Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information:

Anisotropic displacement parameters from dispersion-corrected DFT methods and their experimental validation by temperature-dependent X-ray diffraction

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S1. Powder Patterns

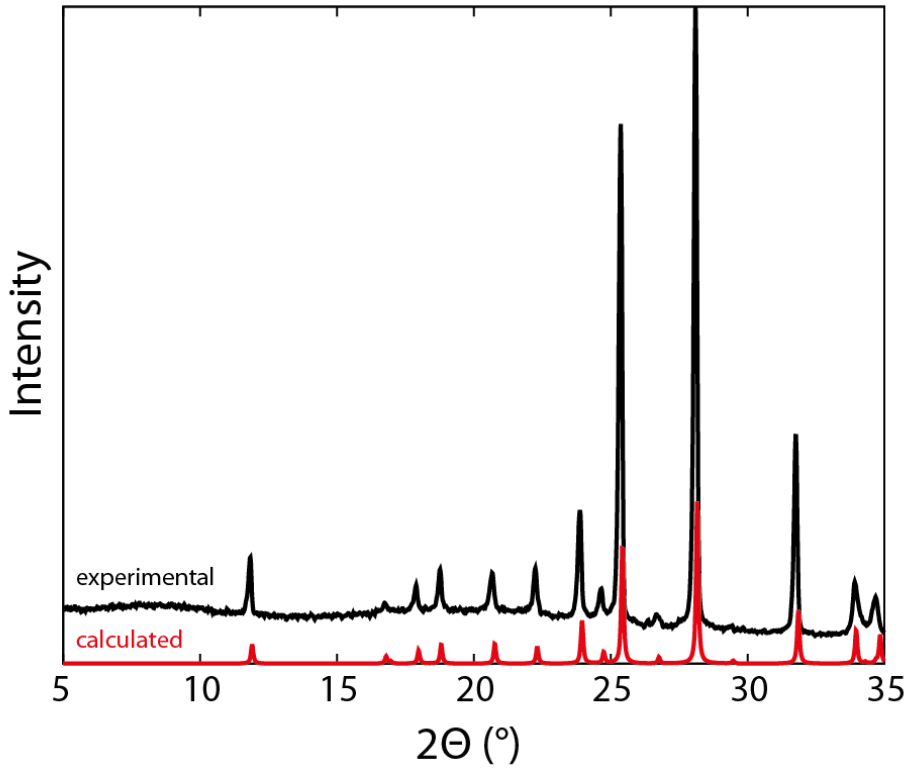

Figure S1. Comparison of the experimental powder pattern of the monoclinic phase to a calculated one from the experimental single crystal structure.

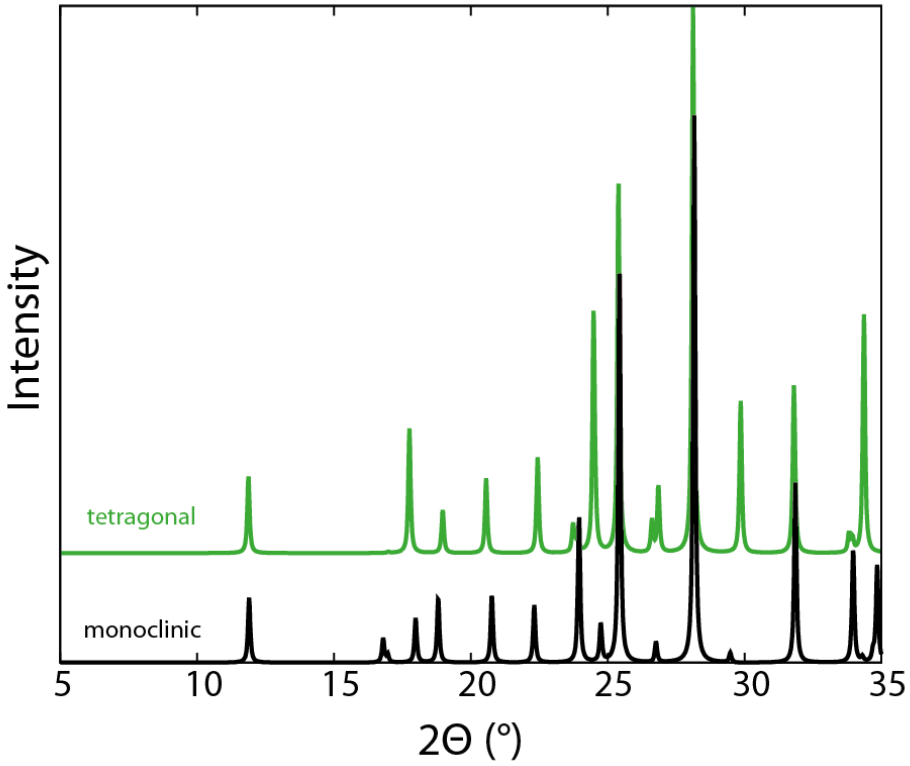

Figure S2. Comparison of the simulated diffraction pattern of the tetragonal polymorph to the simulated diffraction pattern of the monoclinic polymorph. The polymorphs can be easily distinguished.

S2. Shape Criterion

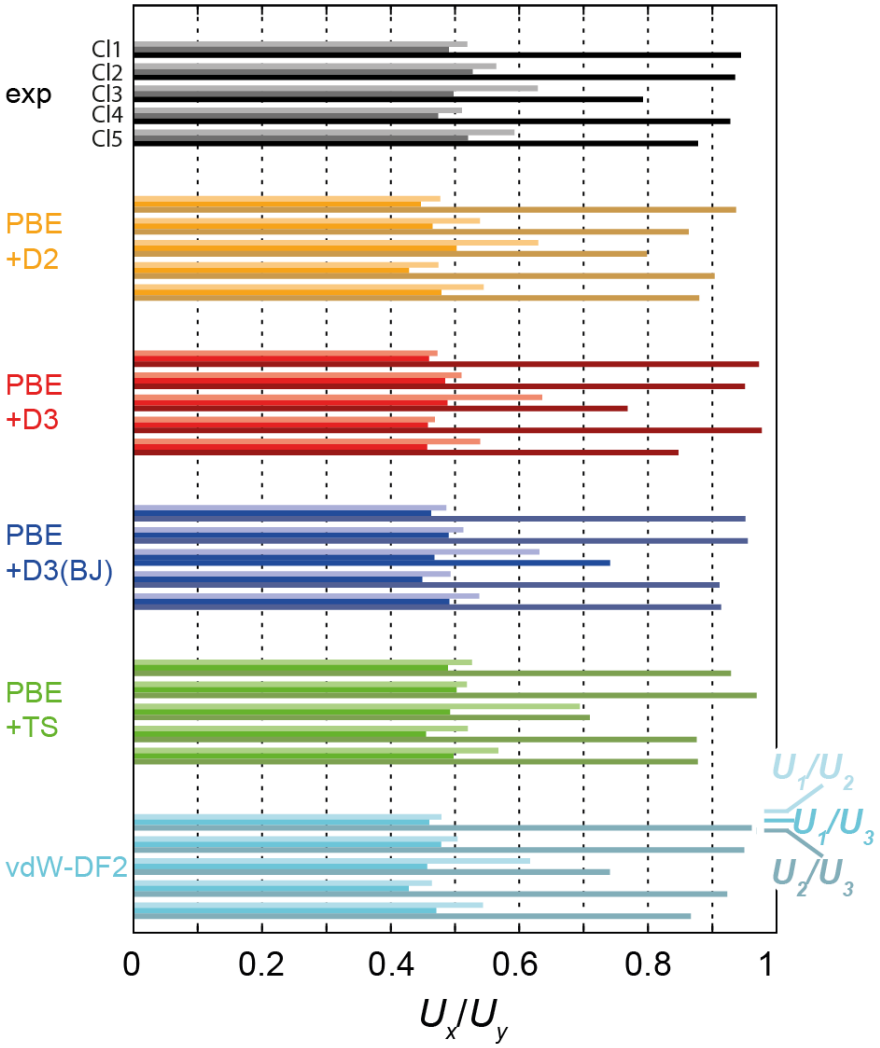

Figure S3. Comparison of the ratio of the main-axis components of the thermal displacement parameters calculated at several levels of theory with the experiment at 100 K. These quotients give information about the shape of the thermal ellipsoids.

S3. k-Point Meshes (for Electronic-Structure Calculations)

Table S1. **k**-point convergence of the electronic energies for the different methods used in our calculation. The energy is obviously converged in terms of the **k**-point mesh size.

Method	Structure	**k**-point mesh for the electronic structure calculation	Energy (eV)
PBE+D2	fully optimised	10×10×4	-129.44726099
PBE+D2	optimised at the PBE+D2 level with a 10×10×4 **k**-point mesh	11×11×5	-129.44727115
PBE+D3	fully optimised	10×10×4	-129.60977572
PBE+D3	optimised at the PBE+D3 level with a 10×10×4 **k**-point mesh	11×11×5	-129.60977719
PBE+D3(BJ)	fully optimised	10×10×4	-130.47687376
PBE+D3(BJ)	optimised at the PBE+D3(BJ) level with a 10×10×4 **k**-point mesh	11×11×5	-130.47687421
PBE+TS	fully optimised	9×10×4	-129.59291623
PBE+TS	optimised at the PBE+TS level with a 9×10×4 **k**-point mesh	11×11×5	-129.59292067
vdW-DF2	fully optimised	10×10×4	-90.71193744
vdW-DF2	optimised at the vdw-DF2 level with a 10×10×4 **k**-point mesh	11×11×5	-90.71196497
PBE	fully optimised	10×10×4	-127.83095426
PBE	optimised at the PBE level with a 10×10×4 **k**-point mesh	11×11×5	-127.83095381

S4. *q*-Point Meshes (for the ADP Calculation within Phonopy)

Please note that the following ADPs refer to a Cartesian coordinate system. This is why we refer to the matrix elements as U_{xx}, U_{yy}, U_{zz} etc. in the following plots.

Diamond

The diamond structure was optimised at the PBE/PAW level of theory. The **k**-point mesh was a 14×14×14 mesh. The convergence criteria for the structures on which the phonon calculation are based are the same as the ones for Cl_5py. Figure S4 clearly shows the convergence of the ADPs with a growing q-point mesh.

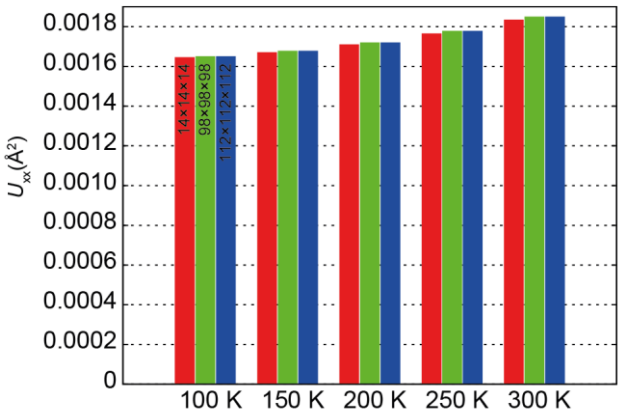

Figure S4. Convergence of the ADPs of diamond when a higher q-point mesh is applied during the ADP calculation. The shown **q**-point meshes are 14×14×14, 98×98×98 and 112×112×112.

Cl_5py

We show the convergence of the U_{xx} parameter of Cl3 at 300 K for every used method with and without cutoff in the following Figures. The ADPs calculated at higher temperatures are more sensitive to different **q**-point mesh sizes. It is also obvious that a small cutoff is needed for the calculation of the ADPs to arrive at reliable ones. During this calculation the force constants were re-symmetrised ("FC_SYMMETRY=1").

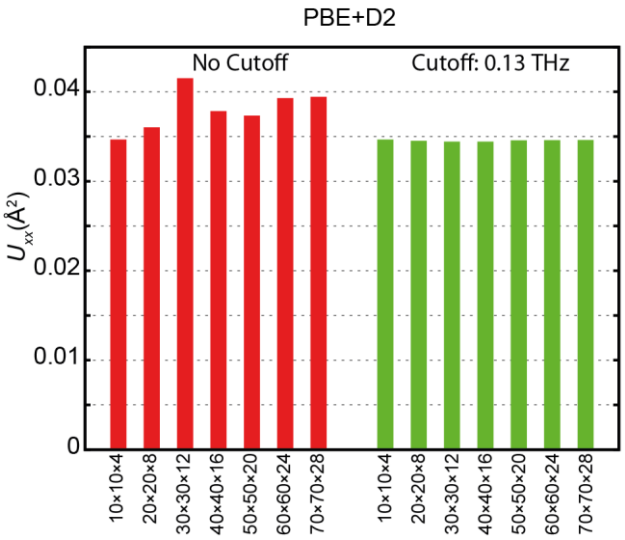

Figure S5. Convergence of the ADPs based on the forces from the PBE+D2 level of theory with an increasing **q**-point mesh size. The cutoff clearly improves the ADP calculation.

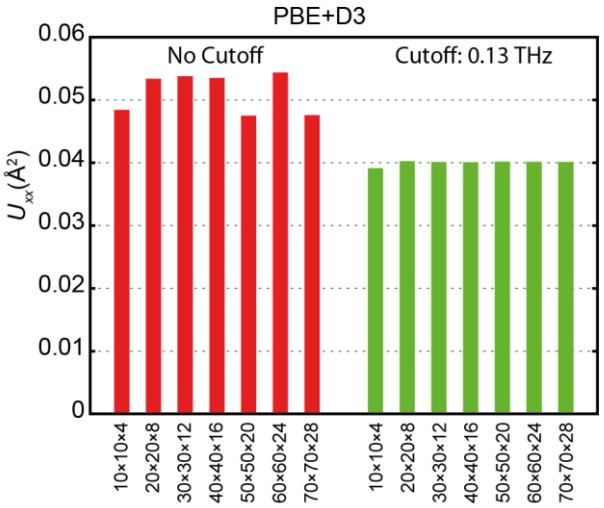

Figure S6. Convergence of the ADPs based on the forces from the PBE+D3 level of theory with an increasing **q**-point mesh size. The cutoff clearly improves the ADP calculation.

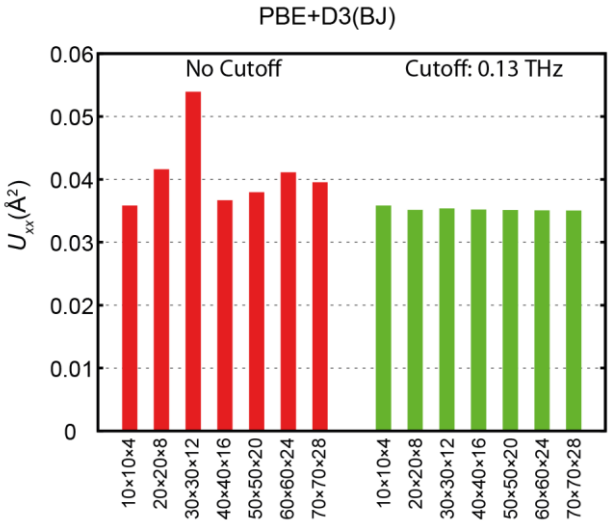

Figure S7. Convergence of the ADPs based on the forces from the PBE+D3(BJ) level of theory with an increasing **q**-point mesh size. The cutoff clearly improves the ADP calculation.

