

Figure S1: Virtual Circular Dichromism (CD) spectrum of ClpK. The primary amino acid sequence of ClpK was passed through the DichroCalc server, the data obtained from the server was then analysed to understand the secondary structures of ClpK (<https://comp.chem.nottingham.ac.uk/dichrocalc/>).

Table S1: Ramachandran analysis of the template ClpB and modelled trimeric ClpK protein obtained from ProCheck.

| Residues in | Ramachandran statistics | |
|----------------------------|-------------------------|--------------|
| | 1QVR | KpClpK Model |
| Most favoured regions | 83.10% | 90.10% |
| Additional allowed regions | 15.20% | 8.30% |
| Generously allowed regions | 1.70% | 1.20% |
| Disallowed regions | 0.00% | 0.40% |
| Total residues | 717 | 2100 |

Table S2: DichroWeb¹ analysis of the secondary structure of ClpK.

| | Helix (%) | Strand (%) | Turns (%) | Unordered (%) | NRMSD ³ |
|-------------------------------|-----------|------------|-----------|---------------|--------------------|
| ClpK (952²) | 35.3 | 22.9 | 20.7 | 21 | 0.12 |

¹[1]

²Number of amino acids

³Normalised root mean square deviation (NRMSD) value is independent of dimensions, and a value of <0.1 is considered acceptable.

Table S3: Properties of the binding pockets in the N-terminal region of ClpB and ClpK identified using DoGSiteScorer¹.

| | ClpB | ClpK |
|---------------------------|---------|-----------|
| Volume (Å ³) | 1767.82 | 1511.88 |
| Surface (Å ²) | 1967.01 | 1626.42 |
| Depth (Å) | 31.30 | 20.80 |
| Hydrophobicity ratio | 0.34 | 0.28 |
| Enclosure | 0.08 | 0.07 |
| Frequent amino acid | Leucine | Glutamine |

¹[2]

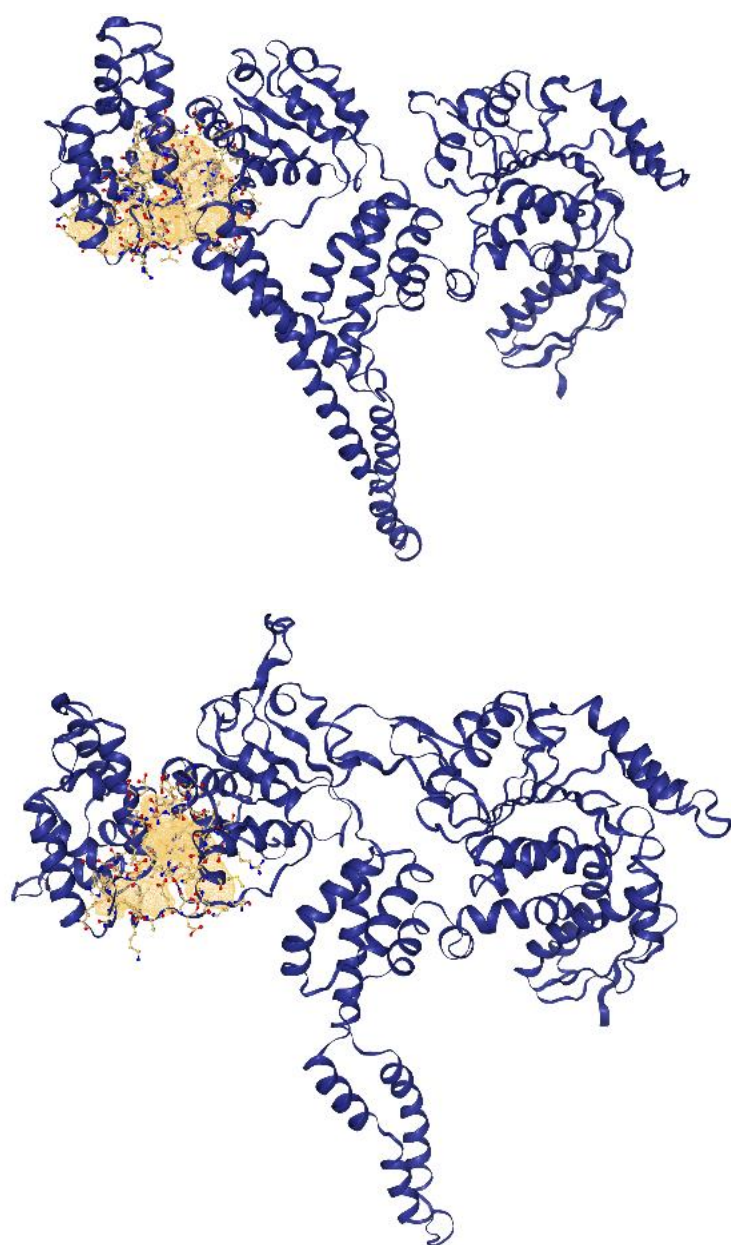


Figure S2: N-terminal binding groove identified in ClpK and ClpB. Top) ClpB with the binding groove shown in yellow. **Bottom)** ClpK with the binding groove identified in yellow. The binding grooves were identified using DoGSiteScorer [2].

