```
data_General
_audit_creation_date              '2009-01-15'
_audit_creation_method            'by CrystalStructure v3.5.1'
_audit_update_record              ?

#=============================================================================
=

# PROCESSING SUMMARY (IUCr Office Use Only)

_journal_date_recd_electronic    ?
_journal_date_from_coeditor      ?
_journal_date_accepted           ?
_journal_coeditor_code           ?

#=============================================================================
=

# SUBMISSION DETAILS

_publ_contact_author_name          'Dr.M.Cgdem Sayil'
_publ_contact_author_email         'sayil@istanbul.edu.tr'
_publ_contact_author_fax           'ENTER FAX NUMBER'
_publ_contact_author_phone         'ENTER PHONE NUMBER'
_publ_contact_letter
;
ENTER TEXT OF LETTER
;
_publ_requested_journal            'ENTER JOURNAL NAME HERE'
_publ_requested_category           'CHOOSE FI FM FO CI CM CO or AD'
_publ_requested_coeditor_name      ?

#=============================================================================
=

# TITLE AND AUTHOR LIST

_publ_section_title
;
ENTER SECTION TITLE
;
_publ_section_title_footnote
```

```
;
ENTER FOOTNOTE TO TITLE OF PAPER
;
loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
'Tavman, Aydin'  .
; Istanbul University
Faculty of Engineering
Department of Chemistry
34320 Avcilar-Istanbul
Turkey
;
'Sayil, Cigdem'  .
; Istanbul University
Faculty of Engineering
Department of Chemistry
34320 Avcilar-Istanbul
Turkey
;
_publ_section_synopsis
;
ENTER SYNOPSIS
;

#==============================================================================
=

# TEXT

_publ_section_abstract
;
ENTER ABSTRACT
;
_publ_section_comment
;
ENTER TEXT
;
_publ_section_references
;
ENTER OTHER REFERENCES
```

Rigaku/MSC and Rigaku Corporation. (2003).
CrystalStructure.
Single Crystal Structure Analysis Software. Version 3.5.1.
Rigaku/MSC, 9009 New Trails Drive, The Woodlands, TX, USA 77381-5209.
Rigaku, 3-9-12 Akishima, Tokyo 196-8666, Japan.

Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. (1996)
CRYSTALS Issue 10, Chemical Crystallography Laboratory, Oxford, UK.

Carruthers, J.R. and Watkin, D.J. (1979), Acta Cryst, A35, 698-699
;
_publ_section_figure_captions
;
ENTER FIGURE CAPTIONS
;
_publ_section_exptl_prep
;
ENTER COMPOUND PREPARATION DETAILS
;
_publ_section_exptl_refinement
;
ENTER SPECIAL DETAILS OF THE REFINEMENT
;

#==========
=

data___AydinTavmanEBB2HClson

#==========
=

CHEMICAL DATA

_chemical_formula_sum	'C16 H16 Cl2 N4 '
_chemical_formula_moiety	'C16 H16 Cl2 N4 '
_chemical_formula_weight	335.23
_chemical_melting_point	?

#==========
=

```
# CRYSTAL DATA
_symmetry_cell_setting              triclinic
_symmetry_space_group_name_H-M      'P -1      '
_symmetry_space_group_name_Hall     '-P 1'
_symmetry_Int_Tables_number         2
loop_
_symmetry_equiv_pos_as_xyz
'x,y,z'
'-x,-y,-z'

#------------------------------------------------------------------------------

_cell_length_a                      7.13500
_cell_length_b                      9.6299(1)
_cell_length_c                      15.3340(7)
_cell_angle_alpha                   80.67(2)
_cell_angle_beta                    79.66(2)
_cell_angle_gamma                   68.395(11)
_cell_volume                        958.33(10)
_cell_formula_units_Z               2
_cell_measurement_reflns_used       4181
_cell_measurement_theta_min         2.7
_cell_measurement_theta_max         25.0
_cell_measurement_temperature       294

#------------------------------------------------------------------------------

_exptl_crystal_description          'block'
_exptl_crystal_colour               'colorless'
_exptl_crystal_size_max             0.40
_exptl_crystal_size_mid             0.30
_exptl_crystal_size_min             0.10
_exptl_crystal_density_diffrn       1.162
_exptl_crystal_density_meas         ?
_exptl_crystal_density_method       'not measured'
_exptl_crystal_F_000                348.00
_exptl_absorpt_coefficient_mu       0.339
_exptl_absorpt_correction_type      multi-scan
_exptl_absorpt_process_details
;
Higashi, T. (1995). Program for Absorption Correction.
```

Rigaku Corporation, Tokyo, Japan.
;
_exptl_absorpt_correction_T_min 0.885
_exptl_absorpt_correction_T_max 0.967

#==========
=

EXPERIMENTAL DATA

_diffrn_ambient_temperature 293.1
_diffrn_radiation_type 'Mo K\a'
_diffrn_radiation_wavelength 0.7107
_diffrn_measurement_device_type 'Rigaku RAXIS-UNKNOWN'
_diffrn_measurement_method \w
_diffrn_detector_area_resol_mean 10.00
_diffrn_reflns_number 47668
_diffrn_reflns_av_R_equivalents 0.109
_diffrn_reflns_theta_max 25.07
_diffrn_measured_fraction_theta_max 0.9953
_diffrn_reflns_theta_full 25.07
_diffrn_measured_fraction_theta_full 0.9953
_diffrn_reflns_limit_h_min -8
_diffrn_reflns_limit_h_max 8
_diffrn_reflns_limit_k_min -11
_diffrn_reflns_limit_k_max 11
_diffrn_reflns_limit_l_min -18
_diffrn_reflns_limit_l_max 18

