# Text S1

Table 1: **The average minimal RMSD ($R_{\min}$) of 8-residue loops on Test Set 2, calculated using DISGRO.**

| PDB | Start | End | Sequence | $R_{\min}$ |
|---|---|---|---|---|
| 1a1h | 107 | 114 | CPVESCDR | 1.38 |
| 1a3c | 92 | 99 | IPVDITDQ | 0.88 |
| 1a62 | 70 | 77 | SSYLAGPD | 0.65 |
| 1a62 | 102 | 109 | RPPKEGER | 0.68 |
| 1aac | 49 | 56 | EAMPHNVH | 0.3 |
| 1aba | 7 | 14 | YDSNIHKC | 0.62 |
| 1ads | 274 | 281 | KVFDFELS | 0.77 |
| 1amm | 69 | 76 | MGFNDSIR | 0.88 |
| 1amm | 158 | 165 | GAMNAKVG | 0.41 |
| 1arb | 136 | 143 | RRDQNYPG | 1.11 |
| 1arb | 212 | 219 | GPSSCSAT | 0.69 |
| 1arb | 249 | 256 | DPASTGAQ | 0.95 |
| 1aru | 234 | 241 | LSPFPGEF | 0.41 |
| 1brt | 205 | 212 | WYTDFRAD | 0.49 |
| 1btk | 67 | 74 | VVPEKNPP | 0.8 |
| 1cex | 73 | 80 | VGGAYRAT | 1.84 |
| 1cvl | 148 | 155 | TLVSSSHN | 0.84 |
| 1cvl | 229 | 236 | TSTGTLDV | 0.39 |
| 1dad | 176 | 183 | DVTPPGKR | 0.55 |
| 1dim | 246 | 253 | RNSGLRRS | 0.7 |
| 1ezm | 92 | 99 | GTSPLTHK | 0.41 |
| 1hfc | 119 | 126 | ENYTPDLP | 1.36 |
| 1kpf | 105 | 112 | GQSVYHVH | 0.71 |
| 1mrp | 68 | 75 | AGLLAPIS | 0.78 |
| 1msi | 26 | 33 | VVTPVGIP | 1.13 |
| 1nfp | 118 | 125 | NVDIANVR | 1.05 |
| 1nif | 221 | 228 | NGAVGALT | 0.87 |
| 1nif | 279 | 286 | ETWLIPGG | 0.8 |
| 1nls | 97 | 104 | TGLYKETN | 0.73 |
| 1nox | 99 | 106 | VIHPGVQG | 1.12 |
| 1opd | 8 | 15 | ITAPNGLH | 0.54 |
| 1plc | 6 | 13 | GADDGSLA | 1.24 |
| 1plc | 32 | 39 | NAGFPHNI | 1.16 |
| 1ppn | 101 | 108 | GPYAAKTD | 0.85 |
| 1ppn | 191 | 198 | RGTGNSYG | 0.58 |

| | | | | |
|---|---|---|---|---|
| 1ra9 | 51 | 58 | GRPLPGRK | 0.77 |
| 1rhs | 235 | 242 | KKVDLTKP | 0.47 |
| 1rro | 18 | 25 | CQDPDTFE | 0.59 |
| 1vwj | 45 | 52 | SAVGNAES | 1.28 |
| 1wer | 824 | 831 | SKQSCELS | 0.37 |
| 1wer | 916 | 923 | NIISDSPS | 0.55 |
| 2arc | 28 | 35 | ANGYLDFF | 0.49 |
| 2ayh | 124 | 131 | TNGVGGHE | 0.65 |
| 2ayh | 194 | 201 | GSYNGANP | 0.66 |
| 2ctc | 53 | 60 | STGGSNRP | 1.45 |
| 3seb | 40 | 47 | SIDQFLYF | 0.5 |
| 5p21 | 144 | 151 | TSAKTRQG | 0.59 |
| 5ptp | 22 | 29 | CGANTVPY | 0.78 |
| 5ptp | 172 | 179 | YPGQITSN | 1.36 |
| 7rsa | 64 | 71 | ACKNGQTN | 0.85 |
| Mean | | | | **0.80** |

Table 2: **The average minimal RMSD ($R_{\min}$) of 11-residue loops on Test Set 2, calculated using** DISGRO**.**

| PDB | Start | End | Sequence | $R_{\min}$ |
|---|---|---|---|---|
| 153l | 154 | 164 | VRSYARMDIGT | 0.94 |
| 1a2p | 74 | 84 | INYTSGFRNSD | 1.47 |
| 1a2y | 91 | 101 | FWSTPRTFGGG | 1.54 |
| 1ads | 290 | 300 | SYNRNWRVCAL | 0.66 |
| 1akz | 130 | 140 | AHQANSHKERG | 1.29 |
| 1aru | 289 | 299 | IPSAVSNNAAP | 1.56 |
| 1awq | 100 | 110 | ANAGPNTNGSQ | 1.41 |
| 1cvl | 254 | 264 | RASGQNDGLVS | 1.16 |
| 1dad | 42 | 52 | GSEKTPEGLRN | 1.52 |
| 1ixh | 120 | 130 | NPGLKLPSQNI | 1.09 |
| 1mla | 7 | 17 | PGQGSQTVGML | 0.96 |
| 1nls | 216 | 226 | NIDSSIPSGST | 1.28 |
| 1rcf | 122 | 132 | TDGYDFNDSKA | 1.3 |
| 2eng | 120 | 130 | IPGGGVGIFDG | 0.5 |
| 2pth | 8 | 18 | LANPGAEYAAT | 1.28 |
| 3pte | 91 | 101 | LPGLLPDDRIT | 1.18 |
| 5pti | 7 | 17 | EPPYTGPCKAR | 1.09 |
| Mean | | | | **1.19** |

Table 3: **The average minimal RMSD ($R_{\min}$) of 12-residue loops on Test Set 2, calculated using** DISGRO**.**

| PDB | Start | End | Sequence | $R_{\min}$ |
|---|---|---|---|---|
| 153l | 98 | 109 | KRSHKPQGTWNG | 1.15 |
| 1akz | 100 | 111 | IEDFVHPGHGDL | 0.86 |
| 1arb | 74 | 85 | NYQNSTCRAPNT | 1.2 |
| 1bkf | 9 | 20 | PGDGRTFPKRGQ | 1.14 |
| 1cex | 24 | 35 | RGSTETGNLGTL | 0.91 |
| 1dim | 212 | 223 | TDGITWSLPSGY | 0.87 |
| 1ixh | 160 | 171 | VGTGSTVKWPIG | 1.86 |
| 1luc | 158 | 169 | LNPSAYTQGGAP | 1.99 |
| 1xyz | 298 | 309 | NPLIYDSNYNPK | 1.15 |
| 2ayh | 21 | 32 | ADGYSNGGVFNC | 1.62 |
| Mean | | | | **1.28** |

Table 4: **Results of 4-residue loops on Test Set 3, calculated using DISGRO.**

| PDB | Start | End | Sequence | $R_{\min}$ | $R_{\text{ave}}$ | $R_{Emin}$ |
|---|---|---|---|---|---|---|
| 1aaj | 82 | 85 | FTEA | 0.08 | 0.44 | 0.39 |
| 1ads | 99 | 102 | LKLD | 0.12 | 0.27 | 0.26 |
| 1cbs | 21 | 24 | VLGV | 0.3 | 0.79 | 0.85 |
| 1fkf | 42 | 45 | RNKP | 0.1 | 0.3 | 0.36 |
| 1frd | 59 | 62 | DQSD | 0.18 | 0.98 | 0.24 |
| 1gpr | 123 | 126 | NVPS | 0.43 | 1.11 | 0.7 |
| 1iab | 100 | 103 | FYHE | 0.11 | 0.52 | 0.11 |
| 1mba | 97 | 100 | GFGV | 0.09 | 0.33 | 0.49 |
| 1nfp | 37 | 40 | EDTS | 0.64 | 1.56 | 0.93 |
| 1pbe | 117 | 120 | GATT | 0.23 | 0.92 | 0.97 |
| 1pgs | 226 | 229 | LGAL | 0.19 | 1.38 | 0.19 |
| 1plc | 74 | 77 | LSNK | 0.1 | 0.45 | 0.26 |
| 1ppn | 42 | 45 | TGNL | 0.13 | 0.5 | 0.33 |
| 1prn | 66 | 69 | GNAA | 0.19 | 0.54 | 0.31 |
| 1rcf | 111 | 114 | QRGG | 0.3 | 0.61 | 0.53 |
| 1tca | 287 | 290 | AGPK | 0.14 | 0.88 | 0.24 |
| 1thw | 194 | 197 | PGSS | 0.15 | 0.39 | 0.22 |
| 1tib | 46 | 49 | KADA | 0.07 | 0.27 | 0.14 |
| 1tml | 42 | 45 | FAHH | 0.66 | 1.19 | 1.08 |
| 1tys | 131 | 134 | SAWN | 0.11 | 0.55 | 1.2 |
| 1xif | 82 | 85 | TGMK | 0.11 | 0.28 | 0.31 |
| 1xnb | 30 | 33 | WSNT | 0.02 | 0.08 | 0.06 |
| 2cmd | 163 | 166 | GKQP | 0.24 | 1.11 | 0.57 |
| 2cy3 | 101 | 104 | KDKK | 0.08 | 0.33 | 0.37 |
| 2exo | 161 | 164 | DPTA | 0.42 | 0.79 | 0.84 |
| 2sga | 44 | 47 | LGFN | 0.17 | 0.79 | 0.17 |
| 2sil | 220 | 223 | LPSG | 0.84 | 1.17 | 1.2 |
| 2tgi | 72 | 75 | ASAS | 0.11 | 0.4 | 0.45 |
| 3cyr | 69 | 72 | HAKG | 0.31 | 0.71 | 0.91 |
| 4enl | 335 | 338 | EKKA | 0.05 | 0.27 | 0.16 |
| 4gcr | 116 | 119 | FHLT | 0.31 | 0.84 | 0.76 |
| 5fd1 | 81 | 84 | ITEK | 0.17 | 0.7 | 0.42 |
| 5p21 | 75 | 78 | GEGF | 0.03 | 0.75 | 0.2 |
| 7rsa | 47 | 50 | VHES | 0.12 | 0.54 | 0.21 |
| 8abp | 55 | 58 | ASGA | 0.1 | 0.32 | 0.22 |
| Mean | | | | **0.21** | **0.66** | **0.48** |

$R_{\min}$, $R_{\text{ave}}$ and $R_{Emin}$ denote the average minimum backbone RMSD, the average ensemble RMSD and the average RMSD of the lowest energy conformations of the 1,000 loop ensemble with the same length, respectively.

Table 5: **Results of 5-residue loops on Test Set 3, calculated using** DISGRO**.**

| PDB | Start | End | Sequence | $R_{\min}$ | $R_{\text{ave}}$ | $R_{Emin}$ |
|---|---|---|---|---|---|---|
| 1ads | 274 | 278 | KVFDF | 0.27 | 1.16 | 1.64 |
| 1alc | 110 | 114 | LCTEK | 0.48 | 2.15 | 0.66 |
| 1art | 346 | 350 | ANRDF | 0.28 | 1.42 | 1.12 |
| 1byb | 223 | 227 | RAGHP | 0.17 | 0.73 | 0.55 |
| 1csh | 98 | 102 | TGQIP | 0.36 | 1.58 | 1.91 |
| 1cus | 31 | 35 | CADVI | 0.27 | 0.96 | 0.3 |
| 1dts | 62 | 66 | SSLQL | 0.36 | 1.2 | 1.35 |
| 1eco | 72 | 76 | ELPNI | 0.55 | 1.72 | 2.11 |
| 1ede | 15 | 19 | LDQYP | 0.38 | 1.95 | 0.43 |
| 1fkf | 10 | 14 | GDGRT | 0.16 | 1.33 | 0.38 |
| 1frd | 83 | 87 | PRSNC | 0.16 | 0.91 | 0.7 |
| 1gof | 430 | 434 | FASNG | 0.22 | 0.82 | 0.44 |
| 1gpr | 54 | 58 | SPVRG | 0.27 | 0.78 | 0.91 |
| 1hbq | 158 | 162 | ELCLA | 0.11 | 0.55 | 0.56 |
| 1nar | 56 | 60 | ESWDV | 0.19 | 0.95 | 0.68 |
| 1onc | 59 | 63 | TTSEF | 0.14 | 0.71 | 0.92 |
| 1pbe | 194 | 198 | PVSHE | 0.1 | 0.7 | 0.36 |
| 1pgs | 36 | 40 | DVTTV | 0.13 | 0.84 | 0.38 |
| 1phf | 277 | 281 | RPERI | 0.33 | 2.05 | 0.92 |
| 1poa | 108 | 112 | NDYNI | 0.08 | 0.61 | 0.62 |
| 1prn | 187 | 191 | GIVDN | 0.16 | 0.8 | 0.3 |
| 1sbp | 181 | 185 | VERGI | 0.3 | 1.77 | 0.57 |
| 1tib | 253 | 257 | PDIPA | 0.07 | 0.51 | 0.31 |
| 1tml | 147 | 151 | GSSQA | 0.13 | 0.48 | 0.46 |
| 1ukz | 94 | 98 | KANKH | 0.12 | 0.68 | 0.46 |
| 1ycc | 74 | 78 | YIPGT | 0.34 | 1.06 | 0.91 |
| 2cmd | 188 | 192 | QVPGV | 0.49 | 1.31 | 1.22 |
| 2cpl | 115 | 119 | CTAKT | 0.29 | 1 | 0.81 |
| 2end | 93 | 97 | ISDIP | 0.22 | 1.52 | 1.49 |
| 2fox | 25 | 29 | ESGKD | 0.25 | 1 | 1.11 |
| 2hbg | 37 | 41 | AHPQM | 0.17 | 1.16 | 0.17 |
| 3tgl | 207 | 211 | HLPPA | 0.86 | 1.52 | 1.16 |
| 7rsa | 75 | 79 | SYSTM | 0.15 | 0.81 | 0.75 |
| 8abp | 300 | 304 | KKGLG | 0.04 | 0.86 | 1.91 |
| Mean | | | | **0.25** | **1.11** | **0.84** |

$R_{\min}$, $R_{\text{ave}}$ and $R_{Emin}$ denote the average minimum backbone RMSD, the average ensemble RMSD and the average RMSD of the lowest energy conformations of the 1,000 loop ensemble with the same length, respectively.

