CIF File of compound 10

```
data_db1

_audit_creation_method                  'SHELXL-2014/7'
_shelx_SHELXL_version_number            '2014/7'
_chemical_name_systematic               ?
_chemical_name_common                   ?
_chemical_melting_point                 ?
_chemical_formula_moiety                'C24 H34 N6 O4'
_chemical_formula_sum                   'C24 H34 N6 O4'
_chemical_formula_weight                470.57

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  _atom_type_scat_dispersion_imag
  _atom_type_scat_source
  'C'    'C'      0.0181      0.0091
  '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'      0.0311      0.0180
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'O'    'O'      0.0492      0.0322
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_space_group_crystal_system             orthorhombic
_space_group_IT_number                  61
_space_group_name_H-M_alt               'P b c a'
_space_group_name_Hall                  '-P 2ac 2ab'

_shelx_space_group_comment
;
The symmetry employed for this shelxl refinement is uniquely defined
by the following loop, which should always be used as a source of
symmetry information in preference to the above space-group names.
They are only intended as comments.
;

loop_
```

_space_group_symop_operation_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'
'-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 22.9241(2)
_cell_length_b 7.32050(10)
_cell_length_c 42.5522(4)
_cell_angle_alpha 90
_cell_angle_beta 90
_cell_angle_gamma 90
_cell_volume 7140.93(13)
_cell_formula_units_Z 12
_cell_measurement_temperature 100(2)
_cell_measurement_reflns_used 14178
_cell_measurement_theta_min 2.8330
_cell_measurement_theta_max 69.7890
_exptl_crystal_description 'cut block'
_exptl_crystal_colour yellow
_exptl_crystal_density_meas ?
_exptl_crystal_density_method ?
_exptl_crystal_density_diffrn 1.313
_exptl_crystal_F_000 3024
_exptl_transmission_factor_min ?
_exptl_transmission_factor_max ?
_exptl_crystal_size_max 0.140
_exptl_crystal_size_mid 0.090
_exptl_crystal_size_min 0.040
_exptl_absorpt_coefficient_mu 0.745
_shelx_estimated_absorpt_T_min 0.903
_shelx_estimated_absorpt_T_max 0.971
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_exptl_crystal_face_index_h
_exptl_crystal_face_index_k
_exptl_crystal_face_index_l
_exptl_crystal_face_perp_dist
1 0 1 0.0200
-1 0 -1 0.0200

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     1       0      -1 0.0250
    -1       0       1 0.0250
     0      -1       0 0.0700
     0       1       0 0.0700
_exptl_absorpt_correction_T_min                  0.892
_exptl_absorpt_correction_T_max                  1.000
_exptl_absorpt_correction_type                   gaussian
_exptl_absorpt_process_details
;
CrysAlisPro 1.171.40.67a (Rigaku Oxford Diffraction, 2019)
Numerical absorption correction based on gaussian integration over
                a multifaceted crystal model
Empirical absorption correction using spherical harmonics,
  implemented in SCALE3 ABSPACK scaling algorithm.
;
#_exptl_absorpt_special_details       ?
_diffrn_ambient_temperature            100(2)
_diffrn_radiation_wavelength           1.54178
_diffrn_radiation_type                 CuK\a
_diffrn_source 'Rotating-anode X-ray tube'
_diffrn_source_type 'Rigaku (Cu) X-ray Source'
_diffrn_radiation_monochromator mirror
_diffrn_measurement_device_type 'XtaLAB AFC11 (RCD3): quarter-chi single'
_diffrn_detector_area_resol_mean    ?
_diffrn_reflns_number                  31395
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_diffrn_reflns_av_R_equivalents        0.0338
_diffrn_reflns_limit_h_min             -24
_diffrn_reflns_limit_h_max             27
_diffrn_reflns_limit_k_min             -8
_diffrn_reflns_limit_k_max             8
_diffrn_reflns_limit_l_min             -51
_diffrn_reflns_limit_l_max             49
_diffrn_reflns_theta_min               2.076
_diffrn_reflns_theta_max               68.243
_diffrn_reflns_theta_full              67.679
_diffrn_measured_fraction_theta_max    0.988
_diffrn_measured_fraction_theta_full   0.989
_diffrn_reflns_Laue_measured_fraction_max      0.988
_diffrn_reflns_Laue_measured_fraction_full     0.989
_diffrn_reflns_point_group_measured_fraction_max    0.988
_diffrn_reflns_point_group_measured_fraction_full   0.989
_reflns_number_total                   6453
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_reflns_number_gt                    5944
_reflns_threshold_expression         'I > 2\s(I)'

_reflns_special_details
;
 Reflections were merged by SHELXL according to the crystal
 class for the calculation of statistics and refinement.

 _reflns_Friedel_fraction is defined as the number of unique
 Friedel pairs measured divided by the number that would be
 possible theoretically, ignoring centric projections and
 systematic absences.
;

_computing_data_collection           'CrysAlisPro 1.171.40.67a (Rigaku OD, 2019)'
_computing_cell_refinement           'CrysAlisPro 1.171.40.67a (Rigaku OD, 2019)'
_computing_data_reduction            'CrysAlisPro 1.171.40.67a (Rigaku OD, 2019)'
_computing_structure_solution        'SHELXT (Sheldrick, 2015'
_computing_structure_refinement      'SHELXL-2014/7 (Sheldrick, 2014)'
_computing_molecular_graphics        'ORTEP-3 (Farrugia, 1997)'
_computing_publication_material      'SHELXL-2014/7 (Sheldrick, 2014)'
_refine_special_details              ?
_refine_ls_structure_factor_coef     Fsqd
_refine_ls_matrix_type               full
_refine_ls_weighting_scheme          calc
_refine_ls_weighting_details
'w=1/[\s^2^(Fo^2^)+(0.0522P)^2^+2.4244P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary       ?
