

# Supporting information

This supplementary information file contains the following:

- Algorithm 1: Side chain filtering and total partial loop conformation energy
- Table S1: Energy sampling comparison between the DiSGro algorithm and PETALS on the LoopBuilder dataset. Includes the case where PETALS samples with the DiSGro energy function.
- Table S2: Full data table of sampling results of PETALS and the DiSGro algorithm on each target of the LoopBuilder set
- Figure S1: Plots of the (DiSGro energy, RMSD) pairs of the lowest DiSGro energy conformation sampled by the DiSGro algorithm and PETALS for each loop target of the LoopBuilder set, by loop length.

## Algorithm 1: Side chain filtering and total partial loop conformation energy

All energies  $E$  are evaluated on the energy function chosen by the user

Let  $E^{bb}$  denote the total energy of the backbone, i.e. the N, C $_{\alpha}$ , C, O, and C $_{\beta}$  atoms

For each partial loop of length  $l_0 + 1$  with backbone energy  $E^{bb}$ :

Sample a maximum of  $n_{rot}$  rotamers for residue  $l_0 + 1$ ,

with probability of rotamer  $i$  selected  $\propto \exp(-E_i^{rot})$  without replacement

For  $j = 1, 2, \dots, n_{rot}$

Attach side chain rotamer  $j$  on residue  $l_0 + 1$  and let  $E_j^{rot}$  denote its energy

If  $l_0 = 0$

Save rotamer  $j$  as a side chain rotamer combination for residue 1

If  $l_0 > 0$

For  $k = 1, 2, \dots, n_{sc}$

Attach saved side chain rotamer combination  $k$  on residues 1 to  $l_0$

and let  $E_k^{tot}$  be its total energy

Calculate the two interaction energies:

$E_k^{bbsc}$  = energy of res  $l_0 + 1$  backbone with rotamer combination  $k$  on 1 to  $l_0$

$E_{j,k}^{scsc}$  = energy of rotamer  $j$  on  $l_0 + 1$  with rotamer combination  $k$  on 1 to  $l_0$

The total side chain energy of this combination is

$$E_{j,k}^{tot} = E_j^{rot} + E_k^{tot} + E_k^{bbsc} + E_{j,k}^{scsc}$$

Endfor

Select lowest  $n_{sc}$  energies to be saved side chain rotamer combinations for res 1 to  $l_0 + 1$

Endif

Endfor

The total energy of the partial loop conformation is  $E^{bb} + \min(E_{j,k}^{tot})$

Endfor

**Table S1.** Energy sampling comparison between the DiSGro algorithm and PETALS on the LoopBuilder dataset. Columns 3-7 represent respectively: average minimum DiSGro energy found by PETALS sampling with the DiSGro energy function, average minimum DiSGro energy found by PETALS sampling with the DiSGro+BBT energy function, average minimum energy found by the DiSGro algorithm, average DiSGro energy of the native loop conformations, number of cases where the minimum DiSGro energy found by PETALS is lower than that found by the DiSGro algorithm.

Length	Targets	PETALS <sup>1</sup>	PETALS <sup>2</sup>	DiSGro	Native	PETALS < DiSGro <sup>3</sup>
8	63	-467	-458	-398	-453	61 (out of 63)
9	56	-529	-517	-432	-530	55 (out of 56)
10	40	-589	-571	-438	-595	40 (out of 40)
11	54	-595	-565	-422	-582	54 (out of 54)
12	40	-652	-628	-445	-663	40 (out of 40)
13	40	-710	-683	-443	-727	40 (out of 40)

<sup>1</sup>: sampled with DiSGro energy

<sup>2</sup>: sampled with DiSGro+BBT energy

<sup>3</sup>: using PETALS results from column 4 for the comparison

**Table S2.** Energy and RMSD comparison between PETALS and the DiSGro algorithm, on each target of the LoopBuilder set. "MinE" is the lowest DiSGro energy conformation sampled, and "RMSD of MinE" is the RMSD to native of that conformation. The DiSGro energy of the native loop conformation is also shown. For sampling, PETALS uses the DiSGro+BBT energy function following the conclusion of Section 3.2.