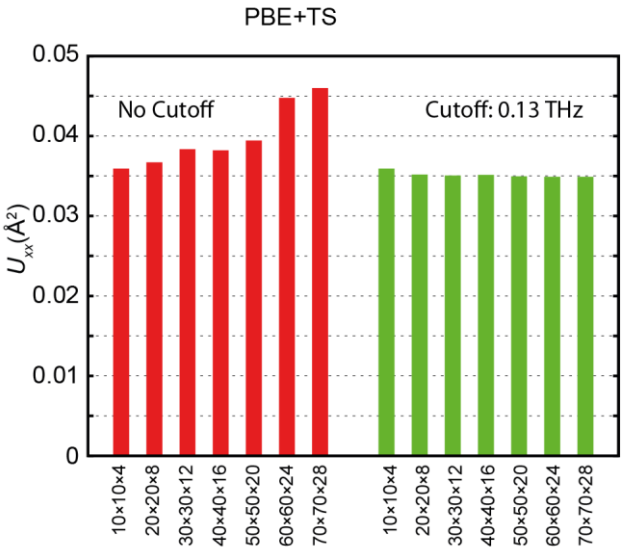

Figure S8. Convergence of the ADPs based on the forces from the PBE+TS level of theory with an increasing **q**-point mesh size. The cutoff clearly improves the ADP calculation.

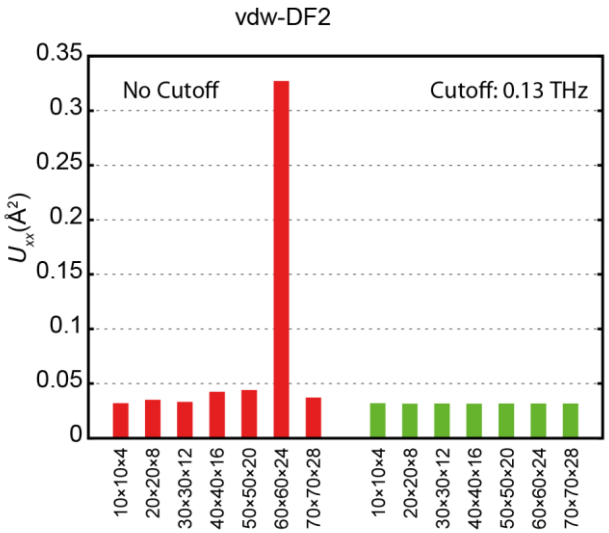

Figure S9. Convergence of the ADPs based on the forces from the vdw-DF2 level of theory with an increasing **q**-point mesh size. The cutoff clearly improves the ADP calculation.

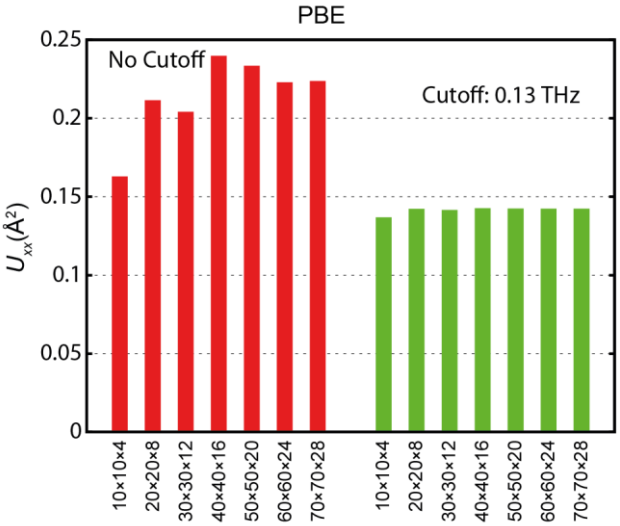

Figure S10. Convergence of the ADPs based on the forces from the PBE level of theory with an increasing **q**-point mesh size. The cutoff clearly improves the ADP calculation. The PBE-ADPs differ strongly from the experimental ones and the ADPs calculated at dispersion-corrected levels of theory.

S5. Free Energy with and without Cutoff

Only a small **q**-point mesh (20×20×8) was used for this calculation within Phonopy. The free energies at 300 K with and without cutoff show no significant difference at 300 K.

Table S2. Influence of the cutoff of 0.13 THz on the free energy F at 300 K.

Method	F(300 K) (kJ/mol) without cutoff	F(300 K) (kJ/mol) with a cutoff of 0.13 THz
PBE+D2	66.99	67.02
PBE+D3	66.09	66.11
PBE+D3(BJ)	67.58	67.58
PBE+TS	68.59	68.61
Vdw-DF2	65.68	65.71
PBE	54.56	54.77

S6. Supercell Size (for ADP Calculation within Phonopy)

The ADPs were calculated with two different supercell sizes (3×3×1 and 4×4×2), only one Γ-point was used for the calculation of the forces. As one can see, the ADPs are slightly but not massively worse when using the 3×3×1 supercell. Whenever possible, one should converge the supercell size with respect to the ADPs. In this case, a larger supercell than a 4×4×2 supercell (which here contains 704 atoms) is computationally not affordable.

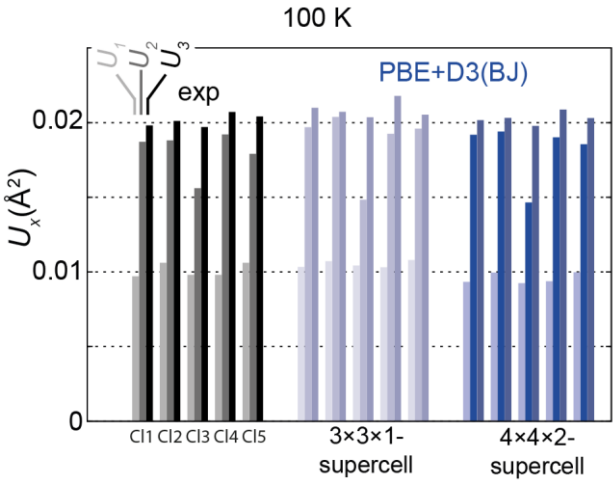

Figure S11. Effect of supercell size on the ADPs. The 4×4×2 setup was used for the computations in the main text.

S7. Structures in POSCAR Format

Pre-Optimized Structures

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PBE+D3

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  0.7257556527171665  0.0619755929211879  0.9926911047618405
  0.7198884716394749  0.8120028676262201  0.5664400449879323
  0.7198726718920593  0.1880168828689523  0.0664377852846909
  0.3738678829318807  0.5876270939181991  0.4921422644554362
  0.3738549492717287  0.4123656013242709  0.9921373053798629
```

Structures for Phonon Calculation

The structures were re-optimised with higher convergence criteria for the following phonon calculation.

```
PBE+D2
   1.00000000000000
     5.3505150960730425    0.0000002237510558    0.0097962277054017
    -0.0000000032055366    5.1924406701029007    0.0000005891109016
    -2.5327621368973490    0.0000007727828706   14.8439180805270166
   Cl   C    N
    10    10     2
Direct
  0.1149071834886541  0.6767238981336590  0.3328008339629065
  0.1149072008740077  0.3232758914572713  0.8328008547076351
  0.5321893216170821  0.1092765347676448  0.3241311953331731
  0.5321893782690310  0.8907232242087559  0.8241312630633573
  0.9618213558063715  0.1771526289428493  0.4921221856264921
  0.9618215778308183  0.8228473816135278  0.9921222341143192
  0.9686868697662376  0.8162026945784575  0.6599632067871255
  0.9686871301192639  0.1837975193136927  0.1599631944961430
  0.5316252276623317  0.3970082058646298  0.6530723070647255
  0.5316254568857985  0.6029920087901530  0.1530722405830645
  0.3582494062624093  0.7256232313851427  0.4215263638659010
  0.3582495055799484  0.2743765329029557  0.9215263142562620
  0.5410356626498753  0.9176834497259492  0.4169086885510609
  0.5410358665263360  0.0823164426235365  0.9169087622722643
  0.5430362682920347  0.6026830433873585  0.5637685447730405
  0.5430363249011805  0.3973170671572035  0.0637684622425212
  0.7340864916251419  0.9476933179652391  0.4921922710933586
  0.7340865909844183  0.0523066184933114  0.9921922200252027
  0.7373837213892145  0.7867611149459464  0.5677903108783227
  0.7373839438255487  0.2132390786025908  0.0677903445550569
  0.3619775500607858  0.5754921596738427  0.4928940184876538
  0.3619778415834887  0.4245079554662965  0.9928941272604632

PBE+D3
  1.00000000000000
     5.3805244183329073    0.0000000445374535   -0.0560823766844859
     0.0000001128344493    5.2091159037598347   -0.0000002626538988
    -2.7313504703433513   -0.0000005102159734   15.1501995837013936
   Cl   C    N
    10    10     2
Direct
  0.1211221160828546  0.6620667874333916  0.3323686398469351
  0.1211220518551589  0.3379332254469038  0.8323686250055613
  0.5373275116720997  0.0904690524397789  0.3240415109453244
  0.5373274179061763  0.9095309322517210  0.8240414850898550
  0.9606939649393639  0.1740982423579038  0.4921427894119949
  0.9606939075840345  0.8259017668420562  0.9921427497170775
  0.9620832136584949  0.8319903292423397  0.6603056095757909
  0.9620831928698991  0.1680096605448871  0.1603055850376874
  0.5277459546020158  0.4142694952435871  0.6533307378752458
  0.5277459194423090  0.5857304806106346  0.1533307376698340
  0.3610384542800863  0.7183420778700995  0.4213666033335237
  0.3610384379928257  0.2816579474360040  0.9213666114926075
  0.5434931404167024  0.9087519251792993  0.4168245867610759
  0.5434929706377908  0.0912481353268593  0.9168245309981510
  0.5409541648468914  0.6098331468152142  0.5638364458830394
  0.5409542734004411  0.3901667900864254  0.0638364697829907
  0.7336443573459934  0.9459849887746461  0.4922329313896610
  0.7336443874054749  0.0540150347270716  0.9922329448130971
  0.7344092224552555  0.7934500379060399  0.5679225242437961
```

```
  0.7344091356150135  0.2065499740677613  0.0679224784915931
  0.3624881145598655  0.5757708585389679  0.4927977145218024
  0.3624879664311961  0.4242291108584575  0.9927976321133275

PBE+D3(BJ)
   1.00000000000000
     5.3271448991819241    0.0000000012333532    0.0000229819805352
     0.0000000011167501    5.1761818976290614   -0.0000000066773809
    -2.7078325907876550   -0.0000000127922121   14.9446074192090581
   Cl   C    N
    10    10     2
Direct
  0.1160024502651523  0.6675764360867843  0.3317276907988507
  0.5344821537945116  0.0994603414955016  0.3234699277166814
  0.9631761050403089  0.1774005986313610  0.4920126981392658
  0.9673185714211312  0.8261042138471093  0.6606384721872102
  0.5303120593264280  0.4059115058077509  0.6541972258198763
  0.1160024488448494  0.3324235640839787  0.8317276902687398
  0.5344821564111029  0.9005396573285579  0.8234699257068477
  0.9631761037157293  0.8225993995161029  0.9920127022505609
  0.9673185670350342  0.1738957852849725  0.1606384754468834
  0.5303120559127734  0.5940884966364486  0.1541972253420286
  0.3583430961522991  0.7205110707603626  0.4211309960650972
  0.5419890949209973  0.9126997478438056  0.4165595754999049
  0.5416224929405917  0.6059379943918155  0.5641851388269851
  0.7345867525730830  0.9474816265346476  0.4921544554845617
  0.7365019551152270  0.7908220579468308  0.5681169890803970
  0.3583431041100325  0.2794889283926852  0.9211309944894434
  0.5419890951995699  0.0873002564278116  0.9165595753734863
  0.5416224924101161  0.3940620021736796  0.0641851378765044
  0.7345867525372206  0.0525183733885521  0.9921544551616646
  0.7365019478624329  0.2091779424670627  0.0681169908950160
  0.3607648057538337  0.5740985945780599  0.4929070627726560
  0.3607648104083847  0.4259014063761192  0.9929070614479316

PBE+TS
   1.00000000000000
     5.3532346825970301    0.0000000651084227   -0.0411855480683922
     0.0000001217428936    5.2273449447838738   -0.0000005519739951
    -2.6743221667420385   -0.0000016898895777   15.3137702626725876
   Cl   C    N
    10    10     2
Direct
  0.1239143921676959  0.6614498473664228  0.3340767961841125
  0.1239144112372167  0.3385501755611342  0.8340767843132550
  0.5401402747921243  0.0898462233272305  0.3263201232056671
  0.5401402331762507  0.9101538301860298  0.8263201078816118
  0.9606577431313340  0.1738086044774520  0.4923140981155940
  0.9606576657368451  0.8261914316650703  0.9923140665883571
  0.9596738427498158  0.8322540369061390  0.6581528983756642
  0.9596737413740687  0.1677459385712008  0.1581528740869755
  0.5254834357808560  0.4149349194497536  0.6513686946096283
  0.5254833690198526  0.5850650229277619  0.1513686942571068
  0.3623107195302151  0.7176260508281228  0.4221797743174898
  0.3623106360282151  0.2823741590774257  0.9221798240568051
  0.5446534236768511  0.9082775477988929  0.4178262614563800
  0.5446533743629768  0.0917224149820810  0.9178261995118331
  0.5394798577335546  0.6100186403524276  0.5629288694581044
  0.5394798766908260  0.3899813681604175  0.0629289026790272
  0.7335194838192524  0.9457791161494257  0.4923188448666510
  0.7335194829518400  0.0542210064945992  0.9923188959255084
  0.7330035265354884  0.7935227863479878  0.5669856782085322
  0.7330035382179367  0.2064770374798044  0.0669856105431925
  0.3621634950218721  0.5753076728942657  0.4926980445058958
```

```
  0.3621633522649050  0.4246921689964048  0.9926979008526081

Vdw-DF2

   1.00000000000000
     5.3705187924880242   -0.0000000317662681   -0.0135647545318876
    -0.0000000976926081    5.2177925206244886    0.0000004078838768
    -2.6095497839694644    0.0000011917906830   14.8900143801326514
   Cl   C    N
    10    10     2
Direct
  0.1114121293048541  0.6696747937641342  0.3310619509771364
  0.1114121139134703  0.3303252212240464  0.8310619451279762
  0.5299538774054323  0.1050861644841828  0.3220240757599159
  0.5299538130041541  0.8949138237542812  0.8220241042659688
  0.9635899907298953  0.1780015952197259  0.4916988364525083
  0.9635899939513370  0.8219984004608707  0.9916988598767046
  0.9724827779622005  0.8199857151226907  0.6615818415406571
  0.9724828160312425  0.1800143150068097  0.1615818305594267
  0.5323495982437391  0.3992951382122875  0.6554830228156137
  0.5323495932052874  0.6007048272679378  0.1554829960443817
  0.3583499964573370  0.7224711412447037  0.4212162625141446
  0.3583499340440365  0.2775288012475465  0.9212162081898577
  0.5404196024313276  0.9135098332227505  0.4165806984014118
  0.5404196715293900  0.0864901266819118  0.9165807367060258
  0.5436694196545541  0.6048271070662579  0.5643759453421563
  0.5436694075045492  0.3951728964029168  0.0643759346138389
  0.7333947224229710  0.9459579124451489  0.4919946738837926
  0.7333946410102177  0.0540421171343445  0.9919946598410948
  0.7371993933164974  0.7880774466486135  0.5679821322805512
  0.7371993922771778  0.2119225473985269  0.0679821195971809
  0.3621784880327938  0.5747894809773413  0.4931705362993547
  0.3621785035675282  0.4252105950128924  0.9931705729102944
```

