Least Square Planes. Two complexes are present in the asymmetric unit. Values for the second molecule are given in blue.



|  |  |  |
| --- | --- | --- |
| plane. | mean deviation in Å | max deviation in Å (atom) |
| N1 C1 C2 C3 C4 C5 C9 C8 C7 C6 ***quin1***  N1B C1B C2B C3B C4B C5B C9B C8B C7B C6B | 0.077  0.090 | 0.136 (N1)  0.153 (C9B) |
| N2 C14 C13 C12 C11 C10 ***pyr1***  N2B C14B C13B C12B C11B C10B | 0.011  0.006 | 0.016 (C14)  0.008 (C13B) |
| N3 C23 C22 C21 C19 C20 C15 C16 C17 C18 ***quin2***  C15B C16B C17B C18B C19B C21B C22B C23B N3B C20B | 0.073  0.065 | 0.137 (N3)  0.123 (N3B) |
| N4 C24 C25 C26 C27 C28 ***pyr2***  N4B C28B C27B C26B C25B C24B | 0.022  0.019 | 0.035 (N4)  0.030 (N4B) |
| N5 C34 C33 C32 C31 C30 ***pyr3***  N5B C30B C31B C32B C33B C34B | 0.004  0.004 | 0.005 (C34)  0.005 (N5B) |
| N6 C36 C37 C38 C39 C40 ***pyr4***  N6B C40B C39B C37B C38B C36B | 0.026  0.023 | 0.039 (N6)  0.037 (N6B) |

Angles between least-square planes (in ˚). Two complexes are present in the asymmetric unit. Values for the second molecule are given in blue

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Pyr1 | Quin2 | Pyr2 | Pyr3 | Pyr4 |
| Quin1 | 36.7  38.3 | 74.7  77.0 | 32.0  31.4 | 41.6  46.1 | 84.2  85.9 |
| Pyr1 |  | 38.1  38.8 | 53.5  52.8 | 22.0  20.3 | 53.1  54.1 |
| Quin2 |  |  | 83.8  84.9 | 42.1  39.2 | 27.7  31.6 |
| Pyr2 |  |  |  | 41.6  45.7 | 77.9  76.7 |
| Pyr3 |  |  |  |  | 42.9  39.9 |