buster-report: convenient summaries of BUSTER output including analysis of ligand geometry

GΦL

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Introduction

BUSTER runs produce relatively large quantities of output, much of it in tabular forms which are not straightforward to understand or parse.

`buster-report` summarises this output in a user-friendly form, including attractive graphs. `buster-report` outputs HTML (for web browsers) or PDF (for printing or electronic lab notebooks).
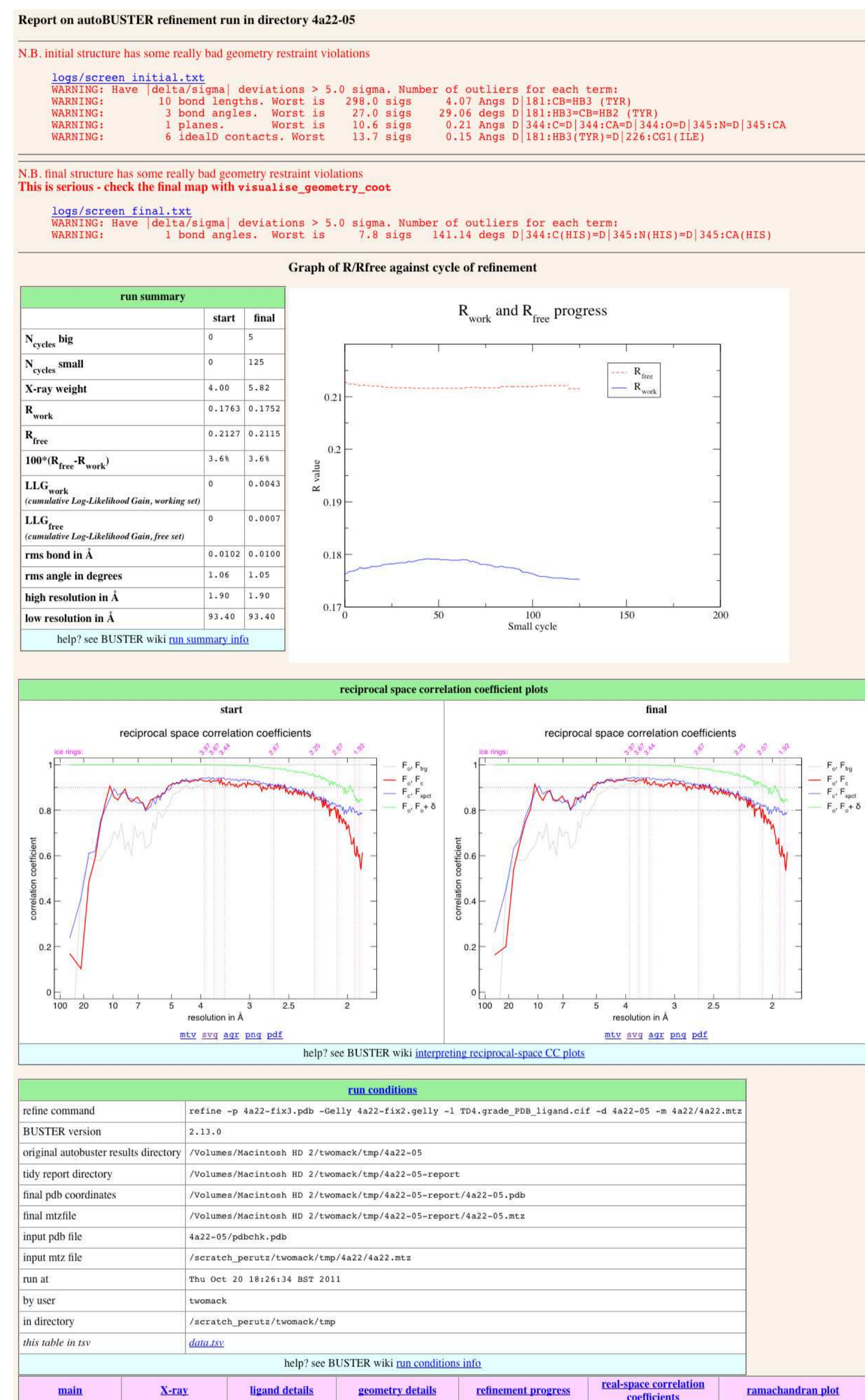
Ligand assessment

MOGUL is the standard tool for assessing ligand poses, but the current MOGUL GUI doesn't readily support the assessment of multiple ligands in a single structure; `buster-report` does all the necessary file manipulation to provide a clear report of ligand problems, and combines the MOGUL output with correlation coefficients and images of the ligand in (standard and difference) density.