Loop		PETALS		DiSGro		Native
Protein	Residues	MinE	RMSD of MinE	MinE	RMSD of MinE	Energy
135l	84-91	-507.31	0.37	-482.74	0.70	-540.43
1a3c	92-99	-360.13	1.72	-315.51	0.80	-374.92
1a62	71-78	-319.44	0.54	-256.77	1.77	-265.00
1a62	103-110	-378.99	1.87	-345.54	2.31	-223.62
1ads	274-281	-683.55	0.56	-526.99	1.16	-725.61
1alc	34-41	-548.01	0.68	-536.13	0.68	-583.80
1amm	81-88	-497.74	1.49	-461.11	1.55	-465.56
1amm	158-165	-416.75	1.86	-384.72	1.63	-398.72
1arb	136-143	-554.22	0.72	-363.77	1.88	-554.95
1arb	212-219	-213.06	1.49	-221.55	1.74	-253.16
1arb	249-256	-321.13	0.29	-266.55	0.72	-317.78
1aru	234-241	-585.61	0.45	-552.87	0.76	-609.54
1btkA	67-74	-353.89	1.27	-326.42	2.76	-339.13
1btkA	133-140	-390.82	1.00	-304.01	8.91	-251.18
1btl	50-57	-323.92	0.97	-286.35	0.85	-322.46
1c52	97-104	-580.22	0.75	-531.55	1.20	-600.82
1cex	73-80	-396.73	2.08	-415.05	3.83	-536.57
1clc	313-320	-740.49	0.57	-629.12	0.80	-757.71
1cvl	148-155	-469.88	2.10	-434.38	1.85	-394.74
1cvl	229-236	-344.01	2.10	-330.86	1.81	-296.55
1ddt	127-134	-557.21	0.74	-459.52	2.37	-533.11
1ezm	92-99	-491.85	0.66	-463.58	0.32	-480.90
1fnd	262-269	-780.62	0.33	-754.88	0.32	-771.80
1gof	606-613	-489.86	2.80	-448.00	0.34	-513.86
1hbq	31-38	-409.59	2.66	-314.30	2.34	-408.37
1iab	48-55	-443.88	0.77	-293.53	2.82	-470.57
1lit	82-89	-524.91	1.21	-413.97	1.85	-542.56
1lst	101-108	-381.81	0.54	-293.14	2.69	-379.59
1mpp	74-81	-441.84	1.46	-396.23	2.92	-386.11
1mrp	68-75	-499.57	0.37	-406.58	0.85	-467.48
1msi	26-33	-475.73	2.86	-391.47	1.64	-433.89
1nar	192-199	-652.36	0.99	-596.01	1.44	-641.75
1nfp	118-125	-394.71	0.73	-361.23	2.00	-397.40
1nif	221-228	-379.05	1.62	-359.20	3.68	-390.51
1nif	279-286	-608.75	1.04	-493.65	0.97	-585.79
1nls	97-104	-364.62	1.03	-241.60	1.36	-382.09
1nwpA	84-91	-407.07	0.43	-395.20	0.83	-436.00
1oyc	80-87	-564.04	0.87	-517.67	0.81	-603.74
1poa	71-78	-358.80	1.99	-337.19	2.08	-341.25

