Neutral and cationic paramagnetic amino-amidinate Iron(II) complexes

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2008

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# CIF-file generated for  C23H32ClFeN3                 CP524

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# 1. SUBMISSION DETAILS

# Name and address of author for correspondence
_publ_contact_author_name
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   Drs. A. Meetsma
;
_publ_contact_author_address
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  Crystal Structure Center, Chemical Physics,
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  University of Groningen,
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  NL-9747 AG Groningen, The Netherlands.

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_publ_contact_author_email          A.Meetsma@rug.nl
_publ_contact_author_fax            '+31 50 3634441'
_publ_contact_author_phone          '+31 50 3634368'

_publ_requested_journal             'Organometallics'
# Publication choise FI FM FO CI CM CO AD
_publ_requested_category            ?
_publ_requested_coeditor_name       ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2007-09-04     10:13:13

 Consider this CIF submission for depostion of compound 1a
 X-ray structure of a manuscript to be submitted to : Organometallics
  (Our Code : CP524)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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# 3. TITLE AND AUTHOR LIST

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;
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;
 ?
;

# The loop structure below should contain the names and adresses of all
# authors, in the required order of publication. Repeat as necessary.


loop_
_publ_author_name
_publ_author_address

   'Meetsma, Auke'

;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;

#=============================================================================
```

```
# 4. TEXT

_publ_section_synopsis
;
 ?
;
_publ_section_abstract
;
 ?
;

# Insert blank lines between paragraphs

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The asymmetric unit consists of a half-formula unit of the title compound.
 The formula unit is a dimer molecule with site symmetry -1.

;
_publ_section_exptl_prep
;
 ?
;
_publ_section_exptl_refinement
;
 The structure was solved by Patterson methods and extension of the model
 was accomplished by direct methods applied to difference structure factors
 using the program DIRDIF. The positional and anisotropic displacement
 parameters for the non-hydrogen atoms were refined.
 A subsequent difference Fourier synthesis resulted in the location of all
 the hydrogen atoms, which coordinates and isotropic displacement parameters
 were refined.
;

# Insert blank lines between references

_publ_section_references
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 Beurskens, P.T., Beurskens, G., Gelder, R. de,
   Garc\'ia-Granda, S., Gould, R.O., Isra\"el, & Smits, J.M.M. (1999).
   The DIRDIF99 program system,
   Technical Report of the Crystallography Laboratory,
   University of Nijmegen, The Netherlands.

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   Utrecht modified version October 1994.
   Enraf-Nonius, Delft, The Netherlands.

