Electronic Supplementary Material (ESI) for RSC Chemical Biology. This journal is © The Royal Society of Chemistry 2021

Supporting Figures





Figure S2









h Tr-NOESY SLBR-H – sTa-Thr C Tr-NOESY SLBR-B – sTa-Thr









d

Protein-ligand H-bonds



Bond	Acceptor	DonorH	Donor	Presence
1	ASP481@O	0SA@H5N	0SA@N5	70.4
2	0SA@O1A	THR483@HG1	THR483@OG1	62.4
3	0SA@O1B	THR483@H	THR483@N	60.9
4	TYR485@OH	3LB@H6O	3LB@O6	54.6
5	0SA@O9	ARG484@HH22	ARG484@NH2	34.4
6	0SA@08	ARG484@HH12	ARG484@NH1	33.6
7	0SA@O1B	THR483@HG1	THR443@OG1	22.9
8	3VA@O2N	TYR443@HH	TYR443@OH	19.3
9	0SA@01A	THR483@H	THR483@N	15.2
10	ARG449@O	0SA@H9O	0SA@O9	14.0



е









4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 ppm

















SLBR-H + 3'SLn