Table 6: **Results of 6-residue loops on Test Set 3, calculated using DISGRO.**

| PDB | Start | End | Sequence | $R_{\min}$ | $R_{\text{ave}}$ | $R_{Emin}$ |
|---|---|---|---|---|---|---|
| 1ads | 149 | 154 | DEGLVK | 0.17 | 0.67 | 0.46 |
| 1arp | 282 | 287 | VLGFDR | 0.41 | 2.73 | 1.24 |
| 1cbs | 66 | 71 | KVGEEF | 0.31 | 0.9 | 1.42 |
| 1dts | 146 | 151 | GVKLGC | 0.61 | 2.35 | 3.16 |
| 1ede | 180 | 185 | VTPSDL | 0.97 | 2.28 | 3.2 |
| 1fnd | 204 | 209 | VPTSSS | 0.36 | 0.88 | 0.41 |
| 1gca | 100 | 105 | DSYDKA | 0.26 | 0.95 | 0.4 |
| 1gpr | 83 | 88 | HFGIDT | 0.63 | 1.5 | 0.93 |
| 1hbq | 15 | 20 | FDKARF | 0.52 | 1.89 | 0.7 |
| 1lst | 109 | 114 | LKGKHV | 0.32 | 1.02 | 0.51 |
| 1onc | 12 | 17 | TNTRDV | 0.28 | 1.72 | 0.28 |
| 1phf | 350 | 355 | FGHGSH | 0.38 | 1.21 | 1.63 |
| 1php | 217 | 222 | IGGGLA | 0.21 | 0.73 | 0.38 |
| 1ppn | 144 | 149 | YRGGIF | 0.44 | 3.43 | 0.7 |
| 1prn | 57 | 62 | DGDAFA | 0.33 | 2.65 | 2.61 |
| 1scs | 19 | 24 | DPSYPH | 0.4 | 1.32 | 0.96 |
| 1tca | 94 | 99 | SGNNKL | 0.33 | 1.48 | 0.7 |
| 1tib | 176 | 181 | VGNRAF | 0.52 | 1.34 | 0.53 |
| 1tys | 66 | 71 | DTNIAY | 0.23 | 0.9 | 0.23 |
| 1xif | 357 | 362 | FEEFDV | 0.85 | 3.78 | 2.9 |
| 1ycc | 85 | 90 | LKKEKD | 0.29 | 1.76 | 0.29 |
| 2ayh | 160 | 165 | VDGVLK | 0.3 | 2.83 | 0.67 |
| 2cpl | 122 | 127 | LDGKHV | 0.19 | 0.91 | 0.4 |
| 3cyr | 25 | 30 | HEKVEC | 0.27 | 0.99 | 0.96 |
| 2mnr | 308 | 313 | AATPTA | 0.39 | 0.91 | 0.47 |
| 2ran | 40 | 45 | LTARSN | 0.26 | 1.37 | 0.47 |
| 2sil | 176 | 181 | GGVGSG | 0.24 | 1.14 | 0.33 |
| 3chy | 12 | 17 | DDFSTM | 0.42 | 2.19 | 3.71 |
| 3grs | 336 | 341 | ALLTPV | 0.81 | 2.91 | 2.14 |
| 3hsc | 227 | 232 | HLGGED | 0.31 | 1.39 | 0.37 |
| 3tgl | 82 | 87 | SSSIRN | 0.63 | 2.46 | 1.74 |
| 5fd1 | 87 | 92 | PLPDAE | 0.86 | 2.58 | 0.99 |
| 5fx2 | 41 | 46 | VEAGGL | 0.95 | 2.02 | 3.65 |
| 5p21 | 104 | 109 | KDSDDV | 0.26 | 1.31 | 1.06 |
| 7rsa | 14 | 19 | DSSTSA | 0.64 | 2.06 | 1.51 |
| 8abp | 65 | 70 | TPDPKL | 0.47 | 2.05 | 1.76 |
| Mean | | | | **0.44** | **1.74** | **1.22** |

$R_{\min}$, $R_{\text{ave}}$ and $R_{Emin}$ denote the average minimum backbone RMSD, the average ensemble RMSD and the average RMSD of the lowest energy conformations of the 1,000 loop ensemble with the same length, respectively.

Table 7: **Results of 7-residue loops on Test Set 3, calculated using DISGRO.**

| PDB | Start | End | Sequence | $R_{\min}$ | $R_{\text{ave}}$ | $R_{Emin}$ |
|---|---|---|---|---|---|---|
| 1amp | 225 | 231 | YACSDHA | 0.54 | 2.12 | 1.13 |
| 1arb | 249 | 255 | DPASTGA | 0.36 | 2.47 | 3.46 |
| 1art | 356 | 362 | QNGMFSF | 0.49 | 1.31 | 0.56 |
| 1byb | 198 | 204 | WEFPRIG | 0.97 | 1.67 | 1.16 |
| 1cbs | 45 | 51 | QEGDTFY | 0.9 | 4.62 | 1.48 |
| 1cyo | 24 | 30 | ILHYKVY | 0.37 | 1.44 | 0.46 |
| 1dts | 76 | 82 | FAEPTSP | 0.67 | 1.5 | 1.25 |
| 1ede | 121 | 127 | VVQDWGG | 0.6 | 2.04 | 1.89 |
| 1gca | 196 | 202 | LSGPNAN | 0.46 | 2.65 | 0.67 |
| 1gpr | 35 | 41 | SGKMMGD | 0.54 | 2.72 | 1.62 |
| 1hbq | 138 | 144 | ARDPSGF | 0.49 | 1.54 | 1.54 |
| 1hfc | 151 | 157 | KVSEGQA | 0.3 | 0.99 | 0.64 |
| 1iab | 142 | 148 | QYYSIMH | 0.38 | 1.44 | 0.44 |
| 1lif | 64 | 70 | FKLGVEF | 0.55 | 2.91 | 1.65 |
| 1lst | 117 | 123 | LQGSTQE | 0.22 | 2.55 | 0.3 |
| 1mbd | 17 | 23 | VEADVAG | 0.43 | 1.67 | 1.02 |
| 1phf | 26 | 32 | FDMYNPS | 0.53 | 1.43 | 1.03 |
| 1php | 135 | 141 | AELADLY | 0.34 | 1.08 | 0.65 |
| 1plc | 87 | 93 | HQGAGMV | 0.4 | 1.39 | 0.52 |
| 1pmy | 25 | 31 | LKPGDSI | 0.42 | 1.3 | 0.42 |
| 1ppn | 166 | 172 | YGPNYIL | 0.75 | 2.54 | 1 |
| 1ptf | 65 | 71 | VDGADEA | 0.5 | 3.15 | 0.61 |
| 1sbp | 169 | 175 | LDSGARG | 0.39 | 4.24 | 1.1 |
| 1thw | 158 | 164 | CCTTGKC | 0.53 | 2.12 | 0.91 |
| 1tml | 20 | 26 | NPNDPRT | 0.59 | 2.69 | 1.45 |
| 1ycc | 57 | 63 | VLWDENN | 0.78 | 2.07 | 0.89 |
| 2alp | 130 | 136 | AAVGAAV | 0.3 | 1.87 | 0.3 |
| 2ayh | 54 | 60 | SAYNKFD | 0.93 | 3.31 | 1.95 |
| 2cba | 61 | 67 | NNGHAFN | 0.54 | 1.81 | 1.49 |
| 2ctc | 53 | 59 | STGGSNR | 0.88 | 2.9 | 1.79 |
| 2mnr | 270 | 276 | DAMKIGG | 0.39 | 1.34 | 0.39 |
| 3grs | 26 | 32 | IGGGSGG | 0.58 | 1.62 | 0.78 |
| 3tgl | 159 | 165 | QREEGLS | 0.6 | 2.99 | 1.9 |
| 4fgf | 58 | 64 | EERGVVS | 1.03 | 3.6 | 1.03 |
| 4gcr | 150 | 156 | EYRRYLD | 0.34 | 2.04 | 0.34 |
| 5fx2 | 27 | 33 | ADAGYEV | 0.4 | 3.85 | 1.05 |
| 5p21 | 83 | 89 | AINNTKS | 0.4 | 1.4 | 0.4 |
| 7rsa | 20 | 26 | ASSSNYC | 0.94 | 2.47 | 1.91 |
| Mean | | | | **0.55** | **2.23** | **1.08** |

$R_{\min}$, $R_{\text{ave}}$ and $R_{Emin}$ denote the average minimum backbone RMSD, the average ensemble RMSD and the average RMSD of the lowest energy conformations of the 1,000 loop ensemble with the same length, respectively.

Table 8: **Results of 8-residue loops on Test Set 3, calculated using DISGRO.**

| PDB | Start | End | Sequence | $R_{\min}$ | $R_{\text{ave}}$ | $R_{Emin}$ |
|---|---|---|---|---|---|---|
| 135l | 84 | 91 | LSSDITAS | 0.53 | 2.37 | 1.98 |
| 1alc | 34 | 41 | SGYDTQAI | 0.5 | 5.02 | 0.53 |
| 1art | 88 | 95 | FGKGSALI | 0.98 | 3.57 | 3.8 |
| 1btl | 50 | 57 | DLNSGKIL | 0.75 | 2.19 | 1.2 |
| 1cbs | 55 | 62 | STTVRTTE | 0.58 | 4.67 | 5.85 |
| 1ddt | 127 | 134 | FGDGASRV | 0.89 | 2.41 | 2.5 |
| 1fnd | 262 | 269 | LKKDNTYV | 0.3 | 2 | 1.49 |
| 1gky | 72 | 79 | QFSGNYYG | 0.7 | 5.22 | 0.72 |
| 1hfc | 142 | 149 | SNVTPLTF | 0.67 | 1.38 | 1.32 |
| 1iab | 48 | 55 | RTTESDYV | 1.17 | 2.89 | 1.45 |
| 1nar | 192 | 199 | FSNQQKPV | 0.61 | 1.67 | 1.03 |
| 1oyc | 80 | 87 | GGYDNAPG | 0.77 | 2.09 | 1.66 |
| 1phf | 85 | 92 | CPFIPREA | 1.11 | 2.32 | 1.95 |
| 1poa | 71 | 78 | CSQGTLTC | 1.03 | 2.42 | 2.05 |
| 1prn | 150 | 157 | DPDQTVDS | 0.59 | 2.81 | 1.75 |
| 1sbp | 107 | 114 | KQIHDWND | 0.49 | 3.27 | 0.5 |
| 1thw | 18 | 25 | SKGDAALD | 0.57 | 2.17 | 1.34 |
| 1tml | 187 | 194 | NTSNYRWT | 0.53 | 1.58 | 0.73 |
| 1tys | 83 | 90 | WADENGDL | 0.99 | 5.11 | 2.77 |
| 1xnb | 99 | 106 | KSDGGTYD | 0.54 | 1.85 | 1.63 |
| 2ayh | 123 | 130 | YTNGVGGH | 0.59 | 1.9 | 0.65 |
| 2cmd | 270 | 277 | LGKNGVEE | 0.65 | 2.64 | 1.12 |
| 2ctc | 89 | 96 | DYGQDPSF | 0.92 | 2.03 | 1.5 |
| 2dri | 161 | 168 | PADFDRIK | 0.65 | 5.92 | 0.65 |
| 2exo | 262 | 269 | MQVTRCQG | 0.42 | 1.53 | 0.89 |
| 2fox | 88 | 95 | YGWGDGKW | 1.07 | 2.58 | 1.41 |
| 2ran | 26 | 33 | MKGLGTDE | 1.43 | 3.08 | 2.92 |
| 2sga | 32 | 43 | TTGGSRCS | 0.9 | 1.8 | 2.09 |
| 3grs | 424 | 431 | ANKEEKVV | 1.82 | 5.77 | 2 |
| 4enl | 24 | 31 | TTEKGVFR | 0.58 | 1.89 | 1.68 |
| 5p21 | 45 | 52 | VIDGETCL | 0.51 | 1.97 | 1.42 |
| 8dfr | 65 | 72 | RPLKDRIN | 1.65 | 3.68 | 2.56 |
| Mean | | | | **0.80** | **2.87** | **1.72** |

$R_{\min}$, $R_{\text{ave}}$ and $R_{Emin}$ denote the average minimum backbone RMSD, the average ensemble RMSD and the average RMSD of the lowest energy conformations of the 1,000 loop ensemble with the same length, respectively.

