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SUPPORTING INFORMATION

for

RING SIZE EFFECT ON THE SOLID STATE ASSEMBLY AND INCLUSION PROPERTIES OF PROPARGYL SUBSTITUTED HEXA AND OCTA CYCLIC PEPTOIDS

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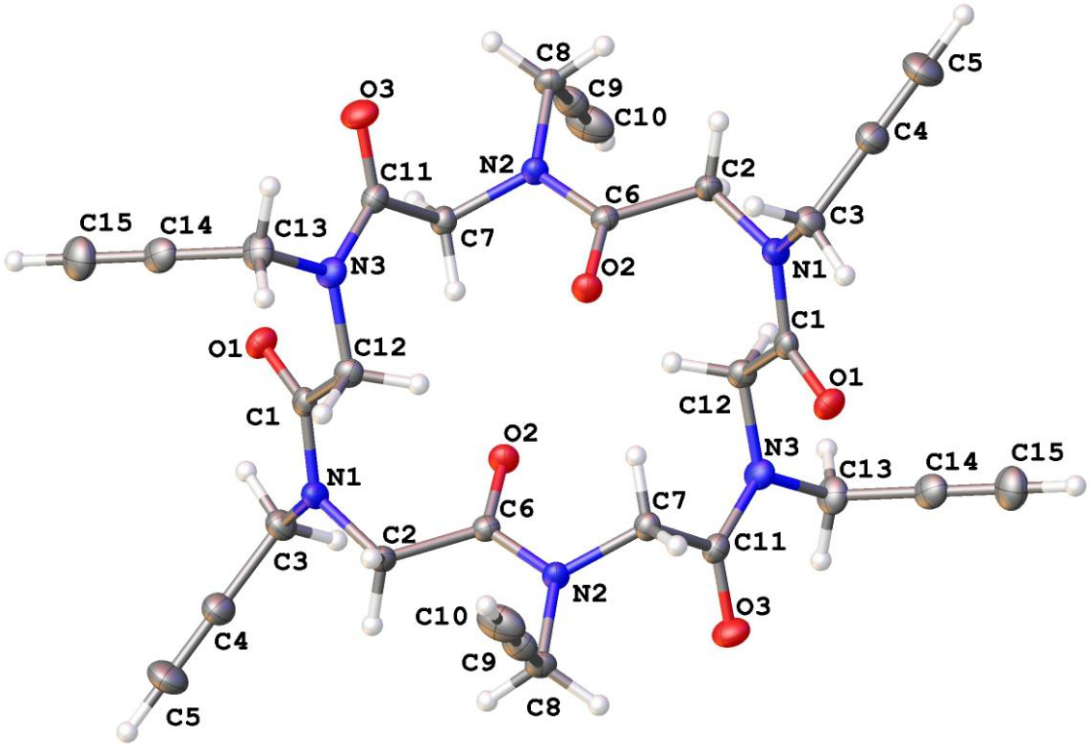
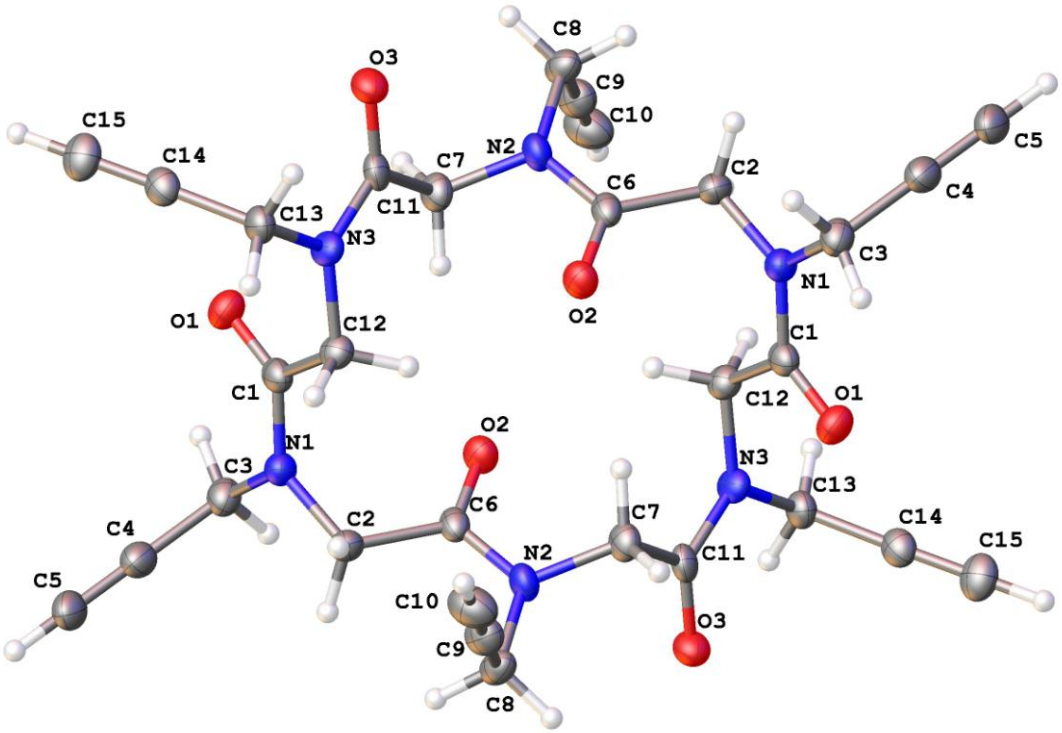
LIST OF ABBREVIATIONS