#==========
=

REFINEMENT DATA

_refine_special_details
;
Refinement using reflections with F^2^ > 3.0 sigma(F^2^).
The weighted R-factor(wR), goodness of fit (S) and R-factor (gt) are
based on F, with F set to zero for negative F. The threshold expression of
F^2^ > 2.0 sigma(F^2^) is used only for calculating R-factor (gt).
;
_reflns_number_total 3414

```
_reflns_number_gt                    2886
_reflns_threshold_expression         F^2^>2.0\s(F^2^)
_refine_ls_structure_factor_coef     F
_refine_ls_R_factor_gt               0.0840
_refine_ls_wR_factor_ref             0.2190
_refine_ls_hydrogen_treatment        riding
_refine_ls_number_reflns             2886
_refine_ls_number_parameters         215
_refine_ls_goodness_of_fit_ref       1.125
_refine_ls_weighting_scheme          calc
_refine_ls_weighting_details
;
Chebychev polynomial with 3 parameters (Carruthers & Watkin, 1979)
15.8680    10.0543    9.9976
;
_refine_ls_shift/su_max              0.0000
_refine_diff_density_max             0.28
_refine_diff_density_min             -0.27
_refine_ls_extinction_method         none
_refine_ls_extinction_coef           ?

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
'C' 'C'  0.003 0.002
;
International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
'H' 'H'  0.000 0.000
;
International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.4)
;
'N' 'N'  0.006 0.003
;
International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
```

'Cl' 'Cl' 0.148 0.159
;
International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;

#==========
=

ATOMIC COORDINATES AND THERMAL PARAMETERS

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

Cl(1)	Cl	0.6845(5)	-0.5289(3)	0.5846(2)	0.0385(9)	Uani	1.00	1	d	.	.
Cl(2)	Cl	0.2679(7)	0.0128(4)	0.9033(3)	0.0543(12)	Uani	1.00	1	d	.	.
N(1)	N	0.256(2)	-0.3131(11)	0.9341(6)	0.033(3)	Uani	1.00	1	d	.	.
N(3)	N	0.327(1)	-0.2184(11)	0.5667(7)	0.028(2)	Uani	1.00	1	d	.	.
N(2)	N	0.311(2)	-0.5170(13)	0.8815(7)	0.037(3)	Uani	1.00	1	d	.	.
N(4)	N	0.124(2)	0.0002(11)	0.6130(6)	0.030(3)	Uani	1.00	1	d	.	.
C(16)	C	0.204(2)	0.0330(12)	0.5252(8)	0.031(3)	Uani	1.00	1	d	.	.
C(1)	C	0.269(2)	-0.5430(13)	0.9737(9)	0.035(3)	Uani	1.00	1	d	.	.
C(7)	C	0.301(2)	-0.3789(13)	0.8589(8)	0.030(3)	Uani	1.00	1	d	.	.
C(10)	C	0.212(2)	-0.150(1)	0.6338(7)	0.030(3)	Uani	1.00	1	d	.	.
C(2)	C	0.232(2)	-0.4140(13)	1.0070(7)	0.029(3)	Uani	1.00	1	d	.	.
C(11)	C	0.320(2)	-0.1059(13)	0.4975(8)	0.029(3)	Uani	1.00	1	d	.	.
C(14)	C	0.259(2)	0.1593(13)	0.3823(9)	0.032(3)	Uani	1.00	1	d	.	.
C(8)	C	0.363(2)	-0.3091(11)	0.7672(6)	0.020(2)	Uani	1.00	1	d	.	.
C(12)	C	0.424(2)	-0.1143(12)	0.4063(8)	0.034(3)	Uani	1.00	1	d	.	.
C(3)	C	0.187(2)	-0.395(1)	1.1001(7)	0.029(3)	Uani	1.00	1	d	.	.
C(5)	C	0.221(3)	-0.655(2)	1.1178(11)	0.053(5)	Uani	1.00	1	d	.	.

C(13)	C	0.384(2)	0.022(2)	0.3531(9)	0.046(4)	Uani	1.00	1	d . . .
C(15)	C	0.169(3)	0.166(2)	0.4706(8)	0.045(4)	Uani	1.00	1	d . . .
C(9)	C	0.157(2)	-0.233(2)	0.7217(7)	0.038(3)	Uani	1.00	1	d . . .
C(6)	C	0.251(2)	-0.6721(13)	1.0277(9)	0.041(4)	Uani	1.00	1	d . . .
C(4)	C	0.180(2)	-0.519(1)	1.1528(9)	0.034(3)	Uani	1.00	1	d . . .
H(1)	H	0.157(2)	-0.301(1)	1.1220(7)	0.034(4)	Uiso	1.00	1	d . . .
H(2)	H	0.162(2)	-0.517(1)	1.2155(9)	0.040(4)	Uiso	1.00	1	d . . .
H(3)	H	0.210(3)	-0.738(2)	1.1585(11)	0.066(6)	Uiso	1.00	1	d . . .
H(4)	H	0.262(2)	-0.7606(13)	1.0043(9)	0.047(4)	Uiso	1.00	1	d . . .
H(5)	H	0.250(2)	-0.2231(11)	0.9372(6)	0.042(4)	Uiso	1.00	1	d . . .
H(6)	H	0.326(2)	-0.5799(13)	0.8447(7)	0.050(4)	Uiso	1.00	1	d . . .
H(7)	H	0.422(2)	-0.2372(11)	0.7720(6)	0.021(3)	Uiso	1.00	1	d . . .
H(8)	H	0.456(2)	-0.3841(11)	0.7319(6)	0.021(3)	Uiso	1.00	1	d . . .
H(9)	H	0.062(2)	-0.161(2)	0.7588(7)	0.044(4)	Uiso	1.00	1	d . . .
H(10)	H	0.102(2)	-0.306(2)	0.7155(7)	0.044(4)	Uiso	1.00	1	d . . .
H(11)	H	0.395(1)	-0.3128(11)	0.5656(7)	0.032(3)	Uiso	1.00	1	d . . .
H(12)	H	0.055(2)	0.0643(11)	0.6503(6)	0.034(3)	Uiso	1.00	1	d . . .
H(13)	H	0.507(2)	-0.2074(12)	0.3843(8)	0.036(4)	Uiso	1.00	1	d . . .
H(14)	H	0.444(2)	0.020(2)	0.2926(9)	0.047(4)	Uiso	1.00	1	d . . .
H(15)	H	0.246(2)	0.2494(13)	0.3439(9)	0.039(4)	Uiso	1.00	1	d . . .
H(16)	H	0.076(3)	0.257(2)	0.4919(8)	0.057(5)	Uiso	1.00	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_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

