Formation of fibrillar structures through self-assembly of designed peptide turns

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Peptide I

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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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C4A C 0.50805(14) 0.31570(18) 0.81710(10) 0.0163(3) Uani 1 1 d . . .

H4A H 0.5295 0.2342 0.8392 0.020 Uiso 1 1 calc R . .

C13A C 1.0123(3) 0.6327(7) 0.9919(3) 0.141(3) Uani 1 1 d . . .

H13A H 1.0669 0.6885 1.0164 0.212 Uiso 1 1 calc R . .

H13B H 0.9957 0.6418 0.9379 0.212 Uiso 1 1 calc R . .

H13C H 1.0340 0.5494 1.0058 0.212 Uiso 1 1 calc R . .

C16A C 0.8621(2) 0.7593(3) 1.1519(2) 0.0672(10) Uani 1 1 d . . .

H16A H 0.8823 0.7748 1.2056 0.101 Uiso 1 1 calc R . .

H16B H 0.8120 0.8194 1.1263 0.101 Uiso 1 1 calc R . .

H16C H 0.9211 0.7650 1.1340 0.101 Uiso 1 1 calc R . .

O12A O 0.92171(15) 0.6606(3) 1.01587(14) 0.0826(9) Uani 1 1 d . . .

O11A O 0.87672(18) 0.4624(3) 1.00298(17) 0.0951(11) Uani 1 1 d . . .

O100 O 0.7683(4) 0.2580(4) 0.9991(2) 0.0594(11) Uani 0.50 1 d P . .

C5A C 0.53065(14) 0.41146(19) 0.88114(10) 0.0175(3) Uani 1 1 d . . .

C7A C 0.51786(15) 0.44103(19) 1.01040(10) 0.0196(4) Uani 1 1 d . . .

C8A C 0.60113(15) 0.54082(19) 1.03271(10) 0.0186(4) Uani 1 1 d . . .

C10A C 0.77614(15) 0.6039(2) 1.05030(12) 0.0260(4) Uani 1 1 d . . .

H10V H 0.7464 0.6802 1.0245 0.031 Uiso 1 1 calc R . .

C41A C 0.39099(14) 0.31466(18) 0.77898(10) 0.0183(4) Uani 1 1 d . . .

H41A H 0.3570 0.3129 0.8182 0.022 Uiso 1 1 calc R . .

H41B H 0.3715 0.3908 0.7507 0.022 Uiso 1 1 calc R . .

C42A C 0.35273(15) 0.20745(19) 0.72596(11) 0.0188(4) Uani 1 1 d . . .

C43A C 0.29030(17) 0.2261(2) 0.65268(12) 0.0261(4) Uani 1 1 d . . .

H43A H 0.2751 0.3061 0.6347 0.031 Uiso 1 1 calc R . .

C44A C 0.24981(19) 0.1266(2) 0.60537(12) 0.0337(5) Uani 1 1 d . . .

H44A H 0.2073 0.1409 0.5564 0.040 Uiso 1 1 calc R . .

C45A C 0.27221(18) 0.0079(2) 0.63053(13) 0.0314(5) Uani 1 1 d . . .

H45A H 0.2447 -0.0584 0.5991 0.038 Uiso 1 1 calc R . .

C46A C 0.33656(18) -0.0120(2) 0.70359(13) 0.0302(5) Uani 1 1 d . . .

H46A H 0.3534 -0.0921 0.7210 0.036 Uiso 1 1 calc R . .

C47A C 0.37551(17) 0.0866(2) 0.75033(12) 0.0260(4) Uani 1 1 d . . .

H47A H 0.4180 0.0720 0.7993 0.031 Uiso 1 1 calc R . .

C2A C 0.66442(15) 0.33451(18) 0.78295(10) 0.0185(4) Uani 1 1 d . . .

C101 C 0.81124(14) 0.3601(2) 0.73379(12) 0.0249(4) Uani 1 1 d . . .

C102 C 0.87120(18) 0.4463(2) 0.79545(15) 0.0375(5) Uani 1 1 d . . .

H10A H 0.8660 0.4189 0.8436 0.056 Uiso 1 1 calc R . .

H10B H 0.8437 0.5282 0.7854 0.056 Uiso 1 1 calc R . .

H10C H 0.9421 0.4467 0.7966 0.056 Uiso 1 1 calc R . .

C103 C 0.81624(17) 0.4031(3) 0.65649(14) 0.0365(6) Uani 1 1 d . . .

H10D H 0.7716 0.3529 0.6176 0.055 Uiso 1 1 calc R . .

H10E H 0.8855 0.3956 0.6543 0.055 Uiso 1 1 calc R . .

H10F H 0.7949 0.4877 0.6488 0.055 Uiso 1 1 calc R . .

C104 C 0.84514(17) 0.2264(2) 0.74780(14) 0.0332(5) Uani 1 1 d . . .

H10G H 0.7984 0.1746 0.7112 0.050 Uiso 1 1 calc R . .

H10H H 0.8455 0.2027 0.7980 0.050 Uiso 1 1 calc R . .

H10I H 0.9130 0.2174 0.7431 0.050 Uiso 1 1 calc R . .

C11A C 0.86231(19) 0.5657(4) 1.01962(15) 0.0526(8) Uani 1 1 d . . .

C14A C 0.81612(17) 0.6314(2) 1.13612(13) 0.0329(5) Uani 1 1 d . . .

H14A H 0.7570 0.6283 1.1559 0.040 Uiso 1 1 calc R . .

C15A C 0.8921(3) 0.5346(3) 1.17799(16) 0.0619(9) Uani 1 1 d . . .

H15A H 0.8635 0.4539 1.1643 0.093 Uiso 1 1 calc R . .

H15B H 0.9064 0.5462 1.2317 0.093 Uiso 1 1 calc R . .

H15C H 0.9547 0.5423 1.1646 0.093 Uiso 1 1 calc R . .

C71A C 0.41186(16) 0.5005(2) 0.98553(12) 0.0274(4) Uani 1 1 d . . .

H71A H 0.3601 0.4374 0.9740 0.041 Uiso 1 1 calc R . .

H71B H 0.4052 0.5500 0.9412 0.041 Uiso 1 1 calc R . .

H71C H 0.4034 0.5517 1.0257 0.041 Uiso 1 1 calc R . .

C72A C 0.52983(18) 0.3563(2) 1.07921(11) 0.0278(4) Uani 1 1 d . . .

H72A H 0.4792 0.2920 1.0660 0.042 Uiso 1 1 calc R . .

H72B H 0.5204 0.4036 1.1206 0.042 Uiso 1 1 calc R . .

H72C H 0.5973 0.3205 1.0940 0.042 Uiso 1 1 calc R . .

O5A O 0.54149(11) 0.52193(13) 0.87026(7) 0.0217(3) Uani 1 1 d . . .

O8A O 0.58151(11) 0.64260(14) 1.05428(8) 0.0250(3) Uani 1 1 d . . .

O2A O 0.71659(11) 0.30059(15) 0.84533(8) 0.0260(3) Uani 1 1 d . . .

O1A O 0.70031(10) 0.36958(14) 0.72567(8) 0.0219(3) Uani 1 1 d . . .

N6A N 0.53261(13) 0.36386(15) 0.94895(8) 0.0186(3) Uani 1 1 d . . .

H6A H 0.5428 0.2860 0.9565 0.022 Uiso 1 1 calc R . .

N9A N 0.69651(12) 0.51111(17) 1.03291(9) 0.0225(3) Uani 1 1 d . . .

H9A H 0.7103 0.4369 1.0227 0.027 Uiso 1 1 calc R . .

N3A N 0.56110(12) 0.34213(16) 0.76178(8) 0.0189(3) Uani 1 1 d . . .

H3A H 0.5273 0.3624 0.7161 0.023 Uiso 1 1 calc R . .

N6B N 0.47808(12) -0.37116(15) 0.54684(8) 0.0179(3) Uani 1 1 d . . .

H6B H 0.4781 -0.2923 0.5419 0.021 Uiso 1 1 calc R . .

N9B N 0.30114(12) -0.49734(16) 0.46853(9) 0.0197(3) Uani 1 1 d . . .

H9B H 0.2929 -0.4197 0.4743 0.024 Uiso 1 1 calc R . .

N3B N 0.43365(12) -0.34995(16) 0.72798(8) 0.0181(3) Uani 1 1 d . . .

H3B H 0.4628 -0.3660 0.7751 0.022 Uiso 1 1 calc R . .

O5B O 0.45849(10) -0.52904(13) 0.62167(7) 0.0201(3) Uani 1 1 d . . .

O8B O 0.39958(11) -0.64460(13) 0.43950(8) 0.0236(3) Uani 1 1 d . . .

O2B O 0.28450(10) -0.32925(14) 0.63357(8) 0.0238(3) Uani 1 1 d . . .

O1B O 0.28773(10) -0.36694(15) 0.75593(8) 0.0249(3) Uani 1 1 d . . .

C5B C 0.47465(13) -0.41907(17) 0.61314(10) 0.0155(3) Uani 1 1 d . . .

C7B C 0.48175(15) -0.44856(18) 0.48275(10) 0.0176(4) Uani 1 1 d . . .

C8B C 0.39129(15) -0.54032(18) 0.46290(10) 0.0183(4) Uani 1 1 d . . .

C10B C 0.21720(15) -0.5838(2) 0.46476(11) 0.0223(4) Uani 1 1 d . . .

H10W H 0.2436 -0.6464 0.5040 0.027 Uiso 1 1 calc R . .

C11B C 0.17928(15) -0.6504(2) 0.38933(11) 0.0229(4) Uani 1 1 d . . .

C41B C 0.60913(14) -0.32464(19) 0.72208(10) 0.0185(4) Uani 1 1 d . . .

