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data_4c

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 'N'  'N'   0.0061   0.0033
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_computing_cell_refinement        ?
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_computing_molecular_graphics     ?
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_refine_special_details
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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^ > 2sigma(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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_refine_ls_weighting_details
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_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
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_refine_ls_extinction_coef        0.031(3)
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_refine_ls_goodness_of_fit_ref    0.955
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 _atom_site_occupancy
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H1B H 1.9289 0.1773 -0.1499 0.061 Uiso 1 1 calc R . .
C11 C 1.7386(9) 0.14168(10) -0.0535(5) 0.0477(11) Uani 1 1 d . . .
C12 C 1.5442(9) 0.12291(12) -0.0839(7) 0.0575(13) Uani 1 1 d . . .
H12 H 1.4234 0.1295 -0.1500 0.069 Uiso 1 1 calc R . .
C13 C 1.5297(11) 0.09394(13) -0.0149(7) 0.0630(14) Uani 1 1 d . . .
H13 H 1.3952 0.0816 -0.0332 0.076 Uiso 1 1 calc R . .
C14 C 1.7064(11) 0.08319(11) 0.0783(7) 0.0613(14) Uani 1 1 d . . .
H14 H 1.6947 0.0635 0.1216 0.074 Uiso 1 1 calc R . .
C15 C 1.9036(11) 0.10180(11) 0.1080(7) 0.0620(14) Uani 1 1 d . . .
H15 H 2.0252 0.0950 0.1732 0.074 Uiso 1 1 calc R . .
C16 C 1.9180(9) 0.13146(11) 0.0377(6) 0.0541(12) Uani 1 1 d . . .
H16 H 2.0524 0.1439 0.0546 0.065 Uiso 1 1 calc R . .
C2 C 1.6670(8) 0.20009(10) -0.0260(5) 0.0454(11) Uani 1 1 d . . .
H2 H 1.7502 0.1996 0.0727 0.054 Uiso 1 1 calc R . .
N1 N 1.4050(8) 0.19792(10) -0.0006(5) 0.0572(11) Uani 1 1 d . . .
H1C H 1.3116 0.2126 -0.0312 0.069 Uiso 1 1 calc R . .
H1D H 1.3453 0.1820 0.0447 0.069 Uiso 1 1 calc R . .
C3 C 1.7297(9) 0.23063(11) -0.1090(5) 0.0488(11) Uani 1 1 d . . .
O3 O 1.6446(7) 0.23727(8) -0.2338(4) 0.0615(9) Uani 1 1 d . . .
N2 N 1.8930(9) 0.24871(9) -0.0385(5) 0.0555(11) Uani 1 1 d D A .
H2A H 1.9344 0.2445 0.0539 0.067 Uiso 1 1 d R . .
C4 C 2.0070(12) 0.27541(13) -0.1137(7) 0.0674(14) Uiso 1 1 d D . .
H4A1 H 2.1668 0.2695 -0.1484 0.081 Uiso 0.621(9) 1 calc PR A 1
H4B2 H 1.9127 0.2812 -0.2026 0.081 Uiso 0.621(9) 1 calc PR A 1
H4C H 1.9548 0.2749 -0.2194 0.081 Uiso 0.379(9) 1 d PR A 2
H4D H 1.9334 0.2937 -0.0688 0.081 Uiso 0.379(9) 1 d PR A 2
C5 C 2.0267(19) 0.30229(18) -0.0112(10) 0.061(3) Uiso 0.621(9) 1 d PD A 1
H5A H 2.1316 0.2966 0.0730 0.073 Uiso 0.621(9) 1 calc PR A 1
H5B H 1.8683 0.3064 0.0311 0.073 Uiso 0.621(9) 1 calc PR A 1
C6 C 2.126(2) 0.3336(2) -0.0844(13) 0.070(3) Uiso 0.621(9) 1 d PD A 1
H6A H 2.0321 0.3390 -0.1739 0.084 Uiso 0.621(9) 1 calc PR A 1
H6B H 2.1138 0.3504 -0.0113 0.084 Uiso 0.621(9) 1 calc PR A 1
C7 C 2.3744(14) 0.32874(15) -0.1260(8) 0.0818(17) Uiso 1 1 d D . .