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   Space-group symmetry, edited by T. Hahn. Dordrecht: Reidel.
```

(Present distributor Kluwer Academic Publishers, Dordrecht).

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Edited by A.J.C Wilson, Kluwer Academic Publishers,
Dordrecht, The Netherlands.

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University, The Netherlands.

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;

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Fig. 1. PLUTO drawing of the molecule illustrating the puckering
and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective ORTEP drawing of the title compound.
All non-hydrogen atoms are represented by thermal vibrational
ellipsoids drawn to encompass 50% of the electron density.
The hydrogen atoms are drawn with an arbitrary radius.
;
_publ_section_acknowledgements
;
?
;

#==

data_c23h32cl

#==

5. CHEMICAL DATA

_chemical_name_systematic
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?

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;
_chemical_name_common                ?
_chemical_melting_point              ?
_chemical_formula_moiety
'C46 H64 Cl2 Fe2 N6'
_chemical_formula_structural         ?
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_sum
'C46 H64 Cl2 Fe2 N6'
_chemical_formula_weight                883.63
_chemical_compound_source           'by syntheses'

loop_
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_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
 N   N    0.0061    0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Fe  Fe    0.3463    0.8444
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl  Cl    0.1484    0.1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 H   H    0.0000    0.0000
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 C   C    0.0033    0.0016
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#==============================================================================

# 6. CRYSTAL DATA

_symmetry_cell_setting                Monoclinic
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_symmetry_space_group_name_H-M       'P 21/c'

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

_cell_length_a                          14.889(2)
_cell_length_b                          9.889(1)
_cell_length_c                          16.661(1)
_cell_angle_alpha                             90
_cell_angle_beta                        116.03(1)
_cell_angle_gamma                             90
_cell_volume                            2204.3(4)
_cell_formula_units_Z                   2
_cell_measurement_temperature        180
_cell_measurement_reflns_used        22
_cell_measurement_theta_min          18.37
_cell_measurement_theta_max          20.11
_cell_special_details
;
 Unit cell parameters (Duisenberg, 1992) and orientation matrix were determined
 from a least-squares treatment of SET4 (de Boer & Duisenberg, 1984) setting.
 Reduced cell calculations did not indicate any higher metric lattice symmetry
```

```
 and examination of the final atomic coordinates of the structure did not yield
 extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

_exptl_crystal_description          parallelepiped
_exptl_crystal_colour               'colorless transparent'
_exptl_crystal_size_max           0.51
_exptl_crystal_size_mid           0.25
_exptl_crystal_size_min           0.12
_exptl_crystal_size_rad              ?
_exptl_crystal_density_meas          ?
_exptl_crystal_density_diffrn            1.331
_exptl_crystal_density_method       ?
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_exptl_absorpt_correction_T_min     ?
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#===============================================================================

# 7. EXPERIMENTAL DATA

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; ?
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_diffrn_ambient_temperature          180
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type               'Mo K\a'
_diffrn_radiation_source             'fine focus sealed Philips Mo tube '
_diffrn_radiation_monochromator      'perpendicular mounted graphite'
_diffrn_radiation_detector
;
     scintillation NaI crystal with photomultiplier
;
_diffrn_measurement_device_type
;
     Enraf Nonius CAD-4F diffractometer
;

_diffrn_measurement_method           '\w/2\q'

_diffrn_special_details
;
 Crystal into the cold nitrogen stream  of the low-temperature unit
   (Bolhuis, 1971), on an Enraf-Nonius CAD-4F diffractometer.
   Graphite-monochromated Mo K\a radiation,
   \w/2\q scan, \D\w = (1.05 + 0.34 tg \q)\%.
;
_diffrn_detector_area_resol_mean     ?

_diffrn_standards_number             3
_diffrn_standards_interval_count     ?
_diffrn_standards_interval_time      180
_diffrn_standards_decay_%            4.3

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_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
```

```
_diffrn_standard_refln_index_l
 0  2  3
 3  2 -2
-2  2  0

# number of measured reflections (redundant set)
_diffrn_reflns_number              5266
_diffrn_reflns_av_R_equivalents    0.0617
_diffrn_reflns_av_sigmaI/netI      0.0270
_diffrn_reflns_limit_h_min         -19
_diffrn_reflns_limit_h_max         17
_diffrn_reflns_limit_k_min         0
_diffrn_reflns_limit_k_max         12
_diffrn_reflns_limit_l_min         0
_diffrn_reflns_limit_l_max         21
_diffrn_reflns_theta_min           1.52
_diffrn_reflns_theta_max           26.99
_diffrn_measured_fraction_theta_max    0.999
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.999

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization  effects, scale
 variation, but not for absorption and reduced to F~o~^2^
;

# number of unique reflections
_reflns_number_total               4802
_reflns_number_gt                  3956
_reflns_threshold_expression       >2sigma(I)


_computing_data_collection           'CAD4-UNIX software Version 5.1, 1994'
_computing_cell_refinement           'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction            'HELENA (Spek, 1997)'
_computing_structure_solution
;
 DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 1999)
 PLATON (Spek, 1994, 1996)
;
_computing_publication_material      'PLATON (Spek, 1990)'

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

# 8. REFINEMENT DATA

_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 w=1/[\s^2^(Fo^2^)+(0.1087P)^2^+0.2692P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    difmap
_refine_ls_hydrogen_treatment     refall
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4792
_refine_ls_number_parameters      381
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0607
_refine_ls_R_factor_gt            0.0482
_refine_ls_wR_factor_ref          0.1443
_refine_ls_wR_factor_gt           0.1340
_refine_ls_goodness_of_fit_ref    1.040
_refine_ls_restrained_S_all       1.040
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max          0.859
_refine_diff_density_min         -0.904
_refine_diff_density_rms          0.108

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# 9. ATOMIC COORDINATES AND THERMAL PARAMETERS

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_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
 Fe     Fe Uani    0.02521(2)   0.64384(3)   0.01136(2)     1.000    0.0152(1)
 Cl     Cl Uani   -0.00081(5)   0.78407(7)  -0.10499(4)     1.000    0.0263(2)
 N1     N  Uani   0.17267(15)    0.5756(2)  0.06085(14)     1.000    0.0157(6)
 N2     N  Uani  -0.06581(16)    0.5390(2)  0.06064(14)     1.000    0.0158(6)
 N3     N  Uani   0.02476(16)    0.7837(2)  0.11079(14)     1.000    0.0178(6)
 C1     C  Uani   0.26820(18)    0.6052(3)  0.13289(17)     1.000    0.0174(7)
 C2     C  Uani   0.32788(19)    0.7155(3)  0.13102(18)     1.000    0.0205(7)
 C3     C  Uani     0.4167(2)    0.7413(3)    0.2076(2)     1.000    0.0281(8)
 C4     C  Uani     0.4470(2)    0.6625(3)    0.2829(2)     1.000    0.0332(9)
 C5     C  Uani     0.3880(2)    0.5555(3)  0.28439(19)     1.000    0.0297(8)
 C6     C  Uani   0.29801(19)    0.5254(3)  0.21074(18)     1.000    0.0217(7)
 C7     C  Uani     0.3032(2)    0.8060(3)    0.0510(2)     1.000    0.0254(8)
 C8     C  Uani     0.3835(3)    0.7893(3)    0.0158(3)     1.000   0.0338(10)
 C9     C  Uani     0.2982(3)    0.9567(3)    0.0713(3)     1.000   0.0345(10)
 C10    C  Uani     0.2351(2)    0.4082(3)  0.21587(19)     1.000    0.0249(8)
 C11    C  Uani     0.2680(3)    0.2725(3)    0.1943(3)     1.000   0.0379(11)
 C12    C  Uani     0.2314(3)    0.3980(4)    0.3054(3)     1.000   0.0400(11)
 C13    C  Uani    -0.0378(2)    0.5788(3)  0.15373(17)     1.000    0.0197(7)
 C14    C  Uani     0.0425(2)    0.6879(3)  0.18386(17)     1.000    0.0197(7)
 C15    C  Uani    -0.0699(2)    0.8572(3)    0.0836(2)     1.000    0.0236(8)
```

