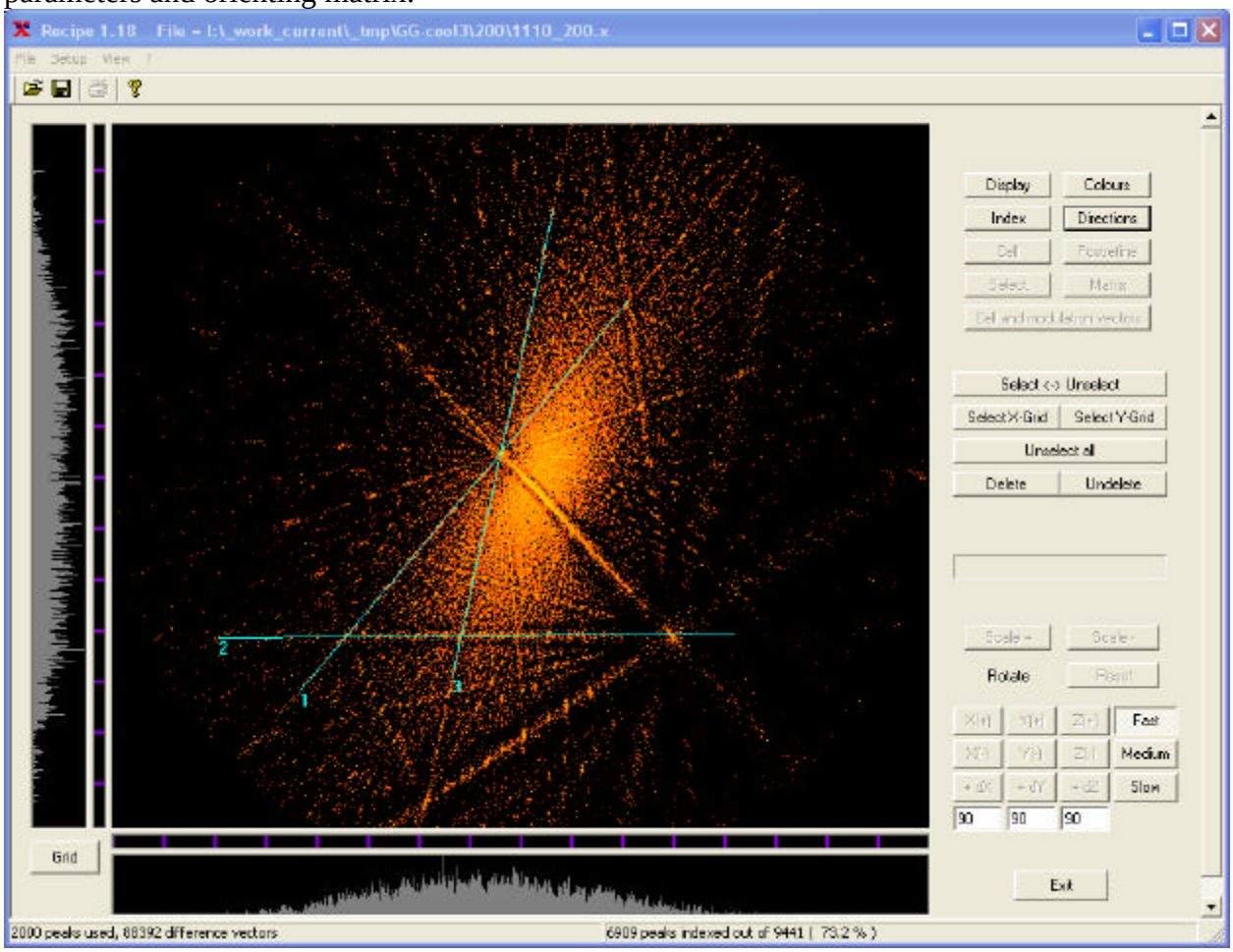
Electronic Supplementary Information

ESI-I. The procedure of indexing diffraction pattern from differently oriented domains in the glycine – glutaric acid co-crystal at 200 K, (phase I)[*]