H41C H 0.6253 -0.4011 0.7505 0.022 Uiso 1 1 calc R . .

H41D H 0.6488 -0.3227 0.6864 0.022 Uiso 1 1 calc R . .

C42B C 0.64167(14) -0.21776(18) 0.77636(10) 0.0173(4) Uani 1 1 d . . .

C43B C 0.61691(16) -0.09763(19) 0.75160(12) 0.0234(4) Uani 1 1 d . . .

H43B H 0.5748 -0.0837 0.7025 0.028 Uiso 1 1 calc R . .

C44B C 0.65394(17) 0.0016(2) 0.79898(13) 0.0297(5) Uani 1 1 d . . .

H44B H 0.6364 0.0815 0.7816 0.036 Uiso 1 1 calc R . .

C45B C 0.71654(18) -0.0173(2) 0.87169(13) 0.0304(5) Uani 1 1 d . . .

H45B H 0.7417 0.0495 0.9034 0.037 Uiso 1 1 calc R . .

C46B C 0.74194(18) -0.1369(2) 0.89744(12) 0.0312(5) Uani 1 1 d . . .

H46B H 0.7846 -0.1502 0.9465 0.037 Uiso 1 1 calc R . .

C47B C 0.70357(16) -0.2374(2) 0.84995(11) 0.0251(4) Uani 1 1 d . . .

H47B H 0.7196 -0.3174 0.8678 0.030 Uiso 1 1 calc R . .

C2B C 0.33025(14) -0.34817(18) 0.69960(10) 0.0180(4) Uani 1 1 d . . .

C105 C 0.17521(15) -0.3653(2) 0.74094(12) 0.0278(4) Uani 1 1 d . . .

C106 C 0.16425(18) -0.3730(3) 0.82019(13) 0.0380(6) Uani 1 1 d . . .

H10J H 0.1982 -0.4459 0.8450 0.057 Uiso 1 1 calc R . .

H10K H 0.0927 -0.3765 0.8170 0.057 Uiso 1 1 calc R . .

H10L H 0.1949 -0.3015 0.8487 0.057 Uiso 1 1 calc R . .

C107 C 0.1303(2) -0.4790(4) 0.69548(17) 0.0608(10) Uani 1 1 d . . .

H10M H 0.1627 -0.5514 0.7220 0.091 Uiso 1 1 calc R . .

H10N H 0.1419 -0.4753 0.6467 0.091 Uiso 1 1 calc R . .

H10O H 0.0577 -0.4824 0.6888 0.091 Uiso 1 1 calc R . .

C71B C 0.47120(17) -0.3627(2) 0.41478(11) 0.0245(4) Uani 1 1 d . . .

H71D H 0.4054 -0.3226 0.4017 0.037 Uiso 1 1 calc R . .

H71E H 0.4769 -0.4100 0.3723 0.037 Uiso 1 1 calc R . .

H71F H 0.5247 -0.3016 0.4278 0.037 Uiso 1 1 calc R . .

C72B C 0.58363(15) -0.5194(2) 0.50244(12) 0.0260(4) Uani 1 1 d . . .

H72D H 0.5885 -0.5729 0.5448 0.039 Uiso 1 1 calc R . .

H72E H 0.6398 -0.4619 0.5153 0.039 Uiso 1 1 calc R . .

H72F H 0.5864 -0.5677 0.4595 0.039 Uiso 1 1 calc R . .

C14B C 0.12928(16) -0.5149(2) 0.48456(12) 0.0287(5) Uani 1 1 d . . .

H14B H 0.1600 -0.4719 0.5327 0.034 Uiso 1 1 calc R . .

C15B C 0.0771(2) -0.4181(3) 0.42700(17) 0.0493(7) Uani 1 1 d . . .

H15D H 0.1274 -0.3608 0.4205 0.074 Uiso 1 1 calc R . .

H15E H 0.0271 -0.3749 0.4446 0.074 Uiso 1 1 calc R . .

H15F H 0.0435 -0.4572 0.3794 0.074 Uiso 1 1 calc R . .

O12B O 0.17794(11) -0.57882(15) 0.33038(8) 0.0261(3) Uani 1 1 d . . .

O11B O 0.14810(14) -0.75464(16) 0.38420(10) 0.0395(4) Uani 1 1 d . . .

C4B C 0.49460(14) -0.32433(18) 0.67765(10) 0.0171(4) Uani 1 1 d . . .

H4B H 0.4762 -0.2423 0.6555 0.021 Uiso 1 1 calc R . .

C108 C 0.1299(2) -0.2466(3) 0.70251(18) 0.0566(9) Uani 1 1 d . . .

H10X H 0.1354 -0.2451 0.6519 0.085 Uiso 1 1 calc R . .

H10Y H 0.1667 -0.1778 0.7306 0.085 Uiso 1 1 calc R . .

H10Z H 0.0589 -0.2415 0.7006 0.085 Uiso 1 1 calc R . .

C16B C 0.05104(19) -0.6059(3) 0.49788(14) 0.0422(6) Uani 1 1 d . . .

H16D H 0.0850 -0.6625 0.5374 0.063 Uiso 1 1 calc R . .

H16E H 0.0198 -0.6509 0.4520 0.063 Uiso 1 1 calc R . .

H16F H -0.0010 -0.5617 0.5126 0.063 Uiso 1 1 calc R . .

C13B C 0.13504(16) -0.6354(3) 0.25721(12) 0.0328(5) Uani 1 1 d . . .

H13D H 0.1460 -0.5826 0.2186 0.049 Uiso 1 1 calc R . .

H13E H 0.0627 -0.6479 0.2481 0.049 Uiso 1 1 calc R . .

H13F H 0.1679 -0.7135 0.2561 0.049 Uiso 1 1 calc R . .

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C13A 0.050(2) 0.281(9) 0.111(4) -0.016(5) 0.054(2) -0.046(4)

C16A 0.0375(15) 0.0416(17) 0.104(3) -0.0275(18) -0.0067(17) -0.0061(13)

O12A 0.0336(10) 0.142(3) 0.0756(15) 0.0202(17) 0.0223(10) -0.0244(14)

O11A 0.0461(13) 0.132(3) 0.114(2) -0.064(2) 0.0328(14) 0.0081(15)

O100 0.081(3) 0.055(3) 0.042(2) 0.0034(19) 0.017(2) 0.024(2)

C5A 0.0149(8) 0.0183(9) 0.0180(8) -0.0017(7) 0.0031(7) -0.0029(7)

C7A 0.0220(9) 0.0190(10) 0.0182(8) -0.0020(7) 0.0068(7) -0.0010(8)

C8A 0.0194(9) 0.0192(9) 0.0156(7) 0.0010(7) 0.0025(7) 0.0012(7)

C10A 0.0176(9) 0.0294(11) 0.0291(10) 0.0033(8) 0.0039(8) 0.0003(8)

C41A 0.0180(9) 0.0162(9) 0.0207(8) -0.0027(7) 0.0057(7) -0.0020(7)

C42A 0.0188(9) 0.0188(9) 0.0203(8) -0.0025(7) 0.0082(7) -0.0028(7)

C43A 0.0302(11) 0.0200(10) 0.0265(10) 0.0003(8) 0.0058(8) -0.0020(9)

C44A 0.0349(12) 0.0386(14) 0.0229(10) -0.0087(9) 0.0015(9) -0.0067(11)

C45A 0.0323(11) 0.0274(12) 0.0359(11) -0.0161(10) 0.0122(9) -0.0111(10)

C46A 0.0357(12) 0.0152(10) 0.0387(11) -0.0013(9) 0.0099(10) -0.0022(9)

C47A 0.0306(11) 0.0193(10) 0.0262(10) 0.0013(8) 0.0054(8) -0.0023(9)

C2A 0.0206(9) 0.0126(8) 0.0226(8) -0.0038(7) 0.0069(7) -0.0004(7)

C101 0.0138(8) 0.0287(11) 0.0335(10) 0.0005(9) 0.0088(8) 0.0013(8)

C102 0.0266(11) 0.0368(13) 0.0485(13) -0.0083(11) 0.0104(10) -0.0096(10)

C103 0.0216(10) 0.0493(15) 0.0430(13) 0.0094(11) 0.0162(9) 0.0012(10)

C104 0.0247(10) 0.0324(12) 0.0433(12) -0.0006(10) 0.0114(9) 0.0065(9)

C11A 0.0235(12) 0.095(3) 0.0386(13) -0.0087(15) 0.0083(10) -0.0051(15)

C14A 0.0268(10) 0.0352(13) 0.0340(11) -0.0103(10) 0.0046(9) -0.0077(9)

C15A 0.070(2) 0.0493(18) 0.0432(15) 0.0095(14) -0.0187(14) -0.0099(16)

C71A 0.0209(10) 0.0309(12) 0.0319(10) -0.0049(9) 0.0101(8) -0.0036(9)

C72A 0.0400(12) 0.0241(11) 0.0198(9) -0.0007(8) 0.0099(8) -0.0076(10)

O5A 0.0268(7) 0.0160(7) 0.0216(6) -0.0014(5) 0.0062(5) -0.0046(6)

O8A 0.0241(7) 0.0169(7) 0.0324(7) -0.0064(6) 0.0062(6) 0.0010(6)

O2A 0.0240(7) 0.0275(8) 0.0251(7) 0.0035(6) 0.0050(6) 0.0014(6)

O1A 0.0164(6) 0.0252(7) 0.0251(6) 0.0036(6) 0.0080(5) 0.0012(6)

N6A 0.0259(8) 0.0119(7) 0.0185(7) -0.0023(6) 0.0075(6) -0.0025(7)

N9A 0.0192(8) 0.0189(8) 0.0277(8) -0.0062(7) 0.0040(6) 0.0011(7)

