Crystal Structure Data

```
data_gkt013

_audit_creation_method          SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common           ?
_chemical_melting_point         ?
_chemical_formula_moiety        ?
_chemical_formula_sum
 'C35 H47 N O5'
_chemical_formula_weight        561.74

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
```

```
_symmetry_cell_setting          'Orthorhombic'
_symmetry_space_group_name_H-M   'P 21 21 21'

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x+1/2, -y, z+1/2'
 'x+1/2, -y+1/2, -z'
 '-x, y+1/2, -z+1/2'

_cell_length_a                 5.6222(3)
_cell_length_b                 14.0127(8)
_cell_length_c                 38.0858(19)
_cell_angle_alpha              90.00
_cell_angle_beta               90.00
_cell_angle_gamma              90.00
_cell_volume                   3000.5(3)
_cell_formula_units_Z          4
_cell_measurement_temperature     120(2)
_cell_measurement_reflns_used   7203
_cell_measurement_theta_min     3.0381
_cell_measurement_theta_max     32.5848

_exptl_crystal_description       plates
_exptl_crystal_colour            colourless
_exptl_crystal_size_max          0.36
_exptl_crystal_size_mid          0.32
_exptl_crystal_size_min          0.28
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.244
_exptl_crystal_density_method    'not measured'
```

_exptl_crystal_F_000 1216

_exptl_absorpt_coefficient_mu 0.082

_exptl_absorpt_correction_T_min 0.9711

_exptl_absorpt_correction_T_max 0.9774

_exptl_absorpt_correction_type 'multi-scan'

_exptl_absorpt_process_details

;

CrysAlis RED, Oxford Diffraction Ltd.,

Version 1.171.29.9 (release 23-03-2006 CrysAlis171 .NET)

(compiled Mar 23 2006,23:39:28)

Empirical absorption correction using spherical harmonics,

implemented in SCALE3 ABSPACK scaling algorithm.

;

_diffrn_ambient_temperature 120(2)

_diffrn_radiation_wavelength 0.71073

_diffrn_radiation_type MoK\a

_diffrn_radiation_source 'Enhance (Mo) X-ray Source'

_diffrn_radiation_monochromator graphite

_diffrn_measurement_device_type ?

_diffrn_measurement_method ?

_diffrn_detector_area_resol_mean 15.9948

_diffrn_standards_number ?

_diffrn_standards_interval_count ?

_diffrn_standards_interval_time ?

_diffrn_standards_decay_% ?

_diffrn_reflns_number 23168

_diffrn_reflns_av_R_equivalents 0.0887

_diffrn_reflns_av_sigmaI/netI 0.0721

```
_diffrn_reflns_limit_h_min       -6
_diffrn_reflns_limit_h_max       6
_diffrn_reflns_limit_k_min       -16
_diffrn_reflns_limit_k_max       16
_diffrn_reflns_limit_l_min       -43
_diffrn_reflns_limit_l_max       45
_diffrn_reflns_theta_min         3.04
_diffrn_reflns_theta_max         24.99
_reflns_number_total             5280
_reflns_number_gt                4137
_reflns_threshold_expression     >2sigma(I)

_computing_data_collection       'CrysAlis CCD, Oxford Diffraction Ltd.,'
_computing_cell_refinement       'CrysAlis RED, Oxford Diffraction Ltd.,'
_computing_data_reduction        'CrysAlis RED, Oxford Diffraction Ltd.,'
_computing_structure_solution    'SHELXS-97 (Sheldrick, 1997)'
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics    'Ortep3'
_computing_publication_material  'Shelx97'

_refine_special_details
;
 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.
;
```

```
_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type           full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0174P)^2^+2.1820P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
_refine_ls_hydrogen_treatment    riding
_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details
 'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack   -1(2)
_refine_ls_number_reflns         5280
_refine_ls_number_parameters     382
_refine_ls_number_restraints     0
_refine_ls_R_factor_all          0.1107
_refine_ls_R_factor_gt           0.0847
_refine_ls_wR_factor_ref         0.1203
_refine_ls_wR_factor_gt          0.1111
_refine_ls_goodness_of_fit_ref   1.178
_refine_ls_restrained_S_all      1.178
_refine_ls_shift/su_max          0.001
_refine_ls_shift/su_mean         0.000

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
```

_atom_site_fract_z

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

_atom_site_symmetry_multiplicity

_atom_site_calc_flag

_atom_site_refinement_flags

_atom_site_disorder_assembly

_atom_site_disorder_group

O1 O 0.7031(7) 0.2696(2) 0.52902(8) 0.0692(11) Uani 1 1 d . . .

O2 O 0.7521(8) 0.4472(3) 0.54286(10) 0.0945(15) Uani 1 1 d . . .

O3 O 0.0943(6) 0.27867(19) 0.70860(7) 0.0478(8) Uani 1 1 d . . .

O4 O -0.0592(6) 0.6526(2) 0.72897(8) 0.0478(8) Uani 1 1 d . . .

O5 O 0.3393(7) 0.2642(3) 0.98909(8) 0.0570(11) Uani 1 1 d . . .