Indexing was done following the procedure described in ***X-Area Software Manual, 2007, STOE & Cie GmbH*** manual. Using the currently selected peaks all difference vectors between all peak positions were calculated, normalised and projected onto the horizontal plane of the Ewald sphere. In case of a single crystal, provided that sufficient number of peaks (100 or more) have been used, a series of more or less sharp 'lines' can be seen. Each pixel represents a direction in reciprocal space. The picture is colour coded, the brighter a pixel the larger is the frequency of difference vectors having that direction. The difference map can be rotated and scaled just as the peaks to provide a better view. Each 'line' corresponds to a set of parallel, equally spaced layers in reciprocal space. After that we as users had to select 3 lines through densely populated regions from which the cell parameters could be determined. The lines must not intersect each other at the same point and they may not be all parallel to each other. Besides this it was not important which lines have been selected.

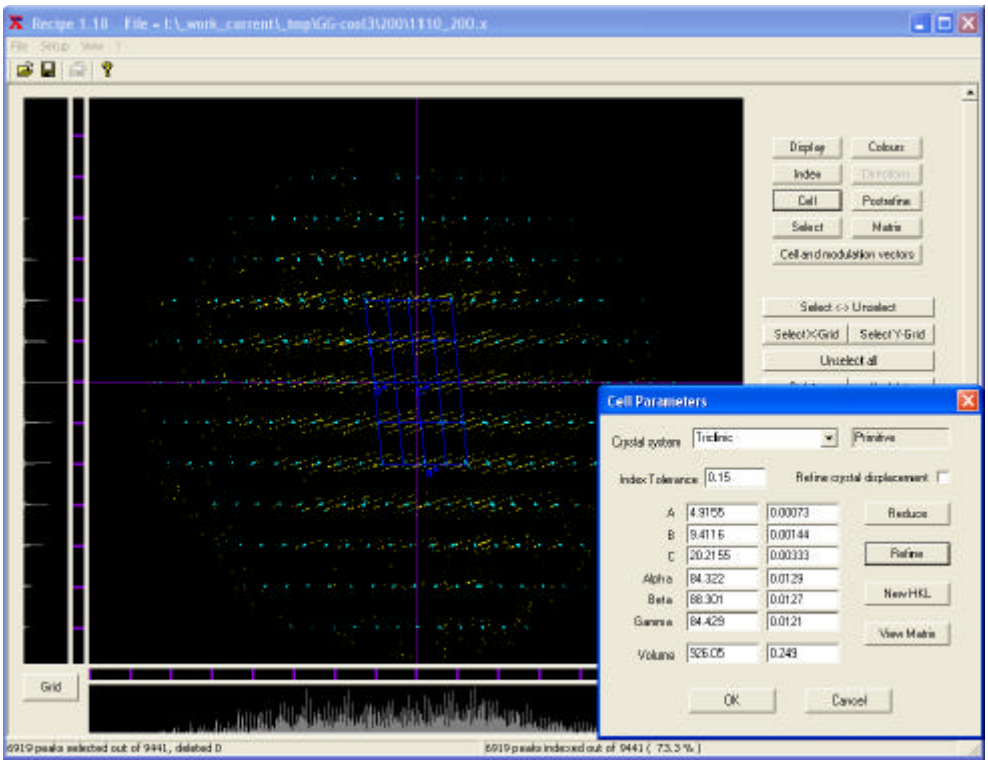
Indexing procedure step by step

1) For indexing procedure we used all peaks on diffraction images with $I > 6s$. After that we projected all difference vectors onto the horizontal plane. After selection of any three lines, which non-intersected in one point and were non-parallel to each other, we could refine unit cell parameters and orienting matrix.

