Supplemental Table 2. Hydrogen bonds (Å) formed by the phosphate anions in the crystal structures of the native form I (2HHC) and II (2HLH). Residues with an asterisk correspond to symmetry-related molecules. Residues shown in bold are predicted to be involved in subtrate binding or in the enzymatic reaction. The contacts of the P_i3 phospahtes are listed separately for form I and form II because these ions are structurally non-equivalent.

Interaction Phosphate anion – Protein/solvent atom (res)		Form I[a]	Form II
(P_i1) O1	Oε2(E110)	2.9	2.6
(P_i1) O1	Nε(R106)	-	3.1
(P_i1) O1	Nη2(R106)	-	2.9
(P_i1) O1	O(Wat93)	-	3.3
(P_i1) O2	Oε1(E110)	2.8	2.7
(P_i1) O2	N(W88)	3.2	3.1
(P_i1) O2	O(Wat148)	-	3.4
(P_i1) O3	O(Wat93)	-	2.7
(P_i1) O3	O(Wat182)	-	2.5
(P_i1) O4	O(Wat102)	-	2.6
(P_i1) O4	Nη2(R91)	2.6	-
(P_i1) O4	Nη1(R106)*	-	2.9
(P_i1) O4	Nη2(R106)*	-	3.1
(P_i2) O1	Oγ(S152)	2.8	2.4
(P_i2) O1	O(Wat268)	-	2.4
(P_i2) O2	Oε2(E59)	3.5	3.4
(P_i2) O2	O(Wat253)	2.4	-
(P_i2) O3	Oε2(E59)	2.5	2.5
(P_i2) O4	Nη1(R151)	2.7	2.7
(P_i3) O1	O(S79)	3.3	-
(P_i3) O2	O(Wat3)*	2.8	-
(P_i3) O2	O(Wat4)	2.7	-
(P_i3) O3	O3(P_i3)*	2.6	-
(P_i3) O4	N(Tris)*	2.4	-
(P_i3) O4	O3(Tris)*	3.3	-
(P_i3) O1	Nη1(**R177**)	-	3.1
(P_i3) O1	O(Wat206)	-	2.6
(P_i3) O1	O(Wat32)	-	3.1
(P_i3) O2	O(Wat206)	-	3.0
(P_i3) O2	N(G16)	-	3.0
(P_i3) O3	Oγ(**S287**)	-	3.4
(P_i3) O3	N(F289)	-	3.0
(P_i3) O3	Nη1(**R177**)	-	3.1
(P_i3) O3	O(Wat196)	-	3.2
(P_i3) O4	O(Wat32)	-	3.1
(P_i3) O4	N(D17)	-	3.0
(P_i4) O3	Nε2(H175)	-	2.6
(P_i4) O3	Nε(**R177**)	-	2.9
(P_i4) O3	Nη1(**R177**)	-	2.4
(P_i4) O4	N(**D224**)	-	3.0

[a]Due to unfortunate PDB renaming conventions, the phosphate ions in the PDB entry 2HHC (form I) are numbered differently than in the entry 2HLH (form II). To simplify discussion, this paper uses a common numbering scheme, as in the entry 2HLH. In the PDB entry 2HHC, the numbers of the phosphate groups 2 and 3 are swapped.