

SUPPLEMENTARY INFORMATION

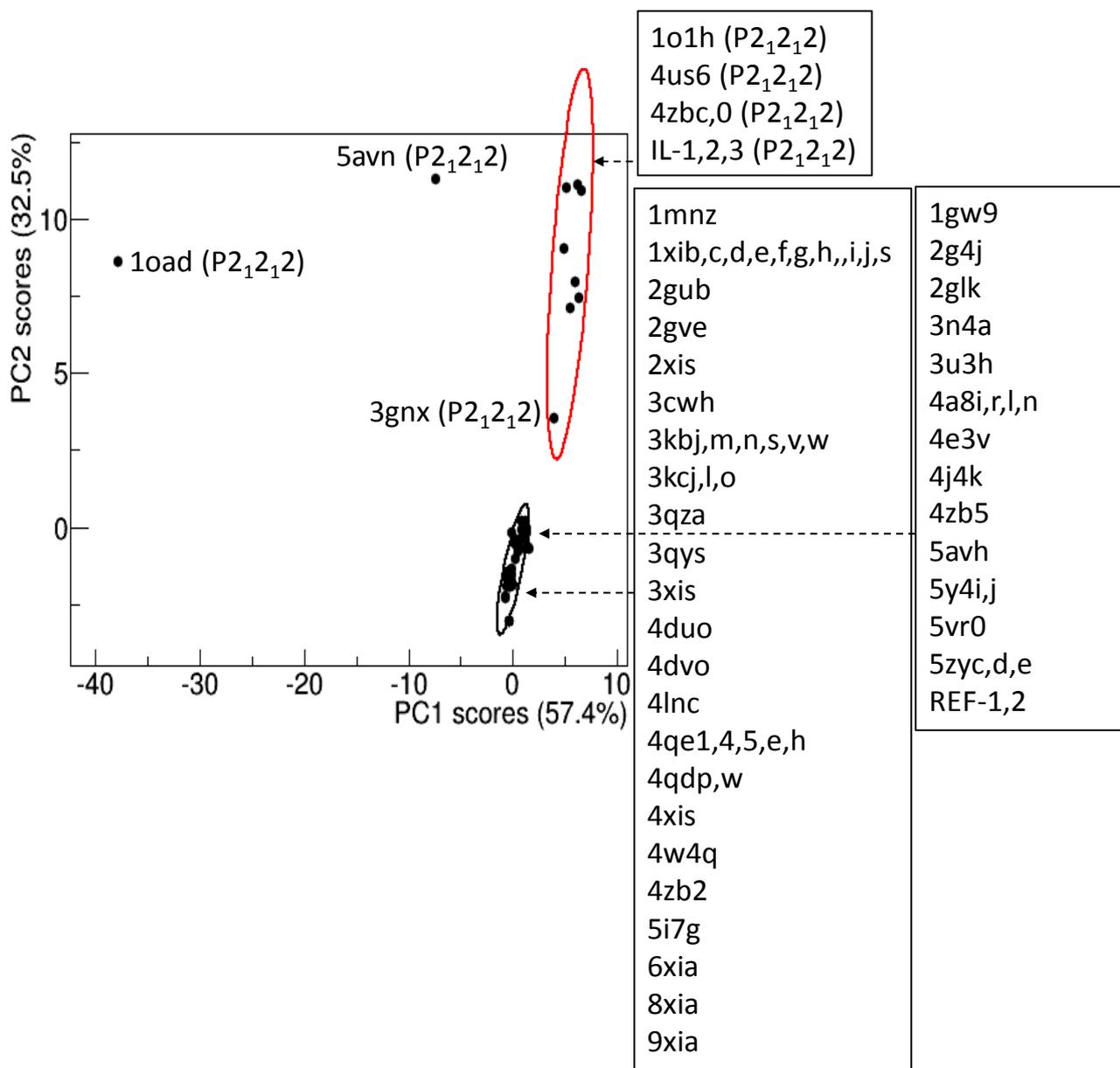


Figure S1. Comparison of the 75 experimental structural models of glucose isomerase from *S. rubiginosus* by principal component analysis applied on crystal cell parameters. Score plot of the first two principal components, where representative points are clustered according to a hierarchic clustering. 85% confidence level ellipses are shown and PDB codes associated to representative points are reported. Space group are indicated if they are P2₁2₁2; in the other cases the space group is I222. The percentage of the total data variance explained by each principal component is shown on the axes.