DMSO dimethylsulfoxide

Npa *N*-(propargyl)glycine

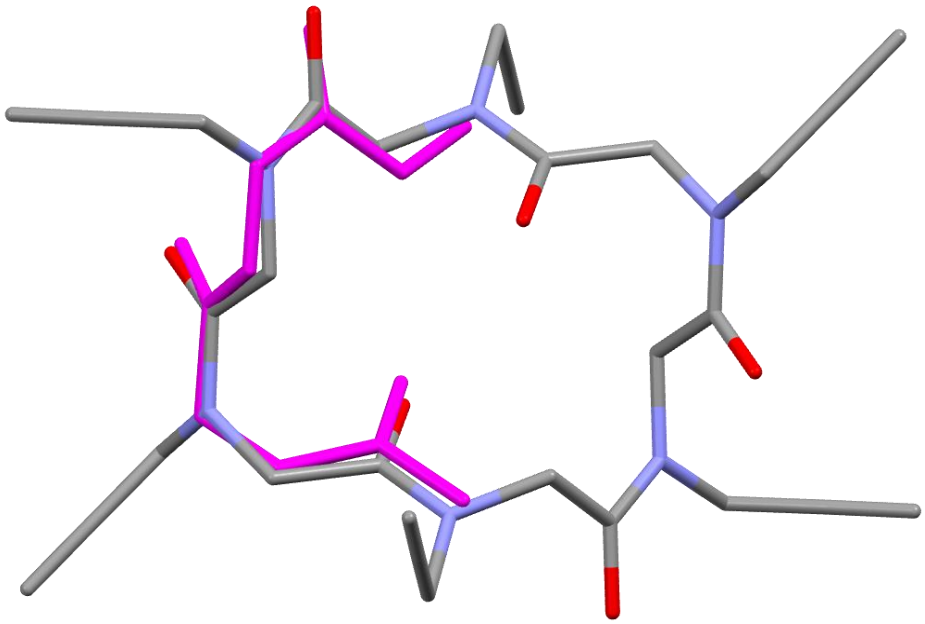


(a)