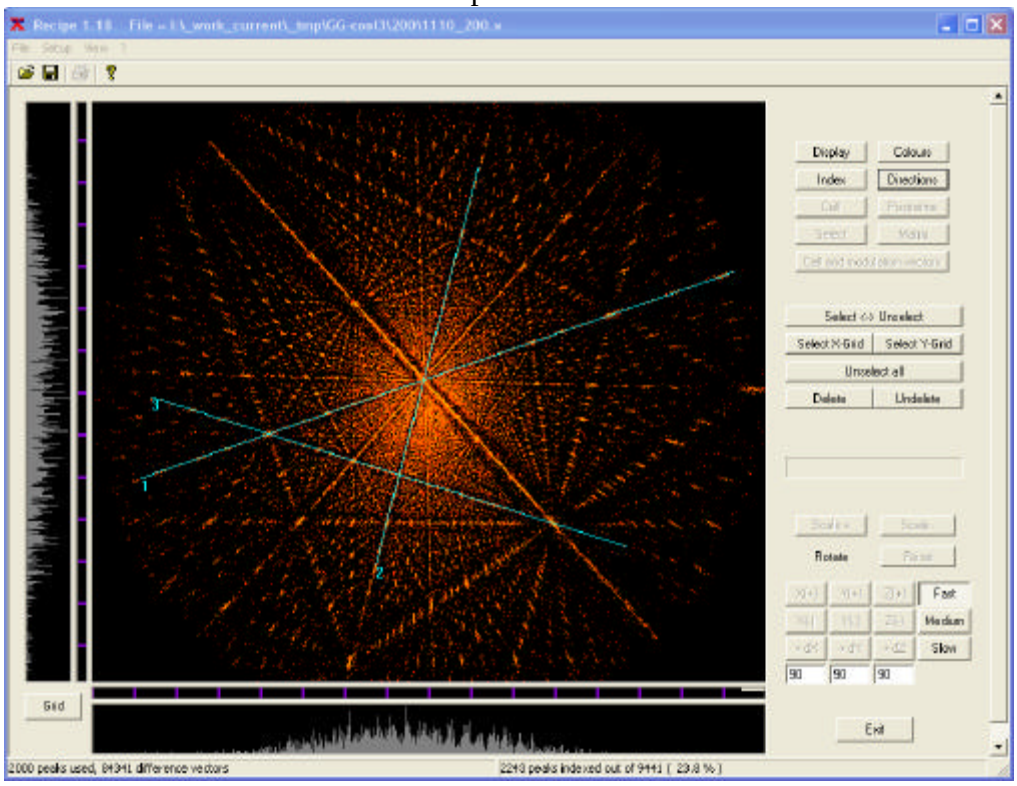


[*] A description of this procedure was requested by a referee, and we have decided that at least some readers may also need it for more clarity