N3A 0.0196(8) 0.0221(8) 0.0157(6) 0.0010(6) 0.0063(6) 0.0002(7)

N6B 0.0224(8) 0.0136(7) 0.0177(7) -0.0006(6) 0.0061(6) -0.0026(6)

N9B 0.0167(7) 0.0137(8) 0.0271(8) -0.0013(6) 0.0040(6) -0.0003(6)

N3B 0.0173(7) 0.0213(8) 0.0164(7) -0.0002(6) 0.0062(6) -0.0023(6)

O5B 0.0250(7) 0.0153(7) 0.0200(6) 0.0005(5) 0.0066(5) -0.0046(6)

O8B 0.0268(7) 0.0153(7) 0.0278(7) -0.0031(6) 0.0068(6) 0.0012(6)

O2B 0.0183(6) 0.0300(8) 0.0228(7) 0.0010(6) 0.0058(5) -0.0006(6)

O1B 0.0190(7) 0.0338(8) 0.0243(6) 0.0036(6) 0.0102(5) 0.0021(6)

C5B 0.0133(8) 0.0151(9) 0.0178(8) -0.0017(7) 0.0044(7) -0.0022(7)

C7B 0.0205(9) 0.0142(9) 0.0186(8) -0.0023(7) 0.0065(7) -0.0020(7)

C8B 0.0233(9) 0.0150(9) 0.0153(7) 0.0013(7) 0.0036(7) 0.0009(7)

C10B 0.0213(9) 0.0230(10) 0.0214(8) 0.0017(7) 0.0045(7) -0.0038(8)

C11B 0.0191(9) 0.0245(10) 0.0252(9) -0.0014(8) 0.0065(7) -0.0016(8)

C41B 0.0167(8) 0.0168(9) 0.0228(9) -0.0030(7) 0.0070(7) 0.0005(7)

C42B 0.0146(8) 0.0179(9) 0.0210(8) -0.0024(7) 0.0076(7) -0.0046(7)

C43B 0.0214(9) 0.0164(10) 0.0310(10) -0.0026(8) 0.0056(8) -0.0018(8)

C44B 0.0283(11) 0.0192(11) 0.0427(12) -0.0066(9) 0.0122(10) -0.0041(9)

C45B 0.0328(12) 0.0290(12) 0.0342(11) -0.0154(9) 0.0170(9) -0.0124(10)

C46B 0.0362(12) 0.0375(13) 0.0201(9) -0.0049(9) 0.0085(8) -0.0125(11)

C47B 0.0269(10) 0.0251(11) 0.0236(9) -0.0004(8) 0.0082(8) -0.0047(9)

C2B 0.0210(9) 0.0131(8) 0.0214(8) -0.0008(7) 0.0089(7) -0.0001(7)

C105 0.0195(9) 0.0373(12) 0.0306(10) -0.0025(9) 0.0135(8) -0.0025(9)

C106 0.0294(11) 0.0556(17) 0.0354(12) -0.0023(11) 0.0194(10) -0.0017(11)

C107 0.0584(18) 0.083(2) 0.0551(16) -0.0357(17) 0.0378(15) -0.0459(18)

C71B 0.0347(11) 0.0201(10) 0.0193(8) -0.0003(8) 0.0091(8) -0.0036(9)

C72B 0.0189(9) 0.0279(11) 0.0328(10) -0.0015(9) 0.0101(8) 0.0016(8)

C14B 0.0234(10) 0.0371(12) 0.0272(9) -0.0083(9) 0.0101(8) -0.0066(9)

C15B 0.0418(14) 0.0535(17) 0.0599(16) 0.0063(14) 0.0265(13) 0.0209(13)

O12B 0.0255(7) 0.0310(8) 0.0207(6) -0.0020(6) 0.0053(5) -0.0010(6)

O11B 0.0472(10) 0.0263(9) 0.0421(9) -0.0059(7) 0.0090(8) -0.0138(8)

C4B 0.0209(9) 0.0141(9) 0.0179(8) -0.0008(7) 0.0080(7) -0.0021(7)

C108 0.0388(14) 0.076(2) 0.0647(18) 0.0278(17) 0.0307(14) 0.0314(15)

C16B 0.0303(12) 0.0606(18) 0.0379(12) -0.0076(12) 0.0134(10) -0.0148(12)

C13B 0.0202(9) 0.0533(15) 0.0247(9) -0.0094(10) 0.0063(8) -0.0047(10)

_geom_special_details

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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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_geom_bond_atom_site_label_1

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_geom_bond_site_symmetry_2

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C4A N3A 1.446(2) . ?

C4A C5A 1.534(3) . ?

C4A C41A 1.540(3) . ?

C4A H4A 0.9800 . ?

C13A O12A 1.463(5) . ?

C13A H13A 0.9600 . ?

C13A H13B 0.9600 . ?

C13A H13C 0.9600 . ?

C16A C14A 1.514(4) . ?

C16A H16A 0.9600 . ?

C16A H16B 0.9600 . ?

C16A H16C 0.9600 . ?

O12A C11A 1.324(5) . ?

O11A C11A 1.192(5) . ?

C5A O5A 1.230(2) . ?

C5A N6A 1.347(2) . ?

C7A N6A 1.471(2) . ?

C7A C71A 1.523(3) . ?

C7A C8A 1.533(3) . ?

C7A C72A 1.536(3) . ?

C8A O8A 1.229(2) . ?

C8A N9A 1.339(2) . ?

C10A N9A 1.444(3) . ?

C10A C11A 1.506(3) . ?

C10A C14A 1.544(3) . ?

C10A H10V 0.9800 . ?

C41A C42A 1.509(3) . ?

C41A H41A 0.9700 . ?

C41A H41B 0.9700 . ?

C42A C43A 1.382(3) . ?

C42A C47A 1.389(3) . ?

C43A C44A 1.394(3) . ?

C43A H43A 0.9300 . ?

C44A C45A 1.371(4) . ?

C44A H44A 0.9300 . ?

C45A C46A 1.389(3) . ?

C45A H45A 0.9300 . ?

C46A C47A 1.377(3) . ?

C46A H46A 0.9300 . ?

C47A H47A 0.9300 . ?

C2A O2A 1.216(2) . ?

C2A O1A 1.346(2) . ?

C2A N3A 1.347(2) . ?

C101 O1A 1.478(2) . ?

C101 C102 1.511(3) . ?

C101 C104 1.520(3) . ?

C101 C103 1.522(3) . ?

C102 H10A 0.9600 . ?

C102 H10B 0.9600 . ?

C102 H10C 0.9600 . ?

C103 H10D 0.9600 . ?

C103 H10E 0.9600 . ?

C103 H10F 0.9600 . ?

C104 H10G 0.9600 . ?

C104 H10H 0.9600 . ?

C104 H10I 0.9600 . ?

C14A C15A 1.515(4) . ?

C14A H14A 0.9800 . ?

C15A H15A 0.9600 . ?

C15A H15B 0.9600 . ?

C15A H15C 0.9600 . ?

C71A H71A 0.9600 . ?

C71A H71B 0.9600 . ?

C71A H71C 0.9600 . ?

C72A H72A 0.9600 . ?

C72A H72B 0.9600 . ?

C72A H72C 0.9600 . ?

N6A H6A 0.8600 . ?

N9A H9A 0.8600 . ?

N3A H3A 0.8600 . ?

N6B C5B 1.344(2) . ?

N6B C7B 1.464(2) . ?

N6B H6B 0.8600 . ?

N9B C8B 1.347(2) . ?

N9B C10B 1.464(2) . ?

N9B H9B 0.8600 . ?

N3B C2B 1.350(2) . ?

N3B C4B 1.447(2) . ?

N3B H3B 0.8600 . ?

O5B C5B 1.231(2) . ?

O8B C8B 1.227(2) . ?

O2B C2B 1.210(2) . ?

O1B C2B 1.349(2) . ?

O1B C105 1.475(2) . ?

C5B C4B 1.534(2) . ?

C7B C72B 1.532(3) . ?

C7B C71B 1.535(3) . ?

C7B C8B 1.541(3) . ?

C10B C11B 1.516(3) . ?

C10B C14B 1.546(3) . ?

C10B H10W 0.9800 . ?

C11B O11B 1.200(3) . ?

C11B O12B 1.333(2) . ?

C41B C42B 1.509(3) . ?

C41B C4B 1.532(3) . ?

C41B H41C 0.9700 . ?

C41B H41D 0.9700 . ?

C42B C47B 1.386(3) . ?

C42B C43B 1.388(3) . ?

C43B C44B 1.383(3) . ?

C43B H43B 0.9300 . ?

C44B C45B 1.375(3) . ?

C44B H44B 0.9300 . ?

C45B C46B 1.387(4) . ?

C45B H45B 0.9300 . ?

C46B C47B 1.399(3) . ?

C46B H46B 0.9300 . ?

C47B H47B 0.9300 . ?

C105 C108 1.509(4) . ?

C105 C107 1.514(4) . ?

C105 C106 1.517(3) . ?

C106 H10J 0.9600 . ?

C106 H10K 0.9600 . ?

C106 H10L 0.9600 . ?

C107 H10M 0.9600 . ?

C107 H10N 0.9600 . ?

C107 H10O 0.9600 . ?

C71B H71D 0.9600 . ?

C71B H71E 0.9600 . ?

C71B H71F 0.9600 . ?

C72B H72D 0.9600 . ?

C72B H72E 0.9600 . ?

C72B H72F 0.9600 . ?

C14B C15B 1.512(4) . ?

C14B C16B 1.526(3) . ?

C14B H14B 0.9800 . ?

C15B H15D 0.9600 . ?

C15B H15E 0.9600 . ?

C15B H15F 0.9600 . ?

O12B C13B 1.440(2) . ?

C4B H4B 0.9800 . ?

C108 H10X 0.9600 . ?