Table 9: **Results of 9-residue loops on Test Set 3, calculated using DISGRO.**

| PDB | Start | End | Sequence | $R_{\min}$ | $R_{\text{ave}}$ | $R_{Emin}$ |
|---|---|---|---|---|---|---|
| 1aba | 69 | 77 | FAPDGSHIG | 0.71 | 2.77 | 1.18 |
| 1amp | 57 | 65 | SASLPNASV | 0.76 | 2.07 | 1.22 |
| 1arp | 127 | 135 | SNCPGSPRL | 0.67 | 1.99 | 1.39 |
| 1btl | 102 | 110 | LVEYSPVTE | 1.15 | 4.99 | 1.64 |
| 1byb | 246 | 254 | GFFKSNGTY | 1.23 | 6.89 | 1.89 |
| 1csh | 252 | 260 | GSALSDPYL | 0.91 | 3.57 | 1.5 |
| 1cyo | 49 | 57 | QAGGDATEN | 0.73 | 2.93 | 0.87 |
| 1ede | 257 | 265 | GMKDKLLGP | 1.07 | 5.69 | 1.44 |
| 1flp | 41 | 49 | AKFSGLFSG | 0.67 | 4.17 | 3.31 |
| 1fnd | 121 | 129 | TNDAGETIK | 0.71 | 4.32 | 5.86 |
| 1fus | 31 | 39 | DTAGSSTYP | 1.3 | 4.44 | 3.22 |
| 1gca | 9 | 17 | IYKYDDNFM | 0.91 | 2.57 | 2.22 |
| 1gky | 6 | 14 | ISGPSGTGK | 0.52 | 2.59 | 0.76 |
| 1gpr | 63 | 71 | VFPTKHAIG | 1.33 | 4.06 | 1.75 |
| 1lif | 73 | 81 | ITADDRKVK | 1.21 | 2.72 | 2.08 |
| 1mrk | 53 | 61 | TNYADETIS | 1.11 | 2.43 | 1.62 |
| 1noa | 76 | 84 | FLFDGTRWG | 1.12 | 3.52 | 1.31 |
| 1npk | 102 | 110 | ASAPGSIRG | 0.61 | 5.29 | 0.61 |
| 1onc | 70 | 78 | VTSRPCKYK | 1.57 | 6.65 | 2.01 |
| 1pgs | 117 | 125 | TETWLAKGR | 0.59 | 1.98 | 1.39 |
| 1php | 91 | 99 | TNEAVGDEV | 0.9 | 4.54 | 1.13 |
| 1ptf | 10 | 18 | AETGIHARP | 0.89 | 3.77 | 2.07 |
| 1tib | 69 | 77 | LDNTNKLIV | 0.74 | 2.05 | 1.82 |
| 1xif | 59 | 67 | IPFGSSDSE | 0.78 | 5.01 | 1.54 |
| 1xnb | 116 | 124 | PSIDGDRTT | 0.96 | 2.58 | 1.89 |
| 2alp | 139 | 159 | SGRTTGYQC | 0.79 | 2.33 | 1.35 |
| 2ayh | 41 | 49 | FTNDGKLKL | 1.05 | 3.47 | 1.51 |
| 2cmd | 81 | 89 | RKPGMDRSD | 0.85 | 4.81 | 2.93 |
| 2cpl | 24 | 32 | LFADKVPKT | 0.74 | 3.34 | 0.97 |
| 2dri | 130 | 138 | QGIAGTSAA | 0.79 | 2.69 | 1.17 |
| 2fox | 5 | 13 | YWSGTGNTE | 0.85 | 3.35 | 3 |
| 2hbg | 18 | 26 | AGADNGAGV | 1.2 | 4.44 | 3.11 |
| 2sil | 183 | 191 | QLNDGKLVF | 0.91 | 2.63 | 0.91 |
| 3chy | 57 | 65 | DWNMPNMDG | 0.84 | 3.01 | 0.84 |
| 3tgl | 56 | 64 | STLIYDTNA | 1.64 | 4.08 | 2.24 |
| 4gcr | 94 | 102 | ERDDFRGQM | 0.96 | 3.75 | 1.68 |
| 5fx2 | 8 | 16 | YGSTTGNTE | 1.06 | 3.19 | 1.81 |
| Mean | | | | **0.94** | **3.64** | **1.82** |

$R_{\min}$, $R_{\text{ave}}$ and $R_{Emin}$ denote the average minimum backbone RMSD, the average ensemble RMSD and the average RMSD of the lowest energy conformations of the 1,000 loop ensemble with the same length, respectively.

Table 10: **Results of 10-residue loops on Test Set 3, calculated using DISGRO.**

| PDB | Start | End | Sequence | $R_{\min}$ | $R_{\text{ave}}$ | $R_{Emin}$ |
|---|---|---|---|---|---|---|
| 135l | 18 | 27 | DNYRGYSLGN | 1.53 | 4.04 | 2.53 |
| 1ads | 170 | 179 | LNKPGLKYKP | 1.09 | 4.24 | 2.13 |
| 1amp | 181 | 190 | TNYKGSAQDV | 1.01 | 2.81 | 1.89 |
| 1arp | 37 | 46 | FYQGSKCESP | 1.02 | 5 | 1.34 |
| 1btl | 170 | 179 | NEAIPNDERD | 0.72 | 2.62 | 2.27 |
| 1ede | 164 | 173 | FVTQPADGFT | 2.09 | 7.23 | 2.3 |
| 1fkf | 63 | 72 | VAQMSVGQRA | 0.48 | 2.97 | 0.48 |
| 1fnd | 185 | 194 | FFEKHDDYKF | 1.69 | 3.32 | 3.73 |
| 1gpr | 133 | 142 | FTNLAEGETV | 1.13 | 3.52 | 2.6 |
| 1hfc | 201 | 210 | ERWTNNFREY | 1.07 | 4.8 | 1.87 |
| 1knt | 35 | 44 | YGGCGGNENK | 1.27 | 4.17 | 2.19 |
| 1lst | 10 | 19 | TDTTYAPFSS | 1.38 | 3.58 | 1.67 |
| 1mbd | 40 | 49 | LEKFDRFKHL | 1.19 | 3.12 | 3.9 |
| 1nfp | 53 | 62 | DKSYNDETKL | 1.6 | 7.43 | 8.15 |
| 1onc | 48 | 57 | CKGIIASKNV | 1.01 | 6.77 | 1.41 |
| 1pbe | 157 | 166 | GCDGFHGISR | 1.52 | 4.28 | 4.02 |
| 1pgs | 68 | 77 | KNKTTGEWYE | 0.99 | 2.69 | 2.23 |
| 1ppn | 190 | 199 | KRGTGNSYGV | 1.48 | 5.08 | 2.5 |
| 1prn | 118 | 127 | NSKYDASGAL | 1.26 | 4.88 | 5.83 |
| 1sbp | 124 | 133 | TPNPKSSGGA | 0.6 | 1.56 | 0.65 |
| 1scs | 65 | 74 | VSYPNADSAT | 0.95 | 2.48 | 1.62 |
| 1tib | 237 | 246 | KIEGIDATGG | 0.67 | 3.2 | 2.31 |
| 1ukz | 21 | 30 | VLGGPGAGKG | 1.16 | 4.27 | 2.72 |
| 2alp | 90 | 105 | RVFPGNDRAW | 1.21 | 3.36 | 2.23 |
| 2ayh | 80 | 89 | KPAKNTGIVS | 0.98 | 2.66 | 1.74 |
| 2cmd | 57 | 66 | GFSGEDATPA | 0.54 | 3.61 | 0.54 |
| 2ctc | 66 | 75 | LGIHSREWIT | 1.23 | 2.57 | 2.01 |
| 2mnr | 91 | 100 | FCLAGYTGLI | 1.32 | 4 | 1.57 |
| 2sil | 197 | 206 | RTKNITTVLN | 1.44 | 3.56 | 1.88 |
| 2sn3 | 30 | 39 | KAKNQGGSYG | 1.06 | 4.51 | 1.72 |
| 3hsc | 28 | 37 | IIANDQGNRT | 1.11 | 3.24 | 2.95 |
| 3tgl | 257 | 266 | HLSYFGINTG | 0.64 | 2.64 | 0.64 |
| 4fgf | 42 | 51 | GVREKSDPHI | 0.69 | 2.95 | 1.3 |
| 5fx2 | 59 | 68 | TWGDDSIELQ | 1.7 | 4.58 | 2.63 |
| 5p21 | 8 | 17 | VVGAGGVGKS | 1.17 | 2.9 | 1.98 |
| 5pti | 23 | 32 | YNAKAGLCQT | 0.77 | 2.71 | 2.36 |
| 7rsa | 110 | 119 | CEGNPYVPVH | 1.83 | 9.08 | 2.28 |
| Mean | | | | **1.15** | **3.96** | **2.33** |

$R_{\min}$, $R_{\text{ave}}$ and $R_{Emin}$ denote the average minimum backbone RMSD, the average ensemble RMSD and the average RMSD of the lowest energy conformations of the 1,000 loop ensemble with the same length, respectively.

Table 11: **Results of 11-residue loops on Test Set 3, calculated using DISGRO.**

| PDB | Start | End | Sequence | $R_{\min}$ | $R_{\text{ave}}$ | $R_{Emin}$ |
|---|---|---|---|---|---|---|
| 1aaj | 91 | 101 | HCTPHPFMRGK | 0.99 | 2.25 | 1.67 |
| 1acf | 58 | 68 | GGFDLAGVHYV | 1.24 | 10.51 | 1.89 |
| 1amp | 32 | 42 | FTNRFYTTTSG | 1.58 | 6.7 | 2.52 |
| 1arb | 212 | 222 | GPSSCSATGTN | 2.18 | 9.1 | 2.18 |
| 1art | 189 | 199 | HGCCHNPTGID | 1.47 | 2.72 | 2.42 |
| 1byb | 22 | 32 | VVNVDNVFEDP | 2.26 | 4.72 | 3.1 |
| 1cid | 121 | 131 | VMGPTSPKMRL | 1.09 | 2.76 | 2.41 |
| 1esl | 144 | 154 | CDPGFSGLKCE | 1.58 | 5.86 | 4.29 |
| 1ezm | 24 | 34 | LIVNDRCEMDD | 1.16 | 4.71 | 2.09 |
| 1iab | 79 | 89 | LQANGCVYHGT | 1.71 | 5.53 | 1.81 |
| 1knb | 521 | 531 | YLNGDKTKPVT | 1.5 | 3.67 | 2.29 |
| 1mrk | 92 | 102 | AKYVFKDAMRK | 1.75 | 3.85 | 2.66 |
| 1noa | 97 | 107 | LSDAAGNGPEG | 1.45 | 4.45 | 5.43 |
| 1phf | 100 | 110 | PTSMDPPEQRQ | 1.56 | 3.77 | 2.73 |
| 1php | 269 | 279 | ADRFANDANTK | 1.5 | 2.89 | 2.94 |
| 1pii | 282 | 292 | IFVATSPRCVN | 1.47 | 5.97 | 2.03 |
| 1plc | 5 | 15 | LGADDGSLAFV | 1.36 | 6.71 | 1.89 |
| 1tca | 68 | 78 | PPPFMLNDTQV | 2.16 | 6.19 | 5.16 |
| 1trb | 87 | 97 | VDLQNRPFRLN | 1.38 | 5.79 | 2.15 |
| 1xnb | 41 | 51 | GWTTGSPFRTI | 1.15 | 3.61 | 1.4 |
| 2exo | 170 | 180 | DYNVEGINAKS | 1.21 | 4.78 | 2 |
| 2hbg | 45 | 55 | FGFSGASDPGV | 0.97 | 4.99 | 1.25 |
| 2pia | 74 | 84 | KRDSNGRGGSI | 1.47 | 3.71 | 2.74 |
| 2pgd | 222 | 232 | WNKTELDSFLI | 1.19 | 4.85 | 6.11 |
| 2rhe | 38 | 48 | QQVPGKAPKLL | 1.3 | 7.01 | 8.26 |
| 3grs | 267 | 277 | TAVPGRLPVMT | 1.37 | 7.36 | 8.88 |
| 3hsc | 56 | 66 | KNQVAMNPTNT | 1.13 | 3.49 | 3.84 |
| 3tgl | 98 | 108 | SYPPVSGTKVH | 1.31 | 3.66 | 2.78 |
| 4enl | 206 | 216 | GNVGDEGGVAP | 1.35 | 5.72 | 1.45 |
| 4i1b | 123 | 133 | STSQAENMPVF | 0.89 | 3.29 | 1.05 |
| 5p21 | 144 | 154 | TSAKTRQGVED | 0.83 | 3.39 | 2.21 |
| 6taa | 150 | 160 | CFIQNYEDQTQ | 1.25 | 6.13 | 2.12 |
| 8dfr | 39 | 49 | STSHVEGKQNA | 1.04 | 3.7 | 2.46 |
| Mean | | | | **1.39** | **4.96** | **2.98** |

$R_{\min}$, $R_{\text{ave}}$ and $R_{Emin}$ denote the average minimum backbone RMSD, the average ensemble RMSD and the average RMSD of the lowest energy conformations of the 1,000 loop ensemble with the same length, respectively.