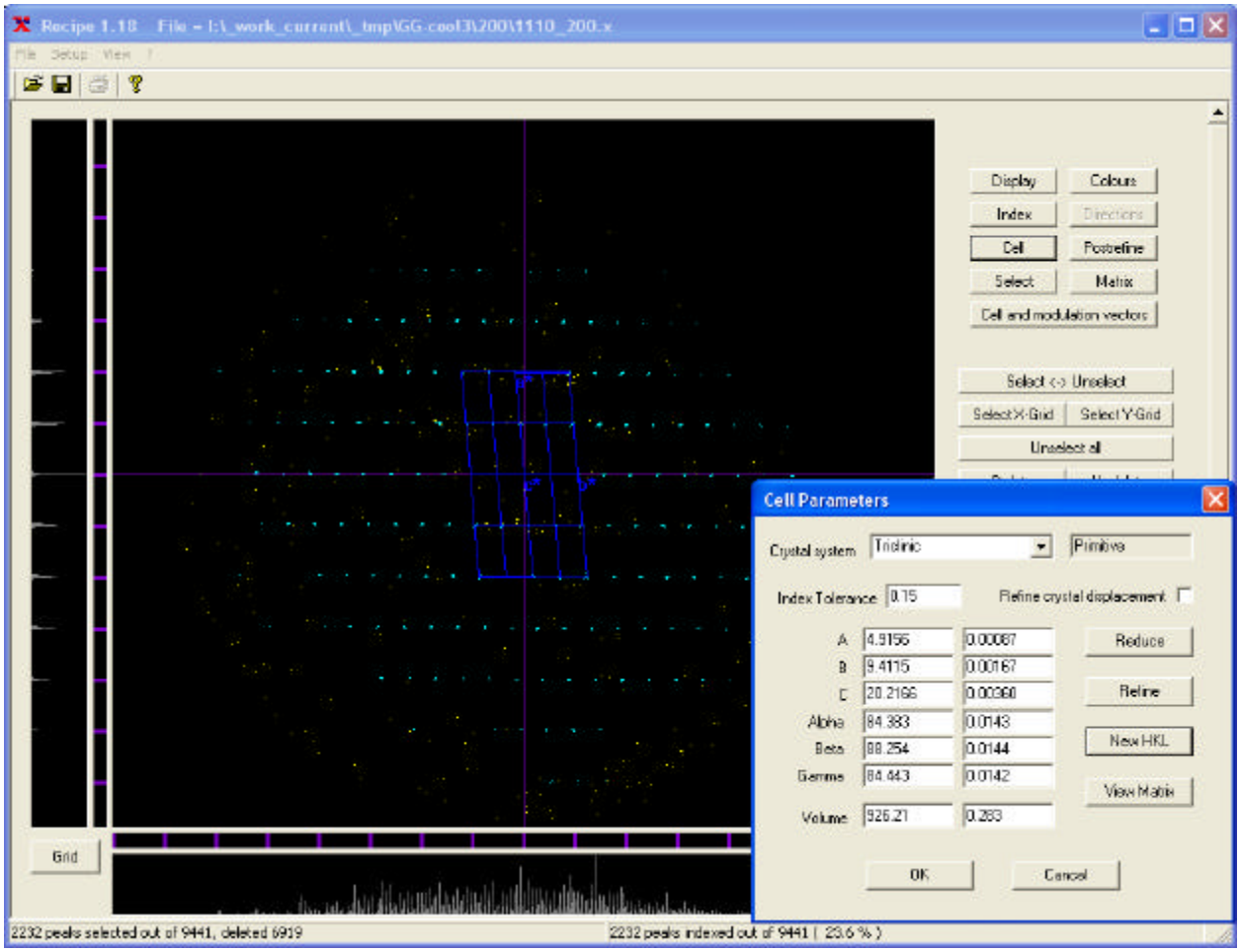
2) After refinement of unit-cell parameters we saw that 6919 out of 9441 (73.3 %) peaks could be described by current orienting matrix. They were marked by blue in the reciprocal space view. Yellow peaks were not yet indexed. At this step refined orienting matrix (obtained using blue-marked peaks) for the first component could be easily saved.



