

Supplementary Materials

Supplementary Table S1. Hydrogen bonds of NS5 dimer with $\geq 100\%$ occupancy.

Donor	Acceptor	Occupancy
ARG391-Side	ASP494-Side	285.43%
ARG673-Side	ASP671-Side	281.79%
ARG594-Side	ASP596-Side	273.51%
ARG364-Side	ASP544-Side	243.38%
ARG438-Side	GLU486-Side	232.78%
ARG815-Side	GLU807-Side	231.13%
ARG722-Side	ASP720-Side	225.83%
ARG391-Side	GLU397-Side	223.18%
ARG598-Side	GLU549-Side	213.58%
ARG352-Side	GLU67-Side	180.13%
ARG76-Side	ASP141-Side	179.80%
ARG395-Side	GLU428-Side	170.20%
SER210-Side	GLU216-Side	160.60%
ARG654-Side	GLU625-Side	159.60%
LYS180-Side	GLU216-Side	151.32%
TYR530-Side	ASP672-Side	150.66%
TYR299-Side	ASP590-Side	148.01%
ALA680-Main	GLU623-Side	146.69%
THR394-Side	GLU397-Side	146.36%
LYS180-Side	ASP146-Side	145.03%
TYR218-Main	VAL205-Main	143.71%
THR8-Side	GLU11-Side	143.05%
THR39-Side	ASP37-Side	141.72%
ARG76-Main	ASP141-Side	140.40%
ARG282-Side	GLU414-Side	140.40%
VAL181-Main	MET217-Main	136.75%
ARG361-Side	ASP596-Side	135.76%
ARG262-Side	GLU267-Side	133.77%
THR828-Side	ASP826-Side	133.77%
ARG729-Side	GLU733-Side	133.44%
VAL205-Main	TYR218-Main	133.11%
THR542-Side	ASP545-Side	133.11%
ARG856-Side	ASP771-Side	133.11%
ARG581-Side	ASP294-Side	132.78%
ARG389-Side	ASP557-Side	132.78%
MET718-Main	ARG722-Main	132.45%
THR161-Side	GLU157-Main	131.13%
TRP219-Main	ILE179-Main	131.13%
SER781-Side	ASN777-Main	130.46%
ARG620-Side	SER697-Side	129.47%
SER235-Side	HSD215-Side	129.47%
LYS125-Main	VAL100-Main	128.81%
ARG370-Side	ASP544-Side	127.48%

Supplementary Table S1 (contd.). Hydrogen bonds of NS5 dimer with $\geq 100\%$ occupancy.

Donor	Acceptor	Occupancy
ARG769-Side	ASP844-Side	127.15%
THR542-Main	ASP545-Side	126.49%
ILE592-Main	VAL577-Main	126.49%
LEU716-Main	LEU724-Main	125.83%
THR301-Side	ASP359-Side	125.50%
THR328-Side	VAL324-Main	125.17%
ARG871-Side	ASP881-Side	124.17%
MET589-Main	TYR308-Main	124.17%
VAL577-Main	ILE592-Main	122.85%
TYR304-Side	SER307-Side	122.19%
TYR218-Side	ASP146-Side	121.85%
ARG519-Side	GLU715-Side	121.85%
THR301-Main	ASP359-Side	121.52%
THR610-Side	TYR606-Main	121.19%
ARG436-Side	GLU439-Side	121.19%
ARG101-Side	GLU99-Side	120.86%
ARG84-Side	GLU111-Side	117.22%
THR399-Side	ARG395-Main	115.56%
THR394-Main	GLU397-Side	114.90%
TYR90-Side	GLN63-Side	114.24%
ARG361-Side	GLU269-Side	113.25%
ARG101-Main	VAL77-Main	112.58%
THR649-Side	GLN645-Main	112.25%
LYS300-Side	ASP359-Side	111.92%
GLU486-Main	TYR482-Main	111.26%
ASP79-Main	ARG101-Main	111.26%
ARG47-Side	GLU49-Side	110.93%
ARG206-Side	THR214-Main	110.60%
ASN321-Main	ARG739-Main	110.26%
TYR482-Side	GLU486-Side	109.93%
TYR89-Side	VAL114-Main	108.94%
ALA528-Main	ASP672-Side	108.28%
TYR572-Side	GLU484-Side	107.95%
ASN609-Main	THR605-Main	107.95%
VAL830-Main	ASN814-Side	107.62%
LYS15-Side	GLU7-Side	107.28%
SER593-Side	HSD305-Side	106.95%
THR8-Main	GLU11-Side	106.95%
LYS719-Side	ASP835-Side	106.29%
ILE591-Main	GLY306-Main	104.97%
LEU257-Main	HSD52-Main	104.30%
LEU193-Main	VAL189-Main	104.30%
ILE162-Main	GLU158-Main	103.97%
GLU648-Main	THR644-Main	103.64%
LEU679-Main	GLU623-Side	103.31%

Supplementary Table S1 (contd.). Hydrogen bonds of NS5 dimer with $\geq 100\%$ occupancy.

Donor	Acceptor	Occupancy
ILE78-Main	THR142-Main	101.66%
TYR89-Main	GLY85-Main	101.66%
ARG206-Side	GLU216-Main	101.66%
THR376-Side	VAL372-Main	100.66%
ARG262-Main	ASN122-Side	100.66%
LEU17-Main	TRP13-Main	100.66%
VAL667-Main	TYR530-Main	100.33%
LEU144-Main	ILE78-Main	100.33%