MS32-03 **Conformational bias in small-molecule crystal structures is rare (and explicable)** Aurora J. Cruz-Cabeza,[a] John W. Liebeschuetz[b] and Frank H. Allen[b] [a]*Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, The Netherlands;* [b] *Cambridge Crystallographic Data Centre, Cambridge, United Kingdom*
E-mail: aurorajosecruz@gmail.com

It is well known that, in the gas phase, biphenyl (BP) adopts a twisted conformation about the ring-ring C-C bond [1] and cyclobutane (CB) adopts a puckered conformation about its ring diagonal [2]. In both cases, though, both BP and CB can adopt higher-energy planar conformations in some crystal structures. These observations, particularly for BP, have led some scientists to infer that conformations observed in crystal structures are biased due to 'crystal packing effects' and that such conformations are not transferrable to other scientific applications.

In the present contribution we compare molecular conformations of BP and CB derivatives as observed in crystal structures taken from the Cambridge Structural Database (CSD) [3] with their optimised geometries in the gas phase. Only ~16% of both BP and CB fragments are exactly planar in relevant crystal structures while >60% have conformations close to the lowest energy conformers in gas-phase. The planar conformers only occur when crystallographic and molecular symmetry elements coincide. Extensive lattice energy scans and crystal structure prediction calculations for parent BP and a CB derivative clearly show how, in very particular cases, higher conformational energies of BP and CB are almost exactly compensated by reductions in the overall lattice energies. Such situations, however, are very rare -due to the symmetry requirements- and only compensate for conformational energy differences of up to 10 kJ/mol. Crystal structure conformations are, therefore, good guides to conformational preferences in other phases [4].

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Keywords: cambridge structural database; conformational analysis; crystal structure prediction

MS32-04 **PDBe - Bringing Structure to Biology.**
S. Velankar,[a] G.J. Kleywegt,[a] [a]*Protein Data Bank in Europe, European Bioinformatics Institute, United Kingdom*
E-mail: sameer@ebi.ac.uk

In 2011, the Protein Data Bank (PDB) celebrated its 40th anniversary. To date, the PDB has essentially been a historic archive capturing structures (and the underpinning experimental data) of biomacromolecules described in the primary literature. As the use of structural data by non-experts becomes commonplace, the demands on the archive (by both these users and funding agencies) and the way it is made accessible will inevitably change. It is therefore necessary to transform sites that serve the archive into resources that are directly relevant for scientists who work in biomedicine and related disciplines, while simultaneously taking care not to alienate the communities that produce the structures. EMBL-EBI's Protein Data Bank in Europe (PDBe; pdbe.org)[1,2], one of the founders of the Worldwide Protein Data Bank (wwPDB; wwpdb.org), is committed to becoming such a resource. PDBe focuses on five areas:

- Advanced services (e.g., SSM, Pisa, PDBeMotif)
- Ligands (e.g., PDBeChem; in the future to include analysis, validation, visualisation and annotation services)
- Integration with other databases and resources (e.g., the SIFTS project carried out in collaboration with UniProt, and various structure browsers and widgets that build on SIFTS data)
- Validation (implementing new tools and resources for X-ray, NMR and 3DEM)
- Experimental data (e.g., the Electron Density Server, which will be ported from Uppsala to PDBe, and Vivaldi, a new tool to visualise experimental NMR data on 3D models)

Some of our recent and current work in these areas, as well as plans for the future will be discussed.

[1] S. Velankar et al. G.J. Kleywegt. (2012). Nucleic Acid Res. 40. D445-452.
[2] S. Velankar, G.J. Kleywegt. (2012) *Acta Cryst. D67. 324-330.*

Keywords: PDB, Protein data Bank in Europe