Electronic Supplementary Information for Dalton Transactions
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Geometrical isomers of [TEAH][Co(L^{Se})$_2$].xH_2O: Synthesis, Structural, Spectroscopic, computational and kinetic studies

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SUP Table **1.** C-H…π interaction in *trans*-**1** and *cis*-**1**

C-H->Cg(J)	Symmetry	H…Cg	X-Perp	Gamma	Y-X…Cg	Y…Cg	Y-X,π
			C-H…π Interaction				
			Complex 1				
C51-H51B-Cg(24)	1+x,y,z	2.97	2.804	19.31	111	3.446(13)	38
C52-H52C-Cg(25)	x,y,z	2.86	2.783	13.04	127	3.518(15)	43

Ring (24) C22-->C23-->C24-->C25-->C26-->C27-->; Ring (25) C32-->C33-->C34-->C35-->C36-->C37-->;

			Complex 2				
C61-H61B-Cg(6)	1/2-X,1/2+Y,3/2-Z	2.63	2.555	13.64	152	3.515(10)	57
C51-H51A-Cg(8)	X,Y,Z	2.70	2.580	17.40	162	3.638(9)	60

Ring (6) C22-->C23-->C24-->C25-->C26-->C27-->; Ring (8) C42-->C43-->C44-->C45-->C46-->C47-->;

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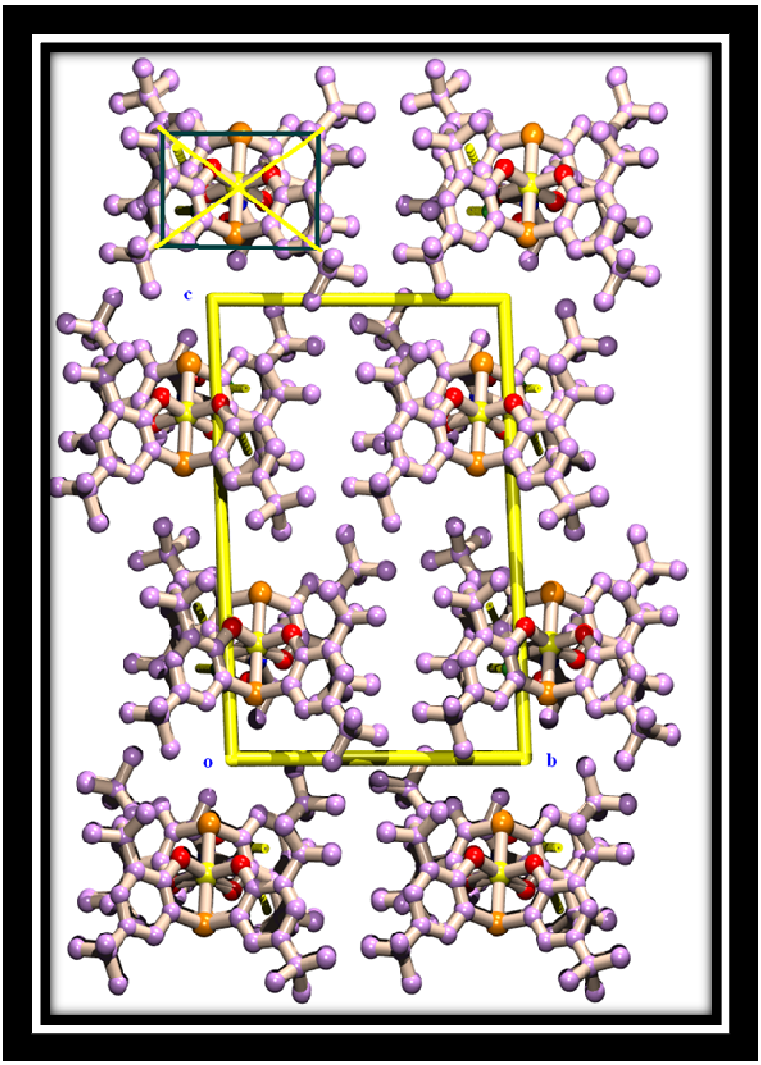

Fig. S1 Packing of adjacent columns in *trans*-**1** throguh van der Waals forces due to the particular arrangement of CH_3 groups along the diagonally opposite corners of each column.