Table 12: **Results of 12-residue loops on Test Set 3, calculated using** DISGRO**.**

| PDB | Start | End | Sequence | $R_{\min}$ | $R_{\text{ave}}$ | $R_{Emin}$ |
|---|---|---|---|---|---|---|
| 154l | 153 | 164 | NVRSYARMDIGT | 1.43 | 4.47 | 3.23 |
| 1arp | 201 | 212 | LDSTPQVFDTQF | 1.23 | 4.38 | 1.48 |
| 1ctm | 9 | 20 | YENPREATGRIV | 1.62 | 5.44 | 1.62 |
| 1cyo | 12 | 23 | IQKHNNSKSTWL | 1.04 | 4.25 | 2.93 |
| 1dts | 41 | 52 | SGSEKTPEGLRN | 1.9 | 11.47 | 6.24 |
| 1eco | 35 | 46 | MAKFTQFAGKDL | 1.58 | 3.63 | 2.45 |
| 1ede | 150 | 161 | CLMTDPVTQPAF | 1.52 | 3.3 | 1.94 |
| 1ezm | 122 | 133 | FGDGATMFYPLV | 1.17 | 3.25 | 1.29 |
| 1hfc | 165 | 176 | RGDHRDNSPFDG | 1.96 | 7.61 | 2.27 |
| 1msc | 9 | 20 | LVDNGGTGDVTV | 1.77 | 6.42 | 7.66 |
| 1onc | 23 | 34 | MSTNLFHCKDKN | 2.41 | 5.37 | 3.77 |
| 1pbe | 129 | 140 | LHDLQGERPYVT | 1.33 | 6.05 | 2.12 |
| 1pmy | 77 | 88 | KCAPHYMMGMVA | 1.42 | 3.15 | 2.56 |
| 1prn | 15 | 26 | VEDRGVGLEDTI | 1.83 | 5.46 | 5.99 |
| 1rcf | 88 | 99 | TGDQIGYADNFQ | 1.44 | 5.46 | 1.49 |
| 1rro | 17 | 28 | ECQDPDTFEPQK | 1.17 | 4.5 | 1.17 |
| 1scs | 199 | 210 | IKSPDSHPADGI | 0.9 | 2.98 | 2.46 |
| 1srp | 311 | 322 | SDVGGLKGNVSI | 0.68 | 2.25 | 0.68 |
| 1tca | 305 | 316 | AVGKRTCSGIVT | 1.65 | 11.17 | 8.24 |
| 1thg | 127 | 138 | WIYGGAFVYGSS | 1.49 | 3.04 | 2.16 |
| 1thw | 178 | 189 | PDAFSYVLDKPT | 1.17 | 6.67 | 1.27 |
| 1tib | 99 | 110 | EINDICSGCRGH | 1.49 | 3.71 | 2.11 |
| 1tml | 243 | 254 | STTNTGDPMIDA | 1.99 | 5.79 | 2.52 |
| 1xif | 203 | 214 | IERLERPELYGV | 1.25 | 3.09 | 1.93 |
| 2cpl | 145 | 156 | FGSRNGKTSKKI | 1.98 | 5.67 | 4.42 |
| 2ebn | 136 | 147 | YQTPPPSGFVTP | 1.72 | 7.88 | 3.21 |
| 2exo | 293 | 304 | LVWDASYAKKPA | 2.27 | 5.46 | 4.61 |
| 2pgd | 361 | 372 | WRGGCIIRSVFL | 1.3 | 5 | 1.75 |
| 2sil | 255 | 266 | ETKDFGKTWTEF | 1.46 | 5.52 | 2.09 |
| 2tgi | 48 | 59 | CPYLWSSDTQHS | 1.38 | 3.89 | 1.57 |
| 3hsc | 72 | 83 | RLIGRRFDDAVV | 1.18 | 4.95 | 1.18 |
| 451c | 16 | 27 | HAIDTKMVGPAY | 1.69 | 6.39 | 6.82 |
| 4enl | 372 | 383 | SHRSGETEDTFI | 1.22 | 2.83 | 2.32 |
| 4i1b | 46 | 57 | FVQGEESNDKIP | 2.29 | 7.3 | 3.98 |
| Mean | | | | **1.53** | **5.23** | **2.99** |

$R_{\min}$, $R_{\text{ave}}$ and $R_{Emin}$ denote the average minimum backbone RMSD, the average ensemble RMSD and the average RMSD of the lowest energy conformations of the 1,000 loop ensemble with the same length, respectively.

Table 13: **The average RMSD of lowest energy conformations ($R_{Emin}$) of 8-residue loops on Test Set 4, obtained by using LOOPY, LOOPY/PLOP, DFIRE, LoopBuilder and DISGRO.**

| PDB | Range | Sequence | LOOPY | LOOPY/PLOP | DFIRE | LoopBuilder | DISGRO |
|---|---|---|---|---|---|---|---|
| 135l | 84-91 | LSSDITAS | 1.46 | 2.61 | 0.40 | 0.40 | 0.83 |
| 1a3c | 92-99 | IPVDITDQ | 3.36 | 2.06 | 1.29 | 3.31 | 1.98 |
| 1a621 | 71-78 | SYLAGPDD | 4.95 | 4.33 | 2.23 | 1.59 | 2.13 |
| 1a622 | 103-110 | PPKEGERY | 3.84 | 2.00 | 2.35 | 3.05 | 1.7 |
| 1ads | 274-281 | KVFDFELS | 1.05 | 1.09 | 0.78 | 0.38 | 1.24 |
| 1alc | 34-41 | SGYDTQAI | 3.06 | 6.51 | 0.82 | 6.45 | 0.84 |
| 1amm2 | 81-88 | IPQHTGTF | 2.00 | 1.27 | 2.47 | 2.13 | 1.95 |
| 1amm3 | 158-165 | GAMNAKVG | 1.14 | 2.37 | 1.24 | 0.36 | 2.42 |
| 1arb1 | 136-143 | RRDQNYPG | 1.93 | 1.65 | 2.88 | 0.46 | 1.38 |
| 1arb2 | 212-219 | GPSSCSAT | 1.63 | 0.44 | 1.30 | 0.77 | 1.97 |
| 1arb3 | 249-256 | DPASTGAQ | 4.06 | 2.11 | 1.79 | 2.24 | 1.03 |
| 1aru | 234-241 | LSPFPGEF | 1.14 | 0.84 | 0.79 | 0.75 | 1 |
| 1btk1 | 67-74 | VVPEKNPP | 2.11 | 1.90 | 1.58 | 1.41 | 2.11 |
| 1btk2 | 133-140 | RYNSDLVQ | 3.73 | 4.86 | 4.35 | 1.54 | 1.4 |
| 1btl | 50-57 | DLNSGKIL | 1.56 | 0.53 | 1.40 | 1.81 | 1.77 |
| 1c52 | 97-104 | VKGFKPFT | 1.78 | 1.65 | 0.80 | 1.19 | 1.32 |
| 1cex | 73-80 | VGGAYRAT | 1.53 | 4.41 | 3.14 | 0.85 | 3.92 |
| 1clc | 313-320 | FRPYDPQY | 0.77 | 2.09 | 1.55 | 0.31 | 1.13 |
| 1cvl1 | 148-155 | TLVSSSHN | 1.58 | 1.09 | 2.50 | 1.46 | 1.17 |
| 1cvl2 | 229-236 | TSTGTLDV | 2.10 | 2.08 | 2.01 | 0.67 | 1.96 |
| 1ddt | 127-134 | FGDGASRV | 2.08 | 1.79 | 2.39 | 0.86 | 1.32 |
| 1ezm1 | 92-99 | GTSPLTHK | 2.04 | 2.09 | 3.05 | 0.33 | 1.16 |
| 1fnd | 262-269 | LKKDNTYV | 0.66 | 0.90 | 2.12 | 0.52 | 0.47 |
| 1gof | 606-613 | VPSDSGVA | 0.88 | 0.53 | 0.65 | 0.51 | 0.69 |
| 1hbq | 31-38 | DPEGLFLQ | 1.36 | 1.72 | 2.64 | 1.27 | 1.14 |
| 1iab | 48-55 | RTTESDYV | 0.73 | 2.42 | 3.25 | 1.83 | 2.57 |
| 1lit | 82-89 | DPKKNRRW | 6.11 | 2.20 | 2.74 | 2.02 | 1.63 |
| 1lst | 101-108 | PIQPTLES | 1.78 | 5.02 | 3.96 | 0.73 | 2.03 |
| 1mpp | 74-81 | TYGTGGAN | 2.91 | 1.24 | 1.18 | 1.25 | 1.56 |
| 1mrp | 68-75 | AGLLAPIS | 0.49 | 0.30 | 0.49 | 1.61 | 1.32 |
| 1msi | 26-33 | VVTPVGIP | 1.44 | 2.53 | 1.18 | 1.01 | 1.25 |
| 1nar | 192-199 | FSNQQKPV | 1.28 | 0.68 | 1.13 | 0.64 | 1.17 |
| 1nfp | 118-125 | NVDIANVR | 1.24 | 3.69 | 1.22 | 0.97 | 1.49 |
| 1nif1 | 221-228 | NGAVGALT | 2.57 | 1.26 | 1.17 | 1.10 | 2.16 |
| 1nif2 | 279-286 | ETWLIPGG | 0.81 | 0.50 | 0.62 | 0.50 | 1.04 |
| 1nls | 97-104 | TGLYKETN | 0.83 | 0.93 | 0.75 | 0.21 | 1.26 |
| 1nwp | 84-91 | TKVIGAGE | 1.81 | 0.79 | 0.79 | 0.20 | 0.82 |
| 1oyc | 80-87 | GGYDNAPG | 1.57 | 0.73 | 0.74 | 0.56 | 0.94 |
| 1poa | 71-78 | CSQGTLTC | 1.66 | 1.44 | 1.15 | 0.89 | 2.03 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 1ppn2 | 191-198 | RGTGNSYG | 3.12 | 1.60 | 3.26 | 3.63 | 2.45 |
| 1prn | 150-157 | DPDQTVDS | 3.16 | 2.26 | 1.17 | 0.78 | 2.16 |
| 1rro | 18-25 | CQDPDTFE | 1.22 | 0.64 | 2.80 | 0.69 | 1.13 |
| 1sbp | 107-114 | KQIHDWND | 0.69 | 0.33 | 1.15 | 0.30 | 1.82 |
| 1thw | 18-25 | SKGDAALD | 1.70 | 1.87 | 1.58 | 0.34 | 1.23 |
| 1tml | 187-194 | NTSNYRWT | 1.48 | 2.14 | 1.31 | 0.72 | 0.58 |
| 1wer1 | 824-831 | SKQSCELS | 1.59 | 0.49 | 1.64 | 1.35 | 0.67 |
| 1wer2 | 916-923 | NIISDSPS | 1.36 | 2.20 | 0.72 | 1.85 | 1.52 |
| 1xnb | 99-106 | KSDGGTYD | 1.34 | 5.05 | 2.57 | 1.32 | 2.21 |
| 2arc | 28-35 | ANGYLDFF | 2.51 | 0.98 | 1.14 | 1.29 | 3.78 |
| 2ayh | 123-130 | YTNGVGGH | 1.70 | 3.35 | 1.52 | 1.01 | 0.7 |
| 2ayh1 | 124-131 | TNGVGGHE | 1.01 | 1.69 | 1.65 | 3.50 | 1.22 |
| 2ayh2 | 194-201 | GSYNGANP | 2.27 | 1.54 | 1.59 | 1.60 | 1.82 |
| 2cmd | 270-277 | LGKNGVEE | 1.40 | 4.96 | 1.99 | 0.36 | 1.48 |
| 2ctc | 53-60 | STGGSNRP | 2.37 | 3.31 | 1.71 | 0.99 | 2.41 |
| 2exo | 262-269 | MQVTRCQG | 0.48 | 0.55 | 0.53 | 0.38 | 1.15 |
| 2sga | 32-43 | TTGGSRCS | 1.53 | 0.95 | 1.22 | 0.97 | 1.41 |
| 3nul | 36-43 | SAKFPQLK | 1.63 | 1.18 | 1.11 | 0.72 | 2.11 |
| 3seb | 40-47 | SIDQFLYF | 1.15 | 0.27 | 0.71 | 0.40 | 0.92 |
| 5p21 | 45-52 | VIDGETCL | 1.21 | 0.61 | 0.93 | 0.56 | 1.97 |
| 5ptp1 | 22-29 | CGANTVPY | 3.42 | 3.12 | 2.37 | 3.98 | 1.35 |
| 5ptp2 | 172-179 | YPGQITSN | 0.57 | 2.02 | 0.96 | 1.30 | 2.83 |
| 7rsa | 64-71 | ACKNGQTN | 2.09 | 2.87 | 3.49 | 3.04 | 1.71 |
| 8dfr | 65-72 | RPLKDRIN | 2.91 | 2.69 | 2.21 | 3.00 | 2.4 |
| Mean | | | 1.89 | 1.96 | 1.69 | 1.31 | **1.59** |

