checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cp1-6, cp1-7, cp2

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: cp1-6

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Bond precision:   C-C = 0.0141 A          Wavelength=1.34138

Cell:             a=28.210(8)     b=33.582(9)          c=14.918(4)
                  alpha=90        beta=105.247(11)     gamma=90
Temperature:      273 K
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	Calculated	Reported
Volume	13635(6)	13635(6)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	C70 H48 Cd2 Cl8 N4 O10
Sum formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	C70 H48 Cd2 Cl8 N4 O10
Mr	1613.55	1613.52
Dx,g cm-3	1.572	1.572
Z	8	8
Mu (mm-1)	5.657	5.657
F000	6464.0	6464.0
F000'	6498.35	
h,k,lmax	33,39,17	33,39,17
Nref	12033	11919
Tmin,Tmax	0.668,0.754	0.535,0.681
Tmin'	0.606	

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Correction method= # Reported T Limits: Tmin=0.535 Tmax=0.681
AbsCorr = NONE

Data completeness= 0.991           Theta(max)= 52.981
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R(reflections)= 0.1268(8624)

wR2(reflections)= 0.3288(11919)

S = 1.201 Npar= 891

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

PLAT420_ALERT_2_B D-H Bond Without Acceptor O9A --H9A . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O10A --H10A . Please Check

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Alert level C

PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.13 Do !
PLAT082_ALERT_2_C High R1 Value ..... 0.13 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.33 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 4.0 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.5 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O3 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cd1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cd2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C29 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C46 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C48 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C50 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C59 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C61 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C62 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cd1 0.138 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01414 Ang.
PLAT361_ALERT_2_C Long C(sp3)-C(sp3) Bond C15 - C36 . 1.74 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C57 - C58 . 1.53 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H3 ..H7 . 1.99 Ang.
x,y,z = 1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 10.686 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.056 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 110 Report

6	0	0,	32	0	0,	3	1	0,	32	2	0,	3	3	0,	0	4	0,
2	4	0,	4	4	0,	32	4	0,	3	5	0,	32	6	0,	2	8	0,
31	11	0,	28	20	0,	25	25	0,	1	1	1,	0	2	1,	2	2	1,
1	3	1,	3	5	1,	1	7	1,	-32	8	1,	2	8	1,	31	9	1,
-31	13	1,	28	18	1,	27	21	1,	24	26	1,	23	27	1,	-2	0	2,
-33	1	2,	31	1	2,	-33	3	2,	-15	3	2,	31	3	2,	-32	10	2,
30	10	2,	27	19	2,	25	23	2,	21	29	2,	-33	1	3,	-5	1	3,
-6	2	3,	-4	2	3,	-33	3	3,	30	4	3,	-33	5	3,	30	6	3,
29	11	3,	-31	15	3,	-20	16	3,	27	17	3,	26	20	3,	23	25	3,
-6	0	4,	-4	0	4,	-1	1	4,	-2	2	4,	-3	3	4,	-33	5	4,
29	5	4,	-33	7	4,	29	7	4,	-32	12	4,	28	12	4,	-31	15	4,
27	15	4,	26	18	4,	24	22	4,	-33	5	5,	28	6	5,	-33	7	5,