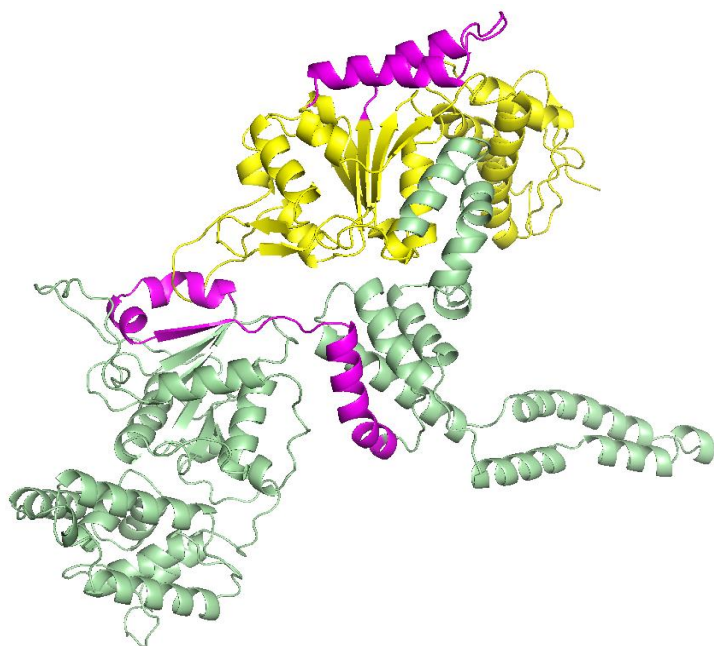


Figure S3: ClpK adopts a RecA-like fold in NBD1 and NBD2. The secondary structural features are coloured as follows; the N-terminal domain and the C-terminal domain are shown as pale green and yellow, respectively. The RecA-like domains are shown in magenta. The protein was visualised using PyMol [3].

MARKQCQVCGQPATVRVEANLNGRNSTMLLCDDHYRQLVRQQKRTVSPLEALFGSRSGLF
EDFLGSDFFRIGEDATPVAADTDDVVDASFGEPATAGSGAPRRRGSGLASRISEQSEALL
QEAAKHAAEFGRSEVDTEHLLLALADSDVVKTIILGQFKIKVDDLKRQIESEAKRGDKPFE
GEIGVSPRVKDALSRAFVASNELGHSYVGPEHFLIGLAEEGEGLAANLLRRYGLTPQALR
QQVSKVVGKGAEDGRAETPTNTPELDKYSRDLTKMARDGKLDPVIGRAQEIETTIEVLAR
RKKNNPVLIGEPGVGKTAIVEGLAQRMVAGEVPETLRDKRLVELNINAMVAGAKYRGEFE
ERVQKVLKEVTEHQGELILFIDEVHTIVGAGQGGGEGGLDVANVFKPMMARGEINLIGAT
TLNEYQKYIEKDAALERRFQPVTVPEPTVAQAIMILRGLRDTFEAHHKVSISEDALIAAA
ELSDRYITARFLPDKAIDLLDQAAARVKLSATARPGAVQELESELHQLRREQDYVAARKQ
YDQAAELGKRIEAKEAELKKLVEDWERERASGSAEVKAEHVAQIVSRLTGIPVNELTVEE
REKLLHLEQRLHERLVGQDEAVRAVADAVRLSRAGLREGGKPVATFLFLGPTGVGKTELA
KALAESIYGDEHALLRIDMSEYGERHTVARLVGAPPGYVGYDEGGQLTEKVRKPYSVLL
LDEIEKAHPDVYNILLQVFDDGRLTDGKGRVVDFTNTII IATSNLGSDIIQRRLKAREAA
GEEYEKTKAEVMDVLRGHRPEFLNRIDEIIVFHALHALGKEEIRHIVGLQLDRVARSA
SQQVTLTFDQTLIDHFAEEGYKPEFGARELKRLIRSELETALAREMLGGGIGKGDHASAR
WDDKAERVVFERKEPPQTPAEPEQPDVAKATETPHGDAGKDSSKKKSASDAS

Figure S4: Primary amino acid sequence of ClpK. The sequence was obtained from GenBank (Uniprot: E0W6V3).