1ppn	191-198	-370.26	3.07	-305.10	1.68	-365.13
1prn	150-157	-241.03	0.51	-190.96	2.60	-223.05
1rro	18-25	-493.74	0.51	-452.39	3.37	-480.02
1sbp	107-114	-783.46	0.67	-625.75	0.47	-805.50
1thw	18-25	-324.55	1.14	-285.20	2.55	-297.67
1tml	187-194	-580.22	1.00	-517.49	1.09	-649.30
1wer	824-831	-465.04	0.48	-364.70	1.38	-447.60
1wer	916-923	-394.30	1.46	-382.26	1.62	-344.62
1xnb	99-106	-475.52	1.38	-418.79	1.48	-496.05
2arcA	28-35	-546.13	2.88	-476.07	3.42	-457.16
2ayh	123-130	-494.77	1.53	-470.00	1.92	-442.38
2ayh	124-131	-389.31	0.66	-369.38	0.60	-340.03
2ayh	194-201	-350.82	1.79	-320.66	1.04	-348.65
2cmd	270-277	-428.59	1.12	-382.25	0.93	-391.25
2ctc	53-60	-267.67	2.24	-215.85	2.47	-256.96
2exo	262-269	-450.83	0.65	-404.95	0.74	-487.23
2sga	32-43	-394.47	3.31	-344.89	1.65	-413.36
3nul	36-43	-505.84	0.95	-493.37	1.82	-487.06
3seb	40-47	-443.72	0.79	-316.71	1.05	-428.45
5p21	45-52	-477.75	0.70	-373.91	0.62	-502.49
5ptp	22-29	-527.43	2.76	-475.76	2.71	-503.14
5ptp	172-179	-534.82	0.82	-440.79	1.64	-564.13
7rsa	64-71	-251.79	3.28	-214.19	3.26	-277.51
8dfr	65-72	-466.63	2.42	-314.41	2.67	-532.01
<b>Length 8 averages</b>		<b>-458.27</b>	<b>1.30</b>	<b>-397.85</b>	<b>1.78</b>	<b>-452.69</b>
1aac	58-66	-343.78	2.54	-296.00	2.81	-347.05
1aba	69-77	-572.18	1.10	-550.61	2.30	-627.53
1amp	57-65	-443.78	0.78	-408.08	1.77	-417.99
1arb	90-98	-347.09	1.22	-310.16	2.03	-315.45
1arb	168-176	-425.58	3.74	-383.48	2.62	-419.73
1arp	127-135	-542.54	0.53	-481.69	1.39	-583.75
1aru	36-44	-601.36	5.81	-398.13	2.96	-693.05
1btl	102-110	-510.78	2.63	-278.13	1.10	-518.67
1byb	246-254	-774.08	0.89	-637.10	1.84	-734.82
1cseE	95-103	-392.03	8.20	-351.89	2.72	-354.91
1csh	252-260	-709.76	0.46	-638.58	0.53	-780.07
1ede	257-265	-493.94	1.32	-270.28	2.59	-560.84
1fus	91-99	-372.97	3.42	-326.63	3.26	-348.36
1fus	31-39	-463.37	4.64	-451.96	3.44	-478.66
1gpr	63-71	-641.75	2.92	-551.75	2.35	-729.11
1isuA	30-38	-232.08	3.93	-222.42	5.80	-189.51
1ivd	244-252	-395.95	2.33	-340.97	4.36	-247.99
1lkkA	142-150	-396.52	1.34	-363.36	0.96	-421.20
1lkkA	193-201	-618.33	0.97	-528.60	1.22	-611.00
1mla	194-202	-502.57	2.82	-412.79	4.55	-515.50

