Dear Sam and Structure Staff:

We emailed our corrections to Sam this morning and we are providing the same again in this fax.

The typesetting for eqn. 3 is particularly important. The subscript \( i \) is an index, and the subscript 'measured' or 'predicted' is a qualifier for the quantity; the two need to be distinct labels on the variable.

Further corrections are below. Please let us know if you have further questions, and CC David Masica on any questions for a faster response. We are happy to review any new proofs rapidly.

Thanks,
Jeffrey J. Gray
Associate Professor
Chemical & Biomolecular Engineering
Johns Hopkins University
Baltimore, Maryland 21218
http://graylab.jhu.edu
Phone: (410) 516-5313
Fax: (410) 516-5510

On Sun, Nov 21, 2010 at 6:27 PM, David Masica <david.masica@gmail.com> wrote:

Hi Sam,

Paper looks great! We noticed a couple of mistakes in two of the tables and two of the equations; please find those mistakes detailed below:

**Table 3:**
Please change the *Table 3* title to the following:

*Table 3. Comparison of all ssNMR measurements, ensemble statistics at each HAp surface from round 2 biased structure prediction, and predicted angles and distances from a representative structure from the final biased structure prediction at the HAp \{001\} surface.*

**Table 4:**
When Table 4 was reformatted, the end (far right) of the header was clipped and is missing (>7). Also, we made a couple font mistakes, namely, two numbers that should have been subscripted that were not, and one superscript that should have been regular font. Rather than explain the changes in words, I have attached a .png (Table4.png) of Table 4 so you can see how the header should read, and make appropriated changes.

**Equation 2:**
Equation 2 and the comma at the end of Equation 2 appear to have a space between them; that space should probably be removed.

**Equation 3:**
Equation 3 changed during reformatting. All occurrences of the word *predicated* should read *predicted*. Also, the subscripting wasn’t accurately formatted. However, it was in Equation 2, compare for instance *iconstraint* in Equation 2 with *imeasured* in Equation 3. In Equation 2, the \( i \) and *constraint* in *iconstraint* are subscripted at different levels, making the meaning clear. Can you possibly recover that subscripting style for all relevant instances in Equation 3. We also made a mistake in Equation 3. In the final component of the piecewise function, the numerator of the fraction should read \( ximeasured - xipredicted \) rather than \( ximeasured - ximeasured \). I have attached a .png (Equation3.png) of Equation 3 so you can see how it should look, and make appropriate changes.
Table 4.png:

<table>
<thead>
<tr>
<th></th>
<th>$E_{S,C^5}$ (4.2 ± 0.3)</th>
<th>$R_{13,C^5}$ (&gt;7)</th>
<th>$F_{14,C6}$ (&gt;7)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Round 1</td>
<td>8.2 ± 2.5</td>
<td>8.1 ± 3.8</td>
<td>13.4 ± 4.1</td>
</tr>
<tr>
<td>Round 2</td>
<td>5.0 ± 0.5</td>
<td>7.6 ± 2.5</td>
<td>12.4 ± 2.8</td>
</tr>
<tr>
<td>Fimal</td>
<td>4.5 ± 0.2</td>
<td>11.4 ± 3.8</td>
<td>13.8 ± 3.4</td>
</tr>
</tbody>
</table>

Equation 3.png

$$E_{i,\text{constraint}} = \begin{cases} 
0, & \text{if } x_{i,\text{measured}} - \sigma < x_{i,\text{predicted}} \\
& \text{and} \\
& x_{i,\text{measured}} + \sigma > x_{i,\text{predicted}} \\
& \text{else} \\
& \left( \frac{x_{i,\text{measured}} - x_{i,\text{predicted}}}{\sigma_i} - 1 \right)^2 
\end{cases}$$