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Supplemental Information

Structural basis for recruitment of the CHK1 DNA damage kinase by the CLASPIN scaffold protein

Matthew Day, Sarah Parry-Morris, Jack Houghton-Gisby, Antony W. Oliver, and Laurence H. Pearl

SUPPLEMENTARY FIGURE 1 – relates to Figure 1 – Disorder prediction for CLASPIN protein

Output from SPOT-Disorder online server https://sparks-lab.org/server/spot-disorder2/ for CLASPIN. SEQ=sequence, p(D) is a score for disorder prediction and Lab is whether the protein is assigned a disordered (D) or ordered (O) label.

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SEQ     MTGEVGSEVHLEINDPNVISQEEADSPSDSGQGSYETIGPLSEGDSDEEIFVSKKLKNRKVLQDSDSETEDTNASPEKTTYDSAEEENKENLYAGKNTKI
P(D)    9999999888888888888899999999999999999999998888888888888888888999999999999999998888888888877766665543
LAB     DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDO

SEQ     KRIYKTVADSDESYMEKSLYQENLEAQVKPCLELSLQSGNSTDFTTDRKSSKKHIHDKEGTAGKAKVKSKRRLEKEERKMEKIRQLKKKETKNQEDDVEQ
P(D)    3333333444443333333333333333333444566778888888888888888888888888888888777666666666666666667777777777
LAB     OOOOOOOOODDOOOOOOOOOOOOOOOOOOOODDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD

SEQ     PFNDSGCLLVDKDLFETGLEDENNSPLEDEESLESIRAAVKNKVKKHKKKEPSLESGVHSFEEGSELSKGTTRKERKAARLSKEALKQLHSETQRLIRES
P(D)    6666554444455556677888888888888888888888888888889999999999999999999988888887766544433333322222211222
LAB     DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOOOOOOOOOOOOOOOOOO

SEQ     ALNLPYHMPENKTIHDFFKRKPRPTCHGNAMALLKSSKYQSSHHKEIIDTANTTEMNSDHHSKGSEQTTGAENEVETNALPVVSKETQIITGSDESCRKD
P(D)    2222222233333222222233333333333333444556667666666777788888999999999999988888777665554444444444444444
LAB     OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOODDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD

SEQ     LVKNEELEIQEKQKQSDIRPSPGDSSVLQQESNFLGNNHSEECQVGGLVAFEPHALEGEGPQNPEETDEKVEEPEQQNKSSAVGPPEKVRRFTLDRLKQL
P(D)    4455555666677777888888888888888888888887776666666666677788888888999999999999999888887765543322222222222
LAB     DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOOOOOOOOOOOO

SEQ     GVDVSIKPRLGADEDSFVILEPETNRELEALKQRFWKHANPAAKPRAGQTVNVNVIVKDMGTDGKEELKADVVPVTLAPKKLDGASHTKPGEKLQVLKAK
P(D)    2222222222222221111111111111111111111112222222222221111111111112222221111111111222333333333322222111111
LAB     OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO

SEQ     LQEAMKLRRFEERQKRQALFKLDNEDGFEEEEEEEEEMTDESEEDGEEKVEKEEKEEELEEEEEKEEEEEEEGNQETAEFLLSSEEIETKDEKEMDKENN
P(D)    2222222222333344444444556677888899999999999999999999999999999999999999999999999999999999999999999999
LAB     OOOOOOOOOOOOOOOOOOOODDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD

SEQ     DGSSEIGKAVGFLSVPKSLSSDSTLLLFKDSSSKMGYFPTEEKSETDENSGKQPSKLDEDDSCSLLTKESSHNSSFELIGSTIPSYQPCNRQTGRGTSFF
P(D)    9999999888888888888888888888888889999999999999999999999999999999999988999999999999888888888999999999
LAB     DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD

SEQ     PTAGGFRSPSPGLFRASLVSSASKSSGKLSEPSLPIEDSQDLYNASPEPKTLFLGAGDFQFCLEDDTQSQLLDADGFLNVRNHRNQYQALKPRLPLASMD
P(D)    9999999999888888899999999999988887777776666555443322222111111111111111111111111111111111111222233334
LAB     DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO

SEQ     ENAMDANMDELLDLCTGKFTSQAEKHLPRKSDKKENMEELLNLCSGKFTSQDASTPASSELNKQEKESSMGDPMEEALALCSGSFPTDKEEEDEEEEFGD
P(D)    4443333222222222333445555566666666655544444455667788889999999999999999999999888888888888999999999999
LAB     DDOOOOOOOOOOOOOOOOODDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD

SEQ     FRLVSNDNEFDSDEDEHSDSGNDLALEDHEDDDEEELLKRSEKLKRQMRLRKYLEDEAEVSGSDVGSEDEYDGEEIDEYEEDVIDEVLPSDEELQSQIKK
P(D)    9999999999999999999999999988888877766666555555555555667778888888888888888877777766666555555554443332
LAB     DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOOOOO

SEQ     IHMKTMLDDDKRQLRLYQERYLADGDLHSDGPGRMRKFRWKNIDDASQMDLFHRDSDDDQTEEQLDESEARWRKERIEREQWLRDMAQQGKITAEEEEEI
P(D)    2222222222111111111111222233333222222122222222222222333444444444433332222222111111222233444455555554
LAB     OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOODDDDDDDDOOOOOOOOOOOOOOOOOOOOOOOODDDDDDDDDDDD

SEQ     GEDSQFMILAKKVTAKALQKNASRPMVIQESKSLLRNPFEAIRPGSAQQVKTGSLLNQPKAVLQKLAALSDHNPSAPRNSRNFVFHTLSPVKAEAAKESS
P(D)    4443222222222333334444433333333333333333344555555544444443333334445566677777666555555556677888889999
LAB     DDOOOOOOOOOOOOOOOODDDDDOOOOOOOOOOOOOOOOOOODDDDDDDDDDDDDDOOOOOOOOODDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD

SEQ     KSQVKKRGPSFMTSPSPKHLKTDDSTSGLTRSIFKYLES
P(D)    999999999999988888888877776654433333445
LAB     DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOOOOOOODD
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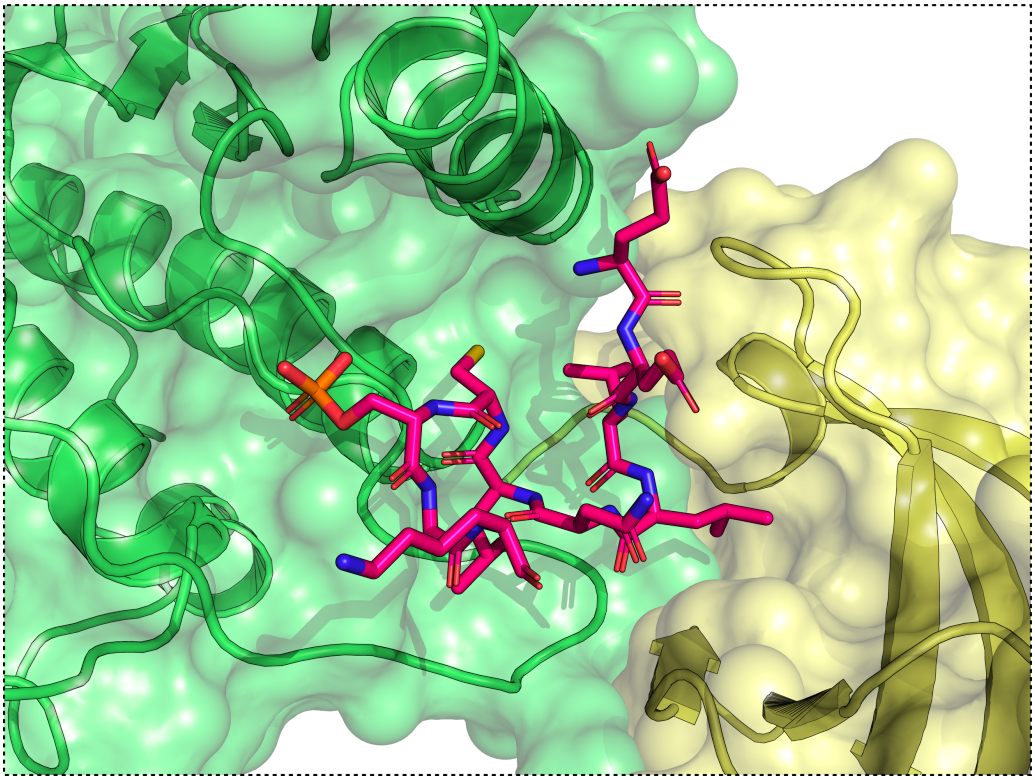
SUPPLEMENTARY FIGURE 2 – relates to Figure 4 – Alternative artefactual CLASPIN confirmation seen in the AU

The two chains of CHK1 in the asymmetric unit are shown in yellow and green with the CLASPIN peptide coloured pink interacting with the phosphate binding pocket of the green CHK1 molecule and making contact with both CHK1 molecules.



SUPPLEMENTARY FIGURE 3 – relates to Figure 5 – Data analysis of CHK1 kinetics from NADH coupled kinase assay

a-d) Fitted lines, and residual plots, for data in Figure 5D. NADH-coupled assay showing ATP turnover by either full length CHK1 or a CHK1 construct consisting of only the kinase domain in the presence of increasing concentrations of the CLASPIN pS945 peptide.

e) Residual plots for fitted lines shown in figure 5E