H7A H 2.3873 0.3146 -0.2118 0.098 Uiso 0.621(9) 1 calc PR A 1
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H7B H 2.4658 0.3204 -0.0409 0.098 Uiso 0.621(9) 1 calc PR A 1
H7C H 2.5178 0.3194 -0.0819 0.098 Uiso 0.379(9) 1 d PR A 2
H7D H 2.2640 0.3318 -0.0414 0.098 Uiso 0.379(9) 1 d PR A 2
C5' C 2.206(2) 0.2789(3) -0.1147(17) 0.058(4) Uiso 0.379(9) 1 d PD A 2
H5'1 H 2.2788 0.2614 -0.1672 0.070 Uiso 0.379(9) 1 calc PR A 2
H5'2 H 2.2629 0.2784 -0.0100 0.070 Uiso 0.379(9) 1 calc PR A 2
C6' C 2.298(3) 0.3084(3) -0.1881(17) 0.066(4) Uiso 0.379(9) 1 d PD A 2
H6'1 H 2.4214 0.3020 -0.2601 0.080 Uiso 0.379(9) 1 calc PR A 2
H6'2 H 2.1654 0.3164 -0.2486 0.080 Uiso 0.379(9) 1 calc PR A 2
N3 N 2.4610(13) 0.36019(12) -0.1679(5) 0.093(2) Uani 1 1 d D A .
H3 H 2.4190 0.3694 -0.2510 0.112 Uiso 1 1 d R . .
C8 C 2.5934(11) 0.37715(11) -0.0763(6) 0.0548(12) Uani 1 1 d . . .
O8 O 2.6281(8) 0.37024(8) 0.0611(4) 0.0663(10) Uani 1 1 d . A .
C9 C 2.5399(11) 0.43362(11) -0.0901(7) 0.0668(16) Uani 1 1 d . . .
H9A H 2.3784 0.4300 -0.1290 0.080 Uiso 1 1 calc R A .
H9B H 2.5308 0.4339 0.0205 0.080 Uiso 1 1 calc R . .
C91 C 2.6257(11) 0.46499(12) -0.1446(6) 0.0558(13) Uani 1 1 d . A .
C92 C 2.5016(11) 0.48137(12) -0.2563(7) 0.0606(13) Uani 1 1 d . . .
H92 H 2.3628 0.4727 -0.2981 0.073 Uiso 1 1 calc R A .
C93 C 2.5768(13) 0.50982(13) -0.3070(7) 0.0718(16) Uani 1 1 d . A .
H93 H 2.4904 0.5204 -0.3815 0.086 Uiso 1 1 calc R . .
C94 C 2.7891(13) 0.52273(13) -0.2433(8) 0.0745(17) Uani 1 1 d . . .
H94 H 2.8456 0.5419 -0.2771 0.089 Uiso 1 1 calc R A .
C95 C 2.9096(11) 0.50702(13) -0.1329(7) 0.0655(15) Uani 1 1 d . A .
H95 H 3.0472 0.5159 -0.0907 0.079 Uiso 1 1 calc R . .
C96 C 2.8362(11) 0.47849(13) -0.0810(7) 0.0663(15) Uani 1 1 d . . .
H96 H 2.9230 0.4682 -0.0056 0.080 Uiso 1 1 calc R A .
C10 C 2.7034(10) 0.40656(11) -0.1400(5) 0.0513(12) Uani 1 1 d . A .
H10 H 2.8639 0.4095 -0.0951 0.062 Uiso 1 1 calc R . .
N4 N 2.7257(9) 0.40537(9) -0.3020(4) 0.0531(10) Uani 1 1 d . . .
H4A H 2.6522 0.4188 -0.3578 0.064 Uiso 1 1 calc R A .
H4B H 2.8128 0.3912 -0.3440 0.064 Uiso 1 1 calc R . .
C1A C 1.0669(12) 0.17229(12) 0.3954(6) 0.0636(15) Uani 1 1 d . . .
H1A1 H 0.9034 0.1746 0.4334 0.076 Uiso 1 1 calc R . .
H1A2 H 1.0592 0.1719 0.2848 0.076 Uiso 1 1 calc R . .
C11A C 1.1657(10) 0.14221(11) 0.4499(6) 0.0539(12) Uani 1 1 d . . .
C12A C 1.3746(10) 0.12987(11) 0.3889(6) 0.0559(12) Uani 1 1 d . . .
H12A H 1.4531 0.1402 0.3100 0.067 Uiso 1 1 calc R . .
C13A C 1.4696(11) 0.10187(12) 0.4450(7) 0.0673(15) Uani 1 1 d . . .
