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Controlling molecular tautomerism through supramolecular selectivity

Epa, K.; Aakeroey, C.B.; Desper, J.; Rayat, S.; Chandra, K.L.; Cruz-Cabeza, A.J.

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anisotropic displacement parameters and molecular geometry data,
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#

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goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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 C26 C 0.1153(5) 0.0464(3) 0.6193(8) 0.0252(13) Uani 1 1 d ...
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 C28 C 0.0220(5) 0.1075(3) 0.7485(8) 0.0268(13) Uani 1 1 d ...
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 C31 C 0.6945(5) -0.0185(3) 0.0759(8) 0.0228(12) Uani 1 1 d ...
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 C32 C 0.7681(5) 0.0139(3) 0.0290(7) 0.0225(12) Uani 1 1 d ...
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 C33 C 0.8287(5) -0.0108(3) -0.0525(8) 0.0233(13) Uani 1 1 d ...
 F33 F 0.8964(3) 0.02296(16) -0.0982(5) 0.0308(9) Uani 1 1 d ...
 C34 C 0.8241(5) -0.0685(3) -0.0814(7) 0.0230(12) Uani 1 1 d ...
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 C35 C 0.7531(5) -0.1012(3) -0.0323(8) 0.0240(13) Uani 1 1 d ...
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 C36 C 0.6891(5) -0.0763(3) 0.0437(8) 0.0255(13) Uani 1 1 d ...
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 C41 C -0.1743(5) 0.3052(3) 0.9535(7) 0.0231(12) Uani 1 1 d ...
 I3 I -0.06454(3) 0.267121(17) 0.85852(5) 0.02455(11) Uani 1 1 d ...
 C42 C -0.2375(6) 0.2719(2) 1.0163(8) 0.0270(14) Uani 1 1 d ...
 F42 F -0.2391(3) 0.21468(16) 1.0009(5) 0.0324(10) Uani 1 1 d ...
 C43 C -0.3017(5) 0.2961(3) 1.0938(8) 0.0239(12) Uani 1 1 d ...
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 C44 C -0.3040(5) 0.3551(3) 1.1110(8) 0.0237(12) Uani 1 1 d ...
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C12 0.032(3) 0.015(2) 0.044(4) -0.005(3) 0.024(3) -0.002(2)

N13 0.025(3) 0.019(2) 0.037(3) -0.001(2) 0.018(2) -0.0004(18)

C14 0.026(3) 0.019(2) 0.026(3) -0.001(2) 0.013(3) -0.001(2)

N15 0.027(3) 0.019(2) 0.033(3) 0.005(2) 0.017(2) 0.0029(19)

C16 0.033(3) 0.014(2) 0.044(4) 0.005(3) 0.019(3) 0.001(2)

C17 0.038(4) 0.023(3) 0.044(4) 0.009(3) 0.024(3) -0.003(3)

C18 0.030(3) 0.031(3) 0.037(4) 0.001(3) 0.021(3) -0.004(3)

C19 0.024(3) 0.024(3) 0.028(3) 0.000(2) 0.012(3) 0.002(2)

N21 0.033(3) 0.023(2) 0.029(3) 0.000(2) 0.020(3) 0.004(2)

C22 0.037(4) 0.019(3) 0.036(4) -0.001(3) 0.021(3) 0.004(2)

N23 0.027(3) 0.018(2) 0.036(3) -0.001(2) 0.019(3) 0.0001(19)

C24 0.022(3) 0.020(3) 0.036(4) 0.007(2) 0.016(3) 0.004(2)

N25 0.029(3) 0.018(2) 0.029(3) 0.003(2) 0.017(2) 0.0025(18)

C26 0.027(3) 0.021(3) 0.032(4) 0.000(2) 0.016(3) 0.000(2)

C27 0.032(3) 0.023(3) 0.031(4) 0.005(3) 0.018(3) 0.000(2)

C28 0.027(3) 0.027(3) 0.033(4) 0.002(3) 0.018(3) 0.000(2)

C29 0.023(3) 0.022(3) 0.028(3) 0.003(2) 0.017(3) 0.003(2)

C31 0.020(3) 0.023(3) 0.028(3) 0.001(2) 0.012(3) 0.002(2)

I1 0.0255(2) 0.02234(18) 0.0295(2) -0.00196(15) 0.01527(17) 0.00134(14)

C32 0.024(3) 0.022(3) 0.026(3) 0.003(2) 0.014(3) 0.005(2)

F32 0.036(2) 0.0177(16) 0.039(2) -0.0028(16) 0.0193(19) -0.0001(14)

C33 0.025(3) 0.021(3) 0.030(3) 0.001(2) 0.018(3) -0.001(2)

