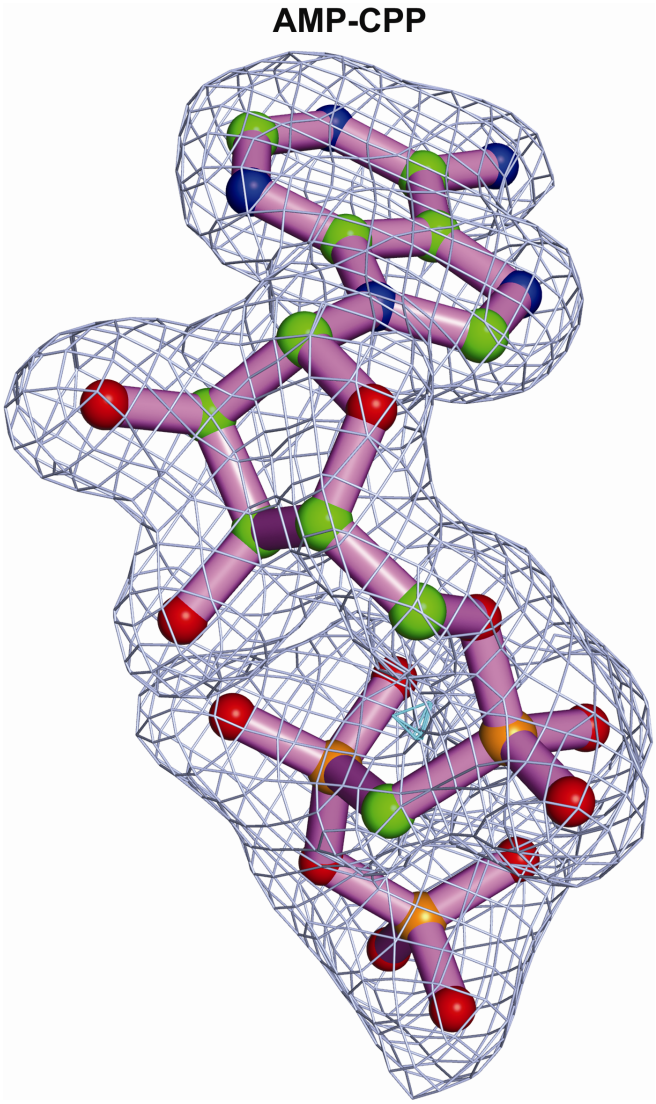
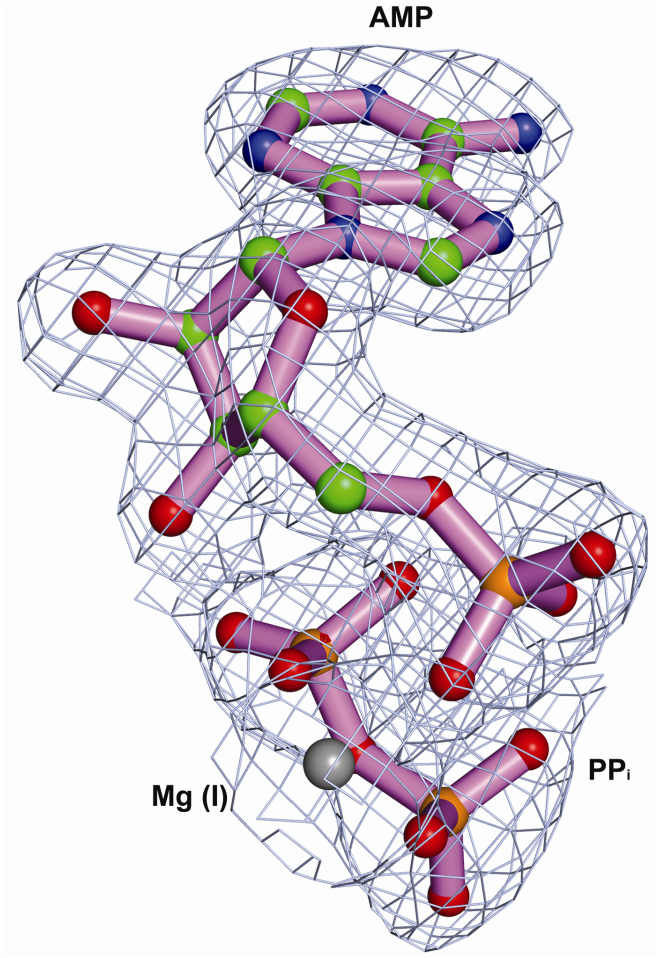
Supplementary material



(*a*)



(*b*)

Figure 11. (*a*) $2F_o$-F_c e lectron density at 1σ (gray), F_o-F_c at 3σ (red) and F_o-F_c at 3σ (cyan) of AMP-CPP ligand *ban*NADS complex form III. (*b*) $2F_o$-F_c electron density at 1σ (blue-gray), F_o-F_c at 3σ (red) and F_o-F_c at 3σ (cyan) of AMP and PP_i ligands and Mg^{2+}-I ion *ban*NADS complex form II. Mg^{2+}-II not shown.

Table 2. NAD^+ Synthetase ATP Binding Site Comparison[1]

PDB Code	Species	Ligands	Mg^{2+} (I, II, or III)	G45	S47	S52	Q50	R79	L80	Q85	T158	K187	T209
Form II	*ban*	AMP + PP_i	I, II	All interactions present									
Form III	*ban*	AMP-CPP	II	All interactions present									
1NSY	*bsu*	ATP, AMP + PP_i	I	All interactions present									
2NSY	*bsu*	NAD-adenylate	I, II	Not applicable									
1FYD	*bsu*	AMP + PP_i	II	All interactions present									
1EE1	*bsu*	NaAD, ATP	II	All interactions present									
1IH8	*bsu*	AMP-CPP	II, III	All interactions present									
1WXE	*eco*	AMP	I	Y G46	N/A	N/A	N/A	N	Y L83	N	Y T160	N/A	No P2 Loop
1WXI	*eco*	AMP + PP_i	I, II	Y G46	Y S48	Y S53	N	Y R82	Y L83	Y Q88	Y T160	Y K189	No P2 Loop
1WXG	*eco*	NaAD	I	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	No P2 Loop
1XNG	*hpy*	NaAD, ATP	II	Y G31	Y S33	Y S38	Y L36	N (L57)	Y M58	N (M64)	Y T132	Y K161	Y S183

[1]Y: Interaction is present between residue and ligand, N: No interaction is seen with homologous residue, N/A: Interaction is not applicable; the relevant ligand atoms (e.g., pyrophosphate groups in 1WXE and entire ATP ligand in 1WXG) are not present in the structure, therefore the respective interaction with the protein cannot exist.

Table 3. Root Mean Squared Deviation Between C_α Atoms[1] (Å)

	Complex *ban*NADS(III)	*bsu*NADS 1IH8.pdb	*eco*NADS 1WXE.pdb	*hpy*NADS 1XNG.pdb	Apo *ban*NADS (I)
Complex *ban*NADS(III)	0	0.42	0.97	1.72	1.18
*bsu*NADS 1IH8.pdb	0.42	0	0.88	1.69	1.22
*eco*NADS 1WXE.pdb	0.97	0.88	0	1.5	1.38
*hpy*NADS 1XNG.pdb	1.72	1.69	1.5	0	2.35
Apo *ban*NADS (I)	1.18	1.22	1.38	2.35	0

[1]RMS deviations were calculated using a C^α atom least squares fit in the software O.