H13A H 1.6111 0.0939 0.4035 0.081 Uiso 1 1 calc R . .
C14A C 1.3542(13) 0.08606(12) 0.5612(7) 0.0700(16) Uani 1 1 d . . .
H14A H 1.4185 0.0676 0.5978 0.084 Uiso 1 1 calc R . .
C15A C 1.1443(12) 0.09764(13) 0.6229(8) 0.0725(16) Uani 1 1 d . . .
H15A H 1.0646 0.0870 0.7004 0.087 Uiso 1 1 calc R . .
C16A C 1.0529(9) 0.12587(13) 0.5663(7) 0.0635(15) Uani 1 1 d . . .
H16A H 0.9118 0.1338 0.6083 0.076 Uiso 1 1 calc R . .
C2A C 1.2165(9) 0.20071(10) 0.4458(5) 0.0448(10) Uani 1 1 d . . .
H2B H 1.3806 0.1990 0.4050 0.054 Uiso 1 1 calc R . .
N1A N 1.2261(8) 0.20159(9) 0.6138(4) 0.0526(10) Uani 1 1 d . . .
H1A3 H 1.1666 0.2172 0.6623 0.063 Uiso 1 1 calc R . .
H1A4 H 1.2911 0.1865 0.6634 0.063 Uiso 1 1 calc R . .
C3A C 1.0971(12) 0.22891(14) 0.3811(6) 0.0668(15) Uani 1 1 d . . .
O3A O 1.1351(8) 0.23663(9) 0.2429(4) 0.0696(11) Uani 1 1 d . . .
N2A N 0.9548(12) 0.24476(13) 0.4723(5) 0.095(2) Uani 1 1 d D B .
H2A1 H 0.9122 0.2371 0.5588 0.115 Uiso 1 1 d R . .
C4A C 0.7565(17) 0.26638(17) 0.4124(10) 0.096(2) Uiso 1 1 d D . .
H4E H 0.8165 0.2851 0.4611 0.116 Uiso 0.401(11) 1 calc PR B 1
H4F H 0.8183 0.2679 0.3091 0.116 Uiso 0.401(11) 1 calc PR B 1
H4G H 0.8085 0.2702 0.3084 0.116 Uiso 0.599(11) 1 d PR B 2
H4H H 0.5899 0.2596 0.4061 0.116 Uiso 0.599(11) 1 d PR B 2
C5A C 0.608(2) 0.2738(2) 0.3915(13) 0.042(3) Uiso 0.401(11) 1 d PD B 1
H5A1 H 0.5258 0.2730 0.4893 0.050 Uiso 0.401(11) 1 calc PR B 1
H5A2 H 0.5346 0.2575 0.3308 0.050 Uiso 0.401(11) 1 calc PR B 1
C6A C 0.513(2) 0.3032(2) 0.3197(11) 0.032(3) Uiso 0.401(11) 1 d PD B 1
H6A1 H 0.6252 0.3094 0.2405 0.038 Uiso 0.401(11) 1 calc PR B 1
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H6A2 H 0.3611 0.2983 0.2700 0.038 Uiso 0.401(11) 1 calc PR B 1
C7A C 0.4758(13) 0.32795(13) 0.4117(8) 0.0737(16) Uiso 1 1 d D . .
H7E H 0.6273 0.3327 0.4622 0.088 Uiso 0.401(11) 1 calc PR B 1
H7F H 0.3625 0.3217 0.4904 0.088 Uiso 0.401(11) 1 calc PR B 1
H7G H 0.4609 0.3294 0.5218 0.088 Uiso 0.599(11) 1 d PR B 2
H7H H 0.3779 0.3106 0.3779 0.088 Uiso 0.599(11) 1 d PR B 2
C5" C 0.870(3) 0.2885(3) 0.4393(19) 0.112(5) Uiso 0.599(11) 1 d PD B 2
H5"1 H 1.0316 0.2865 0.3979 0.134 Uiso 0.599(11) 1 calc PR B 2
H5"2 H 0.8814 0.2917 0.5486 0.134 Uiso 0.599(11) 1 calc PR B 2
C6" C 0.714(4) 0.3198(4) 0.351(2) 0.138(6) Uiso 0.599(11) 1 d PD B 2
H6"1 H 0.8159 0.3381 0.3576 0.166 Uiso 0.599(11) 1 calc PR B 2
H6"2 H 0.6955 0.3149 0.2436 0.166 Uiso 0.599(11) 1 calc PR B 2
N3A N 0.3864(9) 0.35651(9) 0.3435(5) 0.0605(12) Uani 1 1 d D B .