C108 H10Y 0.9600 . ?

C108 H10Z 0.9600 . ?

C16B H16D 0.9600 . ?

C16B H16E 0.9600 . ?

C16B H16F 0.9600 . ?

C13B H13D 0.9600 . ?

C13B H13E 0.9600 . ?

C13B H13F 0.9600 . ?

loop_

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_geom_angle_atom_site_label_3

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N3A C4A C5A 112.52(15) . . ?

N3A C4A C41A 110.31(14) . . ?

C5A C4A C41A 107.44(14) . . ?

N3A C4A H4A 108.8 . . ?

C5A C4A H4A 108.8 . . ?

C41A C4A H4A 108.8 . . ?

O12A C13A H13A 109.5 . . ?

O12A C13A H13B 109.5 . . ?

H13A C13A H13B 109.5 . . ?

O12A C13A H13C 109.5 . . ?

H13A C13A H13C 109.5 . . ?

H13B C13A H13C 109.5 . . ?

C14A C16A H16A 109.5 . . ?

C14A C16A H16B 109.5 . . ?

H16A C16A H16B 109.5 . . ?

C14A C16A H16C 109.5 . . ?

H16A C16A H16C 109.5 . . ?

H16B C16A H16C 109.5 . . ?

C11A O12A C13A 116.1(4) . . ?

O5A C5A N6A 123.68(18) . . ?

O5A C5A C4A 122.60(16) . . ?

N6A C5A C4A 113.66(17) . . ?

N6A C7A C71A 110.11(16) . . ?

N6A C7A C8A 110.35(15) . . ?

C71A C7A C8A 110.03(17) . . ?

N6A C7A C72A 107.05(16) . . ?

C71A C7A C72A 111.07(17) . . ?

C8A C7A C72A 108.17(16) . . ?

O8A C8A N9A 121.34(19) . . ?

O8A C8A C7A 120.34(18) . . ?

N9A C8A C7A 118.17(17) . . ?

N9A C10A C11A 110.1(2) . . ?

N9A C10A C14A 112.00(17) . . ?

C11A C10A C14A 111.29(18) . . ?

N9A C10A H10V 107.7 . . ?

C11A C10A H10V 107.7 . . ?

C14A C10A H10V 107.7 . . ?

C42A C41A C4A 114.37(15) . . ?

C42A C41A H41A 108.7 . . ?

C4A C41A H41A 108.7 . . ?

C42A C41A H41B 108.7 . . ?

C4A C41A H41B 108.7 . . ?

H41A C41A H41B 107.6 . . ?

C43A C42A C47A 117.89(19) . . ?

C43A C42A C41A 121.05(18) . . ?

C47A C42A C41A 121.00(17) . . ?

C42A C43A C44A 120.9(2) . . ?

C42A C43A H43A 119.5 . . ?

C44A C43A H43A 119.5 . . ?

C45A C44A C43A 120.5(2) . . ?

C45A C44A H44A 119.8 . . ?

C43A C44A H44A 119.8 . . ?

C44A C45A C46A 119.1(2) . . ?

C44A C45A H45A 120.4 . . ?

C46A C45A H45A 120.4 . . ?

C47A C46A C45A 120.1(2) . . ?

C47A C46A H46A 119.9 . . ?

C45A C46A H46A 119.9 . . ?

C46A C47A C42A 121.4(2) . . ?

C46A C47A H47A 119.3 . . ?

C42A C47A H47A 119.3 . . ?

O2A C2A O1A 125.64(18) . . ?

O2A C2A N3A 123.97(17) . . ?

O1A C2A N3A 110.39(16) . . ?

O1A C101 C102 109.91(16) . . ?

O1A C101 C104 109.48(16) . . ?

C102 C101 C104 113.13(19) . . ?

O1A C101 C103 102.38(16) . . ?

C102 C101 C103 110.6(2) . . ?

C104 C101 C103 110.79(19) . . ?

C101 C102 H10A 109.5 . . ?

C101 C102 H10B 109.5 . . ?

H10A C102 H10B 109.5 . . ?

C101 C102 H10C 109.5 . . ?

H10A C102 H10C 109.5 . . ?

H10B C102 H10C 109.5 . . ?

C101 C103 H10D 109.5 . . ?

C101 C103 H10E 109.5 . . ?

H10D C103 H10E 109.5 . . ?

C101 C103 H10F 109.5 . . ?

H10D C103 H10F 109.5 . . ?

H10E C103 H10F 109.5 . . ?

C101 C104 H10G 109.5 . . ?

C101 C104 H10H 109.5 . . ?

H10G C104 H10H 109.5 . . ?

C101 C104 H10I 109.5 . . ?

H10G C104 H10I 109.5 . . ?

H10H C104 H10I 109.5 . . ?

O11A C11A O12A 124.4(3) . . ?

O11A C11A C10A 124.2(3) . . ?

O12A C11A C10A 111.4(3) . . ?

C16A C14A C15A 110.8(2) . . ?

C16A C14A C10A 112.0(2) . . ?

C15A C14A C10A 111.6(2) . . ?

C16A C14A H14A 107.4 . . ?

C15A C14A H14A 107.4 . . ?

C10A C14A H14A 107.4 . . ?

C14A C15A H15A 109.5 . . ?

C14A C15A H15B 109.5 . . ?

H15A C15A H15B 109.5 . . ?

C14A C15A H15C 109.5 . . ?

H15A C15A H15C 109.5 . . ?

H15B C15A H15C 109.5 . . ?

C7A C71A H71A 109.5 . . ?

C7A C71A H71B 109.5 . . ?

H71A C71A H71B 109.5 . . ?

C7A C71A H71C 109.5 . . ?

H71A C71A H71C 109.5 . . ?

H71B C71A H71C 109.5 . . ?

C7A C72A H72A 109.5 . . ?

C7A C72A H72B 109.5 . . ?

H72A C72A H72B 109.5 . . ?

C7A C72A H72C 109.5 . . ?

H72A C72A H72C 109.5 . . ?

H72B C72A H72C 109.5 . . ?

C2A O1A C101 120.11(15) . . ?

C5A N6A C7A 122.01(17) . . ?

C5A N6A H6A 119.0 . . ?

C7A N6A H6A 119.0 . . ?

C8A N9A C10A 119.91(18) . . ?

C8A N9A H9A 120.0 . . ?

C10A N9A H9A 120.0 . . ?

C2A N3A C4A 118.88(15) . . ?

C2A N3A H3A 120.6 . . ?

C4A N3A H3A 120.6 . . ?

C5B N6B C7B 122.30(16) . . ?

C5B N6B H6B 118.8 . . ?

C7B N6B H6B 118.8 . . ?

C8B N9B C10B 119.56(17) . . ?

C8B N9B H9B 120.2 . . ?

C10B N9B H9B 120.2 . . ?

C2B N3B C4B 118.78(15) . . ?

C2B N3B H3B 120.6 . . ?

C4B N3B H3B 120.6 . . ?

C2B O1B C105 121.03(15) . . ?

O5B C5B N6B 123.17(17) . . ?

O5B C5B C4B 123.07(16) . . ?

N6B C5B C4B 113.75(16) . . ?

N6B C7B C72B 110.02(15) . . ?

N6B C7B C71B 107.24(15) . . ?

C72B C7B C71B 110.78(16) . . ?

N6B C7B C8B 110.13(15) . . ?

C72B C7B C8B 109.74(16) . . ?

C71B C7B C8B 108.90(15) . . ?

O8B C8B N9B 121.84(19) . . ?

O8B C8B C7B 121.79(18) . . ?

N9B C8B C7B 116.26(17) . . ?

N9B C10B C11B 113.32(15) . . ?

N9B C10B C14B 109.29(18) . . ?

C11B C10B C14B 111.80(16) . . ?

N9B C10B H10W 107.4 . . ?

C11B C10B H10W 107.4 . . ?

C14B C10B H10W 107.4 . . ?

O11B C11B O12B 124.41(19) . . ?

O11B C11B C10B 122.44(19) . . ?

O12B C11B C10B 113.00(17) . . ?

C42B C41B C4B 113.87(15) . . ?

C42B C41B H41C 108.8 . . ?

C4B C41B H41C 108.8 . . ?

C42B C41B H41D 108.8 . . ?

C4B C41B H41D 108.8 . . ?

H41C C41B H41D 107.7 . . ?

C47B C42B C43B 118.96(19) . . ?

C47B C42B C41B 120.39(18) . . ?

C43B C42B C41B 120.45(17) . . ?

C44B C43B C42B 120.9(2) . . ?

C44B C43B H43B 119.5 . . ?

C42B C43B H43B 119.5 . . ?

C45B C44B C43B 120.3(2) . . ?

C45B C44B H44B 119.8 . . ?

C43B C44B H44B 119.8 . . ?

C44B C45B C46B 119.5(2) . . ?

C44B C45B H45B 120.2 . . ?

C46B C45B H45B 120.2 . . ?

C45B C46B C47B 120.3(2) . . ?

C45B C46B H46B 119.9 . . ?

C47B C46B H46B 119.9 . . ?

C42B C47B C46B 120.0(2) . . ?

C42B C47B H47B 120.0 . . ?

C46B C47B H47B 120.0 . . ?

O2B C2B O1B 126.28(17) . . ?

O2B C2B N3B 123.94(16) . . ?

O1B C2B N3B 109.75(15) . . ?

O1B C105 C108 110.81(19) . . ?

O1B C105 C107 108.7(2) . . ?

C108 C105 C107 113.1(2) . . ?

O1B C105 C106 102.39(16) . . ?

C108 C105 C106 110.9(2) . . ?

C107 C105 C106 110.5(2) . . ?

C105 C106 H10J 109.5 . . ?

C105 C106 H10K 109.5 . . ?

H10J C106 H10K 109.5 . . ?

