

# IUCrJ

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**Supporting information for article:**

**fragHAR: towards *ab initio* quantum-crystallographic X-ray structure refinement for polypeptides and proteins**

**Justin Bergmann, Max Davidson, Esko Oksanen, Ulf Ryde and Dylan Jayatilaka**

**S1. GA**

In this section we display the GA dipeptide, and the fragments used.

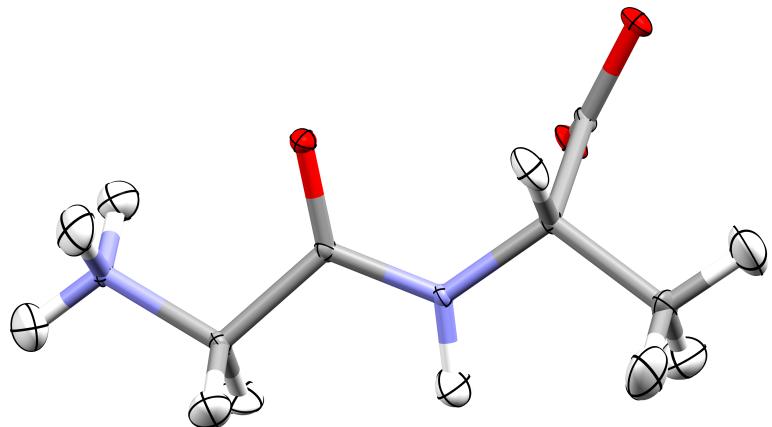


Fig. S1. Gly-Ala (GA)

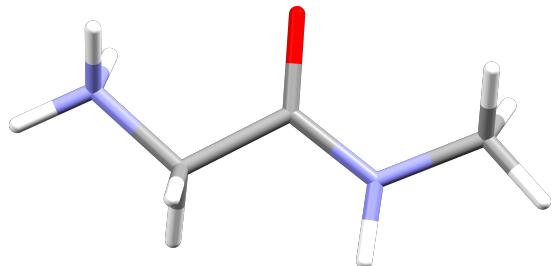


Fig. S2. First fragment of GA, GLY-1

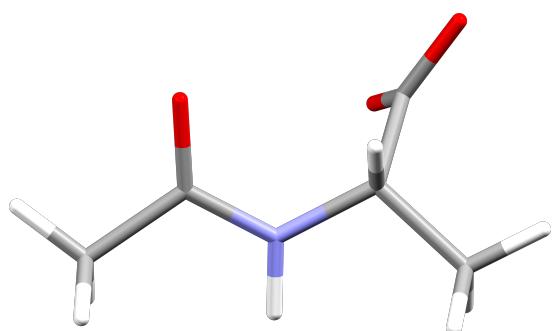


Fig. S3. Second fragment of GA, ALA-2

*S1.1. Bond lengths*

Figures S4–S6 are graphs of the bond lengths from fragHAR vs HAR refinements.

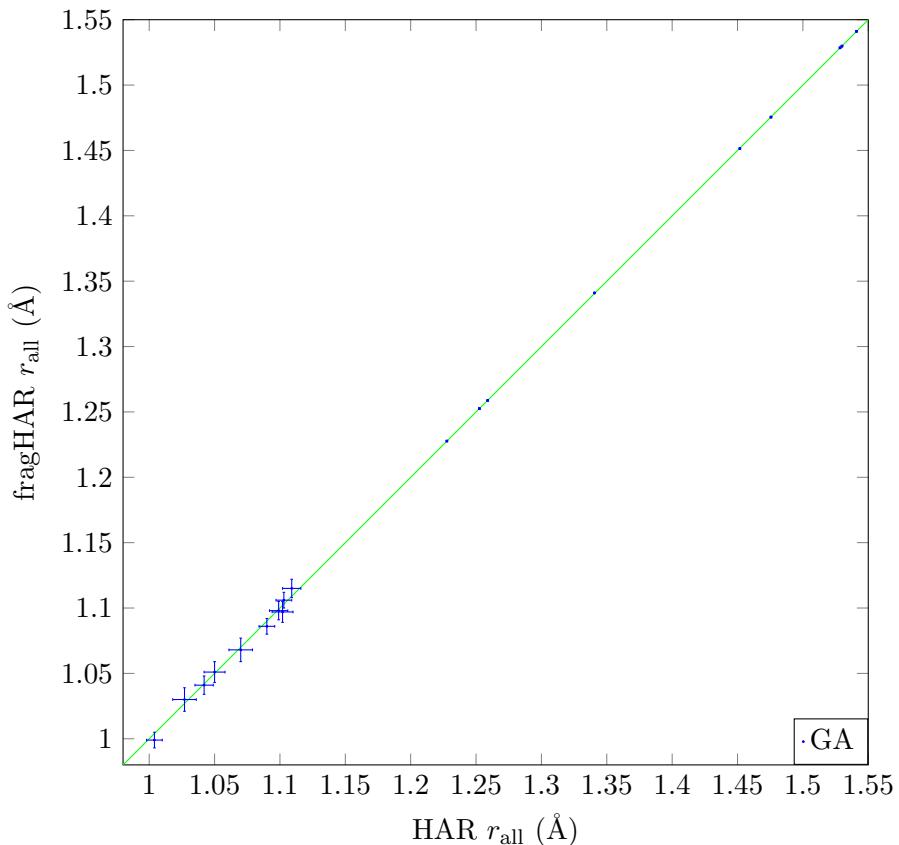


Fig. S4. Bond lengths in GA for fragHAR versus reference HAR calculations, for all atoms.

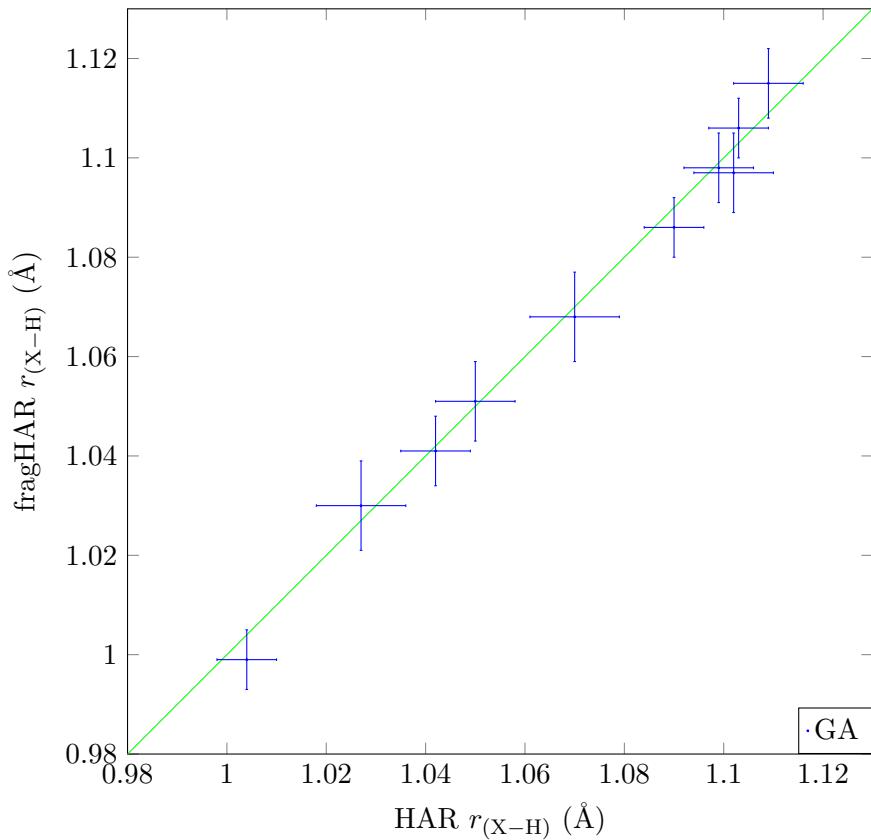


Fig. S5. X–H bond lengths in GA for fragHAR versus reference HAR calculations.