H3A H 0.4362 0.3613 0.2536 0.073 Uiso 1 1 d R . .
C8A C 0.2270(9) 0.37501(11) 0.4153(6) 0.0510(12) Uani 1 1 d . . .
O8A O 0.1431(8) 0.36847(8) 0.5423(4) 0.0623(9) Uani 1 1 d . B .
C9A C 0.2539(10) 0.43170(10) 0.4351(6) 0.0524(12) Uani 1 1 d . . .
H9A1 H 0.1648 0.4316 0.5304 0.063 Uiso 1 1 calc R B .
H9A2 H 0.4220 0.4279 0.4595 0.063 Uiso 1 1 calc R . .
C91A C 0.2342(9) 0.46345(11) 0.3666(5) 0.0479(11) Uani 1 1 d . B .
C92A C 0.4148(9) 0.47520(11) 0.2724(6) 0.0534(12) Uani 1 1 d . . .
H92A H 0.5509 0.4633 0.2511 0.064 Uiso 1 1 calc R B .
C93A C 0.3905(11) 0.50477(13) 0.2102(6) 0.0654(14) Uani 1 1 d . B .
H93A H 0.5072 0.5119 0.1425 0.078 Uiso 1 1 calc R . .
C94A C 0.2015(12) 0.52355(13) 0.2455(8) 0.0716(16) Uani 1 1 d . . .
H94A H 0.1910 0.5435 0.2058 0.086 Uiso 1 1 calc R B .
C95A C 0.0232(11) 0.51201(13) 0.3429(7) 0.0625(14) Uani 1 1 d . B .
H95A H -0.1067 0.5246 0.3695 0.075 Uiso 1 1 calc R . .
C96A C 0.0374(10) 0.48254(11) 0.3995(8) 0.0627(15) Uani 1 1 d . . .
H96A H -0.0862 0.4750 0.4611 0.075 Uiso 1 1 calc R B .
C10A C 0.1618(9) 0.40473(11) 0.3357(6) 0.0480(11) Uani 1 1 d . B .
H10A H 0.2435 0.4054 0.2365 0.058 Uiso 1 1 calc R . .
N4A N -0.0954(8) 0.40871(9) 0.3125(5) 0.0530(10) Uani 1 1 d . . .
H4A1 H -0.1945 0.3947 0.3436 0.064 Uiso 1 1 calc R B .
H4A2 H -0.1490 0.4251 0.2677 0.064 Uiso 1 1 calc R . .

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C11 0.044(3) 0.050(2) 0.049(3) -0.005(2) 0.008(2) -0.002(2)
C12 0.044(3) 0.058(3) 0.071(4) -0.006(3) -0.012(2) -0.008(2)
C13 0.051(3) 0.061(3) 0.077(4) -0.010(3) -0.001(3) -0.001(3)
C14 0.071(4) 0.049(3) 0.064(3) -0.010(2) 0.012(3) 0.010(3)
C15 0.066(3) 0.055(3) 0.064(3) -0.009(2) -0.011(3) 0.019(3)
C16 0.043(3) 0.056(3) 0.063(3) -0.014(2) -0.006(2) 0.004(2)
C2 0.046(2) 0.044(2) 0.046(2) -0.006(2) -0.003(2) -0.008(2)
N1 0.046(2) 0.056(2) 0.070(3) 0.002(2) 0.010(2) -0.006(2)
C3 0.051(3) 0.054(3) 0.041(2) 0.006(2) 0.006(2) 0.003(2)
O3 0.063(2) 0.070(2) 0.051(2) 0.0075(17) -0.0170(19) -0.0142(19)
N2 0.081(3) 0.049(2) 0.037(2) 0.0094(17) -0.013(2) -0.021(2)
N3 0.143(6) 0.087(3) 0.050(3) 0.018(2) -0.027(3) -0.069(4)
C8 0.070(3) 0.054(3) 0.040(3) 0.005(2) 0.002(3) -0.016(3)
O8 0.090(3) 0.077(2) 0.0319(17) 0.0073(16) -0.0067(19) -0.026(2)
C9 0.064(4) 0.060(3) 0.077(4) -0.004(3) 0.016(3) -0.012(3)
C91 0.055(3) 0.057(3) 0.055(3) -0.021(2) 0.012(3) -0.002(2)