C16	C	Uani	0.1063(2)	0.8823(3)	0.1388(2)	1.000	0.0243(8)
C17	C	Uani	0.15954(18)	0.5065(2)	-0.01107(17)	1.000	0.0164(6)
C18	C	Uani	0.24135(18)	0.4869(3)	-0.04045(17)	1.000	0.0186(7)
C19	C	Uani	0.2372(2)	0.5550(3)	-0.1143(2)	1.000	0.0270(8)
C20	C	Uani	0.3102(2)	0.5354(4)	-0.1437(2)	1.000	0.0332(10)
C21	C	Uani	0.3872(2)	0.4464(4)	-0.0994(2)	1.000	0.0324(10)
C22	C	Uani	0.3933(2)	0.3794(3)	-0.0248(2)	1.000	0.0322(9)
C23	C	Uani	0.3204(2)	0.3993(3)	0.0052(2)	1.000	0.0245(8)
H3	H	Uiso	0.456(3)	0.813(4)	0.208(3)	1.000	0.037(10)
H4	H	Uiso	0.504(3)	0.680(4)	0.332(3)	1.000	0.051(12)
H5	H	Uiso	0.415(3)	0.502(4)	0.337(3)	1.000	0.036(10)
H7	H	Uiso	0.241(3)	0.781(3)	0.008(2)	1.000	0.023(8)
H8	H	Uiso	0.442(4)	0.831(4)	0.059(3)	1.000	0.051(12)
H8'	H	Uiso	0.362(4)	0.845(5)	-0.038(4)	1.000	0.066(14)
H8"	H	Uiso	0.401(3)	0.692(4)	0.005(2)	1.000	0.029(9)
H9	H	Uiso	0.239(4)	0.977(5)	0.089(3)	1.000	0.068(14)
H9'	H	Uiso	0.298(3)	1.010(5)	0.023(3)	1.000	0.052(12)
H9"	H	Uiso	0.362(3)	0.988(4)	0.111(3)	1.000	0.037(10)
H10	H	Uiso	0.169(3)	0.426(4)	0.171(2)	1.000	0.030(9)
H11	H	Uiso	0.257(3)	0.271(4)	0.141(3)	1.000	0.032(10)
H11'	H	Uiso	0.222(3)	0.199(4)	0.204(3)	1.000	0.050(11)
H11"	H	Uiso	0.340(4)	0.260(5)	0.233(3)	1.000	0.056(13)
H12	H	Uiso	0.291(3)	0.373(4)	0.355(3)	1.000	0.036(10)
H12'	H	Uiso	0.182(3)	0.330(4)	0.301(3)	1.000	0.042(11)
H12"	H	Uiso	0.205(4)	0.489(5)	0.316(3)	1.000	0.073(16)
H13	H	Uiso	-0.015(2)	0.504(3)	0.193(2)	1.000	0.022(8)
H13'	H	Uiso	-0.094(3)	0.612(3)	0.158(2)	1.000	0.025(8)
H14	H	Uiso	0.042(2)	0.732(3)	0.234(2)	1.000	0.011(7)
H14'	H	Uiso	0.110(3)	0.651(3)	0.201(2)	1.000	0.025(8)
H15	H	Uiso	-0.076(3)	0.908(4)	0.131(3)	1.000	0.034(9)
H15'	H	Uiso	-0.119(3)	0.804(4)	0.068(2)	1.000	0.028(9)
H15"	H	Uiso	-0.084(3)	0.917(4)	0.035(2)	1.000	0.035(9)
H16	H	Uiso	0.105(2)	0.944(3)	0.190(2)	1.000	0.022(8)
H16'	H	Uiso	0.093(3)	0.940(4)	0.087(2)	1.000	0.029(9)
H16"	H	Uiso	0.169(2)	0.831(3)	0.158(2)	1.000	0.018(7)
H19	H	Uiso	0.191(3)	0.609(4)	-0.141(2)	1.000	0.030(9)
H20	H	Uiso	0.308(3)	0.580(4)	-0.192(3)	1.000	0.039(10)
H21	H	Uiso	0.435(3)	0.440(4)	-0.118(3)	1.000	0.043(10)
H22	H	Uiso	0.449(3)	0.322(4)	0.006(2)	1.000	0.030(9)
H23	H	Uiso	0.326(2)	0.350(3)	0.055(2)	1.000	0.021(8)

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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