1mrj	92-100	-631.80	0.90	-587.26	1.36	-631.86
1mrk	53-61	-570.28	2.51	-482.35	1.01	-626.55
1mrp	284-292	-431.52	1.26	-406.99	2.04	-383.75
1nfp	12-20	-648.68	1.27	-558.43	5.65	-470.79
1nif	266-274	-599.96	0.76	-544.61	1.11	-625.38
1nls	131-139	-479.58	0.55	-362.37	2.34	-456.28
1noa	76-84	-617.07	1.51	-492.37	2.00	-575.87
1noa	9-17	-388.56	1.14	-375.77	0.79	-385.63
1noa	99-107	-194.44	1.21	-176.74	4.51	-173.75
1npk	102-110	-463.22	0.75	-391.34	0.99	-465.20
1onc	70-78	-378.38	2.65	-331.45	2.32	-389.91
1pda	108-116	-732.61	1.02	-609.67	0.54	-718.73
1pgs	117-125	-539.90	0.95	-443.00	2.39	-631.86
1php	91-99	-466.17	0.43	-401.33	0.61	-474.64
1ptf	10-18	-414.00	1.02	-373.34	1.77	-427.46
1ra9	142-150	-328.19	2.75	-279.55	2.45	-331.99
1rhs	216-224	-377.98	5.24	-285.41	5.40	-416.55
1sgpE	109-117	-379.53	1.69	-344.90	3.25	-337.66
1tca	170-178	-557.35	1.98	-497.37	1.28	-650.06
1tca	217-225	-659.32	1.75	-396.98	3.30	-660.95
1wer	942-950	-422.35	2.34	-391.60	1.76	-470.35
1xif	59-67	-386.76	0.38	-310.52	2.83	-397.13
1xnb	133-141	-394.67	0.55	-333.01	1.93	-411.09
1xnb	116-124	-435.89	2.87	-369.00	1.80	-426.43
1xyzA	568-576	-651.21	1.29	-504.78	1.56	-661.16
1xyzA	795-803	-1025.92	1.22	-797.86	1.82	-1146.29
2ayh	169-177	-428.92	2.30	-383.19	1.15	-498.18
2cpl	24-32	-660.95	0.52	-531.20	1.07	-752.35
2eng	172-180	-819.02	1.29	-678.66	2.28	-874.49
2hbg	18-26	-424.53	0.42	-376.14	1.44	-460.94
2sil	183-191	-761.73	1.79	-696.84	2.09	-916.44
3pte	78-86	-612.41	0.79	-515.08	0.71	-672.56
3pte	107-115	-1088.02	0.32	-836.84	0.97	-1132.00
3pte	215-223	-301.79	1.52	-295.38	2.24	-271.25
3tgl	56-64	-506.56	2.63	-323.41	2.23	-421.10
4gcr	94-102	-397.51	3.91	-321.14	2.54	-453.49
<b>Length 9 averages</b>		<b>-517.09</b>	<b>1.91</b>	<b>-432.29</b>	<b>2.22</b>	<b>-530.27</b>
135l	18-27	-771.76	0.81	-539.30	2.92	-829.98
1ads	171-180	-531.99	3.65	-381.40	1.80	-562.08
1ads	170-179	-575.05	1.40	-401.09	1.92	-566.06
1amp	181-190	-497.60	2.12	-377.56	2.85	-559.19
1arb	41-50	-684.04	1.67	-566.23	1.11	-744.04
1arp	37-46	-647.09	1.81	-527.18	5.87	-730.81
1aru	128-137	-821.07	0.50	-677.44	1.02	-862.39
1avmA	145-154	-539.66	4.72	-396.03	2.30	-523.69

1btl	170-179	-407.16	1.94	-279.36	1.71	-373.00
1dim	87-96	-505.29	2.18	-330.28	3.13	-526.53
1dim	131-140	-633.38	2.47	-508.37	2.51	-726.05
1ede	164-173	-758.61	2.08	-497.34	4.69	-753.05
1edg	269-278	-660.36	0.93	-517.56	0.74	-667.36
1ezm	237-246	-817.37	0.89	-643.81	1.37	-920.81
1fkf	63-72	-642.56	4.33	-509.78	1.03	-757.68
1gpr	133-142	-610.47	1.84	-536.42	2.71	-558.66
1gvp	49-58	-540.20	0.67	-429.86	1.88	-536.15
1ixh	84-93	-556.71	2.19	-475.15	2.17	-562.41
1knt	35-44	-400.35	2.55	-288.32	5.44	-431.19
1mrj	173-182	-517.55	0.62	-407.93	1.39	-550.65
1onc	48-57	-437.52	3.98	-358.29	4.06	-424.52
1pgs	68-77	-708.92	1.14	-501.57	2.24	-721.23
1plc	42-51	-387.38	1.45	-259.63	2.80	-393.23
1ppn	190-199	-532.90	2.73	-436.43	2.66	-511.67
1scs	65-74	-602.65	3.78	-505.36	1.32	-571.69
1tca	23-32	-322.76	5.75	-313.31	1.32	-361.78
1tca	258-267	-447.59	0.69	-286.72	2.33	-541.72
1whi	47-56	-309.84	1.65	-271.70	3.97	-269.49
2alp	90-105	-759.59	2.28	-225.27	2.46	-875.05
2ayh	80-89	-636.12	2.15	-453.37	1.74	-733.28
2cmd	57-66	-423.28	1.23	-367.63	4.58	-444.02
2mnr	91-100	-727.66	0.60	-686.29	1.04	-738.95
2sil	197-206	-491.15	2.08	-334.10	3.23	-501.29
3hsc	28-37	-483.91	1.56	-421.40	4.36	-499.57
3seb	200-209	-686.34	1.40	-592.54	1.54	-676.03
3tgl	257-266	-899.14	0.65	-734.62	1.31	-947.89
4fgf	42-51	-508.97	0.86	-367.03	1.19	-524.35
7rsa	110-119	-521.53	1.79	-401.18	4.01	-517.11
7rsa	33-42	-520.93	2.32	-432.56	2.81	-527.97
7rsa	87-96	-322.91	9.09	-288.35	6.56	-270.71
<b>Length 10 averages</b>		<b>-571.23</b>	<b>2.16</b>	<b>-438.19</b>	<b>2.60</b>	<b>-594.83</b>
153l	154-164	-555.05	0.78	-449.85	3.31	-661.03
1a2pA	76-86	-635.68	2.07	-419.49	2.08	-575.82
1a2yA	91-101	-702.12	5.02	-538.70	2.52	-632.05
1a8d	195-205	-406.83	1.12	-264.37	2.05	-420.41
1ads	290-300	-1059.84	1.37	-773.33	1.63	-1118.10
1ako	110-120	-574.99	4.18	-439.27	1.73	-643.12
1akz	211-221	-504.32	4.25	-472.79	2.09	-603.75
1aol	152-162	-939.23	1.42	-715.50	1.72	-953.99
1aru	297-307	-418.46	1.09	-370.31	2.20	-358.29
1awqA	1101-1111	-380.48	2.21	-165.76	5.95	-349.80
1bolA	33-43	-896.92	3.10	-725.70	3.09	-907.78
1bx4A	250-260	-459.13	2.92	-292.33	7.81	-460.28