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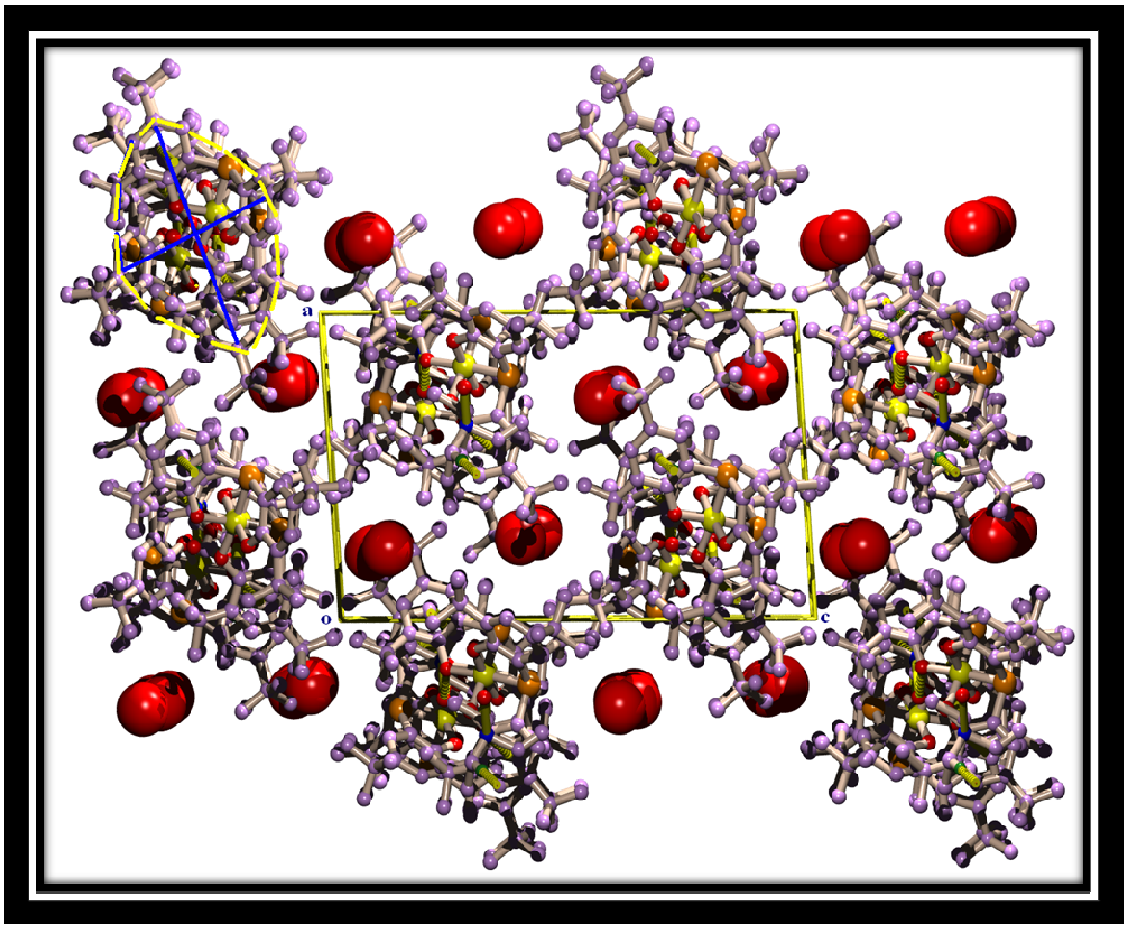

Fig. S2 The packing of helices of *cis*-**1** and the position of the water dimer (shown in CPK) formed by two more water molecules present in *cis*-**1** than the *trans*-**1.**

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checkCIF/PLATON report (basic structural check)

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: 1

Bond precision: C-C = 0.0135 A Wavelength=0.71073
Cell: a=12.4294(17) b=13.837(2) c=19.810(4)
alpha=90.238(14) beta=98.366(15) gamma=106.126(13)
Temperature: 150 K

