Supplementary Table 3

PDB Code	2H3D	3DGR	3DHD	3DHF	3DKJ	3DKL
2H3D	-	0.95	0.85	0.86	0.88	0.88
3DGR		-	0.61	0.61	0.55	0.57
3DHD			-	0.43	0.40	0.43
3DHF				-	0.42	0.33
3DKJ					-	0.39
3DKL						-

Table 3: Root mean square deviation (RMSD) values between different structures (in Å). The alignment and RMSD calculation was done with PyMOL[1]. The structures are 2H3D (human NAMPT) [2], 3DGR (human NAMPT·AMPcP complex) [3], 3DHD (human NAMPT·NMN·Mg_2PPi complex) [3], 3DHF (human BeF_3–-NAMPT·NMN·Mg_2PPi complex) [3], 3DKJ (human NAMPT·PRPP·BzAM complex) [3], and 3DKL (human BeF_3–-NAMPT·Mg_2PRPP·BzAM complex) [3]. The structural resolution of the PDB structures ranges from 1.8 Å to 2.1 Å.

References

[1] Schrödinger, LLC (2010) The {PyMOL} Molecular Graphics System, Version˜1.4.1.

KEY: PyMOL
ANNOTATION: PyMOL The PyMOL Molecular Graphics System, Version 1.3, Schr{ö}dinger, LLC.

[2] Wang T, Zhang X, Bheda P, Revollo JR, Imai Si, et al. (2006) Structure of Nampt/PBEF/visfatin, a mammalian NAD+ biosynthetic enzyme. Nature Structural & Molecular Biology 13: 661–662.

[3] Burgos ES, Ho MC, Almo SC, Schramm VL (2009) A phosphoenzyme mimic, overlapping catalytic sites and reaction coordinate motion for human NAMPT. Proceedings of the National Academy of Sciences 106: 13748–13753.

Supplementary Figure 2

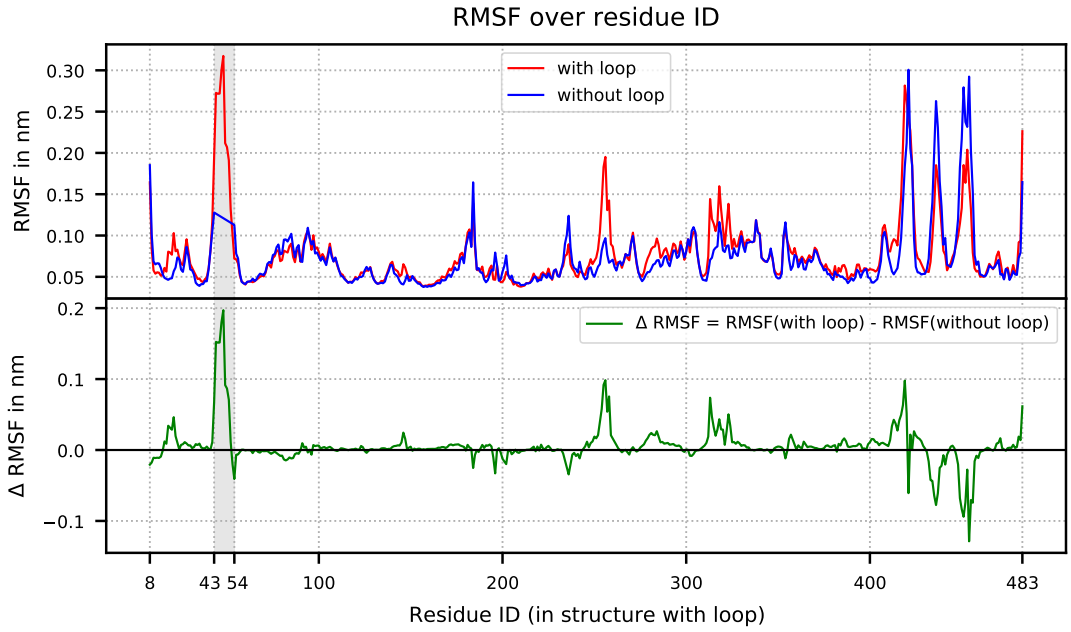

Figure 3: Root mean square fluctuations (RMSF) for every residue of chain A of NamPT with loop insertion (red) and without loop insertion (blue) are shown, respectively (top). The difference RMSF for every residue is shown in the bottom (green). For better comparison the residue IDs for the structure without loop are aligned to accord with the structure with loop and the average RMSF of residues 43 and 54 displayed in the blue curve between these residues. For the RMSF calculation, the first 100 ns of the simulation are omitted to allow equilibration.