crystals

MDPI

Supplementary materials

Table S1. Summary of data collection and refinement statistics.

	Value
Wavelength	1.033300
Resolution range	44.02 - 1.602 (1.659 - 1.602)
Space group	P 1 21 1
Unit cell	63.462 127.775 79.583 90 106.883 90
Total reflections	1095513 (108148)
Unique reflections	155703 (15323)
Multiplicity	7.0 (7.1)
Completeness (%)	97.99 (96.83)
Mean I/sigma(I)	15.82 (2.45)
Wilson B-factor	17.62
R-merge	0.07324 (0.7921)
R-meas	0.07907 (0.8539)
R-pim	0.0295 (0.3158)
CC1/2	0.999 (0.825)
CC*	1 (0.951)
Reflections used in refinement	155555 (15322)
Reflections used for R-free	7892 (772)
R-work	0.1553 (0.2301)
R-free	0.1721 (0.2500)
CC(work)	0.972 (0.907)

CC(free)	0.964 (0.886)
Number of non-hydrogen atoms	9928
macromolecules	8440
ligands	129
solvent	1359
Protein residues	1097
RMS(bonds)	0.009
RMS(angles)	1.25
Ramachandran favored (%)	98.43
Ramachandran allowed (%)	1.57
Ramachandran outliers (%)	0.00
Rotamer outliers (%)	0.81
Clashscore	4.38
Average B-factor	22.99
macromolecules	21.14
ligands	25.67
solvent	34.21

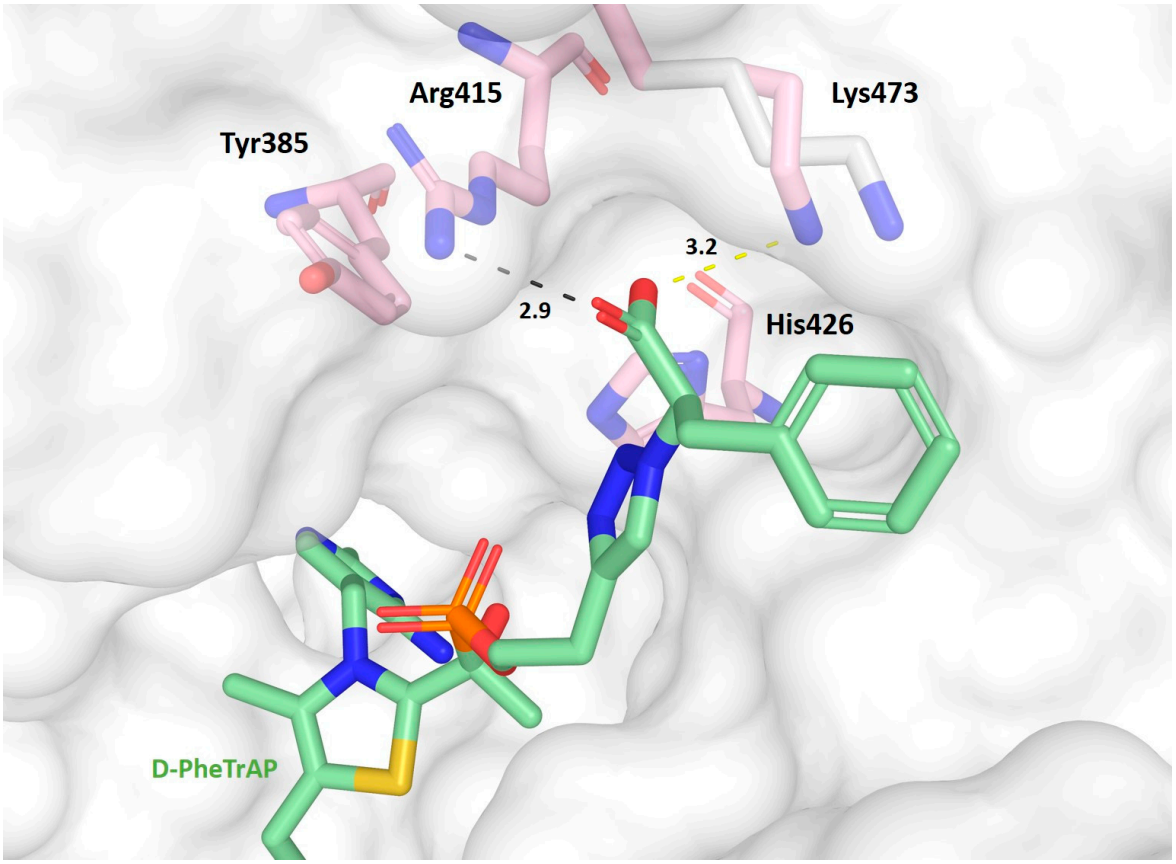

Figure S1. Flexible docking pose of the covalent adduct of D-PheTrAP with ThDP. The docking pose is shown as green sticks. Residues of the MtDXPS structure with the new Lys473 orientation are coloured in pink, while the original Lys473 orientation is highlighted as white sticks. Hydrogen bonds are represented as yellow dashed lines, with distances indicated in Angstroms. Distances are represented as black dashed lines, with distances indicated in Angstroms.