The results of all the methods except DISGRO are obtained from Table A1 in Ref. [1].

Table 14: **The average RMSD of lowest energy conformations ($R_{Emin}$) of 9-residue loops on Test Set 4, obtained by using LOOPY, LOOPY/PLOP, DFIRE, LoopBuilder and DISGRO.**

| PDB | Range | Sequence | LOOPY | LOOPY/PLOP | DFIRE | LoopBuilder | DISGRO |
|---|---|---|---|---|---|---|---|
| 1aac | 58-66 | VAGVLGEAA | 3.97 | 7.17 | 1.65 | 1.62 | 2.51 |
| 1aba | 69-77 | FAPDGSHIG | 1.50 | 0.76 | 0.91 | 0.90 | 1.33 |
| 1amp | 57-65 | SASLPNASV | 1.41 | 4.92 | 1.14 | 0.77 | 1.83 |
| 1arb1 | 90-98 | ANGDGSMSQ | 0.96 | 3.60 | 1.22 | 0.55 | 1.16 |
| 1arb2 | 168-176 | AWGGGAGTT | 6.07 | 7.84 | 6.54 | 6.58 | 1.68 |
| 1arp | 127-135 | SNCPGSPRL | 0.57 | 0.24 | 0.45 | 0.28 | 1.61 |
| 1aru | 36-44 | NFYQGSKCE | 2.67 | 7.59 | 2.06 | 1.30 | 2.52 |
| 1btl | 102-110 | LVEYSPVTE | 6.22 | 1.08 | 1.96 | 3.37 | 2.55 |
| 1byb | 246-254 | GFFKSNGTY | 2.23 | 5.61 | 1.14 | 0.79 | 1.31 |
| 1cse | 95-103 | VLNSSGSGS | 2.81 | 7.02 | 0.39 | 0.62 | 2.49 |
| 1csh | 252-260 | GSALSDPYL | 1.92 | 5.49 | 1.22 | 1.01 | 1.1 |
| 1ede | 257-265 | GMKDKLLGP | 1.59 | 3.37 | 1.24 | 0.76 | 1.83 |
| 1fus | 91-99 | THTGASGNN | 3.59 | 5.22 | 7.39 | 1.90 | 3.3 |
| 1fus1 | 31-39 | DTAGSSTYP | 2.90 | 5.95 | 4.33 | 4.00 | 2.92 |
| 1gpr | 63-71 | VFPTKHAIG | 2.04 | 2.07 | 3.92 | 1.90 | 2.73 |
| 1isu | 30-38 | PGASPTAAG | 6.18 | 4.99 | 4.22 | 6.16 | 3.13 |
| 1ivd | 244-252 | GSASGRADT | 5.48 | 4.45 | 4.94 | 4.37 | 2.55 |
| 1lkk1 | 142-150 | LAPGNTHGS | 1.79 | 0.79 | 2.52 | 0.86 | 0.98 |
| 1lkk2 | 193-201 | ISPRITFPG | 2.32 | 0.73 | 1.34 | 0.91 | 1.88 |
| 1mla | 194-202 | LPVSVPSHC | 2.07 | 3.77 | 3.87 | 4.48 | 2.16 |
| 1mrj | 92-100 | AKYVFKDAM | 2.79 | 5.89 | 1.55 | 2.04 | 2.05 |
| 1mrk | 53-61 | TNYADETIS | 1.22 | 4.06 | 1.30 | 0.63 | 1.81 |
| 1mrp | 284-292 | EAPVVSATT | 2.04 | 1.48 | 2.86 | 2.74 | 1.51 |
| 1nfp | 12-20 | NFYHVGQQE | 1.74 | 4.60 | 3.88 | 3.79 | 5.12 |
| 1nif | 266-274 | ATGKFRNPP | 1.11 | 1.31 | 1.97 | 0.57 | 1.4 |
| 1nls | 131-139 | NQFSKDQKD | 3.55 | 4.92 | 3.14 | 3.86 | 2.03 |
| 1noa | 76-84 | FLFDGTRWG | 4.61 | 7.97 | 2.95 | 2.51 | 0.89 |
| 1noa1 | 9-17 | PSSGLSDGT | 5.99 | 7.72 | 5.43 | 6.00 | 1.65 |
| 1noa2 | 99-107 | DAAGNGPEG | 4.90 | 2.55 | 4.90 | 3.34 | 1.86 |
| 1npk | 102-110 | ASAPGSIRG | 1.27 | 0.30 | 0.74 | 0.23 | 0.82 |
| 1onc | 70-78 | VTSRPCKYK | 10.31 | 7.52 | 3.01 | 1.70 | 1.69 |
| 1pda | 108-116 | FVSNNYDSL | 1.28 | 0.91 | 0.98 | 0.58 | 1.24 |
| 1pgs | 117-125 | TETWLAKGR | 0.72 | 1.84 | 2.13 | 0.59 | 2.14 |
| 1php | 91-99 | TNEAVGDEV | 2.45 | 1.37 | 2.43 | 0.60 | 0.48 |
| 1ptf | 10-18 | AETGIHARP | 3.23 | 3.02 | 1.51 | 2.12 | 1.38 |
| 1ra9 | 142-150 | DADAQNSHS | 2.30 | 2.72 | 3.39 | 1.99 | 2.5 |
| 1rhs | 216-224 | LTEDGFEKS | 2.70 | 5.62 | 2.91 | 1.54 | 2.5 |
| 1sgp | 109-117 | TNTTIPKDG | 1.51 | 2.31 | 2.29 | 0.63 | 2.31 |
| 1tca1 | 170-178 | AGGLTQIVP | 2.04 | 0.99 | 1.76 | 0.47 | 1.24 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 1tca2 | 217-225 | GPLFVIDHA | 1.95 | 0.48 | 1.58 | 0.47 | 1.22 |
| 1wer | 942-950 | NLVEFGAKE | 5.66 | 7.29 | 8.31 | 5.34 | 1.81 |
| 1xif | 59-67 | IPFGSSDSE | 3.71 | 5.59 | 2.99 | 1.04 | 1.65 |
| 1xnb | 133-141 | QSKRPTGSN | 1.06 | 0.87 | 1.95 | 1.02 | 2.05 |
| 1xnb1 | 116-124 | PSIDGDRTT | 3.58 | 0.97 | 1.15 | 1.76 | 2.02 |
| 1xyz1 | 568-576 | QPRQNVFDF | 1.74 | 4.86 | 1.83 | 1.01 | 1.07 |
| 1xyz2 | 795-803 | WGFTDKYTW | 1.67 | 0.98 | 1.80 | 2.55 | 1.16 |
| 2ayh | 169-177 | TANIPSTPG | 0.74 | 1.06 | 2.32 | 0.55 | 2.13 |
| 2cpl | 24-32 | LFADKVPKT | 2.72 | 5.65 | 1.00 | 0.22 | 1.00 |
| 2eng | 172-180 | DWFKNADNP | 1.81 | 1.93 | 1.65 | 2.14 | 0.97 |
| 2hbg | 18-26 | AGADNGAGV | 1.40 | 4.18 | 1.78 | 0.43 | 1.09 |
| 2sil | 183-191 | QLNDGKLVF | 1.74 | 2.72 | 1.32 | 0.33 | 2.24 |
| 3pte1 | 78-86 | EGKLDLDAS | 0.96 | 0.46 | 0.96 | 0.51 | 0.85 |
| 3pte2 | 107-115 | SHRSGLYDY | 1.20 | 0.37 | 1.52 | 0.33 | 2.18 |
| 3pte3 | 215-223 | TPDEAGGAL | 4.19 | 4.28 | 3.87 | 3.29 | 0.59 |
| 3tgl | 56-64 | STLIYDTNA | 1.61 | 6.15 | 3.27 | 3.12 | 2.35 |
| 4gcr | 94-102 | ERDDFRGQM | 1.74 | 7.81 | 2.11 | 1.99 | 2.18 |
| Mean | | | 2.71 | 3.67 | 2.52 | 1.88 | **1.83** |

The results of all the methods except DISGRO are obtained from Table A1 in Ref. [1].

Table 15: **The average RMSD of lowest energy conformations ($R_{Emin}$) of 10-residue loops on Test Set 4, obtained by using LOOPY, LOOPY/PLOP, DFIRE, LoopBuilder and DISGRO.**