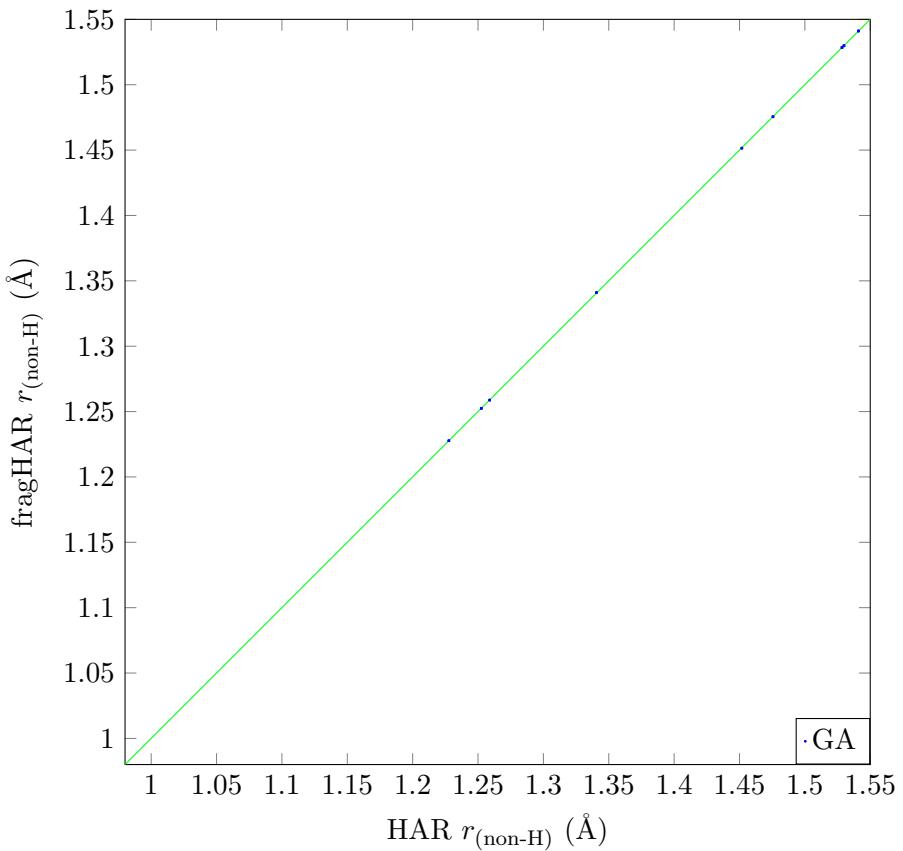


Fig. S6. Non-hydrogen bond lengths in GA, for fragHAR versus reference HAR calculations.

### S1.2. ADPs

Figures S7–S9 show the atomic displacement parameters for Gly-Ala from fragHAR plotted against HAR refinements.

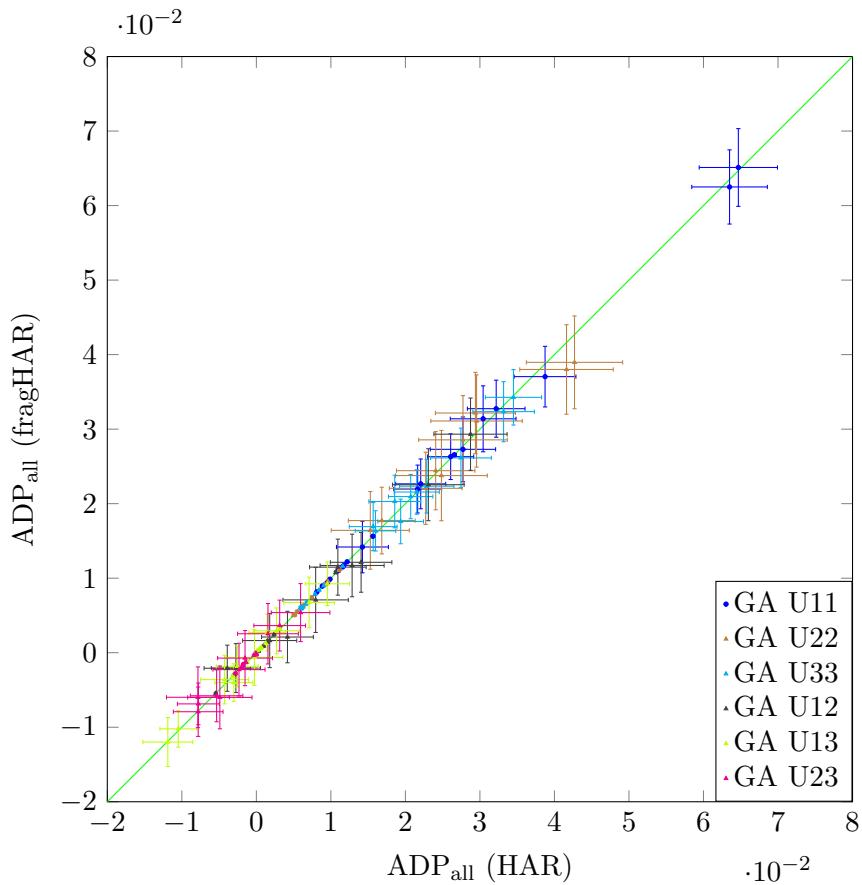


Fig. S7. Atomic displacement parameters in GA for fragHAR versus reference HAR calculations, for all atoms.

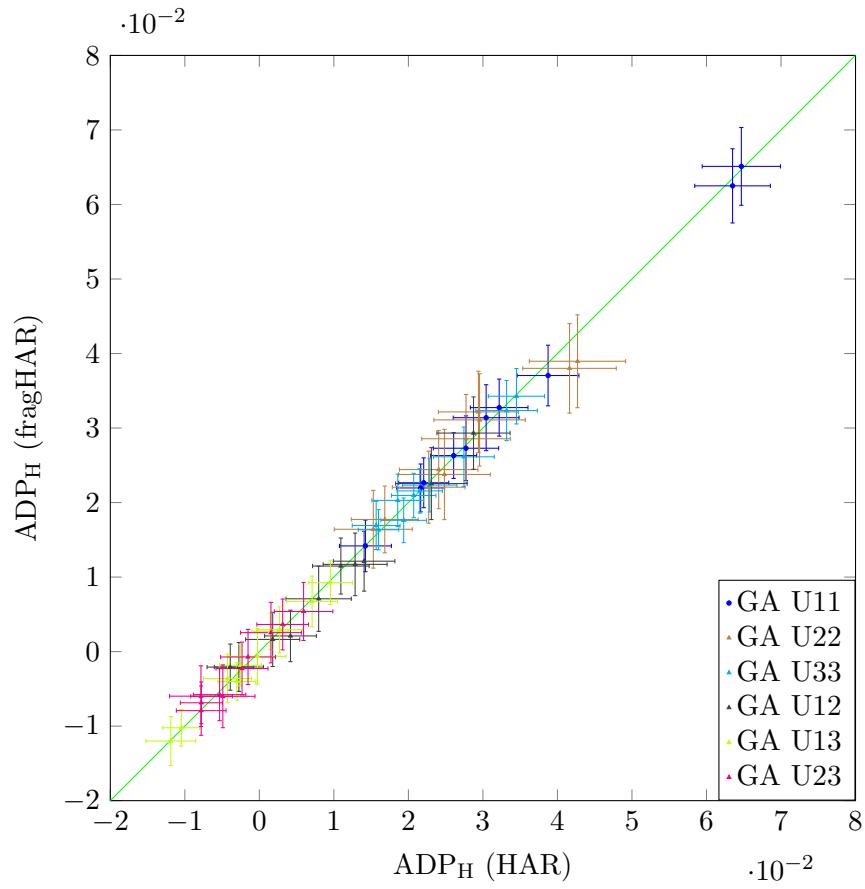


Fig. S8. Hydrogen atomic displacement parameters in GA for fragHAR versus reference HAR calculations.