F33 0.038(2) 0.0221(17) 0.042(3) 0.0002(17) 0.027(2) -0.0039(15)

C34 0.022(3) 0.025(3) 0.026(3) -0.002(2) 0.012(3) 0.000(2)

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C35 0.026(3) 0.017(2) 0.035(4) 0.002(2) 0.019(3) 0.006(2)

F35 0.037(2) 0.0167(16) 0.044(3) 0.0004(16) 0.023(2) 0.0008(14)

C36 0.025(3) 0.021(3) 0.036(4) 0.005(3) 0.018(3) 0.001(2)

F36 0.034(2) 0.0238(18) 0.048(3) 0.0000(17) 0.028(2) -0.0021(15)

C41 0.023(3) 0.019(3) 0.030(3) -0.004(2) 0.012(3) -0.001(2)

I3 0.0260(2) 0.02249(18) 0.0293(2) -0.00325(16) 0.01446(17) -0.00024(14)

C42 0.033(3) 0.013(2) 0.038(4) -0.004(2) 0.014(3) -0.003(2)

F42 0.040(2) 0.0159(16) 0.049(3) -0.0021(17) 0.025(2) -0.0019(15)

C43 0.022(3) 0.026(3) 0.028(3) 0.000(3) 0.013(3) -0.004(2)

F43 0.033(2) 0.0249(18) 0.045(3) 0.0006(17) 0.024(2) -0.0051(15)

C44 0.025(3) 0.021(3) 0.030(3) -0.002(2) 0.014(3) 0.002(2)

I4 0.0297(2) 0.0247(2) 0.0334(3) -0.00097(16) 0.01804(19) 0.00184(14)

C45 0.028(3) 0.016(2) 0.030(4) 0.002(2) 0.013(3) 0.001(2)

F45 0.034(2) 0.0167(16) 0.044(3) -0.0004(16) 0.0189(19) -0.0004(14)

C46 0.024(3) 0.023(3) 0.032(4) 0.001(3) 0.014(3) -0.004(2)

F46 0.038(2) 0.0213(17) 0.043(3) 0.0000(17) 0.026(2) -0.0036(15)

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C14 N15 1.329(8) . ?
C14 C19 1.415(8) . ?
N15 C16 1.346(8) . ?
C16 C17 1.384(10) . ?
C16 H16 0.9500 . ?
C17 C18 1.390(10) . ?
C17 H17 0.9500 . ?
C18 C19 1.399(9) . ?
C18 H18 0.9500 . ?
N21 C22 1.308(8) . ?
N21 C29 1.389(8) . ?
C22 N23 1.356(8) . ?
C22 H22 0.9500 . ?
N23 C24 1.372(8) . ?
N23 H23 0.8800 . ?
C24 N25 1.323(8) . ?
C24 C29 1.407(8) . ?
N25 C26 1.351(8) . ?
C26 C27 1.391(9) . ?
C26 H26 0.9500 . ?
C27 C28 1.400(9) . ?
C27 H27 0.9500 . ?
C28 C29 1.380(8) . ?
C28 H28 0.9500 . ?
C31 C36 1.377(9) . ?
C31 C32 1.386(8) . ?
C31 I1 2.094(6) . ?
C32 F32 1.340(7) . ?
C32 C33 1.381(8) . ?
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C33 C34 1.369(9) . ?
C34 C35 1.376(8) . ?
C34 I2 2.084(6) . ?

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C35 F35 1.343(7) . ?
C35 C36 1.377(8) . ?
C36 F36 1.340(7) . ?
C41 C46 1.380(9) . ?
C41 C42 1.383(9) . ?
C41 I3 2.091(6) . ?
C42 F42 1.338(7) . ?
C42 C43 1.383(9) . ?
C43 F43 1.326(7) . ?
C43 C44 1.383(9) . ?
C44 C45 1.372(9) . ?
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C12 N13 C14 106.5(5) . . ?
C12 N13 H13 126.8 . . ?
C14 N13 H13 126.8 . . ?
N15 C14 N13 127.3(6) . . ?
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C18 C17 H17 119.4 . . ?
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#

Cambridge Crystallographic Data Centre

CCDC

#

#####

#

This CIF contains data from an original supplementary publication

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Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F , and R-factors based on ALL data will be even larger.

