Input parameters

The example of input files are '*.in'. The execution files are '*.sh'. The order of input parameters must follow the input file examples, and blank lines are not allowed. Explanations regarding the input parameters in the input file are provided below.

- n_qv (integer): the number of rows (Q) in the experimental data.
- min_qv_range (integer): the first row of data used for optimization calculation.
- qv_range2 (integer): the last row of data used for optimization calculation.
- n_bin (integer): the number of states on the coordinate system to describe PDD.
- k_gradient (integer): the choice of optimization equation.
  - 0: Eq. (2)
  - 1: Eq. (17)
  - 2: Eq. (18)
- in_exp_file (character): the file name for pseudo-experimental SAXS data.
- bin_header (character): the file header name of SAXS data for each state.
- bin_header (character): the file footer name of SAXS data for each state.
- pdd0_file (character): the file name for an initial ensemble.
- true_pdd_file (character): the file name for a true ensemble.
- k_const (integer): the choice of constraints.
  - 0: No inclusion
  - 1: Included
- conf_fac (real): the value for confidence parameter (required only when k_const = 1).
- trans_rate (real): the value for transformation rate
- n_trans (real): the number of transformation steps.
- n_out (integer): the number of out_trans, which is described below.
- out_trans (integer): the transformation step, at which the data of the refined ensemble and SAXS are outputted.
- out_step (integer): in addition to out_trans, the data of the transformation are outputted at every out_step step.
- out_header (character): the name of file header for the output files.
  - 'out_header'//'_opt.log' : kai2, AREP, KL-divergence from initial PDD are outputted at every transformation.