Cl(1)	0.037(2)	0.027(2)	0.041(2)	-0.0055(12)	0.0014(12)	0.0034(12)
Cl(2)	0.074(3)	0.038(2)	0.060(2)	-0.030(2)	-0.020(2)	0.007(2)
N(1)	0.066(7)	0.025(5)	0.013(4)	-0.024(5)	0.002(4)	-0.004(4)
N(3)	0.025(5)	0.022(5)	0.034(5)	-0.005(4)	-0.001(4)	-0.005(4)
N(2)	0.033(5)	0.061(7)	0.030(5)	-0.025(5)	0.004(4)	-0.027(5)
N(4)	0.033(5)	0.032(5)	0.020(5)	-0.009(4)	-0.005(4)	0.004(4)
C(16)	0.027(6)	0.016(5)	0.044(7)	-0.006(5)	-0.013(5)	0.016(5)
C(1)	0.021(5)	0.030(6)	0.038(7)	-0.004(5)	0.012(5)	0.006(5)
C(7)	0.028(6)	0.030(6)	0.027(6)	-0.014(5)	0.010(4)	0.000(5)
C(10)	0.044(7)	0.034(6)	0.010(5)	-0.017(5)	0.001(4)	0.005(4)
C(2)	0.037(6)	0.031(6)	0.022(6)	-0.008(5)	-0.019(5)	0.002(5)

```
C(11)  0.025(5)   0.027(6)   0.047(7)   -0.018(5)  -0.017(5)  -0.000(5)
C(14)  0.029(6)   0.020(6)   0.047(7)   -0.015(5)  -0.005(5)  0.012(5)
C(8)   0.024(5)   0.017(5)   0.011(5)   -0.005(4)  0.004(4)   0.009(4)
C(12)  0.037(7)   0.016(5)   0.038(7)   0.001(5)   0.007(5)   -0.009(5)
C(3)   0.023(5)   0.043(7)   0.020(5)   -0.010(5)  -0.000(4)  -0.010(5)
C(5)   0.072(10)  0.045(8)   0.049(9)   -0.019(7)  -0.029(8)  -0.006(7)
C(13)  0.052(8)   0.032(7)   0.032(7)   0.016(6)   -0.013(6)  -0.009(5)
C(15)  0.068(9)   0.057(9)   0.017(6)   -0.035(8)  -0.011(6)  0.014(6)
C(9)   0.057(8)   0.046(7)   0.008(5)   -0.018(6)  -0.000(5)  -0.001(5)
C(6)   0.053(8)   0.016(6)   0.049(8)   -0.015(6)  -0.004(6)  0.020(5)
C(4)   0.023(6)   0.034(6)   0.042(7)   -0.009(5)  -0.004(5)  0.004(5)

#==============================================================================
=

_computing_data_collection          'PROCESS'
_computing_cell_refinement          'PROCESS'
_computing_data_reduction           'CrystalStructure'
_computing_structure_solution       'SIR92'
_computing_structure_refinement     'CRYSTALS'
_computing_publication_material     'CrystalStructure Ver. 3.5.1'
_computing_molecular_graphics       ?

#==============================================================================
=

# MOLECULAR GEOMETRY

_geom_special_details
;
ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_publ_flag
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
N(1)    C(7)    1.34(2)   yes  . .
N(1)    C(2)    1.39(1)   yes  . .
```

N(1)	H(5)	0.86(2)	no	. .
N(3)	C(10)	1.30(1)	yes	. .
N(3)	C(11)	1.38(1)	yes	. .
N(3)	H(11)	0.86(1)	no	. .
N(2)	C(1)	1.39(2)	yes	. .
N(2)	C(7)	1.30(2)	yes	. .
N(2)	H(6)	0.86(2)	no	. .
N(4)	C(16)	1.40(1)	yes	. .
N(4)	C(10)	1.35(1)	yes	. .
N(4)	H(12)	0.86(1)	no	. .
C(16)	C(11)	1.38(2)	yes	. .
C(16)	C(15)	1.38(2)	yes	. .
C(1)	C(2)	1.34(2)	yes	. .
C(1)	C(6)	1.41(2)	yes	. .
C(7)	C(8)	1.52(1)	yes	. .
C(10)	C(9)	1.52(2)	yes	. .
C(2)	C(3)	1.43(2)	yes	. .
C(11)	C(12)	1.46(2)	yes	. .
C(14)	C(13)	1.39(2)	yes	. .
C(14)	C(15)	1.39(2)	yes	. .
C(14)	H(15)	0.95(2)	no	. .
C(8)	C(9)	1.61(2)	yes	. .
C(8)	H(7)	0.95(2)	no	. .
C(8)	H(8)	0.95(1)	no	. .
C(12)	C(13)	1.39(2)	yes	. .
C(12)	H(13)	0.95(2)	no	. .
C(3)	C(4)	1.34(2)	yes	. .
C(3)	H(1)	0.95(2)	no	. .
C(5)	C(6)	1.39(2)	yes	. .
C(5)	C(4)	1.40(2)	yes	. .
C(5)	H(3)	0.95(2)	no	. .
C(13)	H(14)	0.95(2)	no	. .
C(15)	H(16)	0.95(2)	no	. .
C(9)	H(9)	0.95(2)	no	. .
C(9)	H(10)	0.95(3)	no	. .
C(6)	H(4)	0.95(2)	no	. .
C(4)	H(2)	0.95(2)	no	. .
H(11)	Cl(1)	2.354(8)	no	. .