| PDB | Range | Sequence | LOOPY | LOOPY/PLOP | DFIRE | LoopBuilder | DISGRO |
|---|---|---|---|---|---|---|---|
| 135l | 18-27 | DNYRGYSLGN | 1.53 | 8.30 | 1.55 | 1.12 | 1.86 |
| 1ads | 171-180 | NKPGLKYKPA | 1.06 | 0.50 | 1.50 | 0.59 | 2.14 |
| 1ads1 | 170-179 | LNKPGLKYKP | 0.96 | 1.29 | 5.05 | 0.68 | 1.6 |
| 1amp | 181-190 | TNYKGSAQDV | 2.30 | 1.80 | 2.78 | 2.21 | 1.53 |
| 1arb | 41-50 | VNNTANDRKM | 1.76 | 3.16 | 0.88 | 1.37 | 1.86 |
| 1arp | 37-46 | FYQGSKCESP | 2.16 | 4.52 | 1.45 | 0.86 | 1.51 |
| 1aru | 128-137 | NCPGSPRLEF | 2.21 | 0.25 | 2.63 | 0.23 | 0.91 |
| 1avm | 145-154 | DHQNNLPAGS | 3.54 | 4.07 | 3.36 | 3.58 | 2.03 |
| 1btl | 170-179 | NEAIPNDERD | 1.84 | 3.38 | 2.34 | 2.57 | 1.72 |
| 1dim1 | 87-96 | YNDRVNSKLS | 2.98 | NA | 2.21 | 2.18 | 2.37 |
| 1dim2 | 131-140 | YRDKAPDTDW | 1.27 | 3.35 | 2.10 | 2.18 | 1.64 |
| 1ede | 164-173 | FVTQPADGFT | 4.19 | 6.86 | 4.21 | 0.92 | 1.99 |
| 1edg | 269-278 | GGTNAWNIND | 1.15 | 1.95 | 0.60 | 0.25 | 0.73 |
| 1ezm | 237-246 | ANSPGWDTRK | 0.56 | 0.75 | 0.67 | 0.42 | 1.27 |
| 1fkf | 63-72 | VAQMSVGQRA | 0.83 | 0.42 | 0.56 | 0.26 | 1.54 |
| 1gpr | 133-142 | FTNLAEGETV | 3.43 | 2.83 | 4.64 | 4.65 | 2.09 |
| 1gvp | 49-58 | LDEGQPAYAP | 2.79 | 1.54 | 2.73 | 3.03 | 1.7 |
| 1ixh | 84-93 | NIPGLKSGEL | 4.67 | 3.63 | 1.57 | 0.39 | 2.74 |
| 1knt | 35-44 | YGGCGGNENK | 1.48 | 5.24 | 1.66 | 4.32 | 2.23 |
| 1mrj | 173-182 | KRVDKTFLPS | 2.85 | 7.86 | 0.77 | 0.36 | 1.03 |
| 1onc | 48-57 | CKGIIASKNV | 3.81 | 2.41 | 5.66 | 5.02 | 3.61 |
| 1pgs | 68-77 | KNKTTGEWYE | 2.30 | 0.76 | 2.74 | 0.74 | 1.25 |
| 1plc | 42-51 | DEDSIPSGVD | 5.38 | 4.28 | 1.35 | 2.30 | 2.16 |
| 1ppn | 190-199 | KRGTGNSYGV | 2.12 | 3.10 | 2.64 | 1.73 | 2.67 |
| 1scs | 65-74 | VSYPNADSAT | 2.00 | 6.34 | 2.57 | 1.48 | 1.56 |
| 1tca1 | 23-32 | QGASPSSVSK | 5.90 | 5.97 | 1.97 | 0.89 | 1.69 |
| 1tca2 | 258-267 | CNPLPANDLT | 1.77 | 0.28 | 0.89 | 0.22 | 2.19 |
| 1whi | 47-56 | TPGGVVKKGQ | 2.15 | 5.70 | 1.46 | 1.56 | 1.46 |
| 2alp | 90-105 | RVFPGNDRAW | 0.70 | NA | 1.61 | 2.13 | 1.56 |
| 2ayh | 80-89 | KPAKNTGIVS | 1.48 | 1.33 | 0.63 | 0.27 | 1.5 |
| 2cmd | 57-66 | GFSGEDATPA | 4.26 | 7.42 | 0.85 | 2.27 | 0.45 |
| 2mnr | 91-100 | FCLAGYTGLI | 4.14 | 3.47 | 2.91 | 2.99 | 1.43 |
| 2sil | 197-206 | RTKNITTVLN | 1.60 | 1.87 | 4.76 | 2.74 | 1.6 |
| 3hsc | 28-37 | IIANDQGNRT | 3.35 | 4.47 | 3.95 | 4.40 | 2.75 |
| 3seb | 200-209 | MMPAPGDKFD | 0.89 | 0.34 | 0.54 | 0.28 | 1.3 |
| 3tgl | 257-266 | HLSYFGINTG | 1.52 | 1.71 | 1.00 | 0.94 | 1.7 |
| 4fgf | 42-51 | GVREKSDPHI | 2.53 | 4.76 | 3.41 | 3.31 | 0.68 |
| 7rsa | 110-119 | CEGNPYVPVH | 2.32 | 2.96 | 2.91 | 2.33 | 2.43 |
| 7rsa1 | 33-42 | RNLTKDRCKP | 2.65 | 4.49 | 3.64 | 3.54 | 3.45 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 7rsa2 | 87-96 | TGSSKYPNCA | 3.16 | 6.32 | 5.21 | 6.29 | 3.22 |
| Mean | | | 2.42 | 3.40 | 2.41 | 1.93 | **1.83** |

The results of all the methods except DISGRO are obtained from Table A1 in Ref. [1].

Table 16: **The average RMSD of lowest energy conformations ($R_{Emin}$) of 11-residue loops on Test Set 4, obtained by using LOOPY, LOOPY/PLOP, DFIRE, LoopBuilder and DISGRO.**

| PDB | Range | Sequence | LOOPY | LOOPY/PLOP | DFIRE | LoopBuilder | DISGRO |
|---|---|---|---|---|---|---|---|
| 153l | 154-164 | VRSYARMDIGT | 2.41 | 3.59 | 3.32 | 0.80 | 2.26 |
| 1a2p | 76-86 | INYTSGFRNSD | 2.13 | 9.30 | 3.05 | 2.68 | 1.78 |
| 1a2y | 91-101 | FWSTPRTFGGG | 2.39 | 2.07 | 2.78 | 1.44 | 2.29 |
| 1a8d | 195-205 | ITGLGAIREDN | 1.97 | 2.45 | 1.64 | 1.51 | 1.79 |
| 1ads | 290-300 | SYNRNWRVCAL | 1.71 | 1.54 | 2.22 | 1.24 | 1.51 |
| 1ako | 110-120 | FPQGESRDHPI | 3.05 | 2.11 | 7.88 | 1.89 | 1.97 |
| 1akz | 211-221 | AHQANSHKERG | 2.56 | 3.05 | 1.23 | 1.16 | 2.75 |
| 1aol | 152-162 | VYWKPSSSWDY | 3.01 | 3.94 | 3.26 | 2.86 | 1.41 |
| 1aru | 297-307 | IPSAVSNNAAP | 2.38 | 1.67 | 2.36 | 2.40 | 1.86 |
| 1awq | 1101-1111 | ANAGPNTNGSQ | 2.03 | 1.67 | 2.11 | 0.77 | 1.38 |
| 1bol | 33-43 | WAPGYGPDNAF | 1.84 | 3.82 | 2.83 | 4.20 | 2.78 |
| 1bx4 | 250-260 | ALPKMNSKRQR | 2.42 | 2.29 | 4.82 | 0.94 | 2.42 |
| 1c5e | 82-92 | YEDVLWPEAAS | 2.36 | 9.04 | 2.70 | 0.37 | 2.12 |
| 1cb0 | 33-43 | YVDTPFGKPSD | 8.16 | 4.22 | 2.21 | 2.91 | 1.35 |
| 1cnv | 162-172 | APGCLSPDEYL | 3.88 | 2.47 | 4.05 | 1.88 | 1.92 |
| 1cs6 | 145-155 | NEFPNFIPADG | 4.31 | 7.95 | 3.68 | 5.11 | 2.58 |
| 1cvl | 257-267 | RASGQNDGLVS | 2.81 | 11.56 | 1.54 | 1.32 | 7.88 |
| 1dad | 42-52 | GSEKTPEGLRN | 4.49 | 4.12 | 13.49 | 3.14 | 3.71 |
| 1dys | 290-300 | FGQPFTTNTNN | 2.37 | 10.06 | 2.23 | 1.90 | 2 |
| 1edt | 93-103 | NHQGAGFANFP | 1.93 | 1.62 | 1.49 | 0.55 | 1.35 |
| 1eur | 87-97 | RPTGIDAPGPN | 2.81 | 5.95 | 5.26 | 4.14 | 3.1 |
| 1exm | 291-301 | RGVSREEVERG | 3.53 | 4.09 | 2.53 | 1.47 | 0.75 |
| 1f46 | 64-74 | MVKPGTFDPEM | 5.06 | 4.18 | 1.78 | 2.23 | 2.53 |
| 1fus | 28-38 | QNDDTAGSSTY | 1.87 | 8.25 | 6.37 | 0.38 | 2.59 |
| 1g6s | 77-87 | GNGGPLHAEGA | 2.92 | 3.94 | 1.04 | 1.45 | 0.91 |
| 1g9g | 125-135 | LDTSQPVGRDP | 2.43 | 2.30 | 1.01 | 2.67 | 1.89 |
| 1gmu | 44-54 | LPRGLLLRGGD | 3.76 | 3.14 | 4.51 | 1.20 | 1.62 |
| 1gqv | 114-124 | RDQRRDPPQYP | 2.79 | 6.46 | 6.38 | 3.03 | 2.38 |
| 1i4j | 86-96 | LPRARGRADII | 4.18 | 4.61 | 8.38 | 4.59 | 1.73 |
| 1iu8 | 85-95 | ARIPDNDGEQP | 2.00 | 9.05 | 9.53 | 4.54 | 1.1 |
| 1ixh | 120-130 | NPGLKLPSQNI | 2.04 | 1.44 | 1.81 | 1.13 | 1.45 |
| 1jp4 | 179-189 | GFQLKEAPAGK | 2.20 | 4.05 | 1.39 | 2.04 | 2.38 |
| 1k7i | 137-147 | TRDASGNLDYG | 3.68 | 8.11 | 5.57 | 7.87 | 4.41 |
| 1lmi | 34-44 | STAVIPGYPVA | 2.54 | 2.64 | 1.76 | 0.90 | 1.68 |
| 1mla | 9-19 | PGQGSQTVGML | 4.13 | 1.84 | 4.68 | 3.60 | 4.06 |
| 1my7 | 254-264 | TPPYADPSLQA | 2.27 | 1.89 | 2.85 | 2.00 | 1.36 |
| 1nln | 26-36 | DKRFPGFVSPH | 1.15 | 1.48 | 1.08 | 0.91 | 1.8 |
| 1nls | 216-226 | NIDSSIPSGST | 3.95 | 1.64 | 1.66 | 3.45 | 1.88 |
| 1nog | 98-108 | GKIELFVVPGG | 2.69 | 2.05 | 2.81 | 2.53 | 2.39 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 1nsc | 383-393 | DGDPWTDSDAL | 4.51 | 8.59 | 3.61 | 4.87 | 3.51 |
| 1ojq | 141-151 | LVSGAALAGRP | 5.12 | 5.92 | 3.43 | 5.35 | 1.4 |
| 1oth | 69-79 | QKGEYLPLLQG | 1.68 | 2.44 | 1.21 | 1.38 | 2.15 |
| 1oyc | 203-213 | DPHSNTRTDEY | 2.82 | 3.72 | 1.55 | 0.56 | 3.55 |
| 1pgs | 83-93 | TPYWVGTEKLP | 1.92 | 3.39 | 3.24 | 4.08 | 2.52 |
| 1pkh | 44-54 | DDEVYDLSKEL | 7.35 | 5.02 | 6.88 | 7.69 | 3.65 |
| 1qlw | 31-41 | ETLSLSPKYDA | 1.91 | 11.88 | 1.98 | 1.82 | 3.53 |
| 1rcf | 122-132 | TDGYDFNDSKA | 1.95 | 7.62 | 1.64 | 3.63 | 2.78 |
| 1t1d | 127-137 | SGGRLRRPVNV | 2.33 | 0.89 | 3.35 | 0.66 | 3.25 |
| 1whi | 25-35 | LGGSGRRYANI | 6.93 | 1.25 | 8.08 | 5.70 | 2.26 |
| 2eng | 124-134 | IPGGGVGIFDG | 3.66 | 3.37 | 1.85 | 3.22 | 2.93 |
| 2pth | 8-18 | LANPGAEYAAT | 2.69 | 3.50 | 2.32 | 1.28 | 2.55 |
| 2tgi | 46-56 | GACPYLWSSDT | 1.86 | 4.67 | 1.88 | 0.95 | 2.73 |
| 3pte | 91-101 | LPGLLPDDRIT | 1.97 | 2.45 | 2.09 | 1.78 | 1.74 |
| 5pti | 7-17 | EPPYTGPCKAR | 2.11 | 4.99 | 2.65 | 3.07 | 3 |
| Mean | | | 3.02 | 4.36 | 3.43 | 2.50 | **2.38** |

The results of all the methods except DISGRO are obtained from Table A1 in Ref. [1].