N1 N 0.0200(6) 0.3606(2) 0.65795(8) 0.0339(8) Uani 1 1 d . . .

C1 C 0.6880(12) 0.1702(4) 0.52137(13) 0.084(2) Uani 1 1 d . . .

H1A H 0.7232 0.1341 0.5422 0.126 Uiso 1 1 calc R . .

H1B H 0.8004 0.1543 0.5033 0.126 Uiso 1 1 calc R . .

H1C H 0.5302 0.1551 0.5135 0.126 Uiso 1 1 calc R . .

C2 C 0.7835(14) 0.5397(5) 0.54602(17) 0.114(3) Uani 1 1 d . . .

H2A H 0.6387 0.5723 0.5401 0.171 Uiso 1 1 calc R . .

H2B H 0.9081 0.5600 0.5305 0.171 Uiso 1 1 calc R . .

H2C H 0.8266 0.5545 0.5698 0.171 Uiso 1 1 calc R . .

C3 C 0.5579(9) 0.3055(3) 0.55483(11) 0.0493(13) Uani 1 1 d . . .

C4 C 0.5816(9) 0.4019(4) 0.56234(10) 0.0528(13) Uani 1 1 d . . .

C5 C 0.4450(8) 0.4420(3) 0.58859(10) 0.0459(12) Uani 1 1 d . . .

H5 H 0.4631 0.5066 0.5937 0.055 Uiso 1 1 calc R . .

C6 C 0.2807(7) 0.3886(3) 0.60774(9) 0.0337(10) Uani 1 1 d . . .

C7 C 0.1318(8) 0.4342(3) 0.63651(9) 0.0334(10) Uani 1 1 d . . .

H7 H 0.0079 0.4738 0.6258 0.040 Uiso 1 1 calc R . .

C8 C -0.1034(8) 0.2849(3) 0.63976(10) 0.0439(11) Uani 1 1 d . . .

H8A H -0.2251 0.3116 0.6246 0.053 Uiso 1 1 calc R . .

H8B H -0.1797 0.2428 0.6566 0.053 Uiso 1 1 calc R . .

C9 C 0.0764(8) 0.2296(3) 0.61809(11) 0.0474(12) Uani 1 1 d . . .

H9A H 0.1634 0.1867 0.6334 0.057 Uiso 1 1 calc R . .

H9B H -0.0076 0.1911 0.6009 0.057 Uiso 1 1 calc R . .

C10 C 0.2503(8) 0.2933(3) 0.59932(10) 0.0380(10) Uani 1 1 d . . .

C11 C 0.3901(8) 0.2532(3) 0.57265(10) 0.0432(12) Uani 1 1 d . . .

H11 H 0.3685 0.1894 0.5668 0.052 Uiso 1 1 calc R . .

C12 C 0.1413(8) 0.3437(3) 0.68826(9) 0.0328(10) Uani 1 1 d . . .

C13 C 0.3414(7) 0.4151(3) 0.69077(9) 0.0300(10) Uani 1 1 d . . .

H13 H 0.4852 0.3851 0.6813 0.036 Uiso 1 1 calc R . .

C14 C 0.2618(7) 0.4928(3) 0.66486(9) 0.0319(10) Uani 1 1 d . . .

H14 H 0.3996 0.5258 0.6549 0.038 Uiso 1 1 calc R . .

C15 C 0.0880(8) 0.5645(3) 0.68156(9) 0.0351(10) Uani 1 1 d . . .

H15A H 0.0809 0.6204 0.6666 0.042 Uiso 1 1 calc R . .

H15B H -0.0692 0.5359 0.6816 0.042 Uiso 1 1 calc R . .

C16 C 0.1437(7) 0.5977(3) 0.71895(9) 0.0312(9) Uani 1 1 d . . .

H16 H 0.2858 0.6382 0.7189 0.037 Uiso 1 1 calc R . .

C17 C 0.1860(7) 0.5105(3) 0.74152(9) 0.0251(9) Uani 1 1 d . . .

H17 H 0.0460 0.4693 0.7392 0.030 Uiso 1 1 calc R . .

C18 C 0.4010(7) 0.4551(3) 0.72663(9) 0.0257(9) Uani 1 1 d . . .

H18 H 0.5286 0.5018 0.7231 0.031 Uiso 1 1 calc R . .

C19 C 0.2466(6) 0.5173(3) 0.78098(9) 0.0228(8) Uani 1 1 d . . .

C20 C 0.4395(7) 0.5931(3) 0.78673(9) 0.0330(10) Uani 1 1 d . . .

H20A H 0.3726 0.6554 0.7833 0.049 Uiso 1 1 calc R . .

H20B H 0.5665 0.5832 0.7703 0.049 Uiso 1 1 calc R . .

H20C H 0.5002 0.5881 0.8102 0.049 Uiso 1 1 calc R . .

C21 C 0.0384(7) 0.5349(3) 0.80563(8) 0.0270(9) Uani 1 1 d . . .

H21A H -0.0913 0.4922 0.7997 0.032 Uiso 1 1 calc R . .

