

# checkCIF/PLATON report

No syntax errors found.    CIF dictionary    Interpreting this report

## Datablock: mont01s

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Bond precision:    C-C = 0.0031 A

Wavelength=0.71073

Cell:            a=10.305(2)            b=11.201(3)            c=11.779(3)  
                  alpha=63.547(4)        beta=65.449(4)        gamma=66.927(4)  
Temperature:    200 K

	Calculated	Reported
Volume	1070.9(4)	1071.0(4)
Space group	P -1	?
Hall group	-P 1	?
Moiety formula	C22 H26 F3 N O3	?
Sum formula	C22 H26 F3 N O3	C22 H26 F3 N O3
Mr	409.44	409.44
Dx,g cm-3	1.270	1.270
Z	2	2
Mu (mm-1)	0.101	0.101
F000	432.0	432.0
F000'	432.27	
h,k,lmax	13,14,15	13,14,15
Nref	5351	5170
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.966

Theta(max)= 28.370

R(reflections)= 0.0586( 3057)

wR2(reflections)= 0.1594( 5170)

S = 0.927

Npar= 293

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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.

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### Alert level A

PLAT213_ALERT_2_A Atom F3B	has ADP max/min Ratio .....	11.70	prola
PLAT052_ALERT_1_A (Proper) Absorption Correction Method Missing ..		?	
PLAT053_ALERT_1_A Minimum Crystal Dimension Missing (or Error) ...		?	
PLAT054_ALERT_1_A Medium Crystal Dimension Missing (or Error) ...		?	
PLAT055_ALERT_1_A Maximum Crystal Dimension Missing (or Error) ...		?	
PLAT093_ALERT_1_A No su's on H-atoms, but refinement reported as .			mixed

PLAT122\_ALERT\_1\_A No \_symmetry\_space\_group\_name\_H-M Given ..... ?

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**Alert level B**

PLAT242\_ALERT\_2\_B Check Low Ueq as Compared to Neighbors for C1

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**Alert level C**

PLAT029\_ALERT\_3\_C \_diffrn\_measured\_fraction\_theta\_full Low ..... 0.97  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for N1 -- C14 .. 5.50 su  
PLAT120\_ALERT\_1\_C Reported SPGR ? Inconsistent with Explicit P-1  
PLAT194\_ALERT\_1\_C Missing \_cell\_measurement\_reflns\_used datum .... ?  
PLAT195\_ALERT\_1\_C Missing \_cell\_measurement\_theta\_max datum .... ?  
PLAT196\_ALERT\_1\_C Missing \_cell\_measurement\_theta\_min datum .... ?

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**Alert level G**

PLAT301\_ALERT\_3\_G Note: Main Residue Disorder ..... 9.00 Perc.  
PLAT154\_ALERT\_1\_G The su's on the Cell Angles are Equal (x 10000) 400 Deg.  
PLAT764\_ALERT\_4\_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.18 Ratio  
PLAT793\_ALERT\_4\_G The Model has Chirality at C8 (Verify) .... R  
PLAT793\_ALERT\_4\_G The Model has Chirality at C9 (Verify) .... S

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- 7 **ALERT level A** = In general: serious problem  
1 **ALERT level B** = Potentially serious problem  
6 **ALERT level C** = Check and explain  
5 **ALERT level G** = General alerts; check

- 11 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
3 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
2 **ALERT type 3** Indicator that the structure quality may be low  
3 **ALERT type 4** Improvement, methodology, query or suggestion  
0 **ALERT type 5** Informative message, check
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Datablock mont01s - ellipsoid plot