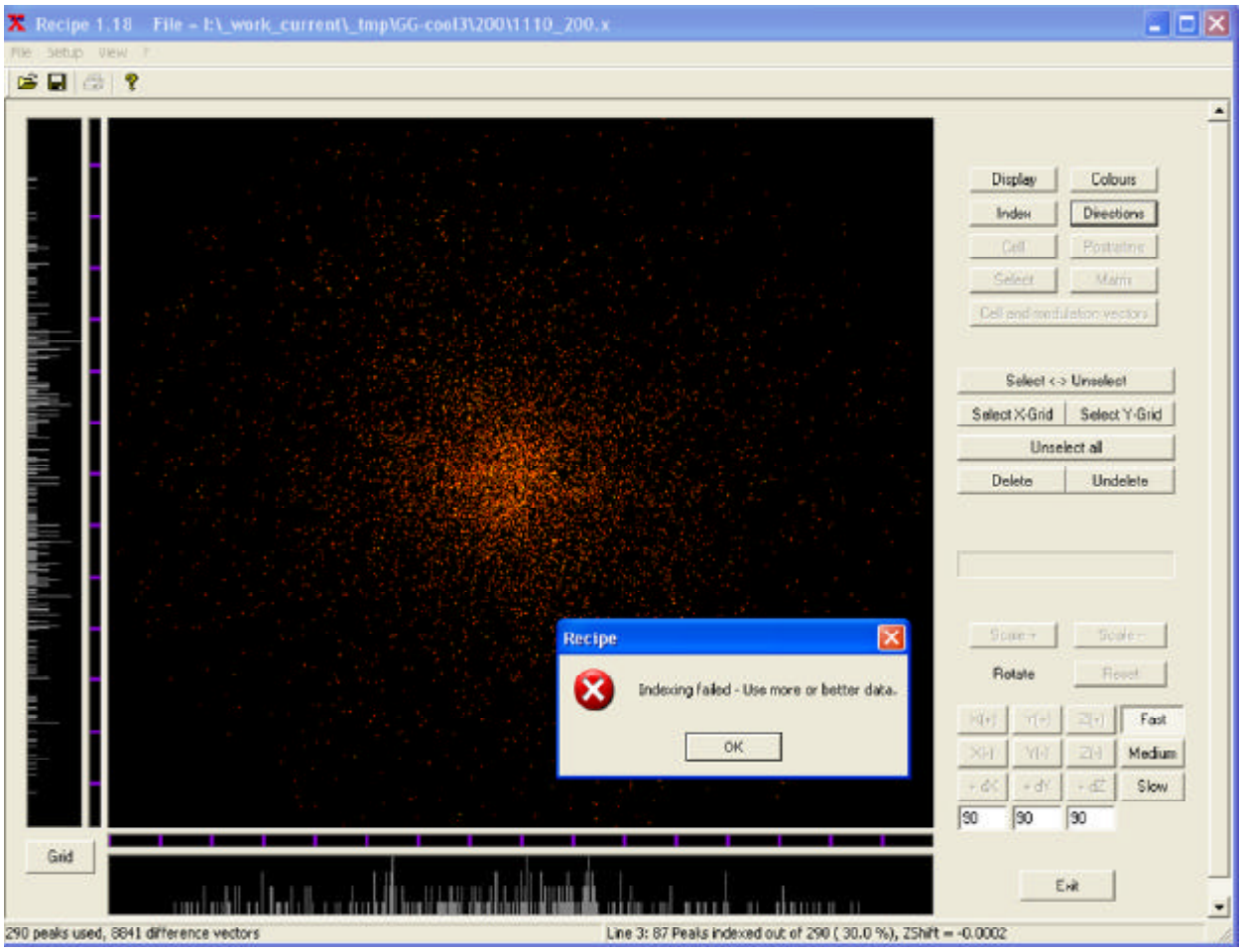
3) At this step we removed all indexed peaks from the reciprocal space view and projected all difference vectors for remaining peaks on the horizontal plane again with selection of 3 independent lines as described for the first step.



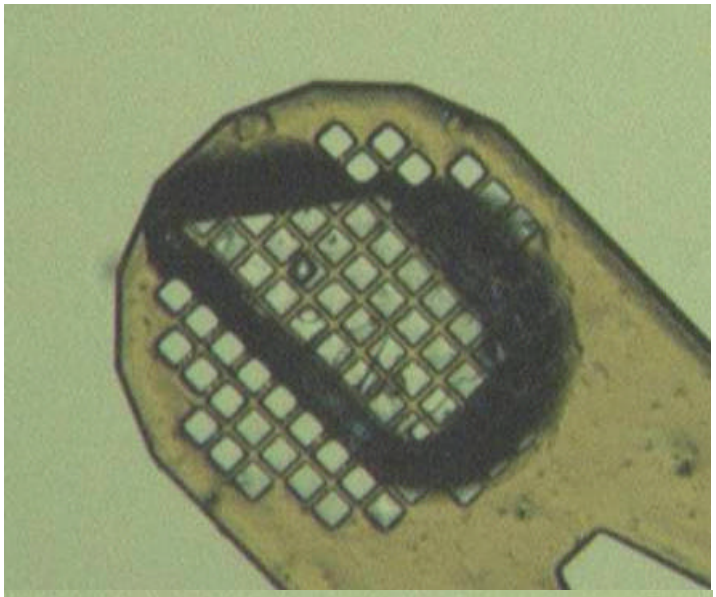
4) After the refinement of unit-cell parameters using this set of reflections, we saw that 2232 out of 9441 (23.6 %) peaks could be described by this orienting matrix. They are marked by blue in the reciprocal space view. Yellow peaks are not yet indexed. At this step refined orienting matrix (obtained using blue-marked peaks) for the second component could be easily saved. As we can see from the pictures presented, cell parameters for both components are in good agreement, and we conclude, that these components belong to the same phase (II).