C92 0.064(3) 0.062(3) 0.056(3) -0.016(3) 0.006(3) -0.008(3)
C93 0.090(5) 0.059(3) 0.066(3) -0.009(3) -0.002(3) -0.003(3)
C94 0.087(4) 0.049(3) 0.087(4) -0.005(3) 0.004(4) -0.010(3)
C95 0.065(4) 0.059(3) 0.072(4) -0.010(3) 0.005(3) -0.012(3)
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C96 0.065(3) 0.078(4) 0.056(3) -0.011(3) -0.003(3) 0.001(3)
C10 0.054(3) 0.061(3) 0.039(2) 0.000(2) 0.000(2) -0.016(2)
N4 0.069(3) 0.055(2) 0.035(2) 0.0071(18) 0.001(2) 0.004(2)
C1A 0.067(3) 0.072(3) 0.052(3) -0.020(3) -0.026(3) 0.011(3)
C11A 0.053(3) 0.057(3) 0.051(3) -0.014(2) -0.010(2) -0.002(2)
C12A 0.061(3) 0.052(3) 0.055(3) -0.011(2) -0.007(3) 0.003(3)
C13A 0.064(3) 0.065(3) 0.073(4) -0.019(3) 0.003(3) 0.010(3)
C14A 0.092(4) 0.052(3) 0.065(3) -0.008(3) 0.000(3) 0.005(3)
C15A 0.077(4) 0.056(3) 0.084(4) 0.002(3) 0.018(4) -0.015(3)
C16A 0.046(3) 0.073(3) 0.071(4) -0.018(3) 0.004(3) -0.011(3)
C2A 0.059(3) 0.047(2) 0.029(2) 0.0006(19) -0.009(2) 0.010(2)
N1A 0.073(3) 0.0483(19) 0.0360(19) -0.0019(17) -0.014(2) 0.013(2)
C3A 0.080(4) 0.081(4) 0.040(3) 0.001(3) 0.010(3) 0.018(4)
O3A 0.089(3) 0.083(2) 0.0368(19) 0.0075(17) 0.006(2) 0.031(2)
N2A 0.145(6) 0.095(3) 0.047(3) 0.018(2) 0.029(3) 0.081(4)
N3A 0.077(3) 0.051(2) 0.053(2) 0.0104(18) 0.020(2) 0.024(2)
C8A 0.050(3) 0.057(3) 0.046(3) 0.008(2) 0.004(2) 0.011(2)
O8A 0.076(2) 0.062(2) 0.0484(19) 0.0058(16) 0.0182(19) 0.0061(19)
C9A 0.058(3) 0.052(3) 0.048(3) -0.001(2) -0.003(3) 0.001(2)
C91A 0.046(3) 0.056(3) 0.041(3) -0.004(2) 0.006(2) 0.002(2)
C92A 0.045(3) 0.055(3) 0.060(3) -0.004(2) 0.004(2) -0.004(2)
C93A 0.066(3) 0.070(3) 0.060(3) 0.005(3) 0.017(3) -0.008(3)
C94A 0.085(4) 0.053(3) 0.077(4) 0.005(3) 0.000(4) 0.005(3)
C95A 0.058(3) 0.055(3) 0.074(4) 0.008(3) 0.006(3) 0.006(3)
C96A 0.050(3) 0.048(3) 0.089(4) 0.000(3) 0.017(3) -0.004(2)
C10A 0.050(3) 0.051(2) 0.043(2) 0.006(2) 0.011(2) 0.007(2)
N4A 0.049(2) 0.048(2) 0.062(3) 0.0054(19) -0.010(2) 0.0070(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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C1 C2 1.533(7) . ?
C1 H1A 0.9700 . ?
C1 H1B 0.9700 . ?
C11 C16 1.349(7) . ?
C11 C12 1.373(7) . ?
C12 C13 1.389(8) . ?
C12 H12 0.9300 . ?
C13 C14 1.356(8) . ?
C13 H13 0.9300 . ?
C14 C15 1.380(8) . ?
C14 H14 0.9300 . ?
C15 C16 1.421(8) . ?
C15 H15 0.9300 . ?
C16 H16 0.9300 . ?
C2 N1 1.472(7) . ?
C2 C3 1.543(6) . ?