H21B H -0.0175 0.6000 0.8029 0.032 Uiso 1 1 calc R . .

C22 C 0.1134(7) 0.5182(3) 0.84389(8) 0.0273(9) Uani 1 1 d . . .

H22A H 0.2249 0.5678 0.8506 0.033 Uiso 1 1 calc R . .

H22B H -0.0258 0.5246 0.8588 0.033 Uiso 1 1 calc R . .

C23 C 0.2274(6) 0.4216(3) 0.85096(8) 0.0230(8) Uani 1 1 d . . .

H23 H 0.1011 0.3740 0.8482 0.028 Uiso 1 1 calc R . .

C24 C 0.4220(7) 0.3952(3) 0.82439(9) 0.0246(8) Uani 1 1 d . . .

H24 H 0.5609 0.4359 0.8286 0.030 Uiso 1 1 calc R . .

C25 C 0.3296(6) 0.4143(3) 0.78730(8) 0.0251(9) Uani 1 1 d . . .

H25 H 0.1860 0.3752 0.7851 0.030 Uiso 1 1 calc R . .

C26 C 0.4859(7) 0.3866(3) 0.75581(9) 0.0313(10) Uani 1 1 d . . .

H26A H 0.4606 0.3205 0.7492 0.038 Uiso 1 1 calc R . .

H26B H 0.6532 0.3961 0.7610 0.038 Uiso 1 1 calc R . .

C27 C 0.3182(6) 0.4121(3) 0.88949(9) 0.0248(9) Uani 1 1 d . . .

C28 C 0.4862(7) 0.4949(3) 0.89925(10) 0.0354(10) Uani 1 1 d . . .

H28A H 0.5577 0.4823 0.9217 0.053 Uiso 1 1 calc R . .

H28B H 0.3972 0.5533 0.9004 0.053 Uiso 1 1 calc R . .

H28C H 0.6082 0.5006 0.8818 0.053 Uiso 1 1 calc R . .

C29 C 0.1013(7) 0.4137(3) 0.91453(9) 0.0347(10) Uani 1 1 d . . .

H29A H 0.0316 0.4771 0.9142 0.042 Uiso 1 1 calc R . .

H29B H -0.0174 0.3694 0.9059 0.042 Uiso 1 1 calc R . .

C30 C 0.1624(7) 0.3876(3) 0.95257(10) 0.0396(11) Uani 1 1 d . . .

H30A H 0.2717 0.4343 0.9622 0.047 Uiso 1 1 calc R . .

H30B H 0.0189 0.3881 0.9667 0.047 Uiso 1 1 calc R . .

C31 C 0.2740(8) 0.2903(3) 0.95378(9) 0.0396(11) Uani 1 1 d . . .

H31 H 0.1603 0.2433 0.9447 0.047 Uiso 1 1 calc R . .

C32 C 0.4968(8) 0.2876(3) 0.93156(9) 0.0395(11) Uani 1 1 d . . .

H32A H 0.5605 0.2232 0.9315 0.047 Uiso 1 1 calc R . .

H32B H 0.6155 0.3294 0.9418 0.047 Uiso 1 1 calc R . .

C33 C 0.4486(7) 0.3184(3) 0.89408(10) 0.0322(10) Uani 1 1 d . . .

C34 C 0.5221(8) 0.2658(3) 0.86752(10) 0.0393(11) Uani 1 1 d . . .

H34 H 0.5963 0.2082 0.8728 0.047 Uiso 1 1 calc R . .

C35 C 0.4951(8) 0.2916(3) 0.82935(9) 0.0381(11) Uani 1 1 d . . .

H35A H 0.3762 0.2506 0.8187 0.046 Uiso 1 1 calc R . .

H35B H 0.6448 0.2806 0.8174 0.046 Uiso 1 1 calc R . .

H104 H -0.029(13) 0.686(5) 0.7473(17) 0.14(3) Uiso 1 1 d . . .

H105 H 0.213(8) 0.255(4) 0.9951(14) 0.06(2) Uiso 1 1 d . . .

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_23

_atom_site_aniso_U_13

_atom_site_aniso_U_12

O1 0.098(3) 0.059(2) 0.0506(19) -0.0008(17) 0.034(2) 0.006(2)

O2 0.137(4) 0.057(3) 0.090(3) 0.004(2) 0.060(3) -0.012(3)

O3 0.074(2) 0.0331(18) 0.0364(16) 0.0101(13) -0.0011(17) -0.0107(18)

O4 0.061(2) 0.046(2) 0.0364(17) -0.0014(15) -0.0052(16) 0.0203(18)

O5 0.058(3) 0.081(3) 0.0311(18) 0.0236(17) 0.0027(18) 0.008(2)

N1 0.041(2) 0.033(2) 0.0268(17) -0.0017(15) -0.0027(17) -0.0055(17)

C1 0.140(6) 0.051(4) 0.062(3) -0.004(3) 0.043(4) 0.021(4)

C2 0.169(8) 0.074(5) 0.100(5) 0.019(4) 0.045(5) -0.021(5)