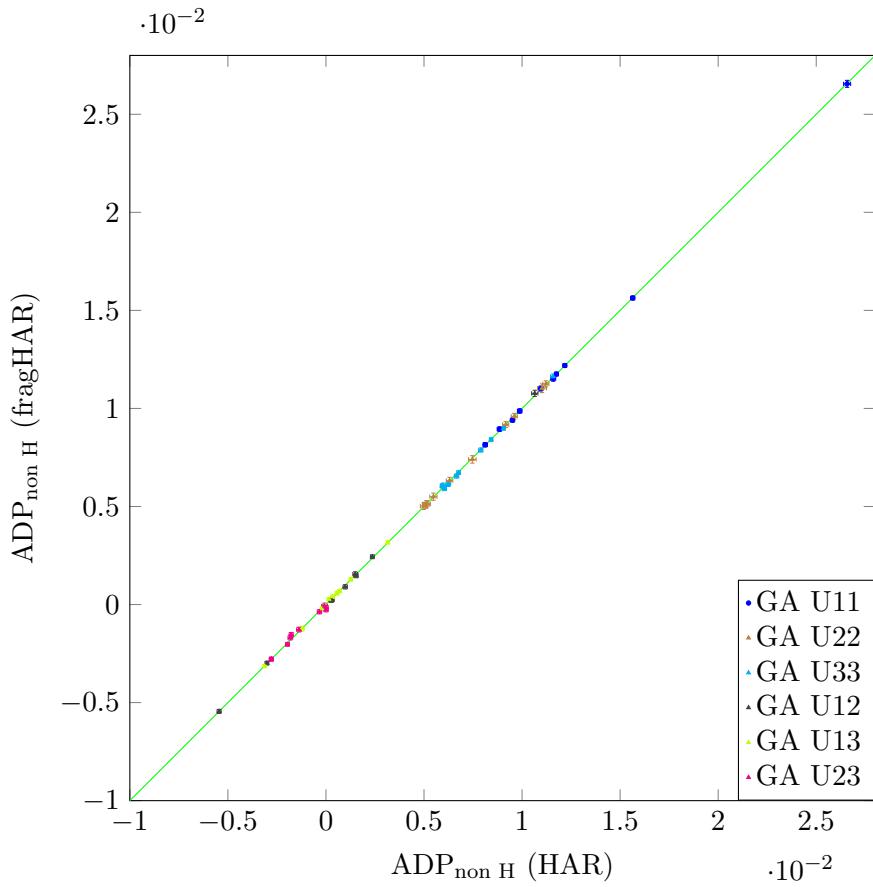


Fig. S9. Non-hydrogen atomic displacement parameters in GA for fragHAR versus reference HAR calculations.

**S2. AHA**

In this section we display the AHA tripeptide, and the fragments used.

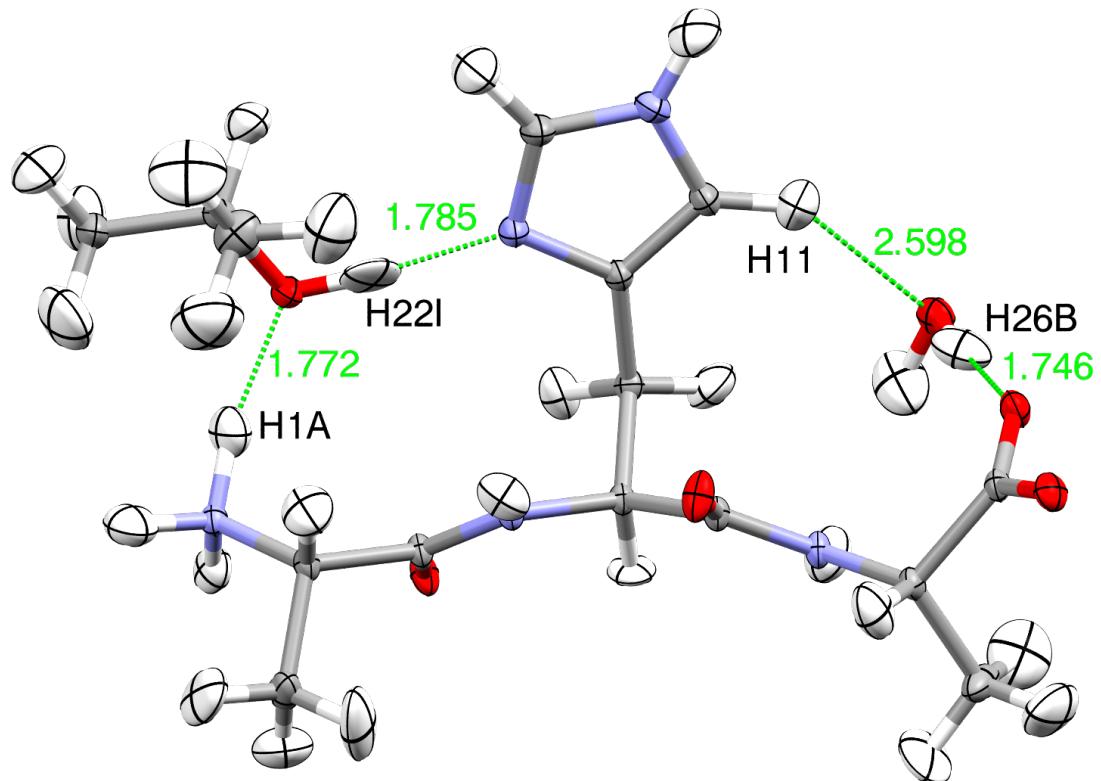


Fig. S10.  $\text{A}_4\text{P}_2$

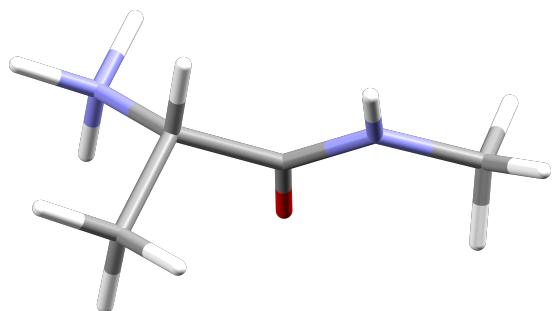


Fig. S11. The ALA-1 fragment

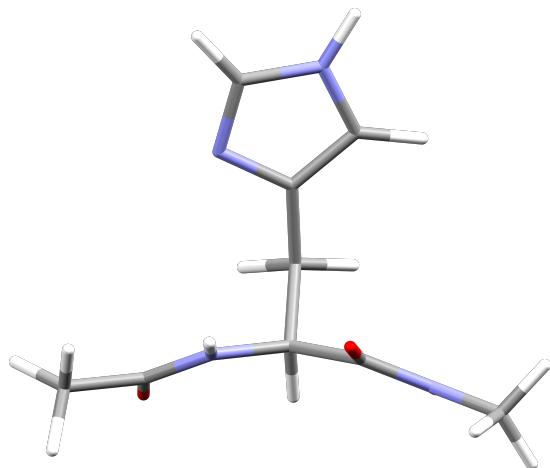


Fig. S12. The HIS-2 fragment

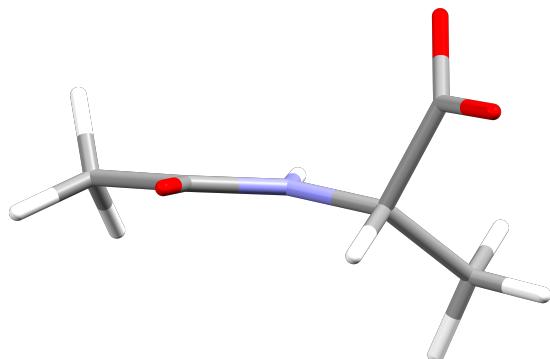


Fig. S13. The ALA-3 fragment

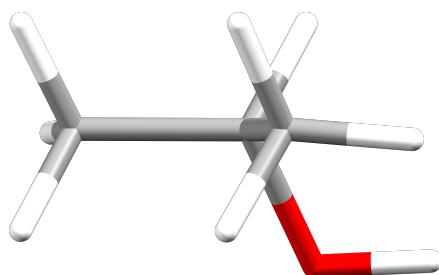


Fig. S14. The PRP-4 fragment

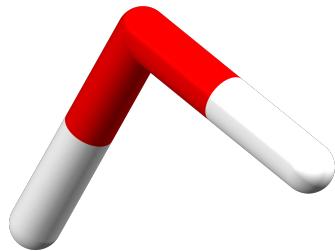


Fig. S15. The WAT-5 fragment

**S3. Bond lengths**

Figures S16–S18 are graphs of the bond lengths from fragHAR vs HAR refinements.