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#####

Cambridge Crystallographic Data Centre
CCDC
#

#####

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anisotropic displacement parameters and molecular geometry data,
as required by the journal to which it was submitted.
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# to carry out CIF format checking respectively.
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Refinement of F^2 against ALL reflections. The weighted R-factor wR and

goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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C12 C 0.1892(3) 0.5418(2) 0.3223(4) 0.0249(7) Uani 1 1 d . . .
H12 H 0.1903 0.5993 0.2744 0.030 Uiso 1 1 calc R . .
N13 N 0.1089(3) 0.52008(19) 0.3988(3) 0.0213(5) Uani 1 1 d . . .
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C16 C 0.1244(3) 0.2990(2) 0.5651(4) 0.0254(6) Uani 1 1 d . . .
H16 H 0.0876 0.2598 0.6207 0.030 Uiso 1 1 calc R . .
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C17 C 0.2233(3) 0.2655(2) 0.5254(5) 0.0257(7) Uani 1 1 d . . .
 H17 H 0.2521 0.2056 0.5561 0.031 Uiso 1 1 calc R . .
 C18 C 0.2797(3) 0.3183(2) 0.4421(4) 0.0240(6) Uani 1 1 d . . .
 H18 H 0.3467 0.2963 0.4136 0.029 Uiso 1 1 calc R . .
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 C23 C 0.8047(3) 0.3393(2) 0.1805(4) 0.0208(6) Uani 1 1 d . . .
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All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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 # Cambridge Crystallographic Data Centre

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Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F , and R-factors based on ALL data will be even larger.

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 N31_1 N 0.7523(3) -0.0217(2) 0.2268(3) 0.0469(8) Uani 1 1 d . . .
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 C32_1 C 0.5477(3) -0.1390(3) 0.0881(3) 0.0497(9) Uani 1 1 d . . .
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 C33_1 C 0.4753(3) -0.2465(3) 0.0075(3) 0.0503(9) Uani 1 1 d . . .
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 C34_1 C 0.5242(3) -0.3405(3) -0.0173(3) 0.0465(9) Uani 1 1 d . . .
 N34_1 N 0.4458(3) -0.4547(2) -0.1029(3) 0.0539(8) Uani 1 1 d . . .
 O34_1 O 0.3358(2) -0.4637(2) -0.1407(2) 0.0656(8) Uani 1 1 d . . .
 O35_1 O 0.4932(2) -0.53694(19) -0.1319(2) 0.0651(8) Uani 1 1 d . . .
 C35_1 C 0.6436(3) -0.3310(3) 0.0361(3) 0.0498(9) Uani 1 1 d . . .
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 C36_1 C 0.7167(3) -0.2236(3) 0.1177(3) 0.0479(9) Uani 1 1 d . . .
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 N41_1 N 0.8305(3) 0.1701(2) 0.3359(3) 0.0485(8) Uani 1 1 d . . .
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 C42_1 C 0.8420(3) 0.3265(3) 0.2991(3) 0.0471(9) Uani 1 1 d . . .
 C43_1 C 0.8514(3) 0.4435(3) 0.3445(3) 0.0485(9) Uani 1 1 d . . .
 H43_1 H 0.8562 0.4727 0.2973 0.058 Uiso 1 1 calc R . .
 C44_1 C 0.8538(3) 0.5172(3) 0.4565(3) 0.0496(9) Uani 1 1 d . . .
 H44_1 H 0.8604 0.5954 0.4846 0.060 Uiso 1 1 calc R . .
 C45_1 C 0.8465(3) 0.4763(3) 0.5269(3) 0.0481(9) Uani 1 1 d . . .
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 C46_1 C 0.8344(3) 0.3603(3) 0.4836(3) 0.0481(9) Uani 1 1 d . . .
 H46_1 H 0.8264 0.3312 0.5303 0.058 Uiso 1 1 calc R . .