C3 0.070(3) 0.046(3) 0.032(2) 0.001(2) 0.007(3) 0.005(3)

C4 0.075(4) 0.051(3) 0.032(2) 0.013(2) 0.016(3) -0.005(3)

C5 0.073(3) 0.037(3) 0.029(2) 0.0052(19) 0.005(2) -0.002(3)

C6 0.046(3) 0.037(3) 0.0179(19) 0.0075(17) 0.001(2) 0.002(2)

C7 0.047(3) 0.025(2) 0.028(2) 0.0077(16) -0.002(2) 0.001(2)

C8 0.048(3) 0.044(3) 0.040(2) 0.001(2) -0.001(2) -0.011(3)

C9 0.061(3) 0.032(3) 0.049(3) -0.006(2) 0.000(3) -0.013(3)

C10 0.052(3) 0.034(3) 0.028(2) -0.0019(19) -0.007(2) -0.001(2)

C11 0.065(3) 0.027(3) 0.037(2) -0.0054(19) -0.003(2) 0.000(3)

C12 0.045(3) 0.028(2) 0.025(2) -0.0023(18) 0.000(2) 0.003(2)

C13 0.034(2) 0.032(2) 0.0240(19) -0.0004(17) 0.0037(18) 0.007(2)

C14 0.039(2) 0.034(2) 0.0232(18) 0.0009(17) 0.0038(19) -0.003(2)

C15 0.051(3) 0.031(2) 0.024(2) 0.0057(16) -0.002(2) -0.007(2)

C16 0.038(2) 0.026(2) 0.030(2) 0.0010(17) 0.0001(19) 0.002(2)

C17 0.026(2) 0.020(2) 0.0291(19) -0.0003(16) -0.0046(18) -0.0057(18)

C18 0.025(2) 0.026(2) 0.0258(19) 0.0012(16) 0.0050(18) -0.0026(19)

C19 0.0208(19) 0.025(2) 0.0228(18) -0.0003(15) -0.0012(17) 0.0035(18)

C20 0.034(2) 0.032(2) 0.033(2) 0.0021(18) -0.0019(19) 0.003(2)

C21 0.026(2) 0.024(2) 0.031(2) 0.0012(16) 0.0019(18) 0.0031(19)

C22 0.026(2) 0.033(2) 0.0228(19) -0.0007(16) 0.0078(18) 0.003(2)

C23 0.0212(19) 0.022(2) 0.0257(18) 0.0016(15) 0.0014(16) -0.0052(18)

C24 0.025(2) 0.023(2) 0.0260(19) 0.0014(16) 0.0012(17) -0.0031(18)

C25 0.024(2) 0.029(2) 0.0221(18) -0.0009(16) -0.0001(17) 0.0034(18)

C26 0.034(2) 0.032(2) 0.027(2) 0.0020(17) 0.0012(19) 0.009(2)

C27 0.024(2) 0.028(2) 0.0229(19) -0.0001(16) 0.0014(16) 0.0071(18)

C28 0.036(2) 0.035(3) 0.035(2) -0.0003(18) 0.002(2) 0.004(2)

C29 0.029(2) 0.044(3) 0.031(2) 0.0045(19) 0.0030(19) 0.005(2)

C30 0.033(2) 0.055(3) 0.030(2) 0.009(2) 0.006(2) 0.000(2)

C31 0.045(3) 0.048(3) 0.025(2) 0.0115(19) 0.000(2) -0.004(2)

C32 0.041(3) 0.043(3) 0.034(2) 0.0078(19) 0.001(2) 0.010(2)

C33 0.031(2) 0.039(3) 0.027(2) 0.0011(18) 0.000(2) 0.001(2)

C34 0.053(3) 0.025(2) 0.040(2) 0.0089(19) -0.007(2) 0.013(2)

C35 0.051(3) 0.036(2) 0.027(2) -0.0036(18) -0.001(2) 0.019(2)

_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.

;

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

O1 C3 1.373(5) . ?

O1 C1 1.426(5) . ?

O2 C2 1.315(6) . ?

O2 C4 1.368(6) . ?

O3 C12 1.225(4) . ?

O4 C16 1.427(5) . ?

O4 H104 0.86(6) . ?

O5 C31 1.442(5) . ?

O5 H105 0.76(5) . ?

N1 C12 1.361(5) . ?

N1 C8 1.444(5) . ?

N1 C7 1.458(5) . ?

C1 H1A 0.9600 . ?

C1 H1B 0.9600 . ?

C1 H1C 0.9600 . ?

C2 H2A 0.9600 . ?

C2 H2B 0.9600 . ?

C2 H2C 0.9600 . ?

C3 C11 1.374(6) . ?

C3 C4 1.387(6) . ?

C4 C5 1.380(6) . ?

C5 C6 1.395(5) . ?

C5 H5 0.9300 . ?

C6 C10 1.384(5) . ?

C6 C7 1.520(5) . ?

C7 C14 1.541(5) . ?

C7 H7 0.9800 . ?

C8 C9 1.518(6) . ?

C8 H8A 0.9700 . ?

C8 H8B 0.9700 . ?