1c5eA	82-92	-707.66	2.01	-666.59	1.53	-831.54
1cb0A	33-43	-555.09	1.87	-388.45	2.16	-694.43
1cnv	162-172	-639.30	3.11	-463.15	2.55	-674.81
1cs6A	145-155	-516.11	2.13	-386.21	3.41	-648.53
1cvl	257-267	-431.51	9.59	-342.15	9.92	-606.35
1dad	42-52	-350.16	4.41	-204.75	7.24	-323.19
1dysA	290-300	-904.85	1.08	-569.65	1.16	-1007.66
1edt	93-103	-668.51	2.95	-610.91	1.51	-806.60
1eur	87-97	-380.64	2.15	-335.06	5.77	-406.98
1exmA	291-301	-492.63	1.64	-307.78	3.64	-463.55
1f46A	64-74	-607.69	1.89	-391.94	1.75	-610.95
1fus	28-38	-498.61	4.80	-487.86	0.98	-525.35
1g6sA	77-87	-419.21	1.56	-370.02	1.12	-469.19
1g9gA	125-135	-492.77	0.71	-364.14	0.91	-534.36
1gmuA	44-54	-546.66	2.25	-324.89	3.92	-510.85
1gqvA	114-124	-432.41	3.49	-240.34	10.57	-385.87
1i4jA	86-96	-332.33	3.36	-239.83	3.44	-197.16
1iu8A	85-95	-363.68	0.69	-267.93	2.11	-377.11
1ixh	120-130	-589.13	0.95	-420.69	2.14	-572.30
1jp4A	179-189	-485.28	1.55	-352.09	3.63	-439.46
1k7iA	137-147	-400.82	6.99	-316.80	7.99	-350.27
1lmiA	34-44	-479.79	1.14	-371.69	2.52	-388.26
1mla	9-19	-578.15	2.76	-494.05	4.14	-586.82
1my7A	254-264	-707.68	0.69	-534.87	4.07	-702.63
1nlnA	26-36	-795.51	1.25	-557.38	1.66	-908.01
1nls	216-226	-416.60	0.96	-241.68	4.29	-439.06
1nogA	98-108	-447.29	3.35	-406.05	2.41	-467.17
1nscA	383-393	-550.14	2.96	-381.60	2.47	-624.17
1ojqA	141-151	-584.26	5.79	-552.43	2.13	-576.77
1othA	69-79	-663.57	0.81	-372.85	2.08	-695.21
1oyc	203-213	-657.48	2.68	-423.77	3.23	-703.78
1pgs	83-93	-631.85	1.49	-496.49	4.00	-737.63
1pkhA	44-54	-446.15	5.52	-317.62	4.26	-286.91
1qlwA	31-41	-428.18	4.35	-304.37	3.77	-296.37
1rcf	122-132	-733.38	0.93	-481.06	1.93	-801.74
1t1dA	127-137	-595.30	3.54	-482.40	2.54	-614.36
1whi	25-35	-547.19	2.26	-419.62	5.69	-529.63
2eng	124-134	-670.50	1.98	-526.62	1.45	-622.60
2pth	8-18	-641.75	3.68	-558.52	3.98	-642.95
2tgi	46-56	-546.27	1.87	-334.63	4.78	-597.63
3pte	91-101	-588.06	0.91	-492.03	2.49	-699.51
5pti	7-17	-457.60	4.30	-368.81	4.61	-384.54
<b>Length 11 averages</b>		<b>-565.09</b>	<b>2.63</b>	<b>-422.17</b>	<b>3.37</b>	<b>-581.98</b>
153l	98-109	-632.32	6.66	-508.98	7.00	-650.76
1a8d	155-166	-776.18	1.91	-486.74	5.34	-925.62