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 H47B_1 H 0.8606 0.2938 0.1456 0.083 Uiso 1 1 calc R . .
 H47C_1 H 0.7687 0.1937 0.1308 0.083 Uiso 1 1 calc R . .
 N11_2 N 0.4919(3) 0.7368(2) 0.7620(2) 0.0463(7) Uani 1 1 d . . .
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 C12_2 C 0.4562(3) 0.6231(3) 0.6824(3) 0.0482(9) Uani 1 1 d . . .
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 N13_2 N 0.5459(3) 0.5689(2) 0.6844(2) 0.0492(8) Uani 1 1 d . . .
 C14_2 C 0.6453(3) 0.6546(3) 0.7685(3) 0.0439(8) Uani 1 1 d . . .
 N15_2 N 0.7580(3) 0.6393(2) 0.7990(3) 0.0500(8) Uani 1 1 d . . .
 C16_2 C 0.8406(3) 0.7354(3) 0.8831(3) 0.0554(10) Uani 1 1 d . . .
 H16_2 H 0.9213 0.7296 0.9066 0.067 Uiso 1 1 calc R . .
 C17_2 C 0.8162(3) 0.8436(3) 0.9385(3) 0.0521(9) Uani 1 1 d . . .
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 C18_2 C 0.6998(3) 0.8578(3) 0.9066(3) 0.0491(9) Uani 1 1 d . . .
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 C36_2 C 0.3463(3) 0.2865(3) 0.4476(3) 0.0469(9) Uani 1 1 d . . .
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 C43_2 C 0.9284(3) 0.3289(3) 0.9157(3) 0.0504(9) Uani 1 1 d . . .
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 O21_1 0.0482(15) 0.0382(13) 0.0593(16) 0.0201(12) 0.0074(12) 0.0155(11)
 C31_1 0.043(2) 0.0387(18) 0.049(2) 0.0215(17) 0.0123(17) 0.0117(15)
 N31_1 0.0409(17) 0.0364(15) 0.0525(18) 0.0201(14) 0.0053(14) 0.0111(13)
 C32_1 0.045(2) 0.0395(19) 0.055(2) 0.0208(18) 0.0113(18) 0.0108(16)
 C33_1 0.040(2) 0.051(2) 0.060(2) 0.0304(19) 0.0113(18) 0.0132(16)
 C34_1 0.045(2) 0.0349(18) 0.050(2) 0.0182(16) 0.0105(17) 0.0083(15)
 N34_1 0.0470(19) 0.0477(18) 0.056(2) 0.0253(16) 0.0064(16) 0.0071(15)
 O34_1 0.0481(16) 0.0545(16) 0.0729(19) 0.0284(15) 0.0005(14) 0.0046(13)
 O35_1 0.0642(18) 0.0363(14) 0.0745(19) 0.0202(13) 0.0110(15) 0.0135(13)
 C35_1 0.051(2) 0.0379(19) 0.054(2) 0.0229(17) 0.0104(18) 0.0124(16)
 C36_1 0.041(2) 0.0425(19) 0.048(2) 0.0197(17) 0.0045(16) 0.0124(15)
 C41_1 0.0417(19) 0.0358(18) 0.048(2) 0.0183(16) 0.0127(16) 0.0122(15)
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 C42_1 0.042(2) 0.0425(19) 0.049(2) 0.0199(17) 0.0128(17) 0.0124(15)
 C43_1 0.044(2) 0.048(2) 0.059(2) 0.0310(19) 0.0168(18) 0.0154(16)
 C44_1 0.047(2) 0.0387(19) 0.054(2) 0.0192(18) 0.0131(18) 0.0131(16)
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 C46_1 0.049(2) 0.0420(19) 0.049(2) 0.0216(17) 0.0128(17) 0.0117(16)
 C47_1 0.068(3) 0.052(2) 0.056(2) 0.0302(19) 0.029(2) 0.0269(19)
 N11_2 0.0427(17) 0.0347(15) 0.0520(18) 0.0188(14) 0.0091(14) 0.0108(13)
 C12_2 0.046(2) 0.0391(19) 0.053(2) 0.0234(17) 0.0078(17) 0.0103(16)
 N13_2 0.0436(17) 0.0389(16) 0.0573(19) 0.0227(15) 0.0096(15) 0.0130(13)
 C14_2 0.042(2) 0.0418(19) 0.045(2) 0.0214(16) 0.0129(16) 0.0146(15)
 N15_2 0.0426(17) 0.0498(17) 0.0539(18) 0.0267(15) 0.0107(15) 0.0136(14)
 C16_2 0.042(2) 0.064(2) 0.057(2) 0.031(2) 0.0111(19) 0.0109(18)
 C17_2 0.053(2) 0.046(2) 0.047(2) 0.0220(18) 0.0083(18) 0.0066(17)
 C18_2 0.053(2) 0.0386(19) 0.048(2) 0.0198(17) 0.0112(18) 0.0103(16)
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 O21_2 0.0525(16) 0.0382(13) 0.0622(17) 0.0184(12) 0.0079(13) 0.0162(11)
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 N31_2 0.0462(17) 0.0334(15) 0.0507(18) 0.0173(14) 0.0072(14) 0.0136(13)
 C32_2 0.052(2) 0.042(2) 0.052(2) 0.0170(18) 0.0131(18) 0.0180(17)
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 C34_2 0.043(2) 0.0390(19) 0.046(2) 0.0191(17) 0.0066(16) 0.0059(15)
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C35_2 0.049(2) 0.042(2) 0.050(2) 0.0212(18) 0.0131(18) 0.0153(16)
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 C44_2 0.053(2) 0.0419(19) 0.044(2) 0.0157(17) 0.0083(18) 0.0172(17)
 C45_2 0.047(2) 0.045(2) 0.047(2) 0.0172(18) 0.0110(18) 0.0119(16)
 C46_2 0.049(2) 0.0404(19) 0.047(2) 0.0164(17) 0.0134(17) 0.0134(16)
 C47_2 0.059(3) 0.058(2) 0.065(3) 0.034(2) 0.022(2) 0.0147(19)

_geom_special_details

;

All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry. An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.