Table 17: **The average RMSD of lowest energy conformations ($R_{Emin}$) of 12-residue loops on Test Set 4, obtained by using LOOPY, LOOPY/PLOP, DFIRE, LoopBuilder and DISGRO.**

| PDB | Range | Sequence | LOOPY | LOOPY/PLOP | DFIRE | LoopBuilder | DISGRO |
|---|---|---|---|---|---|---|---|
| 153l | 98-109 | KRSHKPQGTWNG | 7.80 | 5.80 | 2.63 | 0.82 | 3.27 |
| 1a8d | 155-166 | DLPDKFNAYLAN | 2.14 | 3.17 | 3.00 | 2.36 | 1.84 |
| 1akz | 181-192 | IEDFVHPGHGDL | 1.73 | 3.26 | 2.78 | 3.55 | 2.15 |
| 1aoz | 123-134 | PPQGKKEPFHYD | 2.74 | 4.99 | 2.40 | 4.24 | 2.34 |
| 1arb | 74-85 | NYQNSTCRAPNT | 2.32 | 2.51 | 3.26 | 1.92 | 2.94 |
| 1arb | 182-193 | WQPSGGVTEPGS | 2.97 | 3.07 | 1.62 | 3.12 | 1.38 |
| 1bhe | 121-132 | GQGGVKLQDKKV | 3.37 | 4.12 | 3.37 | 1.00 | 1.26 |
| 1bkf | 9-20 | PGDGRTFPKRGQ | 2.61 | 4.36 | 2.60 | 4.10 | 2.29 |
| 1bn8 | 298-309 | STSSSSYPFSYA | 2.14 | 4.78 | 1.70 | 0.72 | 4.26 |
| 1c5e | 82-93 | YEDVLWPEAASD | 2.51 | 2.68 | 1.50 | 0.59 | 1.07 |
| 1cb0 | 33-44 | YVDTPFGKPSDA | 6.30 | 6.71 | 2.15 | 3.09 | 1.79 |
| 1cb8 | 327-338 | DSTVAAGYKIEP | 3.24 | 4.32 | 3.81 | 4.35 | 3.95 |
| 1cex | 40-51 | RGSTETGNLGTL | 3.18 | 2.29 | 1.90 | 1.46 | 5.43 |
| 1cnv | 188-199 | FYNDRSCQYSTG | 2.46 | 4.35 | 1.71 | 3.98 | 1.87 |
| 1cs6 | 145-156 | NEFPNFIPADGR | 4.93 | 9.14 | 3.74 | 4.06 | 2.47 |
| 1dim | 213-224 | TDGITWSLPSGY | 0.68 | 0.67 | 1.94 | 2.10 | 0.97 |
| 1dqz | 209-220 | CGNGTPSDLGGD | 2.72 | 1.68 | 7.60 | 2.21 | 1.81 |
| 1el5 | 275-286 | IDPDTINREFGV | 3.73 | 4.91 | 2.46 | 1.75 | 2.85 |
| 1exm | 291-302 | RGVSREEVERGQ | 3.79 | 4.59 | 2.94 | 3.88 | 3.08 |
| 1f46 | 64-75 | MVKPGTFDPEMK | 2.72 | 2.54 | 2.46 | 2.31 | 2.91 |
| 1i7p | 63-74 | LPSPQHILGLPI | 3.86 | 3.76 | 7.01 | 1.49 | 2.39 |
| 1ioo | 179-190 | RCPQSDTCDKTANA | 2.04 | NA | 3.05 | 2.17 | 2.37 |
| 1ixh | 160-171 | VGTGSTVKWPIG | 2.15 | 3.05 | 2.34 | 2.46 | 2 |
| 1iye | 103-114 | GDVGMGVNPPAGNA | 4.31 | NA | 2.14 | 4.36 | 3.36 |
| 1jp4 | 179-190 | GFQLKEAPAGKH | 4.22 | 3.74 | 3.04 | 1.93 | 2.32 |
| 1kcm | 118-129 | PDLGTQENVHKL | 2.65 | 5.61 | 2.28 | 2.79 | 2.05 |
| 1luc | 158-169 | LNPSAYTQGGAP | 2.75 | 4.05 | 3.60 | 3.85 | 4.25 |
| 1m3s | 68-79 | VGEILTPPLAEG | 6.15 | 6.36 | 6.03 | 5.89 | 5.03 |
| 1ms9 | 529-540 | GSTPVTPTGSWE | 1.53 | 1.75 | 1.99 | 1.67 | 2.1 |
| 1my7 | 254-265 | TPPYADPSLQAP | 2.27 | 1.65 | 3.64 | 1.91 | 1.39 |
| 1oth | 69-80 | QKGEYLPLLQGK | 1.67 | 1.46 | 3.73 | 0.41 | 2.16 |
| 1oyc | 203-214 | DPHSNTRTDEYG | 4.11 | 3.22 | 2.30 | 3.23 | 3.75 |
| 1pkh | 44-55 | DDEVYDLSKELN | 5.29 | 11.46 | 5.58 | 4.42 | 3.23 |
| 1qlw | 31-42 | ETLSLSPKYDAH | 2.33 | 6.39 | 4.52 | 2.95 | 2.97 |
| 1t1d | 127-138 | SGGRLRRPVNVP | 2.27 | 1.22 | 2.97 | 2.13 | 2.51 |
| 1xyz | 813-824 | NPLIYDSNYNPK | 1.05 | 6.77 | 1.05 | 0.65 | 2.68 |
| 2ayh1 | 21-32 | ADGYSNGGVFNC | 3.24 | 2.01 | 5.65 | 3.08 | 3.61 |
| 2hlc | 91-102 | HSMFNPDTYLND | 3.88 | 5.09 | 4.29 | 5.44 | 3.56 |
| 2pia | 30-41 | DPQGAPLPPFEA | 3.38 | 5.21 | 1.14 | 3.35 | 1.25 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 2ptd | 136-147 | YFVDPIFLKTEG | 2.77 | 5.20 | 1.71 | 1.42 | 1.84 |
| Mean | | | 3.15 | 4.11 | 3.15 | 2.65 | **2.62** |

The results of all the methods except DISGRO are obtained from Table A1 in Ref. [1].

Table 18: **The average RMSD of lowest energy conformations ($R_{Emin}$) of 13-residue loops on Test Set 4, obtained by using LOOPY, LOOPY/PLOP, DFIRE, LoopBuilder and DISGRO.**

| PDB | Range | Sequence | LOOPY | LOOPY/PLOP | DFIRE | LoopBuilder | DISGRO |
|---|---|---|---|---|---|---|---|
| 16pk | 132-144 | ENVRFYKEEGSKK | 3.28 | 6.48 | 4.12 | 2.40 | 4.49 |
| 1a8d | 155-167 | DLPDKFNAYLANK | 3.36 | 4.77 | 2.01 | 1.71 | 3.15 |
| 1a8d1 | 74-86 | KAMDIEYNDMFNN | 3.12 | 4.49 | 3.09 | 6.53 | 3.79 |
| 1arb | 182-194 | WQPSGGVTEPGSS | 2.87 | 3.43 | 2.71 | 3.21 | 1.95 |
| 1bhe | 121-133 | GQGGVKLQDKKVS | 10.18 | 9.63 | 6.31 | 11.02 | 3.91 |
| 1bkp | 51-63 | DNSEVPILTTKKV | 2.37 | 1.11 | 1.30 | 0.82 | 3.91 |
| 1cnv | 110-122 | LSERREGPLGKVA | 10.47 | 10.18 | 2.84 | 12.52 | 1.56 |
| 1cru | 357-369 | YKGGKKAITGWEN | 3.90 | 6.75 | 9.68 | 3.58 | 4.89 |
| 1dpg | 352-364 | KAGTFNFGSEQEA | 5.26 | 6.68 | 2.08 | 1.37 | 8.97 |
| 1dqz | 209-221 | CGNGTPSDLGGDN | 7.72 | 5.77 | 6.98 | 2.40 | 2.68 |
| 1dys | 290-302 | FGQPFTTNTNNPN | 3.17 | 1.45 | 3.77 | 2.42 | 1.46 |
| 1ed8 | 67-79 | GAGGFFKGIDALP | 3.24 | 5.02 | 1.02 | 0.51 | 3.03 |
| 1eok | 147-159 | GYNGWYSGSMAAT | 2.78 | 2.02 | 3.84 | 0.71 | 1.67 |
| 1f46 | 64-76 | MVKPGTFDPEMKD | 3.03 | 3.27 | 3.54 | 2.75 | 2.21 |
| 1g8f | 72-84 | SRLADGTLWTIPI | 6.55 | 7.20 | 2.88 | 6.07 | 1.85 |
| 1gpi | 308-320 | NSVANIPGVDPVN | 2.98 | 11.88 | 2.07 | 0.90 | 4.49 |
| 1hnj | 191-203 | LPNADRVNPENSI | 10.00 | 5.49 | 10.39 | 10.34 | 3.33 |
| 1hxh | 87-99 | NAGILLPGDMETG | 7.70 | 8.15 | 2.09 | 0.61 | 7.48 |
| 1iir | 197-209 | AADPVLAPLQPTD | 4.54 | 4.08 | 5.45 | 10.62 | 1.46 |
| 1jp4 | 153-165 | PYYNYQAGPDAVL | 6.18 | 5.18 | 3.61 | 7.13 | 2.03 |
| 1kbl | 793-805 | KIYESDPFARLDQ | 3.33 | 6.81 | 3.29 | 1.21 | 3.15 |
| 1krh | 131-143 | DDGQPDIHFLAGQ | 3.41 | 6.07 | 2.16 | 0.40 | 2.84 |
| 1l8a | 691-703 | TLNENYHMPAMPE | 1.35 | 3.97 | 2.38 | 2.37 | 0.44 |
| 1lki | 62-74 | PNMTDFPSFHGNG | 1.95 | 8.48 | 8.69 | 6.28 | 2.5 |
| 1m3s | 68-80 | VGEILTPPLAEGD | 5.79 | 1.62 | 4.01 | 1.55 | 5.1 |
| 1mo9 | 107-119 | SGQYWFPDMTEKV | 3.29 | 12.29 | 2.38 | 2.03 | 4.52 |
| 1nln | 26-38 | DKRFPGFVSPHKL | 2.01 | 8.00 | 4.44 | 5.90 | 1.65 |
| 1o6l | 386-398 | KKDPKQRLGGGPS | 6.48 | 8.57 | 4.10 | 2.24 | 5.77 |
| 1ock | 43-55 | DKSARAQASGPLR | 6.96 | 2.77 | 5.28 | 3.97 | 1.53 |
| 1ojq | 167-179 | IDSKELTAYPGQQ | 2.07 | 4.70 | 3.65 | 4.24 | 5.05 |
| 1os8 | 141-153 | WGANREGGSQQR | 4.80 | 10.21 | 6.14 | 3.37 | 2.69 |
| 1p1m | 327-339 | FKSGKIEEGWNAD | 2.07 | 5.28 | 3.26 | 0.99 | 2.15 |
| 1qqp | 161-173 | PFVGVNRYDQYKV | 2.19 | 7.08 | 2.74 | 2.96 | 1.10 |
| 1qsl | 389-401 | YLDAPDQISRERA | 3.54 | 5.60 | 3.59 | 2.03 | 4.55 |
| 1xyz | 645-657 | ECMDDSGNGLRSS | 4.81 | 5.86 | 11.60 | 3.29 | 4.54 |
| 1yge | 452-464 | LPHSAGDLSAAVS | 4.16 | 5.86 | 11.60 | 3.29 | 2.8 |
| 2hlc | 91-103 | HSMFNPDTYLNDV | 3.08 | 5.91 | 4.29 | 3.63 | 4.6 |
| 2olb | 207-219 | NPQYWDNAKTVIN | 3.50 | 4.20 | 4.15 | 3.38 | 2.88 |
| 2ptd | 136-148 | YFVDPIFLKTEGN | 5.91 | 4.00 | 1.91 | 1.48 | 2.32 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 3grs | 404-416 | TPMYHAVTKRKTK | 4.22 | 3.43 | 4.60 | 7.17 | 2.00 |
| Mean | | | 4.44 | 5.84 | 4.35 | 3.74 | **3.26** |

The results of all the methods except DISGRO are obtained from Table A1 in Ref. [1].

Table 19: **Results of 14-residue loops on Test Set 5, obtained by using PLOP [2] and DISGRO.**