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              27 11  5, -32 12  5, -31 15  5,  24 20  5,  21 25  5,  20 26  5,
             -10  0  6, -33  5  6,  27  5  6,  23 19  6,  21 23  6,  20 24  6,
             -33  1  7,  26  2  7, -33  3  7,  26  4  7, -32 10  7,  24 14  7,
              20 22  7, -26  0  8,  24  8  8,  21 17  8,  19 21  8,  23  1  9,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .        6 Check
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.07Ang From C6           -1.67 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.75Ang From O9A     .     0.63 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6        .    -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H12D      .    -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H54       .    -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H12B      .    -0.35 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         46 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          93 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
              H9A   H10A  H9    H10B
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     120.21 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         20 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         47 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          2 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         15 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     0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0001 Report
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PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0002 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        273 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        20% Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C16 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C37 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C15      - C16      .       1.54 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C36      - C37      .       1.55 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C37      - C38      .       1.54 Ang.
PLAT415_ALERT_2_G Short Inter D-H..H-X       H9A      ..H15      .       2.08 Ang.
                                          1-x,1-y,2-z  =      5_667 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H10A     ..H36      .       1.68 Ang.
                                          1-x,1-y,2-z  =      5_667 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O9       ..C29      .       3.02 Ang.
                                          1-x,y,5/2-z  =      2_657 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C29      ..C29      .       3.04 Ang.
                                          1-x,y,5/2-z  =      2_657 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl1      ..Cl6      .       3.22 Ang.
                                            x,y,-1+z  =      1_554 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl2      ..Cl4      .       3.22 Ang.
                                           -x,y,1/2-z  =      2_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl2      ..Cl4A     .       3.31 Ang.
                                           -x,y,1/2-z  =      2_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         95 A**3
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.97000 Dev...        0.01 Ang.
             C12      -H12D           1_555   1_555 ........     #  193 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C37      --C16             1.76 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C15      --C36             1.74 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1       (II)      .       2.09 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       2020 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
               2  0  0,   1  1  0,   0  2  0,
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
               2  0  0,   2  8  1,  -4  0  4,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          5 Note
              -3  3  4,   2  4  0,   3  3  0,   3  5  0,   6  0  0,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      6.276 Note
             Predicted wR2: Based on SigI**2  5.24 or SHELX Weight 27.37
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
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  0 **ALERT level A** = Most likely a serious problem - resolve or explain
  2 **ALERT level B** = A potentially serious problem, consider carefully
 34 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 70 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: cp1-7

Bond precision: C-C = 0.0140 A Wavelength=1.34138

Cell: a=28.300(4) b=33.655(4) c=14.941(2)
alpha=90 beta=105.277(6) gamma=90
Temperature: 273 K

	Calculated	Reported
Volume	13728(3)	13727(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	C70 H48 Cd2 Cl8 N4 O10
Sum formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	C70 H48 Cd2 Cl8 N4 O10
Mr	1613.55	1613.52
Dx,g cm-3	1.561	1.561
Z	8	8
Mu (mm-1)	5.619	5.619
F000	6464.0	6464.0
F000'	6498.35	
h,k,lmax	33,40,17	33,40,17
Nref	12302	12241
Tmin,Tmax	0.599,0.638	0.409,0.686
Tmin'	0.543	

Correction method= # Reported T Limits: Tmin=0.409 Tmax=0.686
AbsCorr = NONE

Data completeness= 0.995 Theta(max)= 53.334

R(reflections)= 0.1251(9337) wR2(reflections)= 0.3086(12241)

S = 1.019 Npar= 863

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
PLAT420_ALERT_2_B D-H Bond Without Acceptor O10 --H10B . Please Check

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Alert level C
PLAT082_ALERT_2_C High R1 Value ..... 0.13 Report