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H15E C15B H15F 109.5 . . ?

C11B O12B C13B 114.92(17) . . ?

N3B C4B C41B 110.16(15) . . ?

N3B C4B C5B 111.57(15) . . ?

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C5B C4B H4B 108.6 . . ?

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C14B C16B H16E 109.5 . . ?

H16D C16B H16E 109.5 . . ?

C14B C16B H16F 109.5 . . ?

H16D C16B H16F 109.5 . . ?

H16E C16B H16F 109.5 . . ?

O12B C13B H13D 109.5 . . ?

O12B C13B H13E 109.5 . . ?

H13D C13B H13E 109.5 . . ?

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C71A C7A C8A O8A 25.2(2) . . . . ?

C72A C7A C8A O8A -96.3(2) . . . . ?

N6A C7A C8A N9A -37.6(2) . . . . ?

C71A C7A C8A N9A -159.28(16) . . . . ?

C72A C7A C8A N9A 79.2(2) . . . . ?

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C5A C4A C41A C42A -167.61(15) . . . . ?

C4A C41A C42A C43A -128.44(19) . . . . ?

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C47A C42A C43A C44A 1.3(3) . . . . ?

C41A C42A C43A C44A -175.92(19) . . . . ?

C42A C43A C44A C45A -0.7(3) . . . . ?

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C41A C42A C47A C46A 176.59(19) . . . . ?

C13A O12A C11A O11A -2.2(5) . . . . ?

C13A O12A C11A C10A 175.8(3) . . . . ?

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C14A C10A C11A O12A -72.4(3) . . . . ?

N9A C10A C14A C16A -155.3(2) . . . . ?

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N9A C10A C14A C15A 79.8(3) . . . . ?

C11A C10A C14A C15A -44.0(3) . . . . ?

O2A C2A O1A C101 4.6(3) . . . . ?

N3A C2A O1A C101 -175.50(16) . . . . ?

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C104 C101 O1A C2A 60.1(2) . . . . ?

C103 C101 O1A C2A 177.65(18) . . . . ?

O5A C5A N6A C7A 18.2(3) . . . . ?

C4A C5A N6A C7A -158.87(16) . . . . ?

C71A C7A N6A C5A 61.6(2) . . . . ?

C8A C7A N6A C5A -60.0(2) . . . . ?

C72A C7A N6A C5A -177.54(17) . . . . ?

O8A C8A N9A C10A -7.2(3) . . . . ?

C7A C8A N9A C10A 177.25(17) . . . . ?

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O2A C2A N3A C4A 3.8(3) . . . . ?

O1A C2A N3A C4A -176.16(16) . . . . ?

C5A C4A N3A C2A 66.8(2) . . . . ?

C41A C4A N3A C2A -173.29(17) . . . . ?

C7B N6B C5B O5B -11.5(3) . . . . ?

C7B N6B C5B C4B 167.48(16) . . . . ?

C5B N6B C7B C72B -66.5(2) . . . . ?

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N6B C7B C8B O8B -145.82(17) . . . . ?

C72B C7B C8B O8B -24.6(2) . . . . ?

C71B C7B C8B O8B 96.9(2) . . . . ?

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C71B C7B C8B N9B -79.5(2) . . . . ?

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C8B N9B C10B C14B 171.54(16) . . . . ?

N9B C10B C11B O11B 146.5(2) . . . . ?

C14B C10B C11B O11B -89.4(3) . . . . ?

N9B C10B C11B O12B -37.8(2) . . . . ?

C14B C10B C11B O12B 86.3(2) . . . . ?

C4B C41B C42B C47B 133.81(18) . . . . ?

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C41B C42B C43B C44B -174.26(18) . . . . ?

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C4B N3B C2B O2B 1.9(3) . . . . ?

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N9B C10B C14B C15B 66.3(2) . . . . ?

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C2B N3B C4B C5B -61.3(2) . . . . ?

C42B C41B C4B N3B -69.0(2) . . . . ?

C42B C41B C4B C5B 168.06(15) . . . . ?

O5B C5B C4B N3B -36.3(2) . . . . ?

N6B C5B C4B N3B 144.68(16) . . . . ?

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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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C2 C 0.52108(16) 0.6442(3) -0.09216(14) 0.0448(7) Uani 1 1 d . . .

O2 O 0.57621(12) 0.6781(2) -0.11278(10) 0.0672(7) Uani 1 1 d . . .

N3 N 0.50689(12) 0.6472(2) -0.03535(11) 0.0455(6) Uani 1 1 d . . .

H3 H 0.4663 0.6264 -0.0229 0.055 Uiso 1 1 calc R . .

C4 C 0.56015(18) 0.6854(3) 0.00361(15) 0.0611(9) Uani 1 1 d . . .

H4 H 0.5767 0.7661 -0.0094 0.073 Uiso 1 1 calc R . .

C5 C 0.62252(15) 0.5992(3) 0.00280(13) 0.0425(7) Uani 1 1 d . . .

C41 C 0.5313(2) 0.7028(4) 0.0609(2) 0.0918(14) Uani 1 1 d . . .

H41A H 0.5696 0.7065 0.0880 0.110 Uiso 1 1 calc R . .

H41B H 0.5033 0.6312 0.0705 0.110 Uiso 1 1 calc R . .

C42 C 0.4853(2) 0.8203(3) 0.06868(17) 0.0669(10) Uani 1 1 d . . .

H42 H 0.4546 0.8264 0.0353 0.080 Uiso 1 1 calc R . .

C43 C 0.4408(3) 0.7845(5) 0.1188(2) 0.1241(19) Uani 1 1 d . . .

H43A H 0.4701 0.7693 0.1514 0.186 Uiso 1 1 calc R . .

H43B H 0.4151 0.7112 0.1097 0.186 Uiso 1 1 calc R . .

H43C H 0.4089 0.8500 0.1274 0.186 Uiso 1 1 calc R . .

C44 C 0.5198(3) 0.9455(5) 0.0769(3) 0.1246(19) Uani 1 1 d . . .

H44A H 0.4844 1.0076 0.0806 0.187 Uiso 1 1 calc R . .

H44B H 0.5486 0.9637 0.0444 0.187 Uiso 1 1 calc R . .

H44C H 0.5480 0.9440 0.1108 0.187 Uiso 1 1 calc R . .

O5 O 0.61673(11) 0.4856(2) -0.00273(10) 0.0551(6) Uani 1 1 d . . .

N6 N 0.68496(12) 0.6537(2) 0.00878(10) 0.0444(6) Uani 1 1 d . . .

H6 H 0.6869 0.7326 0.0063 0.053 Uiso 1 1 calc R . .

C7 C 0.75002(15) 0.5868(3) 0.01934(13) 0.0442(7) Uani 1 1 d . . .

C71 C 0.80802(18) 0.6826(3) 0.02438(17) 0.0673(10) Uani 1 1 d . . .

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H71B H 0.8523 0.6417 0.0277 0.101 Uiso 1 1 calc R . .

H71C H 0.8002 0.7325 0.0576 0.101 Uiso 1 1 calc R . .

C72 C 0.7447(2) 0.5145(4) 0.07619(16) 0.0682(10) Uani 1 1 d . . .

H72A H 0.7399 0.5713 0.1074 0.102 Uiso 1 1 calc R . .

H72B H 0.7861 0.4660 0.0814 0.102 Uiso 1 1 calc R . .

H72C H 0.7047 0.4613 0.0750 0.102 Uiso 1 1 calc R . .

C8 C 0.76858(16) 0.5025(3) -0.03004(13) 0.0432(7) Uani 1 1 d . . .

O8 O 0.80889(13) 0.4159(2) -0.02105(10) 0.0657(7) Uani 1 1 d . . .

N9 N 0.74280(13) 0.5273(2) -0.08223(11) 0.0490(7) Uani 1 1 d . . .

H9 H 0.7160 0.5906 -0.0849 0.059 Uiso 1 1 calc R . .

C10 C 0.75490(15) 0.4614(3) -0.13287(13) 0.0452(8) Uani 1 1 d . . .

C11 C 0.7075(2) 0.4753(4) -0.17756(17) 0.0704(10) Uani 1 1 d . . .

H11 H 0.6700 0.5290 -0.1732 0.085 Uiso 1 1 calc R . .

C12 C 0.7146(2) 0.4134(4) -0.22663(18) 0.0703(10) Uani 1 1 d . . .

H12 H 0.6815 0.4224 -0.2554 0.084 Uiso 1 1 calc R . .

C13 C 0.7708(2) 0.3362(3) -0.23451(16) 0.0633(10) Uani 1 1 d . . .

C14 C 0.81867(19) 0.3234(3) -0.19159(16) 0.0636(10) Uani 1 1 d . . .

H14 H 0.8568 0.2716 -0.1966 0.076 Uiso 1 1 calc R . .

C15 C 0.81099(17) 0.3858(3) -0.14147(15) 0.0561(9) Uani 1 1 d . . .

H15 H 0.8443 0.3768 -0.1128 0.067 Uiso 1 1 calc R . .

N17 N 0.7798(2) 0.2661(4) -0.28724(17) 0.0816(10) Uani 1 1 d . . .

O19 O 0.8301(3) 0.2073(4) -0.29377(18) 0.1332(14) Uani 1 1 d . . .

O18 O 0.7351(2) 0.2717(3) -0.32317(17) 0.1160(12) Uani 1 1 d . . .

C21 C 0.46135(17) 0.6149(3) -0.18354(14) 0.0526(8) Uani 1 1 d . . .

C22 C 0.5189(2) 0.5479(4) -0.21346(19) 0.0883(13) Uani 1 1 d . . .

H22A H 0.5605 0.5973 -0.2130 0.132 Uiso 1 1 calc R . .

H22B H 0.5055 0.5321 -0.2523 0.132 Uiso 1 1 calc R . .

