2-(3,5-dimethyl-1*H*-pyrazol-1-yl)thiazolo[4,5-*b*]pyridine

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checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

```
Bond precision:  C-C = 0.0031 A          Wavelength=0.71073

Cell:             a=11.863(7)     b=10.910(7)     c=16.519(10)
                  alpha=90        beta=90         gamma=90
Temperature:      296 K
```

	Calculated	Reported
Volume	2138(2)	2138(2)
Space group	P b c a	Pbca
Hall group	-P 2ac 2ab	?
Moiety formula	C11 H10 N4 S	?
Sum formula	C11 H10 N4 S	C11 H10 N4 S
Mr	230.29	230.29
Dx,g cm-3	1.431	1.431
Z	8	8
Mu (mm-1)	0.278	0.278
F000	960.0	960.0
F000’	961.23	
h,k,lmax	14,13,20	14,13,19
Nref	1989	1987
Tmin,Tmax	0.882,0.965	0.885,0.965
Tmin’	0.882	

```
Correction method= # Reported T Limits: Tmin=0.885 Tmax=0.965
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 25.500

R(reflections)= 0.0418( 1387)     wR2(reflections)= 0.1166( 1987)

S = 1.027                 Npar= 147
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT048_ALERT_1_C MoietyFormula Not Given (or Incomplete) ........     Please Check
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....     Please Do !
```

Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2018 Note
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
           _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
           _publ_contact_author_phone are all missing.
           At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
           e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
           Abstract of paper in English.
```

Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
           empty.
```

7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

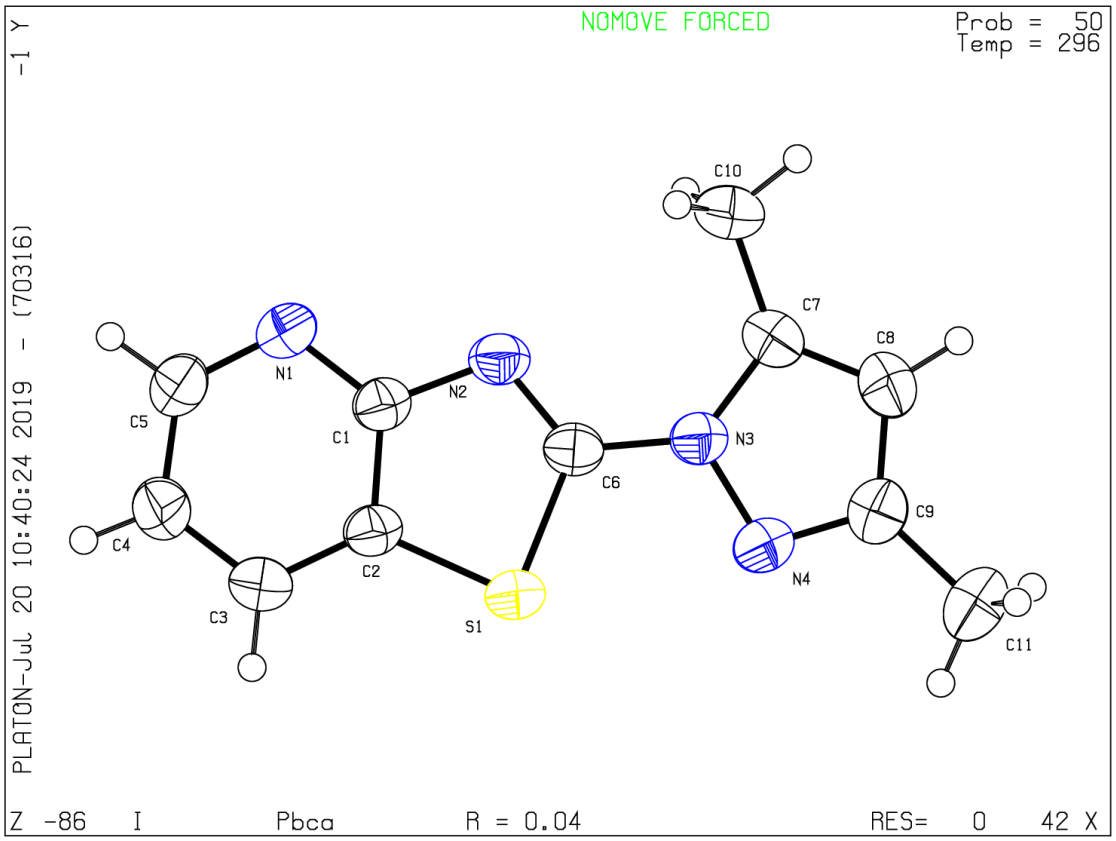
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
```

