Datablock: 1

```
Bond precision:      C-C = 0.0040 A              Wavelength=0.71073
Cell:        a=17.8984(5)    b=12.1563(3)    c=18.9956(5)
             alpha=90          beta=90         gamma=90
Temperature  293 K
:
                 Calculated                   Reported
Volume           4133.03(19)                  4133.03(19)
Space group      P b c a                      P b c a
Hall group       -P 2ac 2ab                   -P 2ac 2ab
Moiety formula   C12 H14 Co N8 S4, B F4, H2 O  ?
Sum formula      C12 H16 B Co F4 N8 O S4       C12 H16 B Co F4 N8 O S4
Mr               562.31                       562.31
Dx,g cm-3        1.807                        1.807
Z                8                            8
Mu (mm-1)        1.295                        1.295
F000             2272.0                       2272.0
F000'            2279.61
h,k,lmax         23,15,24                     23,15,24
Nref             4742                         4739
Tmin,Tmax        0.369,0.772                  0.531,1.000
Tmin'            0.341
Correction method= # Reported T Limits: Tmin=0.531
Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.999       Theta(max)= 27.485
                                 wR2(reflections)=
R(reflections)= 0.0394( 3964)    0.1039( 4739)

S = 1.074              Npar= 288
```

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

PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O1W	0.177	Check
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O1W - H1W .		1.02	Ang.
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O1W - H2W .		1.01	Ang.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N8 --H8NB .		Please	Check
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.89Ang From O1W .		-0.59	eA-3

And 2 other PLAT976 Alerts

PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.62Ang From O1W .		-0.56	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.84Ang From O1W .		-0.52	eA-3

⚪ Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	9	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	Report
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..	0.80	mm
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.85	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	B1	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	4	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1 (III) .	3.59	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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

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

It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.
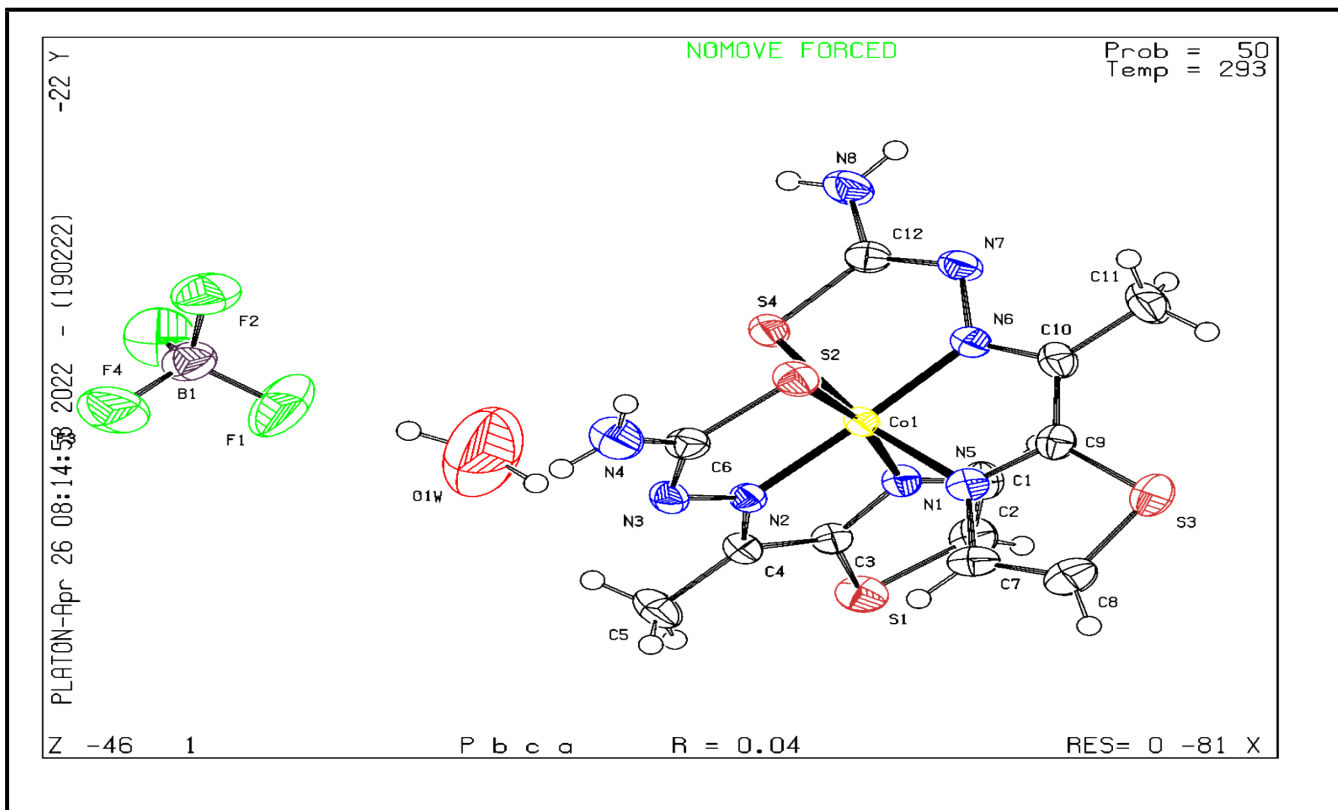
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock 1 - ellipsoid plot