	Calculated	Reported
Volume	3234.6(10)	3234.6(9)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C56 H80 Co O4 Se2, C6 H16 N, O	?
Sum formula	C62 H96 Co N O5 Se2	C62 H98 CO N O5 SE2
Mr	1152.25	1154.26
Dx,g cm-3	1.183	1.185
Z	2	2
Mu (mm-1)	1.434	1.434
F000	1220.0	1224.0
F000'	1220.71	
h,k,lmax	17,19,27	17,19,27
Nref	19058	15144
Tmin,Tmax	0.950,0.958	0.777,1.000
Tmin'	0.689	

Correction method= EMPIRICAL
Data completeness= 0.795 Theta(max)= 30.110
R(reflections)= 0.1021(5761) wR2(reflections)= 0.2568(15144)
S = 0.979 Npar= 667

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

REFLT03_ALERT_3_A Reflection count < 85% complete (theta max?)
From the CIF: _diffrn_reflns_theta_max 30.11
From the CIF: _diffrn_reflns_theta_full 30.11
From the CIF: _reflns_number_total 15144
TEST2: Reflns within _diffrn_reflns_theta_max
Count of symmetry unique reflns 19058
Completeness (_total/calc) 79.46%

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low 0.80
PLAT213_ALERT_2_A Atom C14 has ADP max/min Ratio ..... 5.90 oblat
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 6.33 Ratio
PLAT222_ALERT_3_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 6.19 Ratio
PLAT306_ALERT_2_A Isolated Oxygen Atom (H-atoms Missing ?) O100
PLAT234_ALERT_4_A Large Hirshfeld Difference C61 -- C62 .. 0.30 Ang.
PLAT234_ALERT_4_A Large Hirshfeld Difference C71 -- C72 .. 0.30 Ang.

Alert level B

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections too Low .... 38 Perc.
PLAT213_ALERT_2_B Atom C32 has ADP max/min Ratio ..... 4.40 prola
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C461

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```
PLAT430_ALERT_2_B Short Inter D...A Contact  O41    ..  O100    ..       2.72 Ang.
PLAT224_ALERT_1_B Ueq(Rep) and Ueq(Calc) differ by -0.004 Ang**2 .       C62
```

Alert level C

```
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           reddish
DIFMX01_ALERT_2_C  The maximum difference density is > 0.1*ZMAX*0.75
           _refine_diff_density_max given =      3.318
           Test value =      2.550
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
RFACG01_ALERT_3_C  The value of the R factor is > 0.10
           R factor given   0.102
RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
           Weighted R factor given   0.257
PLAT084_ALERT_2_C High R2 Value ..................................       0.26
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.92
PLAT097_ALERT_2_C Maximum (Positive) Residual Density ............       3.32 eA-3
PLAT213_ALERT_2_C Atom C27     has ADP max/min Ratio .............       3.60 oblat
PLAT213_ALERT_2_C Atom C264    has ADP max/min Ratio .............       3.70 prola
PLAT214_ALERT_2_C Atom C71     (Anion/Solvent) ADP max/min Ratio         4.10 prola
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C361
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.51
PLAT301_ALERT_3_C Main Residue  Disorder .........................       5.00 Perc.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ...         14
PLAT430_ALERT_2_C Short Inter D...A Contact  O31    ..  O100    ..       2.86 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .      43.00 A**3
PLAT041_ALERT_1_C Calc. and Rep. SumFormula Strings    Differ ....          ?
PLAT062_ALERT_4_C Rescale T(min) & T(max) by .....................       0.96
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT152_ALERT_1_C Supplied and Calc Volume s.u. Inconsistent .....          ?
PLAT223_ALERT_4_C Large Solvent/Anion  H     Ueq(max)/Ueq(min) ...       3.26 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O21    --  C23     ..       0.12  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C241   --  C244    ..       0.14  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C341   --  C344    ..       0.14  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C431   --  C433    ..       0.17  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C431   --  C434    ..       0.13  Ang.
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors for        C71
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors for         N5
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors for        C61
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1
           C56 H80 Co O4 Se2
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          2
           C6 H16 N
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          3
           O
```

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:C62 H98 Co1 N1 O5 Se2
           Atom count from the _atom_site data:  C62 H96 Co1 N1 O5 Se2
ABSTM02_ALERT_3_G  When printed, the submitted absorption T values will be
           replaced by the scaled T values. Since the ratio of scaled T's
           is identical to the ratio of reported T values, the scaling
           does not imply a change to the absorption corrections used in
           the study.
           Ratio of Tmax expected/reported      0.958
           Tmax scaled      0.958 Tmin scaled      0.744
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C62 H98 Co N O5 Se2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        124.00    124.00    0.00
          H        196.00    192.00    4.00
```

```
          Co          2.00      2.00     0.00
          N           2.00      2.00     0.00
          O          10.00     10.00     0.00
          Se          4.00      4.00     0.00
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         24
```

```
   8 ALERT level A = In general: serious problem
   5 ALERT level B = Potentially serious problem
  33 ALERT level C = Check and explain
   5 ALERT level G = General alerts; check

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

Datablock: 2