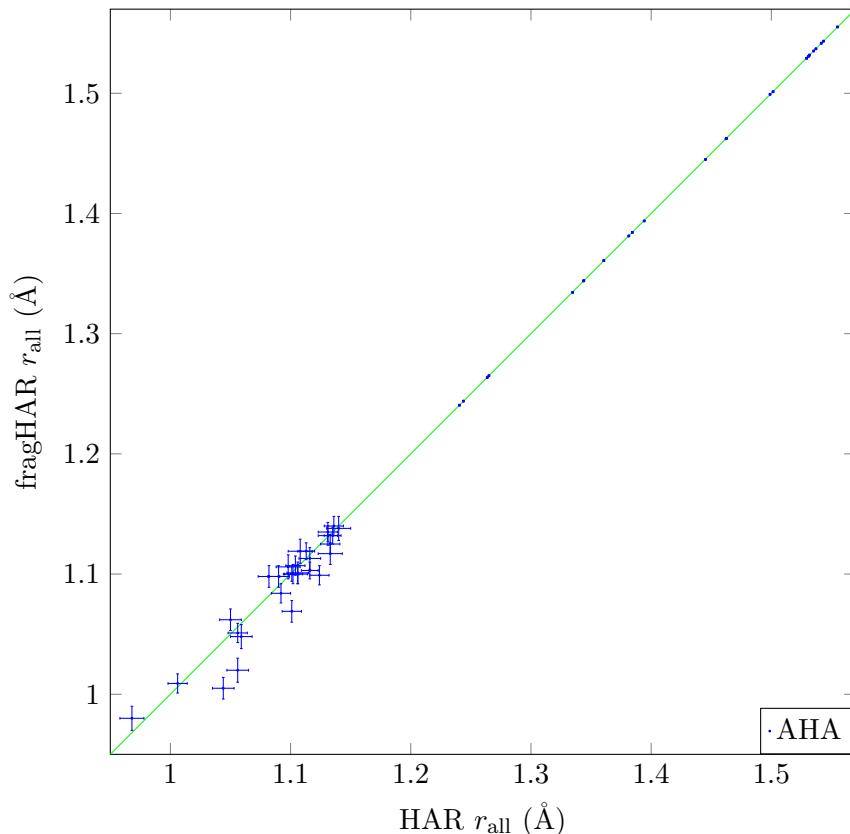


Fig. S16. Bond lengths in AHA for fragHAR versus reference HAR calculations.

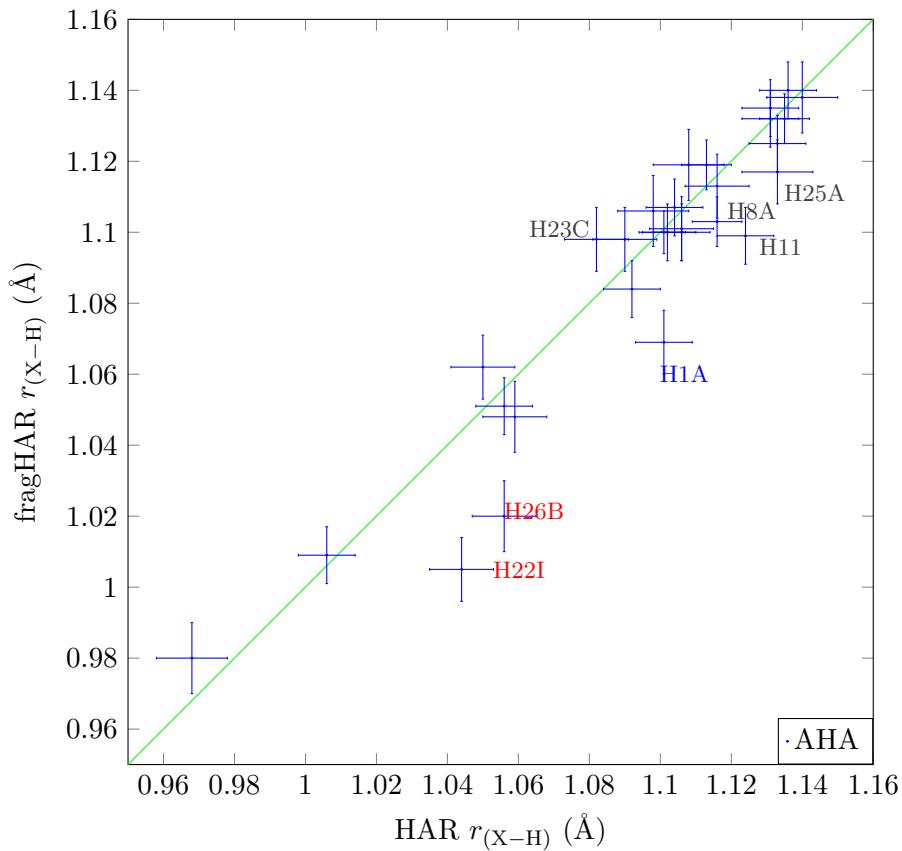


Fig. S17. X–H bond lengths in AHA for fragHAR versus reference HAR calculations.

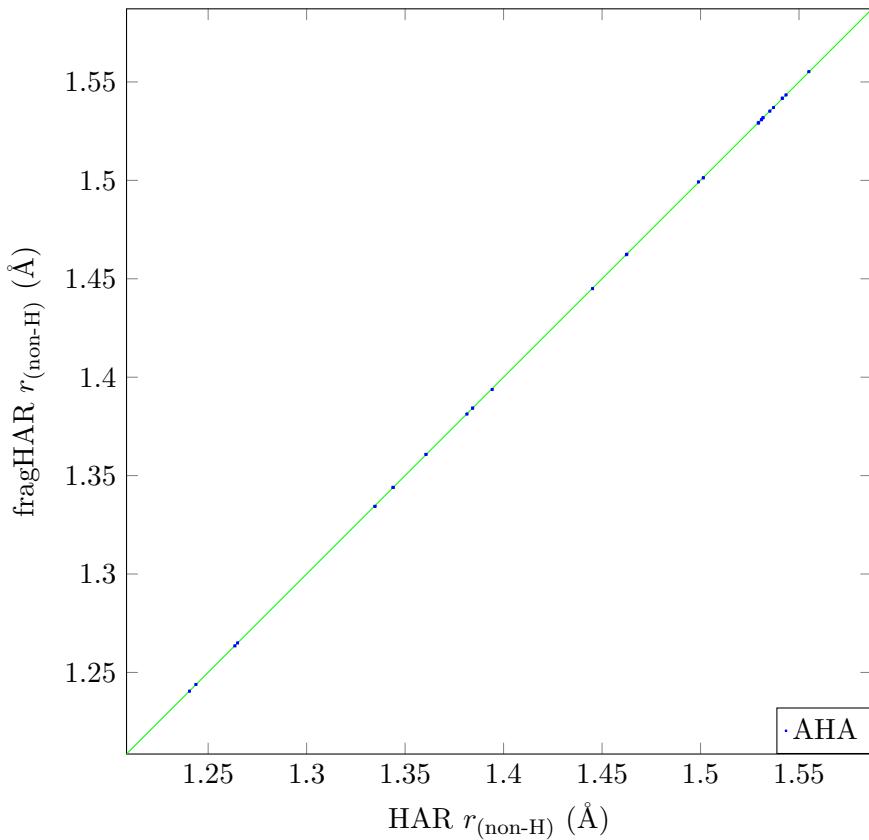


Fig. S18. Non-hydrogen bond lengths in AHA, for fragHAR versus reference HAR calculations.

#### S4. ADPs

Figures S19–S21 show the atomic displacement parameters for AHA from fragHAR plotted against HAR refinements.

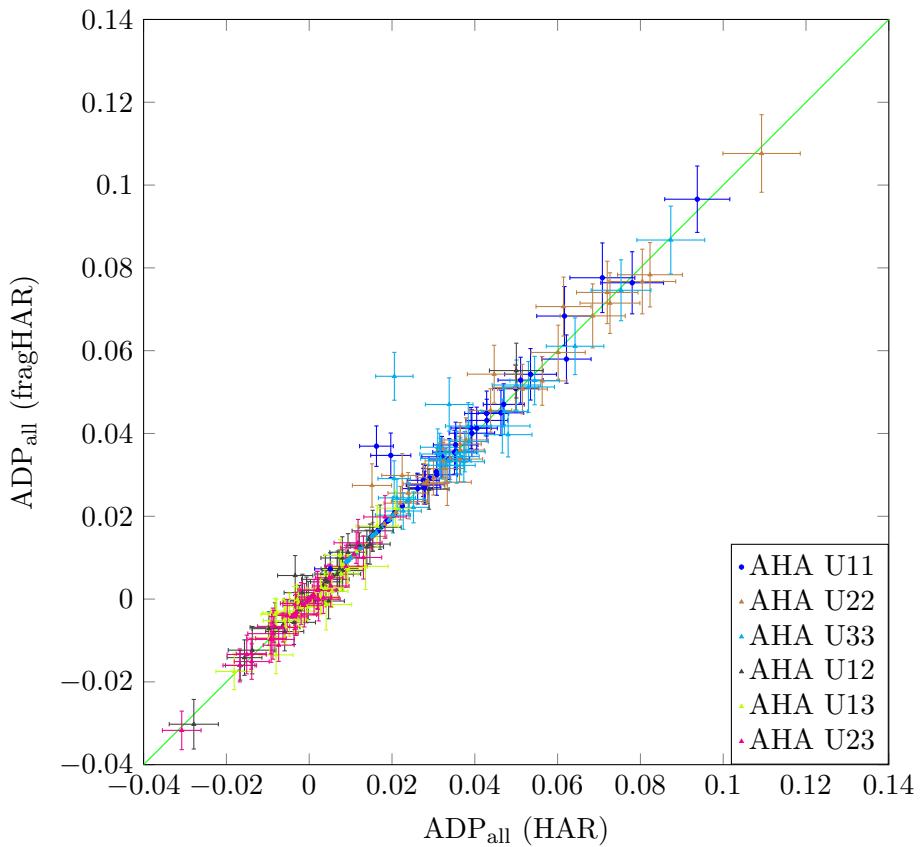


Fig. S19. Atomic displacement parameters in AHA for fragHAR versus reference HAR calculations, for all atoms.