```
PBE
   1.00000000000000
     5.6289701196204449    0.0000000047168496   -0.0000171224973338
     0.0000000048125454    5.5799762491172311   -0.0000000017734526
    -5.1169183682255195   -0.0000000087422168   16.2879528398075557
   Cl   C    N
    10    10     2
Direct
  0.9408803196386373  0.8466587810942201  0.9926897431546138
  0.1727193999611032  0.4241754599133287  0.8337273157797966
  0.5659578234738163  0.0236653225073766  0.8263352423244257
  0.9132124003812194  0.9285134304220790  0.6588286300320760
  0.5047511895148062  0.5294390099993151  0.6509053822803921
  0.9408803188590298  0.1533412184856360  0.4926897437570545
  0.1727194001212666  0.5758245404578020  0.3337273144630615
  0.5659578225334485  0.9763346771595351  0.3263352415430489
  0.9132124005238396  0.0714865692281990  0.1588286294221177
  0.5047511884991707  0.4705609907136292  0.1509053816532955
  0.7254895465478626  0.0618756303289203  0.9925589847567906
  0.3847079922956596  0.3184487366563644  0.9221662206520023
  0.5577739085396729  0.1407303339816863  0.9179207081551368
  0.7136836065442154  0.8378195411262865  0.5670933780706591
  0.5316169378035411  0.6612371828509964  0.5626058898674628
  0.7254895466872924  0.9381243699366948  0.4925589850875838
  0.3847079920777787  0.6815512632501353  0.4221662195502489
  0.5577739089438296  0.8592696663291051  0.4179207074390305
  0.7136836063124505  0.1621804586839062  0.0670933783243584
  0.5316169389971463  0.3387628166995995  0.0626058900562896
  0.3742145764180691  0.4124257684543835  0.9923393937914256
  0.3742145767293081  0.5875742317208150  0.4923393929222826
```

S8. CheckCIF Results for the Computed and Experimental ADPs

We used the calculated ADPs to perform a "least-square refinement" in which only one variable—an overall scale factor—was used. The ADPs calculated by different levels of theory match the experimental intensities to a very different degree. ADPs with very wrong absolute values will cause CheckCIF alerts with respect to R_1,wR_2, GOF, weighting scheme, difference Fourier or a combination thereof. Using calculated ADPs by PBE+D3(BJ) or by the other dispersion-corrected methods to do so does *not* result in such alerts; in contrast, using calculated ADPs at the PBE level of theory does.

We attach the CheckCIF results for the computed and experimental ADPs below. The CheckCIF results are organized in datablocks. The nomenclature of the datablocks is as follows:
PBED3BJ stands for the PBE+D3(BJ) level of theory, PBE stands for the PBE level of theory. The temperatures are indicated in the labels. The datablocks for the experimental ADPs are named "C5CL5N_*K". * stands for the different temperatures.

Calculated Adps !

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PBED3BJ_correct2_100K_r1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: PBED3BJ_correct2_100K_r1

```
Bond precision:  N- C = 0.0001 A          Wavelength=0.71073

Cell:            a=5.3122(2)     b=5.1770(2)         c=14.8307(6)
                 alpha=90        beta=99.493(2)      gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          402.28(3)                 402.28(3)
Space group     P c                       P c
Hall group      P -2yc                    P -2yc
Moiety formula  C5 Cl5 N                  C5 Cl5 N
Sum formula     C5 Cl5 N                  C5 Cl5 N
Mr              251.31                    251.31
Dx,g cm-3       2.075                     2.075
Z               2                         2
Mu (mm-1)       1.724                     1.724
F000            244.0                     244.0
F000'           245.52
h,k,lmax        7,7,21                    7,7,21
Nref            2459[ 1233]               2426
Tmin,Tmax       0.645,0.902               0.787,1.000
Tmin'           0.632

Correction method= # Reported T Limits: Tmin=0.787 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.97/0.99       Theta(max)= 30.482

R(reflections)= 0.0302( 2403)      wR2(reflections)= 0.0813( 2426)

S = 1.185                          Npar= 1
```

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 B

```
PLAT431_ALERT_2_B Short Inter HL..A  Contact Cl3    ..  N1      ..       2.93 Ang.
```

Alert level C

```
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         N1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         N1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         N1
PLAT741_ALERT_1_C Bond    Calc 1.72090(10), Rep     1.72130 ......    Missing su
              CL1  -C1      1.555   1.555 ............. Bond #         1 Check
PLAT741_ALERT_1_C Bond    Calc 1.70980(10), Rep     1.70930 ......    Missing su
              CL2  -C2      1.555   1.555 ............. Bond #         2 Check
PLAT741_ALERT_1_C Bond    Calc 1.70750(10), Rep     1.70770 ......    Missing su
              CL3  -C3      1.555   1.555 ............. Bond #         3 Check
PLAT741_ALERT_1_C Bond    Calc 1.70660(10), Rep     1.70630 ......    Missing su
              CL4  -C4      1.555   1.555 ............. Bond #         4 Check
PLAT741_ALERT_1_C Bond    Calc 1.72510(10), Rep     1.72470 ......    Missing su
              CL5  -C5      1.555   1.555 ............. Bond #         5 Check
PLAT741_ALERT_1_C Bond    Calc 1.32790(10), Rep     1.32780 ......    Missing su
              C1   -N1      1.555   1.555 ............. Bond #         6 Check
PLAT741_ALERT_1_C Bond    Calc 1.39940(10), Rep     1.39960 ......    Missing su
              C1   -C2      1.555   1.555 ............. Bond #         7 Check
PLAT741_ALERT_1_C Bond    Calc 1.39670(10), Rep     1.39670 ......    Missing su
              C2   -C3      1.555   1.555 ............. Bond #         8 Check
PLAT741_ALERT_1_C Bond    Calc 1.39930(10), Rep     1.39860 ......    Missing su
              C3   -C4      1.555   1.555 ............. Bond #         9 Check
PLAT741_ALERT_1_C Bond    Calc 1.39290(10), Rep     1.39340 ......    Missing su
              C4   -C5      1.555   1.555 ............. Bond #        10 Check
PLAT741_ALERT_1_C Bond    Calc 1.32560(10), Rep     1.32570 ......    Missing su
              C5   -N1      1.555   1.555 ............. Bond #        11 Check
PLAT742_ALERT_1_C Angle   Calc   123.06(1), Rep      123.10 ......    Missing su
```

```
              N1   -C1   -C2      1.555   1.555   1.555      #          1
PLAT742_ALERT_1_C Angle   Calc   116.53(1), Rep      116.50 ......    Missing su
              N1   -C1   -CL1     1.555   1.555   1.555      #          2
PLAT742_ALERT_1_C Angle   Calc   120.41(1), Rep      120.40 ......    Missing su
              C2   -C1   -CL1     1.555   1.555   1.555      #          3
PLAT742_ALERT_1_C Angle   Calc   117.69(1), Rep      117.70 ......    Missing su
              C3   -C2   -C1      1.555   1.555   1.555      #          4
PLAT742_ALERT_1_C Angle   Calc   120.79(1), Rep      120.80 ......    Missing su
              C3   -C2   -CL2     1.555   1.555   1.555      #          5
PLAT742_ALERT_1_C Angle   Calc   121.52(1), Rep      121.50 ......    Missing su
              C1   -C2   -CL2     1.555   1.555   1.555      #          6
PLAT742_ALERT_1_C Angle   Calc   119.48(1), Rep      119.50 ......    Missing su
              C2   -C3   -C4      1.555   1.555   1.555      #          7
PLAT742_ALERT_1_C Angle   Calc   120.38(1), Rep      120.30 ......    Missing su
              C2   -C3   -CL3     1.555   1.555   1.555      #          8
PLAT742_ALERT_1_C Angle   Calc   120.15(1), Rep      120.20 ......    Missing su
              C4   -C3   -CL3     1.555   1.555   1.555      #          9
PLAT742_ALERT_1_C Angle   Calc   117.40(1), Rep      117.40 ......    Missing su
              C5   -C4   -C3      1.555   1.555   1.555      #         10
PLAT742_ALERT_1_C Angle   Calc   121.81(1), Rep      121.80 ......    Missing su
              C5   -C4   -CL4     1.555   1.555   1.555      #         11
PLAT742_ALERT_1_C Angle   Calc   120.79(1), Rep      120.80 ......    Missing su
              C3   -C4   -CL4     1.555   1.555   1.555      #         12
PLAT742_ALERT_1_C Angle   Calc   123.68(1), Rep      123.60 ......    Missing su
              N1   -C5   -C4      1.555   1.555   1.555      #         13
PLAT742_ALERT_1_C Angle   Calc   115.96(1), Rep      116.00 ......    Missing su
              N1   -C5   -CL5     1.555   1.555   1.555      #         14
PLAT742_ALERT_1_C Angle   Calc   120.36(1), Rep      120.40 ......    Missing su
              C4   -C5   -CL5     1.555   1.555   1.555      #         15
PLAT742_ALERT_1_C Angle   Calc   118.69(1), Rep      118.70 ......    Missing su
              C5   -N1   -C1      1.555   1.555   1.555      #         16
PLAT927_ALERT_1_C Reported and Calculated  wR2 Differ by .........    -0.0023 Check
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry .....        90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group.      P21/c Check
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds          1 Report
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          1 Units
```

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

  30 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
   0 ALERT type 3 Indicator that the structure quality may be low
  34 ALERT type 4 Improvement, methodology, query or suggestion
   0 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

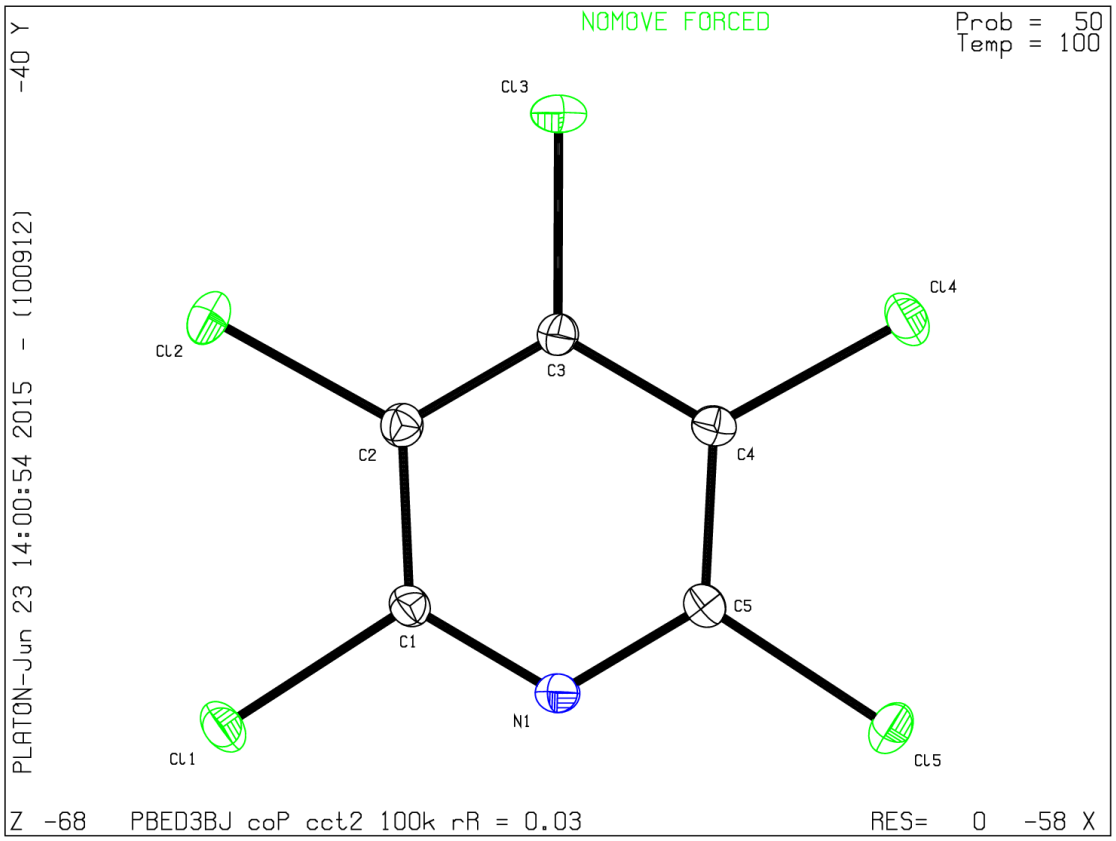
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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 21/06/2015; check.def file version of 21/06/2015

Datablock PBED3BJ_correct2_100K_r1 - ellipsoid plot



Calculated Adps !

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PBED3BJ_correct2_150K_r1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: PBED3BJ_correct2_150K_r1

```
Bond precision:  C-C = 0.0005 A          Wavelength=0.71073

Cell:            a=5.3191(16)     b=5.1827(16)       c=14.894(5)
                 alpha=90         beta=99.704(5)     gamma=90
Temperature:     150 K

                Calculated                Reported
Volume          404.7(2)                  404.7(2)
Space group     P c                       P c
Hall group      P -2yc                    P -2yc
Moiety formula  C5 Cl5 N                  C5 Cl5 N
Sum formula     C5 Cl5 N                  C5 Cl5 N
Mr              251.31                    251.31
Dx,g cm-3       2.062                     2.062
Z               2                         2
Mu (mm-1)       1.713                     1.713
F000            244.0                     244.0
F000'           245.52
h,k,lmax        7,7,21                    7,7,20
Nref            2581[ 1294]               1894
Tmin,Tmax       0.647,0.902               0.590,0.746
Tmin'           0.634

Correction method= # Reported T Limits: Tmin=0.590 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.46/0.73      Theta(max)= 30.904

R(reflections)= 0.0471( 1769)     wR2(reflections)= 0.1127( 1894)

S = 1.244                         Npar= 1
```

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 B

```
PLAT431_ALERT_2_B Short Inter HL..A  Contact Cl3    ..  N1      ..       2.95 Ang.
```

Alert level C

