checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ck-2cf32phn-4nh-qte-new_auto_sq

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: ck-2cf32phn-4nh-qte-new_auto_sq

Bond precision: C-C = 0.0064 A Wavelength=1.54184

Cell: a=43.8664(7) b=27.2131(4) c=22.9748(3)
alpha=90 beta=90 gamma=90
Temperature: 105 K

	Calculated	Reported
Volume	27426.0(7)	27426.0(7)
Space group	F d d 2	F d d 2
Hall group	F 2 -2d	F 2 -2d
Moiety formula	2(C76 H50 F12 N6 O8), 3(C H Cl3) [+ solvent]	C76 H50 F12 N6 O8, 1.5(C H Cl3), 0.5[]
Sum formula	C155 H103 Cl9 F24 N12 O16 [+ solvent]	C77.50 H51.50 Cl4.50 F12 N6 O8
Mr	3164.55	1582.27
Dx,g cm-3	1.533	1.533
Z	8	16
Mu (mm-1)	2.598	2.598
F000	12912.0	12912.0
F000'	12982.39	
h,k,lmax	55,34,28	54,34,28
Nref	14389[7380]	10623
Tmin,Tmax	0.856,0.878	0.588,1.000
Tmin'	0.459	

Correction method= # Reported T Limits: Tmin=0.588 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.44/0.74 Theta(max)= 76.183

R(reflections)= 0.0601(9878) wR2(reflections)= 0.1748(10623)

S = 1.043 Npar= 1020

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax <= 18) .......       6.91 Note
PLAT234_ALERT_4_C Large Hirshfeld Difference Cl5A     --C78      .       0.22 Ang.
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl4      0.272 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl1      0.131 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00643 Ang.
PLAT415_ALERT_2_C Short Inter D-H..H-X       H3       ..H42A     .       2.12 Ang.
                                                1-x,1-y,z  =      2_665 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N4       --H4       .     Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         53 Report
                0 32  0,   2 32  0,   4 32  0,   6 32  0,   8 32  0,  10 32  0,
               12 30  0,  14 30  0,   9 31  1,  11 31  1,   2  0  2,   4  2  2,
                6  0  2,   6 32  2,   8 32  2,  10  0  2,  13  1  3,  15  1  3,
                0 12  4,  52  0  4,   1 13  5,   3 13  5,   5 13  5,  48  0  8,
               23 27  9,  39 19  9,  41 17  9,  24 26 10,  34 20 10,  36 20 10,
                   (   23 More Missing: see the .ckf listing file)
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          3 Check
                5  1 -1,   1  5 -1,   2  2  0,
PLAT987_ALERT_1_C The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C77.5 H51.5 Cl4.5 F12 N6 O8
           Atom count from the _atom_site data:  C77.5 H51.5 Cl4.25 F12 N6 O8
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z   16
          From the CIF: _chemical_formula_sum  C77.50 H51.50 Cl4.50 F12 N6 O8
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C       1240.00   1240.00    0.00
          H        824.00    824.00    0.00
          Cl        72.00     68.00    4.00
          F        192.00    192.00    0.00
          N         96.00     96.00    0.00
```

```
          O        128.00    128.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         11 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         11 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          4 Report
             H1      H3      H4      H6
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C155 H103 Cl9 F24 N12 O16
             Rep.: C77.50 H51.50 Cl4.50 F12 N6 O8
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C76 H50 F12 N6 O8), 3(C H Cl3)
             Rep.: C76 H50 F12 N6 O8, 1.5(C H Cl3), 0.5[]
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.13 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      47.96 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          3 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   Cl4      --C78      .        9.7 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   Cl6      --C78      .       10.1 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C52 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C53 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C71 Check
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
             Cl4     Cl4A    Cl5     Cl5A    Cl6     Cl6A    H78     H78A
             Cl1     Cl2     Cl3     C77     H77
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)         75% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)        100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)       2.50 Check
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C29      -C34      .       1.42 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl4A     ..C78      .       2.10 Ang.
                                          1-x,1-y,z  =      2_665 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl5      ..C78      .       3.07 Ang.
                                          1-x,1-y,z  =      2_665 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl5      ..C1       .       3.07 Ang.
                                             x,y,z   =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl5      ..C2       .       3.23 Ang.
                                             x,y,z   =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C78      ..C78      .       2.61 Ang.
                                          1-x,1-y,z  =      2_665 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        224 A**3
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         13 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          3 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         88 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        280 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage         51 %
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
               2  0 -2,   4  2 -2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.5 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      5.163 Note
             Predicted wR2: Based on SigI**2  3.39 or SHELX Weight 16.79
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