```
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

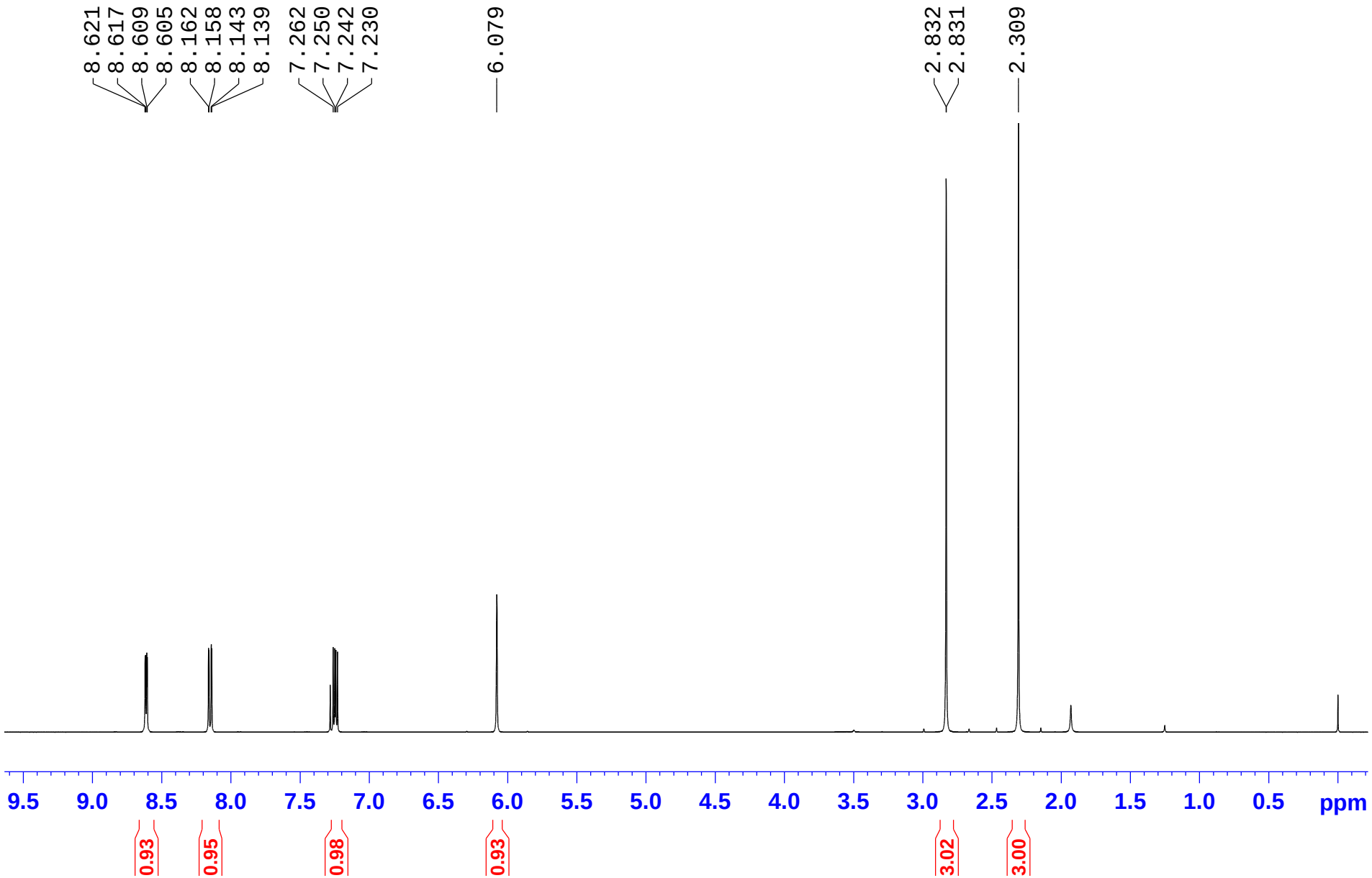
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