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PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.31 Report
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C24 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C57 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Cd1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Cd2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C44 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C48 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C56 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C62 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cd1      0.125 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .........        C30 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01404 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C46      - C49      .       1.53 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     14.464 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.965 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.119 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.598         59 Report
                  2  0  0,   3  3  0,   0  4  0,   2  4  0,   1  1  1,   0  2  1,
                  2  2  1, -33  3  1,   1  3  1,   3  5  1,   2  8  1,   3  9  1,
                 29 17  1,  25 25  1, -23 29  1, -19 33  1,  10 38  1,  -1  1  2,
                -18 34  2,  16 34  2,  -5  1  3,  -6  2  3,  -4  4  3, -18 34  3,
                 12 36  3,  -4  0  4,  15 33  4,  -5 39  4, -20 32  5,  22 22  6,
                 17 27  7,  16 28  7,  15 29  7,  14 30  7, -17 33  7,  -3 37  7,
                 17 25  8,  12 30  8,  15 25  9,  11 29  9,   7 25 12,   2 28 12,
                -21 21 13, -20 22 13,   3 25 13, -14 26 13, -11 27 13,  -2 24 14,
                 -7 25 14,   1 19 15,  -3 21 15, -20 10 16,   4 10 16, -18  4 17,
                -16  8 17, -13 11 17, -10 12 17,  -8 12 17,  -6 12 17,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          4 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H2        .      -0.31 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          38 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms           85 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension           2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
              H9A   H10B  H9    H10A
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large        0.10 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      240.46 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          21 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          31 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records           3 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          13 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used      0.0250 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used      0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used      0.0400 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0020 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        273 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)        17% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H18      ..H32A     .       2.08 Ang.
                                                  x,y,z  =     1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H25      ..H31      .       2.12 Ang.
                                                  x,y,z  =     1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H29A     ..H40      .       1.94 Ang.
                                                  x,y,z  =     1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H30A     ..H37      .       2.05 Ang.
                                                  x,y,z  =     1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H37      ..H30      .       1.79 Ang.
                                                  x,y,z  =     1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H40      ..H29      .       2.12 Ang.
                                                  x,y,z  =     1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H16      ..H9       .       2.09 Ang.
                                                  x,y,z  =     1_555 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H3       ..H10A     .       1.72 Ang.
                                            1-x,1-y,1-z  =     5_666 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H8       ..H9A      .       1.83 Ang.
                                            1-x,1-y,1-z  =     5_666 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H9A      ..H13      .       2.14 Ang.
                                            1-x,1-y,1-z  =     5_666 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H10B     ..H14      .       1.67 Ang.
                                            1-x,1-y,1-z  =     5_666 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl3      ..Cl1      .       3.28 Ang.
                                               x,y,-1+z  =     1_554 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        117 A**3
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C19      --C30              1.80 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      20.00 Deg.
              H27A -C27  -H27A    1_555   1_555   2_655 ......     #  328 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1       (II)      .       2.00 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd2       (II)      .       2.08 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............       2157 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        32% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
                1  1  0,
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
                2  0  0,   2  8  1,  -4  0  4,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          5 Note
               -5  1  3,  -4  4  3,  -1  1  2,   1  1  1,   2  0  0,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..........      6.997 Note
              Predicted wR2: Based on SigI**2  4.41 or SHELX Weight 30.30
```

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

---

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

4 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
30 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
5 ALERT type 5 Informative message, check

Datablock: cp2

Bond precision: C-C = 0.0199 A Wavelength=0.71073

Cell: a=28.0542(14) b=33.5024(15) c=14.7964(10)
alpha=90 beta=105.022(2) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	13431.6(13)	13431.6(13)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	C70 H48 Cd2 Cl8 N4 O10
Sum formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	C70 H48 Cd2 Cl8 N4 O10
Mr	1613.55	1613.52
Dx,g cm-3	1.596	1.596
Z	8	8
Mu (mm-1)	1.014	1.014
F000	6464.0	6464.0
F000'	6462.88	
h,k,lmax	32,38,17	32,38,17
Nref	11058	11028
Tmin,Tmax	0.885,0.904	0.589,0.746
Tmin'	0.885	

Correction method= # Reported T Limits: Tmin=0.589 Tmax=0.746
AbsCorr = NONE

Data completeness= 0.997 Theta(max)= 24.406

R(reflections)= 0.1839(9654)

wR2(reflections)= 0.3821(11028)

S = 1.115 Npar= 946

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

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.46Ang From C23 -4.16 eA-3

Author Response: Majority of residual electron density is located about C23 / C27; surrounding the central heavy Cd1 / Cd2. There is no indication of any additional unassigned atoms or uncalculated twins.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.202

Author Response: Due to the poor diffractions at high theta angles

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.202 Report

Author Response: The high Rint value is caused by the poor crystal data quality.

PLAT082_ALERT_2_B High R1 Value ..... 0.18 Report

Author Response: Poor quality crystals -several tried, best result presented.

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.38 Report

Author Response: Poor crystals - many collected - best result presented.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.40Ang From C27 -3.45 eA-3

Author Response: Majority of residual electron density is located about C23 / C27; surrounding the central heavy Cd1 / Cd2. There is no indication of any additional unassigned atoms or uncalculated twins.

Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590