Fe	0.0156(2)	0.0139(2)	0.0177(2)	0.0004(1)	0.0087(2)	0.0011(1)
Cl	0.0365(4)	0.0192(3)	0.0250(3)	0.0060(2)	0.0152(3)	0.0041(3)
N1	0.0139(9)	0.0152(10)	0.0195(10)	-0.0010(8)	0.0086(8)	-0.0010(8)
N2	0.0189(10)	0.0134(9)	0.0155(10)	0.0008(8)	0.0078(8)	0.0013(8)
N3	0.0190(10)	0.0155(10)	0.0196(10)	-0.0009(8)	0.0091(9)	-0.0011(8)
C1	0.0164(11)	0.0183(12)	0.0171(11)	-0.0028(9)	0.0071(10)	0.0028(9)
C2	0.0167(12)	0.0182(12)	0.0273(13)	-0.0024(10)	0.0103(10)	0.0017(10)
C3	0.0197(13)	0.0258(14)	0.0356(16)	-0.0062(12)	0.0093(12)	-0.0036(11)
C4	0.0224(14)	0.0380(17)	0.0273(15)	-0.0069(13)	-0.0001(12)	-0.0008(12)
C5	0.0250(14)	0.0368(16)	0.0201(13)	0.0044(12)	0.0033(11)	0.0066(12)
C6	0.0209(12)	0.0226(13)	0.0210(12)	0.0005(10)	0.0086(10)	0.0054(10)
C7	0.0222(14)	0.0219(13)	0.0315(14)	0.0020(11)	0.0112(12)	-0.0009(11)

```
  C8      0.0327(16) 0.0325(17) 0.0416(18)  0.0000(14)  0.0213(15) -0.0035(14)
  C9      0.0304(16) 0.0228(14)   0.057(2)  0.0044(14)  0.0254(16) -0.0002(12)
  C10     0.0287(14) 0.0242(14) 0.0236(13)  0.0074(11)  0.0131(12)  0.0035(11)
  C11       0.051(2) 0.0271(17)   0.049(2)  0.0045(14)  0.0342(19)  0.0032(15)
  C12       0.052(2)   0.042(2) 0.0367(18)  0.0103(15)  0.0293(17)  0.0051(17)
  C13     0.0217(12) 0.0215(12) 0.0172(12)  0.0003(10)  0.0097(10) -0.0036(10)
  C14     0.0206(12) 0.0231(13) 0.0153(12) -0.0012(10)  0.0079(10) -0.0009(10)
  C15     0.0234(14) 0.0187(13) 0.0320(15) -0.0014(11)  0.0151(12)  0.0018(11)
  C16     0.0264(14) 0.0186(12) 0.0291(14) -0.0037(11)  0.0134(12) -0.0031(11)
  C17     0.0182(11) 0.0120(11) 0.0187(11)   0.0029(9)   0.0077(9)   0.0025(9)
  C18     0.0162(11) 0.0208(12) 0.0192(12) -0.0044(10)  0.0082(10) -0.0024(10)
  C19     0.0196(13) 0.0331(16) 0.0264(14)  0.0035(12)  0.0083(11)  0.0002(12)
  C20     0.0291(15)   0.051(2) 0.0229(14) -0.0019(13)  0.0145(12) -0.0101(14)
  C21     0.0221(14) 0.0467(19) 0.0356(16) -0.0161(14)  0.0193(13) -0.0061(13)
  C22     0.0225(14) 0.0363(16) 0.0375(16) -0.0055(13)  0.0128(13)  0.0065(13)
  C23     0.0203(12) 0.0272(14) 0.0276(14) -0.0006(11)  0.0119(11)  0.0032(11)

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

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All esds are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

loop_
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_geom_bond_atom_site_label_2
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_geom_bond_site_symmetry_1
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 Fe      Cl        2.2742(8)                    .       .                  yes
 Fe      N1         2.090(2)                    .       .                  yes
 Fe      N2         2.136(2)                    .       .                  yes
 Fe      N3         2.160(2)                    .       .                  yes
 Fe      N2         2.390(2)                    .     3_565                yes
 N1      C1         1.432(4)                    .       .                  yes
 N1      C17        1.317(3)                    .       .                  yes
 N2      C13        1.472(3)                    .       .                  yes
 N2      C17        1.349(4)                    .     3_565                yes
 N3      C14        1.472(3)                    .       .                  yes
 N3      C15        1.470(4)                    .       .                  yes
 N3      C16        1.465(4)                    .       .                  yes
 C1      C2         1.416(4)                    .       .                  no
 C1      C6         1.413(4)                    .       .                  no
 C2      C3         1.400(4)                    .       .                  no
 C2      C7         1.511(4)                    .       .                  no
 C3      C4         1.374(4)                    .       .                  no
 C4      C5         1.382(4)                    .       .                  no
 C5      C6         1.395(4)                    .       .                  no
 C6      C10        1.516(4)                    .       .                  no
 C7      C8         1.554(6)                    .       .                  no
 C7      C9         1.537(4)                    .       .                  no
 C10     C11        1.525(5)                    .       .                  no
 C10     C12        1.520(5)                    .       .                  no
```

```
 C13     C14        1.523(4)                    .      .                 no
 C17     C18        1.511(4)                    .      .                 no
 C18     C19        1.380(4)                    .      .                 no
 C18     C23        1.389(4)                    .      .                 no
 C19     C20        1.388(5)                    .      .                 no
 C20     C21        1.375(5)                    .      .                 no
 C21     C22        1.376(4)                    .      .                 no
 C22     C23        1.394(5)                    .      .                 no
 C3      H3          0.92(4)                    .      .                 no
 C4      H4          0.90(5)                    .      .                 no
 C5      H5          0.95(4)                    .      .                 no
 C7      H7          0.92(4)                    .      .                 no
 C8      H8          0.95(5)                    .      .                 no
 C8      H8'         0.98(6)                    .      .                 no
 C8      H8"         1.03(4)                    .      .                 no
 C9      H9          1.06(6)                    .      .                 no
 C9      H9'         0.96(5)                    .      .                 no
 C9      H9"         0.94(5)                    .      .                 no
 C10     H10         0.96(4)                    .      .                 no
 C11     H11         0.83(5)                    .      .                 no
 C11     H11'        1.06(5)                    .      .                 no
 C11     H11"        0.99(6)                    .      .                 no
 C12     H12         0.94(5)                    .      .                 no
 C12     H12'        0.98(5)                    .      .                 no
 C12     H12"        1.03(5)                    .      .                 no
 C13     H13         0.95(3)                    .      .                 no
 C13     H13'        0.93(5)                    .      .                 no
 C14     H14         0.95(3)                    .      .                 no
 C14     H14'        0.99(4)                    .      .                 no
 C15     H15         0.97(4)                    .      .                 no
 C15     H15'        0.84(4)                    .      .                 no
 C15     H15"        0.95(3)                    .      .                 no
 C16     H16         1.06(3)                    .      .                 no
 C16     H16'        0.98(3)                    .      .                 no
 C16     H16"        0.98(3)                    .      .                 no
 C19     H19         0.83(4)                    .      .                 no
 C20     H20         0.91(4)                    .      .                 no
 C21     H21         0.89(5)                    .      .                 no
 C22     H22         0.95(4)                    .      .                 no
 C23     H23         0.93(3)                    .      .                 no

loop_
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_geom_angle_atom_site_label_3
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_geom_angle_site_symmetry_3
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 Cl      Fe      N1        106.84(6)             .      .       .          yes
 Cl      Fe      N2        136.40(7)             .      .       .          yes
 Cl      Fe      N3        101.92(6)             .      .       .          yes
 Cl      Fe      N2         91.12(5)             .      .     3_565        yes
 N1      Fe      N2        115.19(9)             .      .       .          yes
 N1      Fe      N3        105.10(9)             .      .       .          yes
 N1      Fe      N2         60.02(8)             .      .     3_565        yes
 N2      Fe      N3         78.46(8)             .      .       .          yes
 N2      Fe      N2         99.71(8)             .      .     3_565        yes
 N2      Fe      N3        162.94(8)           3_565    .       .          yes
 Fe      N1      C1       138.57(18)             .      .       .          yes
```