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3	_geom_angle	_geom_angle_publ_flag	_geom_angle_site_symmetry_1	_geom_angle_site_symmetry_2	_geom_angle_site_symmetry_3
C(7)	N(1)	C(2)	110.1(10)	yes	. . .
C(7)	N(1)	H(5)	125(1)	no	. . .
C(2)	N(1)	H(5)	124(1)	no	. . .
C(10)	N(3)	C(11)	104.9(9)	yes	. . .
C(10)	N(3)	H(11)	127(1)	no	. . .
C(11)	N(3)	H(11)	127(1)	no	. . .
C(1)	N(2)	C(7)	110(1)	yes	. . .
C(1)	N(2)	H(6)	124(1)	no	. . .
C(7)	N(2)	H(6)	124(1)	no	. . .
C(16)	N(4)	C(10)	106.7(8)	yes	. . .
C(16)	N(4)	H(12)	126(1)	no	. . .
C(10)	N(4)	H(12)	125(1)	no	. . .
C(11)	C(16)	C(15)	123(1)	yes	. . .
C(11)	C(16)	N(4)	104(1)	yes	. . .
C(15)	C(16)	N(4)	131(1)	yes	. . .
C(2)	C(1)	C(6)	122(1)	yes	. . .
C(2)	C(1)	N(2)	107(1)	yes	. . .
C(6)	C(1)	N(2)	130(1)	yes	. . .
C(8)	C(7)	N(1)	124(1)	yes	. . .
C(8)	C(7)	N(2)	127(1)	yes	. . .
N(1)	C(7)	N(2)	107(1)	yes	. . .
C(9)	C(10)	N(3)	122(1)	yes	. . .
C(9)	C(10)	N(4)	123.6(9)	yes	. . .
N(3)	C(10)	N(4)	113.2(9)	yes	. . .
C(3)	C(2)	N(1)	129(1)	yes	. . .
C(3)	C(2)	C(1)	124(1)	yes	. . .
N(1)	C(2)	C(1)	105(1)	yes	. . .
C(12)	C(11)	N(3)	130(1)	yes	. . .
C(12)	C(11)	C(16)	118(1)	yes	. . .
N(3)	C(11)	C(16)	110(1)	yes	. . .
C(13)	C(14)	C(15)	119(1)	yes	. . .
C(13)	C(14)	H(15)	120(1)	no	. . .
C(15)	C(14)	H(15)	119(1)	no	. . .
C(9)	C(8)	H(7)	111(1)	no	. . .
C(9)	C(8)	H(8)	108(1)	no	. . .
C(9)	C(8)	C(7)	105.6(9)	yes	. . .

H(7)	C(8)	H(8)	109(1)	no	. . .
H(7)	C(8)	C(7)	110(1)	no	. . .
H(8)	C(8)	C(7)	110(1)	no	. . .
C(13)	C(12)	H(13)	122(1)	no	. . .
C(13)	C(12)	C(11)	115(1)	yes	. . .
H(13)	C(12)	C(11)	121(1)	no	. . .
C(4)	C(3)	H(1)	123(1)	no	. . .
C(4)	C(3)	C(2)	113(1)	yes	. . .
H(1)	C(3)	C(2)	122(1)	no	. . .
C(6)	C(5)	C(4)	124(1)	yes	. . .
C(6)	C(5)	H(3)	117(2)	no	. . .
C(4)	C(5)	H(3)	117(1)	no	. . .
H(14)	C(13)	C(14)	117(1)	no	. . .
H(14)	C(13)	C(12)	117(1)	no	. . .
C(14)	C(13)	C(12)	124(1)	yes	. . .
H(16)	C(15)	C(16)	119(1)	no	. . .
H(16)	C(15)	C(14)	121(1)	no	. . .
C(16)	C(15)	C(14)	117(1)	yes	. . .
H(9)	C(9)	H(10)	109(1)	no	. . .
H(9)	C(9)	C(10)	108(1)	no	. . .
H(9)	C(9)	C(8)	107(1)	no	. . .
H(10)	C(9)	C(10)	113(1)	no	. . .
H(10)	C(9)	C(8)	110(1)	no	. . .
C(10)	C(9)	C(8)	106(1)	yes	. . .
H(4)	C(6)	C(1)	123(1)	no	. . .
H(4)	C(6)	C(5)	124(1)	no	. . .
C(1)	C(6)	C(5)	112(1)	yes	. . .
H(2)	C(4)	C(3)	118(1)	no	. . .
H(2)	C(4)	C(5)	119(1)	no	. . .
C(3)	C(4)	C(5)	121(1)	yes	. . .
Cl(1)	H(11)	N(3)	153(1)	no	. . .

```
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_publ_flag
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
```

_geom_torsion_site_symmetry_4

C(2)	N(1)	C(7)	N(2)	-1(1)	yes	. . . .
C(2)	N(1)	C(7)	C(8)	-172(1)	yes	. . . .
H(5)	N(1)	C(7)	N(2)	175(1)	no	. . . .
H(5)	N(1)	C(7)	C(8)	4(2)	no	. . . .
C(7)	N(1)	C(2)	C(1)	1(1)	yes	. . . .
C(7)	N(1)	C(2)	C(3)	178(1)	yes	. . . .
H(5)	N(1)	C(2)	C(1)	-175(1)	no	. . . .
H(5)	N(1)	C(2)	C(3)	1(2)	no	. . . .
C(11)	N(3)	C(10)	N(4)	2(1)	yes	. . . .
C(11)	N(3)	C(10)	C(9)	173(1)	yes	. . . .
H(11)	N(3)	C(10)	N(4)	-179.3(14)	no	. . . .
H(11)	N(3)	C(10)	C(9)	-8(2)	no	. . . .
C(10)	N(3)	C(11)	C(16)	1(1)	yes	. . . .
C(10)	N(3)	C(11)	C(12)	177(1)	yes	. . . .
H(11)	N(3)	C(11)	C(16)	-176(1)	no	. . . .
H(11)	N(3)	C(11)	C(12)	0(2)	no	. . . .
C(10)	N(3)	H(11)	Cl(1)	-86(2)	no	. . . .
C(11)	N(3)	H(11)	Cl(1)	91(2)	no	. . . .
C(7)	N(2)	C(1)	C(2)	0(1)	yes	. . . .
C(7)	N(2)	C(1)	C(6)	175(1)	yes	. . . .
H(6)	N(2)	C(1)	C(2)	-172(1)	no	. . . .
H(6)	N(2)	C(1)	C(6)	3(2)	no	. . . .
C(1)	N(2)	C(7)	N(1)	0(1)	yes	. . . .
C(1)	N(2)	C(7)	C(8)	171(1)	yes	. . . .
H(6)	N(2)	C(7)	N(1)	173(1)	no	. . . .
H(6)	N(2)	C(7)	C(8)	-16(2)	no	. . . .
C(10)	N(4)	C(16)	C(11)	5(1)	yes	. . . .
C(10)	N(4)	C(16)	C(15)	179.9(18)	yes	. . . .
H(12)	N(4)	C(16)	C(11)	172(1)	no	. . . .
H(12)	N(4)	C(16)	C(15)	-12(2)	no	. . . .
C(16)	N(4)	C(10)	N(3)	-5(1)	yes	. . . .
C(16)	N(4)	C(10)	C(9)	-175(1)	yes	. . . .
H(12)	N(4)	C(10)	N(3)	-172(1)	no	. . . .
H(12)	N(4)	C(10)	C(9)	16(2)	no	. . . .
N(4)	C(16)	C(11)	N(3)	-4(1)	yes	. . . .
N(4)	C(16)	C(11)	C(12)	178(1)	yes	. . . .
C(15)	C(16)	C(11)	N(3)	-179.7(16)	yes	. . . .
C(15)	C(16)	C(11)	C(12)	3(2)	yes	. . . .
N(4)	C(16)	C(15)	C(14)	-173(1)	yes	. . . .
N(4)	C(16)	C(15)	H(16)	0(3)	no	. . . .
C(11)	C(16)	C(15)	C(14)	0(2)	yes	. . . .