```
           Calculated sin(theta_max)/wavelength =    0.5814
PLAT147_ALERT_1_C s.u. on Symmetry Constrained Cell Angle(s) .....     Please Check
PLAT220_ALERT_2_C NonSolvent   Resd 1 Cl   Ueq(max)/Ueq(min) Range        3.6 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        4.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        8.5 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C7 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT336_ALERT_2_C Long Bond Distance for ..... C18      -Cl2           1.890 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0199 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C51      - C52      .       1.67 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C53      - C54      .       1.69 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H51      ..H62      .       1.98 Ang.
                                                     x,y,z  =      1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     23.886 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      6.263 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.088 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.047 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.581         27 Report
                3  1  0,   3  3  0,   0  4  0,   2  4  0,   4  4  0,   3  5  0,
                2  8  0,   0 12  0,   0  2  1,   2  2  1,   1  3  1,   0  4  1,
                3  5  1,   1  7  1,   2  8  1,   3  9  1,   5  9  1,  -2  0  2,
               -1  3  2,  -6  2  3,  -4  2  3,  -6  0  4,  -4  0  4,  -2  2  4,
                7  5  5, -25 15 10,  -6  6 12,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          4 Note
                2  0  0,   2  8  1,   5  9  1,  -4  0  4,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.82Ang From C27            2.40 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.51Ang From C23            2.10 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From C27            2.06 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.82Ang From C23            1.96 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.96Ang From C66A           1.96 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.38Ang From O4             1.78 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.76Ang From Cd2            1.70 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.38Ang From Cl4           -1.96 eA-3
```

Author Response: Majority of residual electron density is located about C23 / C27; surrounding the central heavy Cd1 / Cd2. There is no indication of any additional unassigned atoms or uncalculated twins.

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.09Ang From Cd2           -1.90 eA-3
```

Author Response: Majority of residual electron density is located about C23 / C27; surrounding the central heavy Cd1 / Cd2. There is no indication of any additional unassigned atoms or uncalculated twins.

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.01Ang From Cd1           -1.65 eA-3
```

Author Response: Majority of residual electron density is located about C23 / C27; surrounding the central heavy Cd1 / Cd2. There is no indication of any additional unassigned atoms or uncalculated twins.

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.11Ang From Cd2          -1.52 eA-3
```