Fe	N1	C17	95.61(17)	.	.	.	yes
C1	N1	C17	124.4(2)	.	.	.	yes
Fe	N2	C13	109.94(17)	.	.	.	yes
Fe	N2	Fe	80.29(8)	.	.	3_565	yes
Fe	N2	C17	125.93(17)	.	.	3_565	yes
Fe	N2	C13	135.57(17)	3_565	.	.	yes
C13	N2	C17	118.2(2)	.	.	3_565	yes
Fe	N2	C17	82.06(14)	3_565	.	3_565	yes
Fe	N3	C14	99.34(15)	.	.	.	yes
Fe	N3	C15	113.93(17)	.	.	.	yes
Fe	N3	C16	112.92(19)	.	.	.	yes
C14	N3	C15	111.9(2)	.	.	.	yes
C14	N3	C16	110.0(2)	.	.	.	yes
C15	N3	C16	108.5(2)	.	.	.	yes
N1	C1	C2	122.8(2)	.	.	.	yes
N1	C1	C6	116.8(3)	.	.	.	yes
C2	C1	C6	120.2(3)	.	.	.	no
C1	C2	C3	118.1(3)	.	.	.	no
C1	C2	C7	124.3(3)	.	.	.	no
C3	C2	C7	117.6(3)	.	.	.	no
C2	C3	C4	121.9(3)	.	.	.	no
C3	C4	C5	119.6(3)	.	.	.	no
C4	C5	C6	121.3(3)	.	.	.	no
C1	C6	C5	118.8(3)	.	.	.	no
C1	C6	C10	121.7(3)	.	.	.	no
C5	C6	C10	119.5(3)	.	.	.	no
C2	C7	C8	109.9(3)	.	.	.	no
C2	C7	C9	113.4(3)	.	.	.	no
C8	C7	C9	107.8(3)	.	.	.	no
C6	C10	C11	112.9(3)	.	.	.	no
C6	C10	C12	113.3(3)	.	.	.	no
C11	C10	C12	109.1(3)	.	.	.	no
N2	C13	C14	110.8(2)	.	.	.	yes
N3	C14	C13	110.7(2)	.	.	.	yes
N1	C17	C18	122.8(2)	.	.	.	yes
N1	C17	N2	115.5(3)	.	.	3_565	yes
N2	C17	C18	121.5(2)	3_565	.	.	yes
C17	C18	C19	119.9(3)	.	.	.	no
C17	C18	C23	120.8(2)	.	.	.	no
C19	C18	C23	119.2(3)	.	.	.	no
C18	C19	C20	120.7(3)	.	.	.	no
C19	C20	C21	119.8(3)	.	.	.	no
C20	C21	C22	120.1(3)	.	.	.	no
C21	C22	C23	120.2(3)	.	.	.	no
C18	C23	C22	119.9(3)	.	.	.	no
C2	C3	H3	119(3)	.	.	.	no
C4	C3	H3	119(3)	.	.	.	no
C3	C4	H4	121(3)	.	.	.	no
C5	C4	H4	119(3)	.	.	.	no
C4	C5	H5	115(3)	.	.	.	no
C6	C5	H5	123(3)	.	.	.	no
C2	C7	H7	107(2)	.	.	.	no
C8	C7	H7	111(3)	.	.	.	no
C9	C7	H7	108(2)	.	.	.	no
C7	C8	H8	106(3)	.	.	.	no
C7	C8	H8'	107(4)	.	.	.	no
C7	C8	H8"	117(3)	.	.	.	no
H8	C8	H8'	106(4)	.	.	.	no
H8	C8	H8"	109(4)	.	.	.	no
H8'	C8	H8"	112(4)	.	.	.	no

```
 C7      C9      H9          112(3)              .       .       .          no
 C7      C9      H9'         109(3)              .       .       .          no
 C7      C9      H9"         110(3)              .       .       .          no
 H9      C9      H9'         115(4)              .       .       .          no
 H9      C9      H9"         117(4)              .       .       .          no
 H9'     C9      H9"          92(4)              .       .       .          no
 C6      C10     H10         105(2)              .       .       .          no
 C11     C10     H10         108(2)              .       .       .          no
 C12     C10     H10         108(2)              .       .       .          no
 C10     C11     H11         110(3)              .       .       .          no
 C10     C11     H11'        106(2)              .       .       .          no
 C10     C11     H11"        109(3)              .       .       .          no
 H11     C11     H11'        108(4)              .       .       .          no
 H11     C11     H11"        110(5)              .       .       .          no
 H11'    C11     H11"        114(4)              .       .       .          no
 C10     C12     H12         117(3)              .       .       .          no
 C10     C12     H12'        109(3)              .       .       .          no
 C10     C12     H12"        107(3)              .       .       .          no
 H12     C12     H12'        106(4)              .       .       .          no
 H12     C12     H12"        111(4)              .       .       .          no
 H12'    C12     H12"        106(4)              .       .       .          no
 N2      C13     H13      111.7(18)              .       .       .          no
 N2      C13     H13'     109.1(19)              .       .       .          no
 C14     C13     H13      109.5(19)              .       .       .          no
 C14     C13     H13'        109(2)              .       .       .          no
 H13     C13     H13'        107(3)              .       .       .          no
 N3      C14     H14      111.5(18)              .       .       .          no
 N3      C14     H14'        106(2)              .       .       .          no
 C13     C14     H14         108(2)              .       .       .          no
 C13     C14     H14'     112.7(19)              .       .       .          no
 H14     C14     H14'        108(3)              .       .       .          no
 N3      C15     H15         115(3)              .       .       .          no
 N3      C15     H15'        112(3)              .       .       .          no
 N3      C15     H15"        113(3)              .       .       .          no
 H15     C15     H15'        101(4)              .       .       .          no
 H15     C15     H15"        108(3)              .       .       .          no
 H15'    C15     H15"        107(3)              .       .       .          no
 N3      C16     H16      109.6(18)              .       .       .          no
 N3      C16     H16'        107(2)              .       .       .          no
 N3      C16     H16"     107.2(18)              .       .       .          no
 H16     C16     H16'        108(3)              .       .       .          no
 H16     C16     H16"        113(2)              .       .       .          no
 H16'    C16     H16"        113(3)              .       .       .          no
 C18     C19     H19         120(3)              .       .       .          no
 C20     C19     H19         120(3)              .       .       .          no
 C19     C20     H20         121(3)              .       .       .          no
 C21     C20     H20         119(3)              .       .       .          no
 C20     C21     H21         118(3)              .       .       .          no
 C22     C21     H21         122(3)              .       .       .          no
 C21     C22     H22         118(2)              .       .       .          no
 C23     C22     H22         122(2)              .       .       .          no
 C18     C23     H23         122(2)              .       .       .          no
 C22     C23     H23         118(2)              .       .       .          no

loop_
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_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 Cl      Fe      N1      C1          99.8(3)     .       .       .       .   no
 Cl      Fe      N1      C17      -65.89(15)     .       .       .       .   no
 N2      Fe      N1      C1         -92.1(3)     .       .       .       .   no
 N2      Fe      N1      C17      102.20(15)     .       .       .       .   no
 N3      Fe      N1      C1          -8.0(3)     .       .       .       .   no
 N3      Fe      N1      C17     -173.66(14)     .       .       .       .   no
 N2      Fe      N1      C1        -178.9(3)   3_565     .       .       .   no
 N2      Fe      N1      C17       15.42(13)   3_565     .       .       .   no
 Cl      Fe      N2      C13     -122.85(16)     .       .       .       .   no
 Cl      Fe      N2      Fe        102.02(7)     .       .       .     3_565 no
 Cl      Fe      N2      C17         29.3(2)     .       .       .     3_565 no
 N1      Fe      N2      C13       73.80(19)     .       .       .       .   no
 N1      Fe      N2      Fe        -61.33(9)     .       .       .     3_565 no
 N1      Fe      N2      C17     -134.05(19)     .       .       .     3_565 no
 N3      Fe      N2      C13       -27.61(17)    .       .       .       .   no
 N3      Fe      N2      Fe       -162.74(8)     .       .       .     3_565 no
 N3      Fe      N2      C17         124.5(2)    .       .       .     3_565 no
 N2      Fe      N2      C13       135.13(17)  3_565     .       .       .   no
 N2      Fe      N2      Fe          -0.02(7)  3_565     .       .     3_565 no
 N2      Fe      N2      C17         -72.7(2)  3_565     .       .     3_565 no
 Cl      Fe      N3      C14     -179.60(16)     .       .       .       .   no
 Cl      Fe      N3      C15       61.28(19)     .       .       .       .   no
 Cl      Fe      N3      C16       -63.12(18)    .       .       .       .   no
 N1      Fe      N3      C14       -68.28(18)    .       .       .       .   no
 N1      Fe      N3      C15       172.61(18)    .       .       .       .   no
 N1      Fe      N3      C16        48.21(19)    .       .       .       .   no
 N2      Fe      N3      C14        44.97(17)    .       .       .       .   no
 N2      Fe      N3      C15       -74.14(19)    .       .       .       .   no
 N2      Fe      N3      C16       161.46(19)    .       .       .       .   no
 Cl      Fe      N2      C17        93.74(13)    .       .     3_565     .   no
 Cl      Fe      N2      Fe       -137.58(6)     .       .     3_565   3_565 no
 Cl      Fe      N2      C13        -28.9(3)     .       .     3_565   3_565 no
 N1      Fe      N2      C17       -15.12(13)    .       .     3_565     .   no
 N1      Fe      N2      Fe        113.56(10)    .       .     3_565   3_565 no
 N1      Fe      N2      C13       -137.8(3)     .       .     3_565   3_565 no
 N2      Fe      N2      C17     -128.68(14)     .       .     3_565     .   no
 N2      Fe      N2      Fe          0.00(9)     .       .     3_565   3_565 no
 N2      Fe      N2      C13         108.6(3)    .       .     3_565   3_565 no
 Fe      N1      C1      C2         -79.4(4)     .       .       .       .   no
 Fe      N1      C1      C6          95.5(3)     .       .       .       .   no
 C17     N1      C1      C2          83.2(3)     .       .       .       .   no
 C17     N1      C1      C6        -101.9(3)     .       .       .       .   no
 Fe      N1      C17     C18         149.0(2)    .       .       .       .   no
 Fe      N1      C17     N2          -26.9(2)    .       .       .     3_565 no
 C1      N1      C17     C18         -19.5(4)    .       .       .       .   no
 C1      N1      C17     N2          164.6(2)    .       .       .     3_565 no
 Fe      N2      C13     C14           3.4(3)    .       .       .       .   no
 Fe      N2      C13     C14          99.9(3)  3_565     .       .       .   no
 C17     N2      C13     C14        -151.2(2)  3_565     .       .       .   no
 Fe      N2      C17     N1          48.5(3)     .       .     3_565   3_565 no
 Fe      N2      C17     C18       -135.6(2)     .       .     3_565   3_565 no
 C13     N2      C17     N1        -161.4(2)     .       .     3_565   3_565 no
 C13     N2      C17     C18         14.5(3)     .       .     3_565   3_565 no
 Fe      N3      C14     C13       -57.4(2)      .       .       .       .   no
 C15     N3      C14     C13         63.2(3)     .       .       .       .   no
 C16     N3      C14     C13       -176.1(2)     .       .       .       .   no
 C6      C1      C2      C7          179.4(3)    .       .       .       .   no
```