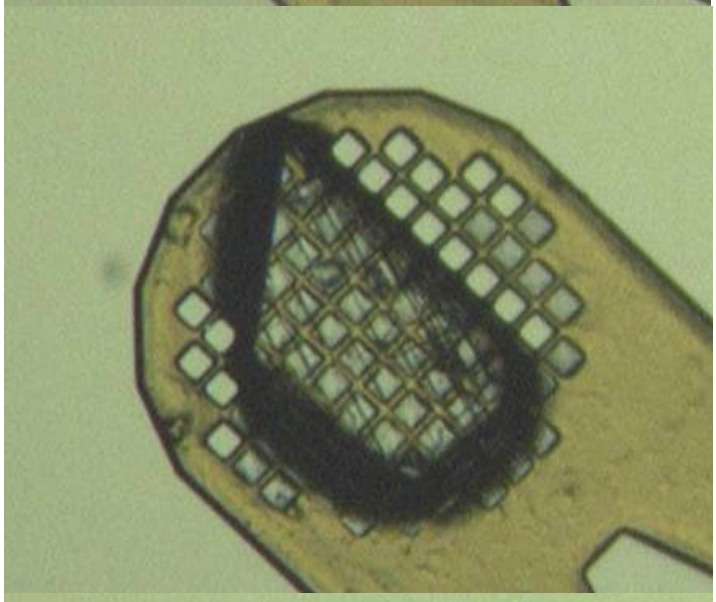
5) At this stage we had 6919 + 2232 = 9151 indexed peaks out of 9441 (73.3 + 23.6 = 96.9 %). 290 peaks (3.1 %) remained non-indexed, and we could see corresponding projections of difference vectors onto the plane. As we can see from the figure below, no clear directions could be found. So one could conclude, that these peaks did not belong to our crystalline phase, and appeared due to scattering from cryo-oil, crystal holder, ice particles, *etc.* which are in X-ray beam. It means, that the crystal contained two components with 73.3 and 23.6 % indexed reflections respectively. Using these values we could roughly estimate the ratio of the domains – it should be ~3:1.



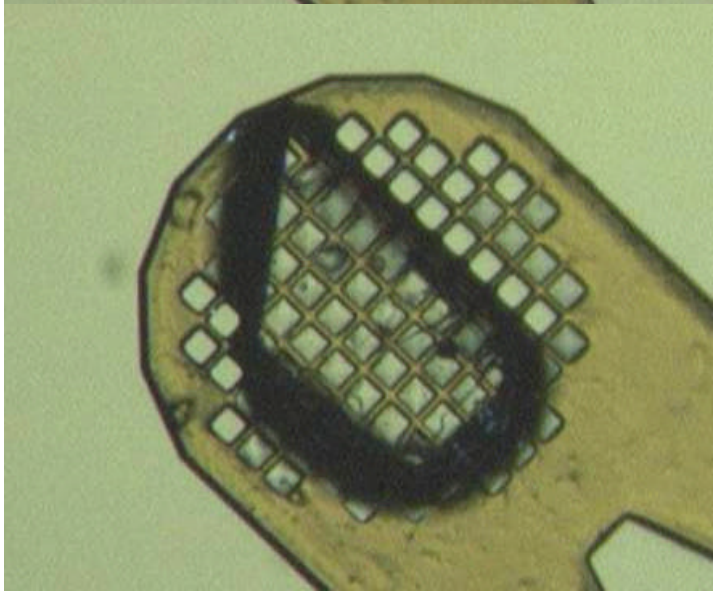
ESI-II. Photographs of a glutaric acid - glycine co-crystal before and after the phase transition into phase II on cooling and after reverse heating



Glutaric acid - glycine co-crystal before starting X-ray measurements at 300 K (*?* = -150º).



Glutaric acid - glycine co-crystal at 200 K after phase transition I ? II. One can see clear black lines on the sample indicating borderlines between domains with different orientations (*?* = 30º).



Glutaric acid - glycine co-crystal at 250 K after phase transition II ? I on heating the sample. One can no longer see the borderlines between domains (*?* = 30º).