list of multiplets section, however does not present it as a tetrad like the other two tetrads. As a result, CIIS-GQ loop

[1] http://g4.x3dna.org/
[2] http://skmatic.x3dna.org/pdb/1oz8/1oz8.out
[3] http://skmatic.x3dna.org/pdb/6t2g/6t2g.out

types and placements are also different. DSSR has found six lateral loops while CIIS-GQ has found three reversal loops.

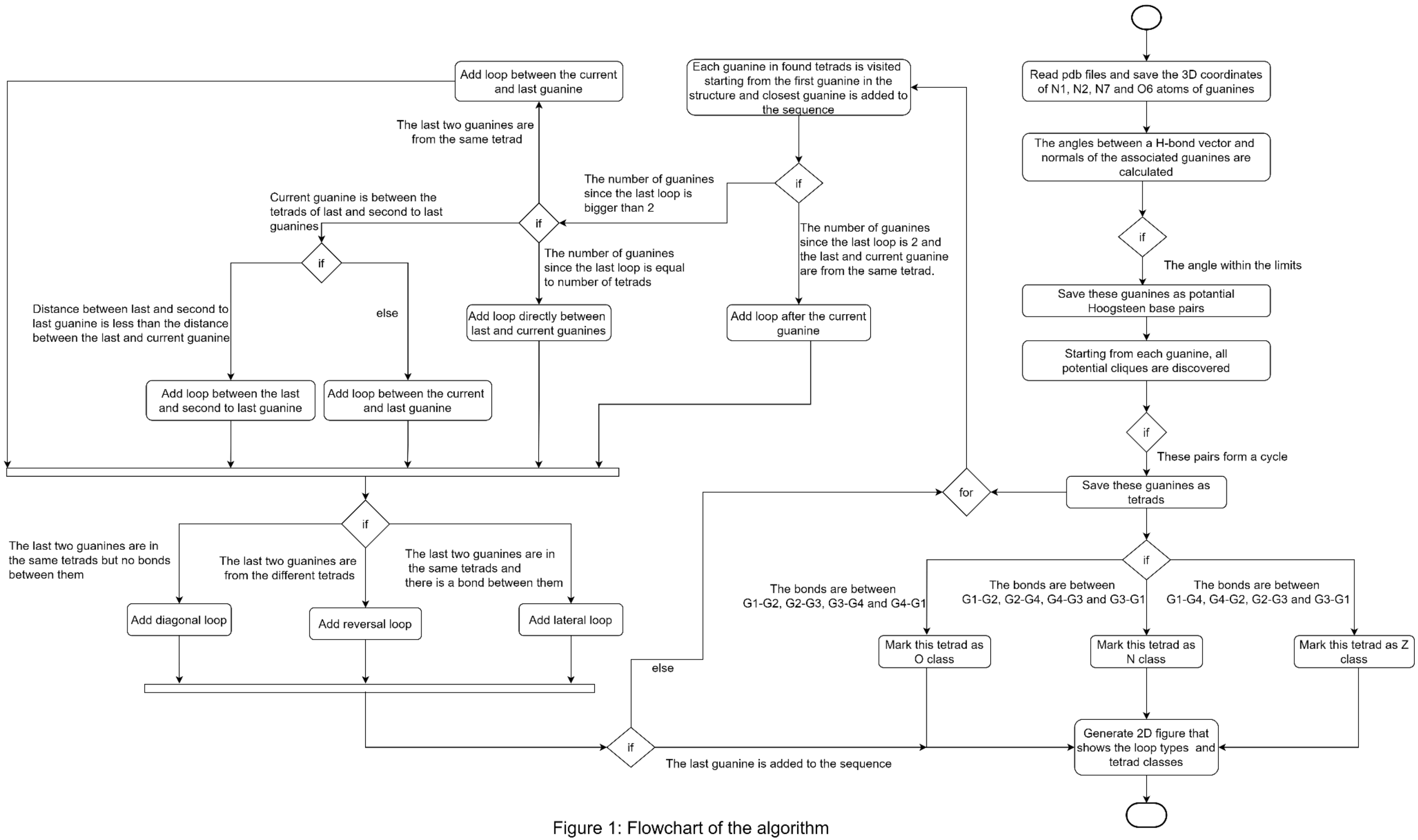

Figure 1: Flowchart of the algorithm

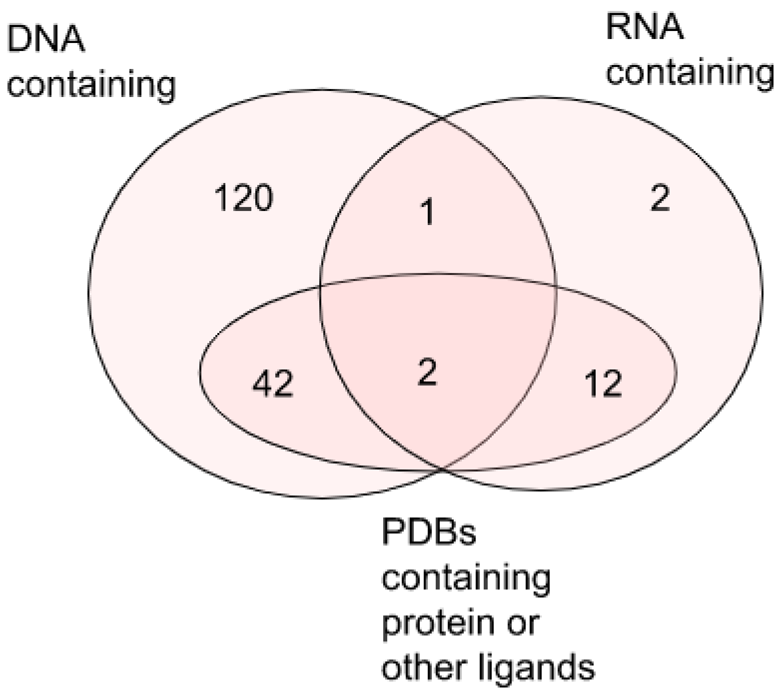

Figure 2. Number of PDB structures based on the backbone of the nucleic acid and presence of ligand.

Table S1: Validation set

Pdb Name	Tetrad	Loops
6h1k	[1,20,16,27], [2,19,15,26], [25,28,17,21] DG1,A.DG20,A.DG16,A.DG27 DG2,A.DG19,A.DG15,A.DG26 DG17,A.DG21,A.DG25,A.DG28	["1,2,d,15,16,17,r,19,20,21,l,25,r,26,27,28"] 1 type=lateral helix=#1 nts=5 GACTG A.DG21,A.DA22,A.DC23,A.DT24,A.DG25 2 type=V-shaped helix=#1 nts=4 GGGG A.DG25,A.DG26,A.DG27,A.DG28
2m91	[2,6,26,29], [1,25,30,7] A.DG1,A.DG7,A.DG30,A.DG25 A.DG2,A.DG6,A.DG29,A.DG26	["1,2,d,15,16,17,r,19,20,21,l,25,r,26,27,28"] loop#1 type=lateral strands=[#1,#2] nts=3 GAA A.DG3,A.DA4,A.DA5 loop#2 type=diagonal strands=[#2,#4] nts=17 GCGCGAAGCATTCGCGA A.DG8,A.DC9,A.DG10,A.DC11,A.DG12,A.DA13,A.DA14,A.DG15,A.DC16,A.DA1