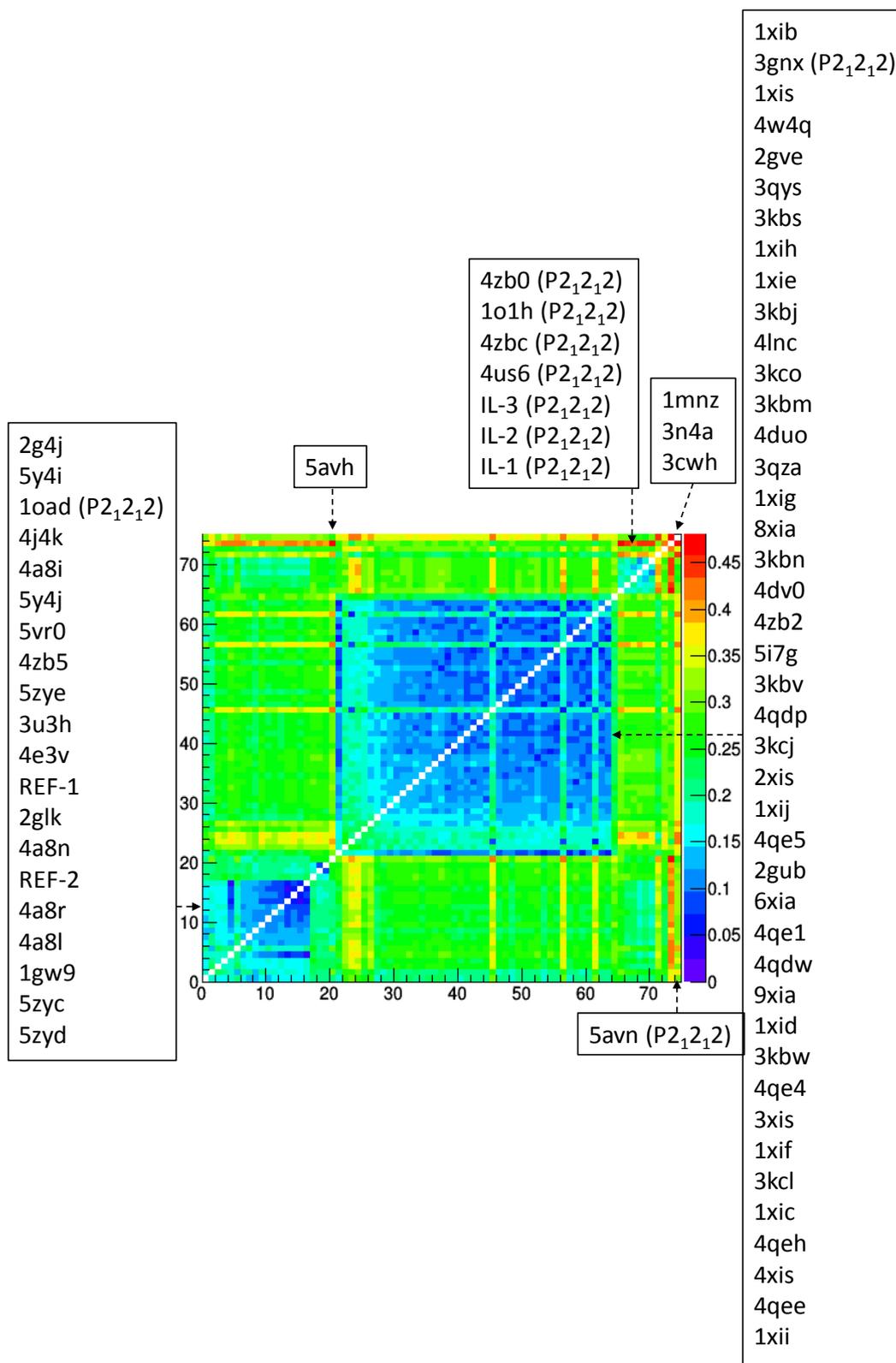


Figure S2. Comparison of the 75 experimental structural models of glucose isomerase from *S. rubiginosus*, carried out by using the root-mean-square deviation of their C α atoms. Distance matrix after application of hierarchical clustering, with PDB codes associated to each row/column reported, ordered according to their occurrence in the matrix and divided according to the clustering results. Space group is indicated if it is P₂₁2₁2, when missing it is I222.