```
Bond precision:      C-C = 0.0101 A              Wavelength=0.71073
Cell:          a=13.4883(12)  b=22.5226(15)  c=22.105(2)
               alpha=90       beta=93.774(8) gamma=90
Temperature: 150 K
```

	Calculated	Reported
Volume	6700.8(10)	6700.8(10)
Space group	P 21/n	P21/n
Hall group	-P 2yn	?
Moiety formula	C56 H77 Co O4 Se2, C6 H15 N, 3(O)	?
Sum formula	C62 H92 Co N O7 Se2	C62 H98 CO N O7 SE2
Mr	1180.22	1186.26
Dx,g cm-3	1.170	1.176
Z	4	4
Mu (mm-1)	1.388	1.388
F000	2488.0	2512.0
F000'	2489.50	
h,k,lmax	18,31,31	18,31,31
Nref	19536	19060
Tmin,Tmax	0.936,0.959	0.882,1.000
Tmin'	0.737	

```
Correction method= EMPIRICAL
Data completeness= 0.976       Theta(max)= 30.000
R(reflections)= 0.0697( 4674)      wR2(reflections)= 0.1720( 19060)
S = 0.965             Npar= 669
```

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

```
PLAT026_ALERT_3_A Ratio Observed / Unique Reflections too Low ....         25 Perc.
PLAT306_ALERT_2_A Isolated Oxygen Atom (H-atoms Missing ?) .......       O100
PLAT306_ALERT_2_A Isolated Oxygen Atom (H-atoms Missing ?) .......       O101
PLAT306_ALERT_2_A Isolated Oxygen Atom (H-atoms Missing ?) .......       O102
```

Alert level B

```
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       3.73 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C151   --  C153    ..      10.14 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C421   --  C424    ..       8.75 su
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond  C71    -   C72    ...       1.30 Ang.
PLAT410_ALERT_2_B Short Intra H...H Contact  H51A   ..  H71B    ..       1.83 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact  O41    ..  O100    ..       2.78 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact  O100   ..  N5      ..       2.74 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact  O101   ..  O102    ..       2.81 Ang.
```

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PLAT231_ALERT_4_B Hirshfeld Test (Solvent)   C61    --  C62     ..      20.82 su
PLAT234_ALERT_4_B Large Hirshfeld Difference C251   --  C252    ..       0.21  Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C71    --  C72     ..       0.27  Ang.
```