C(11)	C(16)	C(15)	H(16)	173(2)	no	. . . .
N(2)	C(1)	C(2)	N(1)	-1(1)	yes	. . . .
N(2)	C(1)	C(2)	C(3)	-178(1)	yes	. . . .
C(6)	C(1)	C(2)	N(1)	-177(1)	yes	. . . .
C(6)	C(1)	C(2)	C(3)	5(2)	yes	. . . .
N(2)	C(1)	C(6)	C(5)	176(1)	yes	. . . .
N(2)	C(1)	C(6)	H(4)	-2(2)	no	. . . .
C(2)	C(1)	C(6)	C(5)	-9(2)	yes	. . . .
C(2)	C(1)	C(6)	H(4)	172(1)	no	. . . .
N(1)	C(7)	C(8)	C(9)	-95(1)	yes	. . . .
N(1)	C(7)	C(8)	H(7)	25(1)	no	. . . .
N(1)	C(7)	C(8)	H(8)	147(1)	no	. . . .
N(2)	C(7)	C(8)	C(9)	95(1)	yes	. . . .
N(2)	C(7)	C(8)	H(7)	-143(1)	no	. . . .
N(2)	C(7)	C(8)	H(8)	-21(2)	no	. . . .
N(3)	C(10)	C(9)	C(8)	69(1)	yes	. . . .
N(3)	C(10)	C(9)	H(9)	-174(1)	no	. . . .
N(3)	C(10)	C(9)	H(10)	-52(2)	no	. . . .
N(4)	C(10)	C(9)	C(8)	-120(1)	yes	. . . .
N(4)	C(10)	C(9)	H(9)	-4(2)	no	. . . .
N(4)	C(10)	C(9)	H(10)	117(1)	no	. . . .
N(1)	C(2)	C(3)	C(4)	-178(1)	yes	. . . .
N(1)	C(2)	C(3)	H(1)	5(2)	no	. . . .
C(1)	C(2)	C(3)	C(4)	-2(1)	yes	. . . .
C(1)	C(2)	C(3)	H(1)	-178(1)	no	. . . .
N(3)	C(11)	C(12)	C(13)	179.6(14)	yes	. . . .
N(3)	C(11)	C(12)	H(13)	3(2)	no	. . . .
C(16)	C(11)	C(12)	C(13)	-4(2)	yes	. . . .
C(16)	C(11)	C(12)	H(13)	179.3(18)	no	. . . .
C(15)	C(14)	C(13)	C(12)	1(2)	yes	. . . .
C(15)	C(14)	C(13)	H(14)	-180(2)	no	. . . .
H(15)	C(14)	C(13)	C(12)	174(1)	no	. . . .
H(15)	C(14)	C(13)	H(14)	-5(3)	no	. . . .
C(13)	C(14)	C(15)	C(16)	-2(2)	yes	. . . .
C(13)	C(14)	C(15)	H(16)	-175(2)	no	. . . .
H(15)	C(14)	C(15)	C(16)	-175(1)	no	. . . .
H(15)	C(14)	C(15)	H(16)	10(3)	no	. . . .
C(7)	C(8)	C(9)	C(10)	174(1)	yes	. . . .
C(7)	C(8)	C(9)	H(9)	58(1)	no	. . . .
C(7)	C(8)	C(9)	H(10)	-61(1)	no	. . . .
H(7)	C(8)	C(9)	C(10)	54(1)	no	. . . .
H(7)	C(8)	C(9)	H(9)	-62(1)	no	. . . .

H(7)	C(8)	C(9)	H(10)	178(1)	no	. . . .
H(8)	C(8)	C(9)	C(10)	-66(1)	no	. . . .
H(8)	C(8)	C(9)	H(9)	177(1)	no	. . . .
H(8)	C(8)	C(9)	H(10)	57(1)	no	. . . .
C(11)	C(12)	C(13)	C(14)	1(2)	yes	. . . .
C(11)	C(12)	C(13)	H(14)	-177(2)	no	. . . .
H(13)	C(12)	C(13)	C(14)	178(1)	no	. . . .
H(13)	C(12)	C(13)	H(14)	-1(3)	no	. . . .
C(2)	C(3)	C(4)	C(5)	2(1)	yes	. . . .
C(2)	C(3)	C(4)	H(2)	175(1)	no	. . . .
H(1)	C(3)	C(4)	C(5)	178(1)	no	. . . .
H(1)	C(3)	C(4)	H(2)	-8(2)	no	. . . .
C(4)	C(5)	C(6)	C(1)	9(2)	yes	. . . .
C(4)	C(5)	C(6)	H(4)	-171(2)	no	. . . .
H(3)	C(5)	C(6)	C(1)	-178(1)	no	. . . .
H(3)	C(5)	C(6)	H(4)	0(3)	no	. . . .
C(6)	C(5)	C(4)	C(3)	-7(2)	yes	. . . .
C(6)	C(5)	C(4)	H(2)	-180(2)	no	. . . .
H(3)	C(5)	C(4)	C(3)	-178(2)	no	. . . .
H(3)	C(5)	C(4)	H(2)	8(3)	no	. . . .