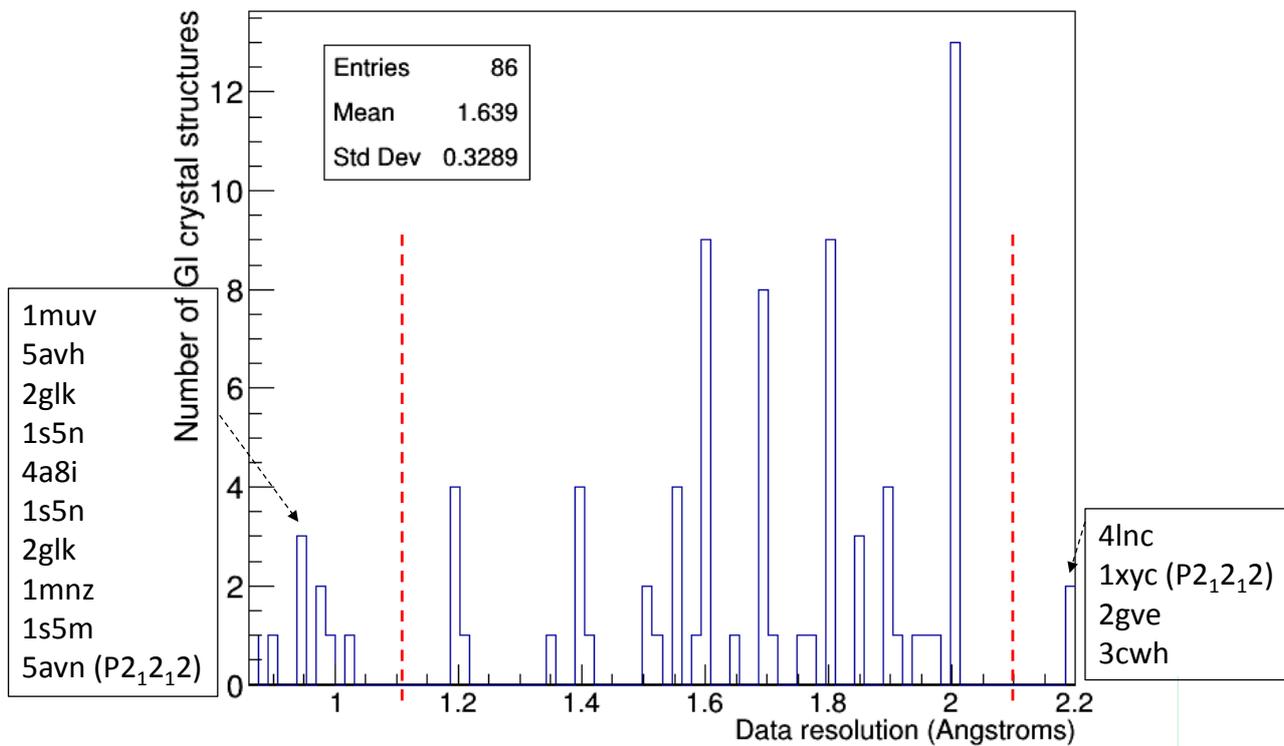


Figure S3. Distribution of data resolution of the 86 glucose isomerase crystal structures considered for comparative analysis. The number of entries (Entries), mean value (Mean) and standard deviation (Str Dev) of the distribution are shown. Two vertical dashed lines indicate threshold to identify outliers, i.e. crystal structures having data resolution better than 1.1 Å or worse than 2.0 Å (corresponding PDB codes are reported in side boxes).