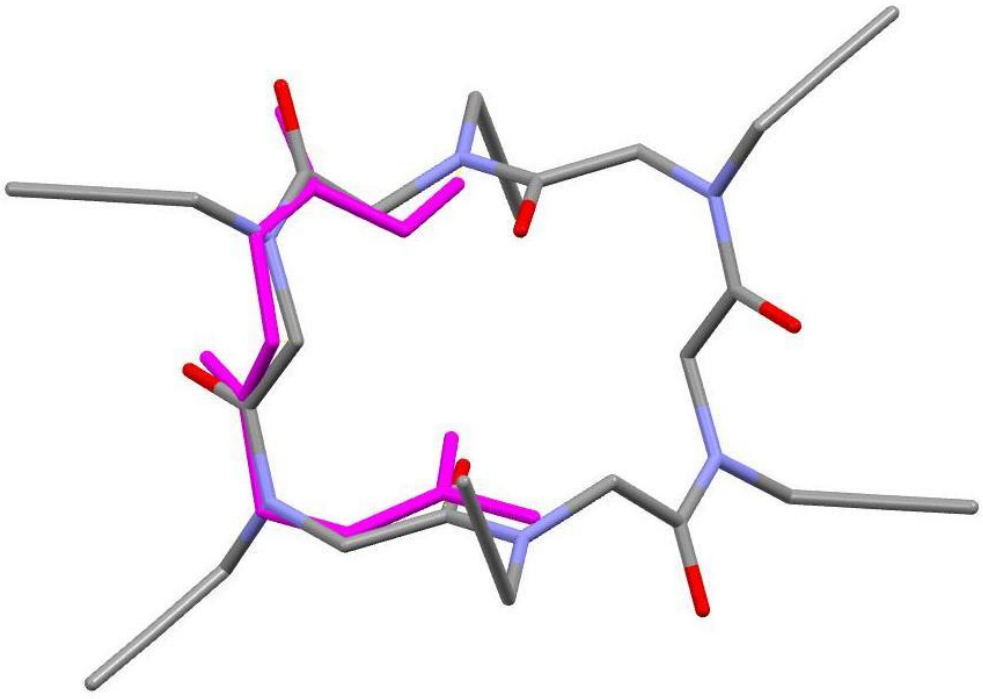


(b)

Figure S1. (**a**) ORTEP with numbering scheme for the cyclopeptoid molecule Cyclo-(*Npa*)$_6$ **1** (a) in crystal form **1A** and (**b**) in crystal form **1B**.



(a)



(b)

Figure S2. (**a**) Superposition of the backbone atoms of cyclopeptoid molecules in crystal form **1A** with idealized type III *beta*-turn peptide (magenta), rmsd 0.344 Å; (**b**) superposition of the backbone atoms of cyclopeptoid molecules in crystal form **1B** with idealized type III *beta*-turn peptide (magenta), rmsd 0.369 Å.

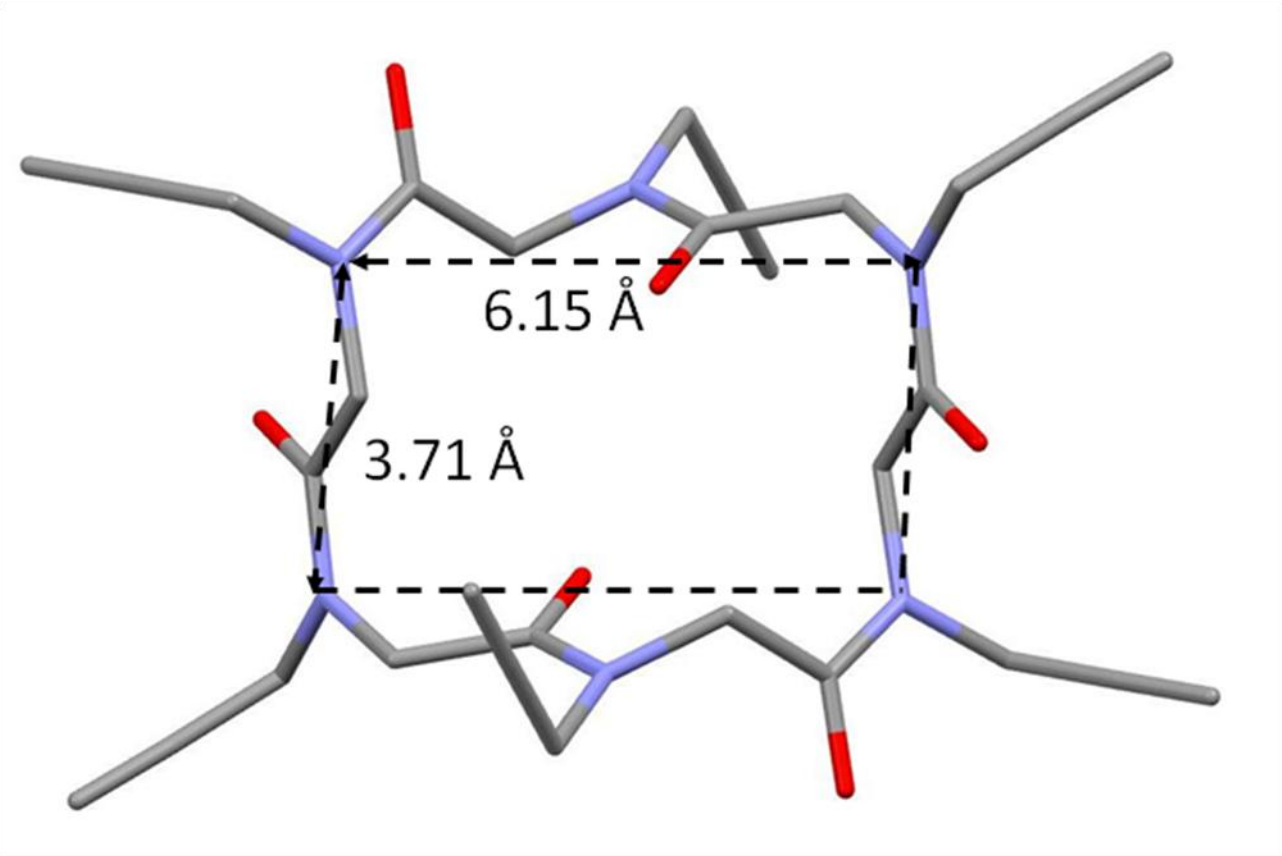


Figure S3. Rectangular shape of cyclic peptoid backbone in crystal form **1B.** Four *cis* amide bonds reside at each corner, *trans* amide bonds are located on two opposing sides.