Alert level C

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......       0.98
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.78
PLAT222_ALERT_3_C Large Non-Solvent    H     Ueq(max)/Ueq(min) ...       3.84 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C16    --  C17     ..       6.28 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C46    --  C47     ..       6.42 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C351   --  C352    ..       5.59 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C351   --  C354    ..       6.17 su
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C151
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C351
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C421
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.06
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ...         10
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C61    -   C62    ...       1.65 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .      68.00 A**3
PLAT041_ALERT_1_C Calc. and Rep. SumFormula Strings    Differ ....          ?
PLAT062_ALERT_4_C Rescale T(min) & T(max) by .....................       0.96
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT231_ALERT_4_C Hirshfeld Test (Solvent)   N5     --  C71     ..       5.67 su
PLAT234_ALERT_4_C Large Hirshfeld Difference O31    --  C32     ..       0.11  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O41    --  C42     ..       0.12  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14    --  C15     ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C15    --  C16     ..       0.13  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C15    --  C151    ..       0.11  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22    --  C23     ..       0.11  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22    --  C27     ..       0.16  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C23    --  C231    ..       0.12  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C25    --  C251    ..       0.13  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C26    --  C27     ..       0.13  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C32    --  C33     ..       0.16  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C35    --  C36     ..       0.17  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C42    --  C43     ..       0.14  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C43    --  C44     ..       0.14  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C43    --  C421    ..       0.13  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C131   --  C133    ..       0.18  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C131   --  C134    ..       0.16  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C151   --  C152    ..       0.14  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C151   --  C154    ..       0.18  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C231   --  C232    ..       0.16  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C251   --  C254    ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C331   --  C333    ..       0.19  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C351   --  C353    ..       0.16  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C421   --  C423    ..       0.14  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C451   --  C452    ..       0.13  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C451   --  C454    ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5     --  C51     ..       0.17  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C51    --  C52     ..       0.18  Ang.
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors for        C51
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors for        C61
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors for        C71
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors for         N5
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          2
             C6 H15 N
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          3
             O
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          4
             O
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          5
             O
```

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:C62 H98 Co1 N1 O7 Se2
           Atom count from the _atom_site data:  C62 H92 Co1 N1 O7 Se2
```

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```
ABSTM02_ALERT_3_G  When printed, the submitted absorption T values will be
           replaced by the scaled T values. Since the ratio of scaled T's
           is identical to the ratio of reported T values, the scaling
           does not imply a change to the absorption corrections used in
           the study.
           Ratio of Tmax expected/reported      0.959
           Tmax scaled      0.959 Tmin scaled      0.846
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C62 H98 Co N O7 Se2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        248.00    248.00    0.00
          H        392.00    368.00   24.00
          Co         4.00      4.00    0.00
          N          4.00      4.00    0.00
          O         28.00     28.00    0.00
          Se         8.00      8.00    0.00
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..      C354
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          6
```

```
  4 ALERT level A = In general: serious problem
 11 ALERT level B = Potentially serious problem
 54 ALERT level C = Check and explain
  6 ALERT level G = General alerts; check

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

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 12/11/2008; check.def file version of 12/11/2008

Datablock 1 - ellipsoid plot

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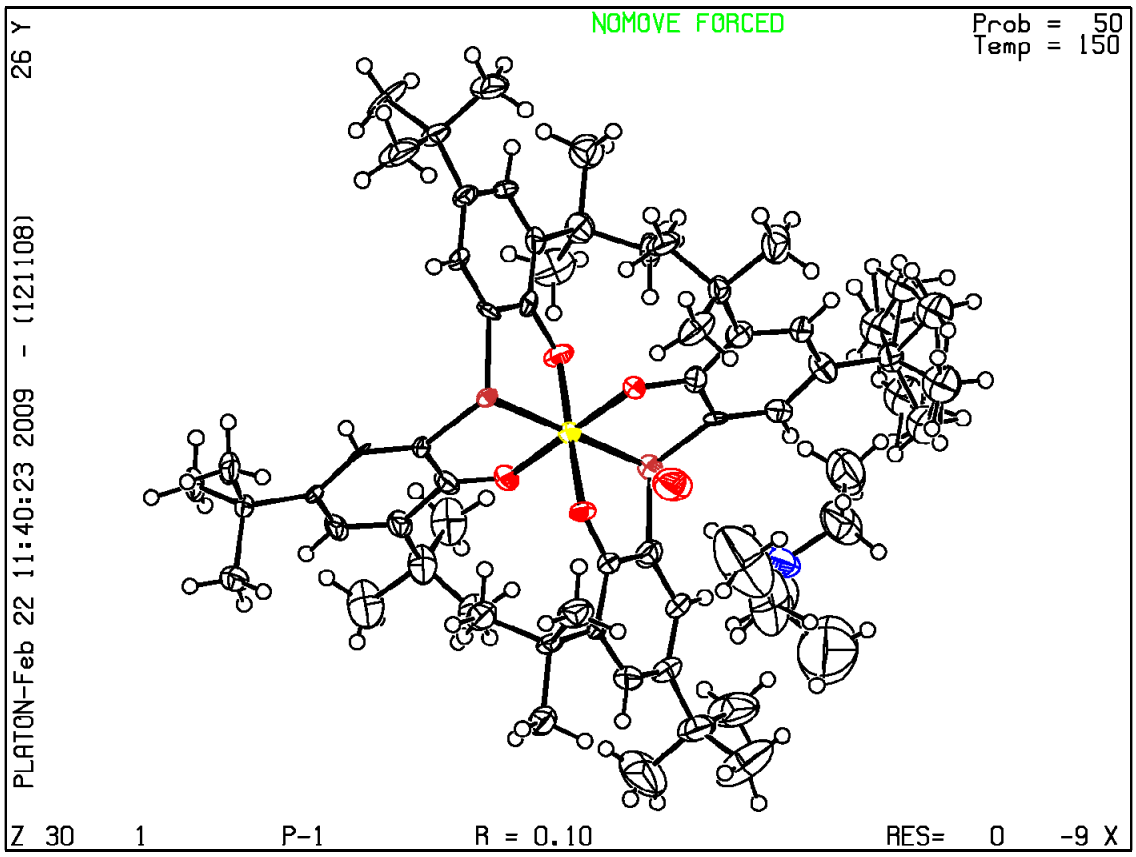