C9 C10 1.505(6) . ?

C9 H9A 0.9700 . ?

C9 H9B 0.9700 . ?

C10 C11 1.402(6) . ?

C11 H11 0.9300 . ?

C12 C13 1.508(5) . ?

C13 C18 1.514(5) . ?

C13 C14 1.536(5) . ?

C13 H13 0.9800 . ?

C14 C15 1.539(5) . ?

C14 H14 0.9800 . ?

C15 C16 1.531(5) . ?

C15 H15A 0.9700 . ?

C15 H15B 0.9700 . ?

C16 C17 1.513(5) . ?

C16 H16 0.9800 . ?

C17 C19 1.544(4) . ?

C17 C18 1.545(5) . ?

C17 H17 0.9800 . ?

C18 C26 1.545(5) . ?

C18 H18 0.9800 . ?

C19 C21 1.520(5) . ?

C19 C20 1.534(5) . ?

C19 C25 1.536(5) . ?

C20 H20A 0.9600 . ?

C20 H20B 0.9600 . ?

C20 H20C 0.9600 . ?

C21 C22 1.535(4) . ?

C21 H21A 0.9700 . ?

C21 H21B 0.9700 . ?

C22 C23 1.522(5) . ?

C22 H22A 0.9700 . ?

C22 H22B 0.9700 . ?

C23 C24 1.535(5) . ?

C23 C27 1.559(4) . ?

C23 H23 0.9800 . ?

C24 C35 1.521(5) . ?

C24 C25 1.529(4) . ?

C24 H24 0.9800 . ?

C25 C26 1.537(5) . ?

C25 H25 0.9800 . ?

C26 H26A 0.9700 . ?

C26 H26B 0.9700 . ?

C27 C33 1.514(5) . ?

C27 C28 1.541(5) . ?

C27 C29 1.549(5) . ?

C28 H28A 0.9600 . ?

C28 H28B 0.9600 . ?

C28 H28C 0.9600 . ?

C29 C30 1.533(5) . ?

C29 H29A 0.9700 . ?

C29 H29B 0.9700 . ?

C30 C31 1.502(6) . ?

C30 H30A 0.9700 . ?

C30 H30B 0.9700 . ?

C31 C32 1.512(5) . ?

C31 H31 0.9800 . ?

C32 C33 1.516(5) . ?

C32 H32A 0.9700 . ?

C32 H32B 0.9700 . ?

C33 C34 1.318(5) . ?

C34 C35 1.506(5) . ?

C34 H34 0.9300 . ?

C35 H35A 0.9700 . ?

C35 H35B 0.9700 . ?

loop_

_geom_angle_atom_site_label_1

_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

_geom_angle

_geom_angle_site_symmetry_1

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

C3 O1 C1 118.0(4) . . ?

C2 O2 C4 120.1(5) . . ?

C16 O4 H104 111(5) . . ?

C31 O5 H105 95(4) . . ?

C12 N1 C8 121.4(3) . . ?

C12 N1 C7 112.4(3) . . ?

C8 N1 C7 117.2(3) . . ?

O1 C1 H1A 109.5 . . ?

O1 C1 H1B 109.5 . . ?

H1A C1 H1B 109.5 . . ?

O1 C1 H1C 109.5 . . ?

H1A C1 H1C 109.5 . . ?

H1B C1 H1C 109.5 . . ?

O2 C2 H2A 109.5 . . ?

O2 C2 H2B 109.5 . . ?

H2A C2 H2B 109.5 . . ?

O2 C2 H2C 109.5 . . ?

H2A C2 H2C 109.5 . . ?

H2B C2 H2C 109.5 . . ?

O1 C3 C11 124.5(4) . . ?

O1 C3 C4 116.6(4) . . ?

C11 C3 C4 118.9(4) . . ?

O2 C4 C5 126.4(4) . . ?

O2 C4 C3 114.0(4) . . ?

C5 C4 C3 119.5(4) . . ?

C4 C5 C6 121.9(4) . . ?

C4 C5 H5 119.1 . . ?

C6 C5 H5 119.1 . . ?

C10 C6 C5 118.6(4) . . ?

C10 C6 C7 120.3(4) . . ?

C5 C6 C7 121.0(4) . . ?

N1 C7 C6 110.1(3) . . ?

N1 C7 C14 100.9(3) . . ?

C6 C7 C14 117.9(4) . . ?

N1 C7 H7 109.2 . . ?

C6 C7 H7 109.2 . . ?

C14 C7 H7 109.2 . . ?

N1 C8 C9 108.4(4) . . ?

N1 C8 H8A 110.0 . . ?

C9 C8 H8A 110.0 . . ?

N1 C8 H8B 110.0 . . ?

C9 C8 H8B 110.0 . . ?

H8A C8 H8B 108.4 . . ?

C10 C9 C8 112.8(4) . . ?

C10 C9 H9A 109.0 . . ?

C8 C9 H9A 109.0 . . ?

C10 C9 H9B 109.0 . . ?

C8 C9 H9B 109.0 . . ?

H9A C9 H9B 107.8 . . ?