Histograms are used to indicate unusual torsions.

Ligand report for 1PMQ refined with the coordinates of the ligand fixed

To make the diagrams of ligands more comprehensible, the HTML version includes small movies, both of the ligand oscillating, and (when there's one or more very bad bond or angle) of the ligand with the atoms involved in the bad features highlighted. Future versions will use `coot`'s upcoming capability to produce 2D diagrams of ligands, to produce clearer PDF output in which animation is not available.

Illustrations of the bond and angle problems found in 1PMQ

The correlation-coefficient plot

One of **BUSTER**'s unique features is the plot of reciprocal-space correlation coefficients as a function of resolution bin.

green $F_o, F_o + \delta$: information content in the observed reflections. If this is not above all the other lines, something has gone very wrong with the scaling

thick red F_o, F_c : how well does the model reflect the data?

blue F_c, F_{xpct} : how well do you expect the model to reflect the data, given both the quality of the data and the estimated reliability of the model?

grey F_o, F_{frg} : correlation coefficient without taking the solvent model into account. This should be below the red line out to 5Å, and exactly the same as the red line at higher resolutions.

This allows very ready recognition of a number of crystal issues which are not easily discerned from other summary information, including

- Ice rings are readily seen as 'icicles' in the green line (from some integration packages), or as downward peaks in the red and blue lines (from others); note that the more diffuse ring at 2.25Å sometimes shows up when the sharper ones around 3.7Å don't

- Anisotropy of diffraction is visible in a departure of the red line from the blue line

- The resolution bin at which the information content of further reflections starts to drop off can be seen