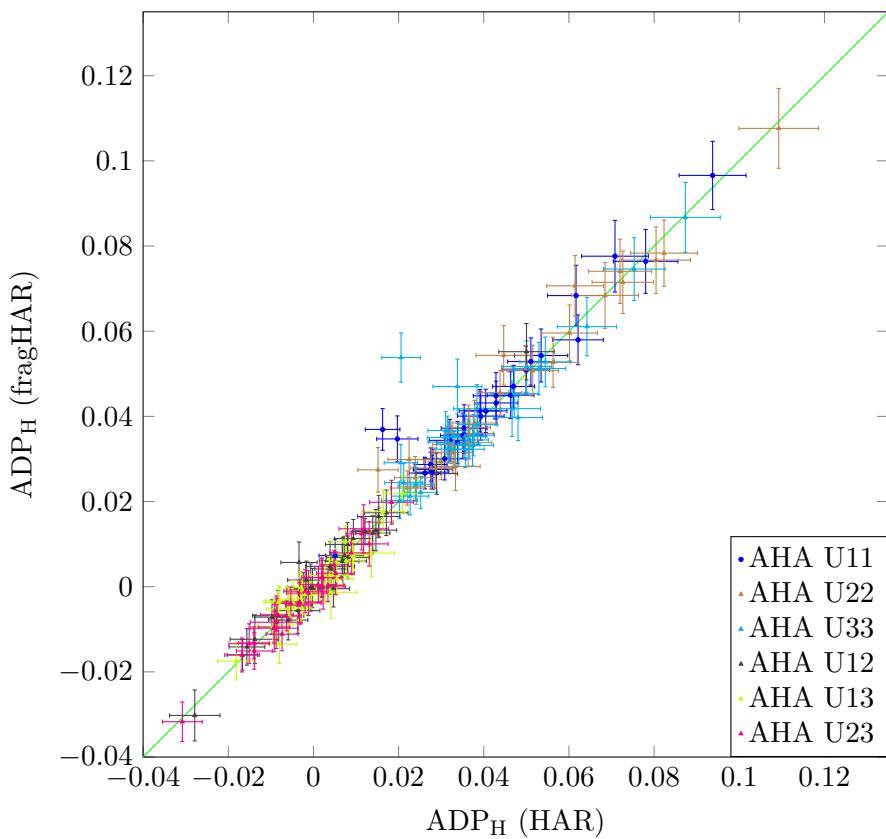


Fig. S20. Hydrogen atomic displacement parameters in AHA for fragHAR versus reference HAR calculations.

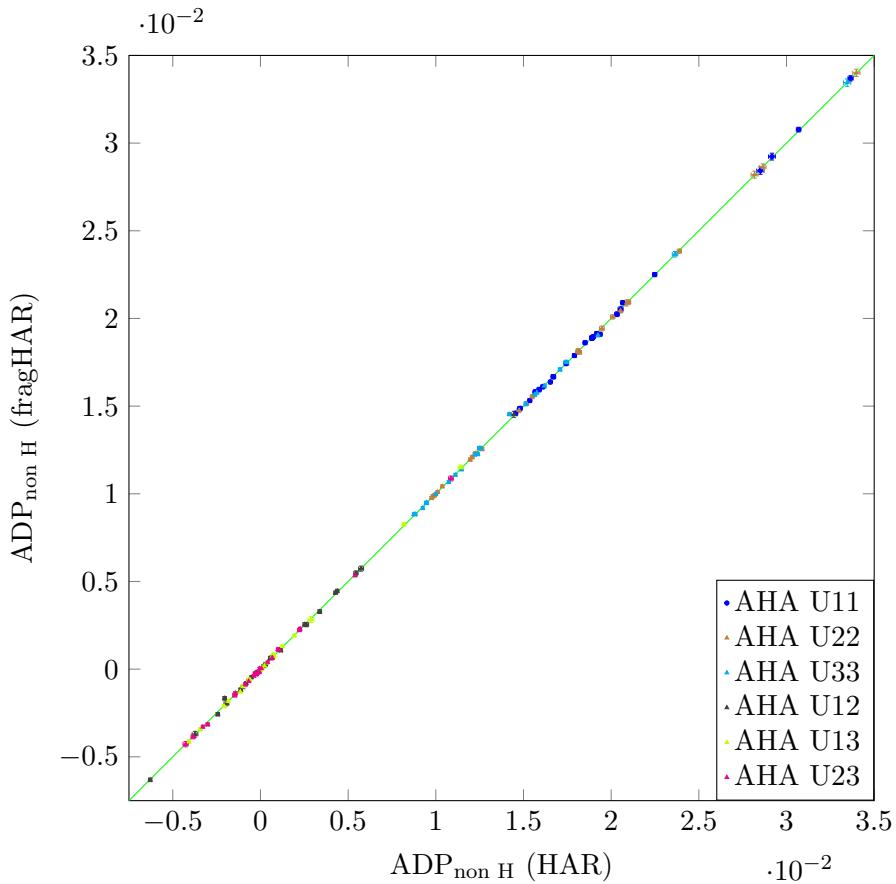


Fig. S21. Non-hydrogen atomic displacement parameters in AHA for fragHAR versus reference HAR calculations.

**S5. A<sub>4</sub>P<sub>2</sub>**

In this section we display the A<sub>4</sub>P<sub>2</sub> hexapeptide, and the fragments used.