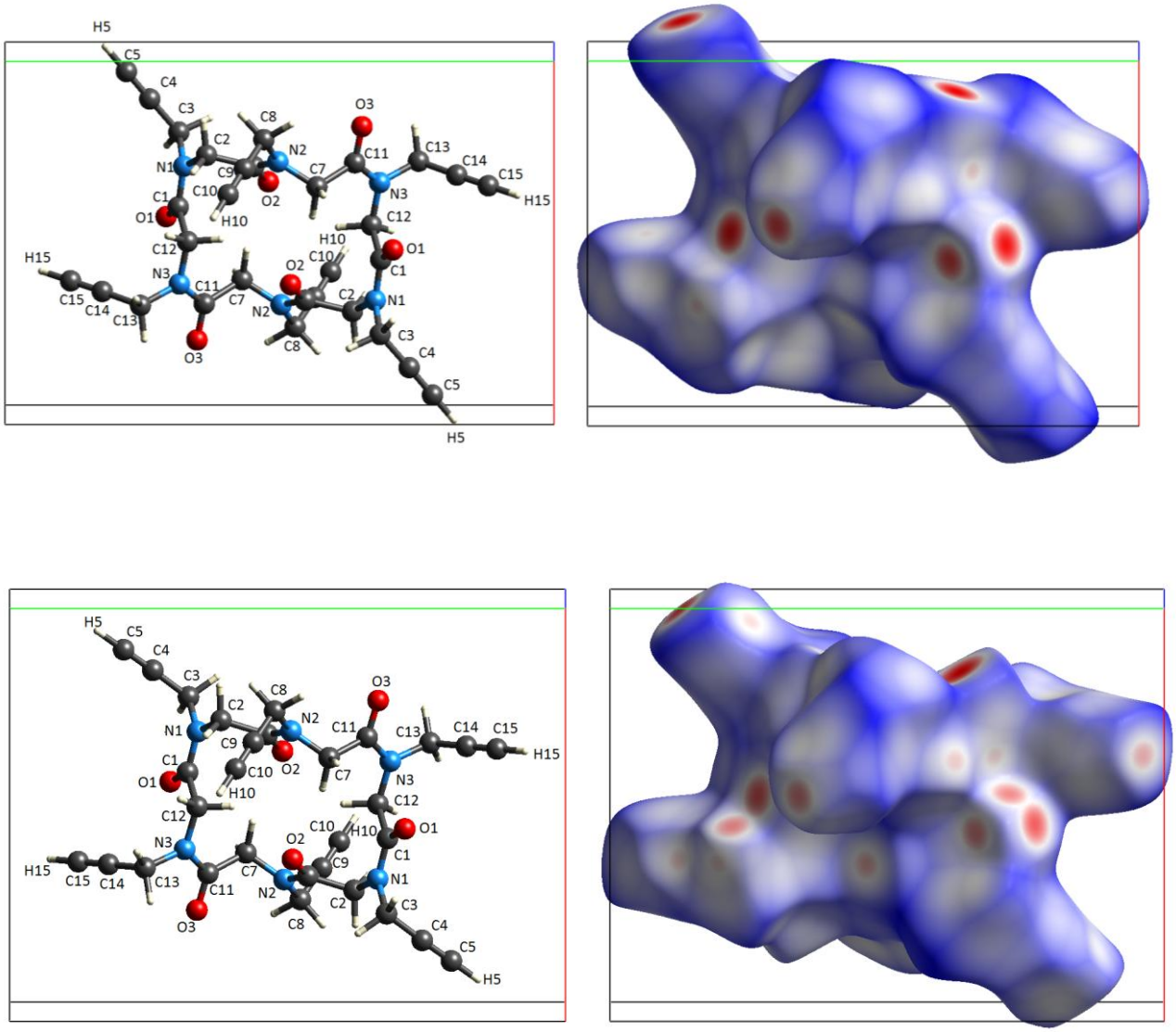
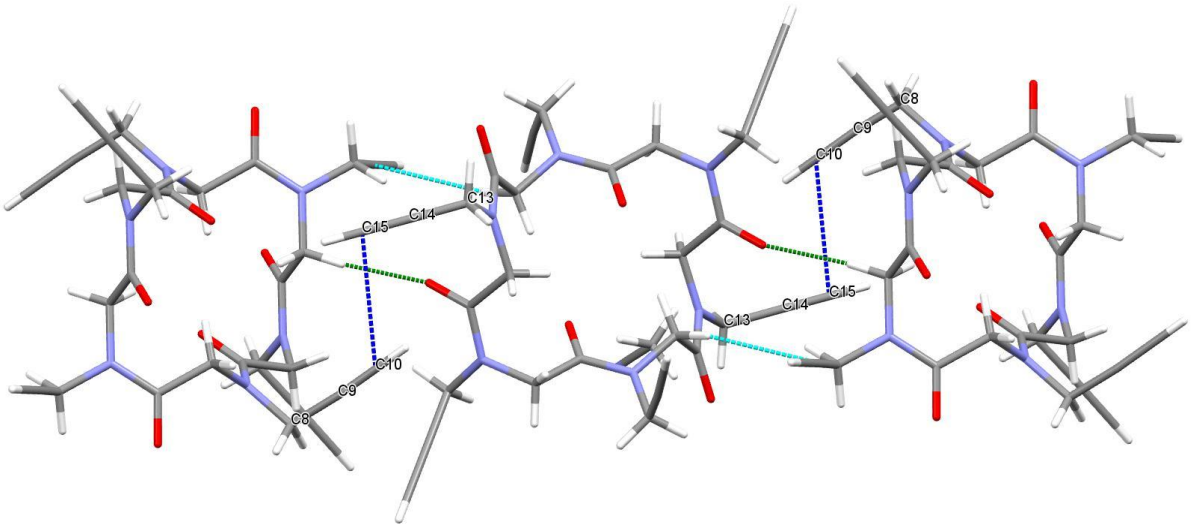