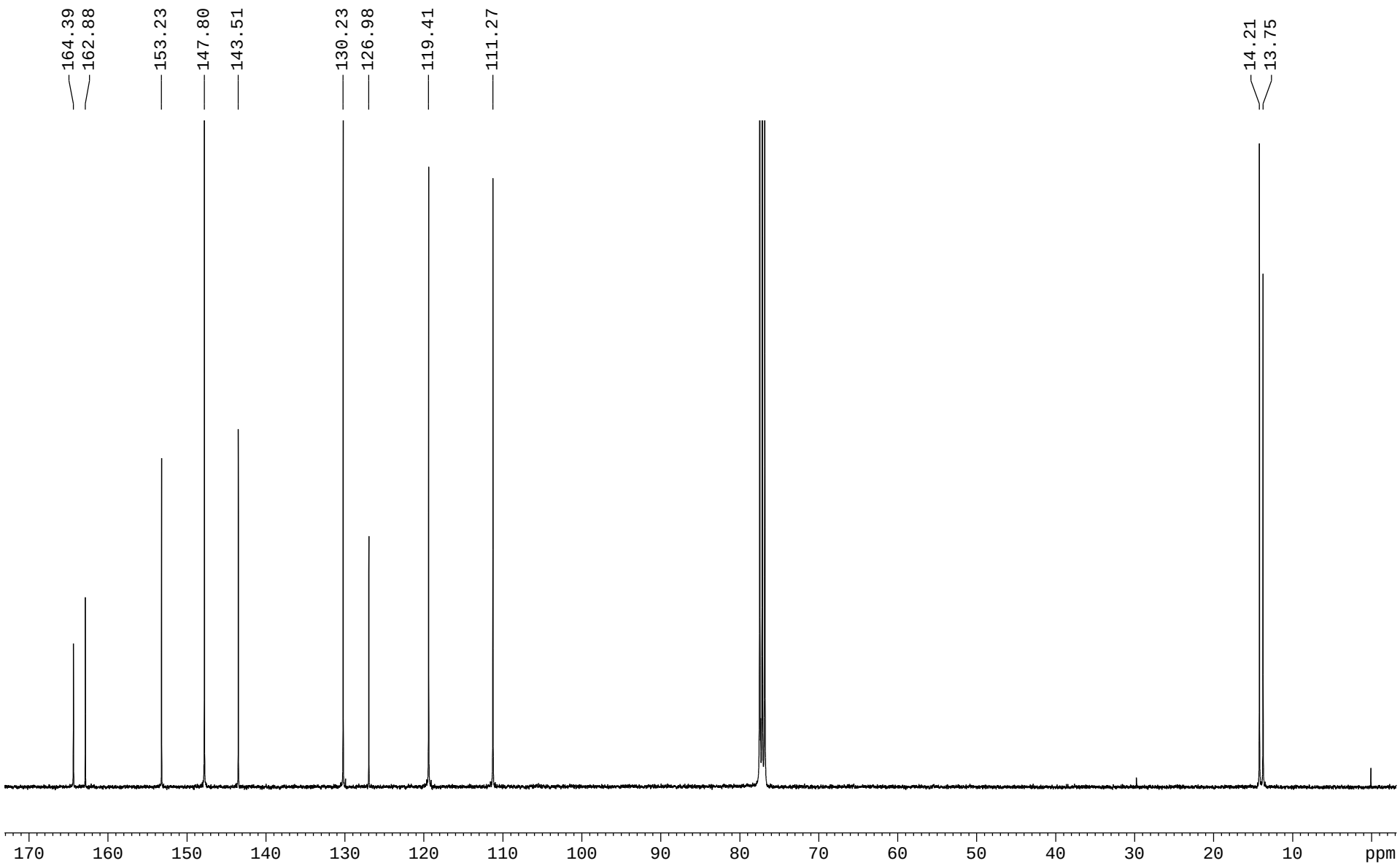
Datablock I - ellipsoid plot



m-01
20190606-13



m-01
20190606-13c



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;
_chemical_name_common                   ?
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_chemical_formula_moiety                ?
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 'C11 H10 N4 S'
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 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'    'C'     0.0033     0.0016
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'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'

'S' 'S' 0.1246 0.1234

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting Orthorhombic

_symmetry_space_group_name_H-M Pbca

loop_

_symmetry_equiv_pos_as_xyz

'x, y, z'

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

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

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

'-x, -y, -z'

'x-1/2, y, -z-1/2'

'x, -y-1/2, z-1/2'

'-x-1/2, y-1/2, z'

_cell_length_a	11.863(7)
_cell_length_b	10.910(7)
_cell_length_c	16.519(10)
_cell_angle_alpha	90.00
_cell_angle_beta	90.00
_cell_angle_gamma	90.00
_cell_volume	2138(2)
_cell_formula_units_Z	8
_cell_measurement_temperature	296(2)
_cell_measurement_reflns_used	1751
_cell_measurement_theta_min	2.82
_cell_measurement_theta_max	20.62

_exptl_crystal_description	block
_exptl_crystal_colour	colourless
_exptl_crystal_size_max	0.45
_exptl_crystal_size_mid	0.38
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_exptl_crystal_F_000	960

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_exptl_absorpt_process_details sadabs

_exptl_special_details

;

?