1akz	181-192	-873.37	1.21	-570.79	1.85	-857.85
1aozA	123-134	-548.54	2.87	-353.09	3.66	-521.24
1arb	74-85	-560.57	1.04	-319.16	2.96	-611.83
1arb	182-193	-706.99	1.55	-421.43	2.02	-755.81
1bhe	121-132	-458.41	2.16	-297.71	2.27	-489.85
1bkf	9-20	-377.22	2.41	-336.96	2.67	-328.64
1bn8A	298-309	-746.37	1.45	-581.44	6.11	-808.86
1c5eA	82-93	-831.05	1.78	-690.18	1.94	-883.48
1cb0A	33-44	-546.31	1.73	-412.73	2.27	-722.60
1cb8A	327-338	-485.41	3.92	-405.60	3.90	-430.29
1cex	40-51	-626.50	7.04	-551.02	6.50	-680.22
1cnv	188-199	-914.53	3.20	-593.36	4.17	-918.12
1cs6A	145-156	-617.95	2.85	-319.85	3.59	-767.51
1dim	213-224	-870.92	0.82	-588.44	1.68	-929.76
1dqzA	209-220	-400.39	0.82	-282.38	2.28	-430.25
1el5A	275-286	-574.62	2.61	-340.30	4.36	-680.03
1exmA	291-302	-531.63	0.99	-309.73	3.70	-525.58
1f46A	64-75	-595.69	2.38	-453.54	3.29	-633.91
1i7pA	63-74	-622.48	1.59	-476.76	1.73	-758.48
1iooA	179-190	-397.21	5.20	-311.07	5.47	-386.64
1ixh	160-171	-785.63	3.11	-650.97	3.80	-837.41
1iyeA	103-114	-418.05	4.75	-329.09	5.72	-396.05
1jp4A	179-190	-624.55	1.93	-473.74	3.01	-580.92
1kcmA	118-129	-699.99	1.67	-539.78	1.30	-756.90
1lucA	158-169	-498.47	4.88	-420.94	5.36	-503.65
1m3sA	68-79	-517.27	2.63	-371.43	6.32	-446.75
1ms9A	529-540	-766.27	0.92	-584.48	2.24	-760.48
1my7A	254-265	-729.78	2.01	-639.27	2.49	-724.32
1othA	69-80	-681.51	1.71	-435.94	3.33	-738.90
1oyc	203-214	-668.31	3.69	-397.22	6.25	-708.14
1pkhA	44-55	-430.07	5.69	-321.49	5.24	-301.23
1qlwA	31-42	-420.85	1.04	-343.26	4.85	-320.21
1t1dA	127-138	-647.58	1.32	-487.48	2.99	-652.64
1xyzA	813-824	-596.31	4.06	-231.22	3.25	-1003.54
2ayh	21-32	-699.83	2.62	-495.61	2.39	-680.24
2hlcA	91-102	-796.38	7.43	-452.51	9.69	-844.70
2pia	30-41	-567.51	2.19	-438.73	1.93	-576.02
2ptd	136-147	-875.51	2.24	-567.49	4.65	-976.61
<b>Length 12 averages</b>		<b>-627.96</b>	<b>2.75</b>	<b>-444.80</b>	<b>3.84</b>	<b>-662.65</b>
16pk	132-144	-653.38	5.23	-326.81	6.35	-885.88
1a8d	155-167	-863.43	2.88	-524.93	5.79	-988.56
1a8d	74-86	-653.08	4.37	-427.38	6.89	-513.41
1arb	182-194	-768.64	1.15	-480.91	4.05	-819.31
1bhe	121-133	-527.46	10.66	-322.72	11.13	-546.16
1bkpA	51-63	-801.76	1.13	-250.15	3.00	-945.31