C2 H2 0.9800 . ?
N1 H1C 0.8600 . ?
N1 H1D 0.8600 . ?
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C3 O3 1.225(6) . ?
C3 N2 1.344(7) . ?
N2 C4 1.469(7) . ?
N2 H2A 0.8600 . ?
C4 C5' 1.114(14) . ?
C4 C5 1.469(10) . ?
C4 H4A1 0.9700 . ?
C4 H4B2 0.9700 . ?
C4 H4C 0.9699 . ?
C4 H4D 0.9698 . ?
C5 C6 1.591(12) . ?
C5 H4D 0.8116 . ?
C5 H5A 0.9700 . ?
C5 H5B 0.9700 . ?
C6 C7 1.439(13) . ?
C6 H6A 0.9700 . ?
C6 H6B 0.9700 . ?
C6 H7D 0.8556 . ?
C7 C6' 1.114(15) . ?
C7 N3 1.483(8) . ?
C7 H7A 0.9700 . ?
C7 H7B 0.9700 . ?
C7 H7C 0.9700 . ?
C7 H7D 0.9700 . ?
C5' C6' 1.513(18) . ?
C5' H5'1 0.9700 . ?
C5' H5'2 0.9700 . ?
C6' H6'1 0.9700 . ?
C6' H6'2 0.9700 . ?
N3 C8 1.310(7) . ?
N3 H3 0.8601 . ?
C8 O8 1.255(6) . ?
C8 C10 1.512(7) . ?
C9 C91 1.510(7) . ?
C9 C10 1.539(7) . ?
C9 H9A 0.9700 . ?
C9 H9B 0.9700 . ?
C91 C92 1.389(9) . ?
C91 C96 1.417(8) . ?
C92 C93 1.368(8) . ?
C92 H92 0.9300 . ?
C93 C94 1.416(9) . ?
C93 H93 0.9300 . ?
C94 C95 1.356(9) . ?
C94 H94 0.9300 . ?
C95 C96 1.372(8) . ?
C95 H95 0.9300 . ?
C96 H96 0.9300 . ?
C10 N4 1.426(6) . ?
C10 H10 0.9800 . ?
N4 H4A 0.8600 . ?
N4 H4B 0.8600 . ?
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C1A C2A 1.543(7) . ?
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C14A H14A 0.9300 . ?
C15A C16A 1.407(9) . ?
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C15A H15A 0.9300 . ?
C16A H16A 0.9300 . ?
C2A N1A 1.473(6) . ?
C2A C3A 1.495(7) . ?
C2A H2B 0.9800 . ?
N1A H1A3 0.8600 . ?
N1A H1A4 0.8600 . ?
C3A O3A 1.273(7) . ?
C3A N2A 1.314(7) . ?
N2A C4A 1.533(10) . ?
N2A H2A1 0.8600 . ?
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C4A H4G 0.9700 . ?
C4A H4H 0.9700 . ?
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C5A H4G 1.3392 . ?
C5A H4H 0.6321 . ?
C5A H5A1 0.9700 . ?
C5A H5A2 0.9700 . ?
C6A C7A 1.352(11) . ?
C6A H6A1 0.9700 . ?
C6A H6A2 0.9700 . ?
C6A H7H 0.9598 . ?
C7A N3A 1.454(7) . ?
C7A C6" 1.47(2) . ?
C7A H7E 0.9700 . ?
C7A H7F 0.9700 . ?
C7A H7G 0.9700 . ?
C7A H7H 0.9698 . ?
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C5" H5"1 0.9700 . ?
C5" H5"2 0.9700 . ?
C6" H6"1 0.9700 . ?
C6" H6"2 0.9700 . ?
N3A C8A 1.346(6) . ?
N3A H3A 0.8600 . ?
C8A O8A 1.238(6) . ?
C8A C10A 1.502(6) . ?
C9A C91A 1.497(7) . ?
C9A C10A 1.539(7) . ?
C9A H9A1 0.9700 . ?
C9A H9A2 0.9700 . ?
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C91A C92A 1.393(7) . ?
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C92A H92A 0.9300 . ?
C93A C94A 1.359(9) . ?
C93A H93A 0.9300 . ?
C94A C95A 1.397(9) . ?
C94A H94A 0.9300 . ?
C95A C96A 1.365(7) . ?
C95A H95A 0.9300 . ?
C96A H96A 0.9300 . ?