loop_

_geom_contact_atom_site_label_1

_geom_contact_atom_site_label_2

_geom_contact_distance

_geom_contact_publ_flag

_geom_contact_site_symmetry_1

_geom_contact_site_symmetry_2

Cl(1)	N(3)	3.146(8)	yes	. 55501
Cl(1)	H(8)	2.781(9)	no	. 55501
Cl(1)	H(11)	2.354(8)	no	. 55501
Cl(1)	H(16)	3.06(1)	no	. 64501
Cl(2)	N(1)	3.13(1)	yes	. 55501
Cl(2)	H(4)	2.86(2)	no	. 56501
Cl(2)	H(5)	2.29(1)	no	. 55501
Cl(2)	H(7)	3.15(1)	no	. 55501
N(1)	Cl(2)	3.13(1)	yes	. 55501
N(1)	N(2)	2.12(2)	yes	. 55501
N(1)	C(1)	2.17(2)	yes	. 55501
N(1)	C(8)	2.53(1)	yes	. 55501
N(1)	C(3)	2.55(1)	yes	. 55501
N(1)	C(9)	3.36(1)	yes	. 55501

N(1)	C(6)	3.53(2)	yes	. 55501
N(1)	H(1)	2.85(1)	no	. 55501
N(1)	H(6)	2.95(2)	no	. 55501
N(1)	H(7)	2.67(1)	no	. 55501
N(1)	H(8)	3.24(1)	no	. 55501
N(1)	H(9)	3.14(2)	no	. 55501
N(3)	Cl(1)	3.146(8)	yes	. 55501
N(3)	N(4)	2.21(1)	yes	. 55501
N(3)	C(16)	2.27(1)	yes	. 55501
N(3)	C(8)	3.09(1)	yes	. 55501
N(3)	C(12)	2.58(2)	yes	. 55501
N(3)	C(15)	3.59(2)	yes	. 55501
N(3)	C(9)	2.47(1)	yes	. 55501
N(3)	H(7)	3.30(1)	no	. 55501
N(3)	H(8)	2.87(1)	no	. 55501
N(3)	H(9)	3.21(1)	no	. 55501
N(3)	H(10)	2.75(2)	no	. 55501
N(3)	H(12)	3.03(1)	no	. 55501
N(3)	H(13)	2.86(2)	no	. 55501
N(2)	N(1)	2.12(2)	yes	. 55501
N(2)	C(2)	2.20(2)	yes	. 55501
N(2)	C(8)	2.53(2)	yes	. 55501
N(2)	C(3)	3.58(2)	yes	. 55501
N(2)	C(9)	3.36(2)	yes	. 55501
N(2)	C(6)	2.54(2)	yes	. 55501
N(2)	H(4)	2.85(2)	no	. 55501
N(2)	H(5)	2.94(2)	no	. 55501
N(2)	H(7)	3.21(2)	no	. 55501
N(2)	H(8)	2.67(1)	no	. 55501
N(2)	H(10)	3.21(2)	no	. 55501
N(4)	N(3)	2.21(1)	yes	. 55501
N(4)	C(11)	2.19(1)	yes	. 55501
N(4)	C(8)	3.58(1)	yes	. 55501
N(4)	C(12)	3.58(1)	yes	. 55501
N(4)	C(15)	2.53(2)	yes	. 55501
N(4)	C(9)	2.53(2)	yes	. 55501
N(4)	H(7)	3.49(1)	no	. 55501
N(4)	H(9)	2.58(1)	no	. 55501
N(4)	H(10)	3.15(2)	no	. 55501
N(4)	H(11)	3.04(1)	no	. 55501
N(4)	H(16)	2.79(2)	no	. 55501
C(16)	N(3)	2.27(1)	yes	. 55501

C(16)	C(10)	2.21(2)	yes	. 55501
C(16)	C(14)	2.37(2)	yes	. 55501
C(16)	C(12)	2.45(2)	yes	. 55501
C(16)	C(13)	2.72(2)	yes	. 55501
C(16)	H(11)	3.10(1)	no	. 55501
C(16)	H(12)	2.03(1)	no	. 55501
C(16)	H(13)	3.31(2)	no	. 55501
C(16)	H(15)	3.23(2)	no	. 55501
C(16)	H(16)	2.03(2)	no	. 55501
C(1)	N(1)	2.17(2)	yes	. 55501
C(1)	C(7)	2.21(2)	yes	. 55501
C(1)	C(3)	2.45(2)	yes	. 55501
C(1)	C(5)	2.32(2)	yes	. 55501
C(1)	C(4)	2.73(2)	yes	. 55501
C(1)	H(1)	3.31(2)	no	. 55501
C(1)	H(3)	3.19(2)	no	. 55501
C(1)	H(4)	2.09(2)	no	. 55501
C(1)	H(5)	3.00(2)	no	. 55501
C(1)	H(6)	2.01(2)	no	. 55501
C(7)	C(1)	2.21(2)	yes	. 55501
C(7)	C(2)	2.23(2)	yes	. 55501
C(7)	C(9)	2.49(2)	yes	. 55501
C(7)	C(6)	3.58(2)	yes	. 55501
C(7)	H(5)	1.96(2)	no	. 55501
C(7)	H(6)	1.92(2)	no	. 55501
C(7)	H(7)	2.06(2)	no	. 55501
C(7)	H(8)	2.06(1)	no	. 55501
C(7)	H(9)	2.63(2)	no	. 55501
C(7)	H(10)	2.69(2)	no	. 55501
C(10)	C(16)	2.21(2)	yes	. 55501
C(10)	C(11)	2.13(2)	yes	. 55501
C(10)	C(8)	2.50(1)	yes	. 55501
C(10)	C(12)	3.56(2)	yes	. 55501
C(10)	C(15)	3.57(2)	yes	. 55501
C(10)	H(7)	2.66(2)	no	. 55501
C(10)	H(8)	2.71(1)	no	. 55501
C(10)	H(9)	2.03(1)	no	. 55501
C(10)	H(10)	2.09(2)	no	. 55501
C(10)	H(11)	1.95(1)	no	. 55501
C(10)	H(12)	1.98(1)	no	. 55501
C(2)	N(2)	2.20(2)	yes	. 55501
C(2)	C(7)	2.23(2)	yes	. 55501