C6 C10 C11 119.0(4) . . ?

C6 C10 C9 122.9(4) . . ?

C11 C10 C9 118.1(4) . . ?

C3 C11 C10 122.0(4) . . ?

C3 C11 H11 119.0 . . ?

C10 C11 H11 119.0 . . ?

O3 C12 N1 123.9(4) . . ?

O3 C12 C13 127.9(4) . . ?

N1 C12 C13 108.2(3) . . ?

C12 C13 C18 117.9(3) . . ?

C12 C13 C14 102.2(3) . . ?

C18 C13 C14 112.5(3) . . ?

C12 C13 H13 107.9 . . ?

C18 C13 H13 107.9 . . ?

C14 C13 H13 107.9 . . ?

C13 C14 C15 112.5(3) . . ?

C13 C14 C7 102.2(3) . . ?

C15 C14 C7 109.6(3) . . ?

C13 C14 H14 110.8 . . ?

C15 C14 H14 110.8 . . ?

C7 C14 H14 110.8 . . ?

C16 C15 C14 117.0(3) . . ?

C16 C15 H15A 108.1 . . ?

C14 C15 H15A 108.1 . . ?

C16 C15 H15B 108.1 . . ?

C14 C15 H15B 108.1 . . ?

H15A C15 H15B 107.3 . . ?

O4 C16 C17 114.1(3) . . ?

O4 C16 C15 104.4(3) . . ?

C17 C16 C15 108.3(3) . . ?

O4 C16 H16 109.9 . . ?

C17 C16 H16 109.9 . . ?

C15 C16 H16 109.9 . . ?

C16 C17 C19 122.5(3) . . ?

C16 C17 C18 108.7(3) . . ?

C19 C17 C18 102.5(3) . . ?

C16 C17 H17 107.4 . . ?

C19 C17 H17 107.4 . . ?

C18 C17 H17 107.4 . . ?

C13 C18 C26 119.2(3) . . ?

C13 C18 C17 110.1(3) . . ?

C26 C18 C17 106.9(3) . . ?

C13 C18 H18 106.7 . . ?

C26 C18 H18 106.7 . . ?

C17 C18 H18 106.7 . . ?

C21 C19 C20 110.1(3) . . ?

C21 C19 C25 106.8(3) . . ?

C20 C19 C25 114.4(3) . . ?

C21 C19 C17 116.2(3) . . ?

C20 C19 C17 109.7(3) . . ?

C25 C19 C17 99.3(3) . . ?

C19 C20 H20A 109.5 . . ?

C19 C20 H20B 109.5 . . ?

H20A C20 H20B 109.5 . . ?

C19 C20 H20C 109.5 . . ?

H20A C20 H20C 109.5 . . ?

H20B C20 H20C 109.5 . . ?

C19 C21 C22 110.5(3) . . ?

C19 C21 H21A 109.6 . . ?

C22 C21 H21A 109.6 . . ?

C19 C21 H21B 109.6 . . ?

C22 C21 H21B 109.6 . . ?

H21A C21 H21B 108.1 . . ?

C23 C22 C21 114.8(3) . . ?

C23 C22 H22A 108.6 . . ?

C21 C22 H22A 108.6 . . ?

C23 C22 H22B 108.6 . . ?

C21 C22 H22B 108.6 . . ?

H22A C22 H22B 107.6 . . ?

C22 C23 C24 113.4(3) . . ?

C22 C23 C27 112.3(3) . . ?

C24 C23 C27 111.5(3) . . ?

C22 C23 H23 106.3 . . ?

C24 C23 H23 106.3 . . ?

C27 C23 H23 106.3 . . ?

C35 C24 C25 111.9(3) . . ?

C35 C24 C23 109.9(3) . . ?

C25 C24 C23 109.0(3) . . ?

C35 C24 H24 108.7 . . ?

C25 C24 H24 108.7 . . ?

C23 C24 H24 108.7 . . ?

C24 C25 C19 114.4(3) . . ?

C24 C25 C26 118.8(3) . . ?

C19 C25 C26 106.8(3) . . ?

C24 C25 H25 105.2 . . ?

C19 C25 H25 105.2 . . ?

C26 C25 H25 105.2 . . ?

C25 C26 C18 103.1(3) . . ?

C25 C26 H26A 111.1 . . ?

C18 C26 H26A 111.1 . . ?

C25 C26 H26B 111.1 . . ?

C18 C26 H26B 111.1 . . ?

H26A C26 H26B 109.1 . . ?

C33 C27 C28 109.2(3) . . ?

C33 C27 C29 108.8(3) . . ?

C28 C27 C29 108.8(3) . . ?

C33 C27 C23 109.9(3) . . ?

C28 C27 C23 111.3(3) . . ?

C29 C27 C23 108.7(3) . . ?

C27 C28 H28A 109.5 . . ?

C27 C28 H28B 109.5 . . ?

H28A C28 H28B 109.5 . . ?

C27 C28 H28C 109.5 . . ?

H28A C28 H28C 109.5 . . ?

H28B C28 H28C 109.5 . . ?