C10A N4A 1.450(7) . ?
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N4A H4A1 0.8600 . ?
N4A H4A2 0.8600 . ?

loop_
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C2 C1 H1B 108.7 . . ?
H1A C1 H1B 107.6 . . ?
C16 C11 C12 120.1(5) . . ?
C16 C11 C1 119.0(4) . . ?
C12 C11 C1 120.9(5) . . ?
C11 C12 C13 119.4(5) . . ?
C11 C12 H12 120.3 . . ?
C13 C12 H12 120.3 . . ?
C14 C13 C12 121.8(5) . . ?
C14 C13 H13 119.1 . . ?
C12 C13 H13 119.1 . . ?
C13 C14 C15 119.1(5) . . ?
C13 C14 H14 120.4 . . ?
C15 C14 H14 120.4 . . ?
C14 C15 C16 119.0(5) . . ?
C14 C15 H15 120.5 . . ?
C16 C15 H15 120.5 . . ?
C11 C16 C15 120.6(5) . . ?
C11 C16 H16 119.7 . . ?
C15 C16 H16 119.7 . . ?
N1 C2 C3 110.3(4) . . ?
N1 C2 C1 111.9(4) . . ?
C3 C2 C1 107.0(4) . . ?
N1 C2 H2 109.2 . . ?
C3 C2 H2 109.2 . . ?
C1 C2 H2 109.2 . . ?
C2 N1 H1C 120.0 . . ?
C2 N1 H1D 120.0 . . ?
H1C N1 H1D 120.0 . . ?
O3 C3 N2 122.3(4) . . ?
O3 C3 C2 122.2(4) . . ?
N2 C3 C2 115.4(4) . . ?
C3 N2 C4 122.5(4) . . ?
C3 N2 H2A 119.3 . . ?
C4 N2 H2A 118.2 . . ?
C5' C4 C5 79.9(10) . . ?
C5' C4 N2 122.4(9) . . ?
C5 C4 N2 112.0(6) . . ?
C5' C4 H4A1 29.4 . . ?
C5 C4 H4A1 109.3 . . ?
N2 C4 H4A1 109.2 . . ?
C5' C4 H4B2 119.6 . . ?
C5 C4 H4B2 109.1 . . ?
N2 C4 H4B2 109.2 . . ?
H4A1 C4 H4B2 107.9 . . ?
C5' C4 H4C 106.9 . . ?
C5 C4 H4C 128.5 . . ?
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H4B2 C4 H4C 23.0 . . ?
C5' C4 H4D 108.1 . . ?
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H4B2 C4 H4D 83.7 . . ?
H4C C4 H4D 106.2 . . ?
C4 C5 C6 116.6(7) . . ?
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H6B C6 H7D 80.8 . . ?
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C6' C7 N3 136.0(10) . . ?
C6 C7 N3 103.9(7) . . ?
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C6' C7 H7B 106.5 . . ?
C6 C7 H7B 111.0 . . ?
N3 C7 H7B 111.0 . . ?
H7A C7 H7B 109.0 . . ?
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C6 C7 H7C 138.0 . . ?
N3 C7 H7C 102.1 . . ?
H7A C7 H7C 89.3 . . ?
H7B C7 H7C 27.6 . . ?
C6' C7 H7D 103.9 . . ?
C6 C7 H7D 35.3 . . ?
N3 C7 H7D 105.7 . . ?
H7A C7 H7D 136.3 . . ?
H7B C7 H7D 77.9 . . ?
H7C C7 H7D 105.5 . . ?
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C6' C5' H5'1 108.2 . . ?
C4 C5' H5'2 108.1 . . ?
C6' C5' H5'2 108.0 . . ?
H5'1 C5' H5'2 107.3 . . ?
C7 C6' C5' 125.5(14) . . ?
C7 C6' H6'1 106.1 . . ?
C5' C6' H6'1 106.0 . . ?
C7 C6' H6'2 105.8 . . ?
C5' C6' H6'2 105.9 . . ?
H6'1 C6' H6'2 106.3 . . ?
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C8 N3 H3 114.4 . . ?
C7 N3 H3 122.8 . . ?
O8 C8 N3 122.8(5) . . ?
O8 C8 C10 119.4(5) . . ?
N3 C8 C10 117.9(4) . . ?
C91 C9 C10 113.7(5) . . ?
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C10 C9 H9A 108.8 . . ?
