

Supplementary material for "Statistical survey of hydrogen bond motifs in crystallographic special symmetry positions, and the influence of chirality of molecules in the crystal on formation of hydrogen bond "ring motifs"

This is a README file for the supplementary materials associated with the paper by Eppel & Bernstein 2008)

The materials described below are incorporated in a separate .zip file.

:The **software** folder contain two softwares, their user instruction and their source code

Chiral finder: Chiral finder is a program that accepts a file with a list of crystal structures and returns four files in which the crystal structures are divided according to their molecular symmetry type: Achiral , Chiral , Meso , Racemic (see Section 2.1 of the paper

Symmetry Finder: A program that accepts files of crystal fragments (motif or molecules correspond to *Conquest* search results), and returns statistics about the number of these fragments that occupy special symmetry sites. It also returns refcode files of all the crystals in which the fragments occupy a specific symmetry site

The **Chiral /Achiral/Meso/Racemic** folders contain all the *Conquest* searches for motifs that were done for Section 3.1 of the paper. In each of these folders there is a folder named **symmetry files** which contains for each motif refcode file of all the structures in which this motif occupies special positions of a specific type (*i.e.* inversion, rotation...) (done with the symmetry finder program

The **structures according to their molecular symmetry type** folder contain four refcode files

Chiral: containing all crystals structures of the chiral molecules/Enatiopure (see Section 2.1 of the paper

(Achiral: containing all crystal structures of Achiral molecules (see Section 2.1 of the paper

(Racemic: Racemic crystals (see Section 2.1 of the paper

(Meso: Crystals of Meso molecules (see Section 2.1 of the paper