C30 C29 C27 113.7(3) . . ?

C30 C29 H29A 108.8 . . ?

C27 C29 H29A 108.8 . . ?

C30 C29 H29B 108.8 . . ?

C27 C29 H29B 108.8 . . ?

H29A C29 H29B 107.7 . . ?

C31 C30 C29 109.9(3) . . ?

C31 C30 H30A 109.7 . . ?

C29 C30 H30A 109.7 . . ?

C31 C30 H30B 109.7 . . ?

C29 C30 H30B 109.7 . . ?

H30A C30 H30B 108.2 . . ?

O5 C31 C30 111.4(3) . . ?

O5 C31 C32 107.7(3) . . ?

C30 C31 C32 110.6(3) . . ?

O5 C31 H31 109.0 . . ?

C30 C31 H31 109.0 . . ?

C32 C31 H31 109.0 . . ?

C31 C32 C33 111.8(3) . . ?

C31 C32 H32A 109.3 . . ?

C33 C32 H32A 109.3 . . ?

C31 C32 H32B 109.3 . . ?

C33 C32 H32B 109.3 . . ?

H32A C32 H32B 107.9 . . ?

C34 C33 C27 123.3(3) . . ?

C34 C33 C32 120.5(4) . . ?

C27 C33 C32 116.3(3) . . ?

C33 C34 C35 125.1(4) . . ?

C33 C34 H34 117.5 . . ?

C35 C34 H34 117.5 . . ?

C34 C35 C24 112.1(3) . . ?

C34 C35 H35A 109.2 . . ?

C24 C35 H35A 109.2 . . ?

C34 C35 H35B 109.2 . . ?

C24 C35 H35B 109.2 . . ?

H35A C35 H35B 107.9 . . ?

loop_

_geom_torsion_atom_site_label_1

_geom_torsion_atom_site_label_2

_geom_torsion_atom_site_label_3

_geom_torsion_atom_site_label_4

_geom_torsion

_geom_torsion_site_symmetry_1

_geom_torsion_site_symmetry_2

_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

_geom_torsion_publ_flag

C1 O1 C3 C11 -3.5(7) . . . . ?

C1 O1 C3 C4 178.2(5) . . . . ?

C2 O2 C4 C5 -6.5(9) . . . . ?

C2 O2 C4 C3 176.2(6) . . . . ?

O1 C3 C4 O2 -1.0(7) . . . . ?

C11 C3 C4 O2 -179.4(4) . . . . ?

O1 C3 C4 C5 -178.4(4) . . . . ?

C11 C3 C4 C5 3.1(7) . . . . ?

O2 C4 C5 C6 -177.8(5) . . . . ?

C3 C4 C5 C6 -0.7(7) . . . . ?

C4 C5 C6 C10 -1.8(6) . . . . ?

C4 C5 C6 C7 -179.9(4) . . . . ?

C12 N1 C7 C6 98.7(4) . . . . ?

C8 N1 C7 C6 -49.1(5) . . . . ?

C12 N1 C7 C14 -26.6(4) . . . . ?

C8 N1 C7 C14 -174.4(3) . . . . ?

C10 C6 C7 N1 15.9(5) . . . . ?

C5 C6 C7 N1 -166.0(4) . . . . ?

C10 C6 C7 C14 130.9(4) . . . . ?

C5 C6 C7 C14 -51.1(5) . . . . ?

C12 N1 C8 C9 -81.1(4) . . . . ?

C7 N1 C8 C9 63.6(5) . . . . ?

N1 C8 C9 C10 -42.7(5) . . . . ?

C5 C6 C10 C11 1.9(6) . . . . ?

C7 C6 C10 C11 179.9(4) . . . . ?

C5 C6 C10 C9 -179.4(4) . . . . ?

C7 C6 C10 C9 -1.4(6) . . . . ?

C8 C9 C10 C6 15.2(6) . . . . ?

C8 C9 C10 C11 -166.1(4) . . . . ?

O1 C3 C11 C10 178.6(4) . . . . ?

C4 C3 C11 C10 -3.1(7) . . . . ?

C6 C10 C11 C3 0.6(6) . . . . ?

C9 C10 C11 C3 -178.1(4) . . . . ?

C8 N1 C12 O3 -26.2(6) . . . . ?

C7 N1 C12 O3 -172.4(4) . . . . ?

C8 N1 C12 C13 151.5(3) . . . . ?

C7 N1 C12 C13 5.3(4) . . . . ?

O3 C12 C13 C18 -40.0(6) . . . . ?

N1 C12 C13 C18 142.5(3) . . . . ?

O3 C12 C13 C14 -163.8(4) . . . . ?

N1 C12 C13 C14 18.6(4) . . . . ?

C12 C13 C14 C15 83.9(4) . . . . ?

C18 C13 C14 C15 -43.5(4) . . . . ?

C12 C13 C14 C7 -33.5(4) . . . . ?

C18 C13 C14 C7 -161.0(3) . . . . ?

N1 C7 C14 C13 36.1(4) . . . . ?

C6 C7 C14 C13 -83.8(4) . . . . ?