```
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         N1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         N1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         N1
PLAT741_ALERT_1_C Bond    Calc   1.7120(6), Rep     1.71270 ......    Missing su
              CL1  -C1      1.555   1.555 ............. Bond #         1 Check
PLAT741_ALERT_1_C Bond    Calc   1.7127(6), Rep     1.71220 ......    Missing su
              CL2  -C2      1.555   1.555 ............. Bond #         2 Check
PLAT741_ALERT_1_C Bond    Calc   1.6972(6), Rep     1.69720 ......    Missing su
              CL3  -C3      1.555   1.555 ............. Bond #         3 Check
PLAT741_ALERT_1_C Bond    Calc   1.7092(6), Rep     1.70930 ......    Missing su
              CL4  -C4      1.555   1.555 ............. Bond #         4 Check
PLAT741_ALERT_1_C Bond    Calc   1.7273(6), Rep     1.72730 ......    Missing su
              CL5  -C5      1.555   1.555 ............. Bond #         5 Check
PLAT741_ALERT_1_C Bond    Calc   1.3399(4), Rep     1.33920 ......    Missing su
              C1   -N1      1.555   1.555 ............. Bond #         6 Check
PLAT741_ALERT_1_C Bond    Calc   1.3889(5), Rep     1.38890 ......    Missing su
              C1   -C2      1.555   1.555 ............. Bond #         7 Check
PLAT741_ALERT_1_C Bond    Calc   1.4094(5), Rep     1.40970 ......    Missing su
              C2   -C3      1.555   1.555 ............. Bond #         8 Check
PLAT741_ALERT_1_C Bond    Calc   1.3943(5), Rep     1.39420 ......    Missing su
              C3   -C4      1.555   1.555 ............. Bond #         9 Check
PLAT741_ALERT_1_C Bond    Calc   1.3929(5), Rep     1.39270 ......    Missing su
              C4   -C5      1.555   1.555 ............. Bond #        10 Check
PLAT741_ALERT_1_C Bond    Calc   1.3014(4), Rep     1.30190 ......    Missing su
              C5   -N1      1.555   1.555 ............. Bond #        11 Check
PLAT742_ALERT_1_C Angle   Calc   122.23(1), Rep      122.30 ......    Missing su
```

```
              N1   -C1   -C2      1.555   1.555   1.555      #          1
PLAT742_ALERT_1_C Angle   Calc   117.11(1), Rep      117.10 ......    Missing su
              N1   -C1   -CL1     1.555   1.555   1.555      #          2
PLAT742_ALERT_1_C Angle   Calc   120.66(1), Rep      120.60 ......    Missing su
              C2   -C1   -CL1     1.555   1.555   1.555      #          3
PLAT742_ALERT_1_C Angle   Calc   118.48(1), Rep      118.40 ......    Missing su
              C1   -C2   -C3      1.555   1.555   1.555      #          4
PLAT742_ALERT_1_C Angle   Calc   121.64(1), Rep      121.70 ......    Missing su
              C1   -C2   -CL2     1.555   1.555   1.555      #          5
PLAT742_ALERT_1_C Angle   Calc   119.88(1), Rep      119.90 ......    Missing su
              C3   -C2   -CL2     1.555   1.555   1.555      #          6
PLAT742_ALERT_1_C Angle   Calc   118.18(1), Rep      118.20 ......    Missing su
              C4   -C3   -C2      1.555   1.555   1.555      #          7
PLAT742_ALERT_1_C Angle   Calc   121.13(1), Rep      121.20 ......    Missing su
              C4   -C3   -CL3     1.555   1.555   1.555      #          8
PLAT742_ALERT_1_C Angle   Calc   120.68(1), Rep      120.70 ......    Missing su
              C2   -C3   -CL3     1.555   1.555   1.555      #          9
PLAT742_ALERT_1_C Angle   Calc   118.10(1), Rep      118.10 ......    Missing su
              C5   -C4   -C3      1.555   1.555   1.555      #         10
PLAT742_ALERT_1_C Angle   Calc   121.98(1), Rep      122.00 ......    Missing su
              C5   -C4   -CL4     1.555   1.555   1.555      #         11
PLAT742_ALERT_1_C Angle   Calc   119.92(1), Rep      119.90 ......    Missing su
              C3   -C4   -CL4     1.555   1.555   1.555      #         12
PLAT742_ALERT_1_C Angle   Calc   123.79(1), Rep      123.80 ......    Missing su
              N1   -C5   -C4      1.555   1.555   1.555      #         13
PLAT742_ALERT_1_C Angle   Calc   116.22(1), Rep      116.20 ......    Missing su
              N1   -C5   -CL5     1.555   1.555   1.555      #         14
PLAT742_ALERT_1_C Angle   Calc   119.98(1), Rep      120.00 ......    Missing su
              C4   -C5   -CL5     1.555   1.555   1.555      #         15
PLAT742_ALERT_1_C Angle   Calc   119.22(1), Rep      119.20 ......    Missing su
              C5   -N1   -C1      1.555   1.555   1.555      #         16
PLAT915_ALERT_3_C Low Friedel Pair Coverage .....                      58 %
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..    Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry .....       90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group.     P21/c Check
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds        1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      146 Note
```

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

  28 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
   1 ALERT type 3 Indicator that the structure quality may be low
  35 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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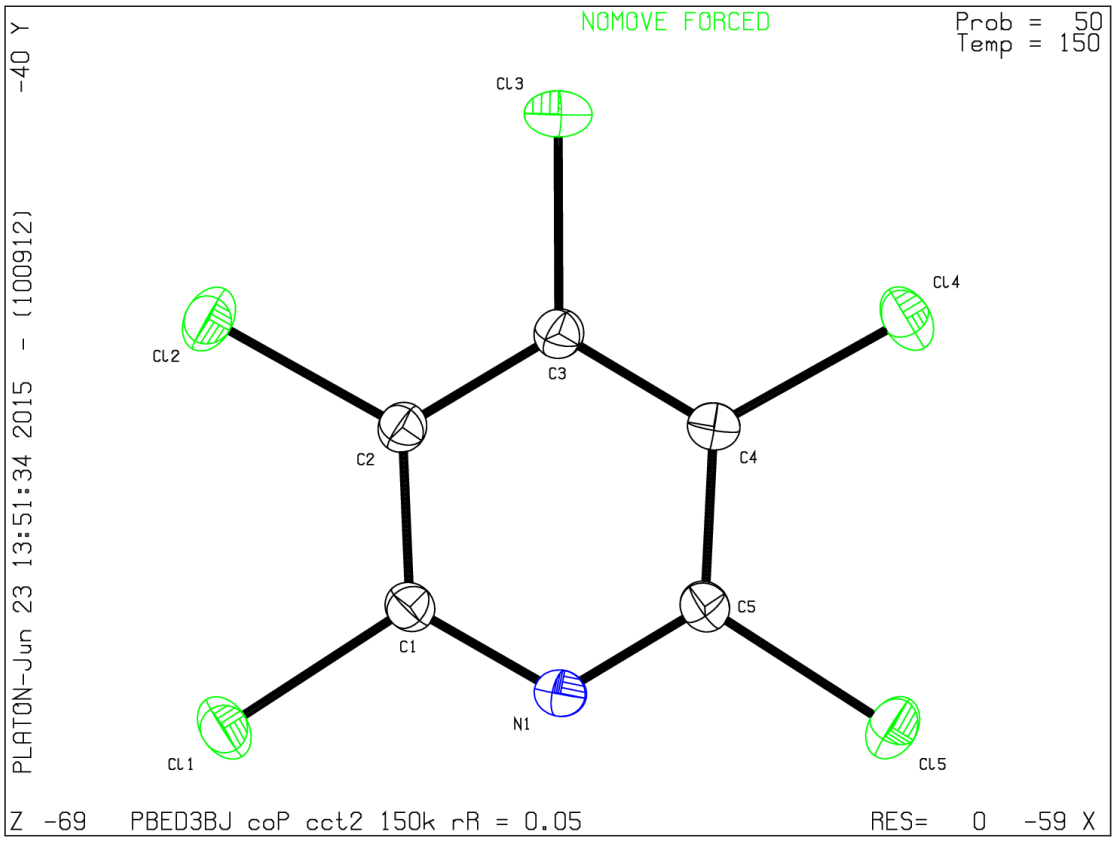
PLATON version of 21/06/2015; check.def file version of 21/06/2015

Datablock PBED3BJ_correct2_150K_r1 - ellipsoid plot



Calculated Adps !

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PBED3BJ_correct2_200K_r1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: PBED3BJ_correct2_200K_r1

```
Bond precision:  C-C = 0.0004 A          Wavelength=0.71073

Cell:            a=5.3290(14)     b=5.1935(13)       c=14.949(4)
                 alpha=90         beta=99.833(5)     gamma=90
Temperature:     200 K

                Calculated                Reported
Volume          407.65(18)                407.66(18)
Space group     P c                       P c
Hall group      P -2yc                    P -2yc
Moiety formula  C5 Cl5 N                  C5 Cl5 N
Sum formula     C5 Cl5 N                  C5 Cl5 N
Mr              251.31                    251.31
Dx,g cm-3       2.047                     2.047
Z               2                         2
Mu (mm-1)       1.701                     1.701
F000            244.0                     244.0
F000'           245.52
h,k,lmax        7,7,21                    7,7,20
Nref            2565[ 1286]               1926
Tmin,Tmax       0.649,0.903               0.609,0.746
Tmin'           0.636

Correction method= # Reported T Limits: Tmin=0.609 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.50/0.75       Theta(max)= 30.771

R(reflections)= 0.0618( 1551)      wR2(reflections)= 0.1304( 1926)

S = 1.303                          Npar= 1
```

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 B

```
PLAT431_ALERT_2_B Short Inter HL..A  Contact Cl3    ..  N1      ..       2.97 Ang.
```

Alert level C

```
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         N1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         N1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         N1
PLAT741_ALERT_1_C Bond    Calc   1.7224(5), Rep     1.72200 ......    Missing su
              CL1  -C1      1.555   1.555 ..............  Bond #         1 Check
PLAT741_ALERT_1_C Bond    Calc   1.7076(5), Rep     1.70810 ......    Missing su
              CL2  -C2      1.555   1.555 ..............  Bond #         2 Check
PLAT741_ALERT_1_C Bond    Calc   1.6988(5), Rep     1.69880 ......    Missing su
              CL3  -C3      1.555   1.555 ..............  Bond #         3 Check
PLAT741_ALERT_1_C Bond    Calc   1.7129(5), Rep     1.71240 ......    Missing su
              CL4  -C4      1.555   1.555 ..............  Bond #         4 Check
PLAT741_ALERT_1_C Bond    Calc   1.7229(5), Rep     1.72320 ......    Missing su
              CL5  -C5      1.555   1.555 ..............  Bond #         5 Check
PLAT741_ALERT_1_C Bond    Calc   1.3230(4), Rep     1.32310 ......    Missing su
              C1   -N1      1.555   1.555 ..............  Bond #         6 Check
PLAT741_ALERT_1_C Bond    Calc   1.3847(4), Rep     1.38420 ......    Missing su
              C1   -C2      1.555   1.555 ..............  Bond #         7 Check
PLAT741_ALERT_1_C Bond    Calc   1.4093(4), Rep     1.40950 ......    Missing su
              C2   -C3      1.555   1.555 ..............  Bond #         8 Check
PLAT741_ALERT_1_C Bond    Calc   1.3927(4), Rep     1.39230 ......    Missing su
              C3   -C4      1.555   1.555 ..............  Bond #         9 Check
PLAT741_ALERT_1_C Bond    Calc   1.3790(4), Rep     1.37900 ......    Missing su
              C4   -C5      1.555   1.555 ..............  Bond #        10 Check
PLAT741_ALERT_1_C Bond    Calc   1.3108(4), Rep     1.31110 ......    Missing su
              C5   -N1      1.555   1.555 ..............  Bond #        11 Check
PLAT742_ALERT_1_C Angle   Calc   123.23(1), Rep      123.20 ......    Missing su
```

```
              N1   -C1   -C2      1.555   1.555   1.555      #          1
PLAT742_ALERT_1_C Angle   Calc   116.58(1), Rep      116.60 ......    Missing su
              N1   -C1   -CL1     1.555   1.555   1.555      #          2
PLAT742_ALERT_1_C Angle   Calc   120.19(1), Rep      120.20 ......    Missing su
              C2   -C1   -CL1     1.555   1.555   1.555      #          3
PLAT742_ALERT_1_C Angle   Calc   117.86(1), Rep      117.90 ......    Missing su
              C1   -C2   -C3      1.555   1.555   1.555      #          4
PLAT742_ALERT_1_C Angle   Calc   122.04(1), Rep      122.00 ......    Missing su
              C1   -C2   -CL2     1.555   1.555   1.555      #          5
PLAT742_ALERT_1_C Angle   Calc   120.09(1), Rep      120.10 ......    Missing su
              C3   -C2   -CL2     1.555   1.555   1.555      #          6
PLAT742_ALERT_1_C Angle   Calc   117.93(1), Rep      117.90 ......    Missing su
              C4   -C3   -C2      1.555   1.555   1.555      #          7
PLAT742_ALERT_1_C Angle   Calc   121.62(1), Rep      121.60 ......    Missing su
              C4   -C3   -CL3     1.555   1.555   1.555      #          8
PLAT742_ALERT_1_C Angle   Calc   120.45(1), Rep      120.40 ......    Missing su
              C2   -C3   -CL3     1.555   1.555   1.555      #          9
PLAT742_ALERT_1_C Angle   Calc   118.70(1), Rep      118.70 ......    Missing su
              C5   -C4   -C3      1.555   1.555   1.555      #         10
PLAT742_ALERT_1_C Angle   Calc   121.90(1), Rep      121.90 ......    Missing su
              C5   -C4   -CL4     1.555   1.555   1.555      #         11
PLAT742_ALERT_1_C Angle   Calc   119.40(1), Rep      119.40 ......    Missing su
              C3   -C4   -CL4     1.555   1.555   1.555      #         12
PLAT742_ALERT_1_C Angle   Calc   123.37(1), Rep      123.30 ......    Missing su
              N1   -C5   -C4      1.555   1.555   1.555      #         13
PLAT742_ALERT_1_C Angle   Calc   116.31(1), Rep      116.30 ......    Missing su
              N1   -C5   -CL5     1.555   1.555   1.555      #         14
PLAT742_ALERT_1_C Angle   Calc   120.31(1), Rep      120.30 ......    Missing su
              C4   -C5   -CL5     1.555   1.555   1.555      #         15
PLAT742_ALERT_1_C Angle   Calc   118.90(1), Rep      118.90 ......    Missing su
              C5   -N1   -C1      1.555   1.555   1.555      #         16
PLAT915_ALERT_3_C Low Friedel Pair Coverage ......................        60 %
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..    Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry .....       90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group.    P21/c Check
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds        1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      119 Note
```

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

  28 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
   1 ALERT type 3 Indicator that the structure quality may be low
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   0 ALERT type 5 Informative message, check
```

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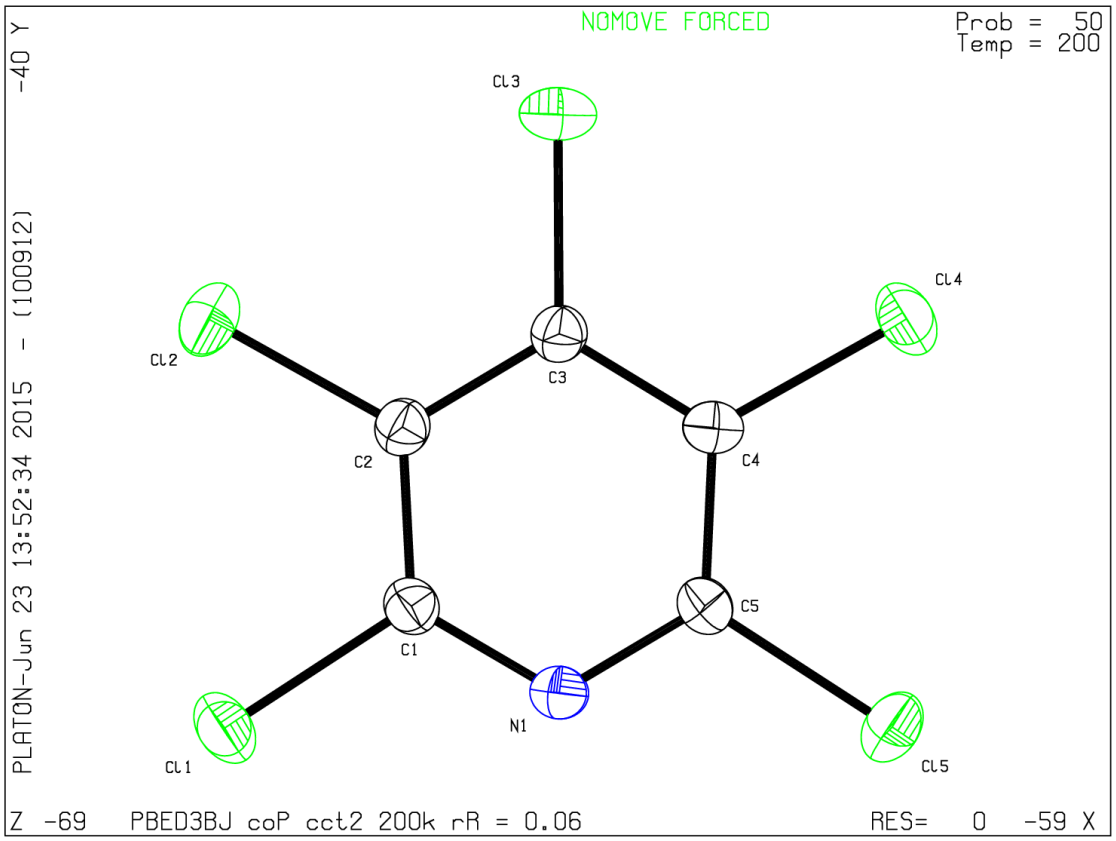
PLATON version of 21/06/2015; check.def file version of 21/06/2015

Datablock PBED3BJ_correct2_200K_r1 - ellipsoid plot



Calculated Adps !