;

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_diffrn_radiation_wavelength 0.71073

_diffrn_radiation_type MoK\a

_diffrn_radiation_source 'fine-focus sealed tube'

_diffrn_radiation_monochromator graphite

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_diffrn_standards_interval_time 0

_diffrn_standards_decay_% 0

_diffrn_reflns_number 14815

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_diffrn_reflns_av_sigmaI/netI 0.0356

_diffrn_reflns_limit_h_min -14

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_diffrn_reflns_limit_k_min -13

_diffrn_reflns_limit_k_max 13

_diffrn_reflns_limit_l_min -19

_diffrn_reflns_limit_l_max 19

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_reflns_number_gt 1387

_reflns_threshold_expression >2sigma(I)

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_computing_cell_refinement 'Bruker SMART'

_computing_data_reduction 'Bruker SAINT'

_computing_structure_solution 'SHELXS-97 (Sheldrick, 1990)'

_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'

_computing_molecular_graphics 'Bruker SHELXTL'

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_computing_publication_material      'Bruker SHELXTL'


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


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_refine_ls_matrix_type                    full
_refine_ls_weighting_scheme            calc
_refine_ls_weighting_details
  'calc w=1/[\s^2^(Fo^2^)+(0.0575P)^2^+0.5423P] 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         constr
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_refine_ls_extinction_method none

_refine_ls_extinction_coef ?

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_refine_ls_number_restraints 0

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_refine_ls_restrained_S_all 1.027

_refine_ls_shift/su_max 0.003

_refine_ls_shift/su_mean 0.000

loop_

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_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

C1 C 0.75038(19) 0.2604(2) 0.75458(14) 0.0407(5) Uani 1 1 d . . .

C2 C 0.63252(18) 0.2526(2) 0.76039(14) 0.0403(5) Uani 1 1 d . . .

C3 C 0.5753(2) 0.3294(2) 0.81208(15) 0.0506(7) Uani 1 1 d . . .

H3 H 0.4973 0.3256 0.8176 0.061 Uiso 1 1 calc R . .

C4 C 0.6389(2) 0.4122(2) 0.85534(17) 0.0545(7) Uani 1 1 d . . .

H4 H 0.6044 0.4657 0.8915 0.065 Uiso 1 1 calc R . .

C5 C 0.7547(2) 0.4152(2) 0.84450(16) 0.0561(7) Uani 1 1 d . . .

H5 H 0.7953 0.4732 0.8737 0.067 Uiso 1 1 calc R . .

C6 C 0.72114(19) 0.1120(2) 0.66926(14) 0.0391(6) Uani 1 1 d . . .

C7 C 0.83690(19) -0.0381(2) 0.58830(14) 0.0436(6) Uani 1 1 d . . .

C8 C 0.8014(2) -0.1276(2) 0.53714(15) 0.0504(6) Uani 1 1 d . . .

H8 H 0.8472 -0.1826 0.5094 0.060 Uiso 1 1 calc R . .

C9 C 0.6839(2) -0.1223(2) 0.53367(15) 0.0477(6) Uani 1 1 d . . .

C10 C 0.9512(2) -0.0053(2) 0.61696(17) 0.0576(7) Uani 1 1 d . . .

H10A H 1.0054 -0.0600 0.5933 0.086 Uiso 1 1 calc R . .

H10B H 0.9542 -0.0121 0.6749 0.086 Uiso 1 1 calc R . .

H10C H 0.9682 0.0774 0.6013 0.086 Uiso 1 1 calc R . .

C11 C 0.6040(3) -0.2008(3) 0.48720(17) 0.0656(8) Uani 1 1 d . . .

H11A H 0.5287 -0.1700 0.4936 0.098 Uiso 1 1 calc R . .

H11B H 0.6078 -0.2834 0.5071 0.098 Uiso 1 1 calc R . .

