checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: klat416s

Bond precision: C-C = 0.0082 A Wavelength=0.71073

Cell: a=9.383(2) b=12.088(3) c=17.463(4)
alpha=77.419(3) beta=74.976(3) gamma=67.314(3)
Temperature: 120 K

	Calculated	Reported
Volume	1749.5(7)	1749.5(7)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C48 H80 B2 Fe2 N14	?
Sum formula	C48 H80 B2 Fe2 N14	C64 H112 B2 FE2 N14 O4
Mr	986.58	1275.00
Dx,g cm-3	0.936	1.210
Z	1	1
Mu (mm-1)	0.450	0.469
F000	528.0	688.0
F000'	528.80	
h,k,lmax	11,14,20	11,14,20
Nref	6162	6144
Tmin,Tmax	0.884,0.968	0.844,0.966
Tmin'	0.837	

Correction method= MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.000

R(reflections)= 0.0721(4220) wR2(reflections)= 0.2163(6144)

S = 1.044 Npar= 340

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 A

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 1
From the CIF: _chemical_formula_weight 1275.00
TEST: Calculate formula weight from _atom_site_*

```
            atom     mass    num     sum
            C        12.01   48.00  576.53
            H         1.01   80.00   80.64
            B        10.81    2.00   21.62
            N        14.01   14.00  196.10
            Fe       55.85    2.00  111.69
            O        16.00    0.00    0.00
            Calculated formula weight              986.58
PLAT043_ALERT_1_A Check Reported Molecular Weight ...............    1275.00
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Alert level B

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PLAT213_ALERT_2_B Atom C10     has ADP max/min Ratio .............       4.10 prola
PLAT213_ALERT_2_B Atom C15'    has ADP max/min Ratio .............       4.80 prola
PLAT213_ALERT_2_B Atom C15     has ADP max/min Ratio .............       4.80 prola
PLAT301_ALERT_3_B Main Residue  Disorder .........................      27.00 Perc.
PLAT049_ALERT_1_B Calculated Density less than 1.0 gcm-3 .........       0.94
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Alert level C

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PLAT213_ALERT_2_C Atom C11     has ADP max/min Ratio .............       3.80 prola
PLAT213_ALERT_2_C Atom C12'    has ADP max/min Ratio .............       3.10 prola
PLAT213_ALERT_2_C Atom C16     has ADP max/min Ratio .............       3.60 prola
PLAT213_ALERT_2_C Atom C22'    has ADP max/min Ratio .............       3.10 prola
PLAT213_ALERT_2_C Atom C24     has ADP max/min Ratio .............       3.40 prola
PLAT213_ALERT_2_C Atom C12     has ADP max/min Ratio .............       3.10 prola
PLAT213_ALERT_2_C Atom C22     has ADP max/min Ratio .............       3.10 prola
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       2.83 Ratio
PLAT222_ALERT_3_C Large Non-Solvent    H     Ueq(max)/Ueq(min) ...       3.03 Ratio
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C10
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C4'
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C19
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C20'
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C4
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C20
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ...          8
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C1     -   C2     ...       1.38 Ang.