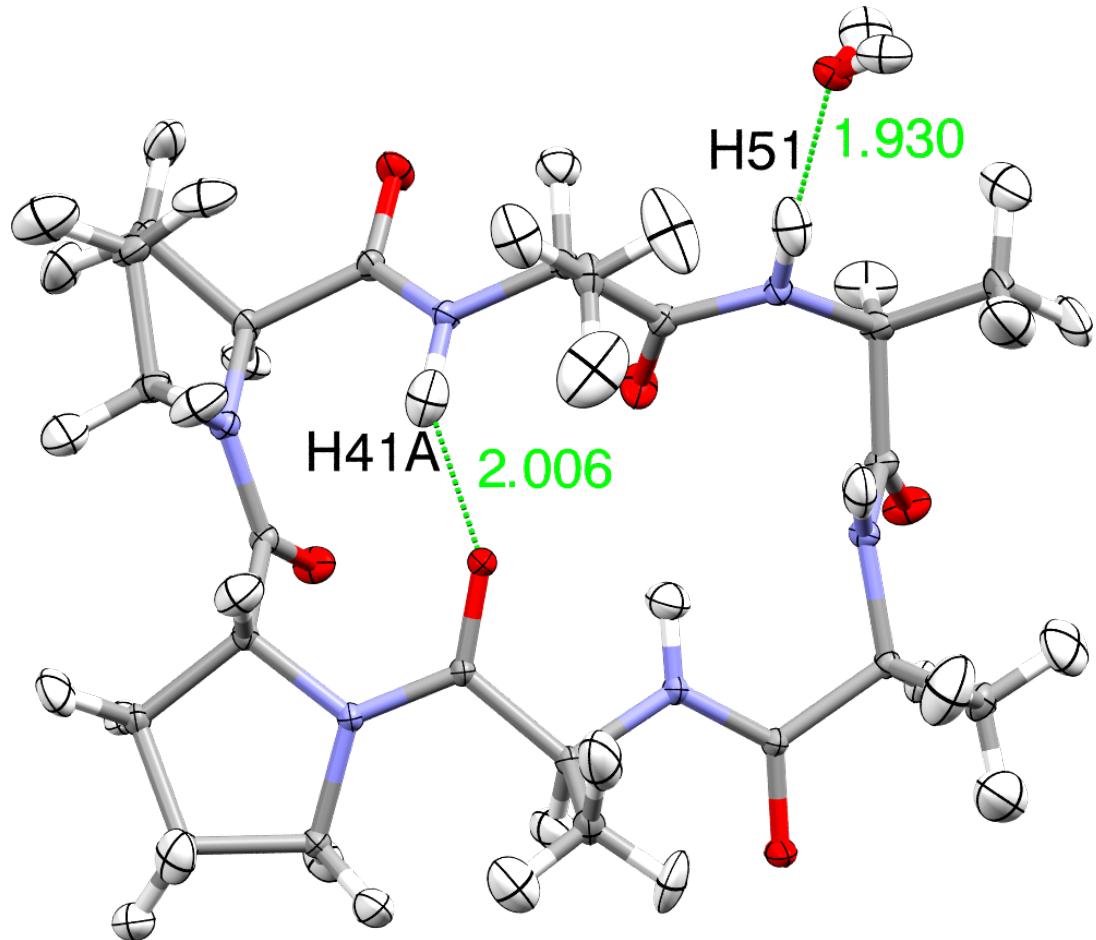


Fig. S22. A<sub>4</sub>P<sub>2</sub>

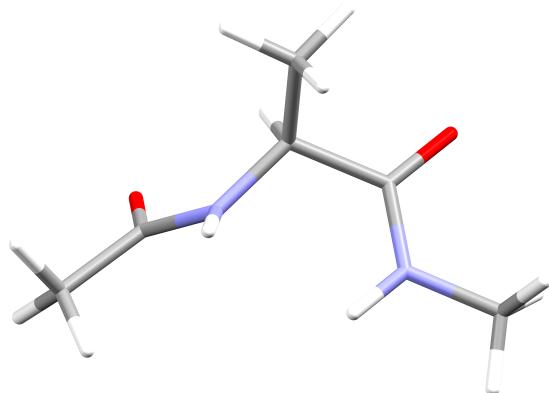


Fig. S23. The ALA-1 fragment in  $\text{A}_4\text{P}_2$

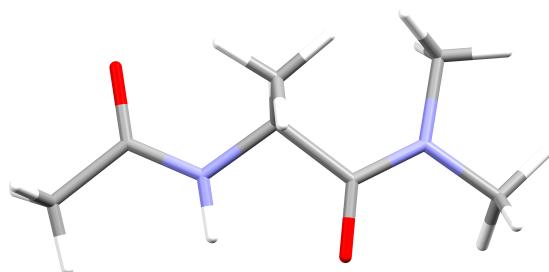


Fig. S24. The ALA-2 fragment in  $\text{A}_4\text{P}_2$

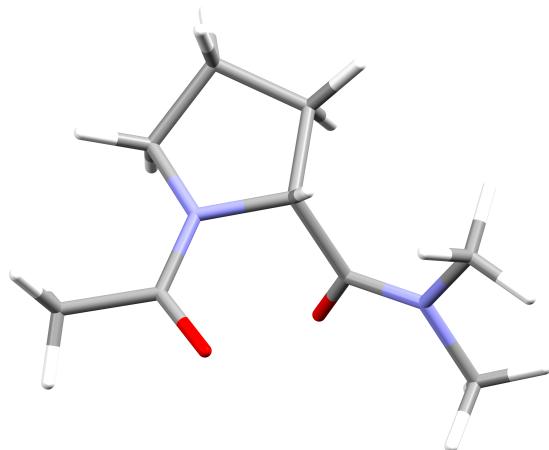


Fig. S25. The PRO-3 fragment in  $\text{A}_4\text{P}_2$

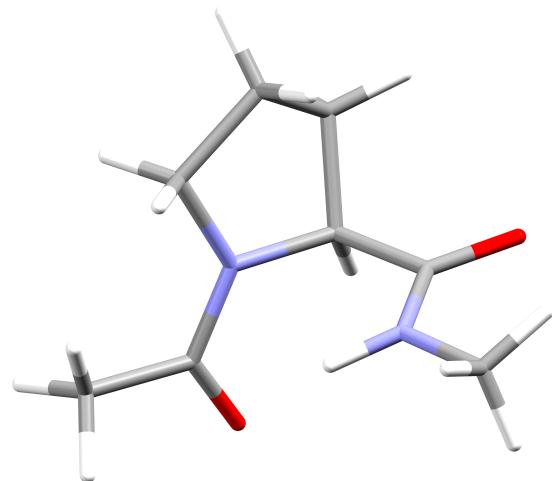


Fig. S26. The PRO-4 fragment in A<sub>4</sub>P<sub>2</sub>

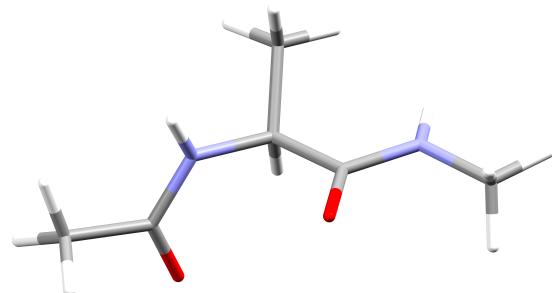


Fig. S27. The ALA-5 fragment in A<sub>4</sub>P<sub>2</sub>

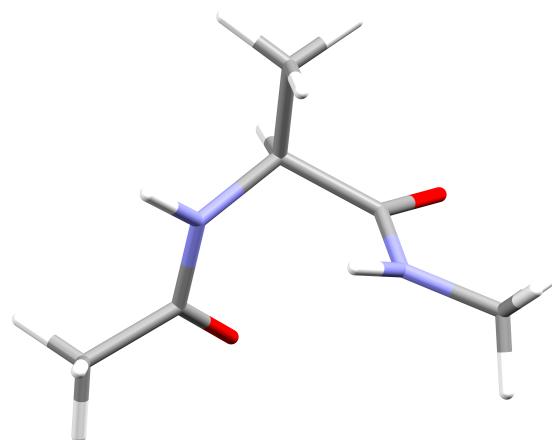


Fig. S28. The ALA-6 fragment in A<sub>4</sub>P<sub>2</sub>

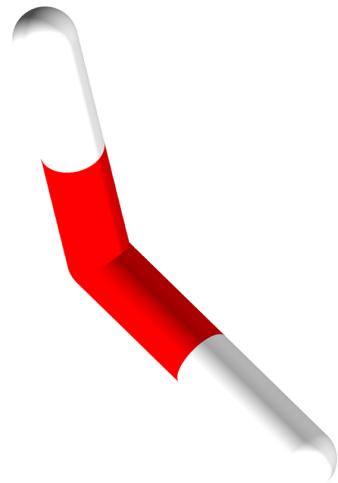


Fig. S29. The WAT-7 fragment in  $\text{A}_4\text{P}_2$

**S6. Bond lengths**

Figures S30–S32 are graphs of the bond lengths from fragHAR vs HAR refinements.

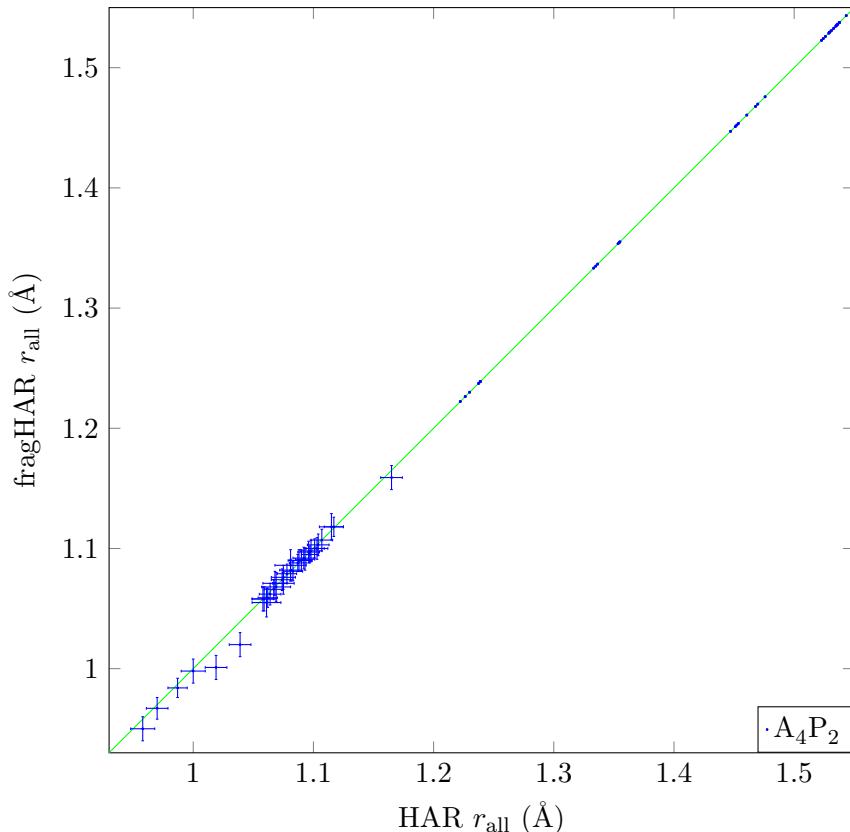


Fig. S30. Bond lengths in  $\text{A}_4\text{P}_2$  for fragHAR versus reference HAR calculations.