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PBE_correct2_100K_r1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: PBE_correct2_100K_r1

```
Bond precision:  N- C = 0.0001 A          Wavelength=0.71073

Cell:            a=5.3122(2)     b=5.1770(2)         c=14.8307(6)
                 alpha=90        beta=99.493(2)      gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          402.28(3)                 402.28(3)
Space group     P c                       P c
Hall group      P -2yc                    P -2yc
Moiety formula  C5 Cl5 N                  C5 Cl5 N
Sum formula     C5 Cl5 N                  C5 Cl5 N
Mr              251.31                    251.31
Dx,g cm-3       2.075                     2.075
Z               2                         2
Mu (mm-1)       1.724                     1.724
F000            244.0                     244.0
F000'           245.52
h,k,lmax        7,7,21                    7,7,21
Nref            2459[ 1233]               2426
Tmin,Tmax       0.645,0.902               0.787,1.000
Tmin'           0.632

Correction method= # Reported T Limits: Tmin=0.787 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.97/0.99       Theta(max)= 30.482

R(reflections)= 0.3569( 2403)      wR2(reflections)= 0.7040( 2426)

S = 10.985                         Npar= 1
```

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

```
DIFMN02_ALERT_2_A  The minimum difference density is < -0.1*ZMAX*2.00
           _refine_diff_density_min given =     -4.817
           Test value =     -3.400
DIFMX01_ALERT_2_A  The maximum difference density is > 0.1*ZMAX*2.00
           _refine_diff_density_max given =      5.667
           Test value =      3.400
GOODF01_ALERT_2_A  The least squares goodness of fit parameter lies
           outside the range 0.40 <> 6.00
           Goodness of fit given =     10.985
RFACG01_ALERT_3_A  The value of the R factor is > 0.20
           R factor given   0.357
RFACR01_ALERT_3_A  The value of the weighted R factor is > 0.45
           Weighted R factor given   0.704
PLAT082_ALERT_2_A High R1 Value ..................................       0.36 Report
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ...................       0.70 Report
PLAT087_ALERT_2_A Unsatisfactory S value (Too High) ..............      10.98 Check
PLAT097_ALERT_2_A Large Reported Max.  (Positive) Residual Density       5.67 eA-3
PLAT098_ALERT_2_A Large Reported Min.  (Negative) Residual Density      -4.82 eA-3
PLAT934_ALERT_3_A Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....        919 Check
PLAT971_ALERT_2_A Check Calcd Residual Density  0.10A From     Cl1       5.93 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.52A From     Cl3      -5.00 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.42A From     Cl4      -4.78 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.50A From     Cl1      -4.65 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.47A From     Cl2      -4.46 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.55A From     Cl4      -4.34 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.49A From     Cl3      -4.23 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.64A From     Cl2      -4.14 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.55A From     Cl5      -4.10 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.45A From     Cl2      -4.09 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.54A From     Cl1      -4.05 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.56A From     Cl3      -3.98 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.50A From     Cl1      -3.83 eA-3
PLAT972_ALERT_2_A Check Calcd Residual Density  0.56A From     Cl5      -3.71 eA-3
```

Alert level B

```
PLAT431_ALERT_2_B Short Inter HL..A  Contact Cl3    ..  N1       ..       2.93 Ang.
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...          1 Check
PLAT971_ALERT_2_B Check Calcd Residual Density  0.12A From     Cl4       3.49 eA-3
PLAT971_ALERT_2_B Check Calcd Residual Density  0.17A From     Cl2       3.44 eA-3
PLAT971_ALERT_2_B Check Calcd Residual Density  0.18A From     Cl3       3.40 eA-3
PLAT971_ALERT_2_B Check Calcd Residual Density  0.12A From     Cl5       3.17 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.54A From     Cl5      -3.45 eA-3
```

Alert level C

```
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.330
          From the CIF: _refine_ls_abs_structure_Flack_su    0.030
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C2
```

```
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         N1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         N1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         N1
PLAT741_ALERT_1_C Bond    Calc 1.72090(10), Rep     1.72130 ......    Missing su
              CL1  -C1      1.555   1.555 ..... Bond #          1 Check
PLAT741_ALERT_1_C Bond    Calc 1.70980(10), Rep     1.70930 ......    Missing su
              CL2  -C2      1.555   1.555 ..... Bond #          2 Check
PLAT741_ALERT_1_C Bond    Calc 1.70750(10), Rep     1.70770 ......    Missing su
              CL3  -C3      1.555   1.555 ..... Bond #          3 Check
PLAT741_ALERT_1_C Bond    Calc 1.70660(10), Rep     1.70630 ......    Missing su
              CL4  -C4      1.555   1.555 ..... Bond #          4 Check
PLAT741_ALERT_1_C Bond    Calc 1.72510(10), Rep     1.72470 ......    Missing su
              CL5  -C5      1.555   1.555 ..... Bond #          5 Check
PLAT741_ALERT_1_C Bond    Calc 1.32790(10), Rep     1.32780 ......    Missing su
              C1   -N1      1.555   1.555 ..... Bond #          6 Check
PLAT741_ALERT_1_C Bond    Calc 1.39940(10), Rep     1.39960 ......    Missing su
              C1   -C2      1.555   1.555 ..... Bond #          7 Check
PLAT741_ALERT_1_C Bond    Calc 1.39670(10), Rep     1.39670 ......    Missing su
              C2   -C3      1.555   1.555 ..... Bond #          8 Check
PLAT741_ALERT_1_C Bond    Calc 1.39930(10), Rep     1.39860 ......    Missing su
              C3   -C4      1.555   1.555 ..... Bond #          9 Check
PLAT741_ALERT_1_C Bond    Calc 1.39290(10), Rep     1.39340 ......    Missing su
              C4   -C5      1.555   1.555 ..... Bond #         10 Check
PLAT741_ALERT_1_C Bond    Calc 1.32560(10), Rep     1.32570 ......    Missing su
              C5   -N1      1.555   1.555 ..... Bond #         11 Check
PLAT742_ALERT_1_C Angle   Calc   123.06(1), Rep      123.10 ......    Missing su
              N1   -C1   -C2      1.555   1.555   1.555      #          1
PLAT742_ALERT_1_C Angle   Calc   116.53(1), Rep      116.50 ......    Missing su
              N1   -C1   -CL1     1.555   1.555   1.555      #          2
PLAT742_ALERT_1_C Angle   Calc   120.41(1), Rep      120.40 ......    Missing su
              C2   -C1   -CL1     1.555   1.555   1.555      #          3
PLAT742_ALERT_1_C Angle   Calc   117.69(1), Rep      117.70 ......    Missing su
              C3   -C2   -C1      1.555   1.555   1.555      #          4
PLAT742_ALERT_1_C Angle   Calc   120.79(1), Rep      120.80 ......    Missing su
              C3   -C2   -CL2     1.555   1.555   1.555      #          5
PLAT742_ALERT_1_C Angle   Calc   121.52(1), Rep      121.50 ......    Missing su
              C1   -C2   -CL2     1.555   1.555   1.555      #          6
PLAT742_ALERT_1_C Angle   Calc   119.48(1), Rep      119.50 ......    Missing su
              C2   -C3   -C4      1.555   1.555   1.555      #          7
```

```
PLAT742_ALERT_1_C Angle   Calc   120.38(1), Rep      120.30 ......    Missing su
             C2   -C3   -CL3     1.555   1.555   1.555      #         8
PLAT742_ALERT_1_C Angle   Calc   120.15(1), Rep      120.20 ......    Missing su
             C4   -C3   -CL3     1.555   1.555   1.555      #         9
PLAT742_ALERT_1_C Angle   Calc   117.40(1), Rep      117.40 ......    Missing su
             C5   -C4   -C3      1.555   1.555   1.555      #        10
PLAT742_ALERT_1_C Angle   Calc   121.81(1), Rep      121.80 ......    Missing su
             C5   -C4   -CL4     1.555   1.555   1.555      #        11
PLAT742_ALERT_1_C Angle   Calc   120.79(1), Rep      120.80 ......    Missing su
             C3   -C4   -CL4     1.555   1.555   1.555      #        12
PLAT742_ALERT_1_C Angle   Calc   123.68(1), Rep      123.60 ......    Missing su
             N1   -C5   -C4      1.555   1.555   1.555      #        13
PLAT742_ALERT_1_C Angle   Calc   115.96(1), Rep      116.00 ......    Missing su
             N1   -C5   -CL5     1.555   1.555   1.555      #        14
PLAT742_ALERT_1_C Angle   Calc   120.36(1), Rep      120.40 ......    Missing su
             C4   -C5   -CL5     1.555   1.555   1.555      #        15
PLAT742_ALERT_1_C Angle   Calc   118.69(1), Rep      118.70 ......    Missing su
             C5   -N1   -C1      1.555   1.555   1.555      #        16
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     15.329 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.965 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      6.284 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.258 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.071 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.828 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.719 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.254 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.320 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.685 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.771 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.218 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.170 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      18.36
PLAT971_ALERT_2_C Check Calcd Residual Density  1.08A From     Cl3       1.87 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.42A From      C4      -1.93 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.66A From      C4      -1.67 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.49A From      C2      -1.67 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.61A From      N1      -1.65 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.58A From      C1      -1.63 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.43A From      C1      -1.59 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.65A From      N1      -1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.47A From      C3      -1.52 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.49A From      C5      -1.52 eA-3
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry .....         90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group.      P21/c Check
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds          1 Report
PLAT916_ALERT_2_G Hooft y and Flack x Parameter values differ by .       0.10 Check
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          1 Units
```

---

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```
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 19 ALERT type 3 Indicator that the structure quality may be low
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  0 ALERT type 5 Informative message, check
```

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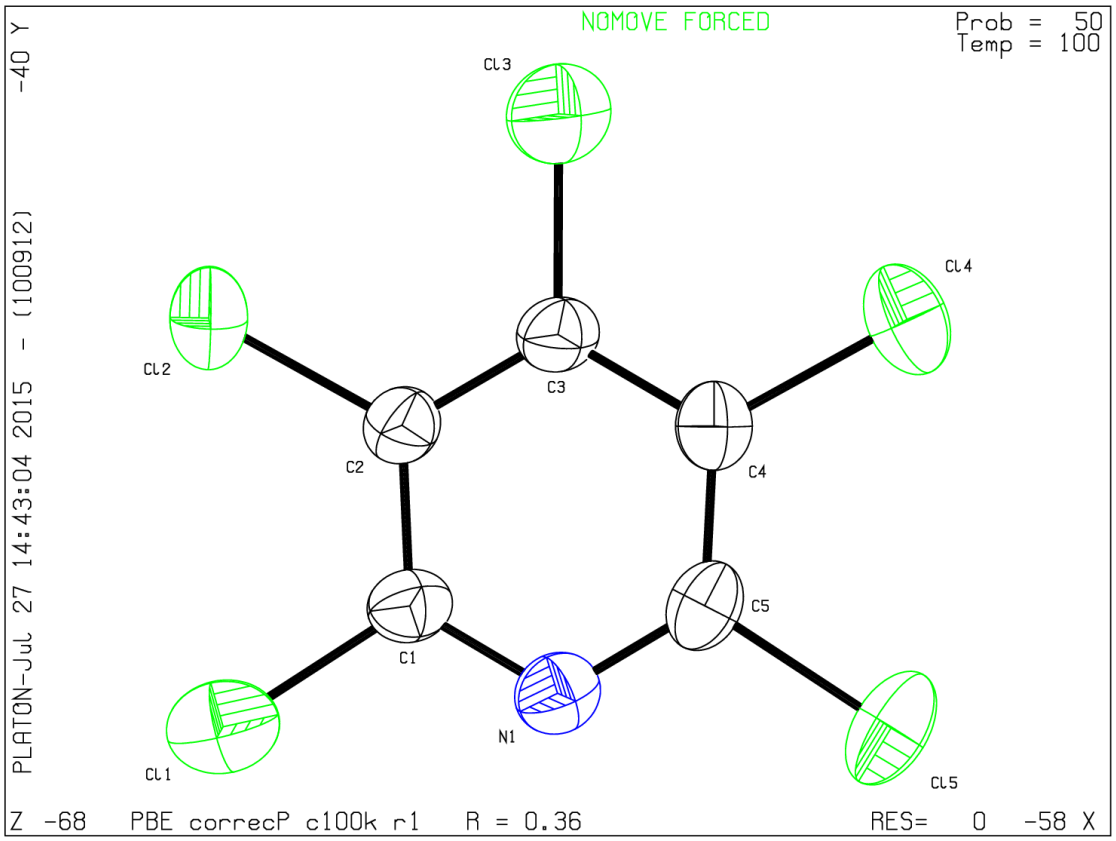
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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 21/06/2015; check.def file version of 21/06/2015

Datablock PBE_correct2_100K_r1 - ellipsoid plot



Calculated Adps !

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PBE_correct2_150K_r1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: PBE_correct2_150K_r1

```
Bond precision:  C-C = 0.0005 A          Wavelength=0.71073

Cell:            a=5.3191(16)     b=5.1827(16)       c=14.894(5)
                 alpha=90         beta=99.704(5)     gamma=90
Temperature:     150 K

