SUPPLEMENTARY APPENDIX

This appendix has been provided by the authors to give readers additional information about their work.

Supplement to:

**Homology modelling and in silico substrate-binding analysis of a *Rhizobium* sp. RC1 haloalkanoic acid permease**

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**Figure S1** Pairwise sequence alignment of *Rhizobium* sp. RC1 haloacid transport (DehrP, Uniprot accession number: Q1M2W6 [1], with the new sequence (DehrP*).

Note: The deleted 13 amino acids (dark grey) and the additional 154 amino acids (light grey) is from the C-terminus of a 98% identical *Agrobacterium* sp. NHG3 haloacid transporter (DehP, Uniprot accession number: Q8KLT0, [2] after the DehrP sequence was aligned with the DehP sequence. The asterisks (*) indicate conserved residues as generated by the Clustal Omega [3] sequence alignment server.

| DehrP | MTTITLVAR11LASS4RMCTREERKVFASSLGIVTFYEFDLWESLALLAIQGATFFKDFPPATQ | 60 |
|-------|-------------------------------------------------|----|
| DehrP | MTTITLVAR11LASS4RMCTREERKVFASSLGIVTFYEFDLWESLALLAIQGATFFKDFPPATQ | 60 |
| DehrP | AITAILLPAAGS15VRTGALFGRGDMGRKNTLVTMSLTFVLLPGSDDTIGL | 120 |
| DehrP*| AITAILLPAAGS15VRTGALFGRGDMGRKNTLVTMSLTFVLLPGSDDTIGL | 120 |
| DehrP | AAPTILL11LLQLQ1A1GSQTKQQAAYEAFAHPFERGKDYTSMIQTTATAGLFLSLTVIL | 180 |
| DehrP*| AAPTILL11LLQLQ1A1GSQTKQQAAYEAFAHPFERGKDYTSMIQTTATAGLFLSLTVIL | 180 |
| DehrP | GTRSLLG15E SF1GNWVR15FLLLLVSLLG15SW11IMQLN15SPF1QRMK15PASKPA15REA | 240 |
| DehrP*| GTRSLLG15E SF1GNWVR15FLLLLVSLLG15SW11IMQLN15SPF1QRMK15PASKPA15REA | 240 |
| DehrP | FAHNPVR15ALVLGQGARQVAVWYTQ15FV15FLQL315LVVGGF15TITL11IC8811LG5S | 300 |
| DehrP*| FAHNPVR15ALVLGQGARQVAVWYTQ15FV15FLQL315LVVGGF15TITL11IC8811LG5S | 300 |
| DehrP | FFVFGKL15LDR15GRKP15MIA15GGLAVT15FPI15FEA15TENA15HT11LAMA11LAVK15SRV15GRL15P | 360 |
| DehrP*| FFVFGKL15LDR15GRKP15MIA15GGLAVT15FPI15FEA15TENA15HT11LAMA11LAVK15SRV15GRL15P | 360 |
| DehrP | SWG11GYS15ISEM15DHL15VLIP15EFL11ILL15R15CM15IV15RQ15LVQ15G15QL15CSS15MRP | 412 |
| DehrP*| SWG11GYS15ISEM15DHL15VLIP15EFL11ILL15R15CM15IV15RQ15LVQ15G15QL15CSS15MRP | 412 |
| DehrP | HPD11QAC15KE15QF11TAA11LAAA15YPKR15Q11D15RM15TH11FLDS15 GRP15Q11PL15GL15 IL15L15AY15T | 412 |
| DehrP*| HPD11QAC15KE15QF11TAA11LAAA15YPKR15Q11D15RM15TH11FLDS15 GRP15Q11PL15GL15 IL15L15AY15T | 412 |
| DehrP | NVYGPMR15ALVLEFLPARI11RYS15SLLPY11TH11CNGW15FGL15L15PAA15FA15H15VA15TD11YF15GL15W15PI | 527 |
| DehrP*| NVYGPMR15ALVLEFLPARI11RYS15SLLPY11TH11CNGW15FGL15L15PAA15FA15H15VA15TD11YF15GL15W15PI | 553 |
Figure S2. Local model quality of DehrP.
Note: The z-score (dark spot) is -2.86 according to the ProSA-web [4], and it falls in the range of the z-score for PDB proteins whose structures are determined by X-ray crystallography (light blue region) and nuclear magnetic resonance (NMR; dark blue region), indicating good quality model [4].

Supplementary Figure S3. Stereochemical analysis of DehrP using Ramachandran plot (re-typed for clarity of the readers).
Note: The plot obtained by the RAMPAGE [5] server shows that 93.6% of the amino acid residues are in the favoured region (blue region), 3.9% of the residues are in the allowed region (brown region) and 2.4% of the residues are outlier residues, indicating good quality model.
Overall quality factor**: 90.511

![Quality graphic](image)

**Figure S4** The overall quality graphic of DehrP using the ERRAT [6] program after refinement by the 3Drefine [7] server.

Note: The overall quality factor (OQF) of the model is ~91%, which is considered to be a good model. The incorrect regions are shown in black, and the correct regions are shown in grey. On the error axis, two lines are drawn to indicate the confidence with which it is possible to reject regions that exceed that error value. **Expressed as the percentage of the protein for which the calculated error value falls below the 95% rejection limit. For low resolutions (2.5 to 3 Å) the average OQF is around 91% [6].

**Table S1** The affinities of DehrP and GlcPse complexes generated by AutoDock Vina 1.1.2 [8].

| Ligand | Affinity (kcal/mol) | Distance from best mode (RMSD) |
|--------|---------------------|---------------------------------|
|        | GlcPse | DehrP | GlcPse | DehrP |
| DGlc   | −4.6   | −4.2  | 37.064/38.093 | 12.051/13.486 |
| MBA    | −2.9   | −2.9  | 53.11/53.426  | 17.618/17.822 |
| MCA    | −3.2   | −2.9  | 10.986/11.084 | 12.488/12.804 |
| DBA    | −      | −3.6  | −          | 17.534/18.321 |
| DCA    | −      | −3.5  | −          | 18.615/19.141 |
| TCA    | −      | −3.9  | −          | 19.169/19.810 |
| 2,2-DCP| −      | −4.0  | −          | 19.556/20.219 |

**References**

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