Below are a few comments for the SAMPL5 comparison paper:

(1) Page 6: "octa-acid OAH host" and "octa-acid OAMe host".

OAH and OAMe are names assigned specifically for the SAMPL5 challenge, but they have different names in the earlier experimental studies. Here is how we described them in the overview paper:

“The first two hosts, OAH [32] and OAMe, from the Gibb laboratory, are also known as octa-acid (OA) and tetra-endo-methyl octa-acid (TEMOA).”

You might want to introduce the compounds along those lines.

The references are:

OAH:

Gibb CLD, Gibb BC (2014) Binding of cyclic carboxylates to octa-acid deep-cavity cavitand.

J Comput Aided Mol Des 28:319–325. doi: 10.1007/s10822-013-9690-2

OAMe:

Gan H, Gibb BC (2013) Guest-mediated switching of the assembly state of a watersoluble

deep-cavity cavitand. Chem Commun 49:1395–1397. doi: 10.1039/c2cc38227j

Jordan JH, Gibb BC (2014) Molecular containers assembled through the hydrophobic

effect. Chem Soc Rev 44:547–585. doi: 10.1039/c4cs00191e

(2) Reference for CBClip:

Zhang B, Isaacs L (2014) Acyclic cucurbit[n]uril-type molecular containers: Influence of

aromatic walls on their function as solubilizing excipients for insoluble drugs. J Med

Chem 57:9554–9563. doi: 10.1021/jm501276u

(3) May need to cite MOE:

Molecular Operating Environment (MOE) 2013.08 (2016) Chemical Computing Group

Inc., 1010 Sherbooke St. West, Suite #910, Montreal, QC, Canada, H3A 2R7.

(4) Reference for AMEBR 14

Case, D. A.; Babin, V. ; Berryman, J. T. ; Betz, R. M.; Cai Q., Cerutti, D. S.; Cheatham, T. E.,

III; Darden, T. A.; Duke RE., Gohlke, H.; Goetz, A. W.; Gusarov, S.; Homeyer, N.; Janowski

P., Kaus, J.; Kolossvary, I.; Kovalenko, A.; Lee, T. S.; LeGrand, S.; Luchko, T.; Luo, R.;

Madej, B.; Merz, K. M.; Paesani, F.; Roe, D. R.; Roitberg, A.; Sagui, C.; Salomon-Ferrer, R.;

Seabra, G.; Simmerling, C. L.; Smith, W.; Swails, J.; Walker, R. C.; Wang, PA AMBER 14;

University of California, San Francisco, 2014.

(5) Also on Page 6, it says “in the figures above”, but the paper does not contain a figure for the compound structures. Is it from the instruction file?

Another thing to note is this paragraph is only a description about how we treated the protonation states of the hosts and guests for the standard input files, but it was totally up to the participants to decide on the protonation states and whether there would be binding shifts in the challenge.

(6) On page 7: “how short? What was done precisely?”

It may be not worth a detailed description in the main text since it is just equilibration for the solvent. But the details are here:

First ran 1 ps NVT at 10 K, then a heating up phase from 10 K to 298.15 K during 50 ps NVT, and finally 1 ns NPT at 298.15 K.

(7) In Table 3, not sure if Antechamber is the right module to be listed along with other programs.

The coulomb constant was actually defined in a module called tleap.

You can find the constant from $AMBERHOME/AmberTools/src/leap/src/leap/unitio.c

"#define ELECTRONTOKCAL  18.2223"

and it is not part of Antechamber. Maybe confirm with AMEBR experts ☺

(8) On page 9: Is this correct on the constraints, or were just H-bonds constrained?

Only bonds involving hydrogen are constrained.