Author Response: Majority of residual electron density is located about C23 / C27; surrounding the central heavy Cd1 / Cd2. There is no indication of any additional unassigned atoms or uncalculated twins.

```
PLAT977_ALERT_2_C Check Negative Difference Density on H11C      .      -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H22       .      -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H24       .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H29       .      -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H46       .      -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H57       .      -0.50 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H64       .      -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H67B      .      -0.38 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        57 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms       113 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension        1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............         4 Report
              H9AA  H10A  H9A   H10
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    1537.88 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       49 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records       11 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    0.0010 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    0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        30% Note
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for        C52 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H24      ..H10      .       1.88 Ang.
                                               -1-x,-y,-z  =      5_455 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H34      ..H10      .       1.69 Ang.
                                               -1-x,-y,-z  =      5_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C49      ..C11      .       3.15 Ang.
                                             -1-x,y,1/2-z  =      2_455 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        87 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          1 Note
            H9AA
PLAT794_ALERT_5_G Tentative Bond Valency for Cd2       (II)      .       2.20 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       3311 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        69% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
               2  0  0,   1  1  0,   0  2  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         22 Note
              -18  2 17,  -6  6 12,  -2  0  2,  -1  3  2,   0  2  1,   0  4  0,
                0 12  0,   1  7  1,   2  2  1,   2  4  0,   2  8  0,   3  1  0,
                3  3  0,   3  5  0,   4  4  0,   7  5  5,  13 33  7,  15 33  7,
               18 24  8,  24 30  0,  34  4  0,  34  6  1,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      7.560 Note
              Predicted wR2: Based on SigI**2  5.05 or SHELX Weight 34.27
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

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

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

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

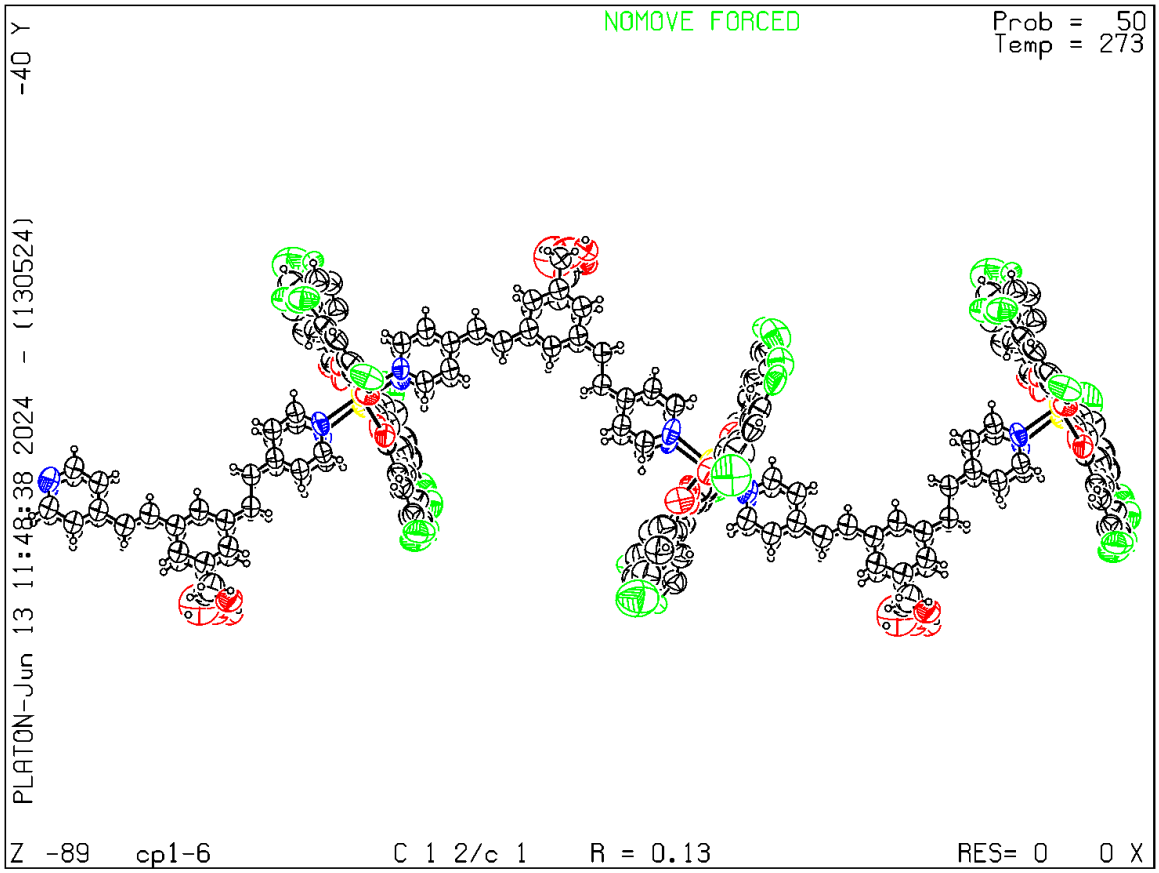
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

Publication of your CIF in other journals

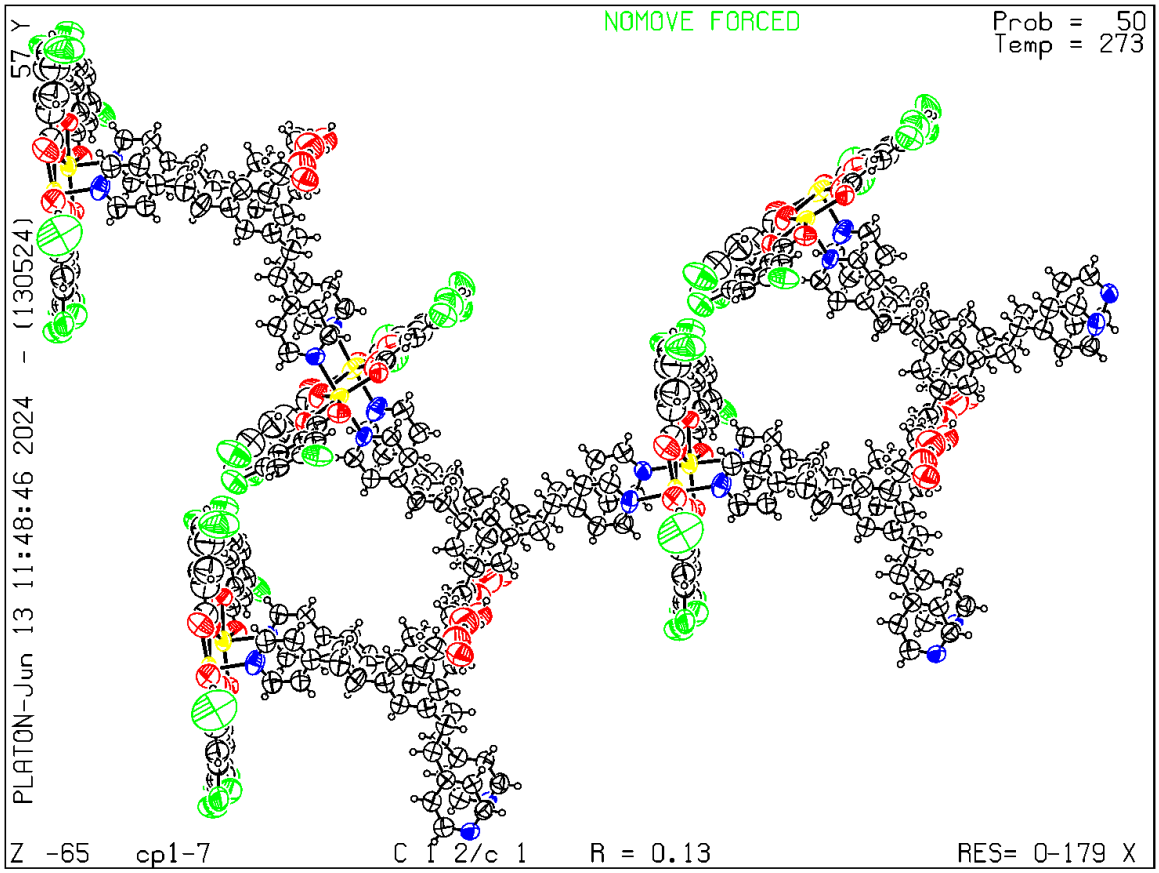
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/05/2024; check.def file version of 04/05/2024

Datablock cp1-6 - ellipsoid plot



Datablock cp1-7 - ellipsoid plot



Datablock cp2 - ellipsoid plot