H22C H 0.5277 0.4712 -0.1943 0.132 Uiso 1 1 calc R . .

C23 C 0.4582(3) 0.7501(4) -0.1961(2) 0.0963(14) Uani 1 1 d . . .

H23A H 0.4159 0.7838 -0.1807 0.145 Uiso 1 1 calc R . .

H23B H 0.4591 0.7627 -0.2367 0.145 Uiso 1 1 calc R . .

H23C H 0.4977 0.7904 -0.1791 0.145 Uiso 1 1 calc R . .

C24 C 0.3914(2) 0.5548(4) -0.19491(19) 0.0913(14) Uani 1 1 d . . .

H24A H 0.3948 0.4679 -0.1880 0.137 Uiso 1 1 calc R . .

H24B H 0.3781 0.5688 -0.2339 0.137 Uiso 1 1 calc R . .

H24C H 0.3568 0.5897 -0.1700 0.137 Uiso 1 1 calc R . .

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C2 0.0463(17) 0.0355(16) 0.0525(19) 0.0012(14) 0.0030(16) -0.0070(14)

O2 0.0603(15) 0.0724(17) 0.0690(16) 0.0025(12) 0.0070(13) -0.0136(13)

N3 0.0394(14) 0.0444(15) 0.0526(16) -0.0050(12) 0.0003(12) -0.0036(12)

C4 0.055(2) 0.063(2) 0.065(2) -0.0171(18) -0.0007(18) 0.0016(17)

C5 0.0390(17) 0.0417(18) 0.0469(18) -0.0079(14) 0.0036(14) -0.0034(13)

C41 0.087(3) 0.098(4) 0.091(3) 0.006(3) -0.005(3) 0.005(3)

C42 0.064(2) 0.067(3) 0.071(3) -0.0147(19) 0.002(2) 0.016(2)

C43 0.144(5) 0.110(4) 0.118(4) 0.010(3) 0.003(4) 0.010(4)

C44 0.145(5) 0.108(4) 0.121(5) -0.008(3) 0.014(4) -0.014(4)

O5 0.0502(13) 0.0484(14) 0.0667(15) -0.0056(11) 0.0061(11) -0.0041(10)

N6 0.0423(14) 0.0376(13) 0.0534(16) -0.0047(11) 0.0024(12) -0.0014(11)

C7 0.0391(16) 0.0390(17) 0.0546(18) -0.0014(14) 0.0005(14) -0.0024(13)

C71 0.059(2) 0.058(2) 0.085(3) -0.0012(19) -0.004(2) -0.0015(18)

C72 0.076(2) 0.058(2) 0.070(2) -0.0017(18) 0.009(2) 0.0020(19)

C8 0.0429(17) 0.0360(16) 0.0507(19) 0.0042(13) 0.0068(15) 0.0023(14)

O8 0.0778(17) 0.0555(14) 0.0639(15) 0.0022(11) 0.0036(13) 0.0191(13)

N9 0.0455(15) 0.0477(16) 0.0537(16) 0.0048(13) 0.0044(13) 0.0081(12)

C10 0.0412(17) 0.0428(17) 0.0515(19) 0.0091(14) 0.0018(15) 0.0019(14)

C11 0.065(2) 0.075(3) 0.072(3) 0.005(2) 0.001(2) 0.006(2)

C12 0.062(2) 0.077(3) 0.072(3) 0.001(2) -0.006(2) -0.001(2)

C13 0.069(2) 0.061(2) 0.060(2) 0.0043(18) -0.0009(19) -0.0088(19)

C14 0.064(2) 0.060(2) 0.066(2) 0.0010(18) 0.000(2) 0.0044(18)

C15 0.0519(19) 0.062(2) 0.054(2) 0.0027(17) 0.0009(16) 0.0081(17)

N17 0.087(3) 0.084(3) 0.073(3) 0.004(2) 0.002(2) -0.005(2)

O19 0.148(3) 0.139(4) 0.112(3) -0.017(3) 0.002(3) 0.010(3)

O18 0.131(3) 0.113(3) 0.104(3) 0.000(2) -0.001(2) -0.010(2)

C21 0.054(2) 0.049(2) 0.054(2) 0.0048(15) -0.0026(16) 0.0005(15)

C22 0.093(3) 0.091(3) 0.080(3) 0.003(2) -0.004(3) 0.001(3)

C23 0.105(3) 0.087(3) 0.097(3) 0.015(3) -0.007(3) 0.006(3)

C24 0.098(3) 0.095(3) 0.081(3) -0.002(2) -0.009(3) -0.014(3)

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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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O1 C21 1.481(4) . ?

C2 O2 1.218(3) . ?

C2 N3 1.357(4) . ?

N3 C4 1.429(4) . ?

N3 H3 0.8600 . ?

C4 C41 1.463(5) . ?

C4 C5 1.518(4) . ?

C4 H4 0.9800 . ?

C5 O5 1.245(3) . ?

C5 N6 1.342(3) . ?

C41 C42 1.561(5) . ?

C41 H41A 0.9700 . ?

C41 H41B 0.9700 . ?

C42 C43 1.501(6) . ?

C42 C44 1.523(6) . ?

C42 H42 0.9800 . ?

C43 H43A 0.9600 . ?

C43 H43B 0.9600 . ?

C43 H43C 0.9600 . ?

C44 H44A 0.9600 . ?

C44 H44B 0.9600 . ?

C44 H44C 0.9600 . ?

N6 C7 1.463(4) . ?

N6 H6 0.8600 . ?

C7 C8 1.516(4) . ?

C7 C71 1.526(4) . ?

C7 C72 1.548(5) . ?

C71 H71A 0.9600 . ?

C71 H71B 0.9600 . ?

C71 H71C 0.9600 . ?

C72 H72A 0.9600 . ?

C72 H72B 0.9600 . ?

C72 H72C 0.9600 . ?

C8 O8 1.235(3) . ?

C8 N9 1.344(4) . ?

N9 C10 1.404(4) . ?

N9 H9 0.8600 . ?

C10 C15 1.367(4) . ?

C10 C11 1.393(5) . ?

C11 C12 1.337(5) . ?

C11 H11 0.9300 . ?

C12 C13 1.377(5) . ?

C12 H12 0.9300 . ?

C13 C14 1.366(5) . ?

C13 N17 1.460(5) . ?

C14 C15 1.362(5) . ?

C14 H14 0.9300 . ?

C15 H15 0.9300 . ?

N17 O19 1.165(5) . ?

N17 O18 1.202(4) . ?

C21 C22 1.495(5) . ?

C21 C23 1.499(5) . ?

C21 C24 1.514(5) . ?

C22 H22A 0.9600 . ?

C22 H22B 0.9600 . ?

C22 H22C 0.9600 . ?

C23 H23A 0.9600 . ?

C23 H23B 0.9600 . ?

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O2 C2 O1 126.1(3) . . ?

O2 C2 N3 123.7(3) . . ?

O1 C2 N3 110.2(3) . . ?

C2 N3 C4 119.3(3) . . ?

C2 N3 H3 120.4 . . ?

C4 N3 H3 120.4 . . ?

N3 C4 C41 110.6(3) . . ?

N3 C4 C5 112.0(3) . . ?

C41 C4 C5 112.9(3) . . ?

N3 C4 H4 107.0 . . ?

C41 C4 H4 107.0 . . ?

C5 C4 H4 107.0 . . ?

O5 C5 N6 121.8(3) . . ?

O5 C5 C4 122.8(3) . . ?

N6 C5 C4 115.3(3) . . ?

C4 C41 C42 115.2(4) . . ?

C4 C41 H41A 108.5 . . ?

C42 C41 H41A 108.5 . . ?

C4 C41 H41B 108.5 . . ?

C42 C41 H41B 108.5 . . ?

H41A C41 H41B 107.5 . . ?

C43 C42 C44 112.3(4) . . ?

C43 C42 C41 101.5(4) . . ?

C44 C42 C41 120.0(4) . . ?

C43 C42 H42 107.5 . . ?

C44 C42 H42 107.5 . . ?

C41 C42 H42 107.5 . . ?

C42 C43 H43A 109.5 . . ?

C42 C43 H43B 109.5 . . ?

H43A C43 H43B 109.5 . . ?

C42 C43 H43C 109.5 . . ?

H43A C43 H43C 109.5 . . ?

H43B C43 H43C 109.5 . . ?

C42 C44 H44A 109.5 . . ?

C42 C44 H44B 109.5 . . ?

H44A C44 H44B 109.5 . . ?

C42 C44 H44C 109.5 . . ?

H44A C44 H44C 109.5 . . ?

H44B C44 H44C 109.5 . . ?

C5 N6 C7 123.9(2) . . ?

C5 N6 H6 118.1 . . ?

C7 N6 H6 118.1 . . ?

N6 C7 C8 111.8(2) . . ?

N6 C7 C71 107.1(2) . . ?

C8 C7 C71 107.4(3) . . ?

N6 C7 C72 109.9(3) . . ?

C8 C7 C72 111.3(3) . . ?

C71 C7 C72 109.1(3) . . ?

C7 C71 H71A 109.5 . . ?

C7 C71 H71B 109.5 . . ?

H71A C71 H71B 109.5 . . ?

C7 C71 H71C 109.5 . . ?

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H71B C71 H71C 109.5 . . ?

C7 C72 H72A 109.5 . . ?

C7 C72 H72B 109.5 . . ?

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C7 C72 H72C 109.5 . . ?

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H72B C72 H72C 109.5 . . ?

O8 C8 N9 122.5(3) . . ?

O8 C8 C7 118.5(3) . . ?

N9 C8 C7 119.0(3) . . ?

C8 N9 C10 127.1(3) . . ?

C8 N9 H9 116.4 . . ?