_atom_sites_solution_hydrogens       mixed
_refine_ls_hydrogen_treatment        mixed
_refine_ls_extinction_method         'SHELXL-2014/7 (Sheldrick 2014'
_refine_ls_extinction_coef           0.00011(3)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns             6453
_refine_ls_number_parameters         473
_refine_ls_number_restraints         0
_refine_ls_R_factor_all              0.0469
_refine_ls_R_factor_gt               0.0425
_refine_ls_wR_factor_ref             0.1125
_refine_ls_wR_factor_gt              0.1095
_refine_ls_goodness_of_fit_ref       1.081
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_refine_ls_shift/su_mean         0.000

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 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_site_symmetry_order
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 _atom_site_refinement_flags_posn
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C1 C 0.17035(7) 0.7284(2) 0.33855(3) 0.0357(3) Uani 1 1 d . . . . .
H1A H 0.1923 0.6140 0.3422 0.043 Uiso 1 1 calc R U . . .
H1B H 0.1726 0.8031 0.3579 0.043 Uiso 1 1 calc R U . . .
C2 C 0.19758(7) 0.8319(2) 0.31164(3) 0.0376(3) Uani 1 1 d . . . . .
H2A H 0.1786 0.9528 0.3097 0.045 Uiso 1 1 calc R U . . .
H2B H 0.2394 0.8524 0.3162 0.045 Uiso 1 1 calc R U . . .
C3 C 0.13076(7) 0.7025(3) 0.27487(4) 0.0448(4) Uani 1 1 d . . . . .
H3A H 0.1275 0.6320 0.2551 0.054 Uiso 1 1 calc R U . . .
H3B H 0.1109 0.8212 0.2718 0.054 Uiso 1 1 calc R U . . .
C4 C 0.10117(7) 0.5986(2) 0.30118(4) 0.0407(4) Uani 1 1 d . . . . .
H4A H 0.0589 0.5898 0.2966 0.049 Uiso 1 1 calc R U . . .
H4B H 0.1170 0.4729 0.3019 0.049 Uiso 1 1 calc R U . . .
C5 C 0.07432(7) 0.6274(2) 0.35670(3) 0.0335(3) Uani 1 1 d . . . . .
C6 C 0.09376(7) 0.6343(2) 0.38763(3) 0.0340(3) Uani 1 1 d . . . . .
H6 H 0.1324 0.6748 0.3916 0.041 Uiso 1 1 calc R U . . .
C7 C 0.05847(7) 0.5839(2) 0.41337(3) 0.0341(3) Uani 1 1 d . . . . .
C8 C 0.00136(7) 0.5178(2) 0.40629(4) 0.0350(3) Uani 1 1 d . . . . .
C9 C -0.01853(7) 0.5152(2) 0.37522(4) 0.0374(3) Uani 1 1 d . . . . .
H9 H -0.0571 0.4748 0.3710 0.045 Uiso 1 1 calc R U . . .
C10 C 0.01589(7) 0.5687(2) 0.35090(4) 0.0374(3) Uani 1 1 d . . . . .
H10 H 0.0011 0.5671 0.3301 0.045 Uiso 1 1 calc R U . . .
C11 C 0.13824(7) 0.6510(2) 0.45134(4) 0.0369(3) Uani 1 1 d . . . . .
H11A H 0.1458 0.7756 0.4433 0.044 Uiso 1 1 calc R U . . .
```

H11B H 0.1670 0.5668 0.4418 0.044 Uiso 1 1 calc R U . . .
C12 C 0.14440(7) 0.6487(2) 0.48681(4) 0.0411(4) Uani 1 1 d . . . . .
H12A H 0.1161 0.7358 0.4960 0.049 Uiso 1 1 calc R U . . .
H12B H 0.1345 0.5252 0.4947 0.049 Uiso 1 1 calc R U . . .
C13 C 0.20500(8) 0.6985(3) 0.49783(4) 0.0479(4) Uani 1 1 d . . . . .
H13A H 0.2154 0.8203 0.4894 0.057 Uiso 1 1 calc R U . . .
H13B H 0.2332 0.6089 0.4893 0.057 Uiso 1 1 calc R U . . .
C14 C 0.21015(10) 0.7019(4) 0.53362(5) 0.0753(7) Uani 1 1 d . . . . .
H14A H 0.2502 0.7336 0.5396 0.113 Uiso 1 1 calc R U . . .
H14B H 0.2004 0.5811 0.5421 0.113 Uiso 1 1 calc R U . . .
H14C H 0.1832 0.7930 0.5422 0.113 Uiso 1 1 calc R U . . .
C15 C 0.23594(6) 0.7055(2) 0.26087(3) 0.0335(3) Uani 1 1 d . . . . .
C16 C 0.22510(7) 0.6514(2) 0.22998(3) 0.0339(3) Uani 1 1 d . . . . .
H16 H 0.1858 0.6477 0.2229 0.041 Uiso 1 1 calc R U . . .
C17 C 0.26945(7) 0.6023(2) 0.20888(3) 0.0340(3) Uani 1 1 d . . . . .
C18 C 0.32825(7) 0.6095(2) 0.22033(4) 0.0368(3) Uani 1 1 d . . . . .
C19 C 0.33887(7) 0.6737(2) 0.25085(4) 0.0381(3) Uani 1 1 d . . . . .
H19 H 0.3781 0.6826 0.2580 0.046 Uiso 1 1 calc R U . . .
C20 C 0.29524(7) 0.7236(2) 0.27060(4) 0.0359(3) Uani 1 1 d . . . . .
H20 H 0.3041 0.7705 0.2909 0.043 Uiso 1 1 calc R U . . .