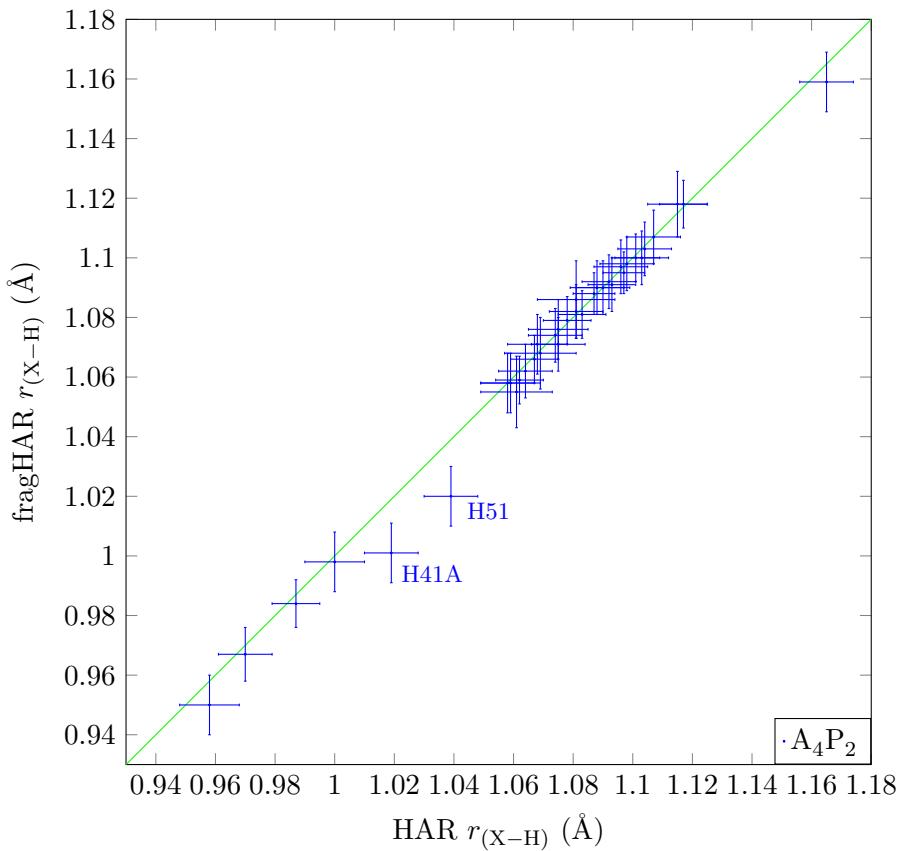


Fig. S31. X–H bond lengths in  $\text{A}_4\text{P}_2$  for fragHAR versus reference HAR calculations.

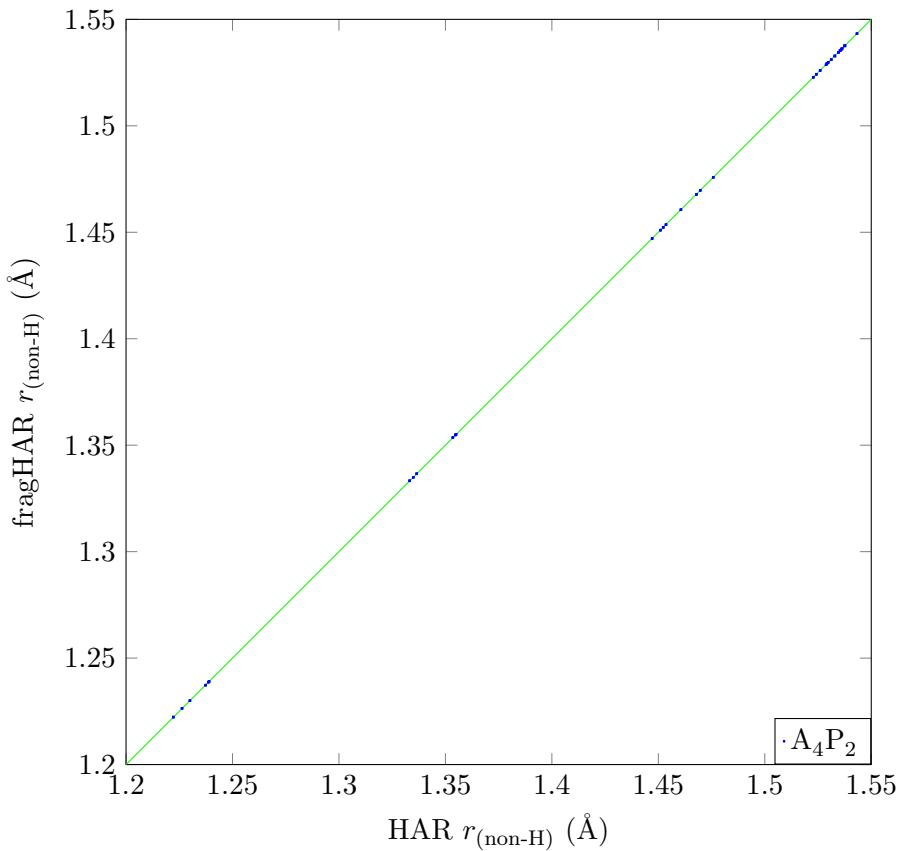


Fig. S32. Non-hydrogen bond lengths in  $\text{A}_4\text{P}_2$ , for fragHAR versus reference HAR calculations.

### S7. ADPs

Figures S33–S35 show the atomic displacement parameters for  $\text{A}_4\text{P}_2$  from fragHAR plotted against HAR refinements.

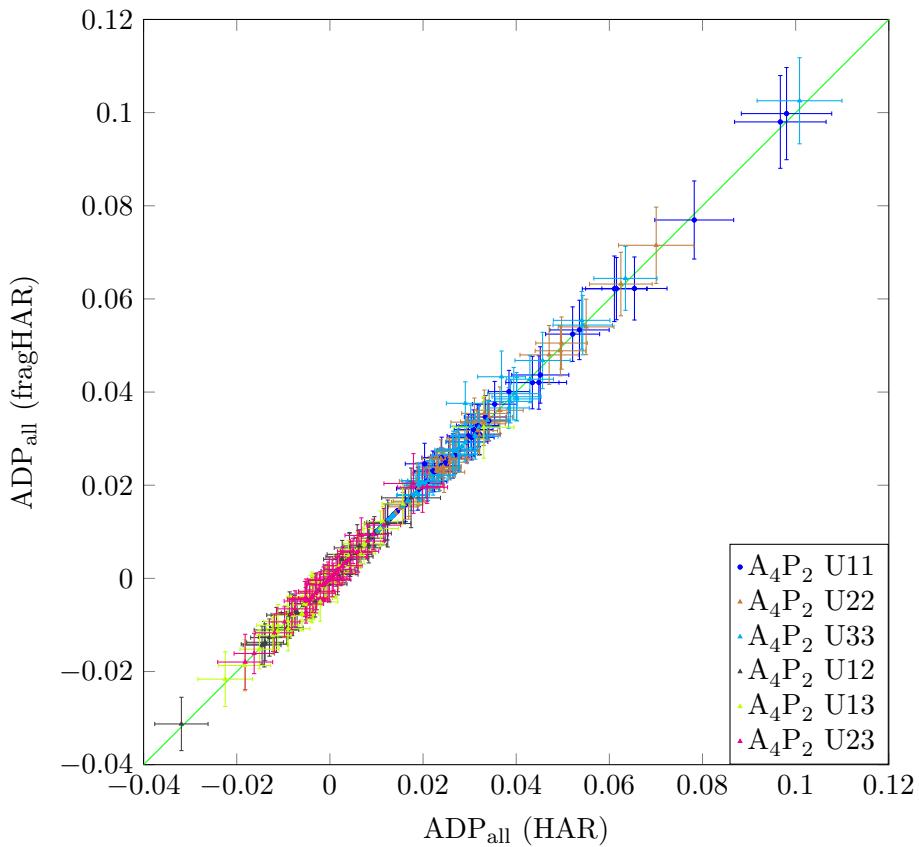


Fig. S33. Atomic displacement parameters in  $\text{A}_4\text{P}_2$  for fragHAR versus reference HAR calculations, for all atoms.