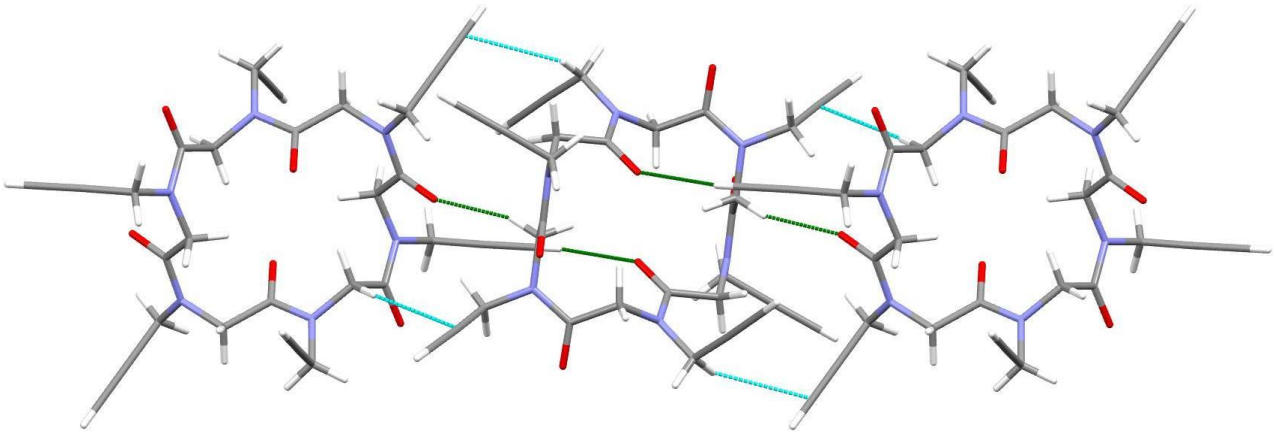