H11C H 0.6241 -0.1996 0.4309 0.098 Uiso 1 1 calc R . .

N1 N 0.81235(17) 0.34121(19) 0.79546(13) 0.0526(6) Uani 1 1 d . . .

N2 N 0.79992(16) 0.17754(18) 0.70149(11) 0.0434(5) Uani 1 1 d . . .

N3 N 0.73945(16) 0.01897(17) 0.61341(11) 0.0423(5) Uani 1 1 d . . .

N4 N 0.64472(16) -0.03325(19) 0.57962(12) 0.0476(5) Uani 1 1 d . . .

S1 S 0.58214(5) 0.14014(6) 0.69659(4) 0.0469(2) 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

C1 0.0368(12) 0.0414(12) 0.0437(13) 0.0010(11) -0.0037(11) -0.0013(11)

C2 0.0343(12) 0.0425(13) 0.0441(14) 0.0011(11) -0.0044(10) -0.0009(11)

C3 0.0369(13) 0.0565(16) 0.0583(16) -0.0049(13) -0.0026(12) 0.0041(12)

C4 0.0503(16) 0.0548(16) 0.0585(17) -0.0129(14) -0.0054(13) 0.0096(13)

C5 0.0513(17) 0.0523(16) 0.0647(17) -0.0158(13) -0.0114(13) 0.0000(13)

C6 0.0356(13) 0.0412(13) 0.0405(13) 0.0054(10) 0.0013(10) -0.0012(10)

C7 0.0414(14) 0.0480(14) 0.0416(13) 0.0047(12) 0.0033(11) 0.0057(11)

C8 0.0546(16) 0.0506(15) 0.0461(15) -0.0040(13) 0.0048(12) 0.0065(12)

C9 0.0555(17) 0.0455(15) 0.0420(14) 0.0022(12) -0.0017(12) -0.0031(12)

C10 0.0368(14) 0.0681(18) 0.0680(17) -0.0042(14) -0.0029(13) 0.0060(13)

C11 0.072(2) 0.0590(18) 0.0656(19) -0.0107(15) -0.0106(15) -0.0116(15)

N1 0.0397(12) 0.0535(13) 0.0647(15) -0.0127(11) -0.0074(10) -0.0033(10)

N2 0.0334(11) 0.0495(12) 0.0473(12) -0.0001(10) 0.0015(9) -0.0035(9)

N3 0.0349(11) 0.0486(12) 0.0435(11) -0.0035(9) 0.0007(9) -0.0026(9)

N4 0.0391(11) 0.0527(13) 0.0511(12) -0.0051(11) -0.0033(9) -0.0059(9)

S1 0.0315(3) 0.0544(4) 0.0549(4) -0.0084(3) 0.0002(3) -0.0046(3)

_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

C1 N1 1.332(3) . ?

C1 N2 1.390(3) . ?

C1 C2 1.404(3) . ?

C2 C3 1.376(3) . ?

C2 S1 1.724(3) . ?

C3 C4 1.377(3) . ?

C3 H3 0.9300 . ?

C4 C5 1.386(3) . ?

C4 H4 0.9300 . ?

C5 N1 1.332(3) . ?

C5 H5 0.9300 . ?

C6 N2 1.291(3) . ?

C6 N3 1.389(3) . ?

C6 S1 1.737(2) . ?

C7 C8 1.359(3) . ?

C7 N3 1.377(3) . ?

C7 C10 1.480(3) . ?

C8 C9 1.397(4) . ?

C8 H8 0.9300 . ?

C9 N4 1.317(3) . ?

C9 C11 1.490(3) . ?

C10 H10A 0.9600 . ?

C10 H10B 0.9600 . ?

C10 H10C 0.9600 . ?

C11 H11A 0.9600 . ?

C11 H11B 0.9600 . ?

C11 H11C 0.9600 . ?

N3 N4 1.378(3) . ?

loop_

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_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

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_geom_angle_site_symmetry_1

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

N1 C1 N2 121.1(2) . . ?

N1 C1 C2 123.7(2) . . ?

N2 C1 C2 115.2(2) . . ?

C3 C2 C1 119.8(2) . . ?

C3 C2 S1 129.93(19) . . ?

C1 C2 S1 110.27(18) . . ?

C2 C3 C4 116.8(2) . . ?

C2 C3 H3 121.6 . . ?

C4 C3 H3 121.6 . . ?

C3 C4 C5 119.4(2) . . ?