                 Calculated                Reported
Volume           404.7(2)                  404.7(2)
Space group      P c                       P c
Hall group       P -2yc                    P -2yc
Moiety formula   C5 Cl5 N                  C5 Cl5 N
Sum formula      C5 Cl5 N                  C5 Cl5 N
Mr               251.31                    251.31
Dx,g cm-3        2.062                     2.062
Z                2                         2
Mu (mm-1)        1.713                     1.713
F000             244.0                     244.0
F000'            245.52
h,k,lmax         7,7,21                    7,7,20
Nref             2581[ 1294]               1894
Tmin,Tmax        0.647,0.902               0.590,0.746
Tmin'            0.634

Correction method= # Reported T Limits: Tmin=0.590 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.46/0.73       Theta(max)= 30.904

R(reflections)= 0.4137( 1769)      wR2(reflections)= 0.6717( 1894)

S = 7.815                          Npar= 1
```

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

```
DIFMX01_ALERT_2_A  The maximum difference density is > 0.1*ZMAX*2.00
           _refine_diff_density_max given =      3.921
           Test value =      3.400
GOODF01_ALERT_2_A  The least squares goodness of fit parameter lies
           outside the range 0.40 <> 6.00
           Goodness of fit given =      7.815
RFACG01_ALERT_3_A  The value of the R factor is > 0.20
           R factor given   0.414
RFACR01_ALERT_3_A  The value of the weighted R factor is > 0.45
           Weighted R factor given   0.672
PLAT082_ALERT_2_A High R1 Value ..................................       0.41 Report
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ...................       0.67 Report
PLAT087_ALERT_2_A Unsatisfactory S value (Too High) ..............       7.82 Check
PLAT097_ALERT_2_A Large Reported Max.  (Positive) Residual Density       3.92 eA-3
PLAT934_ALERT_3_A Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....        386 Check
PLAT971_ALERT_2_A Check Calcd Residual Density  0.11A From     Cl1       5.42 eA-3
PLAT971_ALERT_2_A Check Calcd Residual Density  0.09A From     Cl4       4.09 eA-3
PLAT971_ALERT_2_A Check Calcd Residual Density  0.13A From     Cl5       3.84 eA-3
PLAT971_ALERT_2_A Check Calcd Residual Density  0.19A From     Cl3       3.82 eA-3
PLAT971_ALERT_2_A Check Calcd Residual Density  0.04A From     Cl2       3.76 eA-3
```

Alert level B

```
DIFMN02_ALERT_2_B  The minimum difference density is < -0.1*ZMAX*1.00
           _refine_diff_density_min given =     -2.688
           Test value =     -1.700
PLAT098_ALERT_2_B Large Reported Min.  (Negative) Residual Density      -2.69 eA-3
PLAT431_ALERT_2_B Short Inter HL..A  Contact Cl3    ..  N1      ..       2.95 Ang.
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...          2 Check
PLAT972_ALERT_2_B Check Calcd Residual Density  0.74A From     Cl3      -3.15 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.68A From     Cl2      -3.03 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.69A From     Cl1      -3.03 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.65A From     Cl2      -2.96 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.50A From     Cl4      -2.92 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.60A From     Cl2      -2.90 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.67A From     Cl3      -2.77 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.61A From     Cl2      -2.75 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.68A From     Cl5      -2.74 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.56A From     Cl1      -2.63 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.63A From     Cl4      -2.63 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.65A From     Cl5      -2.57 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density  0.67A From     Cl3      -2.55 eA-3
```

Alert level C

```
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.370
          From the CIF: _refine_ls_abs_structure_Flack_su    0.060
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C3
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PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        C4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        C5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        N1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...       CL1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...       CL2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...       CL3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...       CL4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...       CL5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        C1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        C2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        C3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        C4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        C5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        N1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...       CL1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...       CL2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...       CL3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...       CL4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...       CL5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        C1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        C2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        C3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        C4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        C5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        N1
PLAT741_ALERT_1_C Bond    Calc   1.7120(6), Rep     1.71270 ......    Missing su
              CL1  -C1      1.555   1.555 ..... Bond #         1 Check
PLAT741_ALERT_1_C Bond    Calc   1.7127(6), Rep     1.71220 ......    Missing su
              CL2  -C2      1.555   1.555 ..... Bond #         2 Check
PLAT741_ALERT_1_C Bond    Calc   1.6972(6), Rep     1.69720 ......    Missing su
              CL3  -C3      1.555   1.555 ..... Bond #         3 Check
PLAT741_ALERT_1_C Bond    Calc   1.7092(6), Rep     1.70930 ......    Missing su
              CL4  -C4      1.555   1.555 ..... Bond #         4 Check
PLAT741_ALERT_1_C Bond    Calc   1.7273(6), Rep     1.72730 ......    Missing su
              CL5  -C5      1.555   1.555 ..... Bond #         5 Check
PLAT741_ALERT_1_C Bond    Calc   1.3399(4), Rep     1.33920 ......    Missing su
              C1   -N1      1.555   1.555 ..... Bond #         6 Check
PLAT741_ALERT_1_C Bond    Calc   1.3889(5), Rep     1.38890 ......    Missing su
              C1   -C2      1.555   1.555 ..... Bond #         7 Check
PLAT741_ALERT_1_C Bond    Calc   1.4094(5), Rep     1.40970 ......    Missing su
              C2   -C3      1.555   1.555 ..... Bond #         8 Check
PLAT741_ALERT_1_C Bond    Calc   1.3943(5), Rep     1.39420 ......    Missing su
              C3   -C4      1.555   1.555 ..... Bond #         9 Check
PLAT741_ALERT_1_C Bond    Calc   1.3929(5), Rep     1.39270 ......    Missing su
              C4   -C5      1.555   1.555 ..... Bond #        10 Check
PLAT741_ALERT_1_C Bond    Calc   1.3014(4), Rep     1.30190 ......    Missing su
              C5   -N1      1.555   1.555 ..... Bond #        11 Check
PLAT742_ALERT_1_C Angle   Calc   122.23(1), Rep      122.30 ......    Missing su
              N1   -C1   -C2      1.555   1.555   1.555      #         1
PLAT742_ALERT_1_C Angle   Calc   117.11(1), Rep      117.10 ......    Missing su
              N1   -C1   -CL1     1.555   1.555   1.555      #         2
PLAT742_ALERT_1_C Angle   Calc   120.66(1), Rep      120.60 ......    Missing su
              C2   -C1   -CL1     1.555   1.555   1.555      #         3
PLAT742_ALERT_1_C Angle   Calc   118.48(1), Rep      118.40 ......    Missing su
              C1   -C2   -C3      1.555   1.555   1.555      #         4
PLAT742_ALERT_1_C Angle   Calc   121.64(1), Rep      121.70 ......    Missing su
              C1   -C2   -CL2     1.555   1.555   1.555      #         5
PLAT742_ALERT_1_C Angle   Calc   119.88(1), Rep      119.90 ......    Missing su
              C3   -C2   -CL2     1.555   1.555   1.555      #         6
PLAT742_ALERT_1_C Angle   Calc   118.18(1), Rep      118.20 ......    Missing su
              C4   -C3   -C2      1.555   1.555   1.555      #         7
PLAT742_ALERT_1_C Angle   Calc   121.13(1), Rep      121.20 ......    Missing su
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             C4   -C3   -CL3     1.555   1.555   1.555      #         8
PLAT742_ALERT_1_C Angle   Calc   120.68(1), Rep      120.70 ......    Missing su
             C2   -C3   -CL3     1.555   1.555   1.555      #         9
PLAT742_ALERT_1_C Angle   Calc   118.10(1), Rep      118.10 ......    Missing su
             C5   -C4   -C3      1.555   1.555   1.555      #        10
PLAT742_ALERT_1_C Angle   Calc   121.98(1), Rep      122.00 ......    Missing su
             C5   -C4   -CL4     1.555   1.555   1.555      #        11
PLAT742_ALERT_1_C Angle   Calc   119.92(1), Rep      119.90 ......    Missing su
             C3   -C4   -CL4     1.555   1.555   1.555      #        12
PLAT742_ALERT_1_C Angle   Calc   123.79(1), Rep      123.80 ......    Missing su
             N1   -C5   -C4      1.555   1.555   1.555      #        13
PLAT742_ALERT_1_C Angle   Calc   116.22(1), Rep      116.20 ......    Missing su
             N1   -C5   -CL5     1.555   1.555   1.555      #        14
PLAT742_ALERT_1_C Angle   Calc   119.98(1), Rep      120.00 ......    Missing su
             C4   -C5   -CL5     1.555   1.555   1.555      #        15
PLAT742_ALERT_1_C Angle   Calc   119.22(1), Rep      119.20 ......    Missing su
             C5   -N1   -C1      1.555   1.555   1.555      #        16
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     45.666 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     14.197 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     15.897 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      9.930 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     11.264 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      8.437 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     10.203 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      6.558 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.911 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.231 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      4.854 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.524 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.492 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.627 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.191 Check
PLAT915_ALERT_3_C Low Friedel Pair Coverage ......................         58 %
PLAT925_ALERT_1_C The Reported and Calculated Rho(max) Differ by .       1.50 eA-3
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      14.29
PLAT971_ALERT_2_C Check Calcd Residual Density  1.11A From     Cl3       2.22 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  0.06A From      N1       1.74 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.68A From     Cl4      -2.45 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.52A From     Cl3      -2.44 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.66A From     Cl1      -2.39 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.62A From     Cl5      -2.30 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.63A From      C5      -2.28 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.64A From     Cl5      -2.26 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.68A From     Cl1      -2.18 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.65A From      N1      -1.64 eA-3
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry .....         90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group.      P21/c Check
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds          1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        146 Note
```

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

31 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
 38 ALERT type 2 Indicator that the structure model may be wrong or deficient
 22 ALERT type 3 Indicator that the structure quality may be low
 36 ALERT type 4 Improvement, methodology, query or suggestion
  0 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

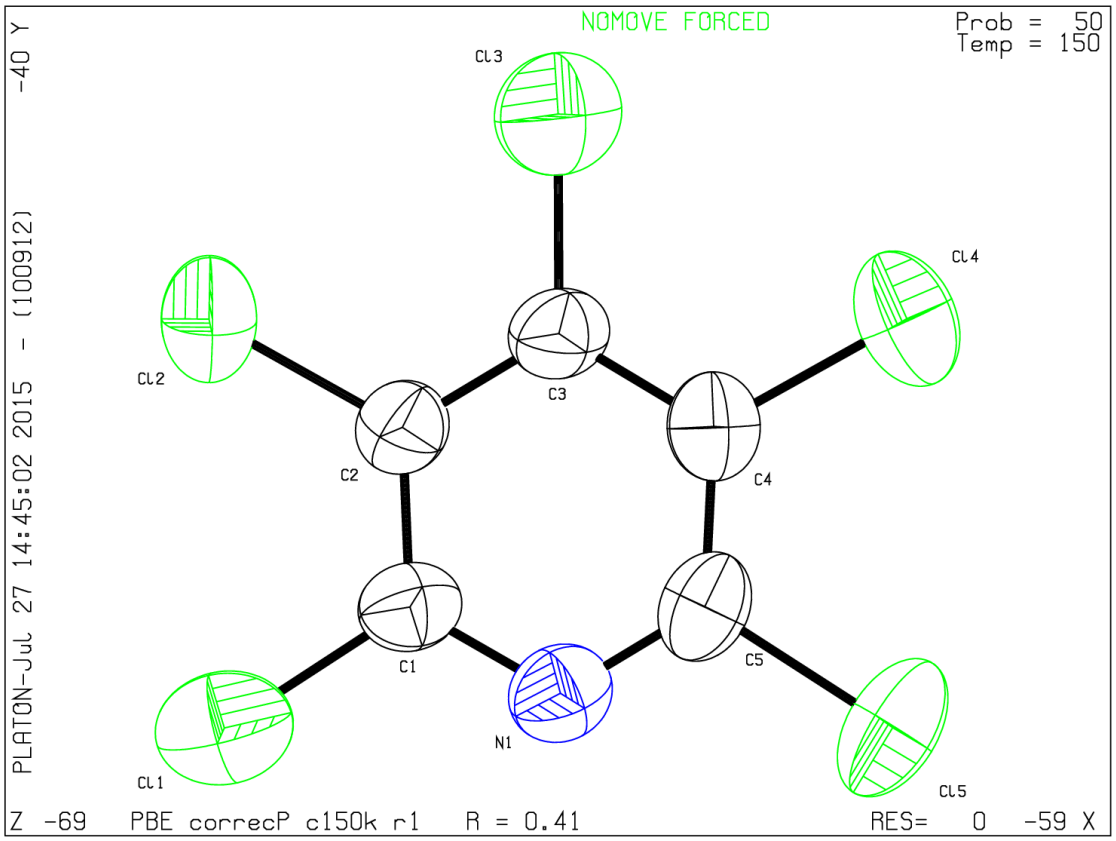
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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 21/06/2015; check.def file version of 21/06/2015

Datablock PBE_correct2_150K_r1 - ellipsoid plot



Calculated Adps !

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PBE_correct2_200K_r1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: PBE_correct2_200K_r1

```
Bond precision:  C-C = 0.0004 A          Wavelength=0.71073

Cell:            a=5.3290(14)     b=5.1935(13)       c=14.949(4)
                 alpha=90         beta=99.833(5)     gamma=90
Temperature:     200 K

                Calculated                Reported
Volume          407.65(18)                407.66(18)
Space group     P c                       P c
Hall group      P -2yc                    P -2yc
Moiety formula  C5 Cl5 N                  C5 Cl5 N
Sum formula     C5 Cl5 N                  C5 Cl5 N
Mr              251.31                    251.31
Dx,g cm-3       2.047                     2.047
Z               2                         2
Mu (mm-1)       1.701                     1.701
F000            244.0                     244.0
F000'           245.52
h,k,lmax        7,7,21                    7,7,20
Nref            2565[ 1286]               1926
Tmin,Tmax       0.649,0.903               0.609,0.746
Tmin'           0.636

Correction method= # Reported T Limits: Tmin=0.609 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.50/0.75       Theta(max)= 30.771

R(reflections)= 0.4762( 1551)      wR2(reflections)= 0.6650( 1926)

S = 7.036                          Npar= 1
```

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

```
GOODF01_ALERT_2_A  The least squares goodness of fit parameter lies
           outside the range 0.40 <> 6.00
           Goodness of fit given =      7.036
RFACG01_ALERT_3_A  The value of the R factor is > 0.20
           R factor given   0.476
RFACR01_ALERT_3_A  The value of the weighted R factor is > 0.45
           Weighted R factor given   0.665
PLAT082_ALERT_2_A High R1 Value ..................................       0.48 Report
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ...................       0.67 Report
PLAT087_ALERT_2_A Unsatisfactory S value (Too High) ..............       7.04 Check
PLAT934_ALERT_3_A Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....        272 Check
PLAT971_ALERT_2_A Check Calcd Residual Density  0.05A From     Cl1       4.07 eA-3
PLAT971_ALERT_2_A Check Calcd Residual Density  0.07A From     Cl4       3.73 eA-3
```

Alert level B

