

***In situ* iodination and X-ray crystal structure of a foldamer helical bundle.**

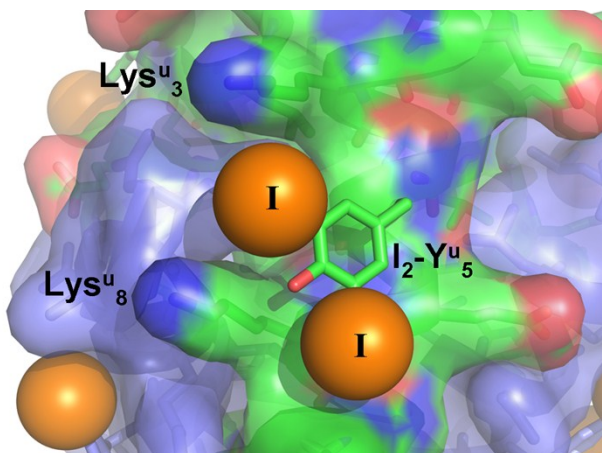
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**Supplementary information**

**Table S1.** X-ray diffraction data collection and refinement statistics for oligourea **H1-I<sub>2</sub>**.

Data Collection	
Space group	$P 6_3$
Unit cell	
a, b, c (Å)	33.92, 33.92, 37.98
$\alpha, \beta, \gamma$ (°)	90.0, 90.0, 120.0
Resolution (Å)	37.98 – 1.64 (1.74 – 1.64)
R <sub>merge</sub> (%)	7.0 (23.7)
I / $\sigma$	8.5 (3.43)
Reflections (total)	12067 (1888)
Reflections (unique)	5602 (902)
Completeness (%)	92.6 (92.9)
Multiplicity	2.15
Refinement	
Resolution (Å)	29.38 – 1.64 (1.68 – 1.64)
R <sub>work</sub> (%)	18.49 (30.00)
R <sub>free</sub> (%)	25.56 (33.00)
Atoms	304
Waters	20
Overall B-factor (Å <sup>2</sup> )	17.37
R.m.s.d. (bond-lengths [Å])	0.013
R.m.s.d. (bond-angles [°])	1.876
CCDC code	1038892*

\* As key information is lost during the .pdb file to .cif file conversion process, the entire .pdb file (including refinement information) has been inserted into the 'comments' section of the .cif file available (free of charge) from the Cambridge Crystallographic Data Centre ([www.ccdc.cam.ac.uk/getstructures](http://www.ccdc.cam.ac.uk/getstructures))



**Figure S1.** Interaction of flexible Lys<sup>u</sup><sub>3</sub> side-chains with 3,5-diiodo-Tyr<sup>u</sup><sub>5</sub> side-chain within the **H1-I<sub>2</sub>** crystal structure.