C10 N9 H9 116.4 . . ?

C15 C10 C11 117.9(3) . . ?

C15 C10 N9 124.1(3) . . ?

C11 C10 N9 118.1(3) . . ?

C12 C11 C10 121.5(4) . . ?

C12 C11 H11 119.2 . . ?

C10 C11 H11 119.2 . . ?

C11 C12 C13 120.1(4) . . ?

C11 C12 H12 120.0 . . ?

C13 C12 H12 120.0 . . ?

C14 C13 C12 119.2(4) . . ?

C14 C13 N17 119.3(4) . . ?

C12 C13 N17 121.5(4) . . ?

C15 C14 C13 120.7(4) . . ?

C15 C14 H14 119.7 . . ?

C13 C14 H14 119.7 . . ?

C14 C15 C10 120.7(3) . . ?

C14 C15 H15 119.7 . . ?

C10 C15 H15 119.7 . . ?

O19 N17 O18 121.7(5) . . ?

O19 N17 C13 119.6(5) . . ?

O18 N17 C13 118.7(4) . . ?

O1 C21 C22 111.2(3) . . ?

O1 C21 C23 107.7(3) . . ?

C22 C21 C23 114.5(3) . . ?

O1 C21 C24 100.9(3) . . ?

C22 C21 C24 111.1(3) . . ?

C23 C21 C24 110.6(3) . . ?

C21 C22 H22A 109.5 . . ?

C21 C22 H22B 109.5 . . ?

H22A C22 H22B 109.5 . . ?

C21 C22 H22C 109.5 . . ?

H22A C22 H22C 109.5 . . ?

H22B C22 H22C 109.5 . . ?

C21 C23 H23A 109.5 . . ?

C21 C23 H23B 109.5 . . ?

H23A C23 H23B 109.5 . . ?

C21 C23 H23C 109.5 . . ?

H23A C23 H23C 109.5 . . ?

H23B C23 H23C 109.5 . . ?

C21 C24 H24A 109.5 . . ?

C21 C24 H24B 109.5 . . ?

H24A C24 H24B 109.5 . . ?

C21 C24 H24C 109.5 . . ?

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C21 O1 C2 N3 165.0(2) . . . . ?

O2 C2 N3 C4 -3.7(5) . . . . ?

O1 C2 N3 C4 176.6(3) . . . . ?

C2 N3 C4 C41 170.2(3) . . . . ?

C2 N3 C4 C5 -62.9(4) . . . . ?

N3 C4 C5 O5 -37.2(4) . . . . ?

C41 C4 C5 O5 88.4(4) . . . . ?

N3 C4 C5 N6 143.1(3) . . . . ?

C41 C4 C5 N6 -91.3(4) . . . . ?

N3 C4 C41 C42 -73.5(4) . . . . ?

C5 C4 C41 C42 160.1(3) . . . . ?

C4 C41 C42 C43 156.4(4) . . . . ?

C4 C41 C42 C44 -79.3(5) . . . . ?

O5 C5 N6 C7 -11.0(4) . . . . ?

C4 C5 N6 C7 168.7(3) . . . . ?

C5 N6 C7 C8 63.5(4) . . . . ?

C5 N6 C7 C71 -179.0(3) . . . . ?

C5 N6 C7 C72 -60.6(4) . . . . ?

N6 C7 C8 O8 -159.1(3) . . . . ?

C71 C7 C8 O8 83.7(3) . . . . ?

C72 C7 C8 O8 -35.7(4) . . . . ?

N6 C7 C8 N9 23.4(4) . . . . ?

C71 C7 C8 N9 -93.8(3) . . . . ?

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O8 C8 N9 C10 1.6(5) . . . . ?

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C8 N9 C10 C15 -21.7(5) . . . . ?

C8 N9 C10 C11 159.5(3) . . . . ?

C15 C10 C11 C12 2.6(5) . . . . ?

N9 C10 C11 C12 -178.4(3) . . . . ?

C10 C11 C12 C13 -1.8(6) . . . . ?

C11 C12 C13 C14 0.4(6) . . . . ?

C11 C12 C13 N17 179.3(4) . . . . ?

C12 C13 C14 C15 0.1(5) . . . . ?

N17 C13 C14 C15 -178.7(3) . . . . ?

C13 C14 C15 C10 0.7(5) . . . . ?

C11 C10 C15 C14 -2.0(5) . . . . ?

N9 C10 C15 C14 179.1(3) . . . . ?

C14 C13 N17 O19 -5.7(6) . . . . ?

C12 C13 N17 O19 175.5(4) . . . . ?

C14 C13 N17 O18 175.1(4) . . . . ?

C12 C13 N17 O18 -3.8(6) . . . . ?

C2 O1 C21 C22 63.8(4) . . . . ?

C2 O1 C21 C23 -62.3(4) . . . . ?

C2 O1 C21 C24 -178.3(3) . . . . ?

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Peptide III

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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
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factors based on ALL data will be even larger.
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C2 C 0.90232(8) 0.64205(17) 0.8239(4) 0.0253(5) Uani 1 1 d . . .
N3 N 0.93961(6) 0.68518(14) 0.9181(3) 0.0257(4) Uani 1 1 d . . .
C4 C 0.94353(8) 0.79547(16) 0.9388(4) 0.0237(5) Uani 1 1 d . . .
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C5 C 0.93151(7) 0.84889(16) 0.7124(4) 0.0223(5) Uani 1 1 d . . .
C7 C 0.89059(7) 0.99775(16) 0.5434(4) 0.0219(5) Uani 1 1 d . . .
C8 C 0.86240(7) 0.94494(16) 0.3517(4) 0.0196(4) Uani 1 1 d . . .
C10 C 0.80795(7) 0.80326(16) 0.2755(4) 0.0227(5) Uani 1 1 d . . .
C11 C 0.79409(8) 0.70894(18) 0.3586(5) 0.0317(6) Uani 1 1 d . . .
H11 H 0.8076 0.6832 0.4919 0.038 Uiso 1 1 calc R . .
C12 C 0.76067(9) 0.65308(18) 0.2467(5) 0.0403(7) Uani 1 1 d . . .
H12 H 0.7522 0.5898 0.3046 0.048 Uiso 1 1 calc R . .
C13 C 0.73961(8) 0.68947(18) 0.0505(5) 0.0336(6) Uani 1 1 d . . .
H13 H 0.7168 0.6524 -0.0251 0.040 Uiso 1 1 calc R . .
C14 C 0.75376(8) 0.78320(16) -0.0295(4) 0.0252(5) Uani 1 1 d . . .
C15 C 0.78747(7) 0.84170(17) 0.0762(4) 0.0237(5) Uani 1 1 d . . .
H15 H 0.7961 0.9044 0.0162 0.028 Uiso 1 1 calc R . .
C31 C 0.98069(8) 0.63105(18) 1.0049(4) 0.0297(6) Uani 1 1 d . . .
H31 H 0.9887 0.5631 0.9859 0.036 Uiso 1 1 calc R . .
C32 C 1.00659(9) 0.71383(18) 1.1330(4) 0.0314(6) Uani 1 1 d . . .
H32 H 1.0254 0.7071 1.2622 0.038 Uiso 1 1 calc R . .

C33 C 0.99475(8) 0.81009(18) 1.0018(4) 0.0324(6) Uani 1 1 d . . .
H33 H 1.0139 0.8649 0.9676 0.039 Uiso 1 1 calc R . .
C71 C 0.93315(9) 1.04689(19) 0.4357(4) 0.0363(6) Uani 1 1 d . . .
H71A H 0.9523 0.9953 0.3679 0.054 Uiso 1 1 calc R . .
H71B H 0.9503 1.0822 0.5528 0.054 Uiso 1 1 calc R . .
H71C H 0.9237 1.0941 0.3186 0.054 Uiso 1 1 calc R . .
C72 C 0.85859(9) 1.07872(17) 0.6440(4) 0.0325(6) Uani 1 1 d . . .
H72A H 0.8750 1.1175 0.7578 0.049 Uiso 1 1 calc R . .
H72B H 0.8324 1.0465 0.7147 0.049 Uiso 1 1 calc R . .
H72C H 0.8482 1.1230 0.5229 0.049 Uiso 1 1 calc R . .
C100 C 0.87307(9) 0.47545(17) 0.6975(4) 0.0342(6) Uani 1 1 d . . .
C101 C 0.87706(9) 0.4993(2) 0.4403(5) 0.0411(6) Uani 1 1 d . . .
H10A H 0.9081 0.4860 0.3893 0.062 Uiso 1 1 calc R . .
H10B H 0.8697 0.5696 0.4144 0.062 Uiso 1 1 calc R . .
H10C H 0.8559 0.4573 0.3554 0.062 Uiso 1 1 calc R . .
C102 C 0.82434(9) 0.4888(2) 0.7918(4) 0.0409(7) Uani 1 1 d . . .
H10D H 0.8134 0.5558 0.7561 0.061 Uiso 1 1 calc R . .
H10E H 0.8246 0.4795 0.9561 0.061 Uiso 1 1 calc R . .
H10F H 0.8042 0.4394 0.7225 0.061 Uiso 1 1 calc R . .
C103 C 0.89011(11) 0.36901(19) 0.7503(6) 0.0587(9) Uani 1 1 d . . .
H10G H 0.8919 0.3599 0.9145 0.088 Uiso 1 1 calc R . .
H10H H 0.9202 0.3595 0.6836 0.088 Uiso 1 1 calc R . .
H10I H 0.8690 0.3202 0.6863 0.088 Uiso 1 1 calc R . .
O1 O 0.90663(6) 0.53979(11) 0.8232(3) 0.0351(4) Uani 1 1 d . . .
O2 O 0.86912(5) 0.69001(12) 0.7539(3) 0.0307(4) Uani 1 1 d . . .
O5 O 0.94814(6) 0.82233(13) 0.5274(3) 0.0333(4) Uani 1 1 d . . .
O8 O 0.85769(5) 0.98769(12) 0.1650(3) 0.0277(4) Uani 1 1 d . . .
O17 O 0.69693(7) 0.78089(14) -0.3109(4) 0.0510(6) Uani 1 1 d . . .
O18 O 0.74681(6) 0.90297(13) -0.3205(3) 0.0389(5) Uani 1 1 d . . .
N6 N 0.90275(6) 0.92896(13) 0.7322(3) 0.0216(4) Uani 1 1 d . . .
H6 H 0.8907 0.9404 0.8654 0.026 Uiso 1 1 calc R . .
N9 N 0.84138(6) 0.85612(14) 0.4069(3) 0.0230(4) Uani 1 1 d . . .
H9 H 0.8492 0.8289 0.5361 0.028 Uiso 1 1 calc R . .
N16 N 0.73086(7) 0.82512(15) -0.2346(4) 0.0305(5) Uani 1 1 d . . .