C(2)	C(5)	2.66(2)	yes	. 55501
C(2)	C(6)	2.41(2)	yes	. 55501
C(2)	C(4)	2.33(2)	yes	. 55501
C(2)	H(1)	2.11(2)	no	. 55501
C(2)	H(2)	3.20(2)	no	. 55501
C(2)	H(4)	3.27(2)	no	. 55501
C(2)	H(5)	2.01(2)	no	. 55501
C(2)	H(6)	3.02(2)	no	. 55501
C(11)	N(4)	2.19(1)	yes	. 55501
C(11)	C(10)	2.13(2)	yes	. 55501
C(11)	C(14)	2.80(2)	yes	. 55501
C(11)	C(13)	2.40(2)	yes	. 55501
C(11)	C(15)	2.43(2)	yes	. 55501
C(11)	C(9)	3.59(2)	yes	. 55501
C(11)	H(11)	2.02(1)	no	. 55501
C(11)	H(12)	3.02(1)	no	. 55501
C(11)	H(13)	2.12(2)	no	. 55501
C(11)	H(14)	3.27(2)	no	. 55501
C(11)	H(16)	3.28(2)	no	. 55501
C(14)	C(16)	2.37(2)	yes	. 55501
C(14)	C(11)	2.80(2)	yes	. 55501
C(14)	C(12)	2.45(2)	yes	. 55501
C(14)	H(3)	3.46(2)	no	. 56401
C(14)	H(13)	3.31(2)	no	. 55501
C(14)	H(14)	2.02(2)	no	. 55501
C(14)	H(16)	2.06(2)	no	. 55501
C(8)	N(1)	2.53(1)	yes	. 55501
C(8)	N(3)	3.09(1)	yes	. 55501
C(8)	N(2)	2.53(2)	yes	. 55501
C(8)	N(4)	3.58(1)	yes	. 55501
C(8)	C(10)	2.50(1)	yes	. 55501
C(8)	C(9)	1.61(2)	yes	. 55501
C(8)	H(5)	2.75(1)	no	. 55501
C(8)	H(6)	2.77(2)	no	. 55501
C(8)	H(9)	2.10(2)	no	. 55501
C(8)	H(10)	2.14(2)	no	. 55501
C(8)	H(11)	3.07(1)	no	. 55501
C(12)	N(3)	2.58(2)	yes	. 55501
C(12)	N(4)	3.58(1)	yes	. 55501
C(12)	C(16)	2.45(2)	yes	. 55501
C(12)	C(10)	3.56(2)	yes	. 55501
C(12)	C(14)	2.45(2)	yes	. 55501

C(12)	C(15)	2.86(2)	yes	. 55501
C(12)	H(11)	2.87(1)	no	. 55501
C(12)	H(14)	2.01(2)	no	. 55501
C(12)	H(15)	3.30(2)	no	. 55501
C(3)	N(1)	2.55(1)	yes	. 55501
C(3)	N(2)	3.58(2)	yes	. 55501
C(3)	C(1)	2.45(2)	yes	. 55501
C(3)	C(5)	2.40(2)	yes	. 55501
C(3)	C(6)	2.91(2)	yes	. 55501
C(3)	H(2)	1.98(2)	no	. 55501
C(3)	H(3)	3.23(2)	no	. 55501
C(3)	H(5)	2.82(1)	no	. 55501
C(5)	C(1)	2.32(2)	yes	. 55501
C(5)	C(2)	2.66(2)	yes	. 55501
C(5)	C(3)	2.40(2)	yes	. 55501
C(5)	H(1)	3.28(2)	no	. 55501
C(5)	H(2)	2.05(2)	no	. 55501
C(5)	H(4)	2.08(2)	no	. 55501
C(13)	C(16)	2.72(2)	yes	. 55501
C(13)	C(11)	2.40(2)	yes	. 55501
C(13)	C(15)	2.40(2)	yes	. 55501
C(13)	H(3)	3.57(2)	no	. 56401
C(13)	H(13)	2.06(2)	no	. 55501
C(13)	H(15)	2.04(2)	no	. 55501
C(13)	H(16)	3.27(2)	no	. 55501
C(15)	N(3)	3.59(2)	yes	. 55501
C(15)	N(4)	2.53(2)	yes	. 55501
C(15)	C(10)	3.57(2)	yes	. 55501
C(15)	C(11)	2.43(2)	yes	. 55501
C(15)	C(12)	2.86(2)	yes	. 55501
C(15)	C(13)	2.40(2)	yes	. 55501
C(15)	H(12)	2.85(2)	no	. 55501
C(15)	H(14)	3.25(2)	no	. 55501
C(15)	H(15)	2.04(2)	no	. 55501
C(9)	N(1)	3.36(1)	yes	. 55501
C(9)	N(3)	2.47(1)	yes	. 55501
C(9)	N(2)	3.36(2)	yes	. 55501
C(9)	N(4)	2.53(2)	yes	. 55501
C(9)	C(7)	2.49(2)	yes	. 55501
C(9)	C(11)	3.59(2)	yes	. 55501
C(9)	C(8)	1.61(2)	yes	. 55501
C(9)	H(5)	3.51(2)	no	. 55501