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

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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT089_ck-2cf32phn-4nh-qte-new_auto_sq
;
PROBLEM: Poor Data / Parameter Ratio (Zmax <= 18) .......       6.91 Note
RESPONSE: ...
;
_vrf_PLAT234_ck-2cf32phn-4nh-qte-new_auto_sq
;
PROBLEM: Large Hirshfeld Difference Cl5A     --C78      .       0.22 Ang.
RESPONSE: ...
;
_vrf_PLAT260_ck-2cf32phn-4nh-qte-new_auto_sq
;
PROBLEM: Large Average Ueq of Residue Including       Cl4      0.272 Check
RESPONSE: ...
;
_vrf_PLAT340_ck-2cf32phn-4nh-qte-new_auto_sq
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.00643 Ang.
RESPONSE: ...
;
_vrf_PLAT415_ck-2cf32phn-4nh-qte-new_auto_sq
;
PROBLEM: Short Inter D-H..H-X       H3       ..H42A     .       2.12 Ang.
RESPONSE: ...
;
_vrf_PLAT420_ck-2cf32phn-4nh-qte-new_auto_sq
;
PROBLEM: D-H Bond Without Acceptor  N4       --H4       .     Please Check
RESPONSE: ...
;
_vrf_PLAT911_ck-2cf32phn-4nh-qte-new_auto_sq
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600         53 Report
RESPONSE: ...
;
_vrf_PLAT918_ck-2cf32phn-4nh-qte-new_auto_sq
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .          3 Check
RESPONSE: ...
```

```
;
_vrf_PLAT987_ck-2cf32phn-4nh-qte-new_auto_sq
;
PROBLEM: The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
RESPONSE: ...
;
# end Validation Reply Form
```

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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

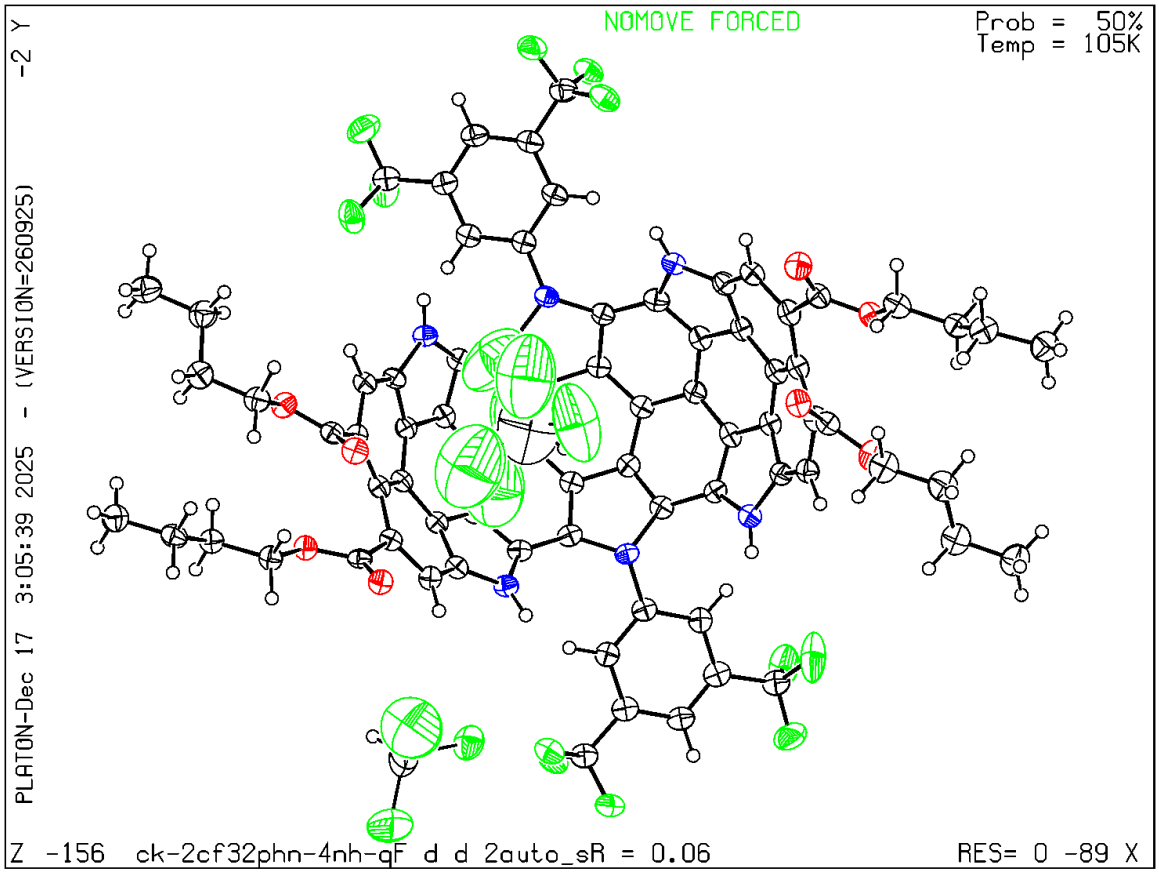
PLATON version of 26/09/2025; check.def file version of 20/09/2025

---

duplicate check

No duplication found

Datablock ck-2cf32phn-4nh-qte-new_auto_sq - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ck-6n-qdi-c60-new_auto

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: ck-6n-qdi-c60-new_auto

