The Representations and Definitions in Table 3.

The Representations and Definitions:

Cg(I) = Plane number I (= ring number in () above)

Cg(J) = Center of gravity of ring J (Plane number above)

α = Dihedral Angle between Planes I and J (o)

β = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (o)

γ = Angle Cg(I)-->Cg(J) vector and normal to plane J (o)

or Angle between Cg-H vector and ring J normal

Cg-Cg = Distance between ring Centroids (Å)

CgI\_Perp = Perpendicular distance of Cg(I) on ring J (Å)

CgJ\_Perp = Perpendicular distance of Cg(J) on ring I (Å)

Slippage = Distance between Cg(I) and Perpendicular Projection of CgH-Perp = Perpendicular distance of H to ring plane J

C-H∙∙∙Cg = C-H-Cg angle (o)

C∙∙∙Cg = Distance of C to Cg (Å)

C-H, π = Angle of the C-H bond with the π-plane (i.e.' Perpendicular = 90o, Parallel = 0o)

5-Membered Ring (1) N1 --> C15 --> N2 --> C16 --> C21 -->

6-Membered Ring (2) C2 --> C3 --> C4 --> C5 --> C6 --> C7 -->

6-Membered Ring (3) C16 --> C17 --> C18 --> C19 --> C20 --> C21 -->

9-Membered Ring (4) N1 --> C15 --> N2 --> C16 --> C17 --> C18 --> C19 --> C20 --> C21

5-Membered Ring (5) N3 --> C22 --> N4 --> C23 --> C28 -->

9-Membered Ring (6) N3 --> C22 --> N4 --> C23 --> C24 --> C25 --> C26 --> C27 --> C28 -->

Symmetry Codes for the Asymmetric Residual Unit (ARU).

[a] = -x, 1/2+y, 1/2-z

[b] = -x, -1/2+y, 1/2-z

[c] = 1/2-x, 1/2+y, z