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N3 0.0217(10) 0.0244(10) 0.0309(10) 0.0004(9) -0.0066(9) 0.0026(8)
C4 0.0229(12) 0.0228(11) 0.0253(11) -0.0032(10) 0.0003(10) 0.0033(9)

C5 0.0209(11) 0.0248(11) 0.0210(11) -0.0048(9) 0.0011(9) -0.0031(9)
C7 0.0270(12) 0.0192(10) 0.0195(10) 0.0009(9) -0.0012(9) -0.0021(10)
C8 0.0183(11) 0.0215(11) 0.0190(10) -0.0014(9) 0.0025(9) 0.0005(9)
C10 0.0155(10) 0.0235(11) 0.0289(12) 0.0008(10) 0.0007(9) 0.0024(9)
C11 0.0261(13) 0.0307(13) 0.0383(13) 0.0093(11) -0.0094(11) -0.0026(10)
C12 0.0349(14) 0.0235(12) 0.0624(18) 0.0111(13) -0.0100(14) -0.0082(11)
C13 0.0296(13) 0.0255(12) 0.0455(15) -0.0018(12) -0.0120(12) -0.0023(11)
C14 0.0218(12) 0.0249(11) 0.0289(12) -0.0044(10) -0.0050(10) 0.0062(10)
C15 0.0214(11) 0.0210(11) 0.0286(12) 0.0013(10) 0.0022(10) -0.0001(9)
C31 0.0235(12) 0.0221(11) 0.0435(15) -0.0050(11) -0.0118(11) 0.0100(10)
C32 0.0312(14) 0.0320(13) 0.0309(13) -0.0059(11) -0.0124(11) 0.0067(11)
C33 0.0239(12) 0.0275(12) 0.0459(15) 0.0014(12) -0.0104(12) -0.0040(10)
C71 0.0369(15) 0.0391(14) 0.0327(13) 0.0052(12) -0.0043(12) -0.0159(12)
C72 0.0508(16) 0.0228(12) 0.0241(12) 0.0003(10) -0.0064(11) 0.0070(12)
C100 0.0389(15) 0.0233(13) 0.0403(15) -0.0004(11) -0.0193(12) -0.0054(10)
C101 0.0403(16) 0.0425(15) 0.0404(15) -0.0080(14) -0.0035(13) -0.0026(13)
C102 0.0458(16) 0.0441(16) 0.0329(14) 0.0117(13) -0.0088(12) -0.0185(13)
C103 0.073(2) 0.0238(14) 0.079(2) 0.0053(15) -0.038(2) -0.0056(14)
O1 0.0365(10) 0.0248(8) 0.0441(10) 0.0004(8) -0.0183(9) -0.0030(8)
O2 0.0264(8) 0.0283(9) 0.0374(9) 0.0052(8) -0.0096(8) 0.0013(7)
O5 0.0365(10) 0.0378(10) 0.0254(8) -0.0051(8) 0.0059(8) 0.0059(8)
O8 0.0345(9) 0.0288(8) 0.0199(7) 0.0023(7) -0.0018(7) -0.0041(7)
O17 0.0483(12) 0.0444(11) 0.0602(14) -0.0009(10) -0.0301(11) -0.0038(10)
O18 0.0500(12) 0.0305(9) 0.0362(10) 0.0011(8) -0.0118(9) 0.0003(9)
N6 0.0240(9) 0.0247(9) 0.0160(9) 0.0007(8) 0.0003(8) 0.0008(8)
N9 0.0236(10) 0.0221(9) 0.0232(9) 0.0051(8) -0.0043(8) -0.0028(8)
N16 0.0295(11) 0.0278(11) 0.0342(11) -0.0061(10) -0.0078(10) 0.0050(9)

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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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C2 N3 1.335(3) . ?

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N3 C4 1.461(3) . ?
N3 C31 1.474(3) . ?
C4 C5 1.528(3) . ?
C4 C33 1.538(3) . ?
C5 O5 1.226(3) . ?
C5 N6 1.347(3) . ?
C7 N6 1.463(3) . ?
C7 C71 1.524(3) . ?
C7 C72 1.527(3) . ?
C7 C8 1.543(3) . ?
C8 O8 1.227(3) . ?
C8 N9 1.356(3) . ?
C10 C11 1.390(3) . ?
C10 C15 1.393(3) . ?
C10 N9 1.414(3) . ?
C11 C12 1.377(3) . ?
C12 C13 1.375(4) . ?
C13 C14 1.380(3) . ?
C14 C15 1.385(3) . ?
C14 N16 1.468(3) . ?
C31 C32 1.516(3) . ?
C32 C33 1.516(3) . ?
C100 O1 1.480(3) . ?
C100 C103 1.516(3) . ?
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O17 N16 1.224(2) . ?
O18 N16 1.229(2) . ?

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O2 C2 O1 126.0(2) . . ?
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C2 N3 C31 125.83(19) . . ?
C4 N3 C31 112.93(18) . . ?
N3 C4 C5 111.65(17) . . ?
N3 C4 C33 102.62(17) . . ?

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O5 C5 N6 122.7(2) . . ?
O5 C5 C4 122.02(19) . . ?
N6 C5 C4 115.27(18) . . ?
N6 C7 C71 111.98(18) . . ?
N6 C7 C72 106.97(17) . . ?
C71 C7 C72 110.48(19) . . ?
N6 C7 C8 112.75(17) . . ?
C71 C7 C8 108.87(18) . . ?
C72 C7 C8 105.59(18) . . ?
O8 C8 N9 123.6(2) . . ?
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C11 C10 N9 116.7(2) . . ?
C15 C10 N9 124.0(2) . . ?
C12 C11 C10 121.1(2) . . ?
C13 C12 C11 120.9(2) . . ?
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C13 C14 C15 123.9(2) . . ?
C13 C14 N16 118.3(2) . . ?
C15 C14 N16 117.81(19) . . ?
C14 C15 C10 117.6(2) . . ?
N3 C31 C32 102.60(18) . . ?
C31 C32 C33 104.09(19) . . ?
C32 C33 C4 103.42(19) . . ?
O1 C100 C103 102.48(19) . . ?
O1 C100 C102 111.4(2) . . ?
C103 C100 C102 109.6(2) . . ?
O1 C100 C101 108.2(2) . . ?
C103 C100 C101 111.2(2) . . ?
C102 C100 C101 113.4(2) . . ?
C2 O1 C100 120.71(17) . . ?
C5 N6 C7 124.65(18) . . ?
C8 N9 C10 127.15(19) . . ?
O17 N16 O18 123.5(2) . . ?
O17 N16 C14 118.4(2) . . ?
O18 N16 C14 118.15(19) . . ?

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O2 C2 N3 C31 -179.8(2) . . . . ?
O1 C2 N3 C31 1.5(3) . . . . ?
C2 N3 C4 C5 -48.2(3) . . . . ?
C31 N3 C4 C5 130.4(2) . . . . ?
C2 N3 C4 C33 -167.6(2) . . . . ?
C31 N3 C4 C33 11.0(2) . . . . ?
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N6 C7 C8 O8 -165.98(19) . . . . ?
C71 C7 C8 O8 -41.1(3) . . . . ?
C72 C7 C8 O8 77.6(2) . . . . ?
N6 C7 C8 N9 18.6(3) . . . . ?
C71 C7 C8 N9 143.5(2) . . . . ?
C72 C7 C8 N9 -97.9(2) . . . . ?
C15 C10 C11 C12 0.2(4) . . . . ?
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C10 C11 C12 C13 -0.7(4) . . . . ?
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C12 C13 C14 C15 -0.1(4) . . . . ?
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C13 C14 C15 C10 -0.3(3) . . . . ?
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C11 C10 C15 C14 0.3(3) . . . . ?
N9 C10 C15 C14 -177.3(2) . . . . ?
C2 N3 C31 C32 -169.0(2) . . . . ?
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C31 C32 C33 C4 38.5(2) . . . . ?
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C103 C100 O1 C2 -178.1(2) . . . . ?
C102 C100 O1 C2 -61.0(3) . . . . ?
C101 C100 O1 C2 64.3(3) . . . . ?
O5 C5 N6 C7 -4.7(3) . . . . ?
C4 C5 N6 C7 173.08(19) . . . . ?
C71 C7 N6 C5 -57.1(3) . . . . ?

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C72 C7 N6 C5 -178.2(2) . . . . ?
C8 C7 N6 C5 66.1(3) . . . . ?
O8 C8 N9 C10 -6.6(3) . . . . ?
C7 C8 N9 C10 168.6(2) . . . . ?
C11 C10 N9 C8 174.8(2) . . . . ?
C15 C10 N9 C8 -7.6(3) . . . . ?
C13 C14 N16 O17 7.9(3) . . . . ?
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