C91 C9 H9B 108.8 . . ?
C10 C9 H9B 108.8 . . ?
H9A C9 H9B 107.7 . . ?
C92 C91 C96 118.4(5) . . ?
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C92 C91 C9 121.4(6) . . ?
C96 C91 C9 120.1(6) . . ?
C93 C92 C91 122.2(6) . . ?
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C91 C92 H92 118.9 . . ?
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C96 C95 H95 118.8 . . ?
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C91 C96 H96 120.6 . . ?
N4 C10 C9 111.2(5) . . ?
N4 C10 C8 111.8(4) . . ?
C9 C10 C8 107.0(4) . . ?
N4 C10 H10 108.9 . . ?
C9 C10 H10 108.9 . . ?
C8 C10 H10 108.9 . . ?
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H4A N4 H4B 120.0 . . ?
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C1A C2A H2B 109.5 . . ?
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C2A N1A H1A4 120.0 . . ?
H1A3 N1A H1A4 120.0 . . ?
O3A C3A N2A 122.8(5) . . ?
O3A C3A C2A 120.0(5) . . ?
N2A C3A C2A 117.2(5) . . ?
C3A N2A C4A 122.5(5) . . ?
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C4A N2A H2A1 109.8 . . ?
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C5A C4A H4F 96.3 . . ?
C5" C4A H4F 86.3 . . ?
N2A C4A H4F 96.3 . . ?
H4E C4A H4F 103.4 . . ?
C5A C4A H4G 91.1 . . ?
C5" C4A H4G 83.7 . . ?
N2A C4A H4G 102.3 . . ?
H4E C4A H4G 100.1 . . ?
H4F C4A H4G 6.5 . . ?
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C5" C4A H4H 140.5 . . ?
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C6A C5A H5A2 103.7 . . ?
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C5A C6A H6A1 107.9 . . ?
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H6A1 C6A H6A2 107.2 . . ?
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C5A C6A H7H 109.2 . . ?
H6A1 C6A H7H 142.0 . . ?
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N3A C7A H7E 107.7 . . ?
C6" C7A H7E 55.6 . . ?
C6A C7A H7F 107.8 . . ?
N3A C7A H7F 107.8 . . ?
C6" C7A H7F 140.8 . . ?
H7E C7A H7F 107.1 . . ?
C6A C7A H7G 131.1 . . ?
N3A C7A H7G 108.9 . . ?
C6" C7A H7G 116.9 . . ?
H7E C7A H7G 67.0 . . ?
H7F C7A H7G 41.9 . . ?
C6A C7A H7H 45.2 . . ?
N3A C7A H7H 109.6 . . ?
C6" C7A H7H 102.1 . . ?
H7E C7A H7H 141.7 . . ?
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C6" C5" H5"1 110.7 . . ?
C4A C5" H5"2 110.4 . . ?
C6" C5" H5"2 110.3 . . ?
H5"1 C5" H5"2 108.7 . . ?
C7A C6" C5" 117.4(13) . . ?
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C5" C6" H6"1 108.1 . . ?
C7A C6" H6"2 107.9 . . ?
C5" C6" H6"2 107.7 . . ?
H6"1 C6" H6"2 107.2 . . ?
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C8A N3A H3A 119.8 . . ?
C7A N3A H3A 118.1 . . ?
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C8A C10A C9A 107.5(4) . . ?
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C11 C12 C13 C14 -2.1(8) . . . . ?
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C13 C14 C15 C16 -1.2(8) . . . . ?
C12 C11 C16 C15 -2.6(8) . . . . ?
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C14 C15 C16 C11 1.8(8) . . . . ?
C11 C1 C2 N1 -65.4(6) . . . . ?
C11 C1 C2 C3 173.6(4) . . . . ?
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C4 C5 C6 C7 -66.7(11) . . . . ?
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C5 C4 C5' C6' -66.7(13) . . . . ?
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C6 C7 C6' C5' -73.0(16) . . . . ?
N3 C7 C6' C5' -175.6(11) . . . . ?
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C6' C7 N3 C8 -163.9(15) . . . . ?
C6 C7 N3 C8 102.0(9) . . . . ?
C7 N3 C8 O8 -10.6(11) . . . . ?
C7 N3 C8 C10 170.7(6) . . . . ?
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C91 C9 C10 C8 179.9(5) . . . . ?
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N3 C8 C10 C9 98.8(7) . . . . ?
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