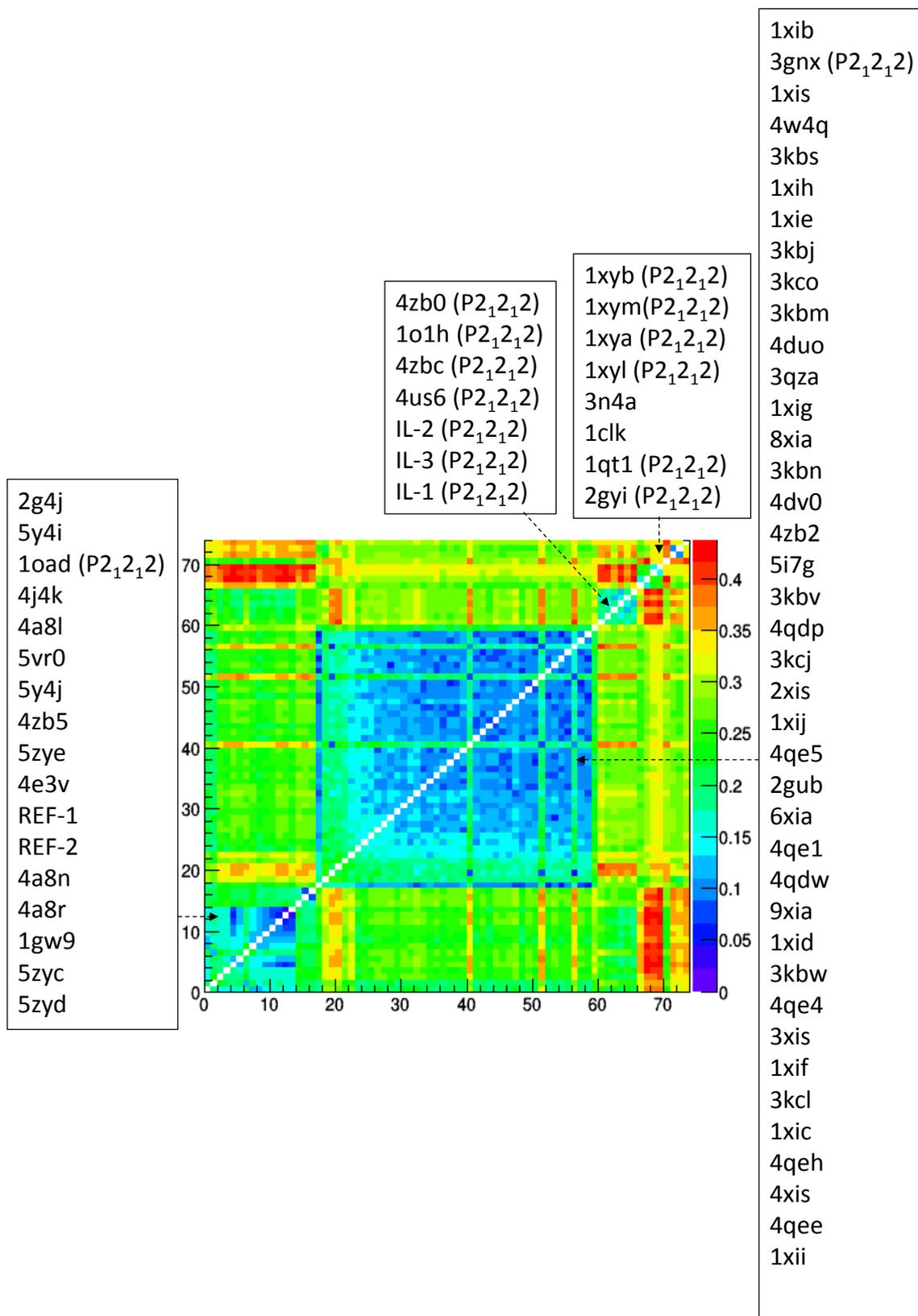


Figure S4. Comparison of the 74 experimental structural models of glucose isomerase obtained after selection on data resolution, carried out by using the root-mean-square deviation of their C α atoms. Distance matrix after application of hierarchical clustering, with PDB codes associated to each row/column reported, ordered according to their occurrence in the matrix and divided according to the clustering results. Space group is indicated if it is P2₁2₁2, when missing it is I222.