C21 C 0.19746(7) 0.5275(2) 0.16726(4) 0.0379(3) Uani 1 1 d . . . . .
H21A H 0.1769 0.6465 0.1676 0.045 Uiso 1 1 calc R U . . .
H21B H 0.1757 0.4418 0.1809 0.045 Uiso 1 1 calc R U . . .
C22 C 0.19874(7) 0.4541(2) 0.13400(4) 0.0399(4) Uani 1 1 d . . . . .
H22A H 0.2218 0.3399 0.1336 0.048 Uiso 1 1 calc R U . . .
H22B H 0.2185 0.5439 0.1202 0.048 Uiso 1 1 calc R U . . .
C23 C 0.13807(8) 0.4157(3) 0.12102(4) 0.0467(4) Uani 1 1 d . . . . .
H23A H 0.1174 0.3320 0.1355 0.056 Uiso 1 1 calc R U . . .
H23B H 0.1158 0.5316 0.1202 0.056 Uiso 1 1 calc R U . . .
C24 C 0.13919(9) 0.3314(3) 0.08844(4) 0.0556(5) Uani 1 1 d . . . . .
H24A H 0.0992 0.3081 0.0814 0.083 Uiso 1 1 calc R U . . .
H24B H 0.1608 0.2160 0.0891 0.083 Uiso 1 1 calc R U . . .
H24C H 0.1583 0.4156 0.0738 0.083 Uiso 1 1 calc R U . . .
N1 N 0.10925(5) 0.68476(18) 0.33182(3) 0.0340(3) Uani 1 1 d . . . . .
N2 N 0.19192(6) 0.7339(2) 0.28205(3) 0.0402(3) Uani 1 1 d . . . . .
N3 N 0.07943(6) 0.59451(19) 0.44295(3) 0.0374(3) Uani 1 1 d . . . . .
H1N H 0.0559(8) 0.550(3) 0.4589(4) 0.045 Uiso 1 1 d . U . . .
N4 N 0.25632(6) 0.55064(19) 0.17927(3) 0.0372(3) Uani 1 1 d . . . . .
H2N H 0.2856(9) 0.513(3) 0.1679(4) 0.045 Uiso 1 1 d . U . . .
N5 N -0.03632(6) 0.44496(19) 0.42960(3) 0.0398(3) Uani 1 1 d . . . . .
N6 N 0.37633(6) 0.5471(2) 0.20271(3) 0.0434(3) Uani 1 1 d . . . . .
O1 O -0.02358(5) 0.46248(17) 0.45809(3) 0.0460(3) Uani 1 1 d . . . . .
O2 O -0.08105(5) 0.36218(19) 0.42151(3) 0.0540(3) Uani 1 1 d . . . . .

O3 O 0.36934(5) 0.49534(19) 0.17479(3) 0.0509(3) Uani 1 1 d . . . . .
O4 O 0.42559(5) 0.5422(2) 0.21515(3) 0.0554(3) Uani 1 1 d . . . . .
C25 C 0.54022(7) 0.1430(2) -0.00554(3) 0.0368(3) Uani 1 1 d . . . . .
H25A H 0.5801 0.1835 -0.0112 0.044 Uiso 1 1 calc R U . . .
H25B H 0.5160 0.2533 -0.0023 0.044 Uiso 1 1 calc R U . . .
C26 C 0.48482(7) -0.0323(2) 0.03215(4) 0.0357(3) Uani 1 1 d . . . . .
H26A H 0.4585 0.0712 0.0370 0.043 Uiso 1 1 calc R U . . .
H26B H 0.4880 -0.1095 0.0512 0.043 Uiso 1 1 calc R U . . .
C27 C 0.57950(7) 0.0946(2) 0.04731(3) 0.0337(3) Uani 1 1 d . . . . .
C28 C 0.56323(7) 0.0892(2) 0.07859(3) 0.0344(3) Uani 1 1 d . . . . .
H28 H 0.5249 0.0497 0.0838 0.041 Uiso 1 1 calc R U . . .
C29 C 0.60129(7) 0.1400(2) 0.10305(3) 0.0346(3) Uani 1 1 d . . . . .
C30 C 0.65768(7) 0.2029(2) 0.09440(4) 0.0366(3) Uani 1 1 d . . . . .
C31 C 0.67469(7) 0.2023(2) 0.06270(4) 0.0379(3) Uani 1 1 d . . . . .
H31 H 0.7132 0.2389 0.0573 0.045 Uiso 1 1 calc R U . . .
C32 C 0.63735(7) 0.1505(2) 0.03954(4) 0.0372(3) Uani 1 1 d . . . . .
H32 H 0.6497 0.1515 0.0182 0.045 Uiso 1 1 calc R U . . .
C33 C 0.52527(7) 0.0777(2) 0.14323(4) 0.0387(4) Uani 1 1 d . . . . .
H33A H 0.5170 -0.0475 0.1356 0.046 Uiso 1 1 calc R U . . .
H33B H 0.4954 0.1610 0.1344 0.046 Uiso 1 1 calc R U . . .
C34 C 0.52308(7) 0.0822(2) 0.17875(4) 0.0421(4) Uani 1 1 d . . . . .
H34A H 0.5283 0.2099 0.1859 0.051 Uiso 1 1 calc R U . . .
H34B H 0.5561 0.0097 0.1871 0.051 Uiso 1 1 calc R U . . .
C35 C 0.46688(8) 0.0087(3) 0.19250(4) 0.0483(4) Uani 1 1 d . . . . .
H35A H 0.4347 0.0945 0.1878 0.058 Uiso 1 1 calc R U . . .
H35B H 0.4575 -0.1100 0.1825 0.058 Uiso 1 1 calc R U . . .
C36 C 0.47156(9) -0.0166(3) 0.22756(4) 0.0567(5) Uani 1 1 d . . . . .
