

## 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<sub>2</sub>PPi complex) [3], 3DHF (human BeF<sub>3</sub>--NAMPT·NMN·Mg<sub>2</sub>PPi complex) [3], 3DKJ (human NAMPT·PRPP·BzAM complex) [3], and 3DKL (human BeF<sub>3</sub>--NAMPT·Mg<sub>2</sub>PRPP·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,  
Schrödinger, LLC.
- [2] Wang T, Zhang X, Bheda P, Revollo JR, Imai Si, et al. (2006) Structure of Nampt/PBEF/visfatin, a mammalian NAD<sup>+</sup> 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.