```
DIFMN02_ALERT_2_B  The minimum difference density is < -0.1*ZMAX*1.00
           _refine_diff_density_min given =     -1.944
           Test value =     -1.700
DIFMX01_ALERT_2_B  The maximum difference density is > 0.1*ZMAX*1.00
           _refine_diff_density_max given =      3.093
           Test value =      1.700
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       3.09 eA-3
PLAT098_ALERT_2_B Large Reported Min.  (Negative) Residual Density      -1.94 eA-3
PLAT431_ALERT_2_B Short Inter HL..A  Contact Cl3    ..  N1      ..       2.97 Ang.
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...          2 Check
PLAT971_ALERT_2_B Check Calcd Residual Density  0.09A From     Cl2       3.41 eA-3
PLAT971_ALERT_2_B Check Calcd Residual Density  0.21A From     Cl3       3.38 eA-3
PLAT971_ALERT_2_B Check Calcd Residual Density  0.12A From     Cl5       3.33 eA-3
```

Alert level C

```
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.340
          From the CIF: _refine_ls_abs_structure_Flack_su    0.140
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...        CL5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C1
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C2
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C3
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C4
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         C5
PLAT161_ALERT_4_C Missing or Zero su (esd) on x-coordinate for ...         N1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...        CL5
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C1
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C2
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C3
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C4
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         C5
```

```
PLAT162_ALERT_4_C Missing or Zero su (esd) on y-coordinate for ...         N1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...        CL5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C1
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C2
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C3
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C4
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         C5
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ...         N1
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         C5 Check
PLAT741_ALERT_1_C Bond    Calc   1.7224(5), Rep     1.72200 ......    Missing su
              CL1  -C1      1.555   1.555 .............. Bond #         1 Check
PLAT741_ALERT_1_C Bond    Calc   1.7076(5), Rep     1.70810 ......    Missing su
              CL2  -C2      1.555   1.555 .............. Bond #         2 Check
PLAT741_ALERT_1_C Bond    Calc   1.6988(5), Rep     1.69880 ......    Missing su
              CL3  -C3      1.555   1.555 .............. Bond #         3 Check
PLAT741_ALERT_1_C Bond    Calc   1.7129(5), Rep     1.71240 ......    Missing su
              CL4  -C4      1.555   1.555 .............. Bond #         4 Check
PLAT741_ALERT_1_C Bond    Calc   1.7229(5), Rep     1.72320 ......    Missing su
              CL5  -C5      1.555   1.555 .............. Bond #         5 Check
PLAT741_ALERT_1_C Bond    Calc   1.3230(4), Rep     1.32310 ......    Missing su
              C1   -N1      1.555   1.555 .............. Bond #         6 Check
PLAT741_ALERT_1_C Bond    Calc   1.3847(4), Rep     1.38420 ......    Missing su
              C1   -C2      1.555   1.555 .............. Bond #         7 Check
PLAT741_ALERT_1_C Bond    Calc   1.4093(4), Rep     1.40950 ......    Missing su
              C2   -C3      1.555   1.555 .............. Bond #         8 Check
PLAT741_ALERT_1_C Bond    Calc   1.3927(4), Rep     1.39230 ......    Missing su
              C3   -C4      1.555   1.555 .............. Bond #         9 Check
PLAT741_ALERT_1_C Bond    Calc   1.3790(4), Rep     1.37900 ......    Missing su
              C4   -C5      1.555   1.555 .............. Bond #        10 Check
PLAT741_ALERT_1_C Bond    Calc   1.3108(4), Rep     1.31110 ......    Missing su
              C5   -N1      1.555   1.555 .............. Bond #        11 Check
PLAT742_ALERT_1_C Angle   Calc   123.23(1), Rep      123.20 ......    Missing su
              N1   -C1   -C2      1.555   1.555   1.555      #         1
PLAT742_ALERT_1_C Angle   Calc   116.58(1), Rep      116.60 ......    Missing su
              N1   -C1   -CL1     1.555   1.555   1.555      #         2
PLAT742_ALERT_1_C Angle   Calc   120.19(1), Rep      120.20 ......    Missing su
              C2   -C1   -CL1     1.555   1.555   1.555      #         3
PLAT742_ALERT_1_C Angle   Calc   117.86(1), Rep      117.90 ......    Missing su
              C1   -C2   -C3      1.555   1.555   1.555      #         4
PLAT742_ALERT_1_C Angle   Calc   122.04(1), Rep      122.00 ......    Missing su
              C1   -C2   -CL2     1.555   1.555   1.555      #         5
PLAT742_ALERT_1_C Angle   Calc   120.09(1), Rep      120.10 ......    Missing su
              C3   -C2   -CL2     1.555   1.555   1.555      #         6
PLAT742_ALERT_1_C Angle   Calc   117.93(1), Rep      117.90 ......    Missing su
              C4   -C3   -C2      1.555   1.555   1.555      #         7
PLAT742_ALERT_1_C Angle   Calc   121.62(1), Rep      121.60 ......    Missing su
              C4   -C3   -CL3     1.555   1.555   1.555      #         8
PLAT742_ALERT_1_C Angle   Calc   120.45(1), Rep      120.40 ......    Missing su
              C2   -C3   -CL3     1.555   1.555   1.555      #         9
PLAT742_ALERT_1_C Angle   Calc   118.70(1), Rep      118.70 ......    Missing su
              C5   -C4   -C3      1.555   1.555   1.555      #        10
PLAT742_ALERT_1_C Angle   Calc   121.90(1), Rep      121.90 ......    Missing su
              C5   -C4   -CL4     1.555   1.555   1.555      #        11
PLAT742_ALERT_1_C Angle   Calc   119.40(1), Rep      119.40 ......    Missing su
              C3   -C4   -CL4     1.555   1.555   1.555      #        12
PLAT742_ALERT_1_C Angle   Calc   123.37(1), Rep      123.30 ......    Missing su
              N1   -C5   -C4      1.555   1.555   1.555      #        13
PLAT742_ALERT_1_C Angle   Calc   116.31(1), Rep      116.30 ......    Missing su
```

```
             N1   -C5   -CL5     1.555   1.555   1.555      #         14
PLAT742_ALERT_1_C Angle   Calc   120.31(1), Rep      120.30 ......    Missing su
             C4   -C5   -CL5     1.555   1.555   1.555      #         15
PLAT742_ALERT_1_C Angle   Calc   118.90(1), Rep      118.90 ......    Missing su
             C5   -N1   -C1      1.555   1.555   1.555      #         16
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......    139.076 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     36.981 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     48.093 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     26.332 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     32.879 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     20.799 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     24.740 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     15.209 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     14.689 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     10.861 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      9.215 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      6.922 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      7.070 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.199 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.859 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.678 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.133 Check
PLAT915_ALERT_3_C Low Friedel Pair Coverage ......................         60 %
PLAT918_ALERT_3_C Reflection(s) with I(obs) much smaller I(calc) .          1 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      12.33
PLAT971_ALERT_2_C Check Calcd Residual Density  0.13A From      N1       1.53 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.64A From     Cl4      -2.35 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.88A From     Cl3      -2.15 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.69A From     Cl1      -2.04 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.76A From     Cl2      -2.03 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.72A From     Cl5      -2.00 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.72A From     Cl3      -1.95 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.70A From     Cl2      -1.94 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.66A From     Cl5      -1.94 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.88A From     Cl3      -1.92 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.84A From     Cl1      -1.87 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.82A From     Cl2      -1.87 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.81A From     Cl1      -1.87 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.84A From     Cl5      -1.82 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.71A From     Cl4      -1.79 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.82A From     Cl4      -1.79 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.82A From     Cl1      -1.77 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.63A From      C5      -1.72 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.79A From     Cl2      -1.68 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.85A From     Cl3      -1.54 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.68A From     Cl3      -1.52 eA-3
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..    Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry .....        90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group.     P21/c Check
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds         1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       119 Note
```

---

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

30 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
 37 ALERT type 2 Indicator that the structure model may be wrong or deficient
 25 ALERT type 3 Indicator that the structure quality may be low
 36 ALERT type 4 Improvement, methodology, query or suggestion
  0 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

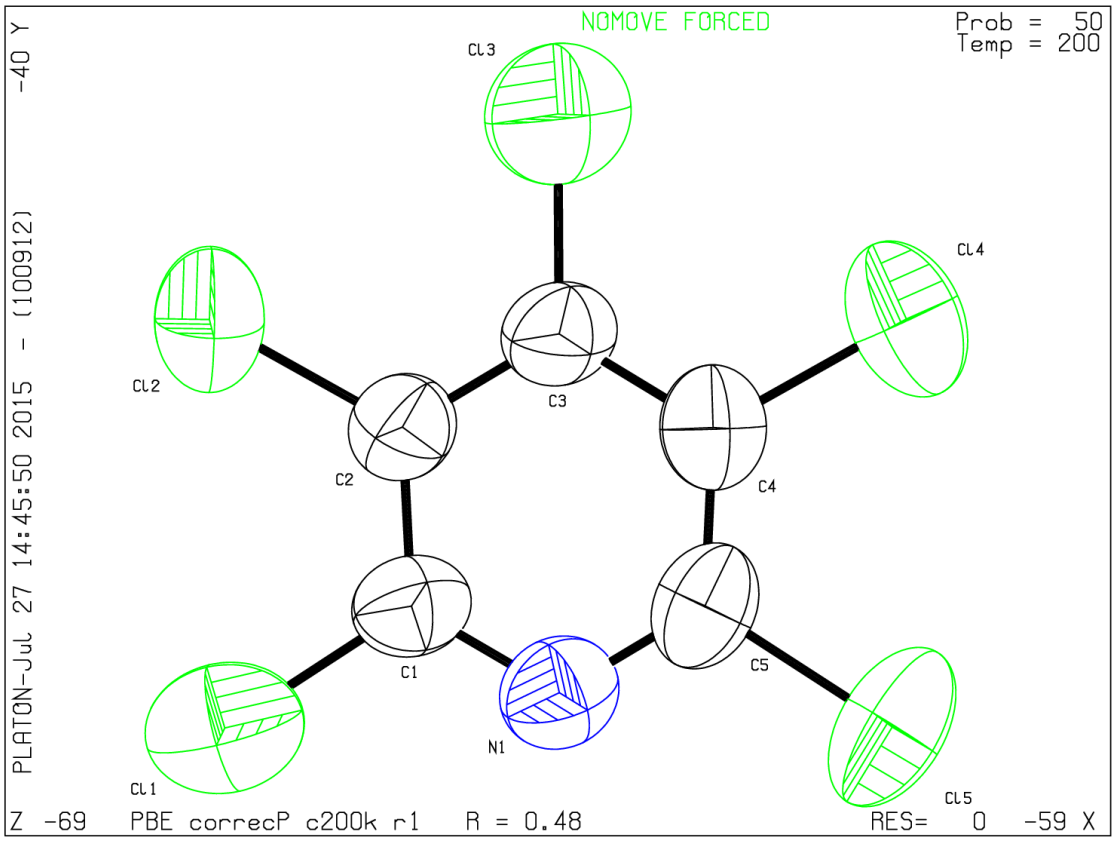
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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 21/06/2015; check.def file version of 21/06/2015

Datablock PBE_correct2_200K_r1 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C5CL5N_100K

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: C5CL5N_100K

```
Bond precision:  C-C = 0.0020 A          Wavelength=0.71073

Cell:            a=5.3122(2)    b=5.1770(2)        c=14.8307(6)
                 alpha=90       beta=99.493(2)     gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	402.28(3)	402.28(3)
Space group	P c	P c
Hall group	P -2yc	P -2yc
Moiety formula	C5 Cl5 N	C5 Cl5 N
Sum formula	C5 Cl5 N	C5 Cl5 N
Mr	251.31	251.31
Dx,g cm-3	2.075	2.075
Z	2	2
Mu (mm-1)	1.724	1.724
F000	244.0	244.0
F000’	245.52	
h,k,lmax	11,11,31	10,11,31
Nref	8293[4152]	7455
Tmin,Tmax	0.645,0.902	0.787,1.000
Tmin’	0.632	

```
Correction method= MULTI-SCAN

Data completeness= 1.80/0.90      Theta(max)= 49.718

R(reflections)= 0.0369( 6543)     wR2(reflections)= 0.0952( 7455)

S = 1.029                 Npar= 100
```

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 B

```
PLAT431_ALERT_2_B Short Inter HL..A  Contact Cl3    ..  N1      ..       2.93 Ang.
```

Alert level C

```
PLAT915_ALERT_3_C Low Friedel Pair Coverage .....................         82 %
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry .....         90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group.      P21/c Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         51 Note
```

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

   1 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
   1 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 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.

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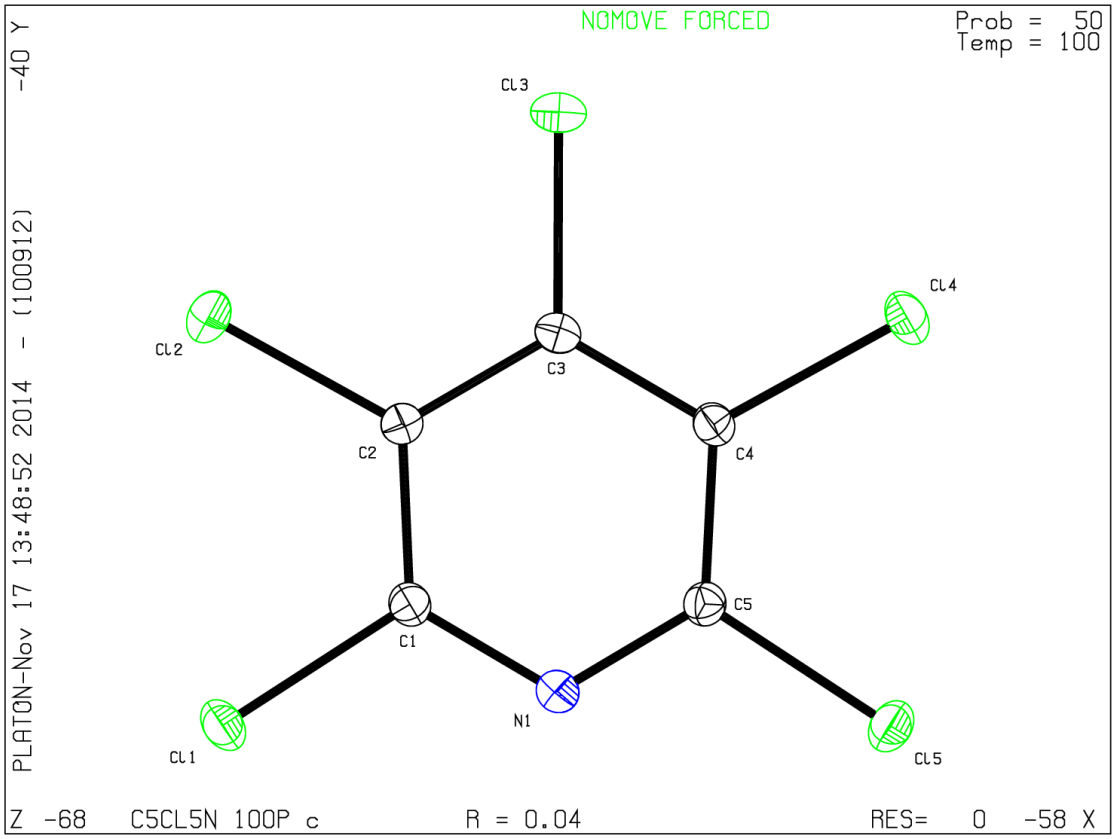
Publication of your CIF in other journals

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

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock C5CL5N_100K - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C5CL5N_150K