- Cases where the standard deviations of the F values have been incorrectly determined produce extremely clear signs in the blue and green lines
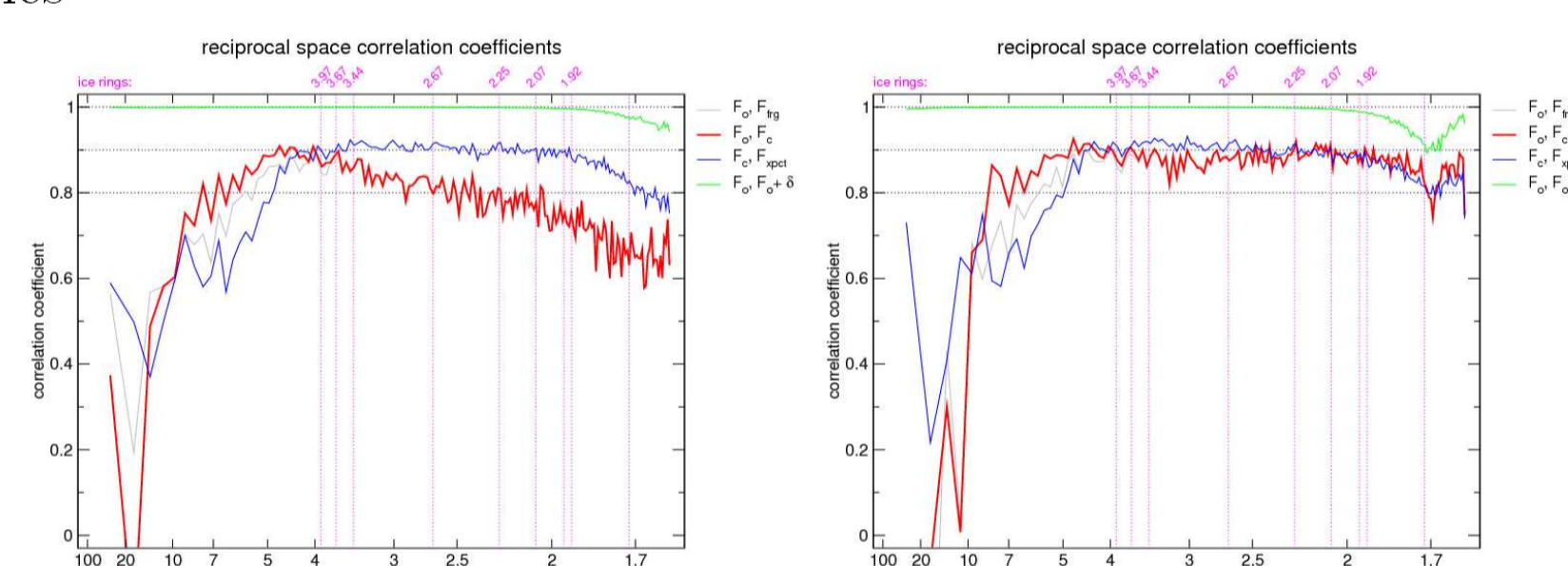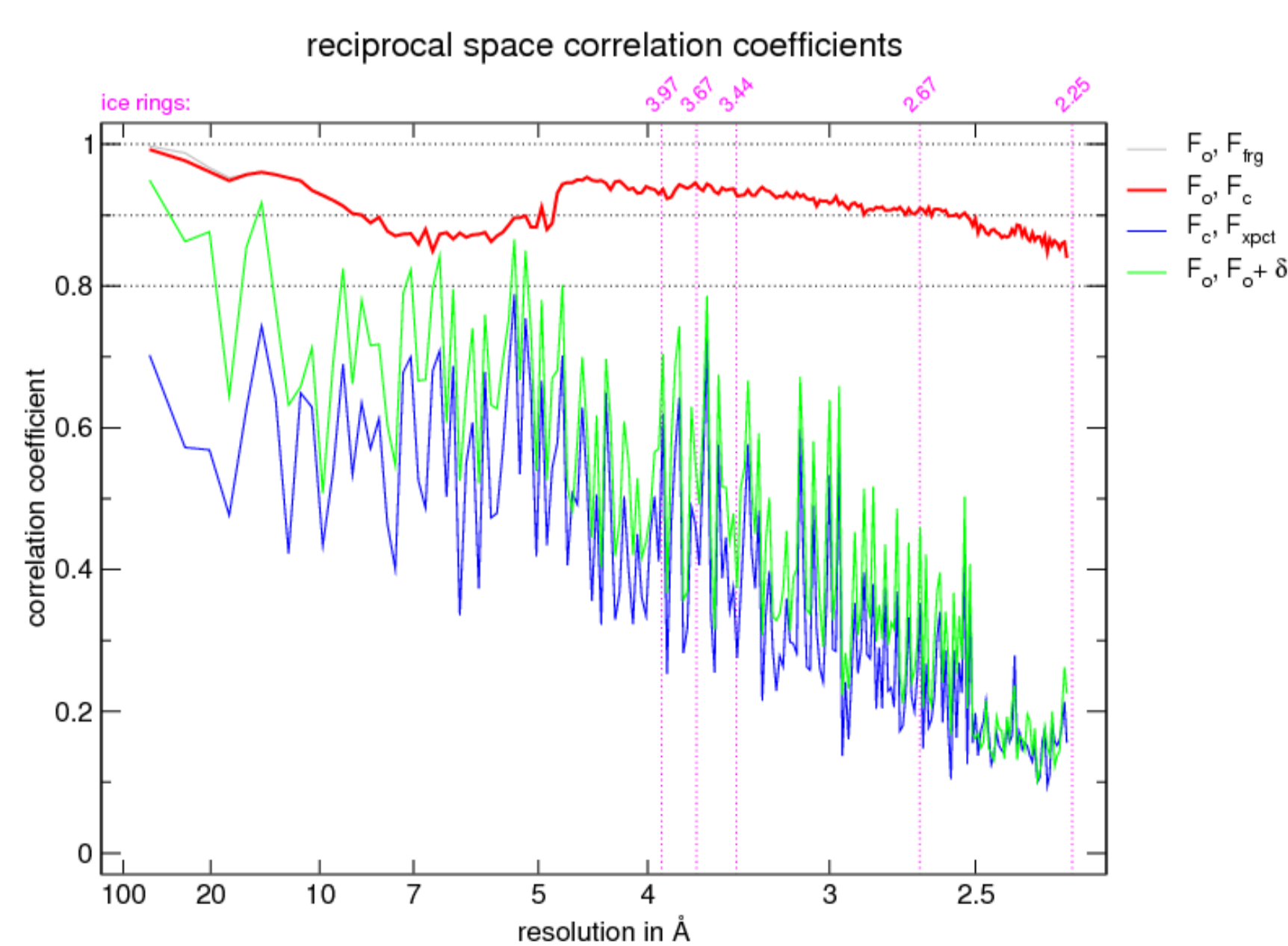