C6	C1	C2	C3	0.7(4)	.	.	.	no
N1	C1	C2	C3	175.4(3)	.	.	.	no
N1	C1	C2	C7	-5.9(5)	.	.	.	no
C2	C1	C6	C5	-1.5(4)	.	.	.	no
N1	C1	C6	C5	-176.5(3)	.	.	.	no
N1	C1	C6	C10	3.8(4)	.	.	.	no
C2	C1	C6	C10	178.8(3)	.	.	.	no
C1	C2	C7	C8	-115.0(3)	.	.	.	no
C1	C2	C3	C4	0.5(5)	.	.	.	no
C7	C2	C3	C4	-178.2(3)	.	.	.	no
C3	C2	C7	C9	-57.0(4)	.	.	.	no
C1	C2	C7	C9	124.3(4)	.	.	.	no
C3	C2	C7	C8	63.7(4)	.	.	.	no
C2	C3	C4	C5	-1.0(5)	.	.	.	no
C3	C4	C5	C6	0.1(5)	.	.	.	no
C4	C5	C6	C10	-179.2(3)	.	.	.	no
C4	C5	C6	C1	1.1(5)	.	.	.	no
C1	C6	C10	C11	95.5(4)	.	.	.	no
C5	C6	C10	C12	40.4(4)	.	.	.	no
C1	C6	C10	C12	-139.9(3)	.	.	.	no
C5	C6	C10	C11	-84.2(4)	.	.	.	no
N2	C13	C14	N3	37.9(3)	.	.	.	no
N2	C17	C18	C19	68.3(3)	3_565	.	.	no
N1	C17	C18	C19	-107.4(3)	.	.	.	no
N1	C17	C18	C23	73.6(3)	.	.	.	no
N2	C17	C18	C23	-110.8(3)	3_565	.	.	no
C23	C18	C19	C20	0.8(4)	.	.	.	no
C17	C18	C19	C20	-178.2(3)	.	.	.	no
C17	C18	C23	C22	177.9(3)	.	.	.	no
C19	C18	C23	C22	-1.1(4)	.	.	.	no
C18	C19	C20	C21	0.5(5)	.	.	.	no
C19	C20	C21	C22	-1.6(5)	.	.	.	no
C20	C21	C22	C23	1.3(5)	.	.	.	no
C21	C22	C23	C18	0.1(5)	.	.	.	no