N1 C7 C14 C15 -83.4(3) . . . . ?

C6 C7 C14 C15 156.8(3) . . . . ?

C13 C14 C15 C16 41.7(5) . . . . ?

C7 C14 C15 C16 154.7(3) . . . . ?

C14 C15 C16 O4 -172.8(3) . . . . ?

C14 C15 C16 C17 -50.8(4) . . . . ?

O4 C16 C17 C19 -64.0(5) . . . . ?

C15 C16 C17 C19 -179.9(3) . . . . ?

O4 C16 C17 C18 176.9(3) . . . . ?

C15 C16 C17 C18 61.0(4) . . . . ?

C12 C13 C18 C26 61.8(5) . . . . ?

C14 C13 C18 C26 -179.6(3) . . . . ?

C12 C13 C18 C17 -62.1(4) . . . . ?

C14 C13 C18 C17 56.4(4) . . . . ?

C16 C17 C18 C13 -66.2(4) . . . . ?

C19 C17 C18 C13 162.8(3) . . . . ?

C16 C17 C18 C26 163.0(3) . . . . ?

C19 C17 C18 C26 31.9(4) . . . . ?

C16 C17 C19 C21 79.5(4) . . . . ?

C18 C17 C19 C21 -158.5(3) . . . . ?

C16 C17 C19 C20 -46.3(5) . . . . ?

C18 C17 C19 C20 75.8(3) . . . . ?

C16 C17 C19 C25 -166.5(3) . . . . ?

C18 C17 C19 C25 -44.5(3) . . . . ?

C20 C19 C21 C22 -66.9(4) . . . . ?

C25 C19 C21 C22 57.9(4) . . . . ?

C17 C19 C21 C22 167.6(3) . . . . ?

C19 C21 C22 C23 -53.5(4) . . . . ?

C21 C22 C23 C24 47.8(4) . . . . ?

C21 C22 C23 C27 175.3(3) . . . . ?

C22 C23 C24 C35 -170.0(3) . . . . ?

C27 C23 C24 C35 62.0(4) . . . . ?

C22 C23 C24 C25 -47.1(4) . . . . ?

C27 C23 C24 C25 -175.0(3) . . . . ?

C35 C24 C25 C19 178.4(3) . . . . ?

C23 C24 C25 C19 56.7(4) . . . . ?

C35 C24 C25 C26 -53.8(5) . . . . ?

C23 C24 C25 C26 -175.6(3) . . . . ?

C21 C19 C25 C24 -62.7(4) . . . . ?

C20 C19 C25 C24 59.5(4) . . . . ?

C17 C19 C25 C24 176.2(3) . . . . ?

C21 C19 C25 C26 163.7(3) . . . . ?

C20 C19 C25 C26 -74.2(4) . . . . ?

C17 C19 C25 C26 42.6(4) . . . . ?

C24 C25 C26 C18 -154.4(3) . . . . ?

C19 C25 C26 C18 -23.2(4) . . . . ?

C13 C18 C26 C25 -131.2(4) . . . . ?

C17 C18 C26 C25 -5.7(4) . . . . ?

C22 C23 C27 C33 -175.0(3) . . . . ?

C24 C23 C27 C33 -46.5(4) . . . . ?

C22 C23 C27 C28 -53.9(4) . . . . ?

C24 C23 C27 C28 74.6(4) . . . . ?

C22 C23 C27 C29 65.9(4) . . . . ?

C24 C23 C27 C29 -165.5(3) . . . . ?

C33 C27 C29 C30 50.2(4) . . . . ?

C28 C27 C29 C30 -68.7(4) . . . . ?

C23 C27 C29 C30 169.9(3) . . . . ?

C27 C29 C30 C31 -57.7(5) . . . . ?

C29 C30 C31 O5 178.6(4) . . . . ?

C29 C30 C31 C32 58.8(4) . . . . ?

O5 C31 C32 C33 -177.4(4) . . . . ?

C30 C31 C32 C33 -55.4(5) . . . . ?

C28 C27 C33 C34 -107.2(5) . . . . ?

C29 C27 C33 C34 134.1(4) . . . . ?

C23 C27 C33 C34 15.1(5) . . . . ?

C28 C27 C33 C32 71.6(4) . . . . ?

C29 C27 C33 C32 -47.1(4) . . . . ?

C23 C27 C33 C32 -166.0(3) . . . . ?

C31 C32 C33 C34 -130.0(4) . . . . ?

C31 C32 C33 C27 51.1(5) . . . . ?

C27 C33 C34 C35 2.0(7) . . . . ?

C32 C33 C34 C35 -176.8(4) . . . . ?

C33 C34 C35 C24 12.5(7) . . . . ?

C25 C24 C35 C34 -164.4(3) . . . . ?

C23 C24 C35 C34 -43.2(5) . . . . ?

_diffrn_measured_fraction_theta_max 0.997

_diffrn_reflns_theta_full 24.99

_diffrn_measured_fraction_theta_full 0.997

_refine_diff_density_max 0.218

_refine_diff_density_min -0.188

_refine_diff_density_rms 0.044