3OUL: before and after ellipsoidal scaling
(rectified using http://services.mbi.ucla.edu/anisoscale/).
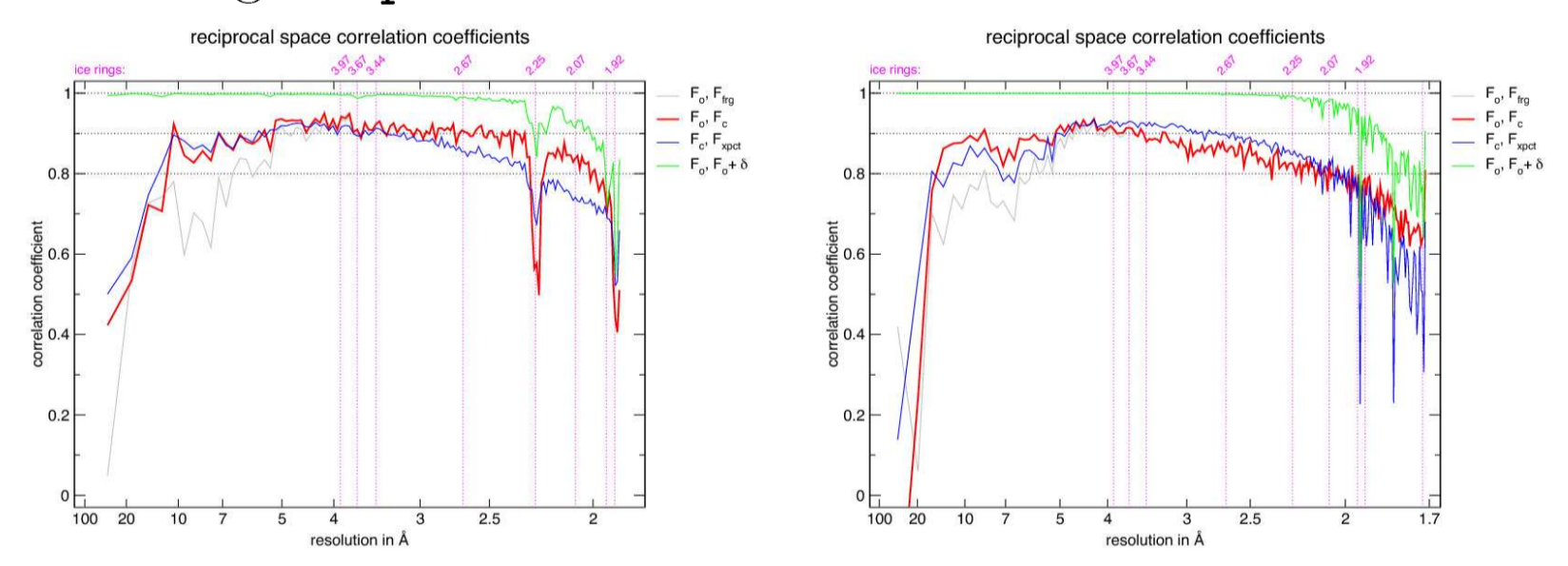