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag

Fe	H7	3.51(4)	.	.	no
Fe	H10	3.36(4)	.	.	no
Fe	H10	3.22(4)	.	3_565	no
Cl	C11	3.627(5)	.	3_565	no
Cl	C16	3.591(3)	.	3_575	no
Cl	H10	3.06(4)	.	3_565	no
Cl	H11'	2.97(5)	.	3_565	no
Cl	H16	3.12(3)	.	3_575	no
Cl	H16'	3.13(4)	.	3_575	no
Cl	H14	3.02(3)	.	4_564	no
N1	H7	2.59(4)	.	.	no
N1	H10	2.38(4)	.	.	no
N2	H15'	2.76(4)	.	.	no
C1	C23	3.275(4)	.	.	no
C2	C18	3.421(4)	.	.	no
C7	C17	3.532(4)	.	.	no
C7	C18	3.449(4)	.	.	no
C7	C19	3.512(4)	.	.	no
C8	C20	3.466(5)	.	.	no

C8	C19	3.266(5)	.	.	no
C8	C18	3.544(5)	.	.	no
C9	C16	3.576(6)	.	.	no
C10	C17	3.574(4)	.	.	no
C11	Cl	3.627(5)	.	3_565	no
C13	C19	3.047(5)	.	3_565	no
C16	C9	3.576(6)	.	.	no
C16	Cl	3.591(3)	.	3_575	no
C17	C10	3.574(4)	.	.	no
C17	C7	3.532(4)	.	.	no
C18	C2	3.421(4)	.	.	no
C18	C8	3.544(5)	.	.	no
C18	C7	3.449(4)	.	.	no
C19	C13	3.047(5)	.	3_565	no
C19	C7	3.512(4)	.	.	no
C19	C8	3.266(5)	.	.	no
C20	C8	3.466(5)	.	.	no
C21	C22	3.463(5)	.	3_665	no
C22	C21	3.463(5)	.	3_665	no
C23	C1	3.275(4)	.	.	no
C1	H16"	2.81(3)	.	.	no
C1	H14'	3.06(5)	.	.	no
C2	H16"	2.83(3)	.	.	no
C3	H8	2.81(5)	.	.	no
C3	H9"	2.84(4)	.	.	no
C5	H12"	3.06(6)	.	.	no
C5	H12	2.87(5)	.	.	no
C5	H11"	3.04(5)	.	.	no
C6	H14'	3.00(4)	.	.	no
C8	H22	2.89(5)	.	3_665	no
C8	H3	2.91(5)	.	.	no
C9	H3	2.83(5)	.	.	no
C10	H14'	2.98(4)	.	.	no
C11	H23	2.91(3)	.	.	no
C12	H5	2.75(5)	.	.	no
C12	H15	2.94(5)	.	2_545	no
C13	H19	2.88(4)	.	3_565	no
C13	H15'	2.64(4)	.	.	no
C15	H12'	3.06(5)	.	2_555	no
C15	H13'	2.82(3)	.	.	no
C16	H9	2.63(6)	.	.	no
C17	H7	2.93(3)	.	.	no
C17	H10	3.08(3)	.	.	no
C18	H8"	2.96(4)	.	.	no
C18	H13'	2.42(4)	.	3_565	no
C18	H7	3.02(3)	.	.	no
C19	H8"	2.73(4)	.	.	no
C19	H13'	2.54(4)	.	3_565	no
C19	H13	3.03(3)	.	3_565	no
C19	H7	3.01(3)	.	.	no
C19	H16	2.98(3)	.	4_564	no
C20	H8"	2.72(3)	.	.	no
C21	H8"	2.94(4)	.	.	no
C22	H8"	3.02(5)	.	3_665	no
C23	H11	3.08(5)	.	.	no
H3	C8	2.91(5)	.	.	no
H3	C9	2.83(5)	.	.	no
H3	H8	2.40(7)	.	.	no
H3	H9"	2.36(6)	.	.	no
H5	C12	2.75(5)	.	.	no
H5	H12	2.37(7)	.	.	no