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C9     -   C10    ...       1.39 Ang.
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C17    -   C18    ...       1.38 Ang.
PLAT041_ALERT_1_C Calc. and Rep. SumFormula Strings    Differ ....          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT154_ALERT_1_C The su's on the Cell Angles are Equal  (x 10000)        300 Deg.
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety         C8
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety        C24
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Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C64 H112 B2 Fe2 N14 O4
            Atom count from the _atom_site data:  C48 H80. B2 Fe2 N14
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    1
           From the CIF: _chemical_formula_sum  C64 H112 B2 Fe2 N14 O4
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         64.00     48.00   16.00
           H        112.00     80.00   32.00
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SQUEEZE - Procedure (cf. BYPASS-procedure - P. van der Sluis & A.L. Spek (1990). Acta Cryst. A46, 194-201)

:: # Accepted Reflns Hmax Kmax Lmax
:: 19747 12 16 23

:: A, B, C (Angstrom) = 9.383 12.088 17.463
:: NX, NY, NZ (SOLV-MAP) = 48 60 84
:: NX, NY, NZ (FFT-MAP) = 32 64 64
:: Resolution (FFT-MAP) = 0.29 0.19 0.27 Angstrom

Missing Reflections below sin(theta)/lambda=0.3

N	H	K	L	Theta
1	3	-1	2	8.07

:: Number of Removed Systematic Extinctions = 0
:: Number of Non-extinction Reflections = 19747
:: Number of Missing Low Order Reflections = 1

:: Fo-scale =0.153884E+00 - SinT/L-Min = 0.20 for Fo/Fc-Scaling

:: Cycle = 1, R(F) = 0.25, Nref(Hemi) = 7894, R(F > 4SIGF) = 0.17 Nref = 4416

Unique Density Minima in Enhanced Difference Map (CutOff level = -0.50 eA-3)

#	x	y	z	(e/A^3)	Shortest Contacts within 3.2 Angstrom (Excl. H)
1	0.990	0.973	0.626	-1.66	Fe1 0.28; N7 1.54; N3 2.30; N1 2.31; N5 2.32; N7 2.74; N4 3.19; N2 3.19;
2	1.005	0.063	0.341	-1.14	Fe1 0.43; N1 1.80; N3 1.95; N7 2.11; N5 2.31; N2 2.63; N4 2.70; B1 2.85; N6 2.94;
3	0.017	0.981	0.347	-1.11	Fe1 0.62; N5 1.56; N7 2.11; N3 2.22; N1 2.43; N6 2.52; C17 2.71; N4 2.91; B1 2.92;
4	0.021	1.000	0.311	-1.09	Fe1 0.91; N5 1.41; N3 1.90; N6 2.05; N1 2.14; B1 2.30; N4 2.36; N2 2.51; N7 2.67;
5	0.623	0.915	0.828	-0.95	C10 0.31; C11 1.21; C9 1.28; N4 2.01; N3 2.10; C12 2.46; C12' 2.46; C16 2.52; C15' 2.88;
6	0.375	0.079	0.315	-0.80	C12 0.26; C12' 0.95; C13' 0.96; C9 1.44; C13 1.49; C14 1.56; C15 1.82; C15' 1.99; N3 2.26;
7	0.403	0.970	0.780	-0.77	C15' 0.92; C15 1.32; C12' 1.86; C12 2.04; C10 2.08; C9 2.19; C14' 2.91; C13' 2.99; C14 3.08;
8	0.652	0.940	0.748	-0.75	C9 0.19; C12 1.33; C12' 1.36; N3 1.42; C10 1.44; C13' 2.21; C11 2.21; N4 2.22; C15' 2.37;
9	0.335	0.643	0.800	-0.69	C2 0.65; C3 1.23; C1 2.02; C8 2.11; N2 2.39; N1 2.74; C4' 3.19;
10	0.553	0.962	0.751	-0.69	C9 0.90; C12' 0.98; C12 1.15; C10 1.51; C15' 1.56; C15 1.75; C13' 2.19; N3 2.23; C14 2.31;
11	0.486	0.871	0.361	-0.69	C14' 0.31; C14 1.26; C12' 1.62; C12 2.29; C13' 2.38; C15' 2.48; C9 2.74; C15 2.77; C6' 3.18;
12	0.033	0.067	0.098	-0.67	B1 1.35; N4 2.27; N6 2.33; N2 2.45; C16 2.48; C24 2.62; C11 2.73; C19 2.77; C8 2.83;
13	0.772	0.799	0.486	-0.67	C23' 0.77; C23 1.10; C20' 2.14; C20 2.62; C13 2.75; C22' 2.80; C13' 2.89;
