Supplementary Table S6.

X-ray data collection and refinement statistics of T41Q/N71S/F124T/M127V NfsB bound to nicotinate.

Protein	**T41Q/N71S/F124T/M127V NfsB**
PDB code	**8CJ0**
Data collection	
Wavelength (Å)	0.934
Resolution range (Å)	35.06-1.99 (2.05-1.99)
Space group	P $4_1 2_1 2$
Unit cell	57.3 Å, 57.3 Å, 266 Å 90°, 90°, 90°
Total reflections	290,689 (19,436)
Unique reflections	31,129 (2,176)
Multiplicity	9.0 (8.93)
Completeness (%)	98.9 (95.3)
$\langle I/\sigma I \rangle$ overall	25.3 (6.2)

Mosaicity	0.141
Wilson B-factor (Å^2)	25.9
Anisotropy	0.167
Rsym[1] (%)	7.5 (55.0)
Refinement and quality	
Reflections used in refinement	31,128 (2168)
Reflections used for R-free	1,575 (5.1%)
R-work[2]	0.170
R-free[3]	0.205
Number of non-hydrogen atoms	3622
macromolecules	3344
ligands	84
solvent	155
Protein residues	
RMSD bond length (Å)	0.011
RMSD bond angles (°)	1.28

RMSD chirality	0.067
RMSD planarity	0.007
F_o-F_c correlation	0.96
Ramachandran plot	
Ramachandran favored (%)	99.5
Ramachandran allowed (%)	0.5
Ramachandran outliers (%)	0
Sidechain outliers (%)	1.7
All atom clash score	2
RSRZ outliers (%)	4.6
Average B-factors (Å^2)	34.0
macromolecules	36
ligands	
FMN	20
Nicotinamide	42

solvent	46.4

- The numbers in parentheses represent statistics in the highest resolution shell.
- *1.* $R_{sym} = \Sigma|I_i - <|>|/\Sigma|I_i|$ where I_i is the intensity of the *i*th measurement, and <|>is the mean intensity for that reflection;
- *2.*$R_{work} = \sum\|F_o| - |F_c|/\sum|F_o|$, where F_o and F_c are the observed and calculated structure factors for data used for refinement, respectively.
- *3.* $R_{free} = \sum\|F_o| - |F_c|/\sum|F_o|$ for 5% of the data not used at any stage of structural refinement.