**left: 2XT0 (serious ice-ring contamination);
right: 3AZR (problems with high-resolution data)**
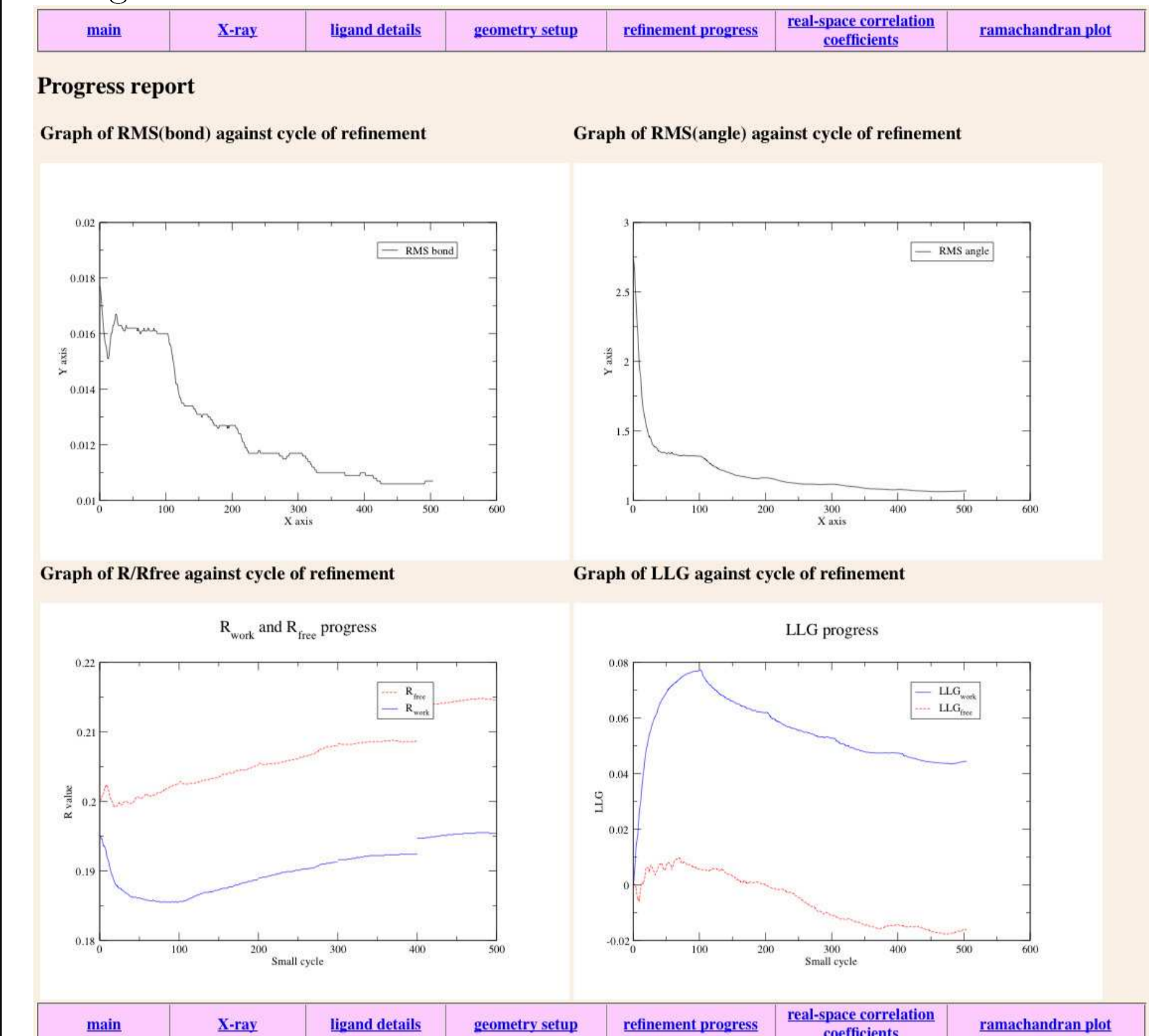