H36A H 0.4350 -0.0676 0.2356 0.085 Uiso 1 1 calc R U . . .
H36B H 0.4790 0.1017 0.2376 0.085 Uiso 1 1 calc R U . . .
H36C H 0.5037 -0.1004 0.2323 0.085 Uiso 1 1 calc R U . . .
N7 N 0.54246(5) 0.03728(17) 0.02366(3) 0.0341(3) Uani 1 1 d . . . . .
N8 N 0.58287(6) 0.13418(19) 0.13306(3) 0.0390(3) Uani 1 1 d . . . . .
H3N H 0.6101(8) 0.175(3) 0.1485(4) 0.047 Uiso 1 1 d . U . . .
N9 N 0.69815(6) 0.2716(2) 0.11643(3) 0.0426(3) Uani 1 1 d . . . . .
O5 O 0.68723(5) 0.25859(17) 0.14532(3) 0.0474(3) Uani 1 1 d . . . . .
O6 O 0.74370(5) 0.34621(19) 0.10699(3) 0.0538(3) Uani 1 1 d . . . . .

loop_
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 _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
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C2 0.0378(8) 0.0410(8) 0.0341(8) -0.0012(6) -0.0007(6) -0.0022(7)
C3 0.0322(8) 0.0670(12) 0.0352(8) -0.0059(8) 0.0001(6) -0.0006(8)
C4 0.0330(8) 0.0500(10) 0.0391(8) -0.0081(7) -0.0011(6) -0.0012(7)
C5 0.0346(8) 0.0281(7) 0.0379(8) 0.0006(6) -0.0012(6) 0.0039(6)
C6 0.0317(7) 0.0321(7) 0.0381(8) -0.0014(6) -0.0013(6) 0.0023(6)
C7 0.0353(8) 0.0289(7) 0.0380(8) -0.0020(6) -0.0001(6) 0.0034(6)
C8 0.0338(8) 0.0319(8) 0.0394(8) 0.0014(6) 0.0018(6) 0.0028(6)
C9 0.0326(8) 0.0345(8) 0.0451(9) -0.0002(7) -0.0021(6) 0.0025(6)
C10 0.0347(8) 0.0370(8) 0.0404(8) -0.0004(6) -0.0037(6) 0.0038(7)
C11 0.0370(8) 0.0357(8) 0.0381(8) -0.0009(6) 0.0008(6) 0.0013(7)
C12 0.0391(9) 0.0458(9) 0.0384(8) -0.0012(7) -0.0004(7) 0.0015(7)
C13 0.0412(9) 0.0551(11) 0.0473(9) 0.0013(8) -0.0042(7) 0.0015(8)
C14 0.0584(13) 0.115(2) 0.0526(11) -0.0108(12) -0.0119(10) -0.0043(13)
C15 0.0343(8) 0.0309(7) 0.0353(7) 0.0053(6) 0.0011(6) -0.0011(6)
C16 0.0313(7) 0.0345(8) 0.0358(8) 0.0039(6) 0.0003(6) -0.0009(6)
C17 0.0374(8) 0.0306(7) 0.0341(7) 0.0064(6) 0.0020(6) -0.0023(6)
C18 0.0326(8) 0.0395(8) 0.0384(8) 0.0068(6) 0.0046(6) -0.0005(6)
C19 0.0327(8) 0.0431(9) 0.0385(8) 0.0082(7) -0.0012(6) -0.0035(7)
C20 0.0359(8) 0.0376(8) 0.0341(7) 0.0044(6) -0.0020(6) -0.0033(7)
C21 0.0371(8) 0.0400(8) 0.0364(8) 0.0024(6) 0.0012(6) -0.0005(7)
C22 0.0401(9) 0.0429(9) 0.0367(8) 0.0012(7) 0.0018(6) -0.0005(7)
C23 0.0423(9) 0.0544(10) 0.0432(9) -0.0020(8) -0.0001(7) -0.0021(8)
C24 0.0527(11) 0.0697(13) 0.0444(10) -0.0039(9) -0.0039(8) -0.0094(10)
N1 0.0326(7) 0.0376(7) 0.0318(6) 0.0003(5) -0.0015(5) 0.0005(5)
N2 0.0325(7) 0.0528(8) 0.0352(7) -0.0052(6) 0.0003(5) -0.0017(6)
N3 0.0363(7) 0.0398(7) 0.0359(7) 0.0004(6) 0.0012(5) -0.0009(6)
N4 0.0344(7) 0.0431(7) 0.0341(6) 0.0014(6) 0.0040(5) 0.0001(6)
N5 0.0372(7) 0.0391(7) 0.0432(7) 0.0018(6) 0.0007(6) 0.0012(6)
N6 0.0355(7) 0.0533(9) 0.0415(8) 0.0041(6) 0.0048(6) -0.0001(6)
O1 0.0456(7) 0.0527(7) 0.0398(6) 0.0005(5) 0.0048(5) -0.0034(6)
O2 0.0417(7) 0.0652(8) 0.0552(7) 0.0064(6) -0.0017(5) -0.0160(6)
O3 0.0407(7) 0.0712(9) 0.0408(6) -0.0042(6) 0.0075(5) 0.0005(6)
O4 0.0325(6) 0.0828(10) 0.0510(7) 0.0009(6) 0.0009(5) 0.0045(6)
C25 0.0381(8) 0.0366(8) 0.0357(8) 0.0028(6) -0.0016(6) -0.0032(7)
C26 0.0355(8) 0.0380(8) 0.0336(7) 0.0024(6) 0.0004(6) -0.0019(7)
C27 0.0352(8) 0.0296(7) 0.0361(8) 0.0003(6) -0.0033(6) 0.0023(6)
C28 0.0331(8) 0.0328(7) 0.0373(8) 0.0004(6) -0.0008(6) 0.0008(6)
C29 0.0381(8) 0.0292(7) 0.0364(8) 0.0011(6) -0.0022(6) 0.0049(6)
C30 0.0338(8) 0.0344(8) 0.0415(8) -0.0002(6) -0.0061(6) 0.0026(7)
C31 0.0321(8) 0.0353(8) 0.0463(9) 0.0010(7) -0.0011(6) 0.0017(6)

C32 0.0369(8) 0.0358(8) 0.0389(8) 0.0013(6) 0.0016(6) 0.0028(7)
C33 0.0391(8) 0.0377(8) 0.0394(8) 0.0008(7) -0.0020(6) 0.0017(7)
C34 0.0415(9) 0.0447(9) 0.0401(8) 0.0004(7) -0.0016(7) 0.0031(7)
C35 0.0437(10) 0.0524(10) 0.0488(10) -0.0047(8) -0.0001(8) 0.0002(8)
C36 0.0505(11) 0.0704(13) 0.0491(10) -0.0010(9) 0.0099(8) 0.0022(10)
N7 0.0349(7) 0.0363(7) 0.0312(6) 0.0021(5) -0.0010(5) -0.0024(6)
N8 0.0385(7) 0.0420(7) 0.0365(7) -0.0003(6) -0.0036(6) -0.0013(6)
N9 0.0395(8) 0.0431(8) 0.0451(8) 0.0016(6) -0.0086(6) 0.0007(6)
O5 0.0467(7) 0.0555(7) 0.0401(6) -0.0016(5) -0.0090(5) -0.0012(6)
O6 0.0401(7) 0.0633(8) 0.0580(7) 0.0066(6) -0.0088(6) -0.0129(6)

_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 H1B 0.9900 . ?