Table S3: *Klebsiella* species and strains used for the genomic analysis of Clp proteins. The species name, web-link and references were obtained from the NCBI genomes database for prokaryotes.

| Strain | Web-link | References |
|---------------------|---|------------|
| <i>K. aerogenes</i> | | |
| CAV1320 | https://www.ncbi.nlm.nih.gov/genome/3417?genome_assembly_id=232549 | [4, 5] |
| FDAARGOS 139 | https://www.ncbi.nlm.nih.gov/genome/327?genome_assembly_id=363711 | [6] |
| G7 | https://www.ncbi.nlm.nih.gov/genome/327?genome_assembly_id=271718 | [7] |
| FDAARGOS 327 | https://www.ncbi.nlm.nih.gov/genome/327?genome_assembly_id=1552 | [6] |

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|-------------------------|---|---------|
| <u>FDAARGOS 152</u> | https://www.ncbi.nlm.nih.gov/genome/327?genome_assembly_id=363028 | [6] |
| <u>FDAARGOS 513</u> | https://www.ncbi.nlm.nih.gov/genome/327?genome_assembly_id=3379 | [6] |
| <u>FDAARGOS 363</u> | https://www.ncbi.nlm.nih.gov/genome/327?genome_assembly_id=34818 | [6] |
| FDAARGOS_641 | https://www.ncbi.nlm.nih.gov/genome/3417?genome_assembly_id=695478 | [6] |
| <i>K. michiganensis</i> | | |
| <u>FDAARGOS 647</u> | https://www.ncbi.nlm.nih.gov/genome/33882?genome_assembly_id=695495 | [6] |
| <i>K. oxytoca</i> | | |
| <u>CAV1015</u> | https://www.ncbi.nlm.nih.gov/genome/1165?genome_assembly_id=291700 | [4, 5] |
| <u>KONIH5</u> | https://www.ncbi.nlm.nih.gov/genome/1165?genome_assembly_id=361932 | [8] |
| CAV1374 | https://www.ncbi.nlm.nih.gov/genome/1165?genome_assembly_id=232487 | [4, 5] |
| CAV1335 | https://www.ncbi.nlm.nih.gov/genome/1165?genome_assembly_id=232486 | [4, 5] |
| <u>FDAARGOS 335</u> | https://www.ncbi.nlm.nih.gov/genome/1165?genome_assembly_id=366590 | [6] |
| <u>CAV1752</u> | https://www.ncbi.nlm.nih.gov/genome/1165?genome_assembly_id=303753 | [4, 5] |
| <u>FDAARGOS 500</u> | https://www.ncbi.nlm.nih.gov/genome/1165?genome_assembly_id=3369 | [6] |
| <i>K. pneumoniae</i> | | |
| <u>2_GR_12</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=56801 | [9, 10] |
| <u>WCHKP649</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=375331 | [11] |
| FDAARGOS_775 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=589914 | [6] |
| <u>TVGHCRE225</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=380774 | [12] |

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|-------------------------------|---|----------|
| <u>BK13043</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=319029 | [13, 14] |
| <u>KP64 DNA</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=16976 | [15] |
| <u>KPNIH48[#]</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=363608 | [8] |
| <u>C2660</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=77054 | [16] |
| <u>WCHKP020037</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=77722 | [11] |
| <u>GSU10-3 DNA</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=17291 | [17-19] |
| <u>WCHKP2</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=382097 | [11] |
| <u>C789</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=74186 | [20] |
| <u>Isolate blood sample 2</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=280776 | [21] |
| <u>WCHKP115068</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=65659 | [11] |
| <u>WCHKP2080</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=65653 | [11] |
| <u>WCHKP36</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=373304 | [11] |
| <u>WCHKP020098</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=65657 | [11] |
| <u>Xen39</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=786792 | [22] |
| <u>WCHKP115069</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=27777 | [11] |
| <u>16 GR 13</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=4137 | [9, 10] |
| <u>FDAARGOS 531</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=3364 | [6] |