```
Bond precision:   C-C = 0.0109 A          Wavelength=1.54184

Cell:           a=13.5694(1)       b=15.6078(1)     c=24.9813(2)
                alpha=102.650(1)   beta=92.214(1)   gamma=100.521(1)
Temperature:    100 K
```

	Calculated	Reported
Volume	5058.46(7)	5058.46(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C92 H64 F12 N8 O4, C60, 2(C H4 O)	C92 H64 F12 N8 O4, 2(C H4 O), C60
Sum formula	C154 H72 F12 N8 O6	C154 H72 F12 N8 O6
Mr	2358.20	2358.19
Dx,g cm-3	1.548	1.548
Z	2	2
Mu (mm-1)	0.912	0.912
F000	2416.0	2416.0
F000'	2424.05	
h,k,lmax	17,19,31	16,19,30
Nref	21285	20310
Tmin,Tmax	0.896,0.930	0.684,1.000
Tmin'	0.796	

```
Correction method= # Reported T Limits: Tmin=0.684 Tmax=1.000
AbsCorr = MULTI-SCAN
```

Data completeness= 0.954 Theta(max)= 76.489

R(reflections)= 0.1187(17137) wR2(reflections)= 0.2463(20310)

S = 1.008 Npar= 1680

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

DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00
_refine_diff_density_min given = -0.979
Test value = -0.900

Author Response: The crystal exhibits a little twinning.

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.79 eA-3

Author Response: The crystal exhibits a little twinning.

PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density -0.98 eA-3

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_B Hirshfeld Test Diff for C4A --C5A . 7.4 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_B Hirshfeld Test Diff for C7A --C8A . 7.6 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_B Hirshfeld Test Diff for C25A --C60A . 7.6 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_B Hirshfeld Test Diff for C43A --C56A . 8.0 s.u.

Author Response: The crystal exhibits a little twinning.

```
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C56A     --C57A     .        8.1 s.u.
```

Author Response: The crystal exhibits a little twinning.

```
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.01093 Ang.
```

Author Response: The crystal exhibits a little twinning.

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.
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C92 H64 F12 N8 O4, C60, 2(C H4 O)
             Rep.: C92 H64 F12 N8 O4, 2(C H4 O), C60
PLAT082_ALERT_2_C High R1 Value ................................       0.12 Report
PLAT213_ALERT_2_C Atom C78A            has ADP max/min Ratio .....        3.1 prolat
PLAT214_ALERT_2_C Atom C8A       (Anion/Solvent) ADP max/min Ratio        4.6 prolat
PLAT214_ALERT_2_C Atom C12A      (Anion/Solvent) ADP max/min Ratio        4.2 prolat
PLAT214_ALERT_2_C Atom C23A      (Anion/Solvent) ADP max/min Ratio        4.8 prolat
PLAT214_ALERT_2_C Atom C28A      (Anion/Solvent) ADP max/min Ratio        4.5 oblate
PLAT214_ALERT_2_C Atom C32A      (Anion/Solvent) ADP max/min Ratio        5.0 prolat
PLAT214_ALERT_2_C Atom C40A      (Anion/Solvent) ADP max/min Ratio        4.1 prolat
PLAT214_ALERT_2_C Atom C50A      (Anion/Solvent) ADP max/min Ratio        4.9 prolat
PLAT214_ALERT_2_C Atom C51A      (Anion/Solvent) ADP max/min Ratio        4.6 oblate
PLAT214_ALERT_2_C Atom C58A      (Anion/Solvent) ADP max/min Ratio        4.5 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.4 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.9 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C21      --C28      .        6.3 s.u.
```