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: C5CL5N_150K

```
Bond precision:  C-C = 0.0080 A          Wavelength=0.71073

Cell:            a=5.3191(16)     b=5.1827(16)       c=14.894(5)
                 alpha=90         beta=99.704(5)     gamma=90
Temperature:     150 K
```

	Calculated	Reported
Volume	404.7(2)	404.7(2)
Space group	P c	P c
Hall group	P -2yc	P -2yc
Moiety formula	C5 Cl5 N	C5 Cl5 N
Sum formula	C5 Cl5 N	C5 Cl5 N
Mr	251.31	251.31
Dx,g cm-3	2.062	2.062
Z	2	2
Mu (mm-1)	1.713	1.713
F000	244.0	244.0
F000’	245.52	
h,k,lmax	7,7,21	7,7,20
Nref	2581[1294]	1894
Tmin,Tmax	0.647,0.902	0.590,0.746
Tmin’	0.634	

```
Correction method= MULTI-SCAN

Data completeness= 1.46/0.73      Theta(max)= 30.904

R(reflections)= 0.0388( 1769)     wR2(reflections)= 0.0945( 1894)

S = 1.062                  Npar= 100
```

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 B

```
PLAT431_ALERT_2_B Short Inter HL..A  Contact Cl3    ..  N1      ..       2.95 Ang.
```

Alert level C

```
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0080 Ang.
PLAT915_ALERT_3_C Low Friedel Pair Coverage .....................        58 %
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry .....         90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group.      P21/c Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        146 Note
```

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

   1 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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Publication of your CIF in other journals

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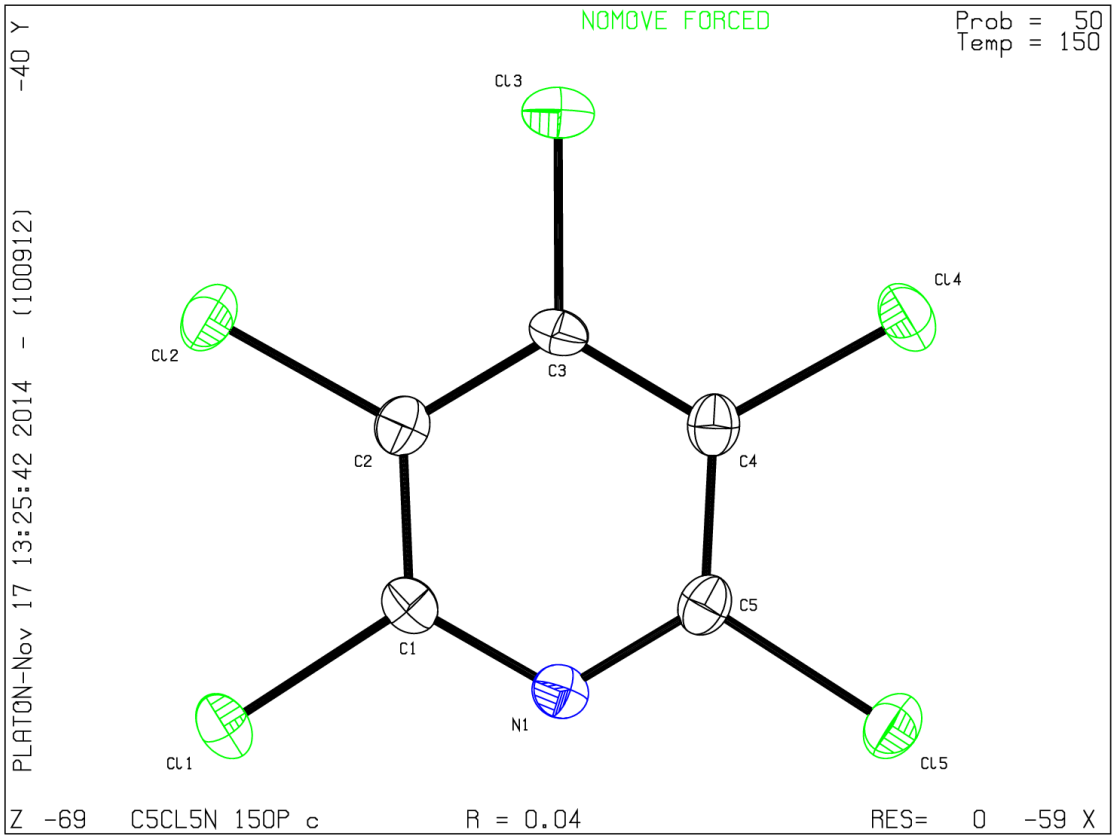
PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock C5CL5N_150K - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C5CL5N_200K

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: C5CL5N_200K

```
Bond precision:  C-C = 0.0100 A          Wavelength=0.71073

Cell:            a=5.3290(14)     b=5.1935(13)       c=14.949(4)
                 alpha=90         beta=99.833(5)     gamma=90
Temperature:     200 K
```

	Calculated	Reported
Volume	407.65(18)	407.66(18)
Space group	P c	P c
Hall group	P -2yc	P -2yc
Moiety formula	C5 Cl5 N	C5 Cl5 N
Sum formula	C5 Cl5 N	C5 Cl5 N
Mr	251.31	251.31
Dx,g cm-3	2.047	2.047
Z	2	2
Mu (mm-1)	1.701	1.701
F000	244.0	244.0
F000’	245.52	
h,k,lmax	7,7,21	7,7,20
Nref	2565[1286]	1926
Tmin,Tmax	0.649,0.903	0.609,0.746
Tmin’	0.636	

```
Correction method= MULTI-SCAN

Data completeness= 1.50/0.75      Theta(max)= 30.771

R(reflections)= 0.0474( 1551)     wR2(reflections)= 0.0979( 1926)

S = 0.992                  Npar= 100
```

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 B

```
PLAT431_ALERT_2_B Short Inter HL..A  Contact Cl3    ..  N1      ..       2.97 Ang.
```

Alert level C

```
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0100 Ang.
PLAT915_ALERT_3_C Low Friedel Pair Coverage .....................        60 %
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry .....         90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group.      P21/c Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        119 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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   1 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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Publication of your CIF in other journals

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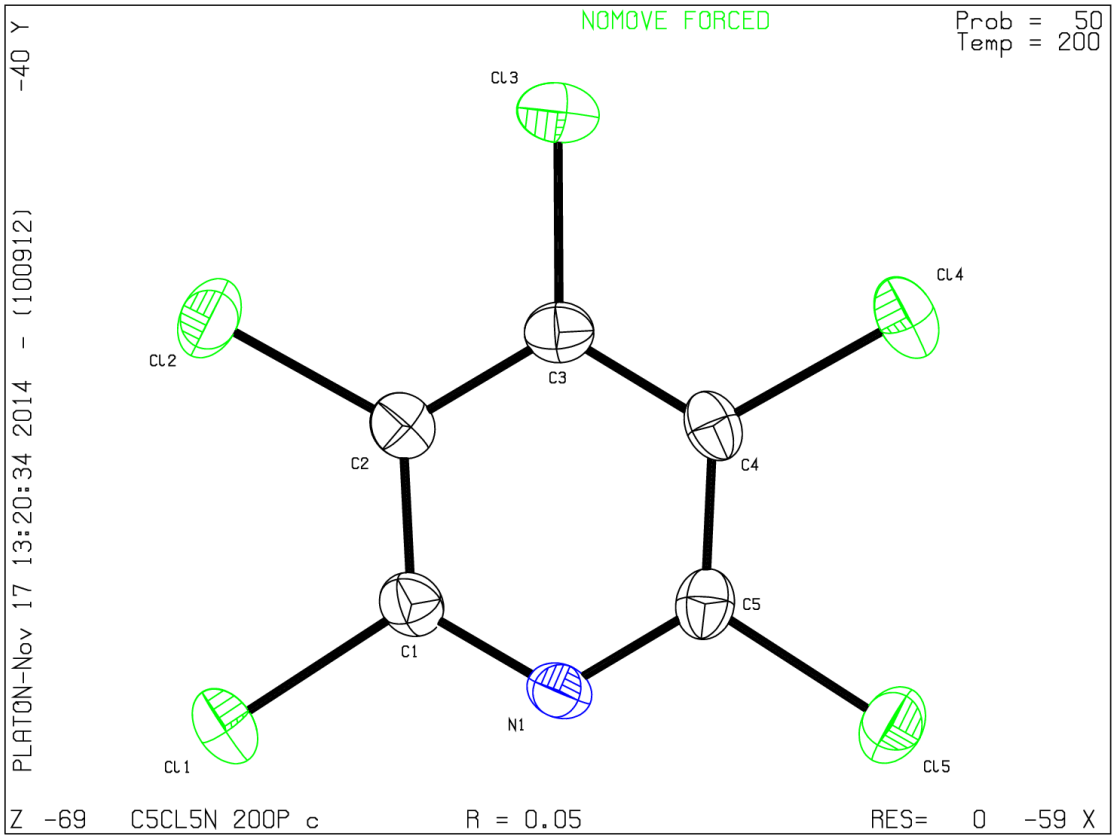
PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock C5CL5N_200K - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C5CL5N_250K

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: C5CL5N_250K

```
Bond precision:  C-C = 0.0110 A          Wavelength=0.71073

Cell:            a=5.3426(15)    b=5.2051(15)        c=15.021(4)
                 alpha=90        beta=100.003(6)     gamma=90
Temperature:     250 K

                 Calculated                Reported
Volume           411.4(2)                  411.4(2)
Space group      P c                       P c
Hall group       P -2yc                    P -2yc
Moiety formula   C5 Cl5 N                  C5 Cl5 N
Sum formula      C5 Cl5 N                  C5 Cl5 N
Mr               251.31                    251.31
Dx,g cm-3        2.029                     2.029
Z                2                         2
Mu (mm-1)        1.686                     1.686
F000             244.0                     244.0
F000'            245.52
h,k,lmax         7,7,21                    7,7,21
Nref             2587[ 1297]               1939
Tmin,Tmax        0.652,0.904               0.609,0.746
Tmin'            0.639

Correction method= # Reported T Limits: Tmin=0.609 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.49/0.75      Theta(max)= 30.760

R(reflections)= 0.0490( 1361)     wR2(reflections)= 0.1001( 1939)

S = 1.008                 Npar= 100
```

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 B

```
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ..............     0.0110 Ang.
PLAT431_ALERT_2_B Short Inter HL..A  Contact Cl3    ..  N1      ..       2.99 Ang.
```

Alert level C

```
PLAT915_ALERT_3_C Low Friedel Pair Coverage .....................         59 %
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry .....         90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group.      P21/c Check
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        119 Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          1 Units
```

```
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   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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```

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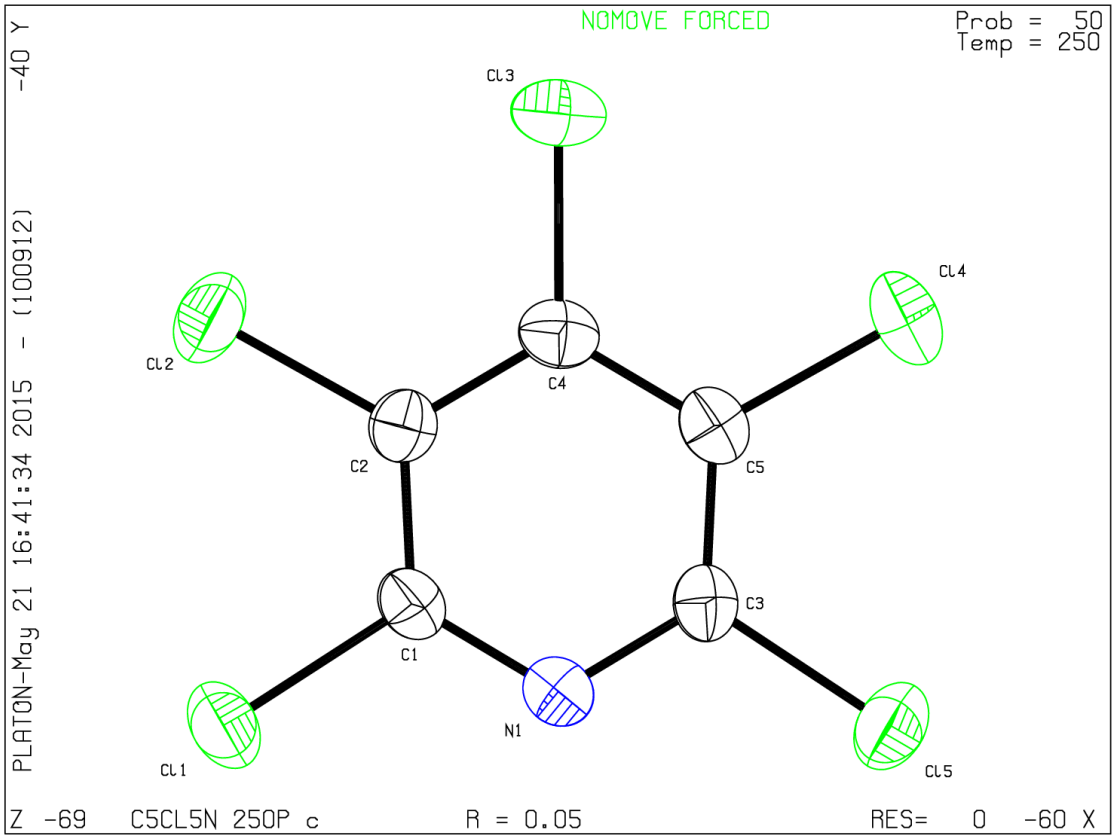
PLATON version of 21/04/2015; check.def file version of 09/03/2015

Datablock C5CL5N_250K - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C5CL5N_300K

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: C5CL5N_300K

```
Bond precision:  C-C = 0.0127 A          Wavelength=0.71073

Cell:            a=5.359(4)    b=5.224(4)            c=15.101(13)
                 alpha=90      beta=100.228(18)      gamma=90
Temperature:     300 K

                Calculated                Reported
Volume          416.0(6)                  416.1(6)
Space group     P c                       P c
Hall group      P -2yc                    P -2yc
Moiety formula  C5 Cl5 N                  C5 Cl5 N
Sum formula     C5 Cl5 N                  C5 Cl5 N
Mr              251.31                    251.31
Dx,g cm-3       2.006                     2.006
Z               2                         2
Mu (mm-1)       1.667                     1.667
F000            244.0                     244.0
F000'           245.52
h,k,lmax        7,7,21                    7,7,20
Nref            2581[ 1294]               1936
Tmin,Tmax       0.655,0.905               0.609,0.746
Tmin'           0.642

Correction method= # Reported T Limits: Tmin=0.609 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.50/0.75      Theta(max)= 30.624

R(reflections)= 0.0525( 1172)     wR2(reflections)= 0.1344( 1936)

S = 0.959                 Npar= 100
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
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Alert level B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0127 Ang.

Alert level C

PLAT431_ALERT_2_C Short Inter HL..A Contact Cl3 .. N1 .. 3.03 Ang.
PLAT915_ALERT_3_C Low Friedel Pair Coverage ..... 59 %
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check

Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.300 Report
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT111_ALERT_2_G ADDSYM Detects (Pseudo) Centre of Symmetry ..... 90 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space group. P21/n Check
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and su .. 0.30 Check
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 112 Note

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PLATON version of 21/04/2015; check.def file version of 09/03/2015

Datablock C5CL5N_300K - ellipsoid plot