Figure S4. Hirshfeld surface for the cyclopeptoid molecule mapped with d_{norm} (a) in crystal form **1A** and (b) in crystal form **1B** as viewed along the *c* axis. *a* and *b* cell axes are, respectively, red and green.



(a)



(b)

Figure S5. (a) Intralayer CO···HC (green dotted lines), CH-pi (light blue dotted lines) and π-π interactions (blue dotted lines) in **1A**; (b) Intralayer CO···HC (green dotted lines) and CH-pi interactions (light blue dotted lines) in **1B**.

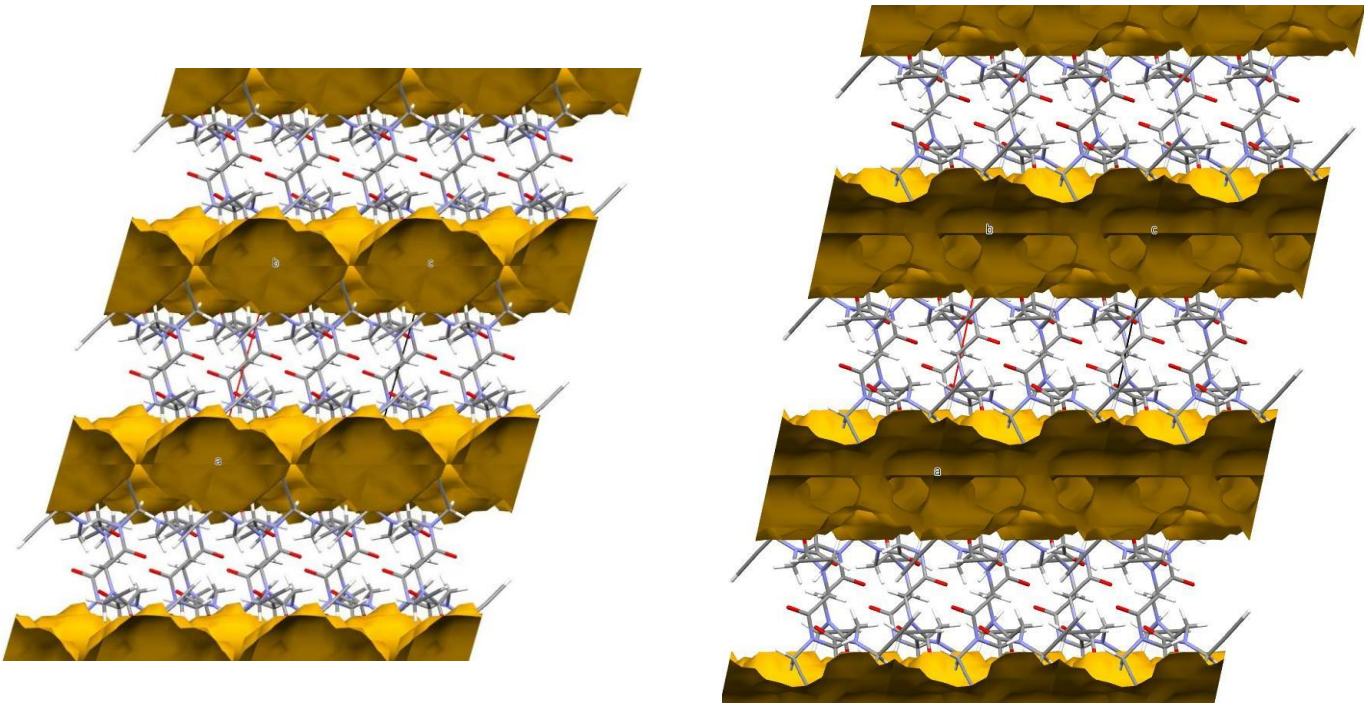


Figure S6. Void space available for guest molecules in crystal forms **1A** (left) and **1B** (right) as viewed along the *b* axis.

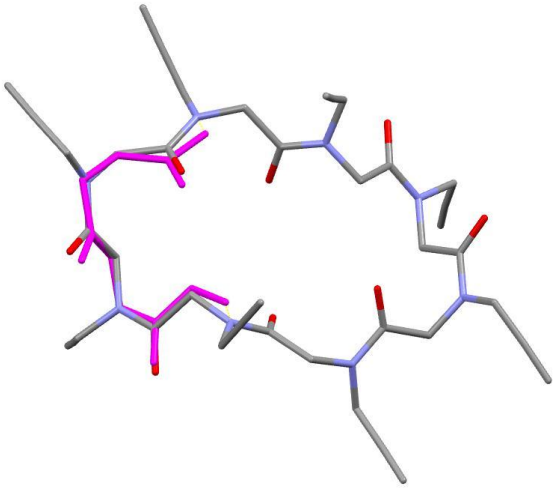


Figure S7. (**a**) Superposition of the backbone atoms of cyclopeptoid molecules in crystal form **2A** with idealized type III *beta*-turn peptide (magenta), rmsd 0.359 Å.