Datablock 2 - ellipsoid plot

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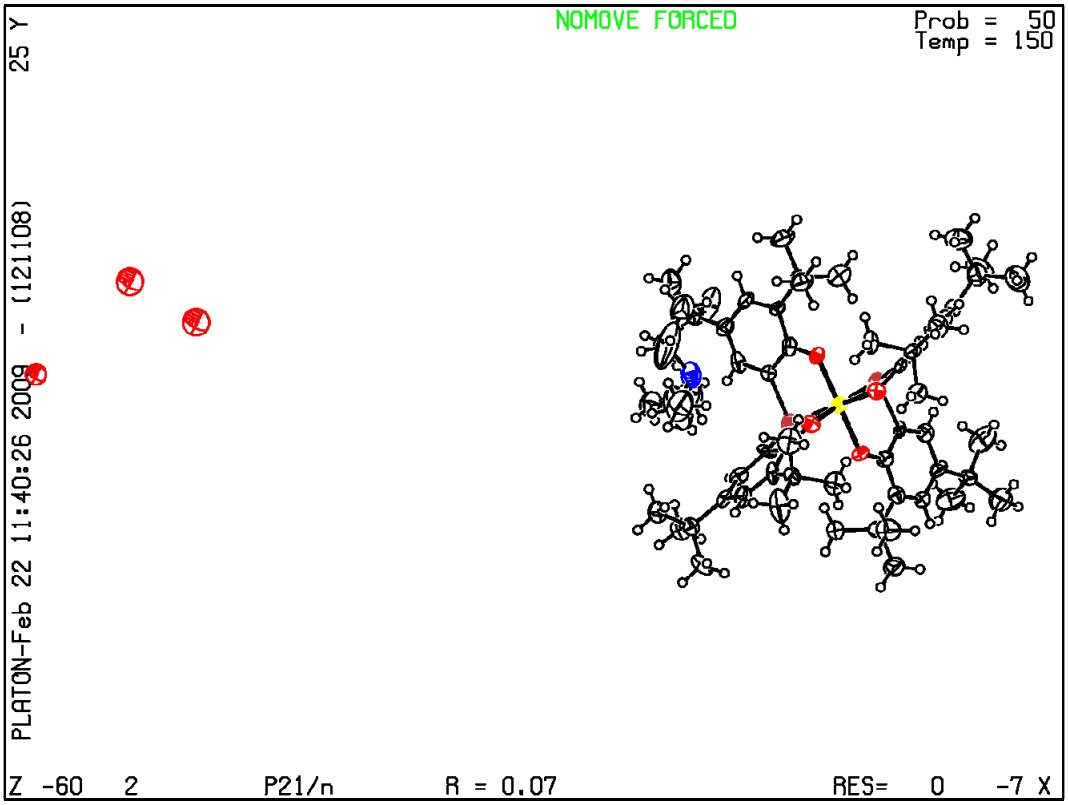

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