H7	Fe	3.51(4)	.	.	no
H7	N1	2.59(4)	.	.	no
H7	C17	2.93(3)	.	.	no
H7	C18	3.02(3)	.	.	no
H7	C19	3.01(3)	.	.	no
H8	C3	2.81(5)	.	.	no
H8	H3	2.40(7)	.	.	no
H8	H9"	2.34(7)	.	.	no
H8'	H9'	2.34(8)	.	.	no
H8"	C18	2.96(4)	.	.	no
H8"	C19	2.73(4)	.	.	no
H8"	C20	2.72(3)	.	.	no
H8"	C21	2.94(4)	.	.	no
H8"	C22	3.02(5)	.	3_665	no
H8"	H22	2.32(7)	.	3_665	no
H9	C16	2.63(6)	.	.	no
H9	H16'	2.19(8)	.	.	no
H9	H16"	2.35(6)	.	.	no
H9	H15"	2.55(6)	.	3_575	no
H9'	H8'	2.34(8)	.	.	no
H9"	C3	2.84(4)	.	.	no
H9"	H3	2.36(6)	.	.	no
H9"	H8	2.34(7)	.	.	no
H10	Fe	3.36(4)	.	.	no
H10	N1	2.38(4)	.	.	no
H10	C17	3.08(3)	.	.	no
H10	H14'	2.52(5)	.	.	no
H10	Fe	3.22(4)	.	3_565	no
H10	Cl	3.06(4)	.	3_565	no
H11	C23	3.08(5)	.	.	no
H11	H23	2.24(6)	.	.	no
H11'	H12'	2.34(6)	.	.	no
H11'	Cl	2.97(5)	.	3_565	no
H11"	C5	3.04(5)	.	.	no
H12	C5	2.87(5)	.	.	no
H12	H5	2.37(7)	.	.	no
H12'	H11'	2.34(6)	.	.	no
H12'	C15	3.06(5)	.	2_545	no
H12'	H15	2.44(7)	.	2_545	no
H12"	C5	3.06(6)	.	.	no
H12"	H14'	2.42(6)	.	.	no
H12"	H15	2.57(8)	.	2_545	no
H13	C19	3.03(3)	.	3_565	no
H13'	C15	2.82(3)	.	.	no
H13'	H15'	2.35(5)	.	.	no
H13'	C18	2.42(4)	.	3_565	no
H13'	C19	2.54(4)	.	3_565	no
H13'	H19	2.57(5)	.	3_565	no
H14	H15	2.53(5)	.	.	no
H14	H16	2.53(4)	.	.	no
H14	Cl	3.02(3)	.	4_565	no
H14'	C1	3.06(5)	.	.	no
H14'	C6	3.00(4)	.	.	no
H14'	C10	2.98(4)	.	.	no
H14'	H10	2.52(5)	.	.	no
H14'	H12"	2.42(6)	.	.	no
H14'	H16"	2.24(5)	.	.	no
H15	H14	2.53(5)	.	.	no
H15	H16	2.46(6)	.	.	no
H15	C12	2.94(5)	.	2_555	no
H15	H12'	2.44(7)	.	2_555	no

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 H15     H12"        2.57(8)                     .     2_555                 no
 H15'    N2          2.76(4)                     .       .                   no
 H15'    C13         2.64(4)                     .       .                   no
 H15'    H13'        2.35(5)                     .       .                   no
 H15"    H16'        2.40(6)                     .       .                   no
 H15"    H9          2.55(6)                     .     3_575                 no
 H15"    H16'        2.43(5)                     .     3_575                 no
 H16     H14         2.53(4)                     .       .                   no
 H16     H15         2.46(6)                     .       .                   no
 H16     Cl          3.12(3)                     .     3_575                 no
 H16     C19         2.98(3)                     .     4_565                 no
 H16     H19         2.58(4)                     .     4_565                 no
 H16'    H9          2.19(8)                     .       .                   no
 H16'    H15"        2.40(6)                     .       .                   no
 H16'    Cl          3.13(4)                     .     3_575                 no
 H16'    H15"        2.43(5)                     .     3_575                 no
 H16"    C1          2.81(3)                     .       .                   no
 H16"    C2          2.83(3)                     .       .                   no
 H16"    H9          2.35(6)                     .       .                   no
 H16"    H14'        2.24(5)                     .       .                   no
 H19     C13         2.88(4)                     .     3_565                 no
 H19     H13'        2.57(5)                     .     3_565                 no
 H19     H16         2.58(4)                     .     4_564                 no
 H22     C8          2.89(5)                     .     3_665                 no
 H22     H8"         2.32(7)                     .     3_665                 no
 H23     C11         2.91(3)                     .       .                   no
 H23     H11         2.24(6)                     .       .                   no

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
C7      H7      N1         0.92(4)    2.59(4)   3.046(4)     111(2)     .   yes
C10     H10     N1         0.96(4)    2.38(4)   2.858(4)     111(3)     .   yes

#===END of Crystallographic Information File
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