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C2 H2A 0.9900 . ?
C2 H2B 0.9900 . ?
C3 N2 1.453(2) . ?
C3 C4 1.514(2) . ?
C3 H3A 0.9900 . ?
C3 H3B 0.9900 . ?
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C4 H4A 0.9900 . ?
C4 H4B 0.9900 . ?
C5 C6 1.391(2) . ?
C5 N1 1.3920(19) . ?

C5 C10 1.428(2) . ?
C6 C7 1.411(2) . ?
C6 H6 0.9500 . ?
C7 N3 1.3495(19) . ?
C7 C8 1.428(2) . ?
C8 C9 1.399(2) . ?
C8 N5 1.419(2) . ?
C9 C10 1.359(2) . ?
C9 H9 0.9500 . ?
C10 H10 0.9500 . ?
C11 N3 1.455(2) . ?
C11 C12 1.516(2) . ?
C11 H11A 0.9900 . ?
C11 H11B 0.9900 . ?
C12 C13 1.511(2) . ?
C12 H12A 0.9900 . ?
C12 H12B 0.9900 . ?
C13 C14 1.528(3) . ?
C13 H13A 0.9900 . ?
C13 H13B 0.9900 . ?
C14 H14A 0.9800 . ?
C14 H14B 0.9800 . ?
C14 H14C 0.9800 . ?
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C15 C20 1.427(2) . ?
C16 C17 1.403(2) . ?
C16 H16 0.9500 . ?
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C17 C18 1.434(2) . ?
C18 C19 1.403(2) . ?
C18 N6 1.409(2) . ?
C19 C20 1.356(2) . ?
C19 H19 0.9500 . ?
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C21 N4 1.453(2) . ?
C21 C22 1.514(2) . ?
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C23 C24 1.518(2) . ?

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C2 C1 H1B 109.5 . . ?
H1A C1 H1B 108.0 . . ?
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N2 C2 H2A 109.2 . . ?
C1 C2 H2A 109.2 . . ?
N2 C2 H2B 109.2 . . ?
C1 C2 H2B 109.2 . . ?
H2A C2 H2B 107.9 . . ?
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N2 C3 H3A 109.5 . . ?
C4 C3 H3A 109.5 . . ?
N2 C3 H3B 109.5 . . ?
C4 C3 H3B 109.5 . . ?
H3A C3 H3B 108.1 . . ?
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N1 C4 H4B 109.0 . . ?
C3 C4 H4B 109.0 . . ?
H4A C4 H4B 107.8 . . ?
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C6 C5 C10 118.35(14) . . ?
N1 C5 C10 119.92(13) . . ?
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C5 C6 H6 118.6 . . ?
C7 C6 H6 118.6 . . ?
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C14 C13 H13A 109.1 . . ?
C12 C13 H13B 109.1 . . ?
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C23 C24 H24C 109.5 . . ?
H24A C24 H24C 109.5 . . ?
H24B C24 H24C 109.5 . . ?
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C5 N1 C1 117.84(12) . . ?
C4 N1 C1 112.96(12) . . ?
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C15 N2 C2 125.36(13) . . ?
C3 N2 C2 110.25(12) . . ?
C7 N3 C11 125.12(13) . . ?
C7 N3 H1N 117.2(12) . . ?

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C27 C28 C29 122.47(14) . . ?
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N8 C29 C30 122.79(14) . . ?
C28 C29 C30 117.25(14) . . ?
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N9 C30 C29 122.79(14) . . ?
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C33 N8 H3N 118.6(11) . . ?
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N5 C8 C9 C10 -174.93(14) . . . . ?
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C28 C29 C30 N9 174.78(14) . . . . ?
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C30 C31 C32 C27 -0.2(2) . . . . ?
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N4 H2N O3    0.87(2) 1.95(2) 2.6291(18) 134.2(16) .
N8 H3N O5    0.95(2) 1.877(19) 2.6126(18) 131.8(15) .