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loop_

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C12_1 H12_1 0.9500 . ?

N13_1 C14_1 1.397(4) . ?

C14_1 N15_1 1.359(4) . ?

C14_1 C19_1 1.411(4) . ?

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C16_1 C17_1 1.402(5) . ?

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C17_1 C18_1 1.406(5) . ?

C17_1 H17_1 0.9500 . ?

C18_1 C19_1 1.391(5) . ?

C18_1 H18_1 0.9500 . ?

C21_1 O21_1 1.251(4) . ?

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C21_1 N31_1 1.391(4) . ?

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 C36_1 H36_1 0.9500 . ?
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 C47_1 H47B_1 0.9800 . ?
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 C17_2 H17_2 0.9500 . ?
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C36_2 H36_2 0.9500 . ?
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C45_2 C46_2 1.401(5) . ?
C45_2 H45_2 0.9500 . ?
C46_2 H46_2 0.9500 . ?
C47_2 H47A_2 0.9800 . ?
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N13_1 C12_1 N11_1 114.5(3) . . ?
N13_1 C12_1 H12_1 122.8 . . ?
N11_1 C12_1 H12_1 122.8 . . ?
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C16_1 N15_1 C14_1 113.2(3) . . ?
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C18_1 C19_1 C14_1 121.3(3) . . ?
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O21_1 C21_1 N41_1 123.8(3) . . ?
O21_1 C21_1 N31_1 123.0(3) . . ?
N41_1 C21_1 N31_1 113.2(3) . . ?
C32_1 C31_1 C36_1 119.3(3) . . ?
C32_1 C31_1 N31_1 124.9(3) . . ?

C36_1 C31_1 N31_1 115.7(3) .. ?
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 C12_2 N11_2 H11_2 121(2) .. ?
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 C42_2 C47_2 H47B_2 109.5 . . ?
 H47A_2 C47_2 H47B_2 109.5 . . ?
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 C12_1 N13_1 C14_1 N15_1 -178.3(3) ?
 C12_1 N13_1 C14_1 C19_1 -0.3(4) ?
 N13_1 C14_1 N15_1 C16_1 178.5(3) ?
 C19_1 C14_1 N15_1 C16_1 0.7(5) ?
 C14_1 N15_1 C16_1 C17_1 0.6(6) ?
 N15_1 C16_1 C17_1 C18_1 -0.8(6) ?
 C16_1 C17_1 C18_1 C19_1 -0.2(5) ?
 C17_1 C18_1 C19_1 N11_1 -179.4(4) ?
 C17_1 C18_1 C19_1 C14_1 1.3(5) ?
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 N15_1 C14_1 C19_1 C18_1 -1.7(6) ?
 N13_1 C14_1 C19_1 C18_1 -179.8(3) ?
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Cambridge Crystallographic Data Centre
CCDC

This CIF contains data from an original supplementary publication

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Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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 C12 C 0.2083(5) 0.1899(5) 0.4733(4) 0.0377(11) Uani 1 1 d . . .
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 H18 H 0.5187 -0.1053 0.7262 0.049 Uiso 1 1 calc R . .
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 C21 C 0.2196(5) 0.6790(4) 0.5439(4) 0.0327(10) Uani 1 1 d . . .
 O21 O 0.1843(3) 0.8074(3) 0.5408(3) 0.0389(8) Uani 1 1 d . . .
 C31 C 0.3814(5) 0.6273(4) 0.7443(4) 0.0326(10) Uani 1 1 d . . .
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 C37 C 0.1166(5) 0.7269(4) 0.8108(4) 0.0340(10) Uani 1 1 d . . .
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 C42 C 0.0336(5) 0.8266(4) 0.2931(4) 0.0351(11) Uani 1 1 d . . .
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 C43 C -0.0479(5) 0.8786(5) 0.1782(4) 0.0374(11) Uani 1 1 d . . .
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 N13 0.029(2) 0.040(2) 0.047(2) -0.0144(18) 0.0014(17) -0.0168(17)
 C14 0.025(2) 0.035(2) 0.031(2) -0.0079(19) 0.0077(18) -0.0094(19)
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All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
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 used when they are defined by crystal symmetry. An approximate (isotropic)
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