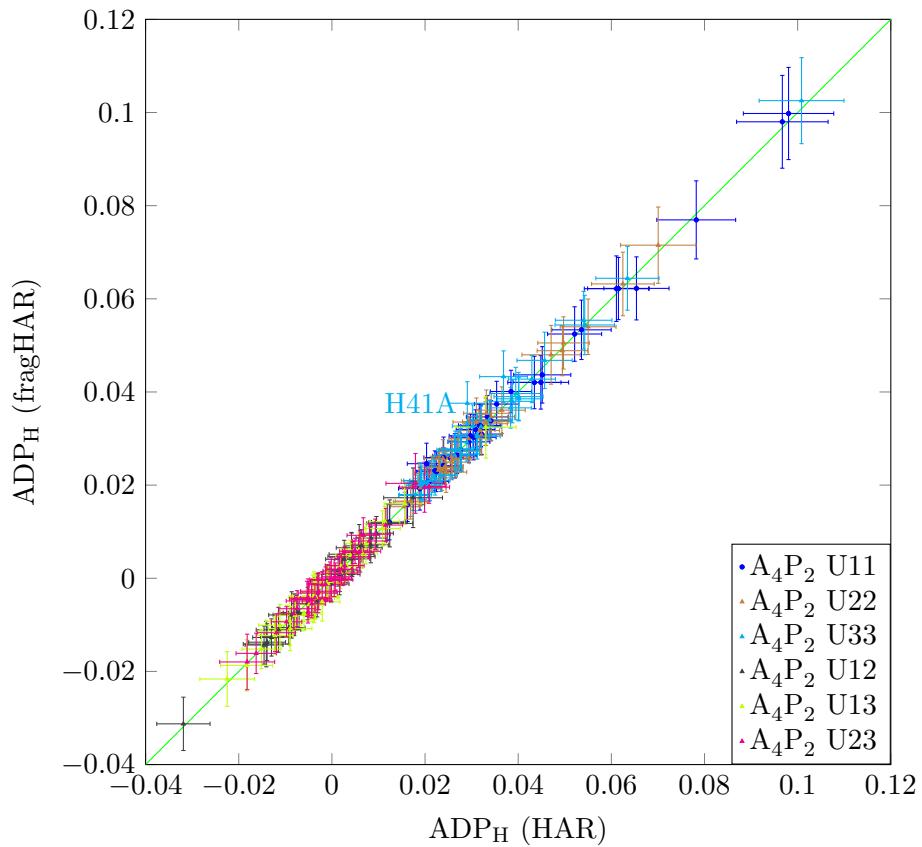


Fig. S34. Hydrogen atomic displacement parameters in  $\text{A}_4\text{P}_2$  for fragHAR versus reference HAR calculations.

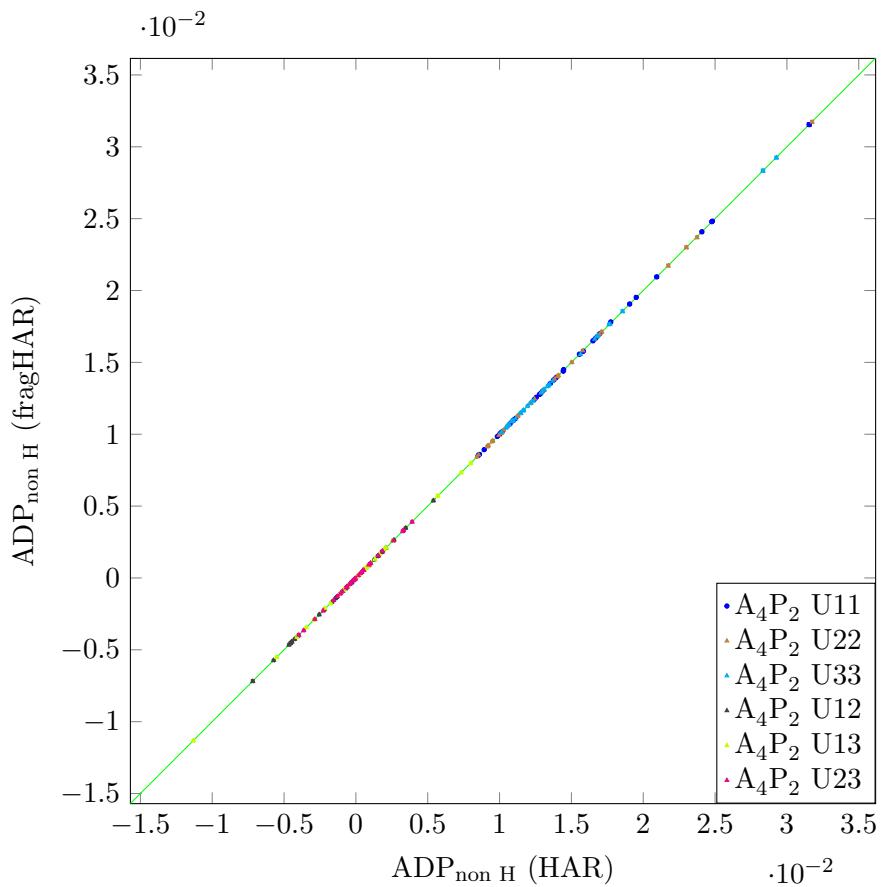


Fig. S35. Non-hydrogen atomic displacement parameters for  $\text{A}_4\text{P}_2$  for fragHAR versus reference HAR calculations.

### S8. Indicative walltime for parallel fragHAR calculations

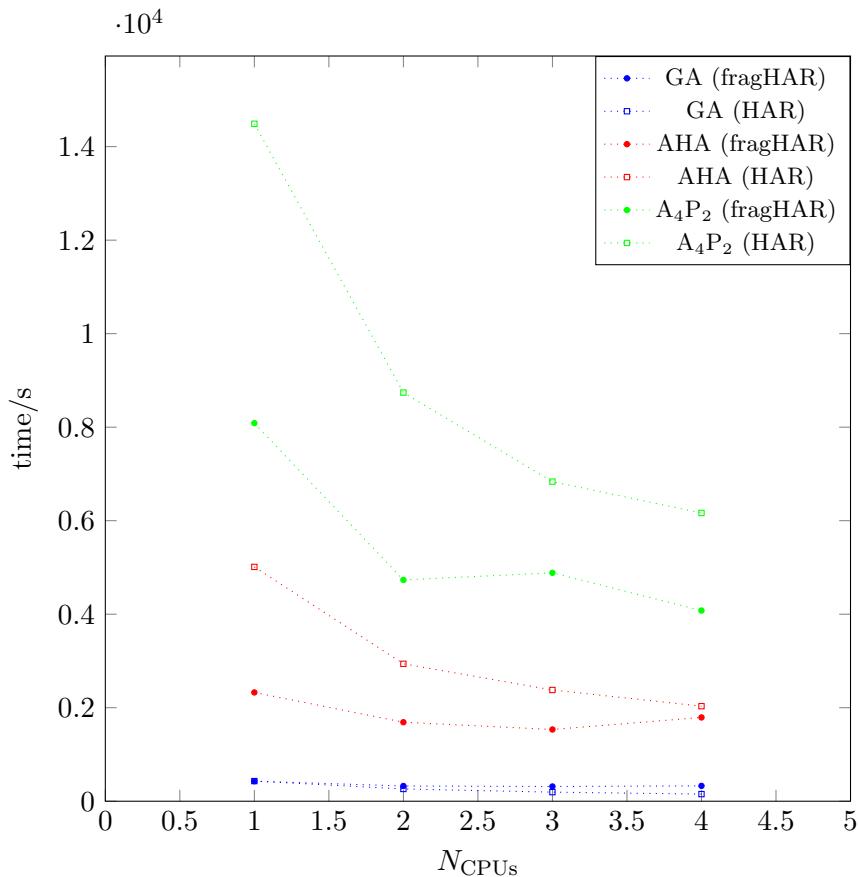


Fig. S36. Indicative walltimes for parallel fragHAR calculations, versus benchmark HAR calculations, as a function of the number of CPUs used.