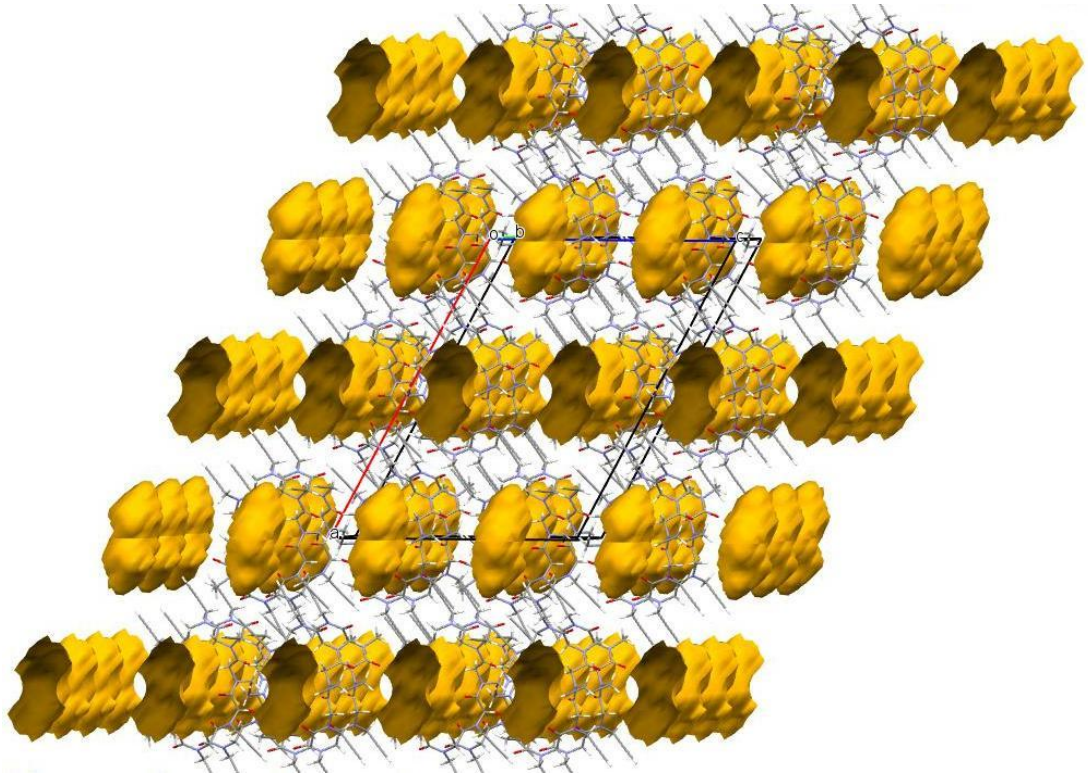
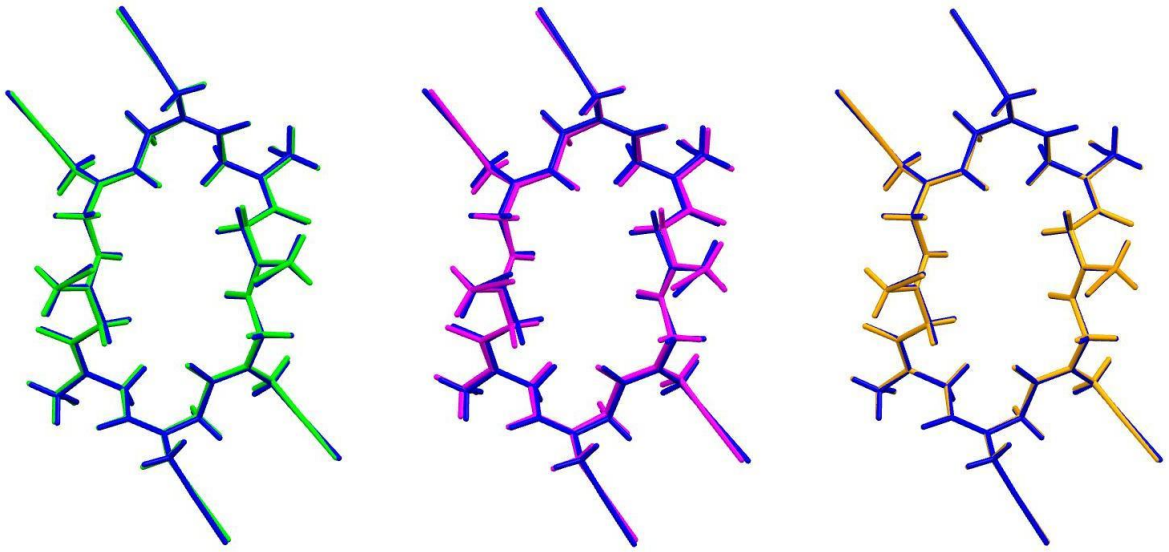


Figure S8. Guest accessible voids in crystal form **2A** as viewed along the *b* axis (perspective view).