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|---------------------|---|----------|
| <u>SCKP020003</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=10198 | [11] |
| <u>KP617</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=249502 | [23] |
| <u>XH209#</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=212989 | [24] |
| <u>CAV1217</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=296907 | [1,2] |
| <u>1 GR 13</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=1578 | [9, 10] |
| <u>121</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=493866 | [25] |
| <u>SCKP020135</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=476671 | [11] |
| <u>WCHKP095845</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=13002 | [11] |
| <u>2-1</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=19 | [26] |
| <u>KP33 DNA</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=16975 | [15] |
| <u>SCKP020049</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=20206 | [11] |
| <u>FDAARGOS 630</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=6954 | [6] |
| <u>FDAARGOS 156</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=36549 | [6] |
| <u>CFSAN054111</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=370067 | [27-31] |
| <u>J1</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=260523 | [32, 33] |
| <u>KpN01</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=27223 | [34] |
| <u>FDAARGOS 566</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=3363 | [6] |

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| <u>Carbapenem-resistant blaNDM-1</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=205032 | [35] |
| <u>WCHKP34</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=382098 | [11] |
| <u>FDAARGOS 631</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=6953 | [3] |
| <u>TA6363</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=771384 | [6] |
| <u>CRKP I</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=521650 | [36] |
| <u>PMK1</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=211364 | [37] |
| <u>1050</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=10329 | [38] |
| <u>KPNIH39</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=277271 | [39] |
| <u>KPN1482</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=319030 | [13, 14] |
| <u>CAV1392</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=232380 | [5] |
| KPNIH45 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=468513 | [8] |
| CAV1344 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=232381 | [4, 5] |
| CAV1042 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=296901 | [4, 5] |
| C2414 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=770443 | [16] |
| 39427 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=908959 | [40] |
| CAV1217 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=296238 | [4, 5] |
| CAV1453 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=296230 | [4, 5] |

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| FDAARGOS_439 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=343753 | [6] |
| FDAARGOS_439 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=343751 | [6] |
| <i>K pneumoniae subsp. pneumoniae</i> | | |
| <u>KPNIH32</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=21262 | [41] |
| <u>WCHKP015093</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=65655 | [11] |
| <u>TGH8</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=272815 | [42-44] |
| <u>KPNIH31</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=213199 | [41] |
| <u>234-12</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=230300 | [45] |
| <u>KPNIH30</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=213198 | [41] |
| <u>KPNIH29</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=213197 | [41] |
| KPNIH33 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=212640 | [41] |
| <u>SCKP020079</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=377125 | [11] |
| SCKP020046 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=373305 | [11] |
| SCKP040074 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=377126 | [11] |
| ST:101960100 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=354684 | [46] |
| <u>TGH10¹</u> | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=272816 | [42-44] |
| TGH13 | https://www.ncbi.nlm.nih.gov/genome/815?genome_assembly_id=283648 | [42-44] |
| <i>K. quasipneumoniae</i> | | |

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|----------------------------|---|----------|
| ATCC 700603 | https://www.ncbi.nlm.nih.gov/genome/38419?genome_assembly_id=294621 | [9, 10] |
| <u>HKUOPLA</u> | https://www.ncbi.nlm.nih.gov/genome/3829?genome_assembly_id=20687 | [47] |
| <u>FDAARGOS 93</u> | https://www.ncbi.nlm.nih.gov/genome/3829?genome_assembly_id=36525 | [6] |
| <i>K. variicola</i> | | |
| <u>WCHKP19</u> | https://www.ncbi.nlm.nih.gov/genome/2121?genome_assembly_id=666503 | [47] |
| <u>DX120E</u> | https://www.ncbi.nlm.nih.gov/genome/2121?genome_assembly_id=280598 | [48] |
| <u>FDAARGOS 627</u> | https://www.ncbi.nlm.nih.gov/genome/2121?genome_assembly_id=695475 | [6] |
| GJ1 | https://www.ncbi.nlm.nih.gov/genome/2121?genome_assembly_id=30584 | [49] |
| GJ3 | https://www.ncbi.nlm.nih.gov/genome/2121?genome_assembly_id=30586 | [49] |
| <u>KP5-1</u> | https://www.ncbi.nlm.nih.gov/genome/2121?genome_assembly_id=20979 | [50] |
| <u>KPN1481</u> | https://www.ncbi.nlm.nih.gov/genome/2121?genome_assembly_id=20630 | [13, 14] |
| 342 | https://www.ncbi.nlm.nih.gov/genome/2121?genome_assembly_id=410978 | [51] |
| <u>WCHKV030666</u> | https://www.ncbi.nlm.nih.gov/genome/2121?genome_assembly_id=666504 | [11] |

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