14	0.754	0.110	0.531	-0.64	C6' 1.91; C14 2.17; N7 2.19; C6 2.29; N7 2.31; C14' 2.61; C13' 2.95; C21 3.01; Fe1 3.07;
15	0.979	0.974	0.219	-0.64	N6 0.37; B1 1.26; N5 1.44; C19 1.65; N2 2.16; N4 2.32; C17 2.40; C18 2.52; C24 2.75;
16	0.947	0.813	0.500	-0.64	C23' 1.42; C23 1.60; C21 2.44; C20' 2.45; C20 2.45; N7 2.52; N7 2.60; C5 2.68; C21' 2.69;
17	0.081	0.218	0.528	-0.63	C23' 0.69; C23 0.78; C20' 1.69; C20 1.84; C21' 2.25; C21 2.30; C17 2.77; C22' 2.88; C22 3.00;
18	0.511	0.994	0.688	-0.63	C12' 0.48; C12 0.87; C15' 1.17; C15 1.28; C14 1.38; C13' 1.51; C14' 1.68; C9 1.81; C13 2.33;
19	0.463	0.940	0.768	-0.62	C15' 1.00; C15 1.18; C12' 1.54; C12 1.57; C9 1.78; C10 1.85; C13' 2.56; C13 2.79; C14 2.80;
20	0.615	0.015	0.780	-0.61	C9 0.87; C10 1.22; N3 1.64; C12' 1.78; C11 1.87; N4 2.04; C12 2.16; C14' 2.50; C15' 2.64;
21	0.018	0.970	0.529	-0.61	N7 0.28; N7 1.15; Fe1 1.93; Fe1 2.95;
22	0.386	0.803	0.548	-0.61	C6' 0.56; C6 0.97; C4' 1.80; C4 2.40; C1 2.64; C7' 2.65; C5' 3.01; N1 3.06; C14 3.13;
23	0.063	0.814	0.391	-0.60	C21 1.35; C20 1.49; C21' 1.80; C20' 1.88; N5 1.90; C17 1.96; C23 1.99; C23' 2.10; Fe1 2.42;
24	0.878	0.163	0.217	-0.60	N2 0.05; N1 1.36; C3 1.39; B1 1.50; C1 2.19; C2 2.22; N6 2.47; N4 2.48; C8 2.55;
25	0.109	0.239	0.559	-0.59	C23 0.11; C23' 0.48; C20' 1.06; C20 1.45; C21' 2.09; C22' 2.17; C17 2.26; C21 2.44; C22 2.50;
26	0.036	0.079	0.235	-0.58	B1 1.17; N4 1.27; N2 1.55; N3 1.62; N1 1.87; N6 1.98; Fe1 2.06; N5 2.32; C11 2.61;
27	0.155	0.056	0.202	-0.57	N4 0.24; N3 1.22; B1 1.49; C11 1.60; C9 2.11; C10 2.32; N6 2.38; N2 2.42; Fe1 2.70;
28	0.586	0.837	0.562	-0.57	C13 1.84; C13' 1.93; C6' 2.62; C23' 2.63; C14 2.71; C12 2.72; C15 2.91; C6 2.92; C23 2.95;
29	0.965	0.903	0.940	-0.57	B1 1.96; C16 2.33; C24 2.63; C8 2.69; N4 2.73; N2 2.87; C24 2.87; C11 2.92; N6 2.99;
30	0.320	0.156	0.094	-0.57	C11 1.11; C16 1.38; C10 1.65; N4 2.28; C9 2.73; N3 3.08;
31	0.804	0.498	0.436	-0.56	C5' 1.84; C22' 1.85; C5 2.05; C7 2.48; C4 2.72; C22 2.73; C21' 3.16;
32	0.880	0.972	0.436	-0.56	N7 1.59; Fe1 1.80; C23' 2.25; N7 2.38; C23 2.55; N5 2.59; N1 3.10; C6' 3.13; C20' 3.15;
33	0.210	0.981	0.060	-0.56	C16 1.77; C11 2.33; B1 2.47; N4 2.53; C24 2.88; N6 3.02; C19 3.17;
34	0.216	0.095	0.236	-0.56	N3 0.72; C9 1.20; N4 1.21; C11 1.79; C10 1.83; C12 2.36; C12' 2.50; B1 2.58; Fe1 2.67;
35	0.198	0.971	0.268	-0.56	N3 0.90; N4 1.59; C9 1.89; Fe1 2.01; N5 2.28; B1 2.45; N6 2.50; C11 2.56; C10 2.71;
36	0.930	0.969	0.331	-0.56	N5 1.02; Fe1 1.44; N6 1.99; C17 2.12; N1 2.35; B1 2.70; N2 2.74; N7 2.78; C23' 2.90;
37	0.877	0.234	0.610	-0.56	C21 0.74; C21' 1.37; C20 1.38; C20' 1.95; C17 2.15; C23 2.24; N5 2.29; C23' 2.44; C22 2.71;
38	0.217	0.091	-0.004	-0.56	C16 1.24; C24 2.48; C11 2.61;
39	0.964	0.898	0.408	-0.55	Fe1 1.80; C23' 1.90; N5 1.91; N7 2.00; C23 2.03; C20 2.26; C20' 2.34; C17 2.35; C21 2.40;
40	1.008	0.070	0.189	-0.55	B1 0.22; N2 1.41; N4 1.48; N6 1.58; N1 2.34; N3 2.39; N5 2.47; C3 2.54; C11 2.64;
41	0.334	0.559	0.877	-0.55	C8 1.99; C2 2.12; C3 2.14;
42	0.959	0.043	0.249	-0.55	B1 1.23; N6 1.37; N2 1.47; N5 1.67; N1 1.79; Fe1 2.02; N4 2.06; N3 2.36; C19 2.66;
43	0.906	0.684	0.309	-0.55	C22' 1.40; C18 1.53; C17 1.66; C20' 1.72; C22 1.88; C20 2.05; C23 2.66; C21' 2.71; C19 2.87;
44	0.678	0.916	0.873	-0.55	C11 0.29; C10 1.11; C16 1.51; N4 1.63; C9 2.10; N3 2.38; B1 2.91;