C1 H1B O6    0.99 2.45 3.1616(19) 128.2 4_655
C2 H2B O5    0.99 2.45 3.2580(19) 138.9 4_655
C9 H9 O3    0.95 2.58 3.3403(19) 137.1 6_556
C10 H10 O4    0.95 2.59 3.496(2) 158.7 6_556
C25 H25B O1    0.99 2.59 3.418(2) 141.4 6_656

_refine_diff_density_max        0.197
_refine_diff_density_min       -0.183
_refine_diff_density_rms        0.033

_shelx_res_file
;

      db1.res created by SHELXL-2014/7


TITL db1_a.res Pbca
CELL    1.54178      22.9241        7.3205      42.5522        90.000        90.000        90.000
ZERR              12        0.0002        0.0001        0.0004         0.000         0.000         0.000
LATT      1
SYMM         0.50000 - X ,                    - Y ,        0.50000 + Z
SYMM         0.50000 + X ,        0.50000 - Y ,                    - Z
SYMM                      - X ,        0.50000 + Y ,        0.50000 - Z
SFAC    C    H    N    O
UNIT    288 408 72 48
```

```
L.S. 4
FMAP 2
temp -173
PLAN 20
size 0.14 0.09 0.04
rem cut yellow block
ACTA
BOND $H
CONF
htab
eqiv $4 1-x,-y,-z
mpla 4 c1 c2 c3 c4 n1 n2
mpla c5 c6 c7 c8 c9 c10
mpla n5 o1 o2
mpla c15 c16 c17 c18 c19 c20
mpla n6 o3 o4
mpla 4 c25 c26 c25_$4 c26_$4 n7
mpla c27 c28 c29 c30 c31 c32
mpla n9 o5 o6
REM Instructions for potential hydrogen bonds
HTAB N3 O1
HTAB N4 O3
HTAB N8 O5
EQIV $1 x-1/2, y, -z+1/2
HTAB C1 O5_$1
EQIV $2 -x+1, y+1/2, -z+1/2
HTAB C1 O6_$2
HTAB C2 O5_$2
HTAB C9 O3_$1
HTAB C10 O4_$1
EQIV $3 x+1/2, y, -z+1/2
HTAB C25 O1_$3
WGHT       0.052200       2.424400
EXTI       0.000110
FVAR             0.17604
mole 1
C1          1          0.170346          0.728441          0.338551          11.00000          0.03393
0.03676 =
                0.03642       0.00138      -0.00393      -0.00166
AFIX    23
H1A      2       0.192348       0.614024       0.342202       11.00000      -1.20000
H1B      2       0.172600       0.803087       0.357914       11.00000      -1.20000
AFIX      0
```

```
C2    1    0.197584    0.831916    0.311635    11.00000    0.03783
0.04097 =
            0.03413    -0.00124    -0.00074    -0.00224
AFIX  23
H2A   2    0.178555    0.952795    0.309701    11.00000   -1.20000
H2B   2    0.239436    0.852411    0.316161    11.00000   -1.20000
AFIX   0
C3    1    0.130763    0.702507    0.274866    11.00000    0.03225
0.06700 =
            0.03521    -0.00593     0.00008    -0.00058
AFIX  23
H3A   2    0.127537    0.632032    0.255086    11.00000   -1.20000
H3B   2    0.110883    0.821207    0.271771    11.00000   -1.20000
AFIX   0
C4    1    0.101173    0.598555    0.301176    11.00000    0.03296
0.04996 =
            0.03909    -0.00806    -0.00107    -0.00120
AFIX  23
H4A   2    0.058911    0.589839    0.296631    11.00000   -1.20000
H4B   2    0.117039    0.472851    0.301925    11.00000   -1.20000
AFIX   0
C5    1    0.074325    0.627404    0.356696    11.00000    0.03460
0.02813 =
            0.03789     0.00063    -0.00120     0.00392
C6    1    0.093761    0.634341    0.387634    11.00000    0.03171
0.03209 =
            0.03812    -0.00145    -0.00129     0.00229
AFIX  43
H6    2    0.132441    0.674785    0.391607    11.00000   -1.20000
AFIX   0
C7    1    0.058469    0.583863    0.413366    11.00000    0.03526
0.02892 =
            0.03800    -0.00196    -0.00011     0.00345
C8    1    0.001362    0.517794    0.406288    11.00000    0.03377
0.03188 =
            0.03939     0.00141     0.00183     0.00278
C9    1   -0.018530    0.515159    0.375216    11.00000    0.03261
0.03451 =
            0.04506    -0.00023    -0.00214     0.00252
AFIX  43
H9    2   -0.057134    0.474847    0.370997    11.00000   -1.20000
AFIX   0
```

```
C10     1       0.015889        0.568720        0.350901        11.00000        0.03468
0.03696 =
             0.04042    -0.00039    -0.00372     0.00377
AFIX  43
H10   2     0.001082     0.567128     0.330051     11.00000    -1.20000
AFIX   0
C11     1       0.138243        0.650996        0.451339        11.00000        0.03697
0.03572 =
             0.03809    -0.00093     0.00078     0.00132
AFIX  23
H11A  2     0.145848     0.775551     0.443255     11.00000    -1.20000
H11B  2     0.167014     0.566777     0.441792     11.00000    -1.20000
AFIX   0
C12     1       0.144397        0.648714        0.486814        11.00000        0.03909
0.04585 =
             0.03841    -0.00120    -0.00035     0.00155
AFIX  23
H12A  2     0.116089     0.735777     0.496000     11.00000    -1.20000
H12B  2     0.134549     0.525211     0.494669     11.00000    -1.20000
AFIX   0
C13     1       0.205000        0.698463        0.497834        11.00000        0.04121
0.05511 =
             0.04728     0.00126    -0.00422     0.00155