| Target | PDB | Start | End | Sequence | $R_{Emin}$(PLOP) | $R_{min}$(DISGRO) | $R_{Emin}$(DISGRO) |
|---|---|---|---|---|---|---|---|
| 1 | 1E6U | A:274 | A:287 | ASKPDGTPRKLLDV | 1.94 | 1.50 | 3.92 |
| 2 | 1JP4 | A:153 | A:166 | PYYNYQAGPDAVLG | 7.26 | 1.67 | 2.50 |
| 3 | 1N0Q | A:24 | A:37 | AGADVNAKDKNGRT | 0.22 | 1.30 | 4.93 |
| 4 | 1N0Q | A:57 | A:70 | AGADVNAKDKNGRT | 0.52 | 1.29 | 2.43 |
| 5 | 1O97 | D:156 | D:169 | RPSVFKPLEGAGSP | 0.82 | 1.36 | 1.72 |
| 6 | 1OCK | A:209 | A:222 | GRSEFSGIVPAKAP | 0.93 | 1.54 | 2.07 |
| 7 | 1P3C | A:112 | A:125 | GYRSIRQVTNLTGT | 0.32 | 0.96 | 2.16 |
| 8 | 1P3D | A:402 | A:415 | DVYAAGEAPIVGAD | 1.74 | 1.73 | 2.39 |
| 9 | 1R6X | A:72 | A:85 | SRLADGTLWTIPIT | 0.30 | 1.99 | 3.05 |
| 10 | 1RDQ | E:273 | E:286 | LQVDLTKRFGNLKN | 1.50 | 1.90 | 4.37 |
| 11 | 1RV9 | A:225 | A:238 | GTHCTVLERDTFFS | 0.26 | 0.71 | 1.09 |
| 12 | 1VYR | A:193 | A:206 | SPSSNQRTDQYGGS | 0.58 | 2.45 | 4.97 |
| 13 | 1VYR | A:235 | A:248 | SPIGTFQNVDNGPN | 1.17 | 1.74 | 2.95 |
| 14 | 1XU1 | A:221 | A:234 | PRANAKLSLSPHGT | 0.47 | 1.19 | 1.90 |
| 15 | 1ZEQ | X:53 | X:66 | ITPQTKMSEIKTGD | 0.27 | 1.67 | 5.28 |
| 16 | 2BWR | A:269 | A:282 | KDFGVNSGWRVEKH | 0.44 | 1.37 | 4.98 |
| 17 | 2BWR | B:158 | B:171 | NNFGYAQGWRLDRH | 4.56 | 2.22 | 3.61 |
| 18 | 2C0H | A:40 | A:53 | QAWVNYARDFGHNQ | 5.96 | 2.19 | 6.74 |
| 19 | 2EX2 | A:139 | A:152 | TSIFASHDKAPGWP | 0.21 | 1.59 | 4.29 |
| 20 | 2GGC | A:79 | A:92 | HGIPDDAKLLKDGD | 0.24 | 1.69 | 4.84 |
| 21 | 2H3L | A:1360 | A:1373 | QPEGPASKLLQPGD | 0.28 | 1.21 | 2.32 |
| 22 | 2O2K | A:1221 | A:1234 | SNLKSKYFAVGKIS | 1.07 | 1.44 | 3.06 |
| 23 | 2PVQ | A:139 | A:152 | LSDKNAYWLGDDFT | 0.66 | 1.44 | 1.44 |
| 24 | 2VFR | A:325 | A:338 | AADAQWLSPAYGRD | 0.34 | 1.90 | 2.71 |
| 25 | 3B40 | A:389 | A:402 | SDFNDGGGVDGWKD | 1.28 | 1.95 | 6.37 |
| 26 | 3B64 | A:44 | A:57 | DSTPMHFFGSTDPV | 0.65 | 2.06 | 4.27 |
| 27 | 3BY9 | A:177 | A:190 | DLSAIEQGWQNKSS | 1.13 | 1.83 | 4.01 |
| 28 | 3BY9 | A:205 | A:218 | SQPAWLFHSVADLS | 0.28 | 1.45 | 3.32 |
| 29 | 3CFZ | A:125 | A:138 | TDKSKYKDEINSTN | 0.68 | 1.36 | 5.80 |
| 30 | 3CNQ | S:50 | S:63 | FVPSETNPFQDNNS | 1.03 | 1.13 | 8.37 |
| 31 | 3CSS | A:163 | A:176 | FGSDGHTASIFPDS | 0.21 | 1.11 | 3.19 |
| 32 | 3DRF | A:550 | A:563 | KRVVGMTLDYGAMN | 1.85 | 2.04 | 3.70 |
| 33 | 3E7H | A:67 | A:80 | GKVSAKDYVNEATG | 1.78 | 1.23 | 3.49 |
| 34 | 3EHR | A:95 | A:108 | NRVGVNGLDKAGST | 0.94 | 2.03 | 5.52 |
| 35 | 3FOT | A:164 | A:177 | DVSTDSTPIPQDAT | 0.30 | 1.18 | 2.21 |
| 36 | 3HXL | A:277 | A:290 | ARVNESLTYQGYDE | 0.79 | 1.60 | 4.51 |
| Mean | | | | | 1.19 | **1.58** | **3.73** |

$R_{min}$ and $R_{Emin}$ are the minimum backbone RMSD and average RMSD of the lowest energy conformations, respectively.

Table 20: **Results of 15-residue loops on Test Set 5, obtained by using PLOP [2] and DISGRO.**

| Target | PDB | Start | End | Sequence | $R_{Emin}$(PLOP) | $R_{min}$(DISGRO) | $R_{Emin}$(DISGRO |
|---|---|---|---|---|---|---|---|
| 1 | 1AH7 | A:157 | A:171 | KVTDGNGYWNWKGTN | 0.32 | 1.21 | 1.73 |
| 2 | 1BHE | A:121 | A:135 | GQGGVKLQDKKVSWW | 0.42 | 1.73 | 5.96 |
| 3 | 1H4A | X:19 | X:33 | SSDHPNLQPYLSRCN | 0.28 | 1.58 | 4.62 |
| 4 | 1JU3 | A:486 | A:500 | RETLVNPTLIEAGEI | 0.35 | 1.96 | 1.96 |
| 5 | 1QAZ | A:298 | A:312 | DKSARAQASGPLRGI | 1.68 | 1.86 | 5.11 |
| 6 | 1QQF | A:1112 | A:1126 | QKPDGVFQEDGPVIH | 0.31 | 1.57 | 2.58 |
| 7 | 1RA0 | A:283 | A:297 | QGRFDTYPKRRGITR | 2.78 | 2.22 | 3.88 |
| 8 | 1RA0 | A:361 | A:375 | LNLQDYGIAAGNSAN | 0.39 | 1.64 | 2.78 |
| 9 | 1RYO | A:172 | A:186 | QLCPGCGCSTLNQYF | 0.88 | 1.21 | 2.4 |
| 10 | 1S95 | A:477 | A:491 | TAVPHPNVKPMAYAN | 0.61 | 2.07 | 3.45 |
| 11 | 1WB4 | A:1033 | A:1047 | ALPHFDYTSDFSKGN | 0.21 | 2.47 | 6.14 |
| 12 | 1WUI | L:454 | L:468 | KGDNVICAPWEMPKQ | 1.81 | 1.18 | 2.46 |
| 13 | 1Y12 | A:10 | A:24 | GDVKGESKDKTHAEE | 0.36 | 2.16 | 11.73 |
| 14 | 1ZHX | A:392 | A:406 | NLSTKNAPSGTLVGD | 7.10 | 1.92 | 4.8 |
| 15 | 2AEB | B:156 | B:170 | IPDVPGFSWVTPCIS | 2.55 | 1.54 | 3.22 |
| 16 | 2B0T | A:701 | A:715 | VQGGATDLGGYYSPN | 1.23 | 1.94 | 3.17 |
| 17 | 2CJP | A:58 | A:72 | DLRGYGDTTGAPLND | 0.46 | 1.22 | 5.63 |
| 18 | 2DSJ | A:354 | A:368 | GGGRKRKGEPIDHGV | 0.51 | 1.56 | 2.96 |
| 19 | 2H3L | A:1339 | A:1353 | GVGGRGNPFRPDDDG | 1.10 | 2.29 | 2.66 |
| 20 | 2O2K | A:1220 | A:1234 | FSNLKSKYFAVGKIS | 1.36 | 1.51 | 2.06 |
| 21 | 2OIT | A:290 | A:304 | FMEPCYGSCTERQHH | 0.54 | 1.75 | 5.17 |
| 22 | 2PKF | A:26 | A:40 | LPEHLHKVSLSFLVD | 2.34 | 2.49 | 4.44 |
| 23 | 2V3V | A:382 | A:396 | WGLPEGRIAPEPGYH | 0.35 | 1.53 | 1.75 |
| 24 | 3A3P | A:286 | A:300 | DSNDNIASFSNRQPE | 0.18 | 1.77 | 2.63 |
| 25 | 3A64 | A:350 | A:364 | SPASHVPAPEAGEWF | 2.55 | 2.37 | 5.53 |
| 26 | 3BB7 | A:231 | A:245 | SEMQYGGPNEGSGAY | 6.26 | 1.61 | 2.72 |
| 27 | 3BF7 | A:49 | A:63 | DVRNHGLSPREPVMN | 5.66 | 1.72 | 5.34 |
| 28 | 3CSS | A:95 | A:109 | LLRDVPSSDVISIDR | 2.36 | 2.3 | 4.41 |
| 29 | 3EA1 | A:136 | A:150 | YFVDPIFLKTEGNIK | 0.49 | 1.91 | 2.21 |
| 30 | 3F1L | A:99 | A:113 | NAGLLGDVCPMSEQN | 1.05 | 1.66 | 3.68 |
| Mean | | | | | 1.55 | **1.80** | **3.91** |

$R_{min}$ and $R_{Emin}$ are the minimum backbone RMSD and average RMSD of the lowest energy conformations, respectively.

Table 21: **Results of 16-residue loops on Test Set 5, obtained by using PLOP [2] and DISGRO.**

| Target | PDB | Start | End | Sequence | $R_{Emin}$(PLOP) | $R_{min}$(DISGRO) | $R_{Emin}$(DISGRO) |
|---|---|---|---|---|---|---|---|
| 1 | 1C1K | A:31 | A:46 | NGKYDVIKYNWCMRVS | 0.66 | 1.62 | 2.3 |
| 2 | 1DJ0 | B:19 | B:34 | DGSKYYGWQRQNEVRS | 7.08 | 2.42 | 5.68 |
| 3 | 1GPI | A:308 | A:323 | NSVANIPGVDPVNSIT | 0.33 | 2.06 | 5.55 |
| 4 | 1UG6 | A:340 | A:355 | GAAYPDLWTGEAVVED | 0.43 | 1.37 | 3.25 |
| 5 | 1WHI | A:88 | A:103 | RDDKSPRGTRIFGPVA | 0.66 | 1.97 | 2.68 |
| 6 | 1WM3 | A:67 | A:82 | INETDTPAQLEMEDED | 0.32 | 2.46 | 3.29 |
| 7 | 1ZHV | A:20 | A:35 | SASEAIPAWADGGGFV | 0.64 | 1.92 | 5.91 |
| 8 | 2BG1 | A:708 | A:723 | SPSIWGNERFALDPSV | 2.15 | 2.11 | 3.7 |
| 9 | 2GGC | A:184 | A:199 | LHYDSRETNVVLKPGM | 1.08 | 1.25 | 3.82 |
| 10 | 2HKJ | A:418 | A:433 | TKIPYKSAGKESIAEV | 0.42 | 1.82 | 5.29 |
| 11 | 2PKF | B:25 | B:40 | LLPEHLHKVSLSFLVD | 0.93 | 1.94 | 3.5 |
| 12 | 2PUH | A:70 | A:85 | DSPGFNKSDAVVMDEQ | 1.52 | 1.56 | 6.62 |
| 13 | 2PYW | A:321 | A:336 | NKDGPGEAYLADIYNN | 2.57 | 1.9 | 4.76 |
| 14 | 3IFE | A:14 | A:29 | KIDTQSNEDSHTVPTT | 1.18 | 1.99 | 1.99 |
| Mean | | | | | 1.43 | **1.88** | **4.16** |

$R_{min}$ and $R_{Emin}$ are the minimum backbone RMSD and average RMSD of the lowest energy conformations, respectively.

Table 22: **Results of 17-residue loops on Test Set 5, obtained by using PLOP [2] and DISGRO.**

| Target | PDB | Start | End | Sequence | $R_{Emin}$(PLOP) | $R_{min}$(DISGRO) | $R_{Emin}$(DISGRO) |
|---|---|---|---|---|---|---|---|
| 1 | 1KWG | A:314 | A:330 | QPGPVNWAPHNPSPAPG | 1.93 | 1.86 | 3.89 |
| 2 | 1QLW | A:145 | A:161 | FRFGPRYPDAFKDTQFP | 0.41 | 2.51 | 5.13 |
| 3 | 1VJU | A:277 | A:293 | LPPRARWGYNWQPEPGT | 0.63 | 1.34 | 3.34 |
| 4 | 2FAO | A:814 | A:830 | AGDDPWADYAGTRQRIS | 0.50 | 2.41 | 4.41 |
| 5 | 2HDW | A:131 | A:147 | DPSYTGESGGQPRNVAS | 2.22 | 1.32 | 4.94 |
| 6 | 2PEF | A:191 | A:207 | TNGMIDKILNKIDPEDV | 1.92 | 1.78 | 1.86 |
| 7 | 3A3P | A:262 | A:278 | SGNEGAPSPSYPAAYPE | 0.52 | 2.31 | 7.34 |
| 8 | 3H2G | A:124 | A:140 | DYLGLGKSNYAYHPYLH | 4.07 | 2.46 | 4.77 |
| 9 | 3HUH | A:71 | A:87 | QEMEFEPKASRPTPGSA | 8.56 | 3.6 | 4.51 |
| Mean | | | | | 2.30 | **2.18** | **4.46** |

$R_{min}$ and $R_{Emin}$ are the minimum backbone RMSD and average RMSD of the lowest energy conformations, respectively.

# References

[1] C.S. Soto, M. Fasnacht, J. Zhu, L. Forrest, and B. Honig. Loop modeling: Sampling, filtering, and scoring. *Proteins: Structure, Function, and Bioinformatics*, 70(3):834–843, 2008.

[2] S. Zhao, K. Zhu, J. Li, and R.A. Friesner. Progress in super long loop prediction. *Proteins: Structure, Function, and Bioinformatics*, 2011.