2HR0: there is clearly something very wrong with these data

The tool `graph_autobuster_recipCC` has been distributed for a couple of releases, but `xmgrace` allows much more user-friendly forms of the graph to be produced.

Progress graphs

Graphs of how R, R_{free}, log-likelihood gain, and RMS bond and angle change over the course of the refinement are available.
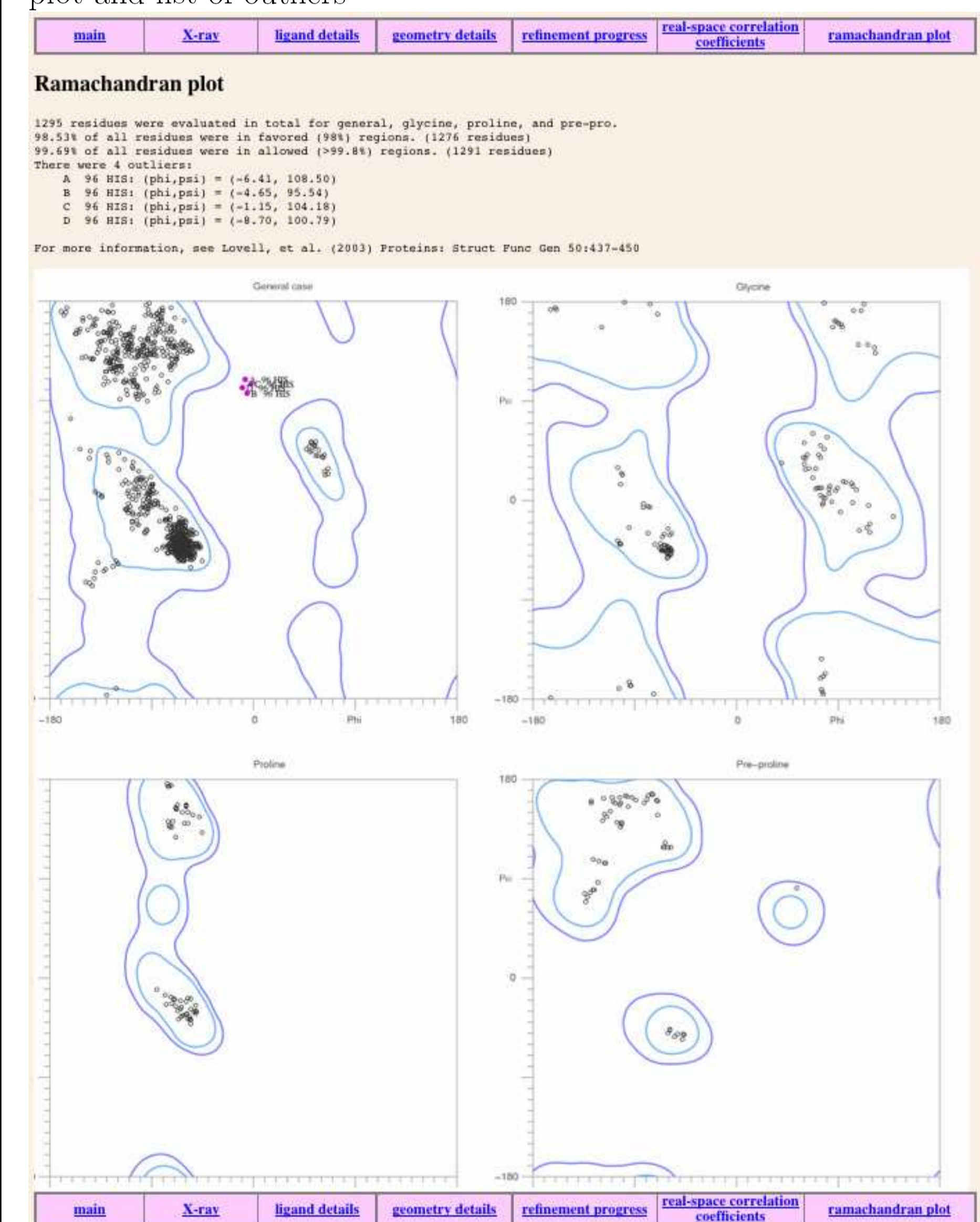

Geometry issues

Serious geometry outliers present at the start of refinement are listed, and serious geometry outliers still present at the end of refinement are listed in large red type.

General assessment using molprobity

Tools from the molprobity toolset are used to produce a Ramachandran plot and list of outliers

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