AFIX  23
H13A  2     0.215415     0.820278     0.489430     11.00000    -1.20000
H13B  2     0.233202     0.608918     0.489282     11.00000    -1.20000
AFIX   0
C14     1       0.210146        0.701862        0.533625        11.00000        0.05839
0.11478 =
             0.05260    -0.01084    -0.01186    -0.00428
AFIX 137
H14A  2     0.250187     0.733591     0.539566     11.00000    -1.50000
H14B  2     0.200368     0.581147     0.542073     11.00000    -1.50000
H14C  2     0.183185     0.793030     0.542195     11.00000    -1.50000
AFIX   0
C15     1       0.235941        0.705505        0.260871        11.00000        0.03426
0.03090 =
             0.03528     0.00531     0.00106    -0.00107
C16     1       0.225097        0.651425        0.229980        11.00000        0.03132
0.03453 =
             0.03581     0.00392     0.00027    -0.00087
AFIX  43
H16   2     0.185819     0.647694     0.222890     11.00000    -1.20000
```

```
AFIX     0
C17      1        0.269450        0.602279        0.208885        11.00000        0.03737
0.03059 =
              0.03413      0.00638      0.00200     -0.00230
C18      1        0.328248        0.609464        0.220330        11.00000        0.03256
0.03954 =
              0.03835      0.00679      0.00456     -0.00053
C19      1        0.338868        0.673710        0.250852        11.00000        0.03272
0.04309 =
              0.03847      0.00816     -0.00122     -0.00346
AFIX    43
H19      2       0.378053        0.682614        0.257955        11.00000     -1.20000
AFIX     0
C20      1        0.295236        0.723592        0.270597        11.00000        0.03588
0.03764 =
              0.03414      0.00444     -0.00201     -0.00333
AFIX    43
H20      2       0.304129        0.770464        0.290857        11.00000     -1.20000
AFIX     0
C21      1        0.197464        0.527537        0.167258        11.00000        0.03714
0.04003 =
              0.03641      0.00240      0.00116     -0.00048
AFIX    23
H21A     2       0.176941        0.646512        0.167576        11.00000     -1.20000
H21B     2       0.175741        0.441839        0.180932        11.00000     -1.20000
AFIX     0
C22      1        0.198736        0.454128        0.133995        11.00000        0.04007
0.04289 =
              0.03673      0.00124      0.00179     -0.00052
AFIX    23
H22A     2       0.221823        0.339862        0.133596        11.00000     -1.20000
H22B     2       0.218511        0.543879        0.120233        11.00000     -1.20000
AFIX     0
C23      1        0.138065        0.415748        0.121018        11.00000        0.04231
0.05443 =
              0.04322     -0.00205     -0.00011     -0.00213
AFIX    23
H23A     2       0.117406        0.332041        0.135510        11.00000     -1.20000
H23B     2       0.115815        0.531558        0.120207        11.00000     -1.20000
AFIX     0
C24      1        0.139186        0.331403        0.088438        11.00000        0.05266
0.06968 =
              0.04444     -0.00388     -0.00387     -0.00940
```

AFIX 137
H24A 2 0.099156 0.308146 0.081416 11.00000 -1.50000
H24B 2 0.160846 0.216049 0.089088 11.00000 -1.50000
H24C 2 0.158281 0.415557 0.073776 11.00000 -1.50000
AFIX 0
N1 3 0.109249 0.684758 0.331820 11.00000 0.03255
0.03763 =
0.03181 0.00035 -0.00149 0.00046
N2 3 0.191919 0.733901 0.282048 11.00000 0.03248
0.05284 =
0.03524 -0.00516 0.00033 -0.00169
N3 3 0.079426 0.594508 0.442946 11.00000 0.03629
0.03982 =
0.03594 0.00040 0.00118 -0.00086
H1N 2 0.055916 0.550438 0.458904 11.00000 -1.20000
N4 3 0.256322 0.550640 0.179271 11.00000 0.03437
0.04311 =
0.03407 0.00142 0.00398 0.00010
H2N 2 0.285571 0.513297 0.167906 11.00000 -1.20000
N5 3 -0.036323 0.444960 0.429601 11.00000 0.03718
0.03910 =
0.04318 0.00177 0.00072 0.00123
N6 3 0.376332 0.547061 0.202706 11.00000 0.03548
0.05332 =
0.04154 0.00407 0.00476 -0.00007
O1 4 -0.023582 0.462483 0.458094 11.00000 0.04562
0.05275 =
0.03975 0.00045 0.00479 -0.00338
O2 4 -0.081049 0.362175 0.421514 11.00000 0.04172
0.06519 =
0.05523 0.00637 -0.00166 -0.01601
O3 4 0.369336 0.495335 0.174795 11.00000 0.04070
0.07123 =
0.04083 -0.00421 0.00746 0.00052
O4 4 0.425589 0.542189 0.215153 11.00000 0.03247
0.08284 =
0.05101 0.00093 0.00085 0.00453
mole 2
C25 1 0.540221 0.143048 -0.005539 11.00000 0.03814
0.03662 =
0.03568 0.00277 -0.00161 -0.00321
AFIX 23
H25A 2 0.580083 0.183507 -0.011167 11.00000 -1.20000

H25B 2 0.515971 0.253312 -0.002256 11.00000 -1.20000
AFIX 0
C26 1 0.484822 -0.032299 0.032153 11.00000 0.03551
0.03801 =
0.03362 0.00240 0.00043 -0.00193
AFIX 23
H26A 2 0.458505 0.071194 0.036978 11.00000 -1.20000