C3 C4 H4 120.3 . . ?

C5 C4 H4 120.3 . . ?

N1 C5 C4 125.0(2) . . ?

N1 C5 H5 117.5 . . ?

C4 C5 H5 117.5 . . ?

N2 C6 N3 124.4(2) . . ?

N2 C6 S1 118.82(18) . . ?

N3 C6 S1 116.76(17) . . ?

C8 C7 N3 104.6(2) . . ?

C8 C7 C10 131.0(2) . . ?

N3 C7 C10 124.3(2) . . ?

C7 C8 C9 107.8(2) . . ?

C7 C8 H8 126.1 . . ?

C9 C8 H8 126.1 . . ?

N4 C9 C8 111.0(2) . . ?

N4 C9 C11 119.8(2) . . ?

C8 C9 C11 129.2(3) . . ?

C7 C10 H10A 109.5 . . ?

C7 C10 H10B 109.5 . . ?

H10A C10 H10B 109.5 . . ?

C7 C10 H10C 109.5 . . ?

H10A C10 H10C 109.5 . . ?

H10B C10 H10C 109.5 . . ?

C9 C11 H11A 109.5 . . ?

C9 C11 H11B 109.5 . . ?

H11A C11 H11B 109.5 . . ?

C9 C11 H11C 109.5 . . ?

H11A C11 H11C 109.5 . . ?

H11B C11 H11C 109.5 . . ?

C5 N1 C1 115.2(2) . . ?

C6 N2 C1 108.30(19) . . ?

C7 N3 N4 112.06(19) . . ?

C7 N3 C6 131.5(2) . . ?

N4 N3 C6 116.34(19) . . ?

C9 N4 N3 104.5(2) . . ?

C2 S1 C6 87.45(11) . . ?

loop_

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_geom_torsion_atom_site_label_4

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_geom_torsion_site_symmetry_2

_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

_geom_torsion_publ_flag

N1 C1 C2 C3 -1.6(4) . . . . ?

N2 C1 C2 C3 179.1(2) . . . . ?

N1 C1 C2 S1 178.32(19) . . . . ?

N2 C1 C2 S1 -0.9(3) . . . . ?

C1 C2 C3 C4 0.7(4) . . . . ?

S1 C2 C3 C4 -179.2(2) . . . . ?

C2 C3 C4 C5 0.6(4) . . . . ?

C3 C4 C5 N1 -1.3(4) . . . . ?

N3 C7 C8 C9 -0.5(3) . . . . ?

C10 C7 C8 C9 177.1(3) . . . . ?

C7 C8 C9 N4 0.5(3) . . . . ?

C7 C8 C9 C11 -179.3(2) . . . . ?

C4 C5 N1 C1 0.5(4) . . . . ?

N2 C1 N1 C5 -179.8(2) . . . . ?

C2 C1 N1 C5 1.0(4) . . . . ?

N3 C6 N2 C1 -179.6(2) . . . . ?

S1 C6 N2 C1 0.4(3) . . . . ?

N1 C1 N2 C6 -178.9(2) . . . . ?

C2 C1 N2 C6 0.4(3) . . . . ?

C8 C7 N3 N4 0.4(3) . . . . ?

C10 C7 N3 N4 -177.5(2) . . . . ?

C8 C7 N3 C6 175.7(2) . . . . ?

C10 C7 N3 C6 -2.1(4) . . . . ?

N2 C6 N3 C7 10.9(4) . . . . ?

S1 C6 N3 C7 -169.1(2) . . . . ?

N2 C6 N3 N4 -173.9(2) . . . . ?

S1 C6 N3 N4 6.1(3) . . . . ?

C8 C9 N4 N3 -0.3(3) . . . . ?

C11 C9 N4 N3 179.6(2) . . . . ?

C7 N3 N4 C9 -0.1(3) . . . . ?

C6 N3 N4 C9 -176.18(19) . . . . ?

C3 C2 S1 C6 -179.2(3) . . . . ?

C1 C2 S1 C6 0.86(18) . . . . ?

N2 C6 S1 C2 -0.8(2) . . . . ?

N3 C6 S1 C2 179.18(18) . . . . ?

_diffrn_measured_fraction_theta_max 0.999

_diffrn_reflns_theta_full 25.50

_diffrn_measured_fraction_theta_full 0.999

_refine_diff_density_max 0.190

_refine_diff_density_min -0.256

_refine_diff_density_rms 0.049