C(9)	H(6)	3.46(2)	no	. 55501
C(9)	H(7)	2.15(2)	no	. 55501
C(9)	H(8)	2.11(2)	no	. 55501
C(9)	H(11)	2.72(1)	no	. 55501
C(9)	H(12)	2.77(2)	no	. 55501
C(6)	N(1)	3.53(2)	yes	. 55501
C(6)	N(2)	2.54(2)	yes	. 55501
C(6)	C(7)	3.58(2)	yes	. 55501
C(6)	C(2)	2.41(2)	yes	. 55501
C(6)	C(3)	2.91(2)	yes	. 55501
C(6)	C(4)	2.47(2)	yes	. 55501
C(6)	H(2)	3.31(2)	no	. 55501
C(6)	H(3)	2.01(2)	no	. 55501
C(6)	H(6)	2.82(2)	no	. 55501
C(4)	C(1)	2.73(2)	yes	. 55501
C(4)	C(2)	2.33(2)	yes	. 55501
C(4)	C(6)	2.47(2)	yes	. 55501
C(4)	H(1)	2.03(2)	no	. 55501
C(4)	H(3)	2.03(2)	no	. 55501
C(4)	H(4)	3.34(2)	no	. 55501
H(1)	N(1)	2.85(1)	no	. 55501
H(1)	C(1)	3.31(2)	no	. 55501
H(1)	C(2)	2.11(2)	no	. 55501
H(1)	C(5)	3.28(2)	no	. 55501
H(1)	C(4)	2.03(2)	no	. 55501
H(2)	C(2)	3.20(2)	no	. 55501
H(2)	C(3)	1.98(2)	no	. 55501
H(2)	C(5)	2.05(2)	no	. 55501
H(2)	C(6)	3.31(2)	no	. 55501
H(3)	C(1)	3.19(2)	no	. 55501
H(3)	C(3)	3.23(2)	no	. 55501
H(3)	C(6)	2.01(2)	no	. 55501
H(3)	C(4)	2.03(2)	no	. 55501
H(4)	Cl(2)	2.86(2)	no	. 54501
H(4)	N(2)	2.85(2)	no	. 55501
H(4)	C(1)	2.09(2)	no	. 55501
H(4)	C(2)	3.27(2)	no	. 55501
H(4)	C(5)	2.08(2)	no	. 55501
H(4)	C(4)	3.34(2)	no	. 55501
H(5)	Cl(2)	2.29(1)	no	. 55501
H(5)	N(2)	2.94(2)	no	. 55501
H(5)	C(1)	3.00(2)	no	. 55501

H(5)	C(7)	1.96(2)	no	. 55501
H(5)	C(2)	2.01(2)	no	. 55501
H(5)	C(8)	2.75(1)	no	. 55501
H(5)	C(3)	2.82(1)	no	. 55501
H(5)	C(9)	3.51(2)	no	. 55501
H(6)	N(1)	2.95(2)	no	. 55501
H(6)	C(1)	2.01(2)	no	. 55501
H(6)	C(7)	1.92(2)	no	. 55501
H(6)	C(2)	3.02(2)	no	. 55501
H(6)	C(8)	2.77(2)	no	. 55501
H(6)	C(9)	3.46(2)	no	. 55501
H(6)	C(6)	2.82(2)	no	. 55501
H(7)	Cl(2)	3.15(1)	no	. 55501
H(7)	N(1)	2.67(1)	no	. 55501
H(7)	N(3)	3.30(1)	no	. 55501
H(7)	N(2)	3.21(2)	no	. 55501
H(7)	N(4)	3.49(1)	no	. 55501
H(7)	C(7)	2.06(2)	no	. 55501
H(7)	C(10)	2.66(2)	no	. 55501
H(7)	C(9)	2.15(2)	no	. 55501
H(8)	Cl(1)	2.781(9)	no	. 55501
H(8)	N(1)	3.24(1)	no	. 55501
H(8)	N(3)	2.87(1)	no	. 55501
H(8)	N(2)	2.67(1)	no	. 55501
H(8)	C(7)	2.06(1)	no	. 55501
H(8)	C(10)	2.71(1)	no	. 55501
H(8)	C(9)	2.11(2)	no	. 55501
H(9)	N(1)	3.14(2)	no	. 55501
H(9)	N(3)	3.21(1)	no	. 55501
H(9)	N(4)	2.58(1)	no	. 55501
H(9)	C(7)	2.63(2)	no	. 55501
H(9)	C(10)	2.03(1)	no	. 55501
H(9)	C(8)	2.10(2)	no	. 55501
H(10)	N(3)	2.75(2)	no	. 55501
H(10)	N(2)	3.21(2)	no	. 55501
H(10)	N(4)	3.15(2)	no	. 55501
H(10)	C(7)	2.69(2)	no	. 55501
H(10)	C(10)	2.09(2)	no	. 55501
H(10)	C(8)	2.14(2)	no	. 55501
H(11)	Cl(1)	2.354(8)	no	. 55501
H(11)	N(4)	3.04(1)	no	. 55501
H(11)	C(16)	3.10(1)	no	. 55501

H(11)	C(10)	1.95(1)	no	. 55501
H(11)	C(11)	2.02(1)	no	. 55501
H(11)	C(8)	3.07(1)	no	. 55501
H(11)	C(12)	2.87(1)	no	. 55501
H(11)	C(9)	2.72(1)	no	. 55501
H(12)	N(3)	3.03(1)	no	. 55501
H(12)	C(16)	2.03(1)	no	. 55501
H(12)	C(10)	1.98(1)	no	. 55501
H(12)	C(11)	3.02(1)	no	. 55501
H(12)	C(15)	2.85(2)	no	. 55501
H(12)	C(9)	2.77(2)	no	. 55501
H(13)	N(3)	2.86(2)	no	. 55501
H(13)	C(16)	3.31(2)	no	. 55501
H(13)	C(11)	2.12(2)	no	. 55501
H(13)	C(14)	3.31(2)	no	. 55501
H(13)	C(13)	2.06(2)	no	. 55501
H(14)	C(11)	3.27(2)	no	. 55501
H(14)	C(14)	2.02(2)	no	. 55501
H(14)	C(12)	2.01(2)	no	. 55501
H(14)	C(15)	3.25(2)	no	. 55501
H(15)	C(16)	3.23(2)	no	. 55501
H(15)	C(12)	3.30(2)	no	. 55501
H(15)	C(5)	3.46(2)	no	. 56401
H(15)	C(13)	2.04(2)	no	. 55501
H(15)	C(15)	2.04(2)	no	. 55501
H(15)	C(4)	3.37(2)	no	. 56401
H(16)	Cl(1)	3.06(1)	no	. 46501
H(16)	N(4)	2.79(2)	no	. 55501
H(16)	C(16)	2.03(2)	no	. 55501
H(16)	C(11)	3.28(2)	no	. 55501
H(16)	C(14)	2.06(2)	no	. 55501
H(16)	C(13)	3.27(2)	no	. 55501

#==========
=

Additional structures and associated data_? identifiers
should be added at this point if there is more than one
structure analysis in the CIF.

#==========
=

End of CIF

#==========
=