Author Response: The crystal exhibits a little twinning.

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C22      --C23      .        6.0 s.u.
```

Author Response: The crystal exhibits a little twinning.

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C22      --C27      .        6.1 s.u.
```

Author Response: The crystal exhibits a little twinning.

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C2A      --C59A     .        6.9 s.u.
```

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C3A --C36A . 5.9 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C8A --C9A . 6.0 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C8A --C52A . 6.7 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C17A --C22A . 6.9 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C19A --C20A . 6.6 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C27A --C32A . 6.4 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C31A --C32A . 6.6 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C35A --C36A . 5.5 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C37A --C48A . 6.2 s.u.

Author Response: The crystal exhibits a little twinning.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C43A --C44A . 6.8 s.u.

Author Response: The crystal exhibits a little twinning.

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C48A     --C49A     .        6.6 s.u.
```

Author Response: The crystal exhibits a little twinning.

```
PLAT234_ALERT_4_C Large Hirshfeld Difference C77      --C78A     .       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1A      --C6A      .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1A      --C13A     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C2A      --C3A      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C5A      --C51A     .       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C6A      --C7A      .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C9A      --C10A     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C10A     --C18A     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11A     --C12A     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C12A     --C13A     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14A     --C15A     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14A     --C60A     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C15A     --C16A     .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C17A     --C18A     .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C18A     --C19A     .       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C19A     --C55A     .       0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C20A     --C57A     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C26A     --C27A     .       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C27A     --C28A     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C28A     --C29A     .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C29A     --C30A     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30A     --C31A     .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30A     --C58A     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C32A     --C33A     .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C33A     --C34A     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C33A     --C38A     .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C36A     --C37A     .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C37A     --C38A     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C40A     --C41A     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C41A     --C42A     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C41A     --C58A     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C42A     --C46A     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C50A     --C51A     .       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C51A     --C52A     .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C52A     --C53A     .       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C57A     --C58A     .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C59A     --C60A     .       0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C13A Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C14A Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C19A Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C27A Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C28A Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C36A Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C41A Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C51A Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C52A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C23 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C4A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C21A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C25A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C44A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C57A Check
```

```
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       C1A      0.121 Check
PLAT601_ALERT_2_C Unit-Cell Contains Solvent Accessible VOIDS .LE.        41 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      9.132 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.247 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        33 Report
               -3  1  0,   3 -2  1,   0 -1  1,   0  1  1,   0 -1  2,   1  0  2,
                1  1  2,  -2  2  2,   1 -1  3,   1  0  3,  -3  2  3,   0 -2  4,
                2  0  4,  -2  1  4,  -1  1  4,   0  1  4,   0 -3  5,   9  9 12,
                7 10 13,   9  3 20,  -2 10 21,   7  4 22,   4  7 22,   6  4 23,
                4  6 23,   5  4 24,   3  4 25,   4  4 25,   2  5 25,   3  3 26,
                   (    3 More Missing: see the .ckf listing file)
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .        16 Check
               -1  1  1,   1  1  1,  -2  2  1,   1  2  1,  -5  4  1,   0 -2  2,
               -2  1  2,   0 -2  3,   1  4  3,  -1  2  4,   1  5  4,  -7  3  5,
                0 -8  6,  -2 -1  8,   2  4  8,  -6 -1 10,
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .     13.20 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.94Ang From C42A           1.82 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.14Ang From C14A           1.69 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.77Ang From C76A           1.62 eA-3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        72 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms        67 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         2 Report
             H5A     H6A
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     32.91 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.001 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         8 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         8 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0100 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C71 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C72 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C87 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C88 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        4% Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C1A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C3A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C5A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C7A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C8A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C9A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C11A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C12A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C14A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C15A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C16A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C18A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C20A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C21A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C22A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C23A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C24A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C25A Check
```

```
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C26A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C28A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C32A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C34A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C35A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C38A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C39A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C40A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C43A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C44A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C45A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C46A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C49A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C50A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C51A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C53A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C55A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C56A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C57A Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C59A Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C7A      ..C12      .       3.19 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C42      ..C47      .       3.18 Ang.
                                               1-x,1-y,1-z  =      2_666 Check
PLAT793_ALERT_4_G Model has Chirality at C1          (Centro SpGr)         S Verify
PLAT793_ALERT_4_G Model has Chirality at C21         (Centro SpGr)         S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       707 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..    Please Do !
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]=      2.96 Note
               0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       882 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        17 Note
              -3  1  0,  -3  2  3,  -2  1  4,  -2  2  2,  -1  1  4,   0 -3  5,
               0 -2  4,   0 -1  1,   0 -1  2,   0  1  1,   0  1  4,   1 -1  3,
               1  0  2,   1  0  3,   1  1  2,   2  0  4,   3 -2  1,
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged    Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........    12.683 Note
             Predicted wR2: Based on SigI**2  1.94 or SHELX Weight 24.43
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 Info
```