(a) (b) (c)

Figure S9. (a) Molecular overlay between crystal forms **2A** (blue) and **2B** (green), rmsd 0.1325 Å; (b) molecular overlay between crystal forms **2A** (blue) and **2C** (magenta), rmsd 0.1956 Å; (c) molecular overlay between crystal forms **2A** (blue) and **2D** (orange), rmsd 0.0563 Å.

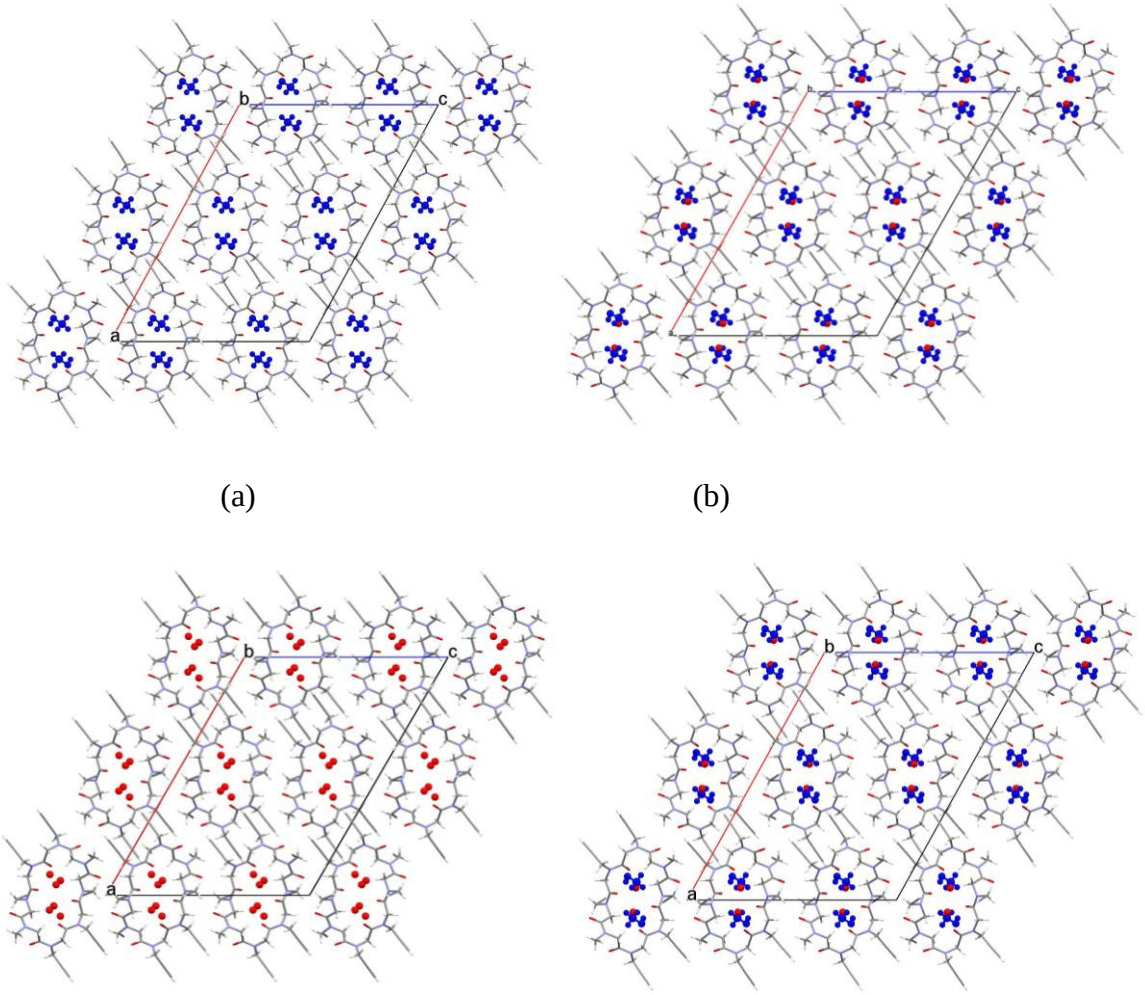


Figure S10. Crystal packing of forms **2A** (a), **2B** (b), **2C** (c), and **2D** (d)as viewed along the *b* axis. Guest molecules are depicted as ball-and-sticks, methanol molecules in blue and water molecules in red.