H26B 2 0.487953 -0.109464 0.051185 11.00000 -1.20000
AFIX 0
C27 1 0.579497 0.094624 0.047306 11.00000 0.03524
0.02965 =
0.03611 0.00030 -0.00326 0.00226
C28 1 0.563230 0.089186 0.078592 11.00000 0.03309
0.03276 =
0.03734 0.00037 -0.00081 0.00085
AFIX 43
H28 2 0.524946 0.049683 0.083774 11.00000 -1.20000
AFIX 0
C29 1 0.601287 0.140005 0.103052 11.00000 0.03810
0.02920 =
0.03638 0.00106 -0.00224 0.00489
C30 1 0.657677 0.202888 0.094403 11.00000 0.03380
0.03444 =
0.04148 -0.00022 -0.00609 0.00264
C31 1 0.674687 0.202285 0.062697 11.00000 0.03209
0.03526 =
0.04626 0.00098 -0.00112 0.00166
AFIX 43
H31 2 0.713168 0.238898 0.057313 11.00000 -1.20000
AFIX 0
C32 1 0.637348 0.150511 0.039542 11.00000 0.03693
0.03583 =
0.03894 0.00125 0.00157 0.00283
AFIX 43
H32 2 0.649740 0.151535 0.018238 11.00000 -1.20000
AFIX 0
C33 1 0.525270 0.077654 0.143225 11.00000 0.03909
0.03772 =
0.03943 0.00076 -0.00202 0.00175
AFIX 23
H33A 2 0.516999 -0.047481 0.135610 11.00000 -1.20000
H33B 2 0.495425 0.161009 0.134442 11.00000 -1.20000
AFIX 0

```
C34     1       0.523076        0.082153        0.178754        11.00000        0.04149
0.04472 =
            0.04006     0.00039     -0.00156    0.00310
AFIX   23
H34A   2    0.528348    0.209873    0.185856    11.00000    -1.20000
H34B   2    0.556082    0.009692    0.187103    11.00000    -1.20000
AFIX    0
C35     1       0.466880        0.008696        0.192497        11.00000        0.04366
0.05243 =
            0.04882     -0.00471    -0.00014    0.00018
AFIX   23
H35A   2    0.434673    0.094541    0.187794    11.00000    -1.20000
H35B   2    0.457509    -0.109964   0.182543    11.00000    -1.20000
AFIX    0
C36     1       0.471556        -0.016597       0.227557        11.00000        0.05052
0.07044 =
            0.04908     -0.00104    0.00992     0.00219
AFIX 137
H36A   2    0.434983    -0.067560   0.235640    11.00000    -1.50000
H36B   2    0.479008    0.101735    0.237550    11.00000    -1.50000
H36C   2    0.503718    -0.100411   0.232277    11.00000    -1.50000
AFIX    0
N7      3       0.542465        0.037284        0.023665        11.00000        0.03490
0.03629 =
            0.03121     0.00215     -0.00100    -0.00245
N8      3       0.582869        0.134176        0.133060        11.00000        0.03849
0.04203 =
            0.03652     -0.00028    -0.00361    -0.00126
H3N    2    0.610098    0.174622    0.148546    11.00000    -1.20000
N9      3       0.698151        0.271562        0.116430        11.00000        0.03952
0.04306 =
            0.04514     0.00158     -0.00857    0.00068
O5      4       0.687233        0.258586        0.145322        11.00000        0.04671
0.05546 =
            0.04013     -0.00156    -0.00901    -0.00124
O6      4       0.743704        0.346215        0.106989        11.00000        0.04014
0.06330 =
            0.05803     0.00661     -0.00879    -0.01288
HKLF 4 1 -1.0000    0.0000    0.0000    0.0000    1.0000    0.0000    0.0000    0.0000 -1.0000

REM    db1_a.res Pbca
REM R1 =    0.0425 for       5944 Fo > 4sig(Fo)    and    0.0469 for all       6453 data
REM       473 parameters refined using          0 restraints
```

```
END

WGHT      0.0522      2.4291

REM Instructions for potential hydrogen bonds
HTAB C1 O5_$1
HTAB C1 O6_$2
HTAB C2 O5_$2
HTAB C9 O3_$1
HTAB C10 O4_$1
HTAB N3 O1
HTAB N4 O3
HTAB C25 O1_$3
HTAB N8 O5

REM Highest difference peak  0.197,  deepest hole -0.183,  1-sigma level  0.033
Q1    1   0.0275  0.5441  0.4096  11.00000  0.05    0.20
Q2    1   0.6498  0.2317  0.1540  11.00000  0.05    0.19
Q3    1  -0.0108  0.5800  0.3952  11.00000  0.05    0.18
Q4    1   0.2999  0.6242  0.2145  11.00000  0.05    0.17
Q5    1   0.4604  0.3028  0.1333  11.00000  0.05    0.17
Q6    1   0.4689 -0.0709  0.0179  11.00000  0.05    0.16
Q7    1   0.1377  0.7032  0.3356  11.00000  0.05    0.16
Q8    1   0.5430  0.0770  0.0105  11.00000  0.05    0.16
Q9    1   0.1802  0.5348  0.4358  11.00000  0.05    0.15
Q10   1   0.2481  0.6694  0.2197  11.00000  0.05    0.15
Q11   1   0.0994  0.6408  0.3427  11.00000  0.05    0.15
Q12   1   0.6447  0.3515  0.0687  11.00000  0.05    0.15
Q13   1   0.4626  0.1361  0.1994  11.00000  0.05    0.15
Q14   1   0.2313  0.7105  0.2445  11.00000  0.05    0.15
Q15   1   0.3327  0.6630  0.2333  11.00000  0.05    0.14
Q16   1  -0.0030  0.4822  0.3932  11.00000  0.05    0.14
Q17   1   0.2679  0.7133  0.2669  11.00000  0.05    0.14
Q18   1   0.1999  0.7418  0.2960  11.00000  0.05    0.14
Q19   1   0.6106  0.2990  0.0453  11.00000  0.05    0.14
Q20   1   0.4503  0.2048  0.1637  11.00000  0.05    0.14
;
_shelx_res_checksum      77399
```