		7,A.DT18,A.DT19,A.DC20,A.DG21,A.DC22,A.DG23,A.DA24 loop#3 type=lateral strands=[#4,#3] nts=2 TA A.DT27,A.DA28
2f8u	[1,9,17,21], [2,8,18,22], [3,7,19,23] A.DG1,A.DG9,A.DG17,A.DG21 A.DG2,A.DG8,A.DG18,A.DG22 A.DG3,A.DG7,A.DG19,A.DG23	["1,2,3,l,7,8,9,l,17,18,19,r,21,22,23"] loop#1 type=lateral strands=[#1,#2] nts=3 CGC A.DC4,A.DG5,A.DC6 loop#2 type=lateral strands=[#2,#3] nts=7 AGGAATT A.DA10,A.DG11,A.DG12,A.DA13,A.DA14,A.DT15,A.DT16 loop#3 type=propeller strands=[#3,#4] nts=1 C A.DC20
7cv3	[3,7,22,25], [4,8,21,26], [5,9,20,27] A.DG3,A.DG7,A.DG22,A.DG25 A.DG4,A.DG8,A.DG21,A.DG26 A.DG5,A.DG9,A.DG20,A.DG27	["3,4,5,r,7,8,9,l,20,21,22,l,25,26,27"] loop#1 type=propeller strands=[#1,#2] nts=1 A A.DA6 loop#2 type=lateral strands=[#2,#3] nts=10 CGCGCCAGCG A.DC10,A.DG11,A.DC12,A.DG13,A.DC14,A.DC15,A.DA16,A.DG17,A.DC18,A.DG19 loop#3 type=lateral strands=[#3,#4] nts=2 TC A.DT23,A.DC24
7cv4	[2,25,18,7], [6,3,24,19] A.DG2,A.DG25,A.DG18,A.DG7 A.DG3,A.DG24,A.DG19,A.DG6	["2,3,l,6,7,l,18,19,l,24,25"] loop#1 type=lateral strands=[#1,#4] nts=2 AG A.DA4,A.DG5 loop#2 type=lateral strands=[#4,#3] nts=10 CGCGCCAGCG A.DC8,A.DG9,A.DC10,A.DG11,A.DC12,A.DC13,A.DA14,A.DG15,A.DC16,A.DG17 loop#3 type=lateral strands=[#3,#2] nts=4

		GTCG A.DG20,A.DT21,A.DC22,A.DG23
5zev	[1,15,10,22], [2,13,9,21], [20,16,11,23]A.DG1,A.DG15,A.DG10,A.DG22 A.DG2,A.DG13,A.DG9,A.DG21 A.DG11,A.DG16,A.DG20,A.DG23	["1,2,d,9,10,11,r,13,15,16,l,20,r,21,22,23"] loop#1 type=diagonal strands=[#1,#3] nts=6 GTACCC A.DG3,A.DT4,A.DA5,A.DC6,A.DC7,A.DC8 loop#2 type=propeller strands=[#3,#2] nts=2 GT A.DG11,A.DT12 loop#3 type=diag-prop strands=[#2,#4] nts=5 GTGCG A.DG16,A.DT17,A.DG18,A.DC19,A.DG20
6kvb	[2,12,9,6], [15,11,5,8], [17,3,23,20],[18,27,24,21] A.DG2,A.DG12,A.DG9,A.DG6 A.DG3,A.DG17,A.DG20,A.DG23 A.DG5,A.DG8,A.DG11,A.DG15 A.DG18,A.DG21,A.DG24,A.DG27	["2,3,r,5,6,r,8,9,r,11,12,r,15,17,18,r,20,21,r,23,24,l,27"] 1 type=V-shaped helix=#1 nts=5 GGTGG A.DG2,A.DG3,A.DT4,A.DG5,A.DG6 2* type=V-shaped helix=#1 nts=5 GGTTG A.DG11,A.DG12,A.DT13,A.DT14,A.DG15 3 type=lateral helix=#1 nts=4 GTTG A.DG24,A.DT25,A.DT26,A.DG27
2lpw	[5,9,21,25], [4,8,20,24], [3,7,19,23] A.DG3,A.DG7,A.DG19,A.DG23 A.DG4,A.DG8,A.DG20,A.DG24 A.DG5,A.DG9,A.DG21,A.DG25	["3,4,5,r,7,8,9,r,19,20,21,r,23,24,25"] loop#1 type=propeller strands=[#1,#2] nts=1 T A.DT6 loop#2 type=propeller strands=[#2,#3] nts=9 TGTAAGTGT A.DT10,A.DG11,A.DT12,A.DA13,A.DA14,A.DG15,A.DT16,A.DG17,A.DT18 loop#3 type=propeller strands=[#3,#4] nts=1 T A.DT22
2n60	[3,7,15,11], [5,8,16,12]	["3,5,r,7,8,r,11,12,r,15,16"]

	A.DG3,A.DG7,A.DG11,A.DG15 A.DG5,A.DG8,A.DG12,A.DG16	loop#1 type=propeller strands=[#1,#2] nts=1 T A.DT6 loop#2 type=propeller strands=[#2,#3] nts=2 GT A.DG9,A.DT10 loop#3 type=propeller strands=[#3,#4] nts=2 GT A.DG13,A.DT14
1hao	[401, 406, 410, 415], [402, 405, 411, 414] D.DG401,D.DG415,D.DG410,D.DG406 D.DG402,D.DG414,D.DG411,D.DG405	["401,402,I,405,406,I,410,411,I,414,415"] loop#1 type=lateral strands=[#1,#4] nts=2 TT D.DT403,D.DT404 loop#2 type=lateral strands=[#4,#3] nts=3 TGT D.DT407,D.DG408,D.DT409 loop#3 type=lateral strands=[#3,#2] nts=2 TT D.DT412,D.DT413
1hap	[401, 406, 410, 415], [402, 405, 411, 414] D.DG401,D.DG406,D.DG410,D.DG415 D.DG402,D.DG405,D.DG411,D.DG414	["401,402,I,405,406,I,410,411,I,414,415"] loop#1 type=lateral strands=[#1,#2] nts=2 TT D.DT403,D.DT404 loop#2 type=lateral strands=[#2,#3] nts=3 TGT D.DT407,D.DG408,D.DT409 loop#3 type=lateral strands=[#3,#4] nts=2 TT D.DT412,D.DT413
1hut	[401, 406, 410, 415], [402, 405, 411, 414] D.DG401,D.DG406,D.DG410,D.DG415 D.DG402,D.DG405,D.DG411,D.DG414	["401,402,I,405,406,I,410,411,I,414,415"] loop#1 type=lateral strands=[#1,#2] nts=2 TT D.DT403,D.DT404 loop#2 type=lateral strands=[#2,#3] nts=3 TGT D.DT407,D.DG408,D.DT409 loop#3 type=lateral strands=[#3,#4] nts=2 TT D.DT412,D.DT413
143d	[2,10,22,14], [3,9,21,15], [4,8,20,16] A.DG2,A.DG10,A.DG22,A.DG14	["2,3,4,I,8,9,10,d,14,15,16,I,20,21,22"]

	A.DG3,A.DG9,A.DG21,A.DG15 A.DG4,A.DG8,A.DG20,A.DG16	loop#1 type=lateral strands=[#1,#2] nts=3 TTA A.DT5,A.DT6,A.DA7 loop#2 type=diagonal strands=[#2,#4] nts=3 TTA A.DT11,A.DT12,A.DA13 loop#3 type=lateral strands=[#4,#3] nts=3 TTA A.DT17,A.DT18,A.DA19
148d	[1,6,10,15], [2,5,11,14] A.DG1,A.DG15,A.DG10,A.DG6 A.DG2,A.DG14,A.DG11,A.DG5	["1,2,l,5,6,l,10,11,l,14,15"] loop#1 type=lateral strands=[#1,#4] nts=2 TT A.DT3,A.DT4 loop#2 type=lateral strands=[#4,#3] nts=3 TGT A.DT7,A.DG8,A.DT9 loop#3 type=lateral strands=[#3,#2] nts=2 TT A.DT12,A.DT13
186d	[3,12,16,21], [4,11,17,22], [5,10,18,23] A.DG3,A.DG12,A.DG16,A.DG21 A.DG4,A.DG11,A.DG17,A.DG22 A.DG5,A.DG10,A.DG18,A.DG23	["3,4,5,l,10,11,12,l,16,17,18,r,21,22,23"] loop#1 type=lateral strands=[#1,#2] nts=4 GTTG A.DG6,A.DT7,A.DT8,A.DG9 loop#2 type=lateral strands=[#2,#3] nts=3 TTG A.DT13,A.DT14,A.DG15 loop#3 type=propeller strands=[#3,#4] nts=2 TT A.DT19,A.DT20
1bub	[1,6,10,15], [2,5,11,14] A.DG1,A.DG15,A.DG10,A.DG6 A.DG2,A.DG14,A.DG11,A.DG5	["1,2,l,5,6,l,10,11,l,14,15"] loop#1 type=lateral strands=[#1,#4] nts=2 TT A.DT3,A.DT4 loop#2 type=lateral strands=[#4,#3] nts=3 TGT A.DT7,A.DG8,A.DT9 loop#3 type=lateral strands=[#3,#2] nts=2 TT A.DT12,A.DT13
1c32	[1,6,10,15], [2,5,11,14] A.DG1,A.DG15,A.DG10,A.DG6 A.DG2,A.DG14,A.DG11,A.DG5	["1,2,l,5,6,l,10,11,l,14,15"] loop#1 type=lateral strands=[#1,#4] nts=2 TT A.DT3,A.DT4

		loop#2 type=lateral strands=[#4,#3] nts=3 TGT A.DT7,A.DG8,A.DT9 loop#3 type=lateral strands=[#3,#2] nts=2 TT A.DT12,A.DT13
1c34	[1,6,10,15], [2,5,11,14] A.DG1,A.DG15,A.DG10,A.DG6 A.DG2,A.DG14,A.DG11,A.DG5	["1,2,l,5,6,l,10,11,l,14,15"] loop#1 type=lateral strands=[#1,#4] nts=2 TT A.DT3,A.DT4 loop#2 type=lateral strands=[#4,#3] nts=3 TGT A.DT7,A.DG8,A.DT9 loop#3 type=lateral strands=[#3,#2] nts=2 TT A.DT12,A.DT13
1c35	[1,6,10,15], [2,5,11,14] A.DG1,A.DG15,A.DG10,A.DG6 A.DG2,A.DG14,A.DG11,A.DG5	["1,2,l,5,6,l,10,11,l,14,15"] loop#1 type=lateral strands=[#1,#4] nts=2 TT A.DT3,A.DT4 loop#2 type=lateral strands=[#4,#3] nts=3 TGT A.DT7,A.DG8,A.DT9 loop#3 type=lateral strands=[#3,#2] nts=2 TT A.DT12,A.DT13
1c38	[1,6,10,15], [2,5,11,14] A.DG1,A.DG15,A.DG10,A.DG6 A.DG2,A.DG14,A.DG11,A.DG5	["1,2,l,5,6,l,10,11,l,14,15"] loop#1 type=lateral strands=[#1,#4] nts=2 TT A.DT3,A.DT4 loop#2 type=lateral strands=[#4,#3] nts=3 TGT A.DT7,A.DG8,A.DT9 loop#3 type=lateral strands=[#3,#2] nts=2 TT A.DT12,A.DT13
1i34	[1,12,8,18], [2,11,7,19] A.DG1,A.DG12,A.DG8,A.DG18 A.DG2,A.DG11,A.DG7,A.DG19	["1,2,d,7,8,r,11,12,d,18,19"] loop#1 type=diagonal strands=[#1,#3] nts=4 TTTT A.DT3,A.DT4,A.DT5,A.DT6 loop#2 type=propeller strands=[#3,#2] nts=2 CA A.DC9,A.DA10 loop#3 type=diagonal strands=[#2,#4] nts=5 GTTTT A.DG13,A.DT14,A.DT15,A.DT16,A.DT17

1k8p	[3,9,15,21], [4,10,16,22], [5,11,17,23] A.DG3,A.DG9,B.DG15,B.DG21 A.DG4,A.DG10,B.DG16,B.DG22 A.DG5,A.DG11,B.DG17,B.DG23	["3,4,5,r,9,10,11,r,15,16,17,r,21,22,23"] loop#1 type=propeller strands=[#1,#2] nts=3 uTA A.BRU6,A.DT7,A.DA8 loop#2 type=propeller strands=[#3,#4] nts=3 uTA B.BRU18,B.DT19,B.DA20
1kf1	[2,8,14,20], [3,9,15,21], [4,10,16,22] A.DG2,A.DG8,A.DG14,A.DG20 A.DG3,A.DG9,A.DG15,A.DG21 A.DG4,A.DG10,A.DG16,A.DG22	["2,3,4,r,8,9,10,r,14,15,16,r,20,21,22"] loop#1 type=propeller strands=[#1,#2] nts=3 TTA A.DT5,A.DT6,A.DA7 loop#2 type=propeller strands=[#2,#3] nts=3 TTA A.DT11,A.DT12,A.DA13 loop#3 type=propeller strands=[#3,#4] nts=3 TTA A.DT17,A.DT18,A.DA19
1oz8	[2,5,8,11], [1,4,7,10], [13,16,19,22], [14,17,20,23] A.DG1,A.DG4,A.DG7,A.DG10 A.DG13,A.DG16,A.DG19,A.DG22 A.DG14,A.DG17,A.DG20,A.DG23	["1,2,r,4,5,r,7,8,r,10,11,r,13,14,r,16,17,r,19,20,r,22,23"] **List of 1 G4-stem** loop#1 type=propeller strands=[#1,#2] nts=1 A A.DA15 loop#2 type=propeller strands=[#2,#3] nts=1 A A.DA18 loop#3 type=propeller strands=[#3,#4] nts=1 A A.DA21 **List of 3 non-stem G4-loops (including the two closing Gs)** 1 type=lateral helix=#1 nts=4 GGAG A.DG1,A.DG2,A.DA3,A.DG4 2 type=lateral helix=#1 nts=4 GGAG A.DG4,A.DG5,A.DA6,A.DG7

		3 type=lateral helix=#1 nts=4 GGAG A.DG7,A.DG8,A.DA9,A.DG10
1qdf	[1,6,10,15], [2,5,11,14] A.DG1,A.DG15,A.DG10,A.DG6 A.DG2,A.DG14,A.DG11,A.DG5	["1,2,l,5,6,l,10,11,l,14,15"] loop#1 type=lateral strands=[#1,#4] nts=2 TT A.DT3,A.DT4 loop#2 type=lateral strands=[#4,#3] nts=3 TGT A.DT7,A.DG8,A.DT9 loop#3 type=lateral strands=[#3,#2] nts=2 TT A.DT12,A.DT13
1qdh	[1,6,10,15], [2,5,11,14] A.DG15,A.DG10,A.DG6 .DG2,A.DG14,A.DG11,A.DG5	["1,2,l,5,6,l,10,11,l,14,15"] loop#1 type=lateral strands=[#1,#4] nts=2 TT A.DT3,A.DT4 loop#2 type=lateral strands=[#4,#3] nts=3 TGT A.DT7,A.DG8,A.DT9 loop#3 type=lateral strands=[#3,#2] nts=2 TT A.DT12,A.DT13
1rde	[1,6,10,15], [2,5,11,14] A.DG1,A.DG15,A.DG10,A.DG6 A.DG2,A.DG14,A.DG11,A.DG5	["1,2,l,5,6,l,10,11,l,14,15"] loop#1 type=lateral strands=[#1,#4] nts=2 TT A.DT3,A.DT4 loop#2 type=lateral strands=[#4,#3] nts=3 TGT A.DT7,A.DG8,A.DT9 loop#3 type=lateral strands=[#3,#2] nts=2 TT A.DT12,A.DT13
1xav	[4,8,13,17], [5,9,14,18], [6,10,15,19] A.DG4,A.DG8,A.DG13,A.DG17 A.DG5,A.DG9,A.DG14,A.DG18	["4,5,6,r,8,9,10,r,13,14,15,r,17,18,19"]
201d	[1,12,28,17], [2,11,27,18], [3,10,26,19], [4,9,25,20]	["1,2,3,4,l,9,10,11,12,d,17,18,19,20,l,25,26,27,28"]

2a5p	[4,8,13,17], [5,9,14,18], [6,24,15,19]	["4,5,6,r,8,9,r,13,14,15,r,17,18,19,d,24"]
2e4i	[2,8,16,20], [3,9,15,21], [4,10,14,22]	["2,3,4,r,8,9,10,l,14,15,16,l,20,21,22"]
2kpr	[1,6,17,13], [2,5,16,12], [7,11,14,18]	["1,2,l,5,6,7,l,11,r,12,13,14,r,16,17,18"]
2m53	[4,11,14,19], [5,7,15,20], [6,8,16,21]	["4,5,6,r,7,8,r,11,l,14,15,16,r,19,20,21"]
2m90	[1,17,30,24], [18,21,25,31], [19,22,26,32]	["1,l,17,18,19,r,21,22,r,24,25,26,r,30,31,32"]
2m92	[2, 6, 10, 13], [3, 7, 14, 33], [4, 8, 15, 34]	["2,3,4,r,6,7,8,r,10,l,13,14,15,r,33,34"]
2m6v	[1, 8, 13, 18], [2, 7, 14, 17]	["1,2,l,7,8,d,13,14,l,17,18"]
2mft	[1, 10, 14, 19], [2, 9, 13, 20], [3, 8, 12, 21]	["1,2,3,d,8,9,10,r,12,13,14,d,19,20,21"]
2n6c	[4, 8, 13, 17], [5, 9, 14, 18], [6, 15, 19, 24]	["4,5,6,r,8,9,r,13,14,15,r,17,18,19,d,24"]
5j6u	[1, 11, 16, 25], [2, 10, 17, 24], [3, 9, 18, 23], [4, 8, 19, 22]	["1,2,3,4,l,8,9,10,11,d,16,17,18,19,l,22,23,24,25"]
5mtg	[3, 10, 25, 30], [4, 11, 24, 31], [5, 12, 23, 32]	["3,4,5,r,10,11,12,d,23,24,25,l,30,31,32"]
5ov2	[3, 8, 14, 22], [2, 7, 15, 21], [1, 6, 16, 20]	["1,2,3,r,6,7,8,d,14,15,16,l,20,21,22"]
6suu	[2, 6, 11, 25], [3, 7, 12, 26], [4, 13, 27, 32]	["2,3,4,r,6,7,r,11,12,13,r,25,26,27,d,32"]
6zte	[18, 22, 25, 29], [19, 23, 26, 30], [20, 27, 31, 36]	["18,19,20,r,22,23,r,25,26,27,r,29,30,31,d,36"]
2mgn	[4, 8, 13, 17], [5, 9, 14, 18], [6, 15, 19, 24]	["4,5,6,r,8,9,r,13,14,15,r,17,18,19,d,24"]
6e84	[12, 15, 22, 25], [13, 16, 23, 26]	["12,13,r,15,16,r,22,23,r,25,26"]
6t2g	[2, 6, 11, 26], [3, 7, 12, 27], [4, 9, 13, 28]	["2,3,4,r,6,7,9,r,11,12,13,r,26,27,28"]
5ob3	[15, 19, 49, 53], [16, 20, 46, 51]	["15,16,r,19,20,d,46,49,r,51,53"]

Pdb Files used for evaluation classified According to the ONZ Classification

DNAs

NNN 13 ['pdb143d', 'pdb2lod', 'pdb2mcc', 'pdb2mco', 'pdb5j05', 'pdb5mcr', 'pdb5mta', 'pdb5mtg', 'pdb5ov2', 'pdb6f4z', 'pdb6ffr', 'pdb6l92', 'pdb6yep'] (21, 25, 27, 39, 48–53)

OO 29 ['pdb148d', 'pdb1bub', 'pdb1c32', 'pdb1c34', 'pdb1c35', 'pdb1c38', 'pdb1hao', 'pdb1hap', 'pdb1hut', 'pdb1qdf', 'pdb1qdh', 'pdb1rde', 'pdb2idn', 'pdb2km3', 'pdb2lyg', 'pdb2m8z', 'pdb2mfu', 'pdb2mwz', 'pdb2n60', 'pdb4wb2', 'pdb4wb3', 'pdb5mjx', 'pdb6eo6', 'pdb6eo7', 'pdb6fc9', 'pdb6gh0', 'pdb6k3y', 'pdb6v0l', 'pdb7cv4'] (24, 54–74)

OOO 79 ['pdb186d', 'pdb1k8p', 'pdb1kf1', 'pdb1xav', 'pdb2e4i', 'pdb2f8u', 'pdb2gku', 'pdb2hy9', 'pdb2jpz', 'pdb2jsk', 'pdb2jsl', 'pdb2jsm', 'pdb2jsq', 'pdb2kqg', 'pdb2kqh', 'pdb2kyp', 'pdb2kzd', 'pdb2kze', 'pdb2l7v', 'pdb2l88', 'pdb2lby', 'pdb2ld8', 'pdb2lee', 'pdb2lk7', 'pdb2lpw', 'pdb2lxq', 'pdb2m27', 'pdb2m4p', 'pdb2m53', 'pdb2m93', 'pdb2may', 'pdb2mb2', 'pdb2mb3', 'pdb2mbj', 'pdb2n4y', 'pdb3r6r', 'pdb3sc8', 'pdb3t5e', 'pdb3uyh', 'pdb4da3', 'pdb4daq', 'pdb4fxm', 'pdb4g0f', 'pdb5ccw', 'pdb5i2v', 'pdb5lig', 'pdb5mbr', 'pdb5mvb', 'pdb5nys', 'pdb5nyt', 'pdb5nyu', 'pdb5w77', 'pdb5yey', 'pdb5z80', 'pdb6ac7', 'pdb6ccw', 'pdb6erl', 'pdb6h5r', 'pdb6ia0', 'pdb6ia4', 'pdb6ip3', 'pdb6ip7', 'pdb6isw', 'pdb6jj0', 'pdb6jkn', 'pdb6jwd', 'pdb6jwe', 'pdb6kfi', 'pdb6kfj', 'pdb6neb', 'pdb6o2l', 'pdb6r9k', 'pdb6r9l', 'pdb6t2g', 'pdb6t51', 'pdb6zl2', 'pdb6zl9', 'pdb7cls', 'pdb7cv3']

(23, 25, 30, 31, 36–38, 44, 64, 73, 75–123)

ZZ 1 ['pdb1i34'](124)

OOOO 9 ['pdb1oz8', 'pdb2ms9', 'pdb2n2d', 'pdb2n3m', 'pdb4u5m', 'pdb5oph', 'pdb6gz6', 'pdb6jce', 'pdb6kvb'] (34, 35, 40, 124–130)

NNNN 3 ['pdb201d', 'pdb2m6w', 'pdb5j6u'] (42, 50)

OOZ 6 ['pdb2a5p', 'pdb2a5r', 'pdb2mgn', 'pdb2n6c', 'pdb6zte', 'pdb6suu'] (44, 121, 131–133)

NN 11 ['pdb2kf7', 'pdb2kf8', 'pdb2kka', 'pdb2kow', 'pdb2m6v', 'pdb2m91', 'pdb5j4p', 'pdb5j4w', 'pdb5lqg', 'pdb5lqh', 'pdb6gzn'] (32, 50, 134–137)

NNO 7 ['pdb2kpr', 'pdb5o4d', 'pdb6l8m', 'pdb6rs3', 'pdb6tc8', 'pdb6tcg', 'pdb6ycv'] (22, 26, 27, 45, 51, 138)

NOO 1 ['pdb2m90'] (64)

ONN 2 ['pdb2m92', 'pdb2o3m'] (64, 139)

ZZZ 1 ['pdb2mft'] (140)

ZZO 2 ['pdb5zev', 'pdb6h1k'] (41, 141)

ZO 1 ['pdb6jcd'] (142)

RNAs

[pdb1s9l, pdb2la5, pdb3ibk, pdb4kzd, pdb4kze, pdb4q9q, pdb4q9r, pdb4wb2, pdb4wb3, pdb5ob3, pdb6e80, pdb6e81, pdb6e84, pdb6e8u, pdb6ffr, pdb6k84, pdb6pq7] (24, 28, 43, 143–151)

Pdb structures used for evaluation and not containing G4s

1a1t, 176d, 168d, 165d, 157d, 124d, 1ap1, 110d, 189d, 187d, 184d, 159d, 138d, 118d, 117d, 116d, 113d, 111d, 103d (152–165)(166)

ONZ Classifications

NNN 13 ['pdb143d', 'pdb2lod', 'pdb2mcc', 'pdb2mco', 'pdb5j05', 'pdb5mcr', 'pdb5mta', 'pdb5mtg', 'pdb5ov2', 'pdb6f4z', 'pdb6ffr', 'pdb6l92', 'pdb6yep']
pdb143d ['2', '3', '4', 'lateral', '8', '9', '10', 'diagonal', '14', '15', '16', 'lateral', '20', '21', '22']
pdb2lod ['1', '2', '3', 'reversal', '6', '7', '8', 'diagonal', '14', '15', '16', 'lateral', '20', '21', '22']
pdb2mcc ['2', '3', '4', 'lateral', '8', '9', '10', 'diagonal', '14', '15', '16', 'lateral', '20', '21', '22']
pdb2mco ['2', '3', '4', 'lateral', '8', '9', '10', 'diagonal', '14', '15', '16', 'lateral', '20', '21', '22']
pdb5j05 ['1', '2', '3', 'lateral', '7', '8', '9', 'diagonal', '14', '15', '16', 'lateral', '18', '19', '20']
pdb5mcr ['1', '2', '3', 'reversal', '6', '7', '8', 'diagonal', '14', '15', '16', 'lateral', '20', '21', '22']
pdb5mta ['3', '4', '5', 'reversal', '10', '11', '12', 'diagonal', '23', '24', '25', 'lateral', '30', '31', '32']
pdb5mtg ['3', '4', '5', 'reversal', '10', '11', '12', 'diagonal', '23', '24', '25', 'lateral', '30', '31', '32']
pdb5ov2 ['1', '2', '3', 'reversal', '6', '7', '8', 'diagonal', '14', '15', '16', 'lateral', '20', '21', '22']
pdb6f4z ['1', '2', '3', 'lateral', '6', '7', '8', 'diagonal', '14', '15', '16', 'lateral', '20', '21', '22']
pdb6ffr__ ['1', '2', '3', 'reversal', '6', '7', '8', 'diagonal', '14', '15', '16', 'lateral', '20', '21', '22']
pdb6l92 ['1', '2', '3', 'lateral', '9', '10', '11', 'diagonal', '16', '17', '18', 'reversal', '20', '21', '22']
pdb6yep ['1', '2', '3', 'lateral', '6', '7', '8', 'diagonal', '14', '15', '16', 'lateral', '20', '21', '22']

OO 29 ['pdb148d', 'pdb1bub', 'pdb1c32', 'pdb1c34', 'pdb1c35', 'pdb1c38', 'pdb1hao_', 'pdb1hap', 'pdb1hut', 'pdb1qdf', 'pdb1qdh', 'pdb1rde', 'pdb2idn', 'pdb2km3', 'pdb2lyg', 'pdb2m8z', 'pdb2mfu', 'pdb2mwz', 'pdb2n60', 'pdb4wb2', 'pdb4wb3', 'pdb5mjx', 'pdb6eo6', 'pdb6eo7', 'pdb6fc9', 'pdb6gh0', 'pdb6k3y', 'pdb6v0l', 'pdb7cv4']
pdb148d ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']

pdb1bub ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb1c32 ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb1c34 ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb1c35 ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb1c38 ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb1hao_ ['401', '402', 'lateral', '405', '406', 'lateral', '410', '411', 'lateral', '414', '415']
pdb1hap ['401', '402', 'lateral', '405', '406', 'lateral', '410', '411', 'lateral', '414', '415']
pdb1hut ['401', '402', 'lateral', '405', '406', 'lateral', '410', '411', 'lateral', '414', '415']
pdb1qdf ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb1qdh ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb1rde ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb2idn ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb2km3 ['3', '4', 'lateral', '9', '10', 'lateral', '15', '16', 'lateral', '21', '22']
pdb2lyg ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb2m8z ['1', '2', 'lateral', '5', '6', 'lateral', '22', '23', 'lateral', '26', '27']
pdb2mfu ['3', '4', 'lateral', '9', '10', 'lateral', '14', '15', 'reversal', '19', '20']
pdb2mwz ['4', '5', 'reversal', '10', '11', 'lateral', '15', '16', 'lateral', '22', '23']
pdb2n60 ['3', '5', 'reversal', '7', '8', 'reversal', '11', '12', 'reversal', '15', '16']
pdb4wb2 ['17', 'reversal', '18', '19', 'reversal', '22', '25', 'reversal', '26', '27', 'reversal', '32']
pdb4wb3 ['17', 'reversal', '18', '19', 'reversal', '22', '25', 'reversal', '26', '27', 'reversal', '32']
pdb5mjx ['1', '2', 'lateral', '5', '6', 'lateral', '10', '11', 'lateral', '14', '15']
pdb6eo6 ['401', '402', 'lateral', '405', '406', 'lateral', '410', '411', 'lateral', '414', '415']
pdb6eo7 ['401', '402', 'lateral', '405', '406', 'lateral', '410', '411', 'lateral', '414', '415']
pdb6fc9 ['1', '2', 'lateral', '5', '6', 'lateral', '22', '23', 'lateral', '26', '27']
pdb6gh0 ['1', '2', 'lateral', '6', '7', 'lateral', '11', '12', 'lateral', '16', '17']
pdb6k3y ['3', '4', 'reversal', '6', '7', 'reversal', '10', '11', 'reversal', '14', '15']
pdb6v0l ['4', '5', 'reversal', '8', '9', 'reversal', '11', '12', 'reversal', '15', '16']
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OOO 79 ['pdb186d', 'pdb1k8p', 'pdb1kf1', 'pdb1xav', 'pdb2e4i', 'pdb2f8u', 'pdb2gku', 'pdb2hy9', 'pdb2jpz', 'pdb2jsk', 'pdb2jsl', 'pdb2jsm', 'pdb2jsq', 'pdb2kqg', 'pdb2kqh', 'pdb2kyp', 'pdb2kzd', 'pdb2kze', 'pdb2l7v', 'pdb2l88', 'pdb2lby', 'pdb2ld8', 'pdb2lee', 'pdb2lk7', 'pdb2lpw', 'pdb2lxq', 'pdb2m27', 'pdb2m4p', 'pdb2m53', 'pdb2m93', 'pdb2may', 'pdb2mb2', 'pdb2mb3', 'pdb2mbj', 'pdb2n4y', 'pdb3r6r', 'pdb3sc8', 'pdb3t5e', 'pdb3uyh', 'pdb4da3', 'pdb4daq', 'pdb4fxm', 'pdb4g0f', 'pdb5ccw', 'pdb5i2v', 'pdb5lig', 'pdb5mbr', 'pdb5mvb', 'pdb5nys', 'pdb5nyt', 'pdb5nyu', 'pdb5w77', 'pdb5yey', 'pdb5z80', 'pdb6ac7', 'pdb6ccw', 'pdb6erl', 'pdb6h5r', 'pdb6ia0', 'pdb6ia4', 'pdb6ip3', 'pdb6ip7', 'pdb6isw', 'pdb6jj0', 'pdb6jkn', 'pdb6jwd', 'pdb6jwe', 'pdb6kfi', 'pdb6kfj', 'pdb6neb', 'pdb6o2l', 'pdb6r9k', 'pdb6r9l', 'pdb6t2g', 'pdb6t51', 'pdb6zl2', 'pdb6zl9', 'pdb7cls', 'pdb7cv3']
pdb186d ['3', '4', '5', 'lateral', '10', '11', '12', 'lateral', '16', '17', '18', 'reversal', '21', '22', '23']
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pdb1kf1 ['2', '3', '4', 'reversal', '8', '9', '10', 'reversal', '14', '15', '16', 'reversal', '20', '21', '22']
pdb1xav ['4', '5', '6', 'reversal', '8', '9', '10', 'reversal', '13', '14', '15', 'reversal', '17', '18', '19']
pdb2e4i ['2', '3', '4', 'reversal', '8', '9', '10', 'lateral', '14', '15', '16', 'lateral', '20', '21', '22']
pdb2f8u ['1', '2', '3', 'lateral', '7', '8', '9', 'lateral', '17', '18', '19', 'reversal', '21', '22', '23']
pdb2gku ['3', '4', '5', 'reversal', '9', '10', '11', 'lateral', '15', '16', '17', 'lateral', '21', '22', '23']
pdb2hy9 ['4', '5', '6', 'reversal', '10', '11', '12', 'lateral', '16', '17', '18', 'lateral', '22', '23', '24']
pdb2jpz ['4', '5', '6', 'lateral', '10', '11', '12', 'lateral', '16', '17', '18', 'reversal', '22', '23', '24']
pdb2jsk ['3', '4', '5', 'reversal', '9', '10', '11', 'lateral', '15', '16', '17', 'lateral', '21', '22', '23']
pdb2jsl ['3', '4', '5', 'lateral', '9', '10', '11', 'lateral', '15', '16', '17', 'reversal', '21', '22', '23']
pdb2jsm ['3', '4', '5', 'reversal', '9', '10', '11', 'lateral', '15', '16', '17', 'lateral', '21', '22', '23']
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pdb2kqg ['2', '3', '4', 'reversal', '6', '7', '8', 'reversal', '14', '15', '16', 'reversal', '18', '19', '20']

pdb2kqh ['2', '3', '4', 'reversal', '6', '7', '8', 'reversal', '14', '15', '16', 'reversal', '18', '19', '20']
pdb2kyp ['2', '3', '4', 'reversal', '6', '7', '8', 'reversal', '14', '15', '16', 'reversal', '18', '19', '20']
pdb2kzd ['2', '3', '4', 'lateral', '8', '9', '10', 'lateral', '13', '14', '15', 'reversal', '17', '18', '19']
pdb2kze ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '13', '14', '15', 'reversal', '17', '18', '19']
pdb2l7v ['7', '8', '9', 'reversal', '11', '12', '13', 'reversal', '16', '17', '18', 'reversal', '20', '21', '22']
pdb2l88 ['1', '2', '3', 'reversal', '7', '8', '9', 'reversal', '11', '12', '13', 'reversal', '17', '18', '19']
pdb2lby ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '12', '13', '14', 'reversal', '16', '17', '18']
pdb2ld8 ['3', '4', '5', 'reversal', '9', '10', '11', 'reversal', '15', '16', '17', 'reversal', '21', '22', '23']
pdb2lee ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '11', '12', '13', 'reversal', '15', '16', '17']
pdb2lk7 ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '11', '12', '13', 'reversal', '15', '16', '17']
pdb2lpw ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '19', '20', '21', 'reversal', '23', '24', '25']
pdb2lxq ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '12', '13', '14', 'reversal', '16', '17', '18']
pdb2m27 ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '14', '15', '16', 'reversal', '18', '19', '20']
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pdb2m53 ['4', '5', '6', 'reversal', '7', '8', 'reversal', '11', 'lateral', '14', '15', '16', 'reversal', '19', '20', '21']
pdb2m93 ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '25', '26', '27', 'reversal', '29', '30', '31']
pdb2may ['3', '4', '5', 'reversal', '9', '10', '11', 'lateral', '15', '16', '17', 'lateral', '21', '22', '23']
pdb2mb2 ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '11', '12', '13', 'reversal', '15', '16', '17']
pdb2mb3 ['3', '4', '5', 'reversal', '9', '10', '11', 'lateral', '15', '16', '17', 'lateral', '21', '22', '23']
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pdb2n4y ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '14', '15', '16', 'reversal', '18', '20', '21']
pdb3r6r ['3', '4', '5', 'reversal', '9', '10', '11', 'reversal', '15', '16', '17', 'reversal', '21', '22', '23']
pdb3sc8 ['2', '3', '4', 'reversal', '8', '9', '10', 'reversal', '14', '15', '16', 'reversal', '20', '21', '22']
pdb3t5e ['2', '3', '4', 'reversal', '8', '9', '10', 'reversal', '14', '15', '16', 'reversal', '20', '21', '22']
pdb3uyh ['2', '3', '4', 'reversal', '8', '9', '10', 'reversal', '14', '15', '16', 'reversal', '20', '21', '22']
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pdb4fxm ['2', '3', '4', 'reversal', '8', '9', '10', 'reversal', '14', '15', '16', 'reversal', '20', '21', '22']
pdb4g0f ['2', '3', '4', 'reversal', '8', '9', '10', 'reversal', '14', '15', '16', 'reversal', '20', '21', '22']
pdb5ccw ['3', '4', '5', 'reversal', '9', '10', '11', 'reversal', '15', '16', '17', 'reversal', '21', '22', '23']
pdb5i2v ['2', '3', '4', 'reversal', '6', '7', '9', 'reversal', '11', '12', '13', 'reversal', '18', '19', '20']
pdb5lig ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '12', '13', '14', 'reversal', '16', '17', '18']
pdb5mbr ['3', '4', '5', 'reversal', '9', '10', '11', 'lateral', '15', '16', '17', 'lateral', '21', '22', '23']
pdb5mvb ['4', '5', '6', 'lateral', '10', '11', '12', 'lateral', '16', '17', '18', 'reversal', '22', '23', '24']
pdb5nys ['3', '4', '5', 'reversal', '8', '9', '10', 'reversal', '12', '13', '14', 'reversal', '17', '18', '19']
pdb5nyt ['3', '4', '5', 'reversal', '8', '9', '10', 'reversal', '12', '13', '14', 'reversal', '17', '18', '19']
pdb5nyu ['3', '4', '5', 'reversal', '8', '9', '10', 'reversal', '12', '13', '14', 'reversal', '17', '18', '19']
pdb5w77 ['7', '8', '9', 'reversal', '11', '12', '13', 'reversal', '16', '17', '18', 'reversal', '20', '21', '22']
pdb5yey ['1', '2', '3', 'lateral', '7', '8', '9', 'lateral', '13', '14', '15', 'lateral', '19', '20', '21']
pdb5z80 ['4', '5', '6', 'reversal', '10', '11', '12', 'lateral', '16', '17', '18', 'lateral', '22', '23', '24']
pdb6ac7 ['3', '4', '5', 'lateral', '9', '11', '12', 'lateral', '15', '16', '17', 'reversal', '21', '22', '23']
pdb6ccw ['4', '5', '6', 'lateral', '10', '11', '12', 'lateral', '16', '17', '18', 'reversal', '22', '23', '24']
pdb6erl ['4', '5', '6', 'reversal', '8', '9', '10', 'reversal', '13', '14', '15', 'reversal', '17', '18', '19']
pdb6h5r ['3', '4', '5', 'reversal', '9', '10', '11', 'reversal', '15', '16', '17', 'reversal', '21', '22', '23']
pdb6ia0 ['3', '4', '5', 'lateral', '9', '10', '11', 'lateral', '15', '16', '17', 'reversal', '21', '22', '23']
pdb6ia4 ['3', '4', '5', 'reversal', '9', '10', '11', 'lateral', '15', '16', '17', 'lateral', '21', '22', '23']
pdb6ip3 ['2', '3', '4', 'reversal', '8', '9', '10', 'reversal', '14', '15', '16', 'reversal', '20', '21', '22']
pdb6ip7 ['2', '3', '4', 'reversal', '8', '9', '10', 'reversal', '14', '15', '16', 'reversal', '20', '21', '22']
pdb6isw ['2', '3', '4', 'reversal', '8', '9', '10', 'reversal', '14', '15', '16', 'reversal', '20', '21', '22']
pdb6jj0 ['7', '8', '9', 'reversal', '11', '12', '13', 'reversal', '16', '17', '18', 'reversal', '20', '21', '22']
pdb6jkn ['1', '2', '3', 'lateral', '7', '8', '9', 'lateral', '13', '14', '15', 'lateral', '19', '20', '21']
pdb6jwd ['1', '2', '3', 'reversal', '7', '8', '9', 'reversal', '11', '12', '13', 'reversal', '17', '18', '19']

pdb6jwe ['1', '2', '3', 'reversal', '7', '8', '9', 'reversal', '11', '12', '13', 'reversal', '17', '18', '19']
pdb6kfi ['4', '5', '6', 'reversal', '10', '11', '12', 'lateral', '16', '17', '18', 'lateral', '22', '23', '24']
pdb6kfj ['4', '5', '6', 'lateral', '10', '11', '12', 'lateral', '16', '17', '18', 'reversal', '22', '23', '24']
pdb6neb ['3', '4', '5', 'reversal', '7', '8', '9', 'reversal', '16', '17', '18', 'reversal', '20', '21', '22']
pdb6o2l ['7', '8', '9', 'reversal', '11', '12', '13', 'reversal', '16', '17', '18', 'reversal', '20', '21', '22']
pdb6r9k ['5', '6', '7', 'lateral', '11', '12', '13', 'reversal', '15', '16', '17', 'reversal', '19', '20', '21']
pdb6r9l ['5', '6', '7', 'lateral', '11', '12', '13', 'reversal', '15', '16', '17', 'reversal', '19', '20', '21']
pdb6t2g ['2', '3', '4', 'reversal', '6', '7', '9', 'reversal', '11', '12', '13', 'reversal', '26', '27', '28']
pdb6t51 ['2', '3', '4', 'reversal', '6', '7', '9', 'reversal', '11', '12', '13', 'reversal', '18', '19', '20']
pdb6zl2 ['4', '5', '6', 'reversal', '8', '9', '10', 'reversal', '13', '14', '15', 'reversal', '17', '18', '19']
pdb6zl9 ['18', '19', '20', 'reversal', '22', '23', '24', 'reversal', '27', '28', '29', 'reversal', '31', '32', '33']
pdb7cls ['3', '4', '20', 'reversal', '22', '23', '24', 'reversal', '26', '27', '28', 'reversal', '30', '31', '32']
pdb7cv3 ['3', '4', '5', 'reversal', '7', '8', '9', 'lateral', '20', '21', '22', 'lateral', '25', '26', '27']

ZZ 1 ['pdb1i34']
pdb1i34 ['1', '2', 'diagonal', '7', '8', 'reversal', '11', '12', 'diagonal', '18', '19']

OOOO 9 ['pdb1oz8', 'pdb2ms9', 'pdb2n2d', 'pdb2n3m', 'pdb4u5m', 'pdb5oph', 'pdb6gz6', 'pdb6jce', 'pdb6kvb']
pdb1oz8 ['1', '2', 'reversal', '4', '5', 'reversal', '7', '8', 'reversal', '10', '11', 'reversal', '13', '14', 'reversal', '16', '17', 'reversal', '19', '20', 'reversal', '22', '23']
pdb2ms9 ['2', '3', 'reversal', '5', '6', 'reversal', '8', '9', 'reversal', '11', '12', '15', 'reversal', '17', '18', 'reversal', '20', '21', 'reversal', '23', '24', 'reversal', '26']
pdb2n2d ['1', '2', '3', '4', 'lateral', '7', '8', '9', '10', 'lateral', '13', '14', '15', '16', 'lateral', '19', '20', '21', '22']
pdb2n3m ['2', '3', 'reversal', '5', '6', 'reversal', '8', '9', 'reversal', '12', '15', '17', '18', 'reversal', '20', '21', 'reversal', '23', '24', 'reversal', '26', '27']
pdb4u5m ['2', '3', 'reversal', '5', '6', 'reversal', '8', '9', 'reversal', '11', '12', '15', 'reversal', '17', '18', 'reversal', '20', '21', 'reversal', '23', '24', 'reversal', '26']
pdb5oph ['1', '2', '3', '4', 'lateral', '7', '8', '9', '10', 'lateral', '13', '14', '15', '16', 'lateral', '19', '20', '21', '22']
pdb6gz6 ['1', 'reversal', '3', '4', 'reversal', '6', '7', 'reversal', '9', '10', 'reversal', '12', '15', 'reversal', '17', '18', 'reversal', '20', '21', 'reversal', '23', '24', 'reversal', '26']
pdb6jce ['1', '2', 'reversal', '5', '6', 'reversal', '10', '11', 'reversal', '14', '15', 'reversal', '18', 'reversal', '20', '21', 'reversal', '23', '24', 'reversal', '26', '27', 'reversal', '29']
pdb6kvb ['2', 'reversal', '3', '5', '6', 'reversal', '8', '9', 'reversal', '11', '12', 'reversal', '15', '17', '18', 'reversal', '20', '21', 'reversal', '23', '24', 'lateral', '27']

NNNN 3 ['pdb201d', 'pdb2m6w', 'pdb5j6u']
pdb201d ['1', '2', '3', '4', 'lateral', '9', '10', '11', '12', 'diagonal', '17', '18', '19', '20', 'lateral', '25', '26', '27', '28']
pdb2m6w ['1', '2', '3', '4', 'lateral', '7', '8', '9', '10', 'diagonal', '15', '16', '17', '18', 'lateral', '21', '22', '23', '24']
pdb5j6u ['1', '2', '3', '4', 'lateral', '8', '9', '10', '11', 'diagonal', '16', '17', '18', '19', 'lateral', '22', '23', '24', '25']

OOZ 6 ['pdb2a5p', 'pdb2a5r', 'pdb2mgn', 'pdb2n6c', 'pdb6suu', 'pdb6zte']
pdb2a5p ['4', '5', '6', 'reversal', '8', '9', 'reversal', '13', '14', '15', 'reversal', '17', '18', '19', 'diagonal', '24']
pdb2a5r ['4', '5', '6', 'reversal', '8', '9', 'reversal', '13', '14', '15', 'reversal', '17', '18', '19', 'diagonal', '24']
pdb2mgn ['4', '5', '6', 'reversal', '8', '9', 'reversal', '13', '14', '15', 'reversal', '17', '18', '19', 'diagonal', '24']
pdb2n6c ['4', '5', '6', 'reversal', '8', '9', 'reversal', '13', '14', '15', 'reversal', '17', '18', '19', 'diagonal', '24']
pdb6suu ['2', '3', '4', 'reversal', '6', '7', 'reversal', '11', '12', '13', 'reversal', '25', '26', '27', 'diagonal', '32']
pdb6zte ['18', '19', '20', 'reversal', '22', '23', 'reversal', '25', '26', '27', 'reversal', '29', '30', '31', 'diagonal', '36']

NN 11 ['pdb2kf7', 'pdb2kf8', 'pdb2kka', 'pdb2kow', 'pdb2m6v', 'pdb2m91', 'pdb5j4p', 'pdb5j4w', 'pdb5lqg', 'pdb5lqh', 'pdb6gzn']
pdb2kf7 ['1', '2', 'lateral', '7', '8', 'diagonal', '14', '15', 'lateral', '19', '20']
pdb2kf8 ['1', '2', 'lateral', '7', '8', 'diagonal', '14', '15', 'lateral', '19', '20']
pdb2kka ['2', '3', 'lateral', '8', '9', 'diagonal', '15', '16', 'lateral', '20', '21']
pdb2kow ['3', '4', 'lateral', '8', '9', 'diagonal', '14', '15', 'lateral', '19', '20']
pdb2m6v ['1', '2', 'lateral', '7', '8', 'diagonal', '13', '14', 'lateral', '17', '18']
pdb2m91 ['1', '2', 'lateral', '6', '7', 'diagonal', '25', '26', 'lateral', '29', '30']
pdb5j4p ['1', '2', 'lateral', '6', '7', 'diagonal', '12', '13', 'lateral', '17', '18']
pdb5j4w ['1', '2', 'lateral', '6', '7', 'diagonal', '12', '13', 'lateral', '16', '17']
pdb5lqg ['3', '4', 'lateral', '9', '10', 'diagonal', '16', '17', 'lateral', '21', '22']
pdb5lqh ['3', '4', 'lateral', '9', '10', 'diagonal', '16', '17', 'lateral', '21', '22']
pdb6gzn ['1', '2', 'lateral', '6', '7', 'diagonal', '13', '14', 'lateral', '18', '19']

NNO 7 ['pdb2kpr', 'pdb5o4d', 'pdb6l8m', 'pdb6rs3', 'pdb6tc8', 'pdb6tcg', 'pdb6ycv']
pdb2kpr ['1', '2', 'lateral', '5', '6', '7', 'lateral', '11', 'reversal', '12', '13', '14', 'reversal', '16', '17', '18']
pdb5o4d ['1', '2', 'lateral', '6', '7', '8', 'lateral', '11', 'reversal', '12', '13', '14', 'reversal', '20', '21', '22']
pdb6l8m ['1', '2', 'lateral', '9', '10', '11', 'lateral', '14', 'reversal', '16', '17', '18', 'reversal', '20', '21', '22']
pdb6rs3 ['1', '2', 'lateral', '6', '7', '8', 'lateral', '14', 'reversal', '15', '16', '17', 'reversal', '20', '21', '22']
pdb6tc8 ['1', '2', 'lateral', '6', '7', '8', 'lateral', '14', 'reversal', '15', '16', '17', 'reversal', '20', '21', '22']
pdb6tcg ['1', '2', 'lateral', '6', '7', '8', 'lateral', '14', 'reversal', '15', '16', '17', 'reversal', '20', '21', '22']
pdb6ycv ['1', '2', 'lateral', '6', '7', '8', 'lateral', '14', 'reversal', '15', '16', '17', 'reversal', '20', '21', '22']

NOO 1 ['pdb2m90']
pdb2m90 ['1', 'lateral', '17', '18', '19', 'reversal', '21', '22', 'reversal', '24', '25', '26', 'reversal', '30', '31', '32']

ONN 2 ['pdb2m92', 'pdb2o3m']
pdb2m92 ['2', '3', '4', 'reversal', '6', '7', '8', 'reversal', '10', 'lateral', '13', '14', '15', 'reversal', '33', '34']
pdb2o3m ['2', '3', '4', 'reversal', '6', '7', '8', 'reversal', '10', 'lateral', '13', '14', '15', 'reversal', '21', '22']

ZZZ 1 ['pdb2mft']
pdb2mft ['1', '2', '3', 'diagonal', '8', '9', '10', 'reversal', '12', '13', '14', 'diagonal', '19', '20', '21']

ZZO 2 ['pdb5zev', 'pdb6h1k']
pdb5zev ['1', '2', 'diagonal', '9', '10', '11', 'reversal', '13', '15', '16', 'lateral', '20', 'reversal', '21', '22', '23']
pdb6h1k ['1', '2', 'diagonal', '15', '16', '17', 'reversal', '19', '20', '21', 'lateral', '25', 'reversal', '26', '27', '28']

ZO 1 ['pdb6jcd']
pdb6jcd ['2', '3', 'lateral', '6', 'reversal', '8', '9', 'lateral', '13', '14', 'diagonal', '19']

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