1cnv	110-122	-592.76	3.21	-394.57	8.88	-664.90
1cruA	357-369	-754.16	2.99	-439.91	4.95	-817.20
1dpgA	352-364	-566.88	9.11	-501.80	12.29	-372.74
1dqzA	209-221	-427.39	2.40	-318.68	2.61	-465.14
1dysA	290-302	-926.68	1.83	-587.94	4.60	-1077.84
1ed8A	67-79	-688.88	1.72	-384.92	8.63	-842.42
1eokA	147-159	-923.16	1.23	-688.02	1.42	-978.50
1f46A	64-76	-578.21	1.62	-442.81	2.21	-633.56
1g8fA	72-84	-897.18	1.13	-715.14	2.26	-1269.84
1gpiA	308-320	-576.42	0.76	-350.23	9.37	-548.44
1hnjA	191-203	-400.98	7.79	-306.64	10.28	-274.19
1hzhA	87-99	-643.48	7.55	-424.98	7.53	-462.13
1iirA	197-209	-700.72	0.63	-418.43	6.06	-802.21
1jp4A	153-165	-659.62	4.82	-504.98	4.62	-646.18
1kblA	793-805	-844.09	2.23	-554.13	1.15	-951.55
1krhA	131-143	-698.88	1.29	-435.20	2.75	-735.67
1l8aA	691-703	-835.90	1.24	-503.45	1.38	-829.35
1lki	62-74	-584.10	5.19	-517.78	2.19	-663.47
1m3sA	68-80	-608.10	3.12	-372.77	5.29	-498.89
1mo9A	107-119	-596.13	3.92	-449.72	4.80	-566.18
1nlnA	26-38	-901.12	4.94	-528.31	3.17	-1018.76
1o6lA	386-398	-416.27	1.63	-220.44	6.20	-565.76
1ockA	43-55	-469.08	2.10	-331.95	6.69	-488.51
1ojqA	167-179	-585.42	4.85	-387.45	3.46	-600.72
1os8A	141-153	-679.50	5.24	-474.10	4.60	-631.31
1p1mA	327-339	-809.70	5.17	-522.67	7.78	-944.03
1qqp2	161-173	-868.03	1.26	-486.63	3.63	-918.02
1qslA	389-401	-620.72	2.60	-332.09	4.90	-686.05
1xyzA	645-657	-604.61	0.91	-379.75	6.31	-619.16
1yge	452-464	-488.45	8.51	-400.43	3.78	-361.70
2hlcA	91-103	-883.65	7.20	-553.46	9.46	-981.26
2olbA	207-219	-761.12	2.55	-454.67	3.67	-796.53
2ptd	136-148	-854.60	3.21	-554.37	6.16	-1005.85
3grs	404-416	-619.90	2.98	-435.07	4.91	-681.47
<b>Length 13 averages</b>		<b>-683.34</b>	<b>3.56</b>	<b>-442.66</b>	<b>5.38</b>	<b>-727.45</b>

**Figure S1.** Plots of the (DiSGro energy, RMSD) pairs of the lowest DiSGro energy conformation sampled by the DiSGro algorithm and PETALS for each loop target of the LoopBuilder set, by loop length.