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

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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_DIFMN03_ck-6n-qdi-c60-new_auto
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMX02_ck-6n-qdi-c60-new_auto
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT042_ck-6n-qdi-c60-new_auto
;
PROBLEM: Calc. and Reported MoietyFormula Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT082_ck-6n-qdi-c60-new_auto
;
PROBLEM: High R1 Value ..............................       0.12 Report
RESPONSE: ...
;
_vrf_PLAT213_ck-6n-qdi-c60-new_auto
;
PROBLEM: Atom C78A            has ADP max/min Ratio .....        3.1 prolat
RESPONSE: ...
;
_vrf_PLAT214_ck-6n-qdi-c60-new_auto
;
PROBLEM: Atom C8A       (Anion/Solvent) ADP max/min Ratio        4.6 prolat
RESPONSE: ...
;
_vrf_PLAT220_ck-6n-qdi-c60-new_auto
;
PROBLEM: NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.4 Ratio
RESPONSE: ...
;
_vrf_PLAT222_ck-6n-qdi-c60-new_auto
;
PROBLEM: NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.9 Ratio
RESPONSE: ...
;
_vrf_PLAT234_ck-6n-qdi-c60-new_auto
;
PROBLEM: Large Hirshfeld Difference C77      --C78A     .       0.22 Ang.
RESPONSE: ...
;
_vrf_PLAT241_ck-6n-qdi-c60-new_auto
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of       C13A Check
RESPONSE: ...
;
_vrf_PLAT242_ck-6n-qdi-c60-new_auto
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of        C23 Check
RESPONSE: ...
```

```
;
_vrf_PLAT260_ck-6n-qdi-c60-new_auto
;
PROBLEM: Large Average Ueq of Residue Including       C1A      0.121 Check
RESPONSE: ...
;
_vrf_PLAT601_ck-6n-qdi-c60-new_auto
;
PROBLEM: Unit-Cell Contains Solvent Accessible VOIDS .LE.         41 Ang**3
RESPONSE: ...
;
_vrf_PLAT906_ck-6n-qdi-c60-new_auto
;
PROBLEM: Large K Value in the Analysis of Variance ......      9.132 Check
RESPONSE: ...
;
_vrf_PLAT911_ck-6n-qdi-c60-new_auto
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600         33 Report
RESPONSE: ...
;
_vrf_PLAT918_ck-6n-qdi-c60-new_auto
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .         16 Check
RESPONSE: ...
;
_vrf_PLAT939_ck-6n-qdi-c60-new_auto
;
PROBLEM: Large Value of Not (SHELXL) Weight Optimized S .      13.20 Check
RESPONSE: ...
;
_vrf_PLAT971_ck-6n-qdi-c60-new_auto
;
PROBLEM: Check Calcd Resid. Dens.  0.94Ang From C42A            1.82 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

---

duplicate check

No duplication found

